



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 06:28 PM UTC

PDB ID : 7B04 / pdb_00007b04
Title : Structure of Nitrite oxidoreductase (Nxr) from the anammox bacterium *Kuenenia stuttgartiensis*.
Authors : Moreno-Chicano, T.; Dietl, A.; Akram, M.; Barends, T.R.M.
Deposited on : 2020-11-18
Resolution : 2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

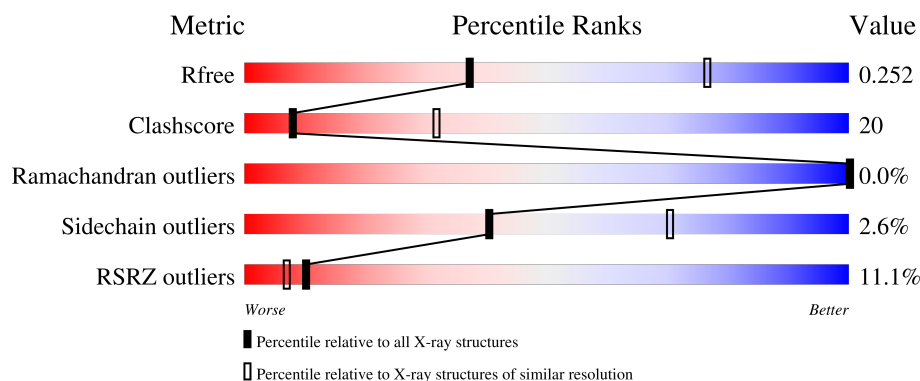
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



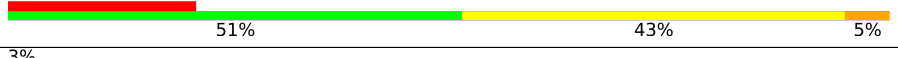
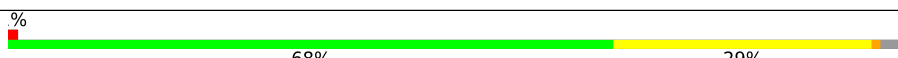
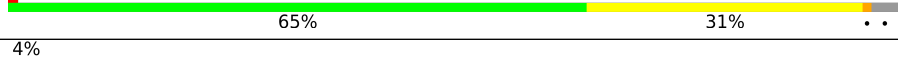
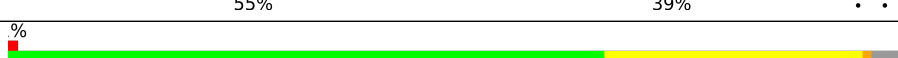
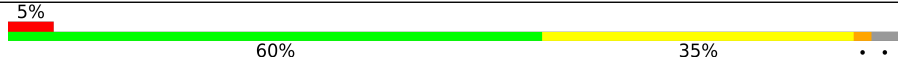
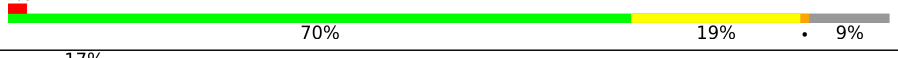
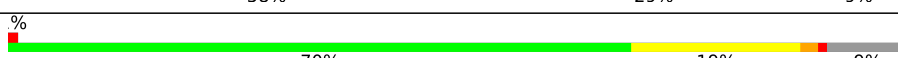
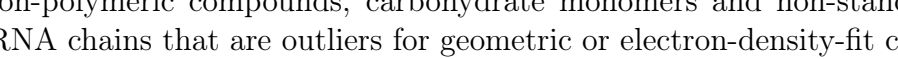
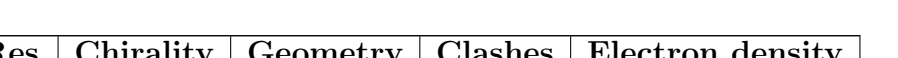
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	410	 74% 25% .
1	D	410	 58% 64% 35%
1	G	410	 % 74% 26%
1	J	410	 77% 22%
1	M	410	 2% 64% 34% .

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Mol	Chain	Length	Quality of chain
1	P	410	
1	S	410	
1	V	410	
2	B	1148	
2	E	1148	
2	H	1148	
2	K	1148	
2	N	1148	
2	Q	1148	
2	T	1148	
2	W	1148	
3	C	322	
3	F	322	
3	I	322	
3	L	322	
3	O	322	
3	R	322	
3	U	322	
3	X	322	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	D	501	-	-	X	-
4	SF4	D	502	-	-	X	-
4	SF4	G	503	-	-	X	-
4	SF4	J	503	-	-	X	-
4	SF4	M	503	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	N	5804	-	-	X	-
4	SF4	P	503	-	-	X	-
4	SF4	Q	5804	-	-	X	-
4	SF4	S	503	-	-	X	-
4	SF4	T	5804	-	-	X	-
4	SF4	V	501	-	-	X	-
4	SF4	V	503	-	-	X	-
4	SF4	W	5804	-	-	X	-
5	F3S	D	504	-	-	X	-
5	F3S	M	504	-	-	X	-
5	F3S	V	504	-	-	X	-
6	MD1	E	5801	X	-	-	-
8	HEM	F	401	-	-	X	-
8	HEM	I	401	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 115931 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitrite oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3349	2138	579	606	26			
1	D	408	Total	C	N	O	S	0	0	0
			2872	1805	508	534	25			
1	G	409	Total	C	N	O	S	0	0	0
			3344	2138	578	602	26			
1	J	409	Total	C	N	O	S	0	0	0
			3361	2147	580	608	26			
1	M	409	Total	C	N	O	S	0	0	0
			3309	2114	572	597	26			
1	P	409	Total	C	N	O	S	0	0	0
			3321	2121	573	601	26			
1	S	409	Total	C	N	O	S	0	0	0
			3333	2131	577	599	26			
1	V	409	Total	C	N	O	S	0	0	0
			3239	2063	556	594	26			

- Molecule 2 is a protein called Nitrite oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1120	Total	C	N	O	S	0	1	0
			9003	5748	1551	1662	42			
2	E	1111	Total	C	N	O	S	0	1	0
			6871	4264	1247	1334	26			
2	H	1118	Total	C	N	O	S	0	1	0
			9028	5760	1561	1665	42			
2	K	1119	Total	C	N	O	S	0	1	0
			9046	5777	1559	1668	42			
2	N	1117	Total	C	N	O	S	0	3	0
			9052	5773	1564	1672	43			
2	Q	1116	Total	C	N	O	S	0	1	0
			8902	5678	1533	1649	42			

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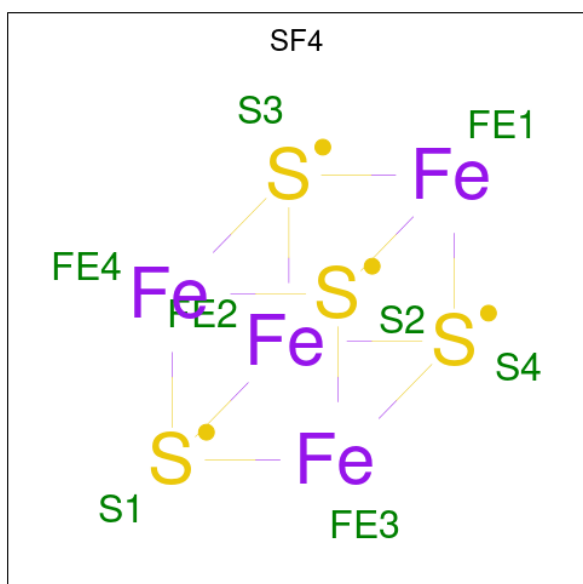
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	1119	Total	C	N	O	S	0	0	0
			9034	5766	1555	1671	42			
2	W	1118	Total	C	N	O	S	0	1	0
			8920	5688	1532	1658	42			

- Molecule 3 is a protein called Nitrite oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	1	0
			2281	1435	400	438	8			
3	F	292	Total	C	N	O	S	0	0	0
			2068	1305	358	398	7			
3	I	292	Total	C	N	O	S	0	0	0
			2216	1401	385	422	8			
3	L	292	Total	C	N	O	S	0	1	0
			2274	1431	396	439	8			
3	O	291	Total	C	N	O	S	0	0	0
			2124	1337	369	410	8			
3	R	291	Total	C	N	O	S	0	0	0
			2261	1423	392	438	8			
3	U	292	Total	C	N	O	S	0	0	0
			2267	1428	393	438	8			
3	X	292	Total	C	N	O	S	0	0	0
			2225	1401	387	429	8			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



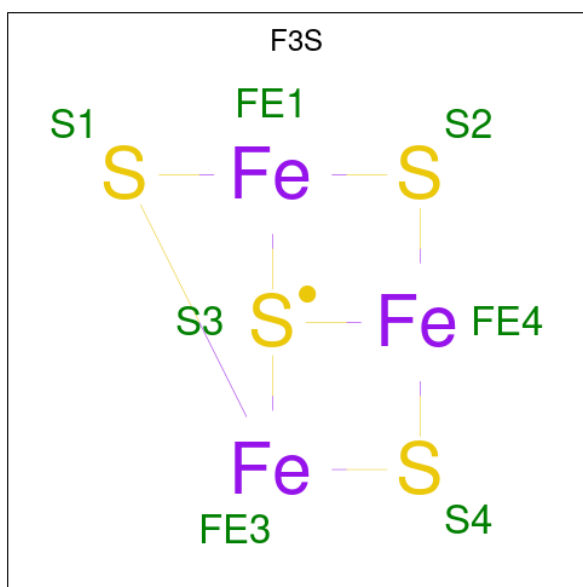
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	E	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	H	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	K	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	N	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	W	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4) (labeled as "Ligand of Interest" by depositor).



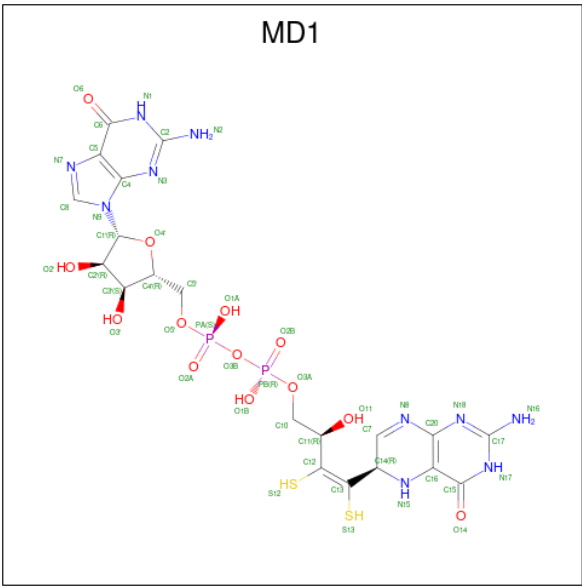
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			7	3	4		
5	G	1	Total	Fe	S	0	0
			7	3	4		
5	J	1	Total	Fe	S	0	0
			7	3	4		
5	M	1	Total	Fe	S	0	0
			7	3	4		
5	P	1	Total	Fe	S	0	0
			7	3	4		
5	S	1	Total	Fe	S	0	0
			7	3	4		
5	V	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 7 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

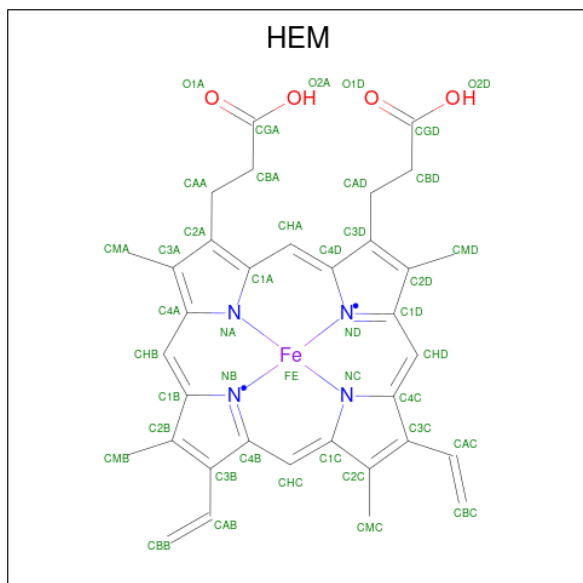
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mo	0	0
			1	1		
7	E	1	Total	Mo	0	0
			1	1		
7	H	1	Total	Mo	0	0
			1	1		
7	K	1	Total	Mo	0	0
			1	1		
7	N	1	Total	Mo	0	0
			1	1		
7	Q	1	Total	Mo	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	T	1	Total Mo 1 1	0	0
7	W	1	Total Mo 1 1	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	2	Total Ca 2 2	0	0
9	F	2	Total Ca 2 2	0	0
9	I	2	Total Ca 2 2	0	0
9	L	2	Total Ca 2 2	0	0
9	O	2	Total Ca 2 2	0	0
9	R	2	Total Ca 2 2	0	0
9	U	2	Total Ca 2 2	0	0
9	X	2	Total Ca 2 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	37	Total O 37 37	0	0
10	B	72	Total O 72 72	0	0
10	C	35	Total O 35 35	0	0
10	D	6	Total O 6 6	0	0
10	E	13	Total O 13 13	0	0
10	F	8	Total O 8 8	0	0
10	G	25	Total O 25 25	0	0
10	H	83	Total O 83 83	0	0
10	I	20	Total O 20 20	0	0
10	J	28	Total O 28 28	0	0
10	K	74	Total O 74 74	0	0
10	L	30	Total O 30 30	0	0

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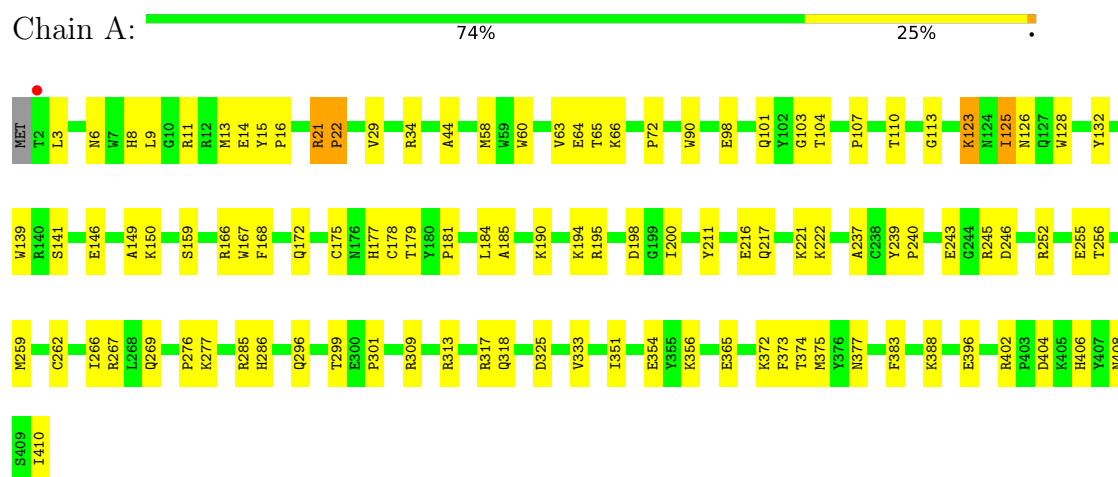
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	10	Total 10	O 10	0	0
10	N	76	Total 76	O 76	0	0
10	O	17	Total 17	O 17	0	0
10	P	16	Total 16	O 16	0	0
10	Q	43	Total 43	O 43	0	0
10	R	22	Total 22	O 22	0	0
10	S	20	Total 20	O 20	0	0
10	T	62	Total 62	O 62	0	0
10	U	25	Total 25	O 25	0	0
10	V	12	Total 12	O 12	0	0
10	W	41	Total 41	O 41	0	0
10	X	24	Total 24	O 24	0	0

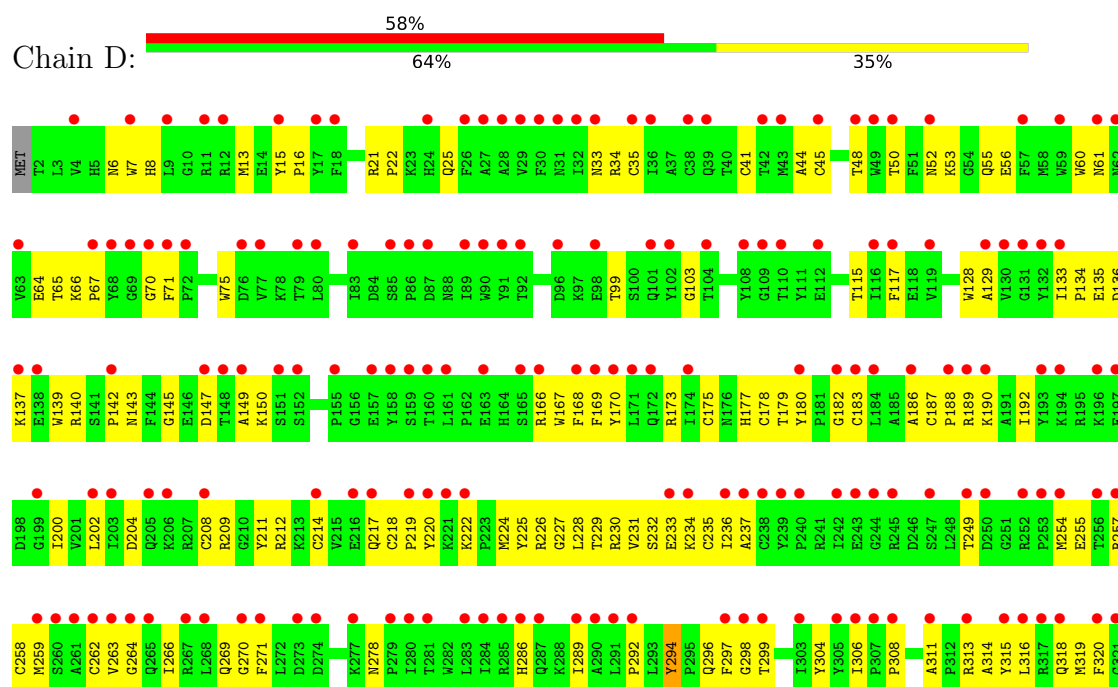
3 Residue-property plots [i](#)

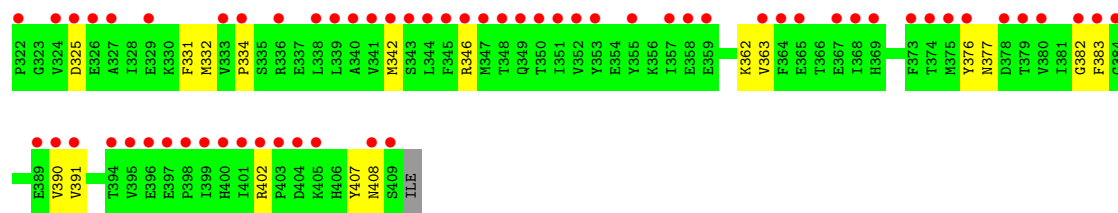
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitrite oxidoreductase subunit B

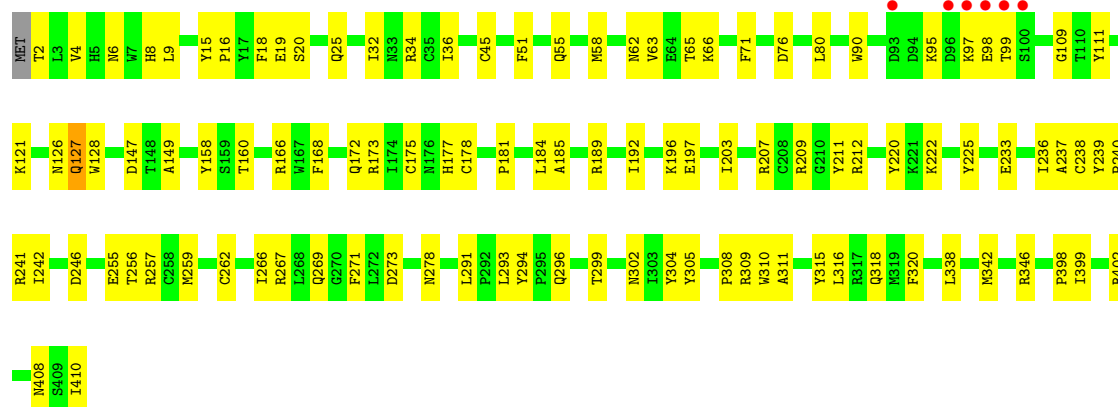
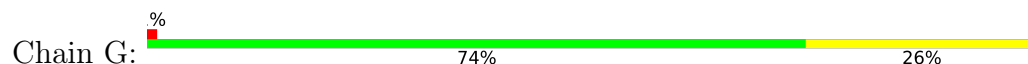


• Molecule 1: Nitrite oxidoreductase subunit B

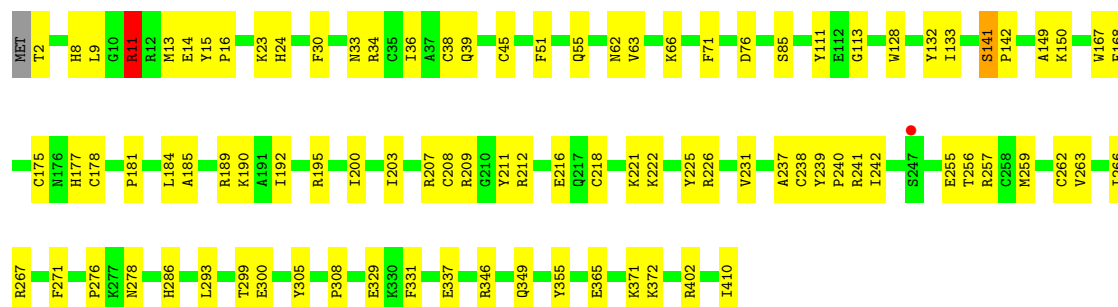
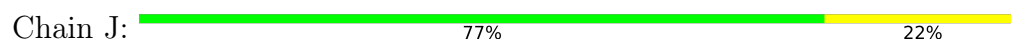




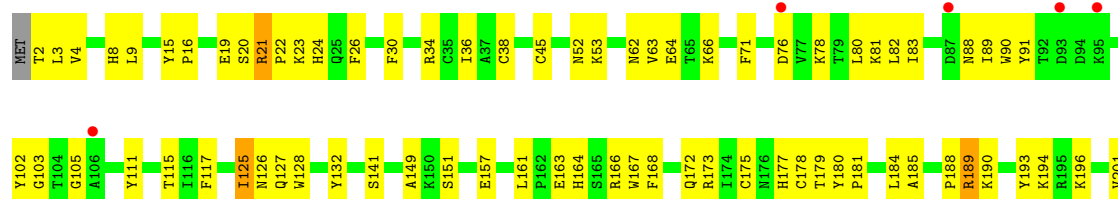
● Molecule 1: Nitrite oxidoreductase subunit B

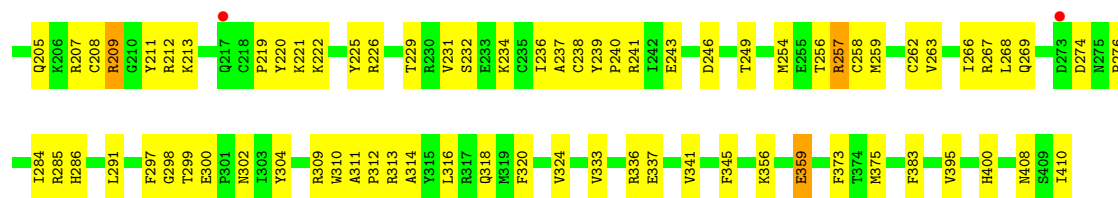


● Molecule 1: Nitrite oxidoreductase subunit B

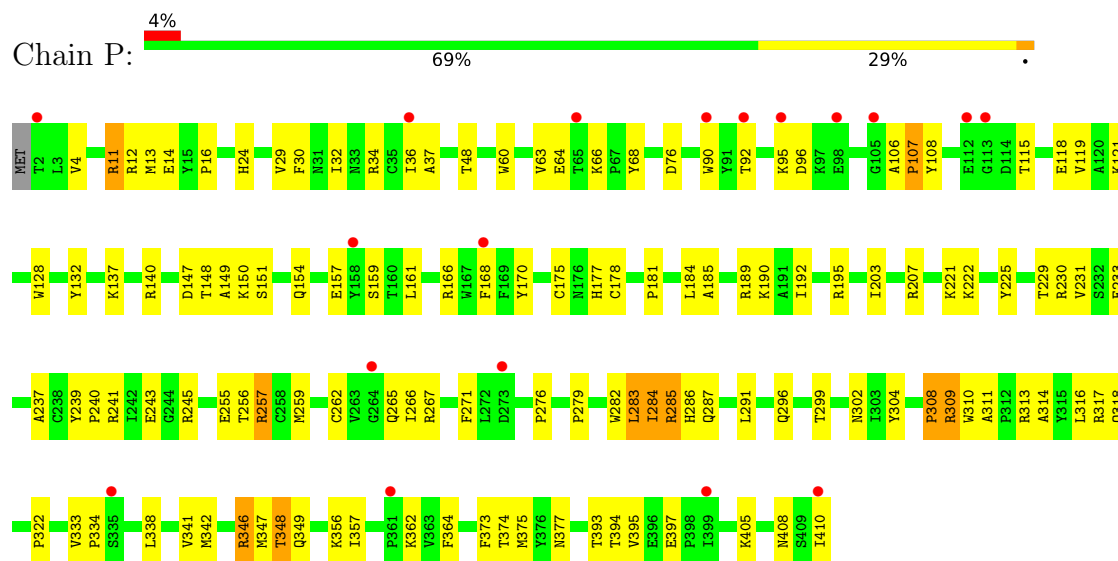


● Molecule 1: Nitrite oxidoreductase subunit B

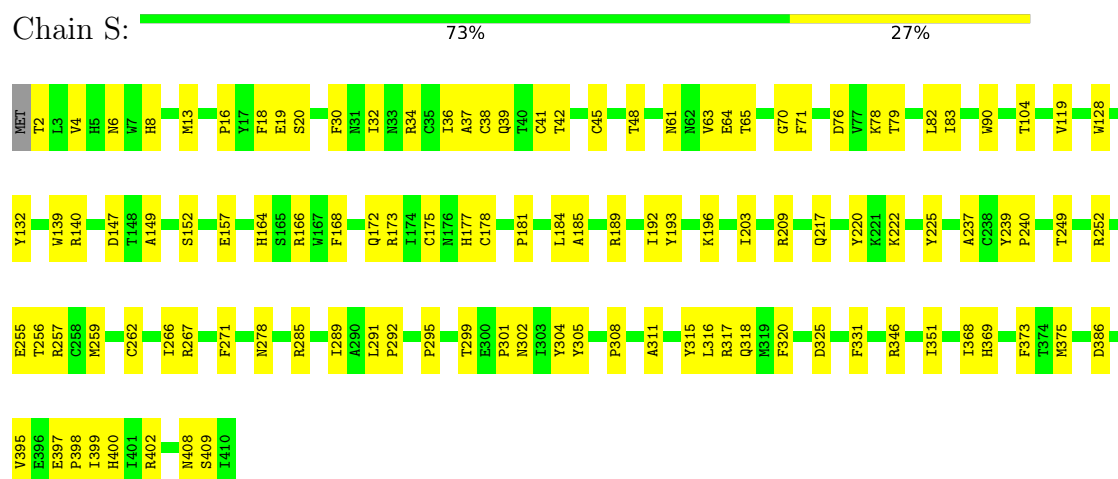




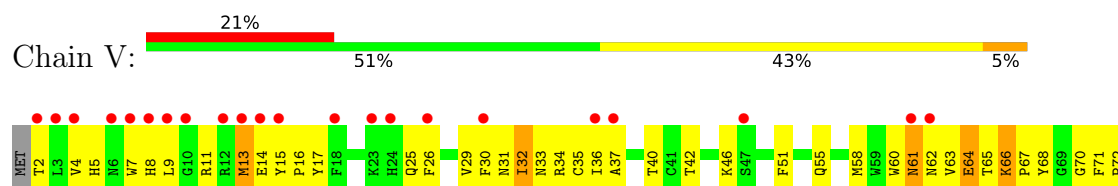
• Molecule 1: Nitrite oxidoreductase subunit B

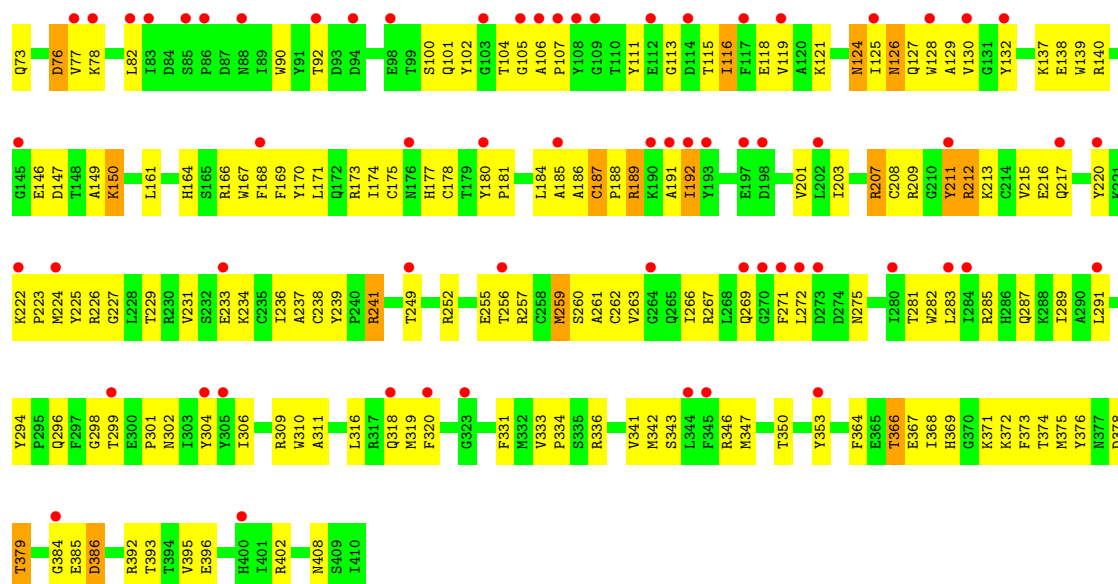


• Molecule 1: Nitrite oxidoreductase subunit B

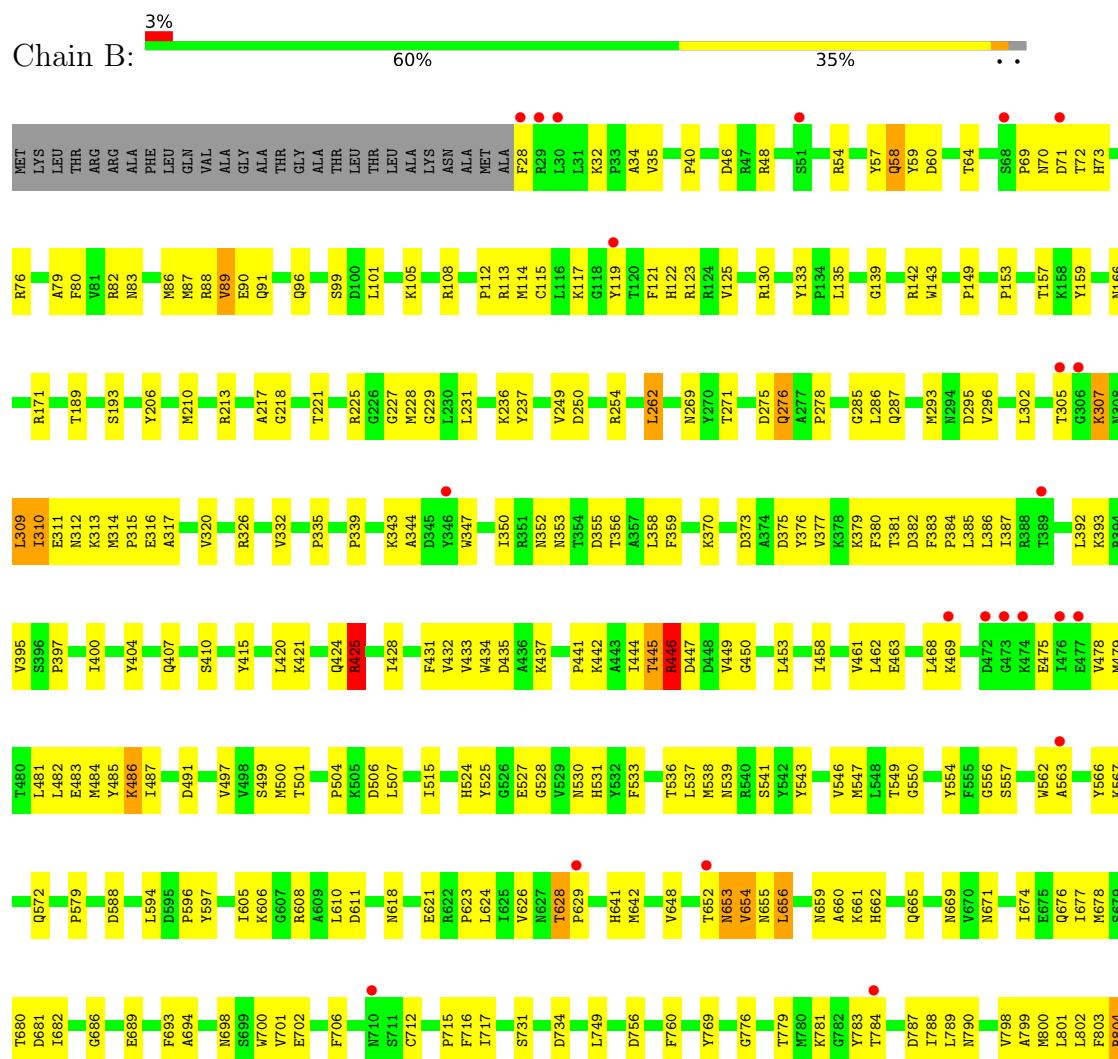


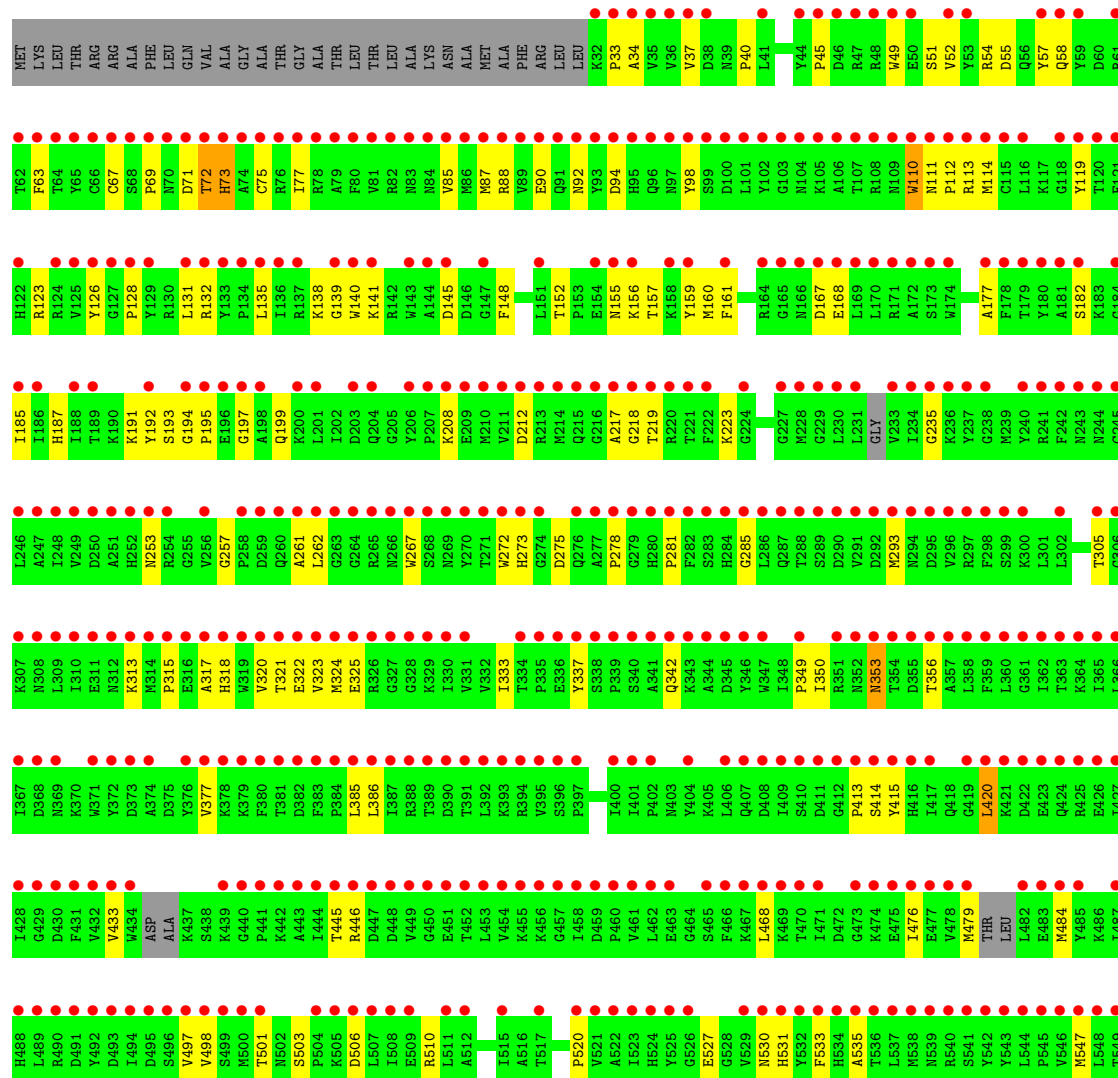
• Molecule 1: Nitrite oxidoreductase subunit B

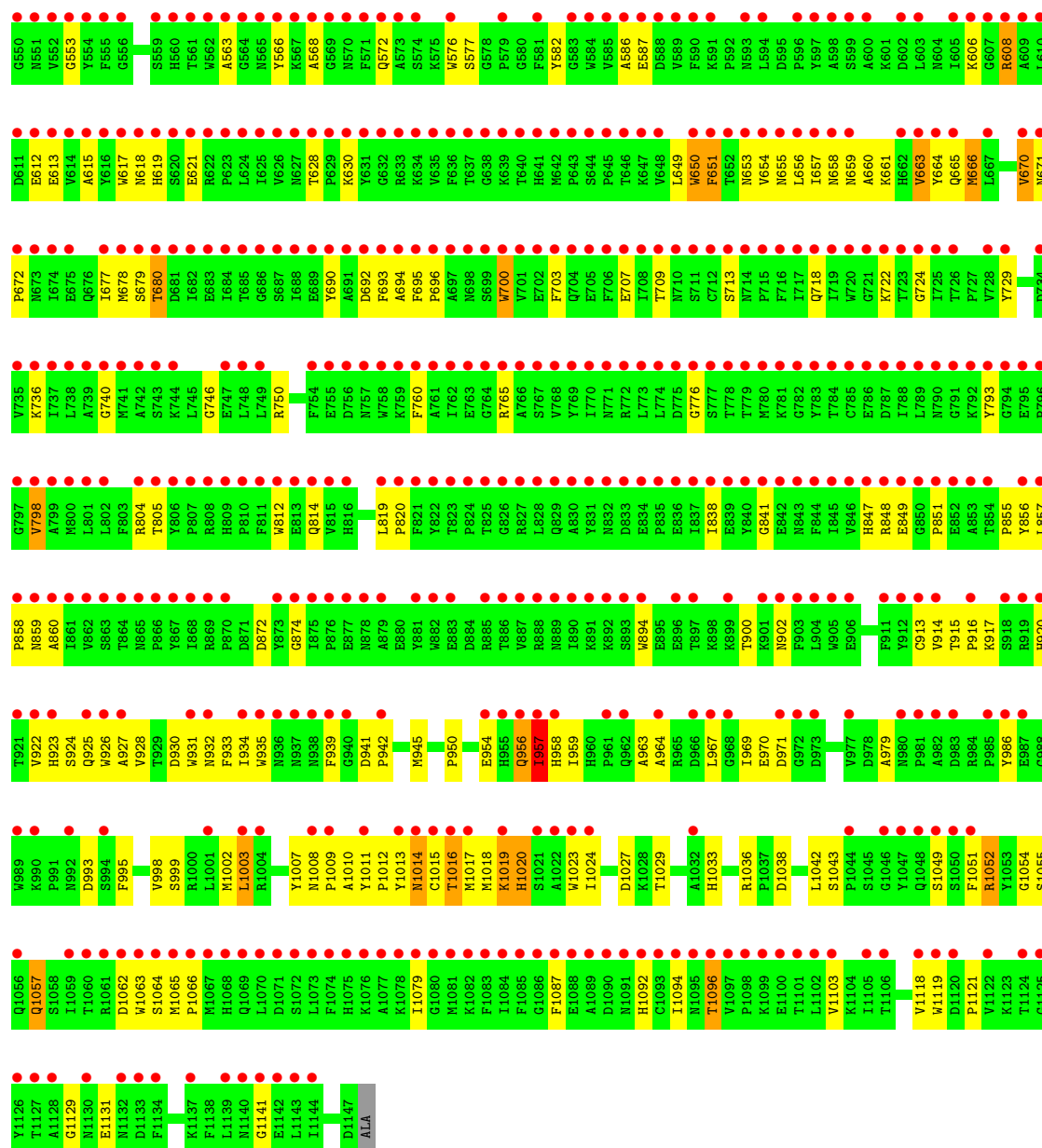




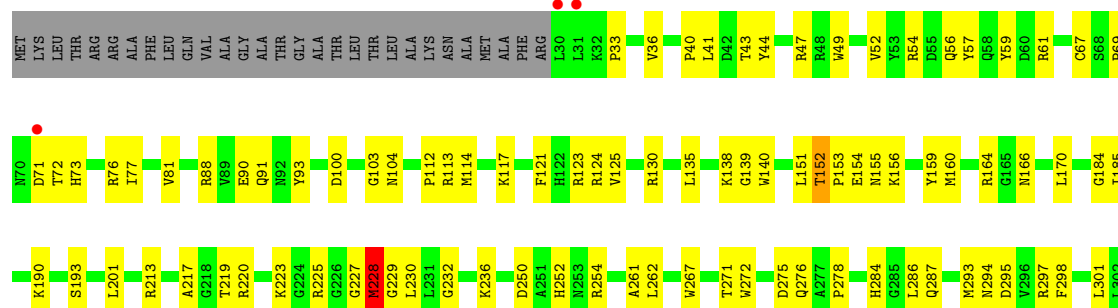
• Molecule 2: Nitrite oxidoreductase subunit A

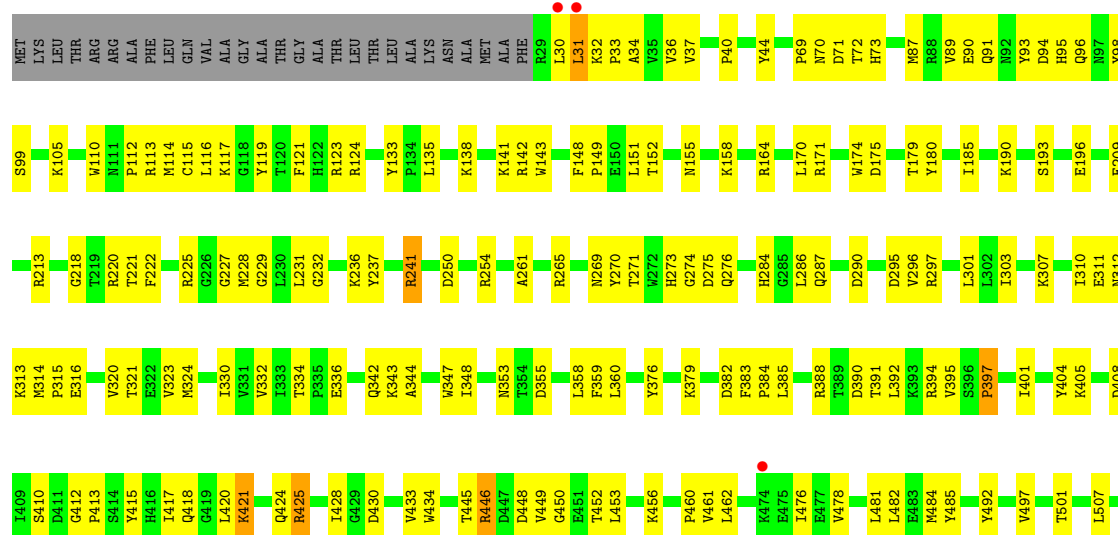






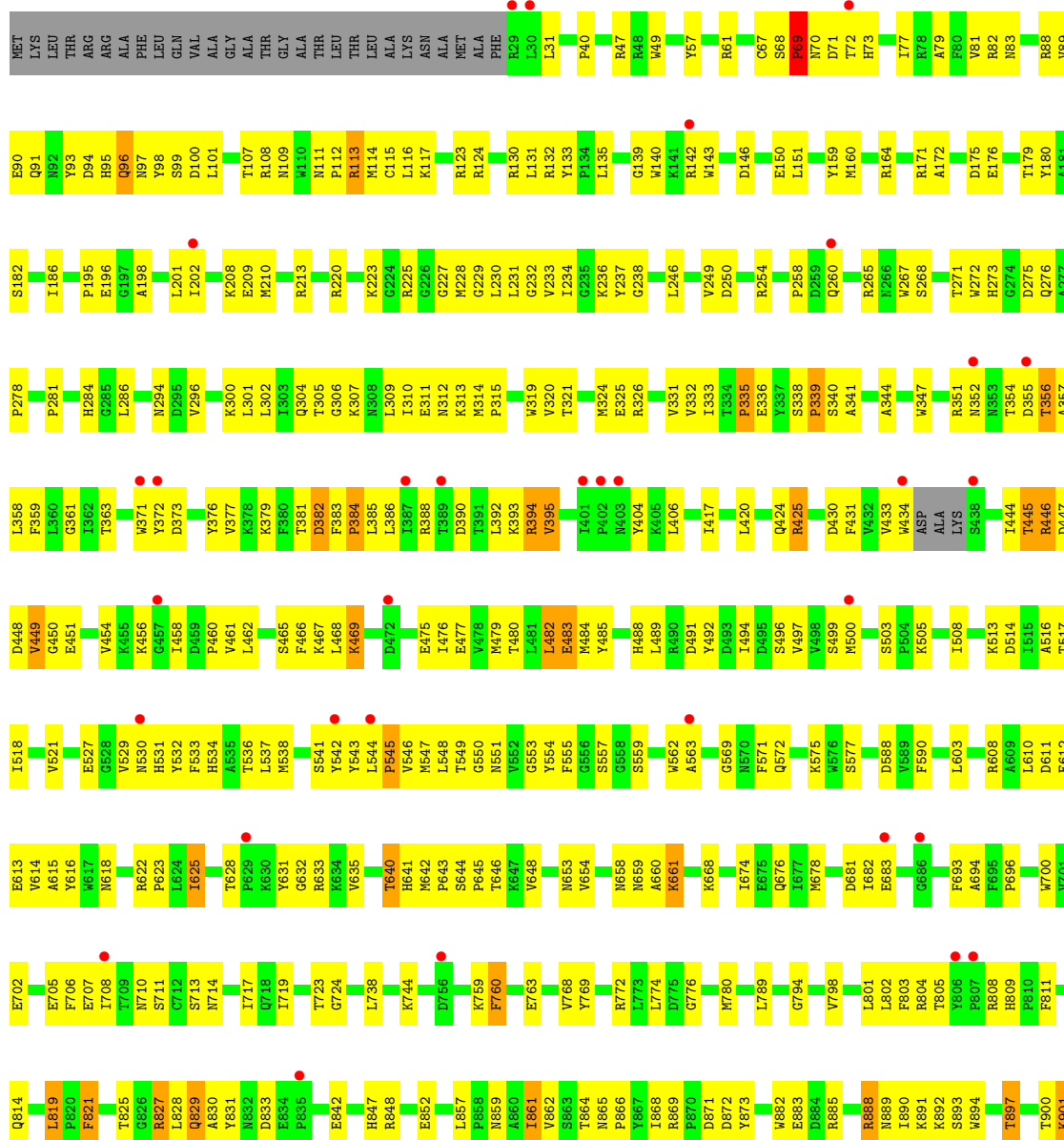
● Molecule 2: Nitrite oxidoreductase subunit A

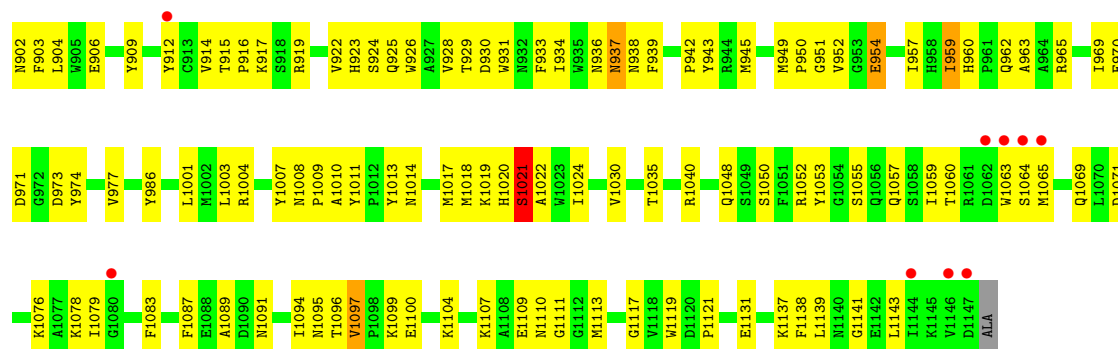




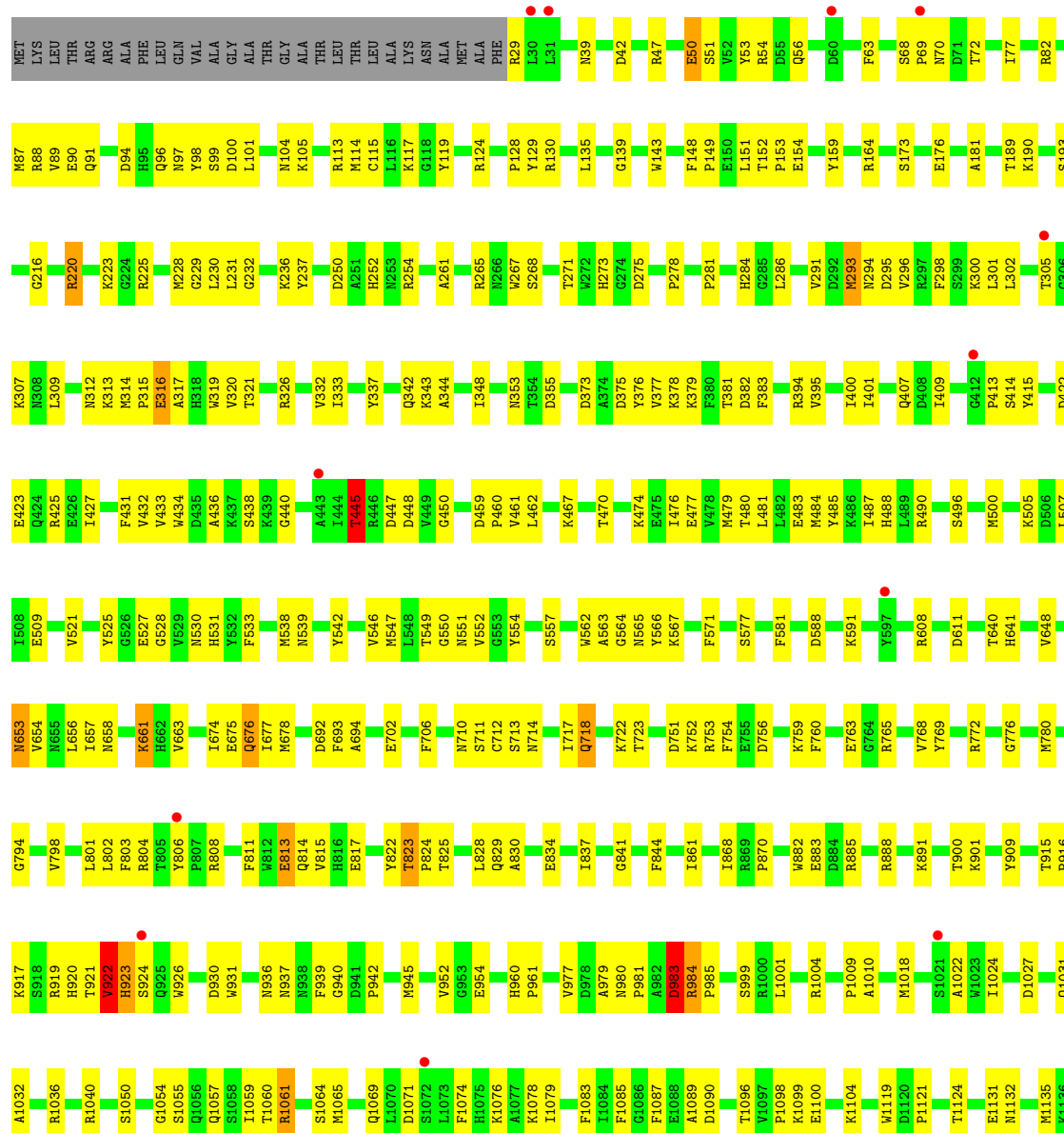


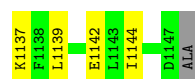
• Molecule 2: Nitrite oxidoreductase subunit A



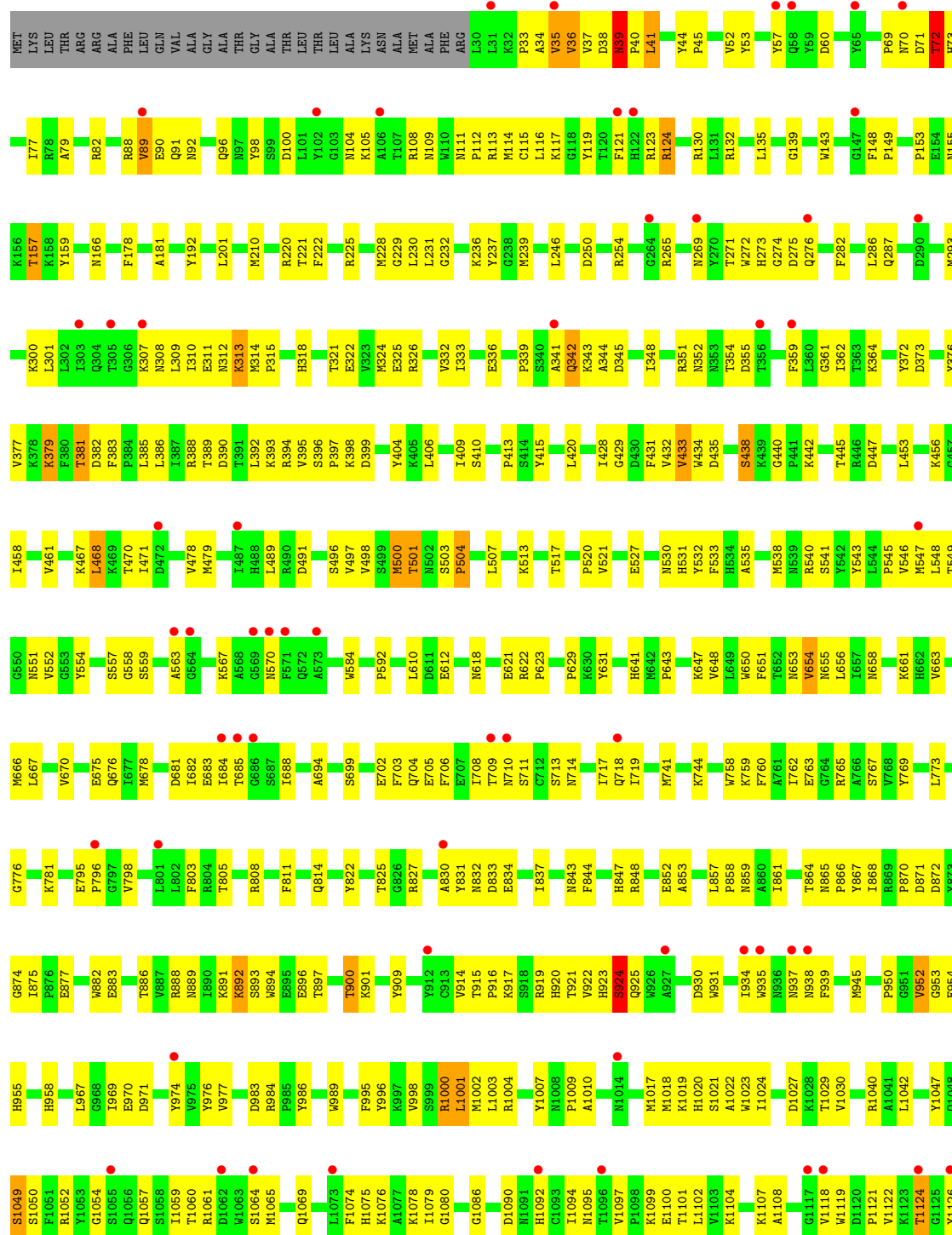


• Molecule 2: Nitrite oxidoreductase subunit A



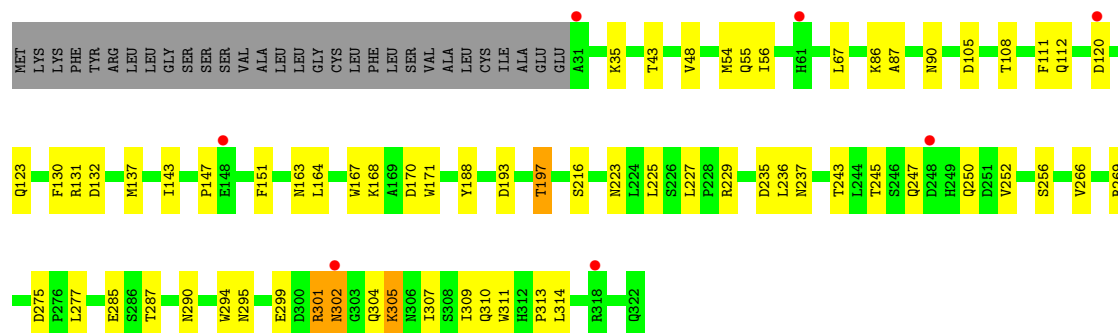


● Molecule 2: Nitrite oxidoreductase subunit A

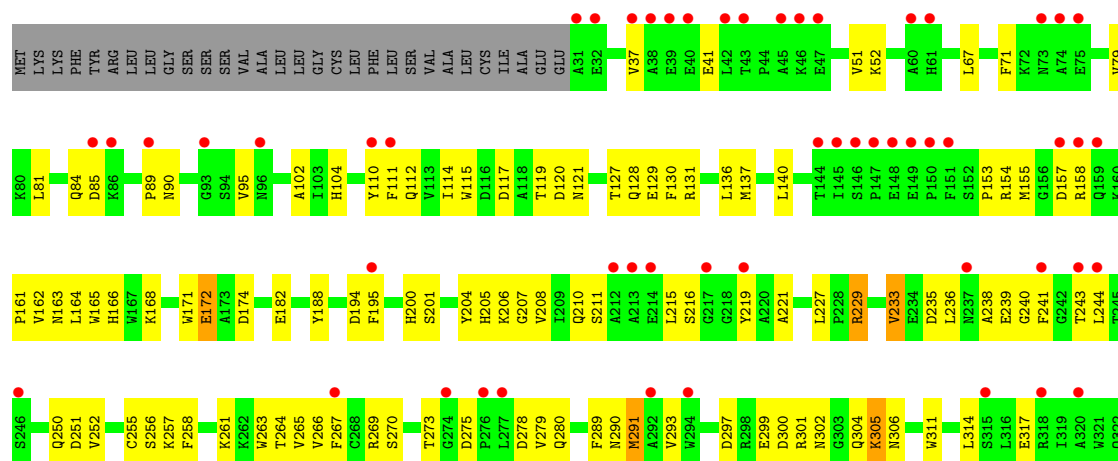




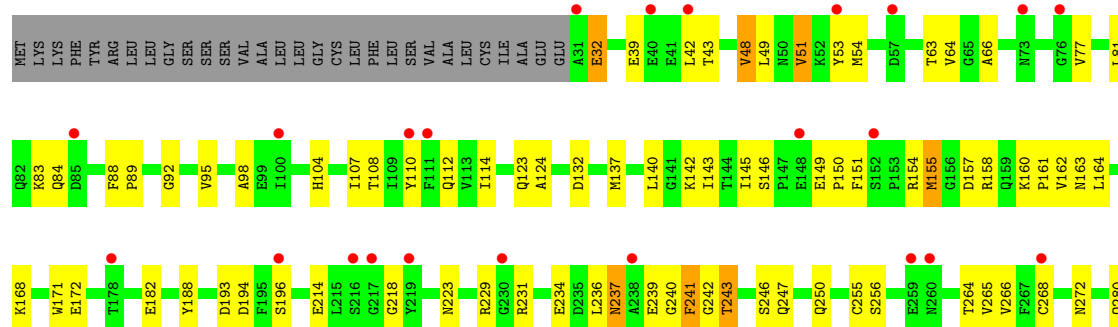
• Molecule 3: Nitrite oxidoreductase subunit C



• Molecule 3: Nitrite oxidoreductase subunit C

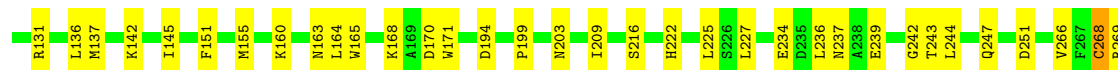
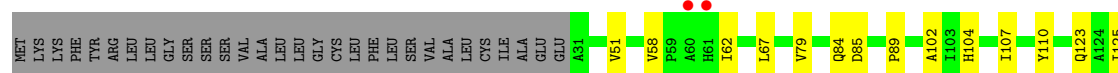


• Molecule 3: Nitrite oxidoreductase subunit C

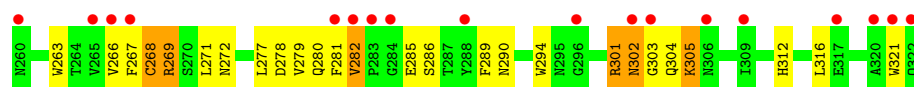
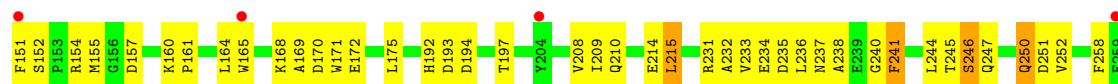
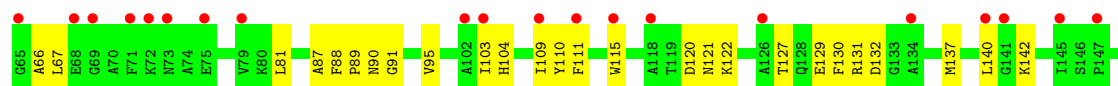
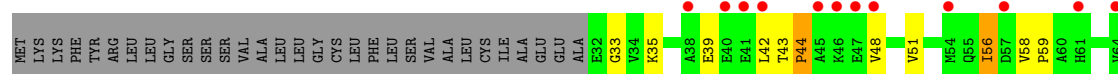




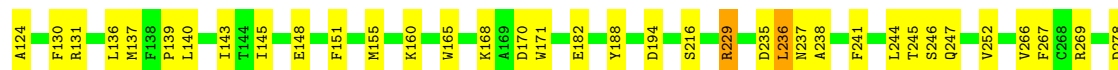
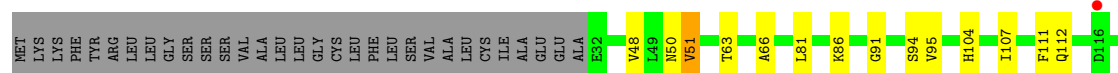
• Molecule 3: Nitrite oxidoreductase subunit C



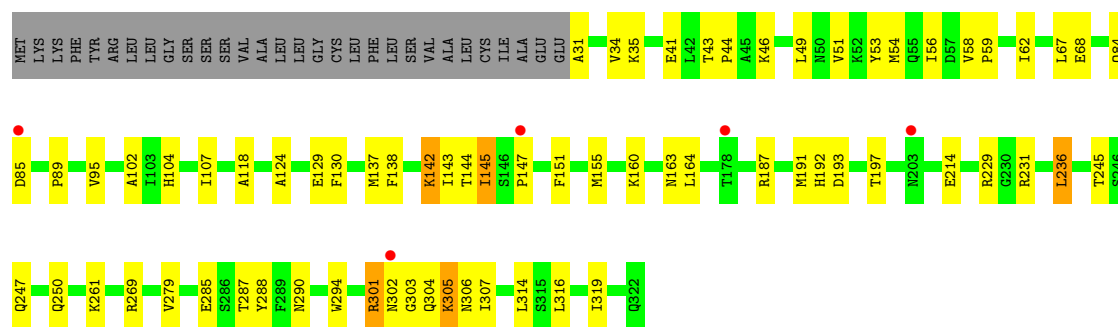
• Molecule 3: Nitrite oxidoreductase subunit C



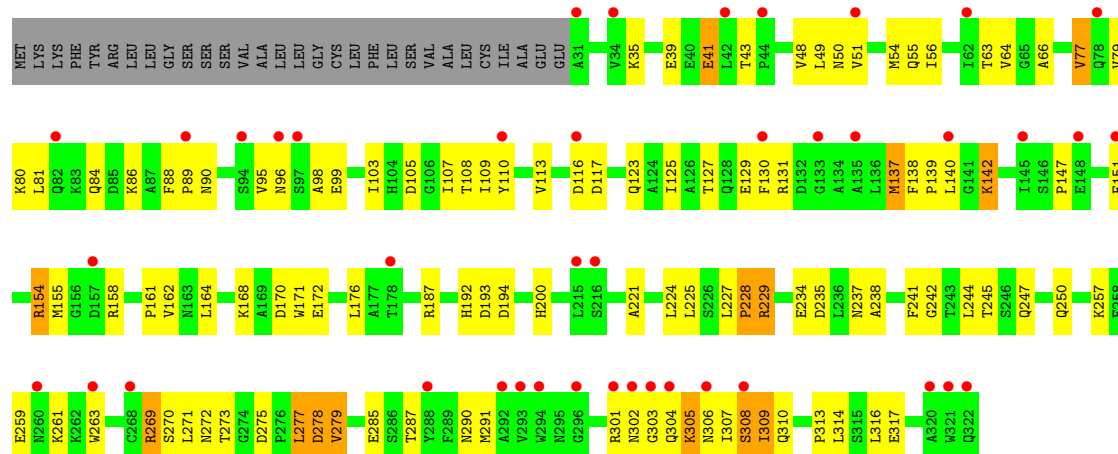
• Molecule 3: Nitrite oxidoreductase subunit C



• Molecule 3: Nitrite oxidoreductase subunit C



• Molecule 3: Nitrite oxidoreductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	177.63Å 206.47Å 527.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.25 – 2.97 192.25 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (192.25-2.97) 95.4 (192.25-2.97)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.14rc1	Depositor
R, R_{free}	0.223 , 0.255 0.221 , 0.252	Depositor DCC
R_{free} test set	21282 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	115931	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MO, MD1, HEM, CA, SF4, F3S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	1/3450 (0.0%)	0.54	0/4676
1	D	0.39	2/2957 (0.1%)	0.53	1/4058 (0.0%)
1	G	0.24	0/3445	0.48	3/4670 (0.1%)
1	J	0.31	2/3462 (0.1%)	0.46	0/4690
1	M	0.32	0/3410	0.60	2/4632 (0.0%)
1	P	0.41	1/3422 (0.0%)	0.64	3/4646 (0.1%)
1	S	0.21	0/3434	0.44	0/4657
1	V	0.58	0/3339	0.90	8/4545 (0.2%)
2	B	0.47	2/9267 (0.0%)	0.66	2/12591 (0.0%)
2	E	0.52	1/7024 (0.0%)	0.89	19/9696 (0.2%)
2	H	0.41	7/9292 (0.1%)	0.62	9/12617 (0.1%)
2	K	0.47	6/9313 (0.1%)	0.62	11/12642 (0.1%)
2	N	0.42	2/9319 (0.0%)	0.62	8/12649 (0.1%)
2	Q	0.58	7/9165 (0.1%)	0.82	11/12465 (0.1%)
2	T	0.43	4/9298 (0.0%)	0.60	7/12625 (0.1%)
2	W	0.51	2/9187 (0.0%)	0.75	11/12501 (0.1%)
3	C	0.45	2/2338 (0.1%)	0.67	4/3175 (0.1%)
3	F	0.48	0/2123	0.81	0/2911
3	I	0.44	0/2272	0.81	7/3093 (0.2%)
3	L	0.57	2/2331 (0.1%)	0.67	2/3169 (0.1%)
3	O	0.54	1/2179 (0.0%)	0.86	4/2983 (0.1%)
3	R	0.50	1/2318 (0.0%)	0.61	2/3151 (0.1%)
3	U	0.44	0/2324	0.65	1/3158 (0.0%)
3	X	0.50	1/2282 (0.0%)	0.78	1/3104 (0.0%)
All	All	0.46	44/116951 (0.0%)	0.68	116/159104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	H	0	1
2	K	0	2
2	W	0	3
All	All	0	7

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	663	VAL	C-N	23.28	1.68	1.33
2	K	148	PHE	C-O	-21.18	1.14	1.23
1	D	294	TYR	C-O	15.02	1.30	1.23
2	W	148	PHE	C-O	-12.71	1.18	1.23
2	T	981	PRO	C-O	-9.13	1.13	1.24
2	H	228	MET	C-O	-7.39	1.14	1.24
2	N	148	PHE	C-O	-7.32	1.20	1.23
3	L	302	ASN	C-O	-7.02	1.17	1.24
2	B	981	PRO	C-O	-6.92	1.15	1.24
2	K	397	PRO	C-O	-6.79	1.15	1.24
2	H	229	GLY	C-O	-6.73	1.16	1.24
2	H	232	GLY	C-O	-6.54	1.15	1.23
2	H	923	HIS	C-O	-6.41	1.18	1.24
2	N	1121	PRO	C-O	-6.36	1.15	1.24
3	R	313	PRO	C-O	-6.17	1.17	1.23
2	B	715	PRO	C-O	-6.11	1.16	1.24
3	X	228	PRO	C-O	-6.03	1.19	1.24
2	Q	1097	VAL	CB-CG2	-5.99	1.32	1.52
2	K	413	PRO	C-O	-5.99	1.16	1.24
2	T	148	PHE	C-O	5.92	1.31	1.24
1	A	22	PRO	C-O	-5.85	1.16	1.23
3	C	304	GLN	C-O	-5.83	1.17	1.23
2	K	923	HIS	C-O	-5.71	1.19	1.24
1	D	133	ILE	CA-C	5.70	1.57	1.53
2	H	153	PRO	C-O	-5.66	1.17	1.24
2	W	592	PRO	C-O	-5.63	1.17	1.23
3	O	44	PRO	C-O	-5.43	1.17	1.23
2	H	760	PHE	C-O	-5.43	1.17	1.24
2	T	922	VAL	C-O	-5.42	1.17	1.24
2	T	923	HIS	C-O	-5.41	1.19	1.24
2	K	33	PRO	C-O	-5.36	1.17	1.24
2	K	148	PHE	CA-C	5.35	1.57	1.53
3	C	302	ASN	C-O	-5.32	1.19	1.24
2	Q	545	PRO	C-O	-5.31	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	195	PRO	C-O	-5.28	1.17	1.24
2	Q	335	PRO	C-O	-5.17	1.17	1.24
3	L	304	GLN	C-O	-5.12	1.18	1.23
1	J	142	PRO	C-O	-5.11	1.17	1.24
2	H	303	ILE	C-O	-5.11	1.18	1.24
1	J	11	ARG	C-O	-5.07	1.17	1.23
2	Q	724	GLY	C-O	-5.03	1.18	1.24
1	P	107	PRO	C-O	-5.03	1.17	1.24
2	Q	69	PRO	C-O	-5.01	1.17	1.24
2	Q	339	PRO	C-O	-5.01	1.18	1.24

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	954	GLU	O-C-N	-22.56	95.87	123.17
3	I	305	LYS	CB-CA-C	12.96	137.23	110.40
2	E	663	VAL	CA-C-N	-12.86	98.64	121.14
2	E	663	VAL	C-N-CA	-12.86	98.64	121.14
2	N	1124	THR	CB-CA-C	-10.24	94.80	110.88
2	Q	69	PRO	N-CA-CB	-10.21	92.53	103.25
2	K	1022	ALA	N-CA-C	10.15	123.43	110.24
3	I	305	LYS	N-CA-C	-9.93	97.72	110.53
2	E	874	GLY	CA-C-N	-9.78	114.82	123.33
2	E	874	GLY	C-N-CA	-9.78	114.82	123.33
2	Q	954	GLU	CB-CA-C	8.80	129.23	112.43
1	V	211	TYR	CB-CA-C	8.29	123.89	110.88
2	K	1021	SER	CA-C-N	8.19	132.86	120.82
2	K	1021	SER	C-N-CA	8.19	132.86	120.82
2	W	651	PHE	CA-C-N	-7.70	113.27	122.44
2	W	651	PHE	C-N-CA	-7.70	113.27	122.44
1	M	257	ARG	CB-CA-C	-7.59	98.20	110.79
2	W	900	THR	CA-CB-OG1	-7.55	98.28	109.60
2	N	115	CYS	CB-CA-C	7.44	123.10	109.71
1	V	124	ASN	CB-CA-C	7.32	122.29	111.89
1	G	97	LYS	N-CA-C	-7.12	103.60	111.36
2	E	608	ARG	CA-C-N	-7.10	111.42	121.72
2	E	608	ARG	C-N-CA	-7.10	111.42	121.72
2	T	50	GLU	CB-CA-C	-7.06	98.22	110.72
3	U	304	GLN	N-CA-C	-7.02	95.54	108.24
2	E	665	GLN	N-CA-C	-6.91	103.75	111.28
2	H	43	THR	CB-CA-C	-6.73	98.10	110.62
3	L	305	LYS	CB-CA-C	6.73	122.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	240	GLY	CA-C-O	-6.63	117.91	122.22
1	V	287	GLN	CA-CB-CG	-6.49	101.13	114.10
2	H	653	ASN	CB-CA-C	6.48	121.44	111.39
2	W	504	PRO	CB-CA-C	-6.39	103.59	111.64
2	K	653	ASN	CA-CB-CG	6.30	118.90	112.60
2	Q	760	PHE	CA-CB-CG	-6.19	107.61	113.80
1	V	17	TYR	CB-CA-C	6.11	119.75	109.48
2	W	221	THR	CA-CB-OG1	-6.11	100.44	109.60
2	K	1022	ALA	CA-C-N	6.09	130.55	121.72
2	K	1022	ALA	C-N-CA	6.09	130.55	121.72
2	K	655	ASN	N-CA-C	-6.04	103.05	110.65
2	Q	356	THR	OG1-CB-CG2	5.99	121.28	109.30
2	T	983	ASP	CA-CB-CG	5.97	118.57	112.60
3	C	302	ASN	CB-CA-C	5.96	123.55	116.63
2	Q	483	GLU	N-CA-C	-5.93	104.50	110.97
1	P	308	PRO	CB-CA-C	-5.91	104.31	111.46
1	V	374	THR	OG1-CB-CG2	5.90	121.10	109.30
1	D	133	ILE	O-C-N	5.86	125.06	121.37
2	Q	653	ASN	CB-CA-C	5.84	120.83	111.66
3	I	305	LYS	CA-C-N	5.84	131.78	123.14
3	I	305	LYS	C-N-CA	5.84	131.78	123.14
2	W	39	ASN	CB-CA-C	-5.71	103.59	110.15
2	T	445	THR	CB-CA-C	-5.69	99.55	110.24
3	I	240	GLY	CA-C-O	-5.67	118.23	122.37
2	Q	936	ASN	CB-CA-C	5.65	121.08	110.63
3	L	278	ASP	CB-CA-C	5.63	118.95	109.48
2	W	924	SER	N-CA-C	-5.62	107.08	114.04
2	B	983	ASP	CB-CA-C	-5.61	100.86	110.24
2	N	51	SER	CA-C-N	-5.60	112.64	120.53
2	N	51	SER	C-N-CA	-5.60	112.64	120.53
2	E	680	THR	N-CA-CB	5.59	119.29	110.23
3	R	235	ASP	CA-CB-CG	5.57	118.17	112.60
1	V	125	ILE	O-C-N	5.51	128.02	121.80
2	T	549	THR	CA-CB-OG1	-5.47	101.40	109.60
2	T	50	GLU	CA-C-N	5.46	131.56	121.52
2	T	50	GLU	C-N-CA	5.46	131.56	121.52
3	O	245	THR	CA-CB-OG1	-5.45	101.43	109.60
3	I	321	TRP	CA-C-O	-5.44	115.53	121.84
3	R	50	ASN	CB-CA-C	-5.43	100.78	109.75
2	E	1016	THR	OG1-CB-CG2	5.41	120.11	109.30
1	M	105	GLY	CA-C-O	-5.40	117.32	122.13
2	W	540	ARG	CA-C-N	5.39	127.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	540	ARG	C-N-CA	5.39	127.50	120.28
2	W	938	ASN	N-CA-C	-5.39	106.88	113.50
3	C	302	ASN	CA-C-N	5.38	133.19	121.19
3	C	302	ASN	C-N-CA	5.38	133.19	121.19
2	E	1057	GLN	N-CA-C	-5.37	106.32	112.92
2	H	921	THR	CA-C-N	-5.36	116.69	122.59
2	H	921	THR	C-N-CA	-5.36	116.69	122.59
2	K	452	THR	CA-CB-OG1	-5.36	101.55	109.60
2	B	425	ARG	CG-CD-NE	-5.33	100.26	112.00
3	O	56	ILE	CA-CB-CG1	5.31	119.42	110.40
1	G	127	GLN	CA-CB-CG	-5.29	103.53	114.10
3	C	302	ASN	CA-CB-CG	5.28	117.88	112.60
2	K	412	GLY	CA-C-N	5.27	124.89	119.56
2	K	412	GLY	C-N-CA	5.27	124.89	119.56
2	W	501	THR	CA-C-O	-5.27	114.72	120.36
2	Q	384	PRO	CB-CA-C	-5.26	103.94	112.62
2	E	1019	LYS	CA-C-N	-5.25	115.55	122.85
2	E	1019	LYS	C-N-CA	-5.25	115.55	122.85
2	N	510	ARG	CB-CA-C	-5.25	102.60	110.90
3	I	304	GLN	CB-CA-C	5.23	118.41	111.14
2	H	1021	SER	N-CA-C	-5.22	99.67	110.80
1	G	99	THR	N-CA-C	-5.21	99.29	108.20
2	E	957	ILE	CA-CB-CG1	5.20	119.24	110.40
2	E	1052	ARG	N-CA-C	-5.19	105.70	111.36
2	E	1011	TYR	CB-CA-C	5.19	116.55	108.61
3	O	302	ASN	CA-CB-CG	5.17	117.77	112.60
1	P	348	THR	CA-CB-OG1	-5.17	101.85	109.60
1	P	154	GLN	CB-CA-C	5.16	116.14	108.87
2	T	983	ASP	CB-CA-C	-5.15	101.99	110.08
2	K	917	LYS	CB-CA-C	5.15	118.20	109.50
1	V	187	CYS	CA-C-N	5.14	124.64	119.19
1	V	187	CYS	C-N-CA	5.14	124.64	119.19
2	H	228	MET	N-CA-C	-5.13	99.87	110.80
2	N	1021	SER	CA-C-N	5.13	131.43	122.81
2	N	1021	SER	C-N-CA	5.13	131.43	122.81
2	N	53	TYR	CB-CA-C	5.09	119.50	110.85
2	Q	861	ILE	CA-C-N	-5.08	116.12	122.48
2	Q	861	ILE	C-N-CA	-5.08	116.12	122.48
2	E	956	GLN	CA-C-N	-5.07	115.89	122.94
2	E	956	GLN	C-N-CA	-5.07	115.89	122.94
2	Q	938	ASN	CB-CA-C	-5.06	100.90	110.01
3	X	107	ILE	N-CA-C	-5.05	107.63	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1020	HIS	CA-C-N	5.03	131.15	121.54
2	H	1020	HIS	C-N-CA	5.03	131.15	121.54
2	E	650	TRP	N-CA-CB	5.02	119.34	111.56
2	E	798	VAL	N-CA-C	5.01	117.22	108.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	446	ARG	Sidechain
2	H	954	GLU	Mainchain
2	K	1021	SER	Mainchain
2	K	446	ARG	Sidechain
2	W	1020	HIS	Peptide
2	W	111	ASN	Peptide
2	W	124	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3349	0	3216	93	0
1	D	2872	0	2267	153	0
1	G	3344	0	3208	93	0
1	J	3361	0	3242	89	0
1	M	3309	0	3136	157	0
1	P	3321	0	3149	122	0
1	S	3333	0	3198	94	0
1	V	3239	0	2948	268	0
2	B	9003	0	8576	375	0
2	E	6871	0	4598	326	0
2	H	9028	0	8644	262	0
2	K	9046	0	8683	310	0
2	N	9052	0	8682	323	0
2	Q	8902	0	8343	454	0
2	T	9034	0	8643	278	0
2	W	8920	0	8364	455	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2281	0	2171	61	0
3	F	2068	0	1752	153	0
3	I	2216	0	2068	157	0
3	L	2274	0	2151	66	0
3	O	2124	0	1863	126	0
3	R	2261	0	2134	61	0
3	U	2267	0	2146	56	0
3	X	2225	0	2060	144	0
4	A	24	0	0	1	0
4	B	8	0	0	0	0
4	D	24	0	0	7	0
4	E	8	0	0	0	0
4	G	24	0	0	3	0
4	H	8	0	0	0	0
4	J	24	0	0	5	0
4	K	8	0	0	1	0
4	M	24	0	0	3	0
4	N	8	0	0	3	0
4	P	24	0	0	3	0
4	Q	8	0	0	3	0
4	S	24	0	0	3	0
4	T	8	0	0	3	0
4	V	24	0	0	6	0
4	W	8	0	0	2	0
5	A	7	0	0	0	0
5	D	7	0	0	3	0
5	G	7	0	0	0	0
5	J	7	0	0	0	0
5	M	7	0	0	2	0
5	P	7	0	0	0	0
5	S	7	0	0	0	0
5	V	7	0	0	5	0
6	B	94	0	43	14	0
6	E	94	0	41	19	0
6	H	94	0	42	14	0
6	K	94	0	43	18	0
6	N	94	0	43	19	0
6	Q	94	0	41	19	0
6	T	94	0	43	13	0
6	W	94	0	44	21	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
7	Q	1	0	0	0	0
7	T	1	0	0	0	0
7	W	1	0	0	0	0
8	C	43	0	30	8	0
8	F	43	0	30	25	0
8	I	43	0	30	29	0
8	L	43	0	30	7	0
8	O	43	0	30	11	0
8	R	43	0	30	5	0
8	U	43	0	30	4	0
8	X	43	0	30	15	0
9	C	2	0	0	0	0
9	F	2	0	0	0	0
9	I	2	0	0	0	0
9	L	2	0	0	0	0
9	O	2	0	0	0	0
9	R	2	0	0	0	0
9	U	2	0	0	0	0
9	X	2	0	0	1	0
10	A	37	0	0	0	0
10	B	72	0	0	7	0
10	C	35	0	0	1	0
10	D	6	0	0	0	0
10	E	13	0	0	1	0
10	F	8	0	0	0	0
10	G	25	0	0	1	0
10	H	83	0	0	2	0
10	I	20	0	0	1	0
10	J	28	0	0	2	0
10	K	74	0	0	3	0
10	L	30	0	0	0	0
10	M	10	0	0	0	0
10	N	76	0	0	5	0
10	O	17	0	0	3	0
10	P	16	0	0	4	0
10	Q	43	0	0	3	0
10	R	22	0	0	1	0
10	S	20	0	0	1	0
10	T	62	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	U	25	0	0	3	0
10	V	12	0	0	1	0
10	W	41	0	0	3	0
10	X	24	0	0	3	0
All	All	115931	0	105822	4324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (4324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:939:PHE:CE2	2:W:1004:ARG:CD	1.78	1.66
1:V:16:PRO:CG	1:V:128:TRP:CE2	1.81	1.62
2:W:939:PHE:CE2	2:W:1004:ARG:HD2	1.10	1.59
1:V:16:PRO:HG3	1:V:128:TRP:CZ2	0.98	1.50
1:V:241:ARG:HH12	1:V:257:ARG:CG	1.20	1.50
1:V:16:PRO:HG3	1:V:128:TRP:CE2	1.38	1.47
2:E:663:VAL:C	2:E:664:TYR:N	1.68	1.46
2:W:939:PHE:CD2	2:W:1004:ARG:HD2	1.50	1.45
1:V:16:PRO:CG	1:V:128:TRP:CZ2	1.85	1.44
1:V:241:ARG:NH1	1:V:257:ARG:CG	1.77	1.41
1:V:16:PRO:CG	1:V:128:TRP:NE1	1.80	1.39
1:V:126:ASN:ND2	3:X:88:PHE:HE1	1.22	1.35
2:E:193:SER:CB	2:E:217:ALA:O	1.78	1.31
2:Q:446:ARG:NH2	2:Q:821:PHE:O	1.59	1.30
1:V:16:PRO:CD	1:V:128:TRP:HE1	1.44	1.29
3:I:302:ASN:OD1	8:I:401:HEM:HAA2	1.29	1.28
1:V:241:ARG:HH12	1:V:257:ARG:CD	1.46	1.28
2:Q:551:ASN:O	2:Q:557:SER:CB	1.81	1.27
2:Q:311:GLU:OE2	2:Q:1019:LYS:NZ	1.64	1.27
1:V:241:ARG:NH2	2:W:90:GLU:OE2	1.67	1.26
1:V:16:PRO:HG2	1:V:128:TRP:NE1	1.39	1.26
1:V:241:ARG:NH1	1:V:257:ARG:HG2	0.91	1.23
2:E:356:THR:OG1	2:E:847:HIS:CB	1.86	1.23
2:E:193:SER:CA	2:E:217:ALA:O	1.89	1.21
2:B:433:VAL:CG1	2:B:444:ILE:HD13	1.71	1.19
1:V:126:ASN:ND2	3:X:88:PHE:CE1	1.99	1.19
1:V:16:PRO:HG2	1:V:128:TRP:CE2	1.56	1.18
1:V:189:ARG:HG3	1:V:211:TYR:HE2	1.02	1.17
2:W:923:HIS:O	2:W:1021:SER:HB3	1.44	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:LYS:HE3	8:C:401:HEM:NB	1.58	1.17
1:M:336:ARG:NH2	1:M:359:GLU:HG2	1.60	1.16
3:X:81:LEU:HD21	3:X:308:SER:CA	1.73	1.16
2:E:192:TYR:O	2:E:197:GLY:HA3	1.46	1.15
3:I:155:MET:CE	3:I:241:PHE:HA	1.76	1.15
3:I:154:ARG:HG2	8:I:401:HEM:HBB1	1.23	1.14
1:V:252:ARG:NH2	1:V:386:ASP:OD2	1.78	1.14
2:W:939:PHE:CE2	2:W:1004:ARG:HD3	1.77	1.14
3:I:154:ARG:CB	8:I:401:HEM:HBB2	1.76	1.14
1:V:189:ARG:HG3	1:V:211:TYR:CE2	1.83	1.13
2:W:937:ASN:ND2	2:W:954:GLU:O	1.80	1.13
3:F:120:ASP:HB3	3:F:258:PHE:CE1	1.84	1.12
1:V:189:ARG:HG2	8:X:401:HEM:HBA2	1.26	1.12
1:V:189:ARG:NH2	1:V:207:ARG:O	1.82	1.12
2:N:1135:MET:CE	2:N:1138:PHE:HD2	1.62	1.12
3:I:154:ARG:HG2	8:I:401:HEM:CBB	1.78	1.12
3:I:305:LYS:NZ	8:I:401:HEM:NB	1.97	1.12
2:W:974:TYR:HE1	2:W:1052:ARG:HD3	1.03	1.12
2:W:924:SER:OG	6:W:5801:MD1:O2A	1.67	1.12
3:I:154:ARG:HB3	8:I:401:HEM:HBB2	1.32	1.11
2:Q:91:GLN:NE2	2:Q:113:ARG:O	1.81	1.11
2:N:1135:MET:HE3	2:N:1138:PHE:HD2	1.03	1.11
1:A:126:ASN:ND2	3:C:90:ASN:OD1	1.83	1.11
1:P:257:ARG:NH1	2:Q:89:VAL:O	1.85	1.10
3:I:154:ARG:CG	8:I:401:HEM:CBB	2.29	1.10
1:M:257:ARG:HH22	2:N:90:GLU:HG3	1.17	1.09
1:M:209:ARG:NH1	3:O:234:GLU:OE1	1.82	1.09
1:V:189:ARG:NH1	1:V:209:ARG:HB2	1.67	1.09
1:V:252:ARG:HH22	1:V:386:ASP:CG	1.60	1.09
1:M:21:ARG:NH2	1:M:180:TYR:OH	1.86	1.08
2:W:435:ASP:HB2	2:W:442:LYS:HD2	1.29	1.08
3:I:48:VAL:HG22	3:I:313:PRO:HB2	1.36	1.07
1:M:189:ARG:NH2	3:O:244:LEU:O	1.87	1.06
2:B:433:VAL:HG11	2:B:444:ILE:HD13	1.31	1.06
2:W:1124:THR:HG23	2:W:1126:TYR:CD2	1.91	1.06
3:I:302:ASN:CG	8:I:401:HEM:HAA2	1.81	1.06
2:Q:394:ARG:HH22	2:Q:829:GLN:NE2	1.54	1.05
2:Q:499:SER:OG	2:Q:894:TRP:NE1	1.89	1.05
3:F:171:TRP:CE2	3:F:229:ARG:NE	2.24	1.05
2:N:1119:TRP:O	2:N:1122:VAL:HG23	1.56	1.05
1:V:212:ARG:NH2	3:X:129:GLU:O	1.90	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:939:PHE:CD2	2:W:1004:ARG:CD	2.22	1.04
2:T:661:LYS:O	2:T:1060:THR:OG1	1.76	1.03
2:T:823:THR:HB	2:T:829:GLN:HE21	1.16	1.03
1:M:257:ARG:NH2	2:N:90:GLU:HG3	1.73	1.03
2:N:1135:MET:HE2	2:N:1139:LEU:HD21	1.07	1.03
2:Q:857:LEU:HB2	2:Q:900:THR:HG21	1.36	1.03
3:X:81:LEU:HD21	3:X:308:SER:N	1.73	1.03
2:N:1135:MET:HE3	2:N:1138:PHE:CD2	1.92	1.02
2:Q:115:CYS:HB2	2:Q:314:MET:HE2	1.34	1.02
2:W:381:THR:HG22	2:W:383:PHE:H	1.21	1.02
2:Q:394:ARG:NH2	2:Q:829:GLN:HE22	1.57	1.02
3:C:305:LYS:HE3	8:C:401:HEM:C1B	1.95	1.01
2:K:937:ASN:ND2	2:K:954:GLU:H	1.56	1.01
1:M:243:GLU:OE1	2:N:54:ARG:NH1	1.93	1.01
2:Q:258:PRO:O	2:Q:608:ARG:NH2	1.93	1.01
2:W:974:TYR:HE1	2:W:1052:ARG:CD	1.72	1.01
2:E:123:ARG:HH11	3:F:194:ASP:HB2	1.23	1.01
3:I:302:ASN:HD22	3:I:303:GLY:N	1.58	1.01
1:D:149:ALA:O	2:E:1009:PRO:HG2	1.58	1.01
2:W:974:TYR:CE1	2:W:1052:ARG:HD3	1.95	1.01
2:K:917:LYS:HZ1	6:K:5801:MD1:H15	1.03	1.01
2:E:193:SER:CB	2:E:217:ALA:C	2.34	1.01
2:Q:937:ASN:ND2	2:Q:954:GLU:O	1.93	1.01
3:X:81:LEU:CD2	3:X:307:ILE:C	2.34	1.01
2:W:38:ASP:O	10:W:5901:HOH:O	1.77	1.00
2:E:848:ARG:CB	2:E:860:ALA:O	2.09	1.00
2:W:857:LEU:HB2	2:W:900:THR:HG21	1.44	1.00
2:Q:937:ASN:HD21	2:Q:954:GLU:N	1.60	1.00
2:W:1124:THR:HG23	2:W:1126:TYR:HD2	1.23	1.00
2:Q:549:THR:OG1	2:Q:551:ASN:OD1	1.80	0.99
2:B:479:MET:HE3	2:B:484:MET:HE3	1.44	0.99
2:N:115:CYS:HB3	4:N:5804:SF4:S2	2.02	0.99
1:V:189:ARG:HH12	1:V:209:ARG:HB2	1.18	0.99
3:I:305:LYS:NZ	8:I:401:HEM:NA	2.09	0.99
1:M:336:ARG:HH22	1:M:359:GLU:HG2	1.24	0.98
1:V:241:ARG:NH2	2:W:90:GLU:CD	2.19	0.98
1:M:239:TYR:OH	2:N:50:GLU:O	1.81	0.98
2:Q:433:VAL:HG21	2:Q:460:PRO:HB3	1.43	0.98
1:V:241:ARG:HH22	2:W:90:GLU:CD	1.71	0.97
3:O:155:MET:SD	8:O:401:HEM:ND	2.38	0.97
2:K:917:LYS:O	2:K:1019:LYS:HE2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:193:SER:O	2:T:216:GLY:O	1.81	0.97
1:V:16:PRO:HD3	1:V:128:TRP:HE1	1.30	0.96
3:X:81:LEU:HD22	3:X:307:ILE:C	1.89	0.96
3:F:171:TRP:CD2	3:F:229:ARG:HD2	2.01	0.96
3:I:155:MET:HE3	3:I:241:PHE:HA	1.46	0.96
2:Q:547:MET:HE1	2:Q:830:ALA:HB2	1.45	0.96
2:H:658:ASN:OD1	2:H:1024:ILE:HG12	1.65	0.96
2:E:663:VAL:C	2:E:664:TYR:CA	2.39	0.95
2:N:1135:MET:CE	2:N:1138:PHE:CD2	2.47	0.95
3:F:120:ASP:HB3	3:F:258:PHE:CD1	2.00	0.95
3:I:53:TYR:CE1	3:I:319:ILE:HA	2.01	0.95
2:N:1135:MET:HE2	2:N:1139:LEU:CD2	1.95	0.95
3:O:303:GLY:O	3:O:305:LYS:HD3	1.67	0.95
1:V:33:ASN:ND2	1:V:331:PHE:CZ	2.34	0.95
3:X:81:LEU:HD21	3:X:308:SER:HA	1.48	0.95
2:N:923:HIS:O	2:N:1021:SER:HB3	1.66	0.95
3:O:130:PHE:CE2	3:O:301:ARG:HD3	2.00	0.95
3:I:302:ASN:ND2	3:I:303:GLY:H	1.64	0.94
2:W:939:PHE:HE2	2:W:1004:ARG:CB	1.80	0.94
1:V:149:ALA:HB2	1:V:168:PHE:HD2	1.31	0.94
2:B:1135:MET:CE	2:B:1138:PHE:CD2	2.50	0.93
3:I:155:MET:HE2	3:I:241:PHE:HB3	1.47	0.93
2:W:293:MET:HE1	2:W:313:LYS:HD2	1.49	0.93
3:O:294:TRP:NE1	3:O:305:LYS:HB3	1.83	0.93
1:V:207:ARG:HG2	1:V:207:ARG:HH11	1.31	0.93
3:I:155:MET:CE	3:I:241:PHE:CA	2.47	0.93
2:W:654:VAL:HG12	6:W:5801:MD1:O2B	1.69	0.92
2:Q:640:THR:OG1	2:Q:1071:ASP:OD1	1.87	0.92
1:M:256:THR:HG21	1:M:259:MET:HE2	1.52	0.92
2:W:438:SER:OG	10:W:5902:HOH:O	1.86	0.91
2:Q:445:THR:HG22	2:Q:448:ASP:OD2	1.70	0.91
1:V:15:TYR:CE2	1:V:185:ALA:HB2	2.03	0.91
3:I:302:ASN:OD1	8:I:401:HEM:CAA	2.16	0.91
2:B:433:VAL:HG13	2:B:444:ILE:HD13	1.50	0.91
1:V:16:PRO:CD	1:V:128:TRP:NE1	2.21	0.91
3:F:229:ARG:HG2	3:F:229:ARG:HH11	1.35	0.91
2:Q:70:ASN:H	2:Q:231:LEU:HD11	1.36	0.91
2:W:435:ASP:CB	2:W:442:LYS:HD2	2.00	0.91
1:P:255:GLU:OE1	1:P:346:ARG:NH2	2.03	0.90
1:V:259:MET:CE	1:V:269:GLN:HG3	2.01	0.90
3:X:275:ASP:HB3	3:X:278:ASP:HB2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:MET:CE	2:B:1138:PHE:HD2	1.83	0.90
2:N:1135:MET:CE	2:N:1139:LEU:HD21	1.98	0.90
2:W:977:VAL:HG22	2:W:1001:LEU:HD23	1.51	0.90
2:Q:69:PRO:O	2:Q:922:VAL:HG11	1.71	0.90
2:B:1135:MET:HE3	2:B:1138:PHE:HD2	1.38	0.89
3:F:155:MET:SD	8:F:401:HEM:NC	2.45	0.89
1:P:276:PRO:HB3	1:P:286:HIS:NE2	1.88	0.89
2:Q:394:ARG:HH22	2:Q:829:GLN:CD	1.81	0.89
2:W:939:PHE:HE2	2:W:1004:ARG:HB3	1.36	0.89
3:I:305:LYS:HD3	3:I:307:ILE:CG2	2.03	0.89
2:W:976:TYR:CD1	2:W:1000:ARG:NH2	2.41	0.89
2:B:101:LEU:HD12	2:B:802:LEU:HD11	1.54	0.89
2:N:1034:GLU:OE2	2:N:1053:TYR:OH	1.88	0.89
2:Q:433:VAL:CG2	2:Q:460:PRO:HB3	2.02	0.89
2:W:893:SER:O	2:W:897:THR:HG23	1.71	0.89
2:Q:394:ARG:NH2	2:Q:829:GLN:NE2	2.17	0.89
2:W:977:VAL:CG2	2:W:1001:LEU:HD23	2.03	0.89
2:K:31:LEU:HD11	3:R:107:ILE:HD11	1.55	0.89
2:Q:759:LYS:O	2:Q:763:GLU:HG3	1.72	0.89
2:B:1135:MET:HE3	2:B:1138:PHE:CD2	2.06	0.88
3:L:302:ASN:O	3:L:305:LYS:HE2	1.71	0.88
3:I:154:ARG:CB	8:I:401:HEM:CBB	2.51	0.88
1:M:336:ARG:NH2	1:M:359:GLU:CG	2.35	0.88
3:O:155:MET:SD	8:O:401:HEM:NC	2.46	0.88
3:L:84:GLN:NE2	3:L:303:GLY:O	2.06	0.88
2:T:653:ASN:O	2:T:653:ASN:ND2	2.07	0.88
2:W:655:ASN:ND2	2:W:685:THR:HB	1.89	0.88
2:E:218:GLY:O	2:E:219:THR:HG22	1.72	0.88
1:V:259:MET:HE3	1:V:269:GLN:HG3	1.54	0.88
3:I:302:ASN:HD22	3:I:303:GLY:H	0.92	0.88
1:V:68:TYR:OH	2:W:1131:GLU:OE2	1.91	0.88
3:X:41:GLU:HB3	3:X:309:ILE:HB	1.55	0.88
3:I:155:MET:CE	3:I:241:PHE:CB	2.51	0.87
3:F:137:MET:HE1	3:F:155:MET:HA	1.54	0.87
3:I:302:ASN:ND2	3:I:303:GLY:N	2.20	0.87
2:W:857:LEU:HB2	2:W:900:THR:CG2	2.04	0.87
3:I:303:GLY:HA2	3:I:305:LYS:HE3	1.57	0.87
2:B:58:GLN:OE1	10:B:5901:HOH:O	1.90	0.87
2:W:153:PRO:O	2:W:157:THR:HG23	1.73	0.87
3:I:48:VAL:CG2	3:I:313:PRO:HB2	2.05	0.87
2:Q:917:LYS:HD2	6:Q:5802:MD1:H15	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:TRP:CE2	3:F:229:ARG:CD	2.58	0.86
2:Q:96:GLN:HG2	2:Q:108:ARG:HG2	1.56	0.86
3:I:154:ARG:CG	8:I:401:HEM:HBB2	2.01	0.86
3:O:303:GLY:HA2	3:O:305:LYS:CD	2.05	0.86
2:E:193:SER:HA	2:E:217:ALA:O	1.75	0.86
1:P:108:TYR:OH	10:P:601:HOH:O	1.93	0.86
3:X:81:LEU:CD2	3:X:308:SER:N	2.38	0.86
2:Q:1138:PHE:HA	2:Q:1143:LEU:HD23	1.55	0.86
2:W:934:ILE:HD11	2:W:952:VAL:HG13	1.55	0.86
2:B:433:VAL:CG1	2:B:444:ILE:CD1	2.54	0.86
3:F:164:LEU:N	3:F:236:LEU:O	2.08	0.85
2:Q:394:ARG:HH12	2:Q:829:GLN:NE2	1.74	0.85
2:Q:821:PHE:HE2	2:Q:828:LEU:HD21	1.41	0.85
3:C:301:ARG:HH21	3:C:301:ARG:HG2	1.41	0.85
3:I:155:MET:HE2	3:I:241:PHE:CB	2.06	0.85
3:I:242:GLY:HA2	8:I:401:HEM:O1A	1.76	0.85
2:W:977:VAL:HG22	2:W:1001:LEU:CD2	2.06	0.85
3:F:157:ASP:C	3:F:239:GLU:O	2.20	0.85
2:E:77:ILE:HD13	2:E:114:MET:CE	2.05	0.85
2:K:917:LYS:NZ	6:K:5801:MD1:H15	1.73	0.85
2:W:974:TYR:CE1	2:W:1052:ARG:CD	2.59	0.85
3:F:171:TRP:CZ2	3:F:229:ARG:NE	2.45	0.84
2:W:919:ARG:HG3	2:W:920:HIS:HD1	1.40	0.84
2:T:983:ASP:OD2	2:T:1061:ARG:NH1	2.10	0.84
1:V:33:ASN:ND2	1:V:331:PHE:CE2	2.46	0.84
2:K:425:ARG:HG2	2:K:425:ARG:HH11	1.42	0.84
2:Q:937:ASN:ND2	2:Q:954:GLU:H	1.75	0.83
2:H:36:VAL:HG12	3:I:243:THR:HG21	1.58	0.83
2:E:1003:LEU:O	2:E:1003:LEU:HD23	1.77	0.83
2:K:937:ASN:ND2	2:K:954:GLU:N	2.26	0.83
2:B:225:ARG:HH11	2:B:656:LEU:HD12	1.44	0.83
2:Q:625:ILE:CD1	2:Q:633:ARG:HE	1.92	0.83
2:E:77:ILE:HD13	2:E:114:MET:HE3	1.57	0.83
2:N:51:SER:O	2:N:52:VAL:C	2.22	0.83
2:B:276:GLN:HE22	2:B:1092:HIS:H	1.27	0.82
2:W:892:LYS:HB3	2:W:897:THR:HG22	1.61	0.82
2:B:641:HIS:CE1	2:B:1087:PHE:HB2	2.14	0.82
2:B:950:PRO:HD2	2:B:954:GLU:HB3	1.62	0.82
2:N:1020:HIS:HE1	6:N:5801:MD1:O11	1.63	0.82
1:V:189:ARG:CG	1:V:211:TYR:HE2	1.88	0.82
3:X:81:LEU:CD2	3:X:308:SER:HA	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:TRP:CZ2	3:F:229:ARG:CD	2.62	0.82
3:L:302:ASN:CG	3:L:303:GLY:H	1.87	0.82
2:E:1063:TRP:H	2:E:1096:THR:HG23	1.43	0.81
2:H:709:THR:HG22	2:H:718:GLN:HB2	1.61	0.81
2:K:379:LYS:HB3	2:K:450:GLY:HA2	1.62	0.81
2:Q:383:PHE:HE2	2:Q:548:LEU:HD21	1.44	0.81
2:T:316:GLU:OE1	10:T:5901:HOH:O	1.97	0.81
1:V:189:ARG:HG2	8:X:401:HEM:CBA	2.07	0.81
3:X:81:LEU:CD2	3:X:308:SER:CA	2.58	0.81
2:Q:115:CYS:HB2	2:Q:314:MET:CE	2.10	0.81
2:B:433:VAL:HG11	2:B:444:ILE:CD1	2.10	0.81
3:I:305:LYS:CD	3:I:307:ILE:HG23	2.11	0.81
2:Q:115:CYS:CB	2:Q:314:MET:HE2	2.10	0.81
2:Q:917:LYS:HZ1	6:Q:5801:MD1:H15	1.24	0.81
1:M:15:TYR:HE1	2:N:41:LEU:HD11	1.45	0.81
2:B:46:ASP:OD1	2:B:48:ARG:HG3	1.81	0.81
2:Q:640:THR:HB	2:Q:1087:PHE:HB3	1.62	0.81
3:I:154:ARG:CG	8:I:401:HEM:HBB1	1.99	0.80
2:T:115:CYS:HB3	4:T:5804:SF4:S2	2.20	0.80
1:V:25:GLN:HG2	1:V:302:ASN:HD22	1.46	0.80
1:V:259:MET:HE3	1:V:269:GLN:HB2	1.61	0.80
2:B:923:HIS:O	2:B:1021:SER:HB3	1.80	0.80
3:I:53:TYR:CE1	3:I:319:ILE:HG23	2.17	0.80
2:T:113:ARG:HG3	2:T:315:PRO:HB2	1.63	0.80
2:E:192:TYR:C	2:E:197:GLY:HA3	2.06	0.80
3:F:171:TRP:CE2	3:F:229:ARG:HD2	2.17	0.80
2:W:974:TYR:O	2:W:1108:ALA:HB3	1.82	0.80
2:N:1124:THR:CG2	2:N:1126:TYR:CD2	2.64	0.80
2:W:153:PRO:O	2:W:157:THR:CG2	2.30	0.80
2:W:937:ASN:CG	2:W:954:GLU:O	2.24	0.80
3:X:139:PRO:HB3	3:X:151:PHE:CE1	2.16	0.80
3:C:305:LYS:HE3	8:C:401:HEM:C4B	2.16	0.80
3:F:305:LYS:HE3	8:F:401:HEM:C4D	1.83	0.80
1:V:101:GLN:O	1:V:104:THR:HG22	1.81	0.80
2:N:305:THR:HG23	2:N:525:TYR:HB3	1.61	0.79
2:Q:307:LYS:HD3	2:Q:562:TRP:HB2	1.63	0.79
2:Q:937:ASN:HD21	2:Q:954:GLU:H	1.24	0.79
2:W:398:LYS:O	2:W:471:ILE:HD11	1.83	0.79
1:M:23:LYS:HD2	1:M:23:LYS:C	2.07	0.79
1:V:262:CYS:SG	1:V:266:ILE:HG12	2.21	0.79
2:E:193:SER:C	2:E:217:ALA:O	2.25	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:275:ASP:HB3	2:H:563:ALA:HB1	1.65	0.79
1:P:107:PRO:HG3	1:P:285:ARG:HH11	1.46	0.79
2:Q:351:ARG:HG3	2:Q:354:THR:HG21	1.64	0.79
3:X:109:ILE:O	3:X:110:TYR:HD1	1.66	0.79
2:B:217:ALA:HB2	2:B:262:LEU:CD1	2.13	0.79
2:E:501:THR:HG23	2:E:503:SER:H	1.46	0.79
2:K:91:GLN:HE21	2:K:114:MET:HB2	1.47	0.79
1:D:263:VAL:HA	2:E:112:PRO:CB	2.13	0.79
2:B:71:ASP:O	2:B:72:THR:HG22	1.82	0.79
2:Q:937:ASN:ND2	2:Q:954:GLU:N	2.30	0.78
2:B:655:ASN:ND2	2:B:924:SER:OG	2.16	0.78
2:T:823:THR:HB	2:T:829:GLN:NE2	1.96	0.78
2:W:939:PHE:CE2	2:W:1004:ARG:HB3	2.18	0.78
2:Q:336:GLU:OE2	6:Q:5802:MD1:O3'	2.02	0.78
2:Q:603:LEU:HD11	2:Q:772:ARG:HD3	1.65	0.78
2:K:433:VAL:HG21	2:K:460:PRO:HB3	1.66	0.78
1:M:4:VAL:HG23	1:M:19:GLU:HB2	1.64	0.78
1:D:149:ALA:O	2:E:1009:PRO:CG	2.31	0.78
3:I:53:TYR:CD1	3:I:319:ILE:HA	2.18	0.78
1:M:194:LYS:HG3	1:M:201:VAL:HG22	1.66	0.78
2:E:1063:TRP:H	2:E:1096:THR:CG2	1.97	0.78
1:V:16:PRO:CB	1:V:128:TRP:CZ2	2.65	0.78
2:W:222:PHE:HD1	2:W:648:VAL:HG13	1.49	0.78
2:W:974:TYR:CE1	2:W:1052:ARG:NH1	2.50	0.78
3:O:110:TYR:CD1	3:O:268:CYS:HB2	2.19	0.77
2:Q:394:ARG:NH1	2:Q:829:GLN:NE2	2.31	0.77
2:B:977:VAL:HG12	2:B:1103:VAL:HG11	1.66	0.77
1:M:190:LYS:HD2	2:N:37:VAL:HG13	1.66	0.77
2:B:1022:ALA:HB1	2:B:1050:SER:HB2	1.66	0.77
1:P:267:ARG:NH1	4:P:503:SF4:S1	2.58	0.77
1:G:25:GLN:HG2	1:G:302:ASN:ND2	1.98	0.77
1:P:231:VAL:CG2	10:P:604:HOH:O	2.31	0.77
1:V:40:THR:HG22	1:V:261:ALA:HB1	1.66	0.77
1:P:262:CYS:HB2	1:P:267:ARG:HD3	1.66	0.77
2:B:225:ARG:NH1	2:B:656:LEU:HD12	2.00	0.77
1:V:9:LEU:HD23	1:V:111:TYR:HD2	1.49	0.77
2:W:853:ALA:HA	2:W:1102:LEU:HD21	1.67	0.77
2:W:91:GLN:NE2	2:W:114:MET:HB2	1.99	0.77
2:W:551:ASN:O	2:W:557:SER:HB2	1.84	0.77
3:X:138:PHE:HB2	3:X:279:VAL:HG21	1.66	0.77
2:K:957:ILE:HB	2:K:1003:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:381:THR:HG22	2:T:383:PHE:H	1.51	0.77
3:U:51:VAL:HG22	3:U:316:LEU:HA	1.67	0.77
3:X:81:LEU:CD2	3:X:307:ILE:O	2.33	0.77
3:X:109:ILE:HB	3:X:271:LEU:CD2	2.15	0.77
2:E:617:TRP:HA	2:E:621:GLU:HG3	1.67	0.76
3:F:171:TRP:CE3	3:F:229:ARG:HD2	2.19	0.76
1:M:259:MET:HG2	1:M:269:GLN:HB2	1.65	0.76
1:P:107:PRO:HG3	1:P:285:ARG:NH1	2.00	0.76
2:Q:357:ALA:HB2	2:Q:847:HIS:CD2	2.20	0.76
1:M:23:LYS:HD2	1:M:23:LYS:O	1.84	0.76
1:S:262:CYS:SG	1:S:266:ILE:HG12	2.25	0.76
3:F:140:LEU:HD21	3:F:163:ASN:HB2	1.68	0.76
3:I:155:MET:HE2	3:I:241:PHE:CA	2.16	0.76
3:U:43:THR:HG22	3:U:147:PRO:HG3	1.66	0.76
1:J:62:ASN:HD22	1:J:71:PHE:HB3	1.50	0.76
1:V:149:ALA:HB2	1:V:168:PHE:CD2	2.18	0.76
1:M:126:ASN:HA	3:O:88:PHE:CE1	2.21	0.76
2:N:923:HIS:O	2:N:1021:SER:CB	2.33	0.76
2:W:321:THR:HG22	2:W:343:LYS:HD2	1.68	0.76
8:X:401:HEM:HBC2	8:X:401:HEM:HHD	1.68	0.76
3:I:51:VAL:HG13	3:I:104:HIS:HD2	1.50	0.76
2:E:926:TRP:HD1	2:E:932:ASN:OD1	1.68	0.75
3:F:155:MET:SD	8:F:401:HEM:ND	2.60	0.75
3:F:305:LYS:HE3	8:F:401:HEM:CHA	2.03	0.75
2:K:31:LEU:N	2:K:31:LEU:HD13	2.02	0.75
1:V:116:ILE:HG13	1:V:129:ALA:HB1	1.67	0.75
2:W:857:LEU:CB	2:W:900:THR:HG21	2.16	0.75
2:W:923:HIS:O	2:W:1021:SER:CB	2.32	0.75
1:J:262:CYS:HB2	1:J:267:ARG:HD3	1.67	0.75
2:Q:575:LYS:HD3	2:Q:575:LYS:H	1.50	0.75
1:V:241:ARG:NH1	1:V:257:ARG:CD	2.31	0.75
2:N:1124:THR:HG22	2:N:1126:TYR:CD2	2.20	0.75
3:C:309:ILE:HG13	3:C:310:GLN:HG3	1.69	0.75
2:K:918:SER:HB2	2:K:1019:LYS:HD3	1.67	0.75
2:N:213:ARG:HD2	2:N:642:MET:HB3	1.66	0.75
2:B:537:LEU:HD21	2:B:842:GLU:HG2	1.66	0.75
2:H:36:VAL:HG12	3:I:243:THR:CG2	2.15	0.75
2:K:917:LYS:O	2:K:1019:LYS:CE	2.34	0.75
1:V:213:LYS:HD2	3:X:301:ARG:HH21	1.52	0.75
2:E:414:SER:O	2:E:420:LEU:HB2	1.87	0.75
1:M:125:ILE:O	1:M:125:ILE:HG12	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:140:LEU:CG	3:O:161:PRO:O	2.34	0.75
3:U:305:LYS:HE2	8:U:401:HEM:C4C	2.17	0.75
1:V:178:CYS:O	1:V:181:PRO:HD3	1.86	0.75
2:W:1124:THR:O	2:W:1126:TYR:CD2	2.39	0.75
3:X:278:ASP:OD2	9:X:402:CA:CA	1.64	0.75
2:B:1088:GLU:HG2	2:B:1091:ASN:HB3	1.69	0.75
2:H:49:TRP:O	2:H:52:VAL:HG23	1.87	0.75
1:M:15:TYR:HE2	1:M:185:ALA:HB2	1.50	0.75
3:O:137:MET:SD	3:O:155:MET:HA	2.27	0.75
3:R:236:LEU:HB2	3:R:245:THR:O	1.86	0.75
2:B:236:LYS:NZ	2:B:734:ASP:OD1	2.20	0.75
3:I:155:MET:CE	3:I:241:PHE:HB3	2.13	0.75
3:O:303:GLY:HA2	3:O:305:LYS:HD2	1.67	0.75
1:V:36:ILE:HG13	2:W:310:ILE:HG23	1.68	0.74
2:B:879:ALA:HB3	2:B:888:ARG:HH21	1.51	0.74
1:V:257:ARG:HD2	2:W:90:GLU:OE1	1.86	0.74
2:K:445:THR:HG22	2:K:448:ASP:OD2	1.86	0.74
1:S:34:ARG:HA	2:T:321:THR:HG21	1.69	0.74
2:N:78:ARG:NH1	2:N:92:ASN:OD1	2.20	0.74
1:D:149:ALA:HB2	1:D:168:PHE:HD2	1.53	0.74
2:Q:950:PRO:HD2	2:Q:954:GLU:HB3	1.68	0.74
1:V:241:ARG:HH11	1:V:257:ARG:HG2	0.91	0.74
2:Q:394:ARG:NH1	2:Q:831:TYR:O	2.21	0.74
3:L:51:VAL:HG22	3:L:316:LEU:HA	1.70	0.74
2:Q:356:THR:HG22	2:Q:538:MET:HA	1.69	0.74
2:Q:1022:ALA:HB1	2:Q:1050:SER:HB2	1.69	0.74
2:E:628:THR:HG22	2:E:630:LYS:H	1.53	0.74
1:M:190:LYS:NZ	2:N:37:VAL:O	2.20	0.74
2:Q:531:HIS:O	2:Q:1099:LYS:HB2	1.86	0.74
2:W:545:PRO:O	2:W:549:THR:HG23	1.87	0.74
2:Q:93:TYR:O	2:Q:96:GLN:NE2	2.21	0.74
3:X:229:ARG:NH1	10:X:502:HOH:O	2.18	0.74
1:G:126:ASN:O	1:G:127:GLN:HG2	1.87	0.74
2:N:1078:LYS:HG3	2:N:1079:ILE:HG12	1.70	0.74
2:E:664:TYR:HB3	2:E:995:PHE:HE2	1.50	0.73
2:B:217:ALA:HB2	2:B:262:LEU:HD12	1.69	0.73
1:D:6:ASN:ND2	1:D:13:MET:SD	2.57	0.73
1:D:190:LYS:HB2	2:E:37:VAL:HG21	1.69	0.73
1:M:149:ALA:HB2	1:M:168:PHE:HD2	1.53	0.73
3:O:301:ARG:HG2	3:O:301:ARG:HH11	1.53	0.73
2:T:546:VAL:HG12	2:T:552:VAL:HG23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:GLY:HA2	2:B:1099:LYS:HZ2	1.53	0.73
1:G:293:LEU:HB2	1:G:305:TYR:HE1	1.51	0.73
1:P:76:ASP:OD2	2:Q:1138:PHE:CZ	2.41	0.73
2:B:135:LEU:HB2	2:B:694:ALA:HB3	1.69	0.73
2:H:267:TRP:NE1	2:H:612:GLU:OE1	2.20	0.73
2:N:1022:ALA:HB1	2:N:1050:SER:CB	2.18	0.73
1:S:257:ARG:NH1	2:T:89:VAL:O	2.20	0.73
3:X:81:LEU:O	3:X:96:ASN:HA	1.89	0.73
3:X:302:ASN:HB2	8:X:401:HEM:HAA1	1.70	0.73
2:H:1024:ILE:HG22	2:H:1055:SER:CB	2.19	0.73
2:N:73:HIS:O	2:N:113:ARG:NH1	2.21	0.73
2:N:880:GLU:O	2:N:885:ARG:NH1	2.21	0.73
1:S:292:PRO:HG2	1:S:295:PRO:HG3	1.69	0.73
2:W:91:GLN:HE21	2:W:114:MET:HB2	1.52	0.73
2:B:302:LEU:HD11	2:B:524:HIS:CD2	2.23	0.73
2:E:385:LEU:HA	2:E:433:VAL:HG11	1.70	0.73
2:Q:332:VAL:HG23	2:Q:344:ALA:HB2	1.70	0.73
1:V:259:MET:HE3	1:V:269:GLN:CG	2.19	0.73
2:E:998:VAL:O	2:E:1054:GLY:HA2	1.88	0.73
8:I:401:HEM:HBA2	8:I:401:HEM:CHA	2.18	0.73
2:K:115:CYS:HB3	4:K:5804:SF4:S2	2.28	0.73
2:N:519:LYS:NZ	2:N:549:THR:O	2.21	0.73
3:L:137:MET:HE1	3:L:155:MET:HA	1.71	0.73
2:K:265:ARG:HE	2:K:612:GLU:HB2	1.53	0.72
3:X:109:ILE:HB	3:X:271:LEU:HD23	1.71	0.72
3:L:271:LEU:HD12	3:L:281:PHE:HB2	1.71	0.72
3:O:155:MET:SD	8:O:401:HEM:FE	1.82	0.72
3:R:148:GLU:OE2	3:R:148:GLU:N	2.20	0.72
2:T:1022:ALA:HB1	2:T:1050:SER:HB2	1.71	0.72
2:W:776:GLY:H	2:W:781:LYS:HZ3	1.35	0.72
2:W:655:ASN:HD21	2:W:685:THR:HB	1.54	0.72
2:K:138:LYS:HG3	2:K:170:LEU:HD11	1.70	0.72
2:K:937:ASN:HD21	2:K:954:GLU:H	1.36	0.72
2:Q:275:ASP:HB3	2:Q:563:ALA:HB1	1.70	0.72
2:Q:394:ARG:CZ	2:Q:829:GLN:HE22	2.02	0.72
3:R:91:GLY:HA3	3:R:304:GLN:HG3	1.71	0.72
2:B:652:THR:HG22	2:B:680:THR:HB	1.71	0.72
2:K:1061:ARG:NH1	2:K:1062:ASP:O	2.22	0.72
1:M:189:ARG:HG2	1:M:189:ARG:NH1	2.03	0.72
2:T:394:ARG:NH2	2:T:829:GLN:OE1	2.23	0.72
1:D:362:LYS:HA	1:D:376:TYR:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:194:GLY:O	2:E:197:GLY:N	2.22	0.72
2:Q:383:PHE:CE2	2:Q:548:LEU:HD21	2.24	0.72
1:V:9:LEU:HD23	1:V:111:TYR:CD2	2.24	0.72
1:A:166:ARG:HD3	2:B:1010:ALA:HA	1.70	0.72
2:B:123:ARG:NH2	2:B:930:ASP:OD2	2.22	0.72
3:F:112:GLN:HG3	3:F:266:VAL:HG22	1.72	0.72
2:K:418:GLN:OE1	2:K:446:ARG:NH2	2.23	0.72
2:N:96:GLN:HB3	2:N:108:ARG:HG2	1.71	0.72
2:Q:492:TYR:CD1	2:Q:500:MET:HE1	2.24	0.72
2:Q:622:ARG:NH1	10:Q:5901:HOH:O	2.23	0.72
3:X:277:LEU:N	3:X:277:LEU:HD23	2.05	0.72
2:H:124:ARG:NH1	2:H:925:GLN:OE1	2.23	0.72
2:H:527:GLU:HG2	6:H:5802:MD1:H101	1.71	0.72
3:I:157:ASP:OD1	3:I:158:ARG:N	2.22	0.72
2:K:241:ARG:HG3	2:K:584:TRP:O	1.89	0.72
2:E:113:ARG:O	2:E:315:PRO:CB	2.38	0.71
2:H:1024:ILE:HG22	2:H:1055:SER:HB2	1.72	0.71
2:N:1135:MET:HE1	2:N:1138:PHE:CD2	2.24	0.71
2:T:824:PRO:HD2	2:T:829:GLN:HE22	1.55	0.71
1:G:309:ARG:HG2	1:G:310:TRP:HE3	1.54	0.71
3:C:301:ARG:HH21	3:C:301:ARG:CG	2.01	0.71
2:K:135:LEU:HB2	2:K:694:ALA:HB3	1.72	0.71
2:K:275:ASP:HB3	2:K:563:ALA:HB1	1.71	0.71
3:R:236:LEU:HA	3:R:247:GLN:HG3	1.73	0.71
1:D:257:ARG:NH1	2:E:90:GLU:OE2	2.24	0.71
2:E:1062:ASP:HA	2:E:1096:THR:CG2	2.20	0.71
2:K:225:ARG:HH21	2:K:269:ASN:HA	1.56	0.71
3:L:142:LYS:NZ	3:L:286:SER:O	2.22	0.71
2:Q:265:ARG:NH2	2:Q:644:SER:OG	2.23	0.71
2:W:648:VAL:HG23	2:W:676:GLN:HB3	1.70	0.71
2:E:414:SER:C	2:E:420:LEU:HB2	2.15	0.71
1:M:15:TYR:CE2	1:M:185:ALA:HB2	2.26	0.71
2:Q:661:LYS:NZ	2:Q:1096:THR:OG1	2.22	0.71
1:D:271:PHE:O	1:D:278:ASN:ND2	2.23	0.71
3:F:241:PHE:HB2	8:F:401:HEM:CHB	2.20	0.71
1:M:16:PRO:HG3	1:M:128:TRP:CE3	2.25	0.71
1:M:207:ARG:NH2	2:N:44:TYR:OH	2.24	0.71
1:V:211:TYR:CE1	3:X:302:ASN:HB3	2.25	0.71
2:E:533:PHE:HA	2:E:1065:MET:HE1	1.73	0.71
3:F:211:SER:O	3:F:215:LEU:HB2	1.91	0.71
2:Q:356:THR:HG23	2:Q:538:MET:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:917:LYS:NZ	6:Q:5801:MD1:H15	1.88	0.71
2:W:1124:THR:O	2:W:1126:TYR:HD2	1.74	0.71
1:G:62:ASN:HD22	1:G:71:PHE:HB3	1.56	0.71
2:K:110:TRP:HZ3	2:K:316:GLU:OE1	1.73	0.71
1:M:256:THR:HG22	1:M:259:MET:HB2	1.73	0.71
2:Q:72:THR:HG21	2:Q:713:SER:HB3	1.73	0.71
2:Q:937:ASN:ND2	2:Q:954:GLU:C	2.48	0.71
2:W:453:LEU:HD11	2:W:827:ARG:HH12	1.55	0.71
2:W:939:PHE:HE2	2:W:1004:ARG:CG	2.04	0.71
2:T:376:TYR:CD2	2:T:550:GLY:HA2	2.26	0.70
2:W:96:GLN:HB3	2:W:108:ARG:HG2	1.71	0.70
2:B:499:SER:OG	2:B:894:TRP:NE1	2.24	0.70
3:I:155:MET:HE1	3:I:241:PHE:CB	2.21	0.70
2:K:917:LYS:NZ	6:K:5801:MD1:S13	2.64	0.70
2:T:135:LEU:HB2	2:T:694:ALA:HB3	1.73	0.70
2:W:547:MET:HE1	2:W:830:ALA:HB2	1.72	0.70
3:L:301:ARG:HH21	3:L:301:ARG:CG	2.03	0.70
2:T:467:LYS:HD3	2:T:477:GLU:OE1	1.91	0.70
2:B:96:GLN:HB3	2:B:108:ARG:HG2	1.71	0.70
2:W:658:ASN:ND2	2:W:1024:ILE:HG23	2.05	0.70
3:O:269:ARG:NH2	3:O:279:VAL:O	2.24	0.70
1:P:149:ALA:HB2	1:P:168:PHE:HD2	1.57	0.70
2:T:407:GLN:O	2:T:425:ARG:NH2	2.21	0.70
1:V:126:ASN:ND2	3:X:88:PHE:CZ	2.49	0.70
2:W:950:PRO:HD2	2:W:954:GLU:HG3	1.73	0.70
3:X:309:ILE:HD13	3:X:309:ILE:N	2.06	0.70
2:B:225:ARG:HH11	2:B:656:LEU:CD1	2.05	0.70
1:D:219:PRO:HB2	1:D:297:PHE:CD1	2.27	0.70
1:M:209:ARG:NH1	3:O:234:GLU:CD	2.49	0.70
1:S:395:VAL:O	2:T:326:ARG:NH1	2.24	0.70
1:V:386:ASP:N	1:V:386:ASP:OD1	2.23	0.70
1:G:408:ASN:ND2	2:H:805:THR:OG1	2.23	0.70
2:W:222:PHE:CD1	2:W:648:VAL:HG13	2.27	0.70
1:J:2:THR:HG22	1:J:15:TYR:O	1.91	0.70
2:W:934:ILE:HD11	2:W:952:VAL:CG1	2.21	0.70
3:I:305:LYS:NZ	8:I:401:HEM:FE	1.58	0.70
3:O:42:LEU:O	3:O:44:PRO:HD3	1.91	0.70
3:O:235:ASP:N	3:O:250:GLN:OE1	2.25	0.70
2:W:434:TRP:HB3	2:W:461:VAL:HG22	1.74	0.70
1:D:65:THR:HG21	1:D:147:ASP:H	1.57	0.70
2:H:225:ARG:HH12	2:H:272:TRP:CD1	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:305:LYS:HD3	3:I:307:ILE:HG23	1.72	0.70
2:K:1078:LYS:HG3	2:K:1079:ILE:HG12	1.73	0.70
1:P:230:ARG:NH2	3:R:182:GLU:O	2.25	0.70
2:Q:179:THR:OG1	2:Q:744:LYS:NZ	2.24	0.70
3:C:305:LYS:CE	8:C:401:HEM:C1B	2.72	0.69
2:N:71:ASP:OD2	2:N:73:HIS:HD2	1.75	0.69
2:B:983:ASP:OD1	2:B:1061:ARG:NH1	2.26	0.69
1:D:53:LYS:O	1:D:226:ARG:NH1	2.25	0.69
2:E:57:TYR:O	2:E:88:ARG:NH1	2.24	0.69
2:E:1012:PRO:HG2	2:E:1015:CYS:HB3	1.74	0.69
1:V:62:ASN:HD22	1:V:71:PHE:HB3	1.57	0.69
2:W:857:LEU:N	2:W:900:THR:HG23	2.08	0.69
1:G:127:GLN:HE22	3:I:89:PRO:HB3	1.55	0.69
3:I:51:VAL:CG1	3:I:104:HIS:HD2	2.06	0.69
1:J:209:ARG:NH2	8:L:401:HEM:O2D	2.25	0.69
1:M:188:PRO:HB2	3:O:302:ASN:OD1	1.92	0.69
8:R:401:HEM:HHD	8:R:401:HEM:HBC2	1.75	0.69
2:W:435:ASP:HB2	2:W:442:LYS:CD	2.15	0.69
2:W:939:PHE:CZ	2:W:1004:ARG:HD3	2.25	0.69
3:C:305:LYS:HE2	8:C:401:HEM:NA	2.07	0.69
2:W:1001:LEU:HA	2:W:1054:GLY:HA3	1.72	0.69
2:B:293:MET:O	2:B:296:VAL:HG12	1.92	0.69
2:B:983:ASP:HB3	2:B:984:ARG:HD3	1.73	0.69
2:B:1022:ALA:HB1	2:B:1050:SER:CB	2.22	0.69
1:D:34:ARG:HA	2:E:321:THR:HG21	1.74	0.69
1:D:346:ARG:O	2:E:111:ASN:HB3	1.93	0.69
2:H:227:GLY:O	2:H:228:MET:C	2.33	0.69
2:H:917:LYS:HE3	6:H:5801:MD1:H15	1.57	0.69
1:M:166:ARG:NH1	2:N:1009:PRO:O	2.25	0.69
1:P:108:TYR:HE2	1:P:291:LEU:HD22	1.58	0.69
1:V:225:TYR:HB3	3:X:127:THR:HG22	1.73	0.69
2:W:857:LEU:H	2:W:900:THR:HG23	1.55	0.69
2:B:628:THR:HG21	2:B:873:TYR:HB3	1.73	0.69
1:G:4:VAL:HG23	1:G:19:GLU:HB2	1.74	0.69
3:I:307:ILE:HD13	8:I:401:HEM:HAB	1.74	0.69
2:Q:394:ARG:CZ	2:Q:829:GLN:NE2	2.56	0.69
1:V:267:ARG:NH1	4:V:503:SF4:S1	2.64	0.69
3:X:139:PRO:HB3	3:X:151:PHE:HE1	1.55	0.69
1:A:21:ARG:NH2	1:A:103:GLY:O	2.26	0.69
3:F:89:PRO:HD2	3:F:302:ASN:HD21	1.58	0.69
2:K:73:HIS:O	2:K:113:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:821:PHE:CE2	2:Q:828:LEU:HD21	2.26	0.69
2:B:57:TYR:O	2:B:88:ARG:NH1	2.26	0.69
1:V:66:LYS:N	1:V:169:PHE:O	2.25	0.69
2:W:228:MET:HE2	2:W:273:HIS:HD2	1.57	0.69
2:B:407:GLN:O	2:B:425:ARG:NH2	2.26	0.68
1:G:262:CYS:SG	1:G:266:ILE:HG12	2.34	0.68
3:I:241:PHE:HD1	3:I:241:PHE:H	1.40	0.68
1:A:313:ARG:O	1:A:317:ARG:HG3	1.94	0.68
2:B:314:MET:HG3	2:B:315:PRO:HD3	1.74	0.68
3:I:51:VAL:HG13	3:I:104:HIS:CD2	2.28	0.68
2:Q:1052:ARG:NH1	2:Q:1109:GLU:OE2	2.24	0.68
1:V:16:PRO:HG3	1:V:128:TRP:HZ2	0.86	0.68
2:B:463:GLU:HG2	2:B:486:LYS:NZ	2.09	0.68
2:K:658:ASN:HD21	2:K:1023:TRP:HA	1.58	0.68
1:V:211:TYR:O	3:X:301:ARG:NE	2.26	0.68
2:W:939:PHE:CD2	2:W:1004:ARG:NE	2.61	0.68
3:X:129:GLU:OE1	3:X:187:ARG:NH1	2.26	0.68
2:B:1135:MET:HE1	2:B:1138:PHE:CD2	2.26	0.68
2:H:858:PRO:O	2:H:888:ARG:NH1	2.25	0.68
1:J:34:ARG:HB3	1:J:266:ILE:HG22	1.75	0.68
2:W:852:GLU:OE2	2:W:984:ARG:NH1	2.23	0.68
3:F:204:TYR:O	3:F:208:VAL:HG23	1.94	0.68
2:K:313:LYS:NZ	2:K:563:ALA:O	2.27	0.68
2:K:880:GLU:O	2:K:885:ARG:NH1	2.27	0.68
1:M:190:LYS:HB3	2:N:37:VAL:HG11	1.74	0.68
1:S:209:ARG:NH2	8:U:401:HEM:O2D	2.26	0.68
1:V:259:MET:HE3	1:V:269:GLN:CB	2.24	0.68
2:W:950:PRO:CD	2:W:954:GLU:HG3	2.24	0.68
8:X:401:HEM:HBB2	8:X:401:HEM:HHC	1.74	0.68
2:E:1003:LEU:HD23	2:E:1003:LEU:C	2.19	0.68
2:H:152:THR:HG22	2:H:155:ASN:H	1.58	0.68
3:I:51:VAL:CG1	3:I:104:HIS:CD2	2.75	0.68
2:N:868:ILE:HB	2:N:891:LYS:HE2	1.76	0.68
2:B:665:GLN:OE1	2:B:987:GLU:N	2.21	0.68
1:D:136:ASP:OD1	1:D:137:LYS:N	2.26	0.68
2:E:986:TYR:OH	2:E:993:ASP:CB	2.42	0.68
2:H:823:THR:HG21	2:H:829:GLN:HG3	1.76	0.68
1:M:15:TYR:CE1	2:N:41:LEU:HD11	2.28	0.68
2:B:275:ASP:HB3	2:B:563:ALA:HB1	1.74	0.68
1:D:408:ASN:HD21	2:E:805:THR:H	1.40	0.68
2:E:135:LEU:HB2	2:E:694:ALA:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:546:VAL:HG13	2:T:551:ASN:HB2	1.76	0.68
2:E:680:THR:HG22	6:E:5801:MD1:N2	2.08	0.68
2:H:227:GLY:O	2:H:228:MET:O	2.12	0.68
2:N:811:PHE:HA	2:N:814:GLN:HG3	1.75	0.68
1:V:15:TYR:HE2	1:V:185:ALA:HB2	1.56	0.68
2:W:275:ASP:HB3	2:W:563:ALA:HB1	1.76	0.68
2:W:865:ASN:O	2:W:891:LYS:NZ	2.23	0.68
3:X:84:GLN:HB2	3:X:307:ILE:HG12	1.75	0.68
2:N:942:PRO:HA	2:N:952:VAL:HG13	1.75	0.68
1:V:211:TYR:O	3:X:301:ARG:CD	2.41	0.68
3:X:309:ILE:HD13	3:X:309:ILE:H	1.59	0.68
2:B:153:PRO:O	2:B:157:THR:HG23	1.94	0.67
2:T:917:LYS:NZ	6:T:5801:MD1:H15	1.91	0.67
2:W:852:GLU:HG2	2:W:1101:THR:HA	1.76	0.67
2:E:52:VAL:HG11	3:F:221:ALA:HB2	1.76	0.67
2:H:166:ASN:HB3	2:Q:1035:THR:HG23	1.76	0.67
2:Q:917:LYS:O	2:Q:1019:LYS:NZ	2.26	0.67
1:S:36:ILE:O	2:T:919:ARG:NH2	2.27	0.67
1:A:356:LYS:HG2	1:A:383:PHE:HE2	1.59	0.67
1:D:212:ARG:N	5:D:504:F3S:S4	2.65	0.67
2:Q:336:GLU:OE1	6:Q:5802:MD1:O2'	2.10	0.67
2:Q:494:ILE:O	2:Q:497:VAL:HG22	1.94	0.67
2:Q:942:PRO:HA	2:Q:952:VAL:HG13	1.75	0.67
2:Q:1138:PHE:HA	2:Q:1143:LEU:CD2	2.24	0.67
2:T:824:PRO:HD2	2:T:829:GLN:NE2	2.09	0.67
1:V:166:ARG:HD3	2:W:1010:ALA:HA	1.75	0.67
2:W:355:ASP:OD2	6:W:5802:MD1:N1	2.26	0.67
3:X:273:THR:HG22	3:X:275:ASP:H	1.60	0.67
3:L:123:GLN:NE2	3:L:125:ILE:HD12	2.08	0.67
2:H:57:TYR:O	2:H:88:ARG:NH1	2.24	0.67
2:K:425:ARG:HG2	2:K:425:ARG:NH1	2.02	0.67
3:F:120:ASP:HB3	3:F:258:PHE:HE1	1.52	0.67
3:I:154:ARG:CD	8:I:401:HEM:CBB	2.73	0.67
3:L:51:VAL:HG12	3:L:102:ALA:HB3	1.77	0.67
3:X:302:ASN:O	3:X:305:LYS:HE3	1.93	0.67
1:A:104:THR:O	1:A:285:ARG:NH1	2.28	0.67
1:D:390:VAL:HG23	1:D:391:VAL:HG23	1.77	0.67
2:E:658:ASN:HD21	2:E:1023:TRP:HA	1.60	0.67
6:E:5802:MD1:O11	6:E:5802:MD1:N15	2.28	0.67
3:F:171:TRP:NE1	3:F:229:ARG:NE	2.43	0.67
1:M:243:GLU:CD	2:N:54:ARG:NH1	2.52	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:301:ARG:HH11	3:O:301:ARG:CG	2.06	0.67
1:P:333:VAL:HG13	1:P:373:PHE:HB2	1.77	0.67
2:Q:1078:LYS:HG3	2:Q:1079:ILE:HG12	1.77	0.67
3:R:237:ASN:OD1	3:R:247:GLN:NE2	2.28	0.67
2:B:442:LYS:HG2	2:B:458:ILE:HD12	1.76	0.67
2:E:160:MET:SD	2:E:167:ASP:HB2	2.35	0.67
2:N:117:LYS:NZ	2:N:919:ARG:O	2.27	0.67
3:R:143:ILE:HD12	3:R:143:ILE:O	1.95	0.67
1:V:336:ARG:HD2	1:V:376:TYR:CE1	2.30	0.67
2:W:381:THR:CG2	2:W:383:PHE:H	2.02	0.67
2:B:395:VAL:HG13	2:B:432:VAL:HB	1.77	0.67
2:H:294:ASN:OD1	2:H:295:ASP:N	2.28	0.67
1:M:80:LEU:HD23	1:M:83:ILE:HD11	1.77	0.67
2:N:653:ASN:C	2:N:653:ASN:HD22	2.01	0.67
3:R:139:PRO:HB3	3:R:151:PHE:HE2	1.59	0.67
1:V:100:SER:OG	1:V:104:THR:HG23	1.94	0.67
2:W:123:ARG:NH2	2:W:930:ASP:OD2	2.26	0.67
2:W:584:TRP:HB2	2:W:773:LEU:HD11	1.77	0.67
2:B:305:THR:HG22	2:B:525:TYR:HB3	1.76	0.67
3:L:123:GLN:HE21	3:L:125:ILE:HD12	1.60	0.67
2:T:445:THR:OG1	2:T:448:ASP:OD2	2.13	0.67
1:V:29:VAL:HG21	1:V:283:LEU:HD23	1.77	0.67
1:G:402:ARG:NH2	10:G:601:HOH:O	2.26	0.66
2:H:681:ASP:OD1	2:H:682:ILE:N	2.28	0.66
3:I:53:TYR:HE1	3:I:319:ILE:HG23	1.59	0.66
2:W:974:TYR:HD1	2:W:1002:MET:SD	2.17	0.66
3:X:130:PHE:CE1	3:X:301:ARG:HD3	2.30	0.66
3:C:294:TRP:NE1	3:C:305:LYS:HB3	2.11	0.66
2:T:1078:LYS:HG3	2:T:1079:ILE:HG12	1.78	0.66
1:V:34:ARG:CB	1:V:266:ILE:HG22	2.25	0.66
1:V:128:TRP:CD1	1:V:185:ALA:HB1	2.30	0.66
2:H:156:LYS:NZ	2:H:673:ASN:OD1	2.28	0.66
2:H:763:GLU:OE1	2:H:765:ARG:NH1	2.28	0.66
3:I:110:TYR:CE1	3:I:268:CYS:HB2	2.31	0.66
1:M:318:GLN:HE22	2:N:1138:PHE:HD1	1.43	0.66
1:V:13:MET:HG3	1:V:118:GLU:OE1	1.95	0.66
2:E:1062:ASP:OD1	2:E:1096:THR:HG21	1.94	0.66
2:H:1078:LYS:HG3	2:H:1079:ILE:HG12	1.75	0.66
3:O:237:ASN:ND2	3:O:277:LEU:O	2.27	0.66
2:Q:977:VAL:HG12	2:Q:1059:ILE:HG21	1.77	0.66
1:M:258:CYS:HB2	1:M:267:ARG:HH12	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:195:ARG:HH12	1:P:239:TYR:HB2	1.60	0.66
2:T:275:ASP:HB3	2:T:563:ALA:HB1	1.77	0.66
2:W:795:GLU:HB3	2:W:798:VAL:HG12	1.76	0.66
2:W:865:ASN:OD1	2:W:866:PRO:HD2	1.95	0.66
1:D:21:ARG:CZ	1:D:179:THR:HG21	2.25	0.66
1:D:187:CYS:HB2	1:D:192:ILE:HD13	1.76	0.66
2:H:922:VAL:HG23	2:H:926:TRP:CE3	2.30	0.66
2:H:922:VAL:HG23	2:H:926:TRP:CZ3	2.31	0.66
1:M:15:TYR:CD2	1:M:16:PRO:HD2	2.29	0.66
1:M:262:CYS:SG	1:M:266:ILE:HG12	2.36	0.66
1:V:207:ARG:HH11	1:V:207:ARG:CG	2.07	0.66
2:E:192:TYR:O	2:E:197:GLY:CA	2.35	0.66
2:H:236:LYS:HG2	2:H:653:ASN:HB3	1.78	0.66
2:Q:491:ASP:OD2	2:Q:864:THR:N	2.24	0.66
2:E:1062:ASP:CG	2:E:1096:THR:CG2	2.69	0.66
1:M:45:CYS:HB2	4:M:501:SF4:S2	2.35	0.66
2:Q:531:HIS:C	2:Q:1097:VAL:HG23	2.21	0.66
1:S:166:ARG:HD3	2:T:1010:ALA:HA	1.78	0.66
1:J:262:CYS:SG	1:J:266:ILE:HG12	2.36	0.66
2:K:175:ASP:O	2:K:179:THR:HG23	1.96	0.66
3:O:303:GLY:C	3:O:305:LYS:HD3	2.21	0.66
2:Q:278:PRO:HB2	2:Q:536:THR:HB	1.76	0.66
2:Q:859:ASN:ND2	2:Q:885:ARG:O	2.27	0.66
2:W:124:ARG:NH2	2:W:925:GLN:OE1	2.29	0.66
2:W:681:ASP:OD1	2:W:682:ILE:N	2.27	0.66
1:J:16:PRO:HG2	1:J:185:ALA:HB1	1.77	0.66
1:P:140:ARG:HD3	2:Q:945:MET:HE3	1.76	0.66
2:T:678:MET:HG2	2:T:693:PHE:HB2	1.77	0.66
2:W:647:LYS:O	2:W:675:GLU:N	2.29	0.66
2:B:790:ASN:OD1	10:B:5902:HOH:O	2.14	0.65
2:B:949:MET:HE2	2:B:953:GLY:HA2	1.78	0.65
2:B:1088:GLU:HB3	2:B:1091:ASN:O	1.95	0.65
2:N:425:ARG:NH2	2:N:430:ASP:OD1	2.27	0.65
2:Q:462:LEU:HB3	2:Q:482:LEU:HD12	1.78	0.65
2:W:868:ILE:HG22	2:W:870:PRO:HD3	1.78	0.65
3:I:305:LYS:HD3	3:I:307:ILE:HG21	1.77	0.65
2:K:941:ASP:HB3	2:K:949:MET:HE1	1.77	0.65
2:N:1061:ARG:NH1	2:N:1062:ASP:O	2.28	0.65
2:Q:57:TYR:O	2:Q:88:ARG:NH1	2.29	0.65
1:V:262:CYS:HA	4:V:503:SF4:S3	2.37	0.65
2:B:1132:ASN:O	2:B:1136:LYS:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:241:ARG:NH1	2:K:757:ASN:O	2.29	0.65
2:Q:91:GLN:HG3	2:Q:114:MET:SD	2.36	0.65
2:Q:220:ARG:HD3	2:Q:265:ARG:HD3	1.78	0.65
1:V:64:GLU:OE2	1:V:70:GLY:HA2	1.96	0.65
2:N:388:ARG:HG3	2:N:395:VAL:HG22	1.77	0.65
2:T:113:ARG:CG	2:T:315:PRO:HB2	2.26	0.65
2:W:57:TYR:O	2:W:88:ARG:NH1	2.25	0.65
1:D:407:TYR:HE2	2:E:576:TRP:HZ2	1.45	0.65
2:H:1024:ILE:HG22	2:H:1055:SER:OG	1.96	0.65
2:K:476:ILE:HD12	2:K:476:ILE:O	1.97	0.65
1:P:262:CYS:SG	1:P:266:ILE:HG12	2.36	0.65
2:Q:124:ARG:NH2	2:Q:925:GLN:OE1	2.30	0.65
2:T:718:GLN:NE2	10:T:5906:HOH:O	2.29	0.65
2:B:373:ASP:OD1	2:B:376:TYR:N	2.20	0.65
3:O:192:HIS:NE2	3:O:194:ASP:OD1	2.28	0.65
1:P:115:THR:O	1:P:119:VAL:HG23	1.97	0.65
1:P:157:GLU:OE1	1:P:166:ARG:NH1	2.20	0.65
1:S:79:THR:HA	1:S:82:LEU:HD12	1.78	0.65
1:V:15:TYR:CD2	1:V:16:PRO:HD2	2.32	0.65
2:W:382:ASP:HA	2:W:385:LEU:HD13	1.78	0.65
2:E:94:ASP:OD2	2:E:98:TYR:CZ	2.50	0.65
2:H:923:HIS:O	2:H:1021:SER:HB2	1.97	0.65
1:J:207:ARG:NH2	2:K:44:TYR:OH	2.29	0.65
2:K:276:GLN:HB3	2:K:1095:ASN:ND2	2.11	0.65
2:K:861:ILE:HB	2:K:891:LYS:HA	1.78	0.65
2:Q:939:PHE:O	2:Q:949:MET:HE2	1.97	0.65
2:B:479:MET:HE3	2:B:484:MET:CE	2.24	0.65
2:E:963:ALA:O	2:E:967:LEU:HD12	1.96	0.65
3:F:158:ARG:N	3:F:239:GLU:O	2.30	0.65
2:Q:658:ASN:OD1	2:Q:1024:ILE:HG23	1.97	0.65
1:V:309:ARG:NH1	2:W:345:ASP:OD1	2.30	0.65
2:W:381:THR:HG22	2:W:383:PHE:N	2.05	0.65
2:W:976:TYR:CD1	2:W:1000:ARG:CZ	2.79	0.65
3:X:117:ASP:HB3	3:X:263:TRP:HD1	1.60	0.65
2:B:641:HIS:CE1	2:B:1069:GLN:HA	2.32	0.65
2:B:686:GLY:HA2	2:B:689:GLU:HB2	1.78	0.65
3:I:305:LYS:HZ3	8:I:401:HEM:FE	1.09	0.65
2:K:250:ASP:OD2	2:K:254:ARG:NH1	2.29	0.65
1:M:91:TYR:HA	2:N:1147:ASP:OD2	1.97	0.65
2:N:51:SER:O	2:N:54:ARG:N	2.30	0.65
1:D:35:CYS:HA	1:D:266:ILE:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:77:ILE:HG23	2:E:114:MET:HE1	1.78	0.65
2:W:857:LEU:H	2:W:900:THR:CG2	2.10	0.65
2:B:446:ARG:NH1	2:B:823:THR:O	2.30	0.64
2:B:527:GLU:HA	2:B:530:ASN:HB2	1.78	0.64
2:E:1029:THR:HG21	2:E:1049:SER:HB2	1.78	0.64
2:N:970:GLU:OE2	2:N:1130:ASN:ND2	2.29	0.64
3:R:131:ARG:NH1	10:R:501:HOH:O	2.29	0.64
2:T:480:THR:HG23	2:T:483:GLU:H	1.61	0.64
2:T:937:ASN:OD1	2:T:940:GLY:N	2.30	0.64
2:W:35:VAL:H	3:X:245:THR:HG21	1.62	0.64
2:W:977:VAL:CG2	2:W:1001:LEU:CD2	2.68	0.64
3:X:287:THR:HG22	3:X:314:LEU:HD11	1.79	0.64
2:B:386:LEU:O	2:B:395:VAL:HG12	1.97	0.64
2:B:913:CYS:HB2	2:B:1103:VAL:HG21	1.80	0.64
2:H:61:ARG:HG2	2:H:81:VAL:HB	1.77	0.64
2:N:1099:LYS:NZ	10:N:5901:HOH:O	2.20	0.64
2:Q:821:PHE:HE2	2:Q:828:LEU:CD2	2.10	0.64
3:R:168:LYS:HD2	3:R:171:TRP:CE2	2.32	0.64
1:V:201:VAL:O	1:V:234:LYS:NZ	2.30	0.64
2:W:123:ARG:HD2	3:X:194:ASP:HB2	1.78	0.64
2:B:852:GLU:OE2	2:B:984:ARG:NH2	2.30	0.64
1:D:292:PRO:HG3	1:D:304:TYR:HE2	1.62	0.64
3:I:112:GLN:HG3	3:I:266:VAL:HG12	1.79	0.64
2:K:533:PHE:HA	2:K:1065:MET:HE3	1.79	0.64
2:Q:625:ILE:HD12	2:Q:633:ARG:HG2	1.77	0.64
2:T:342:GLN:HG3	2:T:343:LYS:HD2	1.79	0.64
2:W:333:ILE:O	6:W:5802:MD1:N2	2.29	0.64
3:C:112:GLN:HG3	3:C:266:VAL:HG12	1.80	0.64
2:E:313:LYS:O	2:E:317:ALA:N	2.30	0.64
3:F:111:PHE:CE1	3:F:165:TRP:HZ3	2.16	0.64
2:Q:357:ALA:HB2	2:Q:847:HIS:HD2	1.59	0.64
1:S:4:VAL:HG23	1:S:19:GLU:HB2	1.79	0.64
2:B:305:THR:CG2	2:B:525:TYR:HB3	2.28	0.64
2:B:661:LYS:HD3	2:B:1098:PRO:HG3	1.79	0.64
2:E:33:PRO:HG3	3:O:321:TRP:CZ3	2.33	0.64
2:E:926:TRP:CD1	2:E:932:ASN:OD1	2.50	0.64
1:G:166:ARG:HD3	2:H:1010:ALA:HA	1.78	0.64
2:H:164:ARG:NH2	2:H:674:ILE:O	2.30	0.64
2:Q:821:PHE:CE2	2:Q:828:LEU:CD2	2.80	0.64
1:V:2:THR:N	1:V:14:GLU:OE1	2.31	0.64
2:E:1014:ASN:ND2	2:E:1014:ASN:H	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:LYS:HD2	2:K:37:VAL:HB	1.78	0.64
2:T:915:THR:HA	2:T:1018:MET:O	1.98	0.64
2:W:969:ILE:HG12	2:W:1107:LYS:HB2	1.80	0.64
2:H:917:LYS:HG2	6:H:5802:MD1:H15	1.62	0.64
1:J:190:LYS:HB3	2:K:40:PRO:HG3	1.80	0.64
1:M:64:GLU:HG3	1:M:66:LYS:HD3	1.80	0.64
2:Q:115:CYS:HB3	4:Q:5804:SF4:S2	2.37	0.64
1:V:4:VAL:N	1:V:13:MET:O	2.27	0.64
2:W:192:TYR:CZ	2:W:647:LYS:HE2	2.33	0.64
2:W:877:GLU:OE2	2:W:892:LYS:NZ	2.30	0.64
3:X:95:VAL:O	3:X:306:ASN:ND2	2.31	0.64
3:X:137:MET:SD	3:X:290:ASN:HB3	2.37	0.64
1:D:60:TRP:HD1	1:D:224:MET:HE3	1.60	0.64
1:M:188:PRO:HG2	3:O:302:ASN:OD1	1.98	0.64
2:Q:811:PHE:HA	2:Q:814:GLN:HG2	1.79	0.64
1:S:36:ILE:HD11	2:T:317:ALA:HB3	1.79	0.64
1:D:263:VAL:HG11	2:E:114:MET:O	1.97	0.64
2:H:381:THR:HG22	2:H:383:PHE:H	1.63	0.64
2:H:446:ARG:NH2	2:H:823:THR:O	2.31	0.64
2:K:314:MET:HE3	6:K:5802:MD1:H162	1.61	0.64
2:K:661:LYS:HA	2:K:1057:GLN:NE2	2.12	0.64
2:Q:1064:SER:OG	2:Q:1069:GLN:NE2	2.25	0.64
1:S:172:GLN:HB3	1:S:267:ARG:HH21	1.62	0.64
2:E:110:TRP:H	2:E:110:TRP:CD1	2.16	0.64
3:F:37:VAL:HA	3:F:154:ARG:NH2	2.13	0.64
2:K:388:ARG:HG3	2:K:395:VAL:HG22	1.78	0.64
3:L:51:VAL:HG21	3:L:316:LEU:HG	1.80	0.64
3:L:151:PHE:CE1	3:L:160:LYS:HB3	2.33	0.64
2:N:353:ASN:ND2	2:N:1100:GLU:OE2	2.31	0.64
2:Q:385:LEU:HD23	2:Q:431:PHE:HB2	1.79	0.64
2:Q:497:VAL:HA	2:Q:500:MET:HG3	1.79	0.64
1:V:296:GLN:NE2	1:V:318:GLN:O	2.30	0.64
2:W:386:LEU:HD12	2:W:432:VAL:HG23	1.79	0.64
2:B:312:ASN:O	6:B:5802:MD1:N8	2.31	0.63
3:C:247:GLN:O	3:C:250:GLN:NE2	2.31	0.63
2:E:915:THR:OG1	6:E:5801:MD1:N17	2.30	0.63
1:M:21:ARG:NH1	1:M:103:GLY:O	2.31	0.63
2:N:505:LYS:NZ	2:N:509:GLU:OE2	2.24	0.63
2:N:653:ASN:ND2	2:N:653:ASN:O	2.30	0.63
2:N:861:ILE:HB	2:N:891:LYS:HA	1.80	0.63
2:E:970:GLU:HG2	2:E:1118:VAL:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1012:PRO:CG	2:E:1015:CYS:HB3	2.28	0.63
3:I:163:ASN:HD22	3:I:164:LEU:N	1.97	0.63
2:Q:1099:LYS:NZ	10:Q:5905:HOH:O	2.28	0.63
2:T:438:SER:O	2:T:440:GLY:N	2.32	0.63
1:V:211:TYR:HB2	5:V:504:F3S:S1	2.38	0.63
3:R:51:VAL:HG23	3:R:104:HIS:HD2	1.63	0.63
3:R:143:ILE:HD13	3:R:145:ILE:HG13	1.81	0.63
2:B:790:ASN:O	2:B:790:ASN:ND2	2.31	0.63
1:D:219:PRO:HB2	1:D:297:PHE:CE1	2.34	0.63
2:E:1033:HIS:NE2	2:E:1052:ARG:HG3	2.14	0.63
2:K:925:GLN:HE21	6:K:5801:MD1:H5'1	1.62	0.63
2:N:120:THR:HG22	2:N:931:TRP:HE3	1.63	0.63
2:B:913:CYS:HB2	2:B:1103:VAL:CG2	2.29	0.63
1:D:150:LYS:O	1:D:166:ARG:HA	1.97	0.63
2:E:959:ILE:HD13	2:E:1016:THR:HG23	1.80	0.63
2:K:31:LEU:H	2:K:31:LEU:HD22	1.64	0.63
2:Q:382:ASP:HA	2:Q:385:LEU:HD13	1.78	0.63
1:S:140:ARG:HD3	2:T:945:MET:HE2	1.79	0.63
2:B:479:MET:CE	2:B:484:MET:HE3	2.25	0.63
1:D:66:LYS:N	1:D:169:PHE:O	2.30	0.63
2:E:1002:MET:O	2:E:1002:MET:HG3	1.97	0.63
1:G:95:LYS:CB	1:G:109:GLY:HA2	2.28	0.63
2:K:117:LYS:HD2	2:K:922:VAL:HG23	1.81	0.63
1:M:102:TYR:N	1:M:274:ASP:OD1	2.21	0.63
2:T:293:MET:HE2	2:T:316:GLU:HB2	1.79	0.63
3:U:191:MET:HG2	3:U:192:HIS:N	2.13	0.63
2:W:265:ARG:HE	2:W:612:GLU:HB2	1.62	0.63
2:B:213:ARG:HD3	2:B:642:MET:HB3	1.80	0.63
1:D:6:ASN:ND2	1:D:298:GLY:O	2.31	0.63
1:D:149:ALA:HB2	1:D:168:PHE:CD2	2.33	0.63
1:G:15:TYR:HE1	2:H:41:LEU:HD11	1.64	0.63
1:M:256:THR:CG2	1:M:259:MET:HE2	2.28	0.63
2:N:179:THR:OG1	2:N:744:LYS:NZ	2.28	0.63
3:X:155:MET:HE2	3:X:241:PHE:HA	1.80	0.63
2:H:389:THR:HG23	2:H:867:TYR:HE1	1.64	0.63
1:J:195:ARG:HD3	1:J:200:ILE:HB	1.80	0.63
2:Q:225:ARG:HH12	2:Q:272:TRP:CD1	2.16	0.63
2:Q:909:TYR:CD1	2:Q:1104:LYS:HB2	2.34	0.63
1:S:252:ARG:NH1	1:S:386:ASP:OD1	2.32	0.63
2:T:640:THR:HB	2:T:1087:PHE:HB3	1.80	0.63
2:K:334:THR:HG22	2:K:336:GLU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:301:ARG:HH21	3:L:301:ARG:HG2	1.63	0.63
2:N:453:LEU:HD11	2:N:827:ARG:HH12	1.62	0.63
2:Q:135:LEU:HB2	2:Q:694:ALA:HB3	1.81	0.63
2:W:684:ILE:O	2:W:684:ILE:HD12	1.99	0.63
2:E:415:TYR:HA	2:E:420:LEU:H	1.64	0.62
2:K:69:PRO:HG2	2:K:71:ASP:HB2	1.81	0.62
2:K:312:ASN:O	6:K:5802:MD1:N8	2.31	0.62
2:W:882:TRP:CD1	2:W:883:GLU:HG2	2.34	0.62
2:W:1001:LEU:HD11	2:W:1003:LEU:HD22	1.81	0.62
2:B:652:THR:O	2:B:654:VAL:HG22	1.99	0.62
1:D:8:HIS:HD2	1:D:292:PRO:HG2	1.63	0.62
3:F:81:LEU:CD2	3:F:293:VAL:HG23	2.30	0.62
2:T:115:CYS:CB	4:T:5804:SF4:S2	2.85	0.62
2:W:844:PHE:HB2	2:W:868:ILE:HD11	1.81	0.62
3:O:121:ASN:N	3:O:132:ASP:OD2	2.28	0.62
2:Q:547:MET:CE	2:Q:830:ALA:HB2	2.25	0.62
2:B:28:PHE:HA	3:U:107:ILE:HD12	1.80	0.62
2:B:491:ASP:OD2	2:B:864:THR:N	2.30	0.62
2:E:680:THR:HG22	6:E:5801:MD1:HN21	1.64	0.62
3:F:81:LEU:HD21	3:F:293:VAL:HG23	1.82	0.62
1:G:158:TYR:CD1	2:H:507:LEU:HD11	2.34	0.62
3:I:294:TRP:CE2	3:I:305:LYS:HB2	2.33	0.62
2:N:1016:THR:HG21	2:N:1105:ILE:HD11	1.80	0.62
1:V:212:ARG:HH11	1:V:212:ARG:CG	2.11	0.62
1:A:159:SER:HB2	2:B:347:TRP:HB3	1.81	0.62
2:E:333:ILE:O	6:E:5802:MD1:N2	2.32	0.62
2:E:930:ASP:O	2:E:934:ILE:HG13	1.99	0.62
2:E:1062:ASP:CG	2:E:1096:THR:HG21	2.25	0.62
2:H:1001:LEU:HA	2:H:1054:GLY:HA3	1.81	0.62
1:M:240:PRO:HG3	2:N:54:ARG:HG2	1.81	0.62
2:Q:705:GLU:HG3	2:Q:706:PHE:N	2.13	0.62
3:I:306:ASN:N	3:I:306:ASN:HD22	1.96	0.62
2:T:763:GLU:OE1	2:T:765:ARG:NH1	2.33	0.62
3:X:81:LEU:N	3:X:96:ASN:O	2.25	0.62
2:E:1036:ARG:NH1	2:E:1038:ASP:OD1	2.33	0.62
3:F:219:TYR:HE2	3:F:227:LEU:HD23	1.65	0.62
2:Q:68:SER:O	2:Q:231:LEU:HD12	1.98	0.62
2:Q:425:ARG:HH11	2:Q:425:ARG:CG	2.12	0.62
2:T:151:LEU:HD12	2:T:675:GLU:HG2	1.80	0.62
2:W:527:GLU:HA	2:W:530:ASN:HB2	1.82	0.62
3:F:171:TRP:NE1	3:F:229:ARG:CZ	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:241:PHE:HB2	8:F:401:HEM:HBB	1.82	0.62
3:I:321:TRP:CE2	3:X:161:PRO:HG3	2.34	0.62
3:O:294:TRP:CE2	3:O:305:LYS:HB3	2.35	0.62
8:R:401:HEM:HBB2	8:R:401:HEM:HMB1	1.82	0.62
3:U:118:ALA:HA	3:U:261:LYS:HG2	1.79	0.62
1:V:64:GLU:HB3	1:V:70:GLY:HA2	1.82	0.62
2:W:939:PHE:CE2	2:W:1004:ARG:CG	2.75	0.62
2:B:271:THR:HG23	2:B:1090:ASP:HA	1.81	0.62
8:C:401:HEM:HBB2	8:C:401:HEM:HMB1	1.81	0.62
3:I:305:LYS:CG	3:I:307:ILE:HG23	2.28	0.62
1:M:125:ILE:HD13	1:M:127:GLN:HB2	1.82	0.62
2:N:275:ASP:HB3	2:N:563:ALA:HB1	1.80	0.62
1:A:365:GLU:OE2	1:A:372:LYS:NZ	2.32	0.62
2:B:435:ASP:OD1	2:B:437:LYS:N	2.29	0.62
2:B:446:ARG:HH11	2:B:446:ARG:CG	2.12	0.62
1:D:137:LYS:HA	1:D:140:ARG:HD2	1.80	0.62
2:E:1033:HIS:CE1	2:E:1052:ARG:HD3	2.35	0.62
3:I:305:LYS:HG2	3:I:307:ILE:HG23	1.81	0.62
8:O:401:HEM:HMB1	8:O:401:HEM:HBB2	1.81	0.62
1:V:211:TYR:HD2	5:V:504:F3S:S1	2.23	0.62
2:B:82:ARG:NH1	10:B:5906:HOH:O	2.32	0.61
1:G:160:THR:HG23	2:H:346:TYR:HB3	1.81	0.61
2:K:421:LYS:HB2	2:K:424:GLN:HG3	1.81	0.61
2:N:100:ASP:OD1	2:N:102:TYR:N	2.31	0.61
2:N:312:ASN:O	6:N:5802:MD1:N8	2.33	0.61
2:T:823:THR:CB	2:T:829:GLN:HE21	2.02	0.61
1:V:36:ILE:O	2:W:919:ARG:NH2	2.33	0.61
2:W:123:ARG:NH2	3:X:193:ASP:OD1	2.33	0.61
2:B:678:MET:HG2	2:B:693:PHE:HB2	1.83	0.61
3:I:231:ARG:NH1	3:I:250:GLN:O	2.33	0.61
3:L:107:ILE:HD11	2:Q:31:LEU:HD11	1.82	0.61
1:M:205:GLN:NE2	1:M:232:SER:O	2.33	0.61
2:Q:865:ASN:O	2:Q:891:LYS:NZ	2.29	0.61
2:T:752:LYS:O	2:T:753:ARG:HG2	2.00	0.61
2:W:759:LYS:O	2:W:763:GLU:HG3	2.01	0.61
3:X:109:ILE:O	3:X:110:TYR:CD1	2.52	0.61
2:B:681:ASP:OD1	2:B:682:ILE:N	2.31	0.61
8:L:401:HEM:HBB2	8:L:401:HEM:HMB1	1.81	0.61
2:Q:760:PHE:HB2	2:Q:769:TYR:CE2	2.36	0.61
1:A:402:ARG:O	2:B:804:ARG:NH2	2.34	0.61
3:C:105:ASP:OD2	2:T:29:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:235:GLY:N	2:E:707:GLU:OE2	2.34	0.61
1:G:15:TYR:CD2	1:G:16:PRO:HD2	2.36	0.61
1:J:133:ILE:HG13	1:J:216:GLU:HG3	1.81	0.61
2:K:123:ARG:HD2	3:L:194:ASP:HB2	1.81	0.61
2:N:1124:THR:HG21	2:N:1126:TYR:CD2	2.35	0.61
2:Q:267:TRP:CD2	2:Q:614:VAL:HG22	2.35	0.61
2:W:311:GLU:OE2	2:W:1019:LYS:NZ	2.33	0.61
2:B:628:THR:CG2	2:B:873:TYR:HB3	2.30	0.61
1:D:292:PRO:HG3	1:D:304:TYR:CE2	2.34	0.61
3:F:155:MET:SD	8:F:401:HEM:FE	1.88	0.61
1:P:302:ASN:HA	1:P:304:TYR:CE2	2.35	0.61
1:V:64:GLU:OE2	1:V:70:GLY:CA	2.49	0.61
1:V:212:ARG:HG3	1:V:212:ARG:NH1	2.14	0.61
1:V:252:ARG:NH2	1:V:386:ASP:CG	2.41	0.61
3:C:235:ASP:HB2	3:C:252:VAL:HG12	1.82	0.61
2:E:275:ASP:HB3	2:E:563:ALA:HB1	1.81	0.61
2:H:974:TYR:CZ	2:H:1004:ARG:HD3	2.36	0.61
1:M:88:ASN:ND2	1:M:111:TYR:OH	2.25	0.61
1:V:16:PRO:CG	1:V:128:TRP:HE1	1.62	0.61
1:V:212:ARG:HH11	1:V:212:ARG:HG3	1.66	0.61
1:V:227:GLY:HA3	3:X:125:ILE:HG22	1.82	0.61
2:W:114:MET:HE2	2:W:119:TYR:CD1	2.36	0.61
2:W:922:VAL:O	2:W:922:VAL:HG12	2.01	0.61
2:E:349:PRO:O	2:E:503:SER:HB3	2.01	0.61
1:G:293:LEU:HB2	1:G:305:TYR:CE1	2.35	0.61
2:H:625:ILE:HG12	2:H:635:VAL:HG22	1.83	0.61
2:K:681:ASP:OD1	2:K:682:ILE:N	2.30	0.61
2:K:915:THR:HA	2:K:1018:MET:O	1.99	0.61
2:K:1076:LYS:NZ	2:K:1080:GLY:O	2.33	0.61
1:M:256:THR:CG2	1:M:259:MET:HB2	2.31	0.61
1:M:256:THR:HG23	1:M:259:MET:H	1.66	0.61
2:N:91:GLN:HE21	2:N:114:MET:HB2	1.65	0.61
2:N:954:GLU:OE1	2:N:1004:ARG:HG3	2.01	0.61
2:Q:641:HIS:CE1	2:Q:1087:PHE:HB2	2.36	0.61
2:Q:678:MET:HG2	2:Q:693:PHE:HB2	1.82	0.61
2:Q:928:VAL:HA	2:Q:933:PHE:CD1	2.35	0.61
1:V:150:LYS:HG2	1:V:167:TRP:NE1	2.16	0.61
2:W:795:GLU:HB3	2:W:798:VAL:CG1	2.31	0.61
2:E:272:TRP:CH2	2:E:618:ASN:HB2	2.36	0.61
2:E:618:ASN:HD21	2:E:661:LYS:CB	2.13	0.61
3:I:98:ALA:HB3	3:I:291:MET:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:ARG:HB2	1:M:266:ILE:HG22	1.81	0.61
2:N:446:ARG:NH2	2:N:821:PHE:O	2.34	0.61
3:O:303:GLY:CA	3:O:305:LYS:CD	2.79	0.61
1:V:37:ALA:HA	1:V:63:VAL:HG11	1.82	0.61
2:W:113:ARG:HG3	2:W:113:ARG:HH11	1.66	0.61
2:W:853:ALA:N	2:W:1100:GLU:OE2	2.22	0.61
2:E:959:ILE:CD1	2:E:1016:THR:HG23	2.30	0.61
3:F:111:PHE:HE1	3:F:165:TRP:HZ3	1.49	0.61
2:H:547:MET:HE1	2:H:830:ALA:HB2	1.82	0.61
2:H:658:ASN:OD1	2:H:1024:ILE:CG1	2.45	0.61
2:K:116:LEU:HD21	2:K:919:ARG:O	2.01	0.61
2:K:918:SER:HA	2:K:1019:LYS:HE2	1.83	0.61
2:N:916:PRO:HA	6:N:5802:MD1:O1A	2.01	0.61
2:Q:307:LYS:NZ	2:Q:313:LYS:NZ	2.48	0.61
2:T:823:THR:HG21	2:T:829:GLN:HG3	1.82	0.61
8:U:401:HEM:HBB2	8:U:401:HEM:HMB1	1.81	0.61
2:E:262:LEU:CG	2:E:608:ARG:CB	2.79	0.61
3:I:143:ILE:HG22	3:I:145:ILE:HG22	1.83	0.61
2:K:865:ASN:O	2:K:891:LYS:NZ	2.33	0.61
1:M:189:ARG:HE	1:M:209:ARG:HG3	1.66	0.61
2:B:91:GLN:HG2	2:B:112:PRO:HB2	1.83	0.60
2:B:353:ASN:ND2	2:B:1100:GLU:OE1	2.34	0.60
3:C:236:LEU:HA	3:C:247:GLN:HG3	1.83	0.60
2:E:51:SER:O	2:E:54:ARG:N	2.34	0.60
3:F:115:TRP:NE1	3:F:293:VAL:HG11	2.15	0.60
2:H:917:LYS:O	2:H:1019:LYS:NZ	2.33	0.60
2:Q:848:ARG:NH1	2:Q:889:ASN:OD1	2.33	0.60
2:Q:1057:GLN:HE22	6:Q:5801:MD1:H162	1.47	0.60
1:V:333:VAL:HG13	1:V:373:PHE:HB2	1.83	0.60
2:W:274:GLY:HA2	2:W:1095:ASN:OD1	2.01	0.60
2:B:113:ARG:NH2	2:B:316:GLU:OE2	2.33	0.60
2:B:469:LYS:HA	2:B:475:GLU:HA	1.82	0.60
2:B:950:PRO:CD	2:B:954:GLU:HB3	2.31	0.60
1:J:149:ALA:HB2	1:J:168:PHE:HD2	1.65	0.60
2:Q:625:ILE:HD13	2:Q:633:ARG:HE	1.65	0.60
2:Q:852:GLU:HG3	2:Q:1063:TRP:HZ2	1.65	0.60
1:V:25:GLN:HG2	1:V:302:ASN:ND2	2.14	0.60
2:E:700:TRP:NE1	6:E:5801:MD1:N7	2.47	0.60
3:F:171:TRP:CH2	3:F:229:ARG:HD3	2.35	0.60
1:G:149:ALA:HB2	1:G:168:PHE:HD2	1.66	0.60
2:K:848:ARG:NH2	2:K:859:ASN:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:HIS:CD2	1:D:292:PRO:HG2	2.36	0.60
1:M:175:CYS:SG	1:M:234:LYS:NZ	2.68	0.60
2:N:917:LYS:O	2:N:1019:LYS:NZ	2.31	0.60
2:E:1020:HIS:CD2	6:E:5801:MD1:C20	2.84	0.60
1:P:4:VAL:O	1:P:13:MET:N	2.29	0.60
2:T:373:ASP:O	2:T:377:VAL:HG23	2.01	0.60
1:V:34:ARG:NH2	2:W:322:GLU:OE2	2.35	0.60
1:V:187:CYS:SG	1:V:191:ALA:HB3	2.42	0.60
1:V:408:ASN:ND2	2:W:805:THR:OG1	2.32	0.60
2:W:113:ARG:HH11	2:W:113:ARG:CG	2.14	0.60
2:H:947:LYS:NZ	10:H:5907:HOH:O	2.34	0.60
1:P:34:ARG:HB2	1:P:266:ILE:HG22	1.84	0.60
1:P:161:LEU:HD21	1:P:309:ARG:HD3	1.84	0.60
2:E:920:HIS:CD2	2:E:935:TRP:O	2.55	0.60
3:F:117:ASP:N	3:F:261:LYS:O	2.35	0.60
1:J:349:GLN:NE2	2:K:90:GLU:OE1	2.35	0.60
1:S:397:GLU:HG3	1:S:398:PRO:HD2	1.83	0.60
2:T:152:THR:HG22	2:T:154:GLU:HG2	1.81	0.60
1:V:60:TRP:HD1	1:V:224:MET:HE3	1.67	0.60
1:V:64:GLU:OE1	1:V:173:ARG:HD3	2.00	0.60
2:W:458:ILE:H	2:W:458:ILE:HD12	1.67	0.60
3:I:154:ARG:HA	8:I:401:HEM:CBB	2.31	0.60
2:K:918:SER:CB	2:K:1019:LYS:HD3	2.31	0.60
1:M:188:PRO:CB	3:O:302:ASN:OD1	2.49	0.60
3:O:165:TRP:CZ2	3:O:269:ARG:HD3	2.37	0.60
3:O:282:VAL:HG23	3:O:285:GLU:CB	2.31	0.60
2:W:438:SER:O	2:W:440:GLY:N	2.35	0.60
2:B:302:LEU:HD23	2:B:320:VAL:HG23	1.84	0.60
2:Q:72:THR:CG2	2:Q:713:SER:OG	2.49	0.60
3:U:129:GLU:CD	3:U:187:ARG:HH12	2.08	0.60
1:A:64:GLU:HG3	1:A:66:LYS:HE3	1.82	0.60
1:G:160:THR:HG21	2:H:510:ARG:HH22	1.67	0.60
2:H:294:ASN:OD1	2:H:807:PRO:HB3	2.01	0.60
2:K:115:CYS:SG	2:K:117:LYS:HE3	2.42	0.60
2:K:1004:ARG:NH2	2:K:1111:GLY:O	2.34	0.60
1:M:166:ARG:HD3	2:N:1010:ALA:HA	1.83	0.60
2:N:533:PHE:HA	2:N:1065:MET:HE3	1.84	0.60
3:O:131:ARG:HE	3:O:170:ASP:CG	2.10	0.60
1:S:83:ILE:HG22	1:S:119:VAL:HG21	1.82	0.60
2:W:315:PRO:HG3	4:W:5804:SF4:S2	2.42	0.60
3:X:48:VAL:HG12	3:X:313:PRO:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:111:PHE:HE1	3:F:165:TRP:CZ3	2.20	0.59
2:K:98:TYR:CE1	2:K:798:VAL:HG21	2.37	0.59
3:L:303:GLY:HA2	3:L:305:LYS:CE	2.32	0.59
2:N:80:PHE:HE1	2:N:90:GLU:HB2	1.67	0.59
2:Q:307:LYS:NZ	2:Q:313:LYS:HZ1	2.00	0.59
2:Q:852:GLU:HG3	2:Q:1063:TRP:CZ2	2.37	0.59
3:U:302:ASN:CG	3:U:303:GLY:H	2.09	0.59
1:A:90:TRP:HB2	2:B:1146:VAL:HG12	1.85	0.59
2:E:582:TYR:O	2:E:586:ALA:N	2.29	0.59
2:E:971:ASP:HB2	2:E:1007:TYR:CD2	2.38	0.59
3:F:219:TYR:CE2	3:F:227:LEU:HD23	2.36	0.59
2:H:528:GLY:HA2	2:H:1099:LYS:HZ2	1.67	0.59
3:L:305:LYS:HE3	8:L:401:HEM:C4A	2.30	0.59
2:B:1088:GLU:HB3	2:B:1091:ASN:HB3	1.84	0.59
2:E:77:ILE:CD1	2:E:114:MET:CE	2.79	0.59
2:K:546:VAL:HG13	2:K:551:ASN:HB2	1.83	0.59
2:N:915:THR:HA	2:N:1018:MET:O	2.02	0.59
2:Q:82:ARG:NH1	10:Q:5904:HOH:O	2.27	0.59
2:Q:383:PHE:N	2:Q:384:PRO:HD2	2.17	0.59
3:R:112:GLN:HG3	3:R:266:VAL:HG12	1.84	0.59
3:R:305:LYS:HE2	8:R:401:HEM:ND	2.16	0.59
1:A:404:ASP:HA	2:B:804:ARG:NH2	2.17	0.59
2:B:117:LYS:NZ	2:B:919:ARG:O	2.35	0.59
1:D:6:ASN:HB2	1:D:13:MET:HG2	1.83	0.59
1:D:262:CYS:SG	1:D:266:ILE:HD12	2.42	0.59
3:F:79:VAL:HG11	3:F:291:MET:SD	2.42	0.59
1:G:121:LYS:NZ	3:I:32:GLU:OE2	2.32	0.59
2:H:312:ASN:O	6:H:5802:MD1:N8	2.35	0.59
2:H:759:LYS:O	2:H:763:GLU:HG3	2.03	0.59
3:I:282:VAL:O	3:I:316:LEU:HD12	2.02	0.59
1:M:190:LYS:CB	2:N:37:VAL:HG11	2.32	0.59
2:N:434:TRP:O	2:N:461:VAL:HG22	2.03	0.59
1:P:296:GLN:NE2	1:P:318:GLN:O	2.34	0.59
2:Q:404:TYR:HE2	2:Q:406:LEU:HD23	1.67	0.59
1:V:353:TYR:CE2	1:V:385:GLU:HG3	2.37	0.59
2:W:406:LEU:CD2	2:W:429:GLY:HA2	2.33	0.59
2:K:577:SER:O	2:K:781:LYS:NZ	2.34	0.59
2:Q:306:GLY:HA3	2:Q:529:VAL:HG22	1.84	0.59
2:Q:445:THR:CG2	2:Q:448:ASP:OD2	2.46	0.59
2:T:822:TYR:CE1	2:T:1076:LYS:HD2	2.38	0.59
2:W:388:ARG:HG3	2:W:395:VAL:HB	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:410:SER:HA	2:W:415:TYR:CD2	2.37	0.59
2:W:834:GLU:OE1	2:W:837:ILE:HD12	2.03	0.59
3:X:140:LEU:HD22	3:X:161:PRO:HB2	1.84	0.59
3:C:302:ASN:O	3:C:305:LYS:CG	2.50	0.59
2:E:110:TRP:CD1	2:E:110:TRP:N	2.71	0.59
1:G:192:ILE:HG12	1:G:203:ILE:HG12	1.84	0.59
8:L:401:HEM:HHD	8:L:401:HEM:HBC2	1.83	0.59
2:N:1124:THR:HG22	2:N:1126:TYR:CG	2.38	0.59
2:Q:70:ASN:H	2:Q:231:LEU:CD1	2.14	0.59
2:B:217:ALA:HB2	2:B:262:LEU:HD13	1.85	0.59
2:E:663:VAL:C	2:E:664:TYR:HA	2.26	0.59
1:M:184:LEU:HD21	2:N:40:PRO:HB2	1.85	0.59
1:P:266:ILE:HG13	1:P:267:ARG:HG3	1.84	0.59
1:P:276:PRO:CB	1:P:286:HIS:NE2	2.62	0.59
2:T:922:VAL:O	2:T:922:VAL:HG12	2.02	0.59
2:W:332:VAL:HG23	2:W:344:ALA:HB2	1.84	0.59
2:B:355:ASP:HB2	2:B:538:MET:HE2	1.84	0.59
1:D:212:ARG:NH2	3:F:129:GLU:O	2.36	0.59
2:E:913:CYS:HA	2:E:1016:THR:O	2.03	0.59
1:G:178:CYS:HB3	1:G:299:THR:O	2.02	0.59
2:K:353:ASN:ND2	2:K:1100:GLU:OE2	2.36	0.59
2:N:1022:ALA:HB1	2:N:1050:SER:HB2	1.83	0.59
2:T:375:ASP:OD2	2:T:379:LYS:NZ	2.34	0.59
1:V:149:ALA:O	2:W:1009:PRO:HG2	2.02	0.59
2:W:382:ASP:OD2	2:W:394:ARG:NH2	2.36	0.59
2:B:485:TYR:OH	2:B:830:ALA:O	2.21	0.59
3:C:302:ASN:O	3:C:305:LYS:HG2	2.03	0.59
2:E:746:GLY:O	2:E:750:ARG:N	2.35	0.59
8:F:401:HEM:HBA1	8:F:401:HEM:HMA1	1.84	0.59
1:G:197:GLU:OE1	2:H:47:ARG:NH2	2.33	0.59
2:H:803:PHE:CG	2:H:808:ARG:HG3	2.37	0.59
2:N:1124:THR:HB	2:N:1126:TYR:H	1.68	0.59
3:O:231:ARG:HD3	3:O:233:VAL:O	2.02	0.59
3:O:241:PHE:HD2	3:O:241:PHE:N	2.01	0.59
1:S:192:ILE:HG12	1:S:203:ILE:HG12	1.85	0.59
2:W:96:GLN:O	2:W:105:LYS:NZ	2.36	0.59
2:W:621:GLU:O	2:W:622:ARG:HD3	2.03	0.59
2:W:996:TYR:CE2	2:W:1000:ARG:HD2	2.38	0.59
2:B:922:VAL:HG12	2:B:922:VAL:O	2.02	0.59
3:C:294:TRP:CE2	3:C:305:LYS:HB3	2.37	0.59
1:G:16:PRO:HG3	1:G:128:TRP:CE3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:678:MET:HG2	2:H:693:PHE:HB2	1.84	0.59
3:L:318[B]:ARG:HE	3:R:143:ILE:HG22	1.68	0.59
1:M:188:PRO:CG	3:O:302:ASN:OD1	2.51	0.59
2:Q:394:ARG:HH12	2:Q:829:GLN:HE21	1.50	0.59
2:W:666:MET:HE3	2:W:670:VAL:HG21	1.84	0.59
2:B:882:TRP:CD1	2:B:883:GLU:HG2	2.38	0.58
2:E:916:PRO:O	2:E:1020:HIS:N	2.33	0.58
2:E:956:GLN:C	2:E:1003:LEU:HD11	2.27	0.58
2:N:135:LEU:HB2	2:N:694:ALA:HB3	1.83	0.58
2:Q:865:ASN:HB3	2:Q:868:ILE:HD12	1.85	0.58
2:T:640:THR:OG1	2:T:1071:ASP:OD1	2.20	0.58
2:W:130:ARG:HH12	2:W:702:GLU:CD	2.11	0.58
2:W:130:ARG:NH1	2:W:702:GLU:OE2	2.36	0.58
2:W:684:ILE:HA	2:W:688:ILE:HD12	1.85	0.58
2:W:858:PRO:O	2:W:888:ARG:NH2	2.27	0.58
3:C:87:ALA:O	3:C:90:ASN:ND2	2.36	0.58
2:E:916:PRO:HA	6:E:5802:MD1:O1A	2.02	0.58
3:F:171:TRP:CH2	3:F:229:ARG:CD	2.86	0.58
2:K:152:THR:HG22	2:K:155:ASN:HB2	1.85	0.58
2:K:1087:PHE:HD1	2:K:1093:CYS:HB3	1.68	0.58
2:N:856:TYR:O	2:N:902:ASN:HB2	2.03	0.58
2:Q:1001:LEU:HD11	2:Q:1018:MET:HE1	1.84	0.58
2:T:1027:ASP:O	2:T:1031:GLN:HG3	2.03	0.58
1:V:209:ARG:NH1	3:X:234:GLU:OE1	2.36	0.58
2:B:113:ARG:HG3	2:B:315:PRO:HB2	1.86	0.58
2:B:375:ASP:OD1	2:B:379:LYS:HE3	2.02	0.58
1:D:52:ASN:ND2	3:F:215:LEU:HA	2.18	0.58
2:E:1129:GLY:N	2:E:1131:GLU:OE2	2.31	0.58
3:F:300:ASP:HA	3:F:304:GLN:CB	2.34	0.58
1:G:51:PHE:HZ	3:I:214:GLU:HG3	1.68	0.58
2:H:250:ASP:OD2	2:H:254:ARG:NH1	2.35	0.58
1:M:90:TRP:HB2	2:N:1146:VAL:HG22	1.86	0.58
2:Q:532:TYR:C	2:Q:1097:VAL:HG21	2.28	0.58
2:W:433:VAL:N	2:W:442:LYS:O	2.36	0.58
3:X:35:LYS:HG3	3:X:86:LYS:HA	1.85	0.58
1:D:294:TYR:HB3	1:D:297:PHE:CE2	2.39	0.58
3:F:157:ASP:C	3:F:239:GLU:C	2.71	0.58
8:F:401:HEM:HBC2	8:F:401:HEM:HHD	1.85	0.58
2:H:138:LYS:HB2	2:H:170:LEU:HD21	1.84	0.58
2:E:527:GLU:HA	2:E:530:ASN:HB2	1.86	0.58
2:H:100:ASP:OD2	2:H:103:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:922:VAL:CG2	2:H:926:TRP:CZ3	2.86	0.58
2:K:937:ASN:ND2	2:K:954:GLU:O	2.35	0.58
2:Q:101:LEU:HD12	2:Q:802:LEU:HD11	1.86	0.58
2:Q:335:PRO:HG3	2:Q:352:ASN:OD1	2.03	0.58
2:Q:485:TYR:O	2:Q:489:LEU:HG	2.03	0.58
2:T:77:ILE:HG23	2:T:114:MET:SD	2.44	0.58
2:T:814:GLN:OE1	2:T:814:GLN:N	2.36	0.58
1:V:15:TYR:OH	1:V:181:PRO:O	2.17	0.58
2:W:498:VAL:HG12	2:W:503:SER:O	2.03	0.58
3:C:132:ASP:OD2	3:C:295:ASN:HA	2.04	0.58
6:E:5801:MD1:N8	10:E:5902:HOH:O	2.32	0.58
2:H:123:ARG:NH2	2:H:930:ASP:OD2	2.37	0.58
2:H:236:LYS:HG2	2:H:653:ASN:CB	2.34	0.58
2:H:314:MET:HE2	2:H:919:ARG:HB2	1.86	0.58
2:K:434:TRP:HB3	2:K:461:VAL:HG22	1.86	0.58
1:M:193:TYR:CE2	2:N:47:ARG:HD3	2.38	0.58
2:N:61:ARG:HH11	2:N:61:ARG:HG3	1.67	0.58
2:Q:373:ASP:O	2:Q:377:VAL:HG23	2.03	0.58
3:L:303:GLY:HA2	3:L:305:LYS:CD	2.34	0.58
1:M:163:GLU:HG2	1:M:312:PRO:HA	1.86	0.58
2:Q:95:HIS:ND1	2:Q:111:ASN:OD1	2.34	0.58
2:Q:100:ASP:HB2	2:Q:802:LEU:HD21	1.85	0.58
2:T:353:ASN:ND2	2:T:1100:GLU:OE2	2.37	0.58
1:V:34:ARG:HB2	1:V:266:ILE:HG22	1.86	0.58
2:W:758:TRP:O	2:W:762:ILE:HG13	2.03	0.58
2:E:651:PHE:N	2:E:651:PHE:CD1	2.71	0.58
2:E:700:TRP:N	2:E:700:TRP:CD1	2.72	0.58
1:G:15:TYR:CE1	2:H:41:LEU:HD11	2.38	0.58
1:M:309:ARG:HG2	1:M:310:TRP:HE3	1.67	0.58
2:Q:47:ARG:HG2	2:Q:47:ARG:O	2.03	0.58
2:Q:388:ARG:HG2	2:Q:476:ILE:HD12	1.84	0.58
2:T:611:ASP:HB3	2:T:1089:ALA:HB2	1.85	0.58
2:W:533:PHE:HA	2:W:1065:MET:HE3	1.86	0.58
3:X:89:PRO:HG3	3:X:302:ASN:HD21	1.69	0.58
2:B:533:PHE:HA	2:B:1065:MET:HE3	1.85	0.58
2:B:1078:LYS:HG3	2:B:1079:ILE:HG12	1.85	0.58
1:D:65:THR:HG21	1:D:147:ASP:N	2.17	0.58
2:E:498:VAL:HA	2:E:501:THR:HG22	1.86	0.58
3:F:130:PHE:CE1	3:F:301:ARG:HD3	2.38	0.58
8:F:401:HEM:HBB2	8:F:401:HEM:HMB1	1.84	0.58
1:J:132:TYR:O	1:J:221:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1078:LYS:HB3	2:Q:1091:ASN:ND2	2.18	0.58
3:X:81:LEU:HD21	3:X:308:SER:CB	2.33	0.58
2:E:760:PHE:HB3	2:E:765:ARG:O	2.03	0.58
2:H:69:PRO:HD2	2:H:71:ASP:OD1	2.03	0.58
2:Q:67:CYS:HB2	2:Q:77:ILE:HD11	1.84	0.58
2:Q:73:HIS:CD2	2:Q:73:HIS:N	2.68	0.58
2:T:376:TYR:CE2	2:T:550:GLY:HA2	2.39	0.58
3:U:305:LYS:HD2	3:U:307:ILE:HG22	1.85	0.58
2:W:861:ILE:HB	2:W:891:LYS:HA	1.85	0.58
2:B:566:TYR:OH	2:B:567:LYS:NZ	2.36	0.57
2:E:69:PRO:HB3	2:E:700:TRP:HH2	1.68	0.57
3:I:32:GLU:HG3	3:I:32:GLU:O	2.01	0.57
2:K:209:GLU:OE1	2:K:209:GLU:N	2.34	0.57
1:P:279:PRO:O	1:P:283:LEU:HB2	2.04	0.57
3:U:145:ILE:HG12	3:U:288:TYR:CE2	2.39	0.57
1:V:336:ARG:NH1	1:V:376:TYR:CD1	2.72	0.57
2:W:501:THR:O	2:W:501:THR:OG1	2.12	0.57
2:W:1078:LYS:HG3	2:W:1079:ILE:N	2.19	0.57
2:B:629:PRO:HG2	2:B:874:GLY:O	2.04	0.57
3:F:110:TYR:HA	3:F:267:PHE:O	2.04	0.57
2:K:390:ASP:OD1	2:K:391:THR:N	2.32	0.57
3:L:303:GLY:C	3:L:305:LYS:HD2	2.28	0.57
1:M:189:ARG:HG2	1:M:189:ARG:HH11	1.67	0.57
1:M:373:PHE:CE2	1:M:375:MET:HB2	2.39	0.57
2:N:311:GLU:OE2	2:N:1019:LYS:NZ	2.35	0.57
2:N:917:LYS:HD2	6:N:5802:MD1:H15	1.69	0.57
3:R:137:MET:SD	3:R:155:MET:HA	2.44	0.57
2:W:72:THR:HG21	2:W:313:LYS:HE3	1.86	0.57
2:W:388:ARG:NH2	2:W:390:ASP:OD2	2.34	0.57
2:W:504:PRO:HG3	2:W:507:LEU:HD12	1.86	0.57
3:C:269:ARG:NH2	10:C:501:HOH:O	2.36	0.57
1:D:173:ARG:NH2	1:D:220:TYR:O	2.37	0.57
1:D:211:TYR:N	5:D:504:F3S:S4	2.77	0.57
2:E:192:TYR:CA	2:E:197:GLY:HA3	2.34	0.57
2:E:915:THR:HA	2:E:1018:MET:O	2.04	0.57
2:H:332:VAL:HG23	2:H:344:ALA:HB2	1.87	0.57
2:H:983:ASP:OD2	2:H:1061:ARG:HD2	2.04	0.57
3:I:42:LEU:HD21	3:I:150:PRO:HA	1.86	0.57
2:K:678:MET:HG2	2:K:693:PHE:HB2	1.86	0.57
3:O:235:ASP:CB	3:O:250:GLN:OE1	2.52	0.57
1:P:267:ARG:HD2	4:P:503:SF4:S1	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:1022:ALA:HB1	2:Q:1050:SER:CB	2.34	0.57
2:W:377:VAL:CG2	2:W:548:LEU:HA	2.34	0.57
2:B:463:GLU:OE2	2:B:486:LYS:NZ	2.37	0.57
2:E:110:TRP:H	2:E:110:TRP:HD1	1.52	0.57
1:J:365:GLU:HG2	1:J:372:LYS:HZ1	1.69	0.57
2:N:117:LYS:HB3	2:N:926:TRP:CD2	2.39	0.57
2:N:678:MET:HG2	2:N:693:PHE:HB2	1.85	0.57
1:P:262:CYS:O	2:Q:112:PRO:HG3	2.04	0.57
2:Q:425:ARG:HG3	2:Q:425:ARG:NH1	2.19	0.57
2:T:528:GLY:HA2	2:T:1099:LYS:HZ2	1.69	0.57
2:W:52:VAL:HG11	3:X:221:ALA:HB2	1.86	0.57
2:W:897:THR:O	2:W:900:THR:HG22	2.04	0.57
2:B:376:TYR:CD2	2:B:550:GLY:HA2	2.39	0.57
1:D:13:MET:HE3	1:D:115:THR:HG21	1.86	0.57
1:J:30:PHE:CE1	1:J:267:ARG:HG2	2.39	0.57
1:J:55:GLN:HG3	1:J:226:ARG:HD2	1.87	0.57
3:O:241:PHE:N	3:O:241:PHE:CD2	2.71	0.57
2:Q:1119:TRP:CD2	2:Q:1121:PRO:HD2	2.40	0.57
2:Q:1131:GLU:OE1	2:Q:1131:GLU:N	2.33	0.57
3:R:151:PHE:CE1	3:R:160:LYS:HB3	2.39	0.57
2:W:930:ASP:OD1	2:W:931:TRP:N	2.38	0.57
1:D:249:THR:HG21	1:D:254:MET:HB3	1.87	0.57
1:D:331:PHE:CE1	2:E:325:GLU:HG2	2.40	0.57
3:F:252:VAL:HG12	3:F:269:ARG:HB2	1.85	0.57
2:K:190:LYS:HA	2:K:193:SER:HB2	1.85	0.57
2:N:984:ARG:NH1	10:N:5912:HOH:O	2.38	0.57
2:Q:225:ARG:HB2	2:Q:267:TRP:HB2	1.86	0.57
2:Q:534:HIS:O	2:Q:538:MET:HG3	2.05	0.57
2:Q:681:ASP:OD2	2:Q:682:ILE:N	2.37	0.57
2:Q:882:TRP:CD1	2:Q:883:GLU:HG2	2.40	0.57
2:T:528:GLY:HA2	2:T:1099:LYS:NZ	2.18	0.57
3:U:58:VAL:HG22	3:U:59:PRO:HD2	1.86	0.57
2:B:400:ILE:HG21	2:B:468:LEU:HD23	1.87	0.57
2:E:337:TYR:HB3	2:E:1010:ALA:HB1	1.86	0.57
3:I:247:GLN:O	3:I:250:GLN:NE2	2.38	0.57
3:O:303:GLY:HA2	3:O:305:LYS:CE	2.35	0.57
1:A:178:CYS:HB3	1:A:299:THR:O	2.05	0.57
1:D:149:ALA:HA	1:D:168:PHE:HB3	1.86	0.57
2:H:139:GLY:O	2:H:159:TYR:HB3	2.05	0.57
2:H:336:GLU:OE2	6:H:5802:MD1:O3'	2.22	0.57
3:L:51:VAL:CG2	3:L:316:LEU:HG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:PRO:HB2	1:M:297:PHE:CD1	2.40	0.57
2:Q:503:SER:HB2	2:Q:508:ILE:HD11	1.86	0.57
1:V:149:ALA:HA	1:V:168:PHE:HB3	1.86	0.57
1:V:189:ARG:HD2	8:X:401:HEM:CGA	2.34	0.57
2:W:456:LYS:HB2	2:W:458:ILE:HD12	1.86	0.57
2:E:1063:TRP:N	2:E:1096:THR:HG23	2.17	0.57
3:I:321:TRP:O	3:I:322:GLN:OXT	2.21	0.57
2:N:82:ARG:NH1	3:O:214:GLU:OE2	2.38	0.57
2:T:917:LYS:HZ1	6:T:5801:MD1:H15	1.49	0.57
2:W:976:TYR:CD2	2:W:1108:ALA:HB2	2.38	0.57
1:A:259:MET:HA	1:A:267:ARG:HD3	1.87	0.57
2:E:386:LEU:H	2:E:433:VAL:HG12	1.70	0.57
2:E:920:HIS:HD2	2:E:935:TRP:O	1.87	0.57
3:F:273:THR:HG22	3:F:275:ASP:H	1.68	0.57
2:N:961:PRO:O	2:N:965:ARG:HG3	2.04	0.57
2:Q:544:LEU:HB2	2:Q:545:PRO:HD3	1.86	0.57
2:Q:648:VAL:HG13	2:Q:676:GLN:HB3	1.85	0.57
1:V:252:ARG:HD2	1:V:350:THR:HG21	1.87	0.57
2:W:924:SER:OG	6:W:5801:MD1:PA	2.63	0.57
2:B:302:LEU:HD11	2:B:524:HIS:HD2	1.65	0.56
2:E:1062:ASP:OD1	2:E:1096:THR:CG2	2.53	0.56
2:E:1062:ASP:CG	2:E:1096:THR:HG23	2.30	0.56
3:F:121:ASN:HB3	3:F:130:PHE:O	2.05	0.56
1:G:399:ILE:HD11	2:H:298:PHE:CE2	2.40	0.56
2:K:930:ASP:OD1	2:K:931:TRP:N	2.38	0.56
3:O:235:ASP:HB3	3:O:250:GLN:OE1	2.05	0.56
2:Q:514:ASP:O	2:Q:518:ILE:HG22	2.05	0.56
3:U:236:LEU:N	3:U:236:LEU:HD23	2.19	0.56
1:V:150:LYS:HG2	1:V:167:TRP:CE2	2.40	0.56
2:W:916:PRO:HA	6:W:5802:MD1:O1A	2.04	0.56
1:A:402:ARG:NH1	2:B:803:PHE:O	2.31	0.56
2:B:433:VAL:HG13	2:B:444:ILE:CD1	2.28	0.56
1:D:41:CYS:N	4:D:503:SF4:S3	2.76	0.56
3:F:301:ARG:H	3:F:304:GLN:CB	2.18	0.56
3:I:321:TRP:CE3	3:I:321:TRP:HA	2.39	0.56
2:T:533:PHE:CD1	2:T:1065:MET:HE3	2.40	0.56
2:W:467:LYS:O	2:W:468:LEU:HD13	2.04	0.56
2:B:392:LEU:HD11	2:B:869:ARG:HG3	1.88	0.56
3:C:285:GLU:CD	3:U:142:LYS:HD3	2.31	0.56
3:C:285:GLU:OE1	3:U:142:LYS:HD3	2.06	0.56
1:D:407:TYR:CE2	2:E:576:TRP:HZ2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:666:MET:HE3	2:E:670:VAL:HG21	1.87	0.56
2:E:851:PRO:O	2:E:858:PRO:HB3	2.05	0.56
2:H:418:GLN:OE1	2:H:446:ARG:NH1	2.38	0.56
3:L:236:LEU:HA	3:L:247:GLN:HG3	1.86	0.56
1:M:78:LYS:O	1:M:82:LEU:HD13	2.05	0.56
1:P:34:ARG:CB	1:P:266:ILE:HG22	2.36	0.56
2:Q:311:GLU:HG3	2:Q:919:ARG:HB3	1.86	0.56
2:Q:312:ASN:O	6:Q:5802:MD1:N8	2.38	0.56
1:S:164:HIS:HD1	2:T:337:TYR:HH	1.51	0.56
2:T:91:GLN:HE21	2:T:114:MET:HB2	1.69	0.56
2:T:115:CYS:SG	2:T:117:LYS:NZ	2.76	0.56
1:V:213:LYS:HB2	5:V:504:F3S:S2	2.45	0.56
2:W:438:SER:OG	2:W:438:SER:O	2.24	0.56
1:A:98:GLU:O	1:A:98:GLU:HG3	2.05	0.56
2:B:86:MET:HE1	2:B:701:VAL:HG11	1.87	0.56
2:B:528:GLY:HA2	2:B:1099:LYS:NZ	2.20	0.56
2:E:586:ALA:O	2:E:606:LYS:O	2.23	0.56
2:E:617:TRP:HA	2:E:621:GLU:CG	2.35	0.56
2:K:709:THR:HG22	2:K:718:GLN:HB2	1.87	0.56
1:M:188:PRO:HG2	3:O:302:ASN:CG	2.29	0.56
3:R:51:VAL:CG2	3:R:104:HIS:HD2	2.18	0.56
2:T:921:THR:O	6:T:5802:MD1:N17	2.39	0.56
2:W:79:ALA:HA	2:W:89:VAL:HG23	1.86	0.56
2:W:228:MET:HE2	2:W:273:HIS:CD2	2.39	0.56
2:W:709:THR:HG22	2:W:718:GLN:HB2	1.87	0.56
2:W:976:TYR:HD2	2:W:1108:ALA:HB2	1.70	0.56
2:B:923:HIS:CG	6:B:5801:MD1:H102	2.40	0.56
2:E:527:GLU:OE2	6:E:5802:MD1:H101	2.04	0.56
2:H:916:PRO:HA	6:H:5802:MD1:O1A	2.06	0.56
1:J:178:CYS:HB3	1:J:299:THR:O	2.06	0.56
1:M:243:GLU:CD	2:N:54:ARG:HH12	2.11	0.56
2:N:51:SER:O	2:N:53:TYR:N	2.39	0.56
3:O:103:ILE:CG2	3:O:110:TYR:HB2	2.36	0.56
2:Q:142[A]:ARG:NH1	2:Q:146:ASP:OD1	2.39	0.56
1:V:16:PRO:CG	1:V:128:TRP:HZ2	1.65	0.56
2:B:117:LYS:HE3	2:B:922:VAL:HG23	1.88	0.56
1:J:192:ILE:HG12	1:J:203:ILE:HG12	1.88	0.56
2:K:164:ARG:NH2	2:K:674:ILE:O	2.35	0.56
2:K:227:GLY:HA3	2:K:654:VAL:HG13	1.87	0.56
2:K:388:ARG:NH2	2:K:390:ASP:OD2	2.39	0.56
2:K:938:ASN:ND2	10:K:5904:HOH:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:136:LEU:HD23	3:L:291:MET:HB3	1.86	0.56
3:L:303:GLY:HA2	3:L:305:LYS:HE3	1.87	0.56
2:N:996:TYR:CE2	2:N:1000:ARG:HB2	2.41	0.56
2:N:1132:ASN:O	2:N:1136:LYS:HG3	2.05	0.56
3:O:137:MET:HE3	3:O:290:ASN:HB3	1.88	0.56
2:Q:123:ARG:HH21	3:R:194:ASP:HB2	1.69	0.56
3:U:236:LEU:HB2	3:U:245:THR:O	2.04	0.56
1:V:126:ASN:HA	3:X:88:PHE:CZ	2.41	0.56
2:W:98:TYR:CE1	2:W:798:VAL:HG11	2.40	0.56
2:W:222:PHE:HD1	2:W:648:VAL:CG1	2.18	0.56
2:W:919:ARG:HG3	2:W:920:HIS:ND1	2.16	0.56
2:E:139:GLY:HA3	2:E:160:MET:HB2	1.88	0.56
3:F:258:PHE:HB2	3:F:263:TRP:CZ3	2.39	0.56
1:G:242:ILE:HD11	1:G:256:THR:HG22	1.87	0.56
1:M:81:LYS:HB2	2:N:1134:PHE:CE1	2.41	0.56
2:N:71:ASP:O	2:N:72:THR:HG22	2.06	0.56
3:O:285:GLU:OE1	3:O:285:GLU:HA	2.04	0.56
1:P:195:ARG:NH2	1:P:243:GLU:OE2	2.36	0.56
2:Q:900:THR:O	2:Q:901:LYS:HD2	2.05	0.56
1:S:34:ARG:CB	1:S:266:ILE:HG22	2.36	0.56
2:T:225:ARG:HH11	2:T:656:LEU:HD12	1.69	0.56
2:W:970:GLU:OE2	2:W:1130:ASN:ND2	2.38	0.56
2:B:941:ASP:OD2	2:B:944:ARG:N	2.39	0.56
1:G:2:THR:HG21	1:G:18:PHE:HD2	1.70	0.56
1:G:25:GLN:CG	1:G:302:ASN:ND2	2.69	0.56
2:Q:94:ASP:OD1	2:Q:94:ASP:N	2.39	0.56
2:Q:386:LEU:HD23	2:Q:480:THR:HG22	1.88	0.56
2:Q:641:HIS:ND1	2:Q:1087:PHE:HB2	2.20	0.56
1:S:38:CYS:HB3	2:T:314:MET:HE2	1.88	0.56
2:T:431:PHE:CE1	2:T:825:THR:HA	2.41	0.56
2:T:1132:ASN:HB3	2:T:1135:MET:H	1.70	0.56
1:V:58:MET:HE1	1:V:233:GLU:HG3	1.88	0.56
2:B:32:LYS:HE3	2:B:35:VAL:HA	1.87	0.56
1:D:15:TYR:HE1	1:D:180:TYR:HA	1.71	0.56
1:M:16:PRO:HG3	1:M:128:TRP:CZ3	2.40	0.56
2:N:305:THR:CG2	2:N:525:TYR:HB3	2.34	0.56
2:Q:616:TYR:CE2	2:Q:623:PRO:HA	2.41	0.56
3:R:86:LYS:HE2	3:R:309:ILE:CD1	2.36	0.56
2:T:1064:SER:OG	2:T:1069:GLN:NE2	2.32	0.56
1:V:15:TYR:HE1	2:W:41:LEU:HD11	1.70	0.56
2:W:33:PRO:HA	3:X:277:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:915:THR:HA	2:W:1018:MET:O	2.05	0.56
2:W:976:TYR:HD1	2:W:1000:ARG:NE	2.03	0.56
2:B:671:ASN:HA	2:B:674:ILE:HG13	1.86	0.56
2:B:841:GLY:HA3	2:B:870:PRO:HB3	1.88	0.56
1:D:143:ASN:ND2	2:E:920:HIS:NE2	2.54	0.56
1:D:192:ILE:HD11	5:D:504:F3S:S3	2.46	0.56
2:H:90:GLU:HG2	2:H:91:GLN:H	1.71	0.56
2:H:135:LEU:HB2	2:H:694:ALA:HB3	1.87	0.56
10:J:601:HOH:O	2:K:1145:LYS:NZ	2.28	0.56
1:M:34:ARG:CB	1:M:266:ILE:HG22	2.36	0.56
2:Q:588:ASP:OD2	2:Q:590:PHE:N	2.39	0.56
2:W:44:TYR:CG	2:W:45:PRO:HD2	2.40	0.56
2:W:631:TYR:OH	2:W:871:ASP:OD1	2.20	0.56
3:X:55:GLN:HG3	3:X:55:GLN:O	2.06	0.56
3:X:242:GLY:H	8:X:401:HEM:HBA1	1.70	0.56
2:B:913:CYS:CB	2:B:1103:VAL:HG21	2.35	0.55
3:F:171:TRP:CZ2	3:F:229:ARG:HD3	2.41	0.55
2:H:977:VAL:HB	2:H:1001:LEU:HD23	1.87	0.55
2:K:937:ASN:HD21	2:K:954:GLU:N	1.99	0.55
2:Q:900:THR:HG22	2:Q:901:LYS:H	1.70	0.55
2:Q:969:ILE:HG12	2:Q:1107:LYS:HB2	1.87	0.55
1:D:209:ARG:HH12	3:F:244:LEU:HD23	1.71	0.55
1:D:314:ALA:HB1	2:E:1141:GLY:HA3	1.88	0.55
2:H:1057:GLN:HA	2:H:1060:THR:HG22	1.88	0.55
2:K:342:GLN:HG3	2:K:343:LYS:HD2	1.88	0.55
1:M:115:THR:HG23	1:M:298:GLY:HA3	1.87	0.55
2:T:551:ASN:O	2:T:557:SER:HB2	2.06	0.55
1:V:42:THR:HG23	1:V:61:ASN:O	2.06	0.55
1:V:184:LEU:HD21	2:W:40:PRO:HB2	1.88	0.55
2:B:928:VAL:CG2	2:B:1048:GLN:HG2	2.36	0.55
2:T:268:SER:HB2	2:T:1090:ASP:OD2	2.05	0.55
3:U:43:THR:HG22	3:U:147:PRO:CG	2.36	0.55
1:V:211:TYR:CD2	5:V:504:F3S:S1	2.99	0.55
1:A:259:MET:HG3	1:A:269:GLN:HB2	1.88	0.55
2:B:916:PRO:HA	6:B:5802:MD1:O1A	2.06	0.55
3:F:210:GLN:HB2	2:Q:208:LYS:HE2	1.86	0.55
3:I:145:ILE:HG23	3:I:288:TYR:CE2	2.42	0.55
2:K:462:LEU:HB3	2:K:482:LEU:HD23	1.88	0.55
3:O:258:PHE:HB2	3:O:263:TRP:CE3	2.41	0.55
1:P:30:PHE:CD1	1:P:267:ARG:HG2	2.41	0.55
1:P:76:ASP:OD2	2:Q:1138:PHE:HZ	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:96:ASP:OD2	1:P:106:ALA:N	2.29	0.55
2:W:178:PHE:HB3	2:W:744:LYS:HG3	1.87	0.55
2:B:468:LEU:O	2:B:475:GLU:HG3	2.05	0.55
3:F:166:HIS:CE1	3:F:168:LYS:HE3	2.42	0.55
2:N:250:ASP:OD2	2:N:254:ARG:NH1	2.39	0.55
2:Q:554:TYR:O	2:Q:555:PHE:C	2.46	0.55
2:T:296:VAL:HG11	2:T:320:VAL:HG22	1.89	0.55
2:T:312:ASN:O	6:T:5802:MD1:N8	2.40	0.55
2:T:804:ARG:NH2	2:T:817:GLU:OE2	2.40	0.55
1:V:72:PRO:HG3	1:V:139:TRP:CZ3	2.42	0.55
2:W:428:ILE:HD11	2:W:1074:PHE:CG	2.41	0.55
3:X:84:GLN:O	3:X:90:ASN:HB2	2.06	0.55
3:C:227:LEU:O	3:C:229:ARG:NH2	2.39	0.55
2:E:618:ASN:HD21	2:E:661:LYS:H	1.52	0.55
2:E:917:LYS:HE2	6:E:5801:MD1:S13	2.46	0.55
1:M:400:HIS:CD2	2:N:104:ASN:HB3	2.41	0.55
2:N:47:ARG:HH21	2:N:47:ARG:HG3	1.70	0.55
2:Q:321:THR:O	2:Q:324:MET:HG2	2.06	0.55
2:Q:372:TYR:HD2	2:Q:377:VAL:HG21	1.71	0.55
2:W:139:GLY:O	2:W:159:TYR:HB3	2.06	0.55
2:W:1023:TRP:CD1	2:W:1023:TRP:N	2.72	0.55
3:X:50:ASN:ND2	3:X:317:GLU:OE1	2.38	0.55
2:E:664:TYR:CD1	2:E:999:SER:HA	2.42	0.55
2:E:917:LYS:HZ1	6:E:5801:MD1:C16	2.20	0.55
3:I:107:ILE:HG13	3:I:108:THR:HG23	1.87	0.55
3:I:132:ASP:OD1	3:I:295:ASN:HA	2.06	0.55
1:J:329:GLU:OE1	1:J:371:LYS:NZ	2.37	0.55
2:K:124:ARG:NH1	2:K:925:GLN:OE1	2.40	0.55
2:K:270:TYR:CE2	2:K:276:GLN:HG3	2.42	0.55
3:O:122:LYS:HB3	3:O:169:ALA:HB1	1.89	0.55
2:Q:424:GLN:NE2	2:Q:1083:PHE:O	2.39	0.55
2:B:868:ILE:HG22	2:B:870:PRO:HD3	1.88	0.55
2:B:915:THR:HA	2:B:1018:MET:O	2.06	0.55
1:D:178:CYS:HB3	1:D:299:THR:O	2.07	0.55
1:D:313:ARG:NH1	1:D:325:ASP:HA	2.22	0.55
2:E:709:THR:N	2:E:718:GLN:O	2.39	0.55
3:F:229:ARG:HG2	3:F:229:ARG:NH1	2.08	0.55
3:F:305:LYS:CE	8:F:401:HEM:C4D	2.64	0.55
1:G:66:LYS:NZ	1:G:76:ASP:OD2	2.38	0.55
3:I:83:LYS:HE2	3:I:92:GLY:O	2.06	0.55
3:I:231:ARG:NH1	3:I:250:GLN:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:124:ARG:NH2	2:K:683:GLU:OE2	2.39	0.55
2:K:276:GLN:HB3	2:K:1095:ASN:HD21	1.71	0.55
2:K:382:ASP:HA	2:K:385:LEU:HD13	1.88	0.55
2:K:834:GLU:HB2	2:K:837:ILE:HD12	1.89	0.55
2:W:976:TYR:HD1	2:W:1000:ARG:HE	1.55	0.55
1:A:317:ARG:NH1	1:A:325:ASP:OD2	2.40	0.55
2:B:415:TYR:CD1	2:B:420:LEU:HB3	2.42	0.55
2:E:964:ALA:HB3	2:E:1007:TYR:HE1	1.70	0.55
3:F:172:GLU:OE1	3:F:255:CYS:HA	2.07	0.55
2:K:1011:TYR:CE2	2:K:1017:MET:HB2	2.42	0.55
1:M:262:CYS:HA	4:M:503:SF4:S3	2.47	0.55
2:N:77:ILE:HD11	4:N:5804:SF4:S1	2.47	0.55
2:N:485:TYR:HA	2:N:488:HIS:HB3	1.88	0.55
1:P:346:ARG:HA	1:P:346:ARG:NE	2.22	0.55
2:Q:381:THR:O	2:Q:827:ARG:NH1	2.39	0.55
2:Q:434:TRP:HB3	2:Q:461:VAL:HG12	1.88	0.55
3:R:269:ARG:NH1	3:R:279:VAL:O	2.40	0.55
2:W:974:TYR:C	2:W:1108:ALA:HB3	2.32	0.55
1:A:259:MET:SD	1:A:267:ARG:HD3	2.47	0.55
2:E:1062:ASP:HA	2:E:1096:THR:HG21	1.88	0.55
3:F:302:ASN:O	3:F:305:LYS:HD2	2.06	0.55
3:I:298:ARG:O	3:I:299:GLU:HB2	2.07	0.55
2:K:916:PRO:HA	6:K:5802:MD1:O1A	2.07	0.55
1:M:115:THR:HG22	1:M:117:PHE:H	1.72	0.55
2:N:977:VAL:HG11	2:N:1001:LEU:HD23	1.89	0.55
1:P:137:LYS:HE2	2:Q:1113:MET:HE1	1.89	0.55
2:Q:77:ILE:HD13	2:Q:114:MET:HE3	1.88	0.55
2:Q:310:ILE:CG1	2:Q:340:SER:HA	2.37	0.55
2:Q:654:VAL:HG12	6:Q:5801:MD1:O2B	2.06	0.55
3:R:305:LYS:HE2	8:R:401:HEM:C1D	2.41	0.55
3:X:109:ILE:C	3:X:110:TYR:CD1	2.85	0.55
2:B:971:ASP:HB2	2:B:1007:TYR:CG	2.42	0.54
2:B:972:GLY:O	2:B:1004:ARG:NH1	2.40	0.54
2:K:925:GLN:NE2	6:K:5801:MD1:H5'1	2.22	0.54
1:S:34:ARG:HA	2:T:321:THR:CG2	2.37	0.54
2:W:236:LYS:HG2	2:W:653:ASN:HB2	1.89	0.54
3:X:235:ASP:O	3:X:250:GLN:NE2	2.40	0.54
2:B:515:ILE:HG22	2:B:549:THR:HG21	1.89	0.54
1:D:257:ARG:HB3	4:D:501:SF4:S2	2.46	0.54
2:E:305:THR:O	6:E:5802:MD1:N2	2.39	0.54
3:F:155:MET:CG	8:F:401:HEM:NC	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:100:ASP:OD2	2:H:104:ASN:N	2.40	0.54
2:H:236:LYS:HE3	2:H:734:ASP:OD2	2.06	0.54
2:H:1061:ARG:HG2	2:H:1062:ASP:N	2.22	0.54
2:K:394:ARG:NH1	2:K:831:TYR:O	2.40	0.54
2:K:984:ARG:NH2	10:K:5907:HOH:O	2.39	0.54
2:N:1001:LEU:HD22	2:N:1055:SER:O	2.07	0.54
2:N:1020:HIS:CE1	6:N:5801:MD1:O11	2.52	0.54
2:Q:223:LYS:NZ	2:Q:646:THR:OG1	2.39	0.54
2:T:72:THR:HG22	2:T:564:GLY:C	2.32	0.54
2:W:250:ASP:OD2	2:W:254:ARG:NH1	2.39	0.54
2:W:293:MET:CE	2:W:313:LYS:HD2	2.30	0.54
2:B:1087:PHE:CD1	2:B:1087:PHE:C	2.85	0.54
1:D:168:PHE:HE1	2:E:342:GLN:HE21	1.56	0.54
1:G:271:PHE:O	1:G:278:ASN:ND2	2.39	0.54
1:J:189:ARG:HH12	3:L:244:LEU:HB3	1.73	0.54
2:K:900:THR:O	2:K:901:LYS:HG3	2.07	0.54
2:K:1001:LEU:HA	2:K:1054:GLY:HA3	1.89	0.54
2:N:882:TRP:CZ3	2:N:983:ASP:OD1	2.60	0.54
1:P:284:ILE:CD1	1:P:304:TYR:CD2	2.91	0.54
2:Q:213:ARG:NE	2:Q:642:MET:HB3	2.22	0.54
1:S:177:HIS:NE2	1:S:237:ALA:HB2	2.22	0.54
1:V:16:PRO:HD3	1:V:128:TRP:NE1	2.08	0.54
2:W:300:LYS:H	2:W:520:PRO:HD2	1.72	0.54
2:W:917:LYS:HZ3	6:W:5801:MD1:H15	1.55	0.54
2:W:974:TYR:O	2:W:1108:ALA:CB	2.54	0.54
3:X:302:ASN:HB2	8:X:401:HEM:CAA	2.38	0.54
2:B:706:PHE:CD1	2:B:789:LEU:HD11	2.42	0.54
2:B:1027:ASP:O	2:B:1031:GLN:HG3	2.07	0.54
2:E:73:HIS:HD2	2:E:315:PRO:CB	2.21	0.54
2:E:479:MET:HG3	2:E:484:MET:HE2	1.90	0.54
3:I:53:TYR:CZ	3:I:319:ILE:HG23	2.42	0.54
2:K:977:VAL:HB	2:K:1001:LEU:HD23	1.90	0.54
2:N:533:PHE:HB2	2:N:1100:GLU:HG3	1.89	0.54
1:P:231:VAL:HG22	10:P:604:HOH:O	2.03	0.54
2:Q:527:GLU:O	2:Q:531:HIS:HB2	2.07	0.54
2:T:983:ASP:HB3	2:T:984:ARG:HD3	1.89	0.54
2:T:1032:ALA:HB1	2:T:1036:ARG:HD2	1.87	0.54
2:B:89:VAL:CG1	2:B:114:MET:HE1	2.38	0.54
2:B:213:ARG:NH2	2:B:642:MET:O	2.40	0.54
2:B:314:MET:HE1	2:B:919:ARG:HB2	1.89	0.54
2:H:434:TRP:CZ3	2:H:441:PRO:HD3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:571:PHE:HB2	2:H:581:PHE:HB2	1.90	0.54
2:K:222:PHE:CD1	2:K:648:VAL:HG22	2.42	0.54
2:K:497:VAL:O	2:K:501:THR:OG1	2.23	0.54
3:O:103:ILE:HG22	3:O:110:TYR:HB2	1.90	0.54
2:Q:229:GLY:HA3	2:Q:237:TYR:CD1	2.42	0.54
2:Q:974:TYR:CZ	2:Q:1004:ARG:HD3	2.43	0.54
2:W:135:LEU:HB2	2:W:694:ALA:HB3	1.89	0.54
1:A:58:MET:HE3	1:A:60:TRP:HE1	1.73	0.54
3:C:54:MET:O	3:C:56:ILE:HG13	2.07	0.54
1:D:117:PHE:CE1	1:D:129:ALA:HB2	2.43	0.54
2:E:445:THR:HG22	2:E:446:ARG:H	1.73	0.54
2:H:923:HIS:O	2:H:1021:SER:CB	2.55	0.54
1:M:225:TYR:HD1	3:O:127:THR:HA	1.73	0.54
2:N:394:ARG:NH1	2:N:831:TYR:O	2.40	0.54
2:N:641:HIS:CE1	2:N:1087:PHE:HB2	2.43	0.54
1:P:282:TRP:CE3	1:P:283:LEU:HD12	2.43	0.54
1:S:104:THR:O	1:S:285:ARG:NH1	2.41	0.54
3:X:81:LEU:O	3:X:96:ASN:O	2.24	0.54
2:E:657:ILE:HD12	2:E:657:ILE:H	1.70	0.54
2:E:924:SER:HB3	6:E:5801:MD1:O2A	2.08	0.54
2:K:71:ASP:O	2:K:72:THR:HG22	2.07	0.54
2:K:376:TYR:CD2	2:K:550:GLY:HA2	2.43	0.54
2:W:124:ARG:NH1	2:W:683:GLU:OE1	2.40	0.54
2:W:228:MET:O	2:W:231:LEU:HG	2.08	0.54
2:W:1040:ARG:HH12	3:X:192:HIS:CE1	2.26	0.54
1:A:16:PRO:HG3	1:A:128:TRP:CE3	2.43	0.54
2:B:227:GLY:HA3	2:B:654:VAL:HG22	1.90	0.54
2:E:651:PHE:HD2	2:E:654:VAL:HA	1.73	0.54
3:I:154:ARG:CA	8:I:401:HEM:CBB	2.86	0.54
2:N:321:THR:HG22	2:N:343:LYS:HG2	1.90	0.54
2:Q:1030:VAL:HG13	2:Q:1053:TYR:HE2	1.72	0.54
1:S:45:CYS:HB2	4:S:501:SF4:S2	2.47	0.54
1:S:289:ILE:HD11	1:S:331:PHE:HB2	1.90	0.54
3:U:138:PHE:HB3	3:U:279:VAL:HG21	1.88	0.54
1:V:396:GLU:HA	1:V:396:GLU:OE2	2.07	0.54
2:W:661:LYS:O	2:W:1060:THR:OG1	2.25	0.54
2:W:909:TYR:CD2	2:W:1104:LYS:HB2	2.43	0.54
2:W:974:TYR:CE1	2:W:1052:ARG:HD2	2.42	0.54
2:B:64:THR:CG2	2:B:76:ARG:HD2	2.38	0.54
2:B:276:GLN:HB3	2:B:1095:ASN:OD1	2.08	0.54
2:B:497:VAL:O	2:B:501:THR:OG1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:776:GLY:H	2:B:781:LYS:HZ2	1.55	0.54
2:E:656:LEU:O	2:E:660:ALA:N	2.41	0.54
1:M:356:LYS:HB3	1:M:383:PHE:HE2	1.71	0.54
2:N:648:VAL:HG13	2:N:676:GLN:HB3	1.90	0.54
3:O:87:ALA:CB	3:O:241:PHE:HE1	2.20	0.54
2:Q:115:CYS:CB	4:Q:5804:SF4:S2	2.96	0.54
2:Q:937:ASN:HD22	2:Q:954:GLU:C	2.15	0.54
2:T:752:LYS:C	2:T:754:PHE:H	2.16	0.54
2:T:753:ARG:HA	2:T:756:ASP:HB2	1.90	0.54
2:T:909:TYR:CD1	2:T:1104:LYS:HB2	2.42	0.54
2:W:354:THR:HA	2:W:847:HIS:HE1	1.73	0.54
3:X:81:LEU:HD23	3:X:307:ILE:O	2.07	0.54
2:B:984:ARG:HH11	2:B:1061:ARG:HB2	1.73	0.54
2:E:33:PRO:HG2	3:F:161:PRO:HB3	1.90	0.54
3:F:114:ILE:HA	3:F:263:TRP:O	2.07	0.54
2:K:321:THR:O	2:K:324:MET:HG2	2.08	0.54
2:N:814:GLN:HA	2:N:819:LEU:HB2	1.91	0.54
2:N:917:LYS:NZ	6:N:5801:MD1:H15	2.06	0.54
1:P:178:CYS:HB3	1:P:299:THR:O	2.08	0.54
3:U:137:MET:HB2	8:U:401:HEM:CBC	2.38	0.54
1:V:318:GLN:OE1	2:W:1143:LEU:HB2	2.07	0.54
2:W:976:TYR:HD1	2:W:1000:ARG:NH2	2.03	0.54
2:B:970:GLU:HG2	2:B:1118:VAL:HG21	1.90	0.53
3:F:299:GLU:O	3:F:301:ARG:NH1	2.41	0.53
2:H:314:MET:HE3	6:H:5802:MD1:N16	2.24	0.53
3:I:53:TYR:OH	3:I:319:ILE:HG23	2.07	0.53
3:I:95:VAL:HG22	3:I:306:ASN:OD1	2.08	0.53
2:K:453:LEU:HD11	2:K:827:ARG:HH12	1.72	0.53
2:K:531:HIS:CG	2:K:1098:PRO:HD2	2.43	0.53
2:N:308:ASN:HD21	2:N:339:PRO:HD2	1.73	0.53
2:Q:533:PHE:CE2	2:Q:1065:MET:HG3	2.43	0.53
2:T:409:ILE:HG21	2:T:445:THR:HG21	1.90	0.53
2:T:434:TRP:HB3	2:T:461:VAL:HG22	1.91	0.53
2:W:308:ASN:ND2	2:W:311:GLU:OE1	2.40	0.53
2:B:311:GLU:OE2	2:B:339:PRO:HG2	2.08	0.53
2:B:949:MET:HE2	2:B:953:GLY:CA	2.38	0.53
1:D:225:TYR:HB3	3:F:127:THR:HG23	1.89	0.53
2:E:1051:PHE:CD2	2:E:1055:SER:HA	2.43	0.53
2:H:140:TRP:HZ2	2:H:676:GLN:HE21	1.54	0.53
3:I:154:ARG:CA	8:I:401:HEM:HBB2	2.38	0.53
3:I:236:LEU:HD23	3:I:246:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:30:LEU:HD12	2:K:31:LEU:HD22	1.90	0.53
1:M:212:ARG:N	5:M:504:F3S:S4	2.72	0.53
2:N:114:MET:HG2	4:N:5804:SF4:S1	2.47	0.53
2:N:1135:MET:HE1	2:N:1138:PHE:CE2	2.43	0.53
2:Q:842:GLU:OE2	2:Q:848:ARG:NH2	2.41	0.53
3:F:41:GLU:OE1	3:F:154:ARG:NH2	2.42	0.53
2:H:663:VAL:HG21	2:H:1024:ILE:HD13	1.89	0.53
3:I:155:MET:HE1	3:I:241:PHE:HB2	1.90	0.53
2:K:415:TYR:HE1	2:K:420:LEU:HD23	1.73	0.53
1:S:38:CYS:CB	2:T:314:MET:HE2	2.38	0.53
2:W:390:ASP:N	2:W:390:ASP:OD1	2.37	0.53
3:X:137:MET:HG2	8:X:401:HEM:CBC	2.38	0.53
2:B:225:ARG:NE	2:B:269:ASN:OD1	2.31	0.53
2:B:588:ASP:OD1	2:B:608:ARG:NH2	2.41	0.53
2:K:116:LEU:H	2:K:116:LEU:HD23	1.74	0.53
2:K:286:LEU:HD12	2:K:287:GLN:H	1.73	0.53
2:K:1064:SER:OG	2:K:1069:GLN:NE2	2.42	0.53
1:V:34:ARG:HB3	1:V:266:ILE:HG22	1.89	0.53
2:W:381:THR:O	2:W:827:ARG:HD3	2.09	0.53
3:X:224:LEU:O	10:X:501:HOH:O	2.18	0.53
2:E:128:PRO:HD3	3:F:194:ASP:HB3	1.91	0.53
2:E:506:ASP:O	2:E:510:ARG:N	2.40	0.53
2:E:572:GLN:HA	2:E:1079:ILE:O	2.09	0.53
2:E:587:GLU:C	2:E:606:LYS:O	2.52	0.53
2:H:76:ARG:HD3	2:H:718:GLN:OE1	2.08	0.53
2:H:1016:THR:HG21	2:H:1105:ILE:HD11	1.89	0.53
2:N:265:ARG:NH1	2:N:643:PRO:HA	2.23	0.53
2:N:1069:GLN:HE21	2:N:1094:ILE:HD11	1.74	0.53
2:Q:659:ASN:OD1	2:Q:1021:SER:OG	2.26	0.53
2:Q:768:VAL:O	2:Q:772:ARG:HG3	2.08	0.53
2:T:114:MET:HG2	4:T:5804:SF4:S1	2.48	0.53
2:B:1088:GLU:CG	2:B:1091:ASN:HB3	2.38	0.53
2:B:1119:TRP:CD2	2:B:1121:PRO:HD2	2.44	0.53
2:E:85:VAL:HG12	2:E:87:MET:HG2	1.90	0.53
2:E:957:ILE:CB	2:E:1018:MET:HG2	2.39	0.53
3:R:143:ILE:HD12	3:R:143:ILE:C	2.34	0.53
3:R:238:ALA:HB2	3:R:244:LEU:HD12	1.90	0.53
1:S:20:SER:HG	1:S:196:LYS:HZ1	1.52	0.53
2:W:551:ASN:O	2:W:558:GLY:N	2.42	0.53
2:B:373:ASP:O	2:B:377:VAL:HG23	2.08	0.53
2:H:528:GLY:HA2	2:H:1099:LYS:NZ	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:307:LYS:HZ3	2:Q:313:LYS:HE2	1.74	0.53
2:Q:433:VAL:HG21	2:Q:460:PRO:CB	2.29	0.53
2:Q:1024:ILE:HG22	2:Q:1055:SER:HB2	1.90	0.53
2:T:164:ARG:NH1	2:T:677:ILE:HD12	2.24	0.53
2:W:34:ALA:HA	3:X:245:THR:HG21	1.90	0.53
1:A:6:ASN:OD1	1:A:8:HIS:N	2.41	0.53
2:B:434:TRP:HB3	2:B:461:VAL:HG22	1.90	0.53
3:C:237:ASN:OD1	3:C:247:GLN:NE2	2.41	0.53
2:E:1051:PHE:CE2	2:E:1055:SER:HA	2.43	0.53
2:H:462:LEU:O	2:H:480:THR:HG21	2.09	0.53
3:I:98:ALA:CB	3:I:291:MET:HE1	2.39	0.53
3:I:142:LYS:HG2	3:X:285:GLU:OE1	2.08	0.53
1:J:207:ARG:HD3	2:K:44:TYR:OH	2.09	0.53
2:N:641:HIS:CE1	2:N:1069:GLN:HA	2.44	0.53
2:N:823:THR:HG21	2:N:829:GLN:HG3	1.91	0.53
2:N:991:PRO:HA	2:N:996:TYR:CD1	2.44	0.53
1:P:284:ILE:HD11	1:P:304:TYR:CD2	2.44	0.53
2:Q:69:PRO:HB3	2:Q:700:TRP:CH2	2.43	0.53
2:Q:660:ALA:O	2:Q:1057:GLN:OE1	2.27	0.53
2:Q:915:THR:HA	2:Q:1018:MET:O	2.09	0.53
2:T:484:MET:HE2	2:T:844:PHE:HZ	1.74	0.53
2:T:1001:LEU:HA	2:T:1054:GLY:HA3	1.91	0.53
1:V:291:LEU:HB2	1:V:320:PHE:HB3	1.91	0.53
2:W:883:GLU:O	2:W:886:THR:OG1	2.26	0.53
6:W:5801:MD1:H11	6:W:5801:MD1:H7	1.90	0.53
2:B:662:HIS:H	2:B:1060:THR:HG23	1.74	0.53
3:O:247:GLN:CB	10:O:502:HOH:O	2.56	0.53
2:Q:915:THR:OG1	6:Q:5801:MD1:N16	2.40	0.53
2:T:1057:GLN:OE1	6:T:5801:MD1:N16	2.37	0.53
1:V:116:ILE:HA	1:V:119:VAL:HG12	1.90	0.53
2:W:513:LYS:O	2:W:517:THR:OG1	2.23	0.53
2:B:166:ASN:ND2	2:B:1031:GLN:OE1	2.42	0.53
2:E:793:TYR:HB2	2:E:798:VAL:O	2.08	0.53
2:E:1131:GLU:H	2:E:1131:GLU:CD	2.13	0.53
2:H:868:ILE:HG22	2:H:870:PRO:HD3	1.90	0.53
2:K:227:GLY:O	2:K:653:ASN:HB3	2.09	0.53
2:K:314:MET:HE1	2:K:919:ARG:HB2	1.90	0.53
2:N:61:ARG:HG2	2:N:81:VAL:HB	1.91	0.53
2:N:547[A]:MET:HE1	2:N:830:ALA:HB2	1.91	0.53
2:Q:611:ASP:HB3	2:Q:1089:ALA:HB2	1.91	0.53
2:Q:903:PHE:CE2	2:Q:904:LEU:HG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:957:ILE:HB	2:Q:1003:LEU:HD21	1.90	0.53
2:T:711:SER:HB3	2:T:714:ASN:OD1	2.09	0.53
3:U:51:VAL:HG23	3:U:104:HIS:HD2	1.74	0.53
1:V:126:ASN:HA	3:X:88:PHE:CE1	2.44	0.53
3:C:163:ASN:HD22	3:C:164:LEU:H	1.57	0.52
1:D:331:PHE:HZ	2:E:324:MET:HG3	1.73	0.52
1:J:36:ILE:HD12	2:K:314:MET:HB2	1.91	0.52
2:N:117:LYS:HB3	2:N:926:TRP:CE2	2.44	0.52
2:N:916:PRO:O	2:N:1020:HIS:N	2.42	0.52
2:Q:228:MET:HB3	2:Q:231:LEU:HD23	1.90	0.52
2:Q:902:ASN:O	2:Q:906:GLU:HG2	2.08	0.52
2:Q:973:ASP:OD1	2:Q:1111:GLY:N	2.37	0.52
1:S:149:ALA:HB2	1:S:168:PHE:HD2	1.73	0.52
2:T:128:PRO:HG2	2:T:129:TYR:CE2	2.44	0.52
2:T:546:VAL:CG1	2:T:552:VAL:HG23	2.39	0.52
1:V:285:ARG:NH2	10:V:603:HOH:O	2.41	0.52
1:V:311:ALA:HB3	1:V:316:LEU:HD11	1.91	0.52
1:V:336:ARG:HD2	1:V:376:TYR:CD1	2.43	0.52
2:W:892:LYS:HB3	2:W:897:THR:CG2	2.37	0.52
1:A:296:GLN:NE2	1:A:318:GLN:O	2.43	0.52
1:D:229:THR:OG1	1:D:231:VAL:HG12	2.09	0.52
2:E:651:PHE:CD2	2:E:654:VAL:HA	2.44	0.52
2:H:113:ARG:HD2	2:H:316:GLU:OE2	2.09	0.52
1:J:11:ARG:NH1	1:J:113:GLY:O	2.42	0.52
2:K:985:PRO:HB2	2:K:999:SER:HB3	1.92	0.52
1:M:178:CYS:O	1:M:194:LYS:NZ	2.43	0.52
2:N:872:ASP:OD1	2:N:890:ILE:HG12	2.10	0.52
3:O:234:GLU:OE2	3:O:246:SER:OG	2.20	0.52
2:Q:625:ILE:CD1	2:Q:633:ARG:CG	2.88	0.52
3:R:302:ASN:CG	3:R:303:GLY:N	2.67	0.52
1:S:4:VAL:N	1:S:13:MET:O	2.34	0.52
2:T:117:LYS:HB3	2:T:926:TRP:CD2	2.43	0.52
3:X:138:PHE:CB	3:X:279:VAL:HG21	2.39	0.52
3:X:229:ARG:CD	3:X:229:ARG:H	2.21	0.52
2:H:661:LYS:O	2:H:1057:GLN:HB3	2.08	0.52
2:N:977:VAL:HG12	2:N:1001:LEU:HB3	1.91	0.52
3:O:58:VAL:HG22	3:O:59:PRO:HD2	1.91	0.52
1:P:108:TYR:CE2	1:P:291:LEU:HD22	2.40	0.52
1:P:282:TRP:CH2	1:P:287:GLN:HG3	2.45	0.52
1:P:347:MET:HE1	2:Q:109:ASN:HA	1.91	0.52
2:Q:916:PRO:HA	6:Q:5802:MD1:O1A	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:LEU:HD22	2:B:1055:SER:O	2.08	0.52
2:E:957:ILE:HA	2:E:1017:MET:O	2.09	0.52
2:E:998:VAL:O	2:E:1054:GLY:CA	2.57	0.52
2:N:228:MET:SD	2:N:269:ASN:HB3	2.50	0.52
3:O:236:LEU:HD23	3:O:246:SER:HA	1.91	0.52
1:P:64:GLU:HG3	1:P:66:LYS:HD3	1.91	0.52
2:Q:571:PHE:CE1	2:Q:780:MET:HE1	2.45	0.52
2:T:641:HIS:CG	2:T:1087:PHE:HB2	2.44	0.52
1:V:126:ASN:O	1:V:127:GLN:HG2	2.08	0.52
1:V:189:ARG:HD2	8:X:401:HEM:O2A	2.09	0.52
2:W:409:ILE:HD11	2:W:445:THR:HG21	1.91	0.52
1:A:356:LYS:HG2	1:A:383:PHE:CE2	2.41	0.52
2:B:483:GLU:O	2:B:487:ILE:HG13	2.08	0.52
2:B:665:GLN:NE2	2:B:669:ASN:OD1	2.42	0.52
2:E:1012:PRO:HG2	2:E:1012:PRO:O	2.09	0.52
3:F:215:LEU:HD13	3:F:219:TYR:CE1	2.45	0.52
1:J:16:PRO:HG3	1:J:128:TRP:CE3	2.44	0.52
3:L:137:MET:HE3	8:L:401:HEM:C3C	2.45	0.52
3:L:290:ASN:OD1	3:L:308:SER:OG	2.26	0.52
1:M:38:CYS:O	2:N:116:LEU:HD22	2.10	0.52
1:P:395:VAL:O	2:Q:326:ARG:NH1	2.30	0.52
2:Q:114:MET:HG2	4:Q:5804:SF4:S1	2.50	0.52
2:Q:124:ARG:NH1	2:Q:683:GLU:OE2	2.42	0.52
2:Q:537:LEU:HD11	2:Q:842:GLU:CD	2.34	0.52
2:T:433:VAL:HG21	2:T:460:PRO:HB3	1.91	0.52
2:T:834:GLU:HB2	2:T:837:ILE:HD12	1.90	0.52
1:V:7:TRP:HB2	1:V:105:GLY:O	2.09	0.52
2:B:317:ALA:O	2:B:320:VAL:HG12	2.09	0.52
2:B:924:SER:OG	2:B:924:SER:O	2.28	0.52
1:D:296:GLN:NE2	1:D:318:GLN:O	2.42	0.52
2:K:872:ASP:OD1	2:K:890:ILE:HG12	2.09	0.52
3:L:51:VAL:HG12	3:L:102:ALA:CB	2.38	0.52
6:N:5802:MD1:N15	6:N:5802:MD1:O11	2.43	0.52
1:P:184:LEU:HA	1:P:192:ILE:HB	1.90	0.52
2:T:661:LYS:HE3	2:T:1096:THR:HG21	1.92	0.52
2:B:943:TYR:HB3	3:C:188:TYR:HB3	1.91	0.52
2:B:1074:PHE:HB2	2:B:1085:PHE:CE1	2.45	0.52
1:D:363:VAL:HG13	1:D:377:ASN:HB2	1.92	0.52
3:F:111:PHE:CE1	3:F:165:TRP:CZ3	2.96	0.52
3:F:115:TRP:CE2	3:F:293:VAL:HG11	2.45	0.52
1:G:34:ARG:HB2	1:G:266:ILE:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:ARG:NH2	1:G:255:GLU:O	2.31	0.52
2:H:882:TRP:CD1	2:H:883:GLU:HG2	2.44	0.52
8:I:401:HEM:CHA	8:I:401:HEM:CBA	2.85	0.52
1:J:365:GLU:HG2	1:J:372:LYS:NZ	2.24	0.52
2:N:611:ASP:HB3	2:N:1089:ALA:HB2	1.92	0.52
2:Q:496:SER:O	2:Q:500:MET:HG3	2.08	0.52
3:U:137:MET:SD	3:U:155:MET:HA	2.50	0.52
2:W:389:THR:HG23	2:W:867:TYR:HE1	1.75	0.52
2:B:271:THR:HB	2:B:1094:ILE:O	2.10	0.52
2:B:641:HIS:ND1	2:B:1087:PHE:HB2	2.24	0.52
2:B:665:GLN:HE21	2:B:669:ASN:HB2	1.75	0.52
2:E:156:LYS:O	2:E:161:PHE:HB2	2.10	0.52
2:E:218:GLY:O	2:E:219:THR:CG2	2.53	0.52
3:F:155:MET:HG3	8:F:401:HEM:CHC	2.40	0.52
3:I:81:LEU:HD11	3:I:291:MET:HE2	1.91	0.52
3:I:321:TRP:HA	3:I:321:TRP:HE3	1.73	0.52
2:K:174:TRP:HE1	2:K:730:GLU:HG2	1.75	0.52
2:K:311:GLU:HG3	2:K:919:ARG:HB3	1.91	0.52
1:P:60:TRP:HZ2	1:P:233:GLU:HB3	1.74	0.52
2:Q:1020:HIS:CE1	6:Q:5801:MD1:N8	2.78	0.52
3:U:151:PHE:CE1	3:U:160:LYS:HB3	2.45	0.52
2:W:376:TYR:O	2:W:379:LYS:O	2.27	0.52
2:B:381:THR:O	2:B:827:ARG:NH2	2.39	0.52
2:E:920:HIS:N	2:E:920:HIS:HD1	2.07	0.52
1:G:126:ASN:C	1:G:127:GLN:HG2	2.30	0.52
2:H:219:THR:HG21	2:H:250:ASP:HB2	1.92	0.52
2:H:435:ASP:HB3	2:H:438:SER:HB3	1.92	0.52
3:I:272:ASN:ND2	3:X:272:ASN:OD1	2.43	0.52
2:K:116:LEU:HD11	2:K:920:HIS:HA	1.92	0.52
2:N:527:GLU:HA	2:N:530:ASN:HB2	1.90	0.52
2:N:882:TRP:CD1	2:N:883:GLU:HG2	2.44	0.52
3:O:91:GLY:HA3	3:O:304:GLN:HB3	1.91	0.52
3:O:294:TRP:CE2	3:O:305:LYS:CB	2.93	0.52
2:Q:625:ILE:CD1	2:Q:633:ARG:NE	2.69	0.52
2:T:706:PHE:CZ	2:T:722:LYS:HD2	2.45	0.52
1:V:252:ARG:CZ	1:V:386:ASP:OD2	2.54	0.52
1:D:177:HIS:NE2	1:D:237:ALA:HB2	2.24	0.52
3:I:39:GLU:O	3:I:43:THR:HG23	2.10	0.52
2:K:448:ASP:OD1	2:K:456:LYS:NZ	2.28	0.52
2:K:485:TYR:OH	2:K:830:ALA:O	2.22	0.52
1:V:226:ARG:HD2	1:V:233:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:239:MET:HE1	2:W:650:TRP:CD2	2.45	0.52
2:W:351:ARG:HB3	2:W:354:THR:HG21	1.91	0.52
1:A:65:THR:HG23	1:A:168:PHE:HD1	1.75	0.51
2:B:117:LYS:HB3	2:B:926:TRP:CD2	2.45	0.51
2:B:629:PRO:CG	2:B:874:GLY:O	2.58	0.51
2:E:613:GLU:HG3	2:E:615:ALA:H	1.75	0.51
2:H:389:THR:HG23	2:H:867:TYR:CE1	2.46	0.51
2:K:287:GLN:NE2	2:K:1090:ASP:O	2.38	0.51
3:L:84:GLN:NE2	3:L:89:PRO:O	2.42	0.51
1:M:257:ARG:NH2	2:N:90:GLU:CG	2.60	0.51
1:P:177:HIS:NE2	1:P:237:ALA:HB2	2.25	0.51
2:Q:182:SER:O	2:Q:186:ILE:HD12	2.08	0.51
2:Q:862:VAL:HA	2:Q:892:LYS:O	2.10	0.51
3:R:165:TRP:CD1	3:R:252:VAL:HG21	2.45	0.51
2:T:117:LYS:HB3	2:T:926:TRP:CE2	2.45	0.51
2:T:395:VAL:HG23	2:T:432:VAL:HB	1.91	0.51
3:U:129:GLU:OE2	3:U:187:ARG:NH1	2.36	0.51
1:V:178:CYS:HB3	1:V:299:THR:O	2.10	0.51
1:V:212:ARG:CG	1:V:212:ARG:NH1	2.72	0.51
2:W:658:ASN:C	2:W:658:ASN:HD22	2.18	0.51
2:W:976:TYR:CD1	2:W:1000:ARG:NE	2.78	0.51
2:W:1057:GLN:HE22	6:W:5801:MD1:H162	1.57	0.51
1:A:245:ARG:O	2:H:790:ASN:ND2	2.40	0.51
2:B:89:VAL:HG13	2:B:114:MET:HE1	1.91	0.51
2:H:33:PRO:HD2	3:I:239:GLU:OE2	2.10	0.51
2:K:654:VAL:HG12	6:K:5801:MD1:O2B	2.11	0.51
3:L:168:LYS:HE2	3:L:225:LEU:HD21	1.91	0.51
1:M:149:ALA:HA	1:M:168:PHE:HB3	1.92	0.51
2:N:273:HIS:HB3	6:N:5801:MD1:C13	2.40	0.51
3:O:289:PHE:CE1	3:O:312:HIS:HB2	2.45	0.51
1:P:302:ASN:HA	1:P:304:TYR:HE2	1.74	0.51
2:T:69:PRO:O	2:T:922:VAL:HG11	2.10	0.51
2:T:152:THR:CG2	2:T:154:GLU:HG2	2.40	0.51
3:U:229:ARG:HG2	3:U:231:ARG:HB2	1.92	0.51
1:V:68:TYR:CE1	2:W:1128:ALA:HA	2.45	0.51
1:V:294:TYR:CE1	1:V:319:MET:HG3	2.44	0.51
3:X:168:LYS:HD2	3:X:171:TRP:CE2	2.45	0.51
1:A:256:THR:CG2	1:A:259:MET:HG2	2.40	0.51
2:B:130:ARG:NH1	2:B:702:GLU:OE1	2.35	0.51
2:B:665:GLN:NE2	2:B:669:ASN:HB2	2.24	0.51
3:F:238:ALA:HB2	3:F:244:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:SER:OG	1:G:196:LYS:NZ	2.38	0.51
1:G:311:ALA:HB3	1:G:316:LEU:HD11	1.92	0.51
2:H:301:LEU:HB3	2:H:521:VAL:HG22	1.92	0.51
3:I:154:ARG:HD2	8:I:401:HEM:CBB	2.41	0.51
1:J:218:CYS:O	1:J:221:LYS:HE2	2.10	0.51
3:L:110:TYR:CD1	3:L:268:CYS:HB2	2.46	0.51
1:P:241:ARG:NH1	2:Q:90:GLU:OE2	2.43	0.51
2:Q:857:LEU:HB2	2:Q:900:THR:CG2	2.23	0.51
2:T:261:ALA:O	2:T:608:ARG:HD3	2.10	0.51
2:T:485:TYR:HA	2:T:488:HIS:HB3	1.93	0.51
1:V:187:CYS:HA	5:V:504:F3S:S2	2.50	0.51
1:V:310:TRP:CZ2	2:W:342:GLN:HG3	2.45	0.51
1:D:33:ASN:OD1	1:D:308:PRO:HA	2.10	0.51
2:E:851:PRO:HA	2:E:858:PRO:HB2	1.93	0.51
2:K:937:ASN:HD21	2:K:953:GLY:CA	2.23	0.51
1:M:166:ARG:HD2	2:N:337:TYR:HB2	1.92	0.51
2:N:597:TYR:CZ	2:Q:49:TRP:HA	2.45	0.51
2:Q:388:ARG:HG3	2:Q:395:VAL:HG23	1.93	0.51
2:T:930:ASP:OD1	2:T:931:TRP:N	2.42	0.51
2:T:977:VAL:HB	2:T:1001:LEU:HD23	1.92	0.51
1:V:241:ARG:HD3	1:V:255:GLU:O	2.11	0.51
2:W:971:ASP:HB2	2:W:1007:TYR:CD2	2.45	0.51
2:W:996:TYR:CZ	2:W:1000:ARG:HG3	2.44	0.51
3:X:51:VAL:CG1	3:X:316:LEU:HA	2.41	0.51
2:B:449:VAL:CG2	10:B:5919:HOH:O	2.59	0.51
2:B:579:PRO:HB3	2:B:605:ILE:HG13	1.92	0.51
3:C:137:MET:HB3	3:C:164:LEU:HD13	1.93	0.51
1:D:190:LYS:HD3	2:E:40:PRO:HD3	1.93	0.51
2:E:959:ILE:HB	2:E:1016:THR:CG2	2.41	0.51
3:F:155:MET:HG3	8:F:401:HEM:C1C	2.46	0.51
2:H:1132:ASN:OD1	2:H:1135:MET:N	2.34	0.51
3:I:51:VAL:O	3:I:51:VAL:HG12	2.09	0.51
3:I:321:TRP:CD1	3:X:161:PRO:HD2	2.46	0.51
2:N:241:ARG:NH1	2:N:757:ASN:O	2.43	0.51
2:Q:431:PHE:CE2	2:Q:825:THR:HG22	2.45	0.51
2:Q:625:ILE:HD12	2:Q:633:ARG:CG	2.41	0.51
2:T:577:SER:O	2:T:776:GLY:HA2	2.09	0.51
1:A:333:VAL:HG13	1:A:373:PHE:HB2	1.92	0.51
3:C:236:LEU:HB2	3:C:245:THR:O	2.10	0.51
2:E:177:ALA:HB1	2:E:695:PHE:HE2	1.75	0.51
2:E:208:LYS:O	2:E:212:ASP:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:468:LEU:HB3	2:E:476:ILE:H	1.74	0.51
2:E:1029:THR:HG21	2:E:1049:SER:CB	2.41	0.51
3:F:95:VAL:H	3:F:306:ASN:ND2	2.09	0.51
2:H:1119:TRP:CD2	2:H:1121:PRO:HD2	2.45	0.51
2:K:611:ASP:HB3	2:K:1089:ALA:HB2	1.93	0.51
2:K:711:SER:HB3	2:K:714:ASN:OD1	2.11	0.51
1:M:291:LEU:HB2	1:M:320:PHE:HB3	1.93	0.51
1:M:311:ALA:HB3	1:M:316:LEU:HD11	1.93	0.51
2:N:1001:LEU:HA	2:N:1054:GLY:HA3	1.91	0.51
3:O:193:ASP:N	3:O:197:THR:OG1	2.28	0.51
2:Q:355:ASP:HB3	2:Q:542:TYR:OH	2.10	0.51
1:S:311:ALA:HB3	1:S:316:LEU:HD11	1.93	0.51
2:T:527:GLU:HA	2:T:530:ASN:HB2	1.93	0.51
1:V:207:ARG:HG2	1:V:207:ARG:NH1	2.11	0.51
3:X:108:THR:HA	3:X:270:SER:HA	1.92	0.51
3:C:285:GLU:OE1	3:U:285:GLU:HG3	2.10	0.51
1:D:16:PRO:HG3	1:D:128:TRP:CE3	2.44	0.51
2:E:950:PRO:HD2	2:E:954:GLU:HB3	1.92	0.51
1:G:36:ILE:HG22	2:H:310:ILE:HG23	1.93	0.51
3:I:305:LYS:CD	3:I:307:ILE:CG2	2.73	0.51
2:K:909:TYR:CZ	2:K:1104:LYS:HD3	2.45	0.51
2:Q:131:LEU:HD13	2:Q:683:GLU:C	2.35	0.51
2:Q:445:THR:O	2:Q:448:ASP:HB2	2.11	0.51
2:E:131:LEU:HG	2:E:696:PRO:HB3	1.93	0.51
3:F:157:ASP:HA	3:F:240:GLY:CA	2.41	0.51
1:G:55:GLN:NE2	1:G:233:GLU:OE1	2.38	0.51
1:G:212:ARG:HD2	1:G:225:TYR:CD1	2.46	0.51
1:J:238:CYS:SG	1:J:257:ARG:HB2	2.50	0.51
2:N:476:ILE:HG13	2:N:478:VAL:CG1	2.40	0.51
1:P:313:ARG:O	1:P:317:ARG:HG2	2.11	0.51
2:Q:117:LYS:HD2	2:Q:922:VAL:HG23	1.93	0.51
2:Q:533:PHE:CE2	2:Q:1063:TRP:HB3	2.46	0.51
2:T:39:ASN:HB3	2:T:42:ASP:HB3	1.91	0.51
2:W:848:ARG:NH2	2:W:859:ASN:OD1	2.44	0.51
1:A:34:ARG:HB2	1:A:266:ILE:HG22	1.92	0.51
2:B:597:TYR:OH	2:H:52:VAL:HG22	2.11	0.51
2:E:356:THR:HG1	2:E:847:HIS:CB	2.16	0.51
1:G:177:HIS:NE2	1:G:237:ALA:HB2	2.25	0.51
3:I:51:VAL:HB	3:I:316:LEU:HA	1.93	0.51
3:I:53:TYR:HE1	3:I:319:ILE:HG12	1.76	0.51
3:I:98:ALA:HB3	3:I:291:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:114:ILE:HG12	3:I:264:THR:HG23	1.91	0.51
2:K:519:LYS:HG3	2:K:551:ASN:HD21	1.74	0.51
1:M:249:THR:HG21	1:M:254:MET:HB2	1.93	0.51
2:Q:140:TRP:HZ3	2:Q:180:TYR:HB3	1.76	0.51
2:Q:307:LYS:HZ3	2:Q:313:LYS:CE	2.24	0.51
2:T:885:ARG:HG2	2:T:888:ARG:HH21	1.75	0.51
2:T:1074:PHE:CE1	2:T:1083:PHE:HB3	2.46	0.51
2:W:307:LYS:HA	6:W:5802:MD1:H5'1	1.93	0.51
2:W:1124:THR:CG2	2:W:1126:TYR:HB2	2.40	0.51
1:A:195:ARG:NH2	1:A:243:GLU:OE2	2.44	0.51
1:A:375:MET:SD	2:B:326:ARG:HB3	2.51	0.51
2:B:250:ASP:OD2	2:B:254:ARG:NH2	2.43	0.51
2:B:1088:GLU:HG2	2:B:1091:ASN:CB	2.38	0.51
1:D:67:PRO:HB3	1:D:315:TYR:CE1	2.46	0.51
2:E:34:ALA:HB1	3:F:243:THR:O	2.11	0.51
2:H:681:ASP:OD1	6:H:5801:MD1:H1'	2.11	0.51
2:K:1119:TRP:O	2:K:1122:VAL:HG22	2.11	0.51
3:L:79:VAL:HG21	3:L:291:MET:HE3	1.92	0.51
2:N:143:TRP:CD1	2:N:149:PRO:HD2	2.46	0.51
1:P:149:ALA:HA	1:P:168:PHE:HB3	1.93	0.51
1:S:318:GLN:HA	2:T:1144:ILE:HG21	1.92	0.51
2:T:89:VAL:CG1	2:T:119:TYR:HA	2.41	0.51
2:T:101:LEU:HD21	2:T:802:LEU:HD11	1.92	0.51
2:T:985:PRO:HB2	2:T:999:SER:HB3	1.93	0.51
2:W:875:ILE:HG23	2:W:888:ARG:HG3	1.91	0.51
2:B:648:VAL:HG13	2:B:676:GLN:HB3	1.91	0.50
2:B:990:LYS:HB2	2:B:993:ASP:OD2	2.10	0.50
2:H:117:LYS:NZ	2:H:921:THR:O	2.44	0.50
2:H:447:ASP:O	2:H:449:VAL:N	2.44	0.50
3:I:137:MET:SD	3:I:162:VAL:HG11	2.51	0.50
2:K:660:ALA:C	2:K:1057:GLN:HE21	2.18	0.50
2:N:355:ASP:OD2	6:N:5802:MD1:N2	2.44	0.50
2:Q:268:SER:OG	2:Q:613:GLU:OE1	2.23	0.50
2:W:406:LEU:HD21	2:W:429:GLY:HA2	1.93	0.50
2:W:500:MET:HA	2:W:894:TRP:CH2	2.45	0.50
1:A:377:ASN:OD1	1:A:396:GLU:HB3	2.11	0.50
2:B:99:SER:HB3	2:B:105:LYS:HG2	1.93	0.50
2:B:923:HIS:NE2	6:B:5801:MD1:S12	2.85	0.50
3:C:302:ASN:HB2	8:C:401:HEM:HAA1	1.92	0.50
2:E:923:HIS:HB3	6:E:5801:MD1:H101	1.93	0.50
2:E:957:ILE:N	2:E:1003:LEU:HD11	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1008:ASN:OD1	2:E:1009:PRO:HD2	2.12	0.50
1:G:172:GLN:HB3	1:G:267:ARG:HH21	1.76	0.50
3:L:51:VAL:HG23	3:L:104:HIS:HD2	1.77	0.50
1:M:241:ARG:HG2	1:M:254:MET:SD	2.52	0.50
2:N:468:LEU:O	2:N:475:GLU:HG2	2.11	0.50
2:N:629:PRO:HG2	2:N:874:GLY:O	2.11	0.50
3:O:171:TRP:O	3:O:175:LEU:HG	2.11	0.50
3:O:282:VAL:HG23	3:O:285:GLU:HB2	1.93	0.50
2:Q:175:ASP:O	2:Q:179:THR:OG1	2.24	0.50
2:Q:569:GLY:O	2:Q:572:GLN:HB2	2.11	0.50
3:R:131:ARG:NE	3:R:170:ASP:OD2	2.36	0.50
1:S:173:ARG:NH2	1:S:220:TYR:O	2.42	0.50
1:S:402:ARG:O	2:T:804:ARG:NH1	2.44	0.50
2:T:423:GLU:O	2:T:427:ILE:HG13	2.12	0.50
2:T:822:TYR:CD1	2:T:1076:LYS:HD2	2.46	0.50
2:T:916:PRO:HA	6:T:5802:MD1:O1A	2.10	0.50
1:V:61:ASN:C	1:V:61:ASN:HD22	2.19	0.50
2:W:359:PHE:HA	2:W:362:ILE:HG22	1.93	0.50
2:W:397:PRO:HB2	2:W:404:TYR:CE2	2.47	0.50
2:W:532:TYR:CZ	2:W:1099:LYS:HG2	2.46	0.50
3:X:244:LEU:HB3	8:X:401:HEM:O2A	2.11	0.50
1:A:216:GLU:HG2	1:A:217:GLN:HG3	1.92	0.50
1:A:262:CYS:HB2	1:A:267:ARG:HD2	1.93	0.50
2:B:536:THR:OG1	2:B:1068:HIS:NE2	2.41	0.50
1:D:167:TRP:HH2	1:D:315:TYR:CE1	2.30	0.50
1:D:234:LYS:NZ	4:D:502:SF4:S1	2.72	0.50
1:D:258:CYS:N	4:D:501:SF4:S2	2.84	0.50
2:E:964:ALA:O	2:E:969:ILE:N	2.27	0.50
2:H:72:THR:O	2:H:72:THR:OG1	2.28	0.50
3:I:53:TYR:CE1	3:I:319:ILE:CA	2.86	0.50
1:M:246:ASP:OD1	2:N:59:TYR:OH	2.20	0.50
2:N:33:PRO:HA	3:O:277:LEU:HD21	1.91	0.50
2:Q:227:GLY:HA3	2:Q:654:VAL:HG13	1.92	0.50
2:Q:310:ILE:HG12	2:Q:340:SER:HA	1.92	0.50
2:Q:710:ASN:HD22	2:Q:801:LEU:HD21	1.77	0.50
1:S:4:VAL:O	1:S:13:MET:N	2.34	0.50
1:V:211:TYR:O	3:X:301:ARG:HD2	2.10	0.50
2:W:915:THR:OG1	6:W:5801:MD1:N17	2.44	0.50
1:A:141:SER:OG	2:B:938:ASN:O	2.22	0.50
2:B:113:ARG:HG2	2:B:113:ARG:O	2.11	0.50
2:B:271:THR:HG21	2:B:1093:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:THR:HG22	2:B:680:THR:CB	2.41	0.50
3:C:43:THR:HG22	3:C:147:PRO:HG3	1.93	0.50
1:D:50:THR:HA	1:D:55:GLN:OE1	2.11	0.50
2:E:671:ASN:N	2:E:672:PRO:CD	2.73	0.50
2:K:596:PRO:HG3	2:K:760:PHE:HE1	1.76	0.50
3:O:193:ASP:O	3:O:197:THR:OG1	2.29	0.50
1:P:231:VAL:HG21	10:P:604:HOH:O	2.04	0.50
3:R:301:ARG:H	3:R:304:GLN:HB2	1.75	0.50
1:S:178:CYS:HB3	1:S:299:THR:O	2.11	0.50
2:T:250:ASP:OD2	2:T:254:ARG:NH1	2.44	0.50
1:V:15:TYR:HE2	1:V:185:ALA:CB	2.24	0.50
1:V:66:LYS:HG2	1:V:171:LEU:HB2	1.92	0.50
2:B:69:PRO:HB3	2:B:700:TRP:CH2	2.46	0.50
2:E:736:LYS:O	2:E:740:GLY:N	2.31	0.50
3:F:95:VAL:HG22	3:F:306:ASN:ND2	2.26	0.50
3:F:305:LYS:NZ	8:F:401:HEM:C1C	2.47	0.50
1:G:173:ARG:NH2	1:G:220:TYR:O	2.40	0.50
2:H:714:ASN:ND2	10:H:5912:HOH:O	2.45	0.50
2:K:196:GLU:OE1	2:K:196:GLU:N	2.35	0.50
3:L:302:ASN:CG	3:L:303:GLY:N	2.55	0.50
2:N:201:LEU:HD13	2:N:645:PRO:HG2	1.94	0.50
2:N:435:ASP:HB3	2:N:438:SER:O	2.12	0.50
2:N:527:GLU:OE1	2:N:527:GLU:N	2.45	0.50
2:N:790:ASN:ND2	1:P:245:ARG:O	2.33	0.50
1:S:16:PRO:HG2	1:S:185:ALA:HB1	1.93	0.50
1:S:400:HIS:H	2:T:806:TYR:HB3	1.75	0.50
1:V:15:TYR:CD2	1:V:16:PRO:CD	2.94	0.50
2:W:504:PRO:HG2	2:W:507:LEU:HB2	1.93	0.50
2:W:843:ASN:OD1	2:W:868:ILE:HD13	2.12	0.50
2:B:948:ARG:NH2	2:B:1112:GLY:O	2.44	0.50
2:B:984:ARG:HH11	2:B:1061:ARG:CB	2.25	0.50
2:E:69:PRO:HB3	2:E:700:TRP:CH2	2.45	0.50
2:E:356:THR:OG1	2:E:847:HIS:CA	2.58	0.50
2:K:241:ARG:NH2	2:K:587:GLU:OE1	2.44	0.50
2:N:1135:MET:CE	2:N:1139:LEU:CD2	2.74	0.50
2:Q:625:ILE:HD11	2:Q:633:ARG:HG3	1.93	0.50
2:T:69:PRO:HB2	2:T:922:VAL:HG11	1.94	0.50
3:U:95:VAL:HG22	3:U:306:ASN:CG	2.37	0.50
2:W:113:ARG:CG	2:W:113:ARG:NH1	2.73	0.50
2:E:814:GLN:O	2:E:819:LEU:N	2.42	0.50
3:F:171:TRP:CZ3	3:F:229:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:572:GLN:HB3	2:K:778:THR:HB	1.93	0.50
3:L:251:ASP:OD2	3:L:273:THR:HG21	2.12	0.50
1:P:11:ARG:NH2	1:P:118:GLU:OE2	2.45	0.50
1:P:166:ARG:HD3	2:Q:1010:ALA:HA	1.94	0.50
2:Q:71:ASP:O	2:Q:73:HIS:CD2	2.64	0.50
2:Q:72:THR:HG21	2:Q:713:SER:CB	2.40	0.50
2:Q:198:ALA:O	2:Q:202:ILE:HG13	2.11	0.50
2:Q:385:LEU:H	2:Q:385:LEU:HD12	1.77	0.50
3:R:139:PRO:HB3	3:R:151:PHE:CE2	2.45	0.50
1:S:16:PRO:HG3	1:S:128:TRP:CE3	2.47	0.50
1:V:192:ILE:HD13	1:V:203:ILE:HG12	1.94	0.50
1:V:263:VAL:CG2	2:W:315:PRO:HA	2.41	0.50
2:W:435:ASP:OD2	2:W:442:LYS:HE2	2.11	0.50
2:W:1119:TRP:CZ2	2:W:1121:PRO:HG2	2.47	0.50
3:X:81:LEU:HD22	3:X:307:ILE:O	2.06	0.50
3:X:125:ILE:HD12	3:X:187:ARG:HB2	1.93	0.50
1:A:63:VAL:HG13	1:A:172:GLN:HG3	1.94	0.50
1:A:195:ARG:HD3	1:A:200:ILE:HB	1.94	0.50
2:B:72:THR:HG21	2:B:313:LYS:HE3	1.92	0.50
2:B:86:MET:HE3	2:B:122:HIS:HB3	1.92	0.50
2:B:547:MET:HG2	2:B:828:LEU:HD13	1.93	0.50
2:B:698:ASN:OD1	2:B:731:SER:OG	2.24	0.50
3:C:35:LYS:HD3	3:C:86:LYS:HA	1.94	0.50
1:D:117:PHE:HZ	1:D:182:GLY:HA2	1.75	0.50
1:D:226:ARG:NH2	3:F:216:SER:OG	2.40	0.50
2:E:855:PRO:O	2:E:902:ASN:N	2.37	0.50
3:F:257:LYS:N	3:F:264:THR:O	2.45	0.50
2:H:185:ILE:HD12	2:H:741:MET:HE2	1.94	0.50
2:H:640:THR:HB	2:H:1087:PHE:HB3	1.93	0.50
3:I:140:LEU:HD12	3:I:161:PRO:HB2	1.94	0.50
1:M:52:ASN:HD22	3:O:215:LEU:HA	1.76	0.50
2:N:294:ASN:HA	2:N:319:TRP:CD2	2.47	0.50
1:P:192:ILE:O	2:Q:40:PRO:HB3	2.12	0.50
1:S:193:TYR:OH	2:T:50:GLU:OE2	2.19	0.50
3:X:95:VAL:H	3:X:306:ASN:HD21	1.58	0.50
2:B:143:TRP:CD1	2:B:149:PRO:HD2	2.47	0.50
2:B:424:GLN:O	2:B:428:ILE:CG1	2.59	0.50
3:C:167:TRP:NE1	3:C:256:SER:OG	2.45	0.50
1:D:48:THR:HG23	2:E:88:ARG:HD3	1.94	0.50
1:D:228:LEU:O	1:D:230:ARG:NH2	2.45	0.50
2:E:553:GLY:O	2:E:812:TRP:HE3	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:945:MET:HE3	3:F:188:TYR:HE1	1.77	0.50
1:G:273:ASP:OD2	1:G:278:ASN:ND2	2.45	0.50
1:J:200:ILE:HD12	1:J:237:ALA:HB3	1.93	0.50
2:K:91:GLN:NE2	2:K:114:MET:HB2	2.21	0.50
2:N:189:THR:O	2:N:193:SER:OG	2.27	0.50
2:N:267:TRP:CD2	2:N:614:VAL:HG22	2.47	0.50
2:T:487:ILE:O	2:T:490:ARG:HG3	2.10	0.50
2:T:753:ARG:HA	2:T:756:ASP:CG	2.37	0.50
2:W:456:LYS:HB2	2:W:458:ILE:CD1	2.41	0.50
2:B:463:GLU:HG2	2:B:486:LYS:HZ1	1.77	0.49
2:B:681:ASP:OD1	6:B:5801:MD1:H1'	2.12	0.49
1:D:255:GLU:OE1	1:D:346:ARG:NH1	2.45	0.49
2:E:267:TRP:HA	2:E:612:GLU:O	2.12	0.49
2:E:655:ASN:O	2:E:659:ASN:N	2.39	0.49
2:H:284:HIS:HD2	2:H:543:TYR:CE2	2.30	0.49
2:N:917:LYS:CD	6:N:5802:MD1:H15	2.24	0.49
2:N:941:ASP:OD2	2:N:944:ARG:N	2.45	0.49
2:Q:425:ARG:HH22	2:Q:430:ASP:CG	2.20	0.49
2:T:712:CYS:O	2:T:808:ARG:NH2	2.45	0.49
2:W:491:ASP:OD2	2:W:864:THR:N	2.44	0.49
2:W:681:ASP:OD1	6:W:5801:MD1:H1'	2.12	0.49
2:W:939:PHE:HE2	2:W:1004:ARG:CD	1.54	0.49
1:A:3:LEU:HD22	1:A:3:LEU:N	2.27	0.49
2:B:69:PRO:HB3	2:B:700:TRP:HH2	1.75	0.49
2:B:213:ARG:HH21	2:B:642:MET:HB3	1.78	0.49
1:D:129:ALA:HB3	1:D:217:GLN:HB3	1.93	0.49
2:E:126:TYR:O	3:F:195:PHE:HE1	1.94	0.49
2:E:707:GLU:OE1	2:E:707:GLU:HA	2.12	0.49
3:F:52:LYS:HA	3:F:317:GLU:CD	2.37	0.49
1:G:63:VAL:HG21	4:G:503:SF4:S4	2.52	0.49
2:H:514:ASP:O	2:H:518:ILE:HG13	2.12	0.49
1:J:149:ALA:HA	1:J:168:PHE:HB3	1.95	0.49
1:J:177:HIS:NE2	1:J:237:ALA:HB2	2.27	0.49
2:K:383:PHE:HA	2:K:481:LEU:HD23	1.93	0.49
1:P:149:ALA:HB2	1:P:168:PHE:CD2	2.44	0.49
1:P:373:PHE:CE2	1:P:375:MET:HB2	2.46	0.49
2:Q:213:ARG:NH2	2:Q:610:LEU:HD21	2.27	0.49
2:Q:390:ASP:OD1	2:Q:390:ASP:N	2.44	0.49
2:Q:923:HIS:ND1	6:Q:5801:MD1:H102	2.26	0.49
2:T:68:SER:OG	10:T:5903:HOH:O	2.20	0.49
1:V:63:VAL:HG21	4:V:503:SF4:S4	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:73:GLN:HG3	1:V:138:GLU:O	2.12	0.49
1:V:186:ALA:O	1:V:188:PRO:HD3	2.12	0.49
2:W:917:LYS:HG3	6:W:5802:MD1:H15	1.77	0.49
1:A:15:TYR:OH	1:A:181:PRO:O	2.29	0.49
1:A:259:MET:HA	1:A:267:ARG:CD	2.42	0.49
2:B:888:ARG:HD3	2:B:890:ILE:HD12	1.94	0.49
2:B:941:ASP:OD2	2:B:943:TYR:N	2.46	0.49
2:E:123:ARG:NH1	3:F:194:ASP:HB2	2.07	0.49
2:H:230:LEU:O	2:H:709:THR:OG1	2.27	0.49
3:O:56:ILE:HD11	3:O:103:ILE:CG1	2.42	0.49
2:Q:449:VAL:HG23	2:Q:827:ARG:HD2	1.94	0.49
3:R:130:PHE:CE1	3:R:301:ARG:HD3	2.47	0.49
3:R:282:VAL:O	3:R:285:GLU:HG2	2.13	0.49
2:T:382:ASP:OD2	2:T:830:ALA:N	2.44	0.49
3:U:137:MET:HE2	3:U:290:ASN:HB3	1.94	0.49
1:V:175:CYS:HA	1:V:222:LYS:HG3	1.94	0.49
2:W:535:ALA:HA	2:W:538:MET:HE3	1.94	0.49
2:W:917:LYS:NZ	6:W:5801:MD1:N15	2.60	0.49
2:B:971:ASP:HB2	2:B:1007:TYR:CD2	2.47	0.49
2:B:978:ASP:OD1	2:B:1000:ARG:NH2	2.32	0.49
1:G:240:PRO:HB3	2:H:54:ARG:HG2	1.95	0.49
2:H:511:LEU:HG	2:H:515:ILE:HD11	1.94	0.49
2:K:295:ASP:OD2	2:K:556:GLY:N	2.39	0.49
2:K:795:GLU:HB3	2:K:798:VAL:HG22	1.95	0.49
1:M:189:ARG:NE	1:M:209:ARG:HG3	2.26	0.49
2:Q:73:HIS:CE1	2:Q:315:PRO:HD2	2.48	0.49
2:Q:130:ARG:NH2	2:Q:702:GLU:OE2	2.40	0.49
2:Q:276:GLN:O	2:Q:1095:ASN:ND2	2.44	0.49
2:Q:1030:VAL:HG13	2:Q:1053:TYR:CE2	2.47	0.49
2:Q:1110:ASN:HB3	2:Q:1117:GLY:O	2.12	0.49
2:T:228:MET:HB3	2:T:231:LEU:CD2	2.43	0.49
1:V:378:ASP:O	1:V:395:VAL:HG23	2.12	0.49
2:W:229:GLY:HA3	2:W:237:TYR:CD1	2.47	0.49
2:B:64:THR:HG23	2:B:76:ARG:HD2	1.93	0.49
2:B:302:LEU:CD2	2:B:320:VAL:HG23	2.43	0.49
1:G:225:TYR:OH	3:I:124:ALA:O	2.26	0.49
2:H:707:GLU:O	2:H:719:ILE:HA	2.12	0.49
2:H:834:GLU:HB2	2:H:837:ILE:HD12	1.93	0.49
1:J:66:LYS:NZ	1:J:76:ASP:OD2	2.45	0.49
2:K:95:HIS:NE2	2:K:113:ARG:HD3	2.27	0.49
2:K:917:LYS:HZ3	6:K:5801:MD1:C13	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:917:LYS:C	2:K:1019:LYS:HE2	2.35	0.49
2:N:446:ARG:NH2	2:N:823:THR:O	2.38	0.49
3:O:120:ASP:HB3	3:O:258:PHE:CD2	2.47	0.49
3:O:305:LYS:HE3	8:O:401:HEM:C4B	2.47	0.49
2:Q:425:ARG:HH11	2:Q:425:ARG:HG3	1.76	0.49
2:Q:711:SER:HB3	2:Q:714:ASN:OD1	2.12	0.49
1:S:71:PHE:HE1	1:S:139:TRP:O	1.96	0.49
1:S:255:GLU:HG2	1:S:351:ILE:HG12	1.94	0.49
2:T:527:GLU:OE1	6:T:5802:MD1:H101	2.13	0.49
1:V:137:LYS:O	1:V:140:ARG:HG2	2.12	0.49
2:W:704:GLN:HA	2:W:704:GLN:NE2	2.26	0.49
2:B:779:THR:HB	2:B:801:LEU:HB2	1.94	0.49
1:D:259:MET:CE	1:D:269:GLN:CB	2.91	0.49
2:E:126:TYR:HB3	3:F:205:HIS:CD2	2.47	0.49
2:E:941:ASP:OD2	2:E:945:MET:HG3	2.11	0.49
3:F:85:ASP:HA	3:F:90:ASN:OD1	2.12	0.49
2:H:284:HIS:HD1	2:H:286:LEU:HB3	1.78	0.49
2:H:513:LYS:O	2:H:517:THR:HG23	2.13	0.49
2:K:218:GLY:O	2:K:221:THR:OG1	2.30	0.49
2:K:647:LYS:HE3	2:K:673:ASN:O	2.12	0.49
3:O:51:VAL:HB	3:O:316:LEU:HA	1.95	0.49
1:P:30:PHE:CE1	1:P:267:ARG:HG2	2.47	0.49
2:Q:265:ARG:NH1	2:Q:612:GLU:HB2	2.27	0.49
2:Q:533:PHE:HB2	2:Q:1100:GLU:OE1	2.13	0.49
2:Q:575:LYS:HD3	2:Q:575:LYS:N	2.23	0.49
2:Q:924:SER:OG	6:Q:5801:MD1:O2A	2.30	0.49
1:S:48:THR:HG23	2:T:88:ARG:HD3	1.95	0.49
2:T:51:SER:HA	2:T:54:ARG:CG	2.43	0.49
2:T:531:HIS:CG	2:T:1098:PRO:HD2	2.48	0.49
2:T:566:TYR:CZ	2:T:567:LYS:HG3	2.47	0.49
2:W:276:GLN:HB3	2:W:1095:ASN:ND2	2.27	0.49
1:D:192:ILE:O	2:E:40:PRO:HB3	2.12	0.49
2:E:618:ASN:ND2	2:E:661:LYS:H	2.11	0.49
2:E:1064:SER:O	2:E:1066:PRO:HD3	2.12	0.49
3:F:130:PHE:CD1	3:F:301:ARG:HD3	2.48	0.49
1:G:175:CYS:HA	1:G:222:LYS:HG3	1.95	0.49
1:G:262:CYS:HA	4:G:503:SF4:S3	2.52	0.49
2:H:466:PHE:HB2	2:H:478:VAL:CG2	2.42	0.49
2:H:595:ASP:O	2:H:772:ARG:NH2	2.46	0.49
2:K:1059:ILE:O	2:K:1101:THR:HG21	2.11	0.49
2:Q:131:LEU:HB3	2:Q:696:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:496:SER:C	2:Q:500:MET:HG3	2.37	0.49
1:V:177:HIS:NE2	1:V:237:ALA:HB2	2.28	0.49
1:V:208:CYS:HB3	1:V:231:VAL:CG1	2.43	0.49
2:W:73:HIS:ND1	2:W:315:PRO:HG2	2.28	0.49
1:A:44:ALA:HB2	2:B:119:TYR:HE2	1.78	0.49
1:A:132:TYR:O	1:A:221:LYS:NZ	2.45	0.49
1:A:262:CYS:SG	1:A:266:ILE:HG12	2.52	0.49
2:B:60:ASP:OD1	2:B:83:ASN:N	2.26	0.49
2:B:504:PRO:HG2	2:B:507:LEU:HD12	1.94	0.49
2:B:783:TYR:OH	2:B:800:MET:O	2.28	0.49
2:H:213:ARG:O	2:H:220:ARG:NH1	2.45	0.49
3:I:285:GLU:HA	3:I:285:GLU:OE2	2.12	0.49
2:K:332:VAL:HG23	2:K:344:ALA:HB2	1.94	0.49
2:K:428:ILE:HD11	2:K:1074:PHE:CG	2.48	0.49
2:N:60:ASP:OD2	2:N:83:ASN:N	2.31	0.49
3:C:163:ASN:HD22	3:C:164:LEU:N	2.11	0.49
3:F:81:LEU:HB3	3:F:306:ASN:HB3	1.95	0.49
3:F:241:PHE:CB	8:F:401:HEM:CHB	2.91	0.49
2:K:445:THR:OG1	2:K:446:ARG:N	2.46	0.49
2:K:681:ASP:OD1	6:K:5801:MD1:H1'	2.13	0.49
2:K:1022:ALA:HB1	2:K:1050:SER:HB2	1.93	0.49
3:L:239:GLU:HB2	3:L:243:THR:HG21	1.95	0.49
1:M:284:ILE:HG22	1:M:285:ARG:HG2	1.93	0.49
2:N:225:ARG:HH22	2:N:273:HIS:CE1	2.31	0.49
2:N:882:TRP:CE3	2:N:983:ASP:OD1	2.65	0.49
2:N:949:MET:HE2	2:N:953:GLY:HA2	1.93	0.49
2:Q:213:ARG:HE	2:Q:642:MET:HB3	1.78	0.49
2:Q:425:ARG:HG3	2:Q:425:ARG:O	2.13	0.49
2:W:286:LEU:HD23	2:W:287:GLN:N	2.28	0.49
2:W:708:ILE:HD12	2:W:719:ILE:HG12	1.94	0.49
2:W:760:PHE:HB2	2:W:769:TYR:CE2	2.48	0.49
2:B:99:SER:HA	2:B:800:MET:HE2	1.94	0.49
1:D:175:CYS:SG	1:D:234:LYS:HE2	2.53	0.49
2:E:934:ILE:HD13	2:E:942:PRO:HD3	1.93	0.49
2:H:706:PHE:CZ	2:H:722:LYS:HD2	2.47	0.49
3:I:110:TYR:CD1	3:I:268:CYS:HB2	2.48	0.49
3:I:123:GLN:NE2	3:I:182:GLU:OE1	2.45	0.49
3:L:305:LYS:HG2	3:L:307:ILE:HG23	1.95	0.49
1:M:211:TYR:O	3:O:301:ARG:NE	2.44	0.49
2:N:71:ASP:OD2	2:N:73:HIS:CD2	2.63	0.49
2:N:462:LEU:O	2:N:480:THR:HG21	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:711:SER:HB3	2:N:714:ASN:OD1	2.13	0.49
1:P:175:CYS:HA	1:P:222:LYS:HG3	1.95	0.49
2:Q:96:GLN:HG2	2:Q:108:ARG:CG	2.36	0.49
2:Q:909:TYR:CE1	2:Q:1104:LYS:HB2	2.48	0.49
3:R:137:MET:HE2	3:R:290:ASN:HB3	1.95	0.49
1:S:78:LYS:HD3	1:S:132:TYR:CZ	2.48	0.49
2:T:63:PHE:HB2	2:T:723:THR:HG22	1.95	0.49
1:V:373:PHE:CZ	2:W:326:ARG:HA	2.48	0.49
2:W:312:ASN:O	6:W:5802:MD1:N8	2.46	0.49
2:W:950:PRO:HD3	2:W:954:GLU:HG3	1.95	0.49
2:W:1040:ARG:CZ	2:W:1042:LEU:HD13	2.43	0.49
1:A:262:CYS:HA	4:A:503:SF4:S3	2.53	0.48
2:B:497:VAL:HA	2:B:500:MET:HG3	1.95	0.48
1:G:408:ASN:N	2:H:813:GLU:OE2	2.27	0.48
2:K:760:PHE:HB2	2:K:769:TYR:CE2	2.48	0.48
2:N:531:HIS:CG	2:N:1098:PRO:HD2	2.48	0.48
3:O:303:GLY:O	3:O:305:LYS:N	2.41	0.48
2:Q:123:ARG:NH2	2:Q:930:ASP:OD2	2.46	0.48
2:T:229:GLY:HA3	2:T:237:TYR:CD1	2.47	0.48
2:T:232:GLY:O	2:T:236:LYS:HB2	2.13	0.48
3:U:43:THR:CG2	3:U:147:PRO:HG3	2.40	0.48
2:W:1029:THR:HB	2:W:1049:SER:OG	2.13	0.48
2:B:310:ILE:CD1	2:B:310:ILE:N	2.76	0.48
2:B:453:LEU:HD11	2:B:827:ARG:NH1	2.27	0.48
2:B:499:SER:HG	2:B:894:TRP:HE1	1.59	0.48
2:B:851:PRO:O	2:B:858:PRO:HB3	2.13	0.48
2:E:152:THR:O	2:E:156:LYS:N	2.40	0.48
2:H:71:ASP:OD2	2:H:73:HIS:ND1	2.45	0.48
2:H:535:ALA:HA	2:H:538:MET:HE3	1.95	0.48
6:H:5802:MD1:N15	6:H:5802:MD1:O11	2.46	0.48
2:K:314:MET:HE3	6:K:5802:MD1:N16	2.26	0.48
3:L:309:ILE:HG13	3:L:310:GLN:HG3	1.95	0.48
2:N:57:TYR:O	2:N:88:ARG:NH1	2.42	0.48
3:O:241:PHE:HB2	8:O:401:HEM:C3A	2.47	0.48
1:P:265:GLN:NE2	2:Q:111:ASN:O	2.29	0.48
1:P:309:ARG:HG3	1:P:310:TRP:HE3	1.78	0.48
2:Q:94:ASP:OD2	2:Q:98:TYR:OH	2.25	0.48
2:Q:974:TYR:CE1	2:Q:1004:ARG:HD3	2.48	0.48
2:T:554:TYR:O	2:T:557:SER:OG	2.29	0.48
1:V:8:HIS:O	1:V:90:TRP:HH2	1.95	0.48
1:V:189:ARG:NH1	1:V:209:ARG:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:225:ARG:HH11	2:W:656:LEU:HD12	1.78	0.48
2:W:520:PRO:HD2	2:W:520:PRO:O	2.12	0.48
2:W:543:TYR:CE1	2:W:559:SER:HB3	2.48	0.48
2:W:882:TRP:O	2:W:886:THR:HG23	2.13	0.48
2:W:937:ASN:ND2	2:W:954:GLU:C	2.66	0.48
3:X:235:ASP:OD1	3:X:278:ASP:OD2	2.32	0.48
1:A:72:PRO:HG3	1:A:139:TRP:CZ3	2.47	0.48
1:A:252:ARG:HH12	1:A:388:LYS:HB3	1.78	0.48
2:B:499:SER:HG	2:B:894:TRP:NE1	2.10	0.48
2:E:272:TRP:CH2	2:E:618:ASN:ND2	2.82	0.48
2:E:1062:ASP:CA	2:E:1096:THR:CG2	2.91	0.48
2:H:67:CYS:HB2	2:H:77:ILE:HD12	1.95	0.48
2:H:293:MET:HE3	2:H:316:GLU:HG3	1.95	0.48
2:K:123:ARG:NH1	2:K:930:ASP:OD2	2.46	0.48
2:K:445:THR:HG22	2:K:448:ASP:CG	2.38	0.48
2:K:595:ASP:HB3	2:K:598:ALA:HB2	1.95	0.48
3:O:303:GLY:C	3:O:305:LYS:CD	2.86	0.48
2:Q:172:ALA:HB1	2:Q:176:GLU:HG2	1.95	0.48
2:Q:210:MET:SD	2:Q:623:PRO:HD3	2.54	0.48
3:U:130:PHE:CE2	3:U:301:ARG:HD3	2.48	0.48
1:V:150:LYS:CG	1:V:167:TRP:NE1	2.76	0.48
1:V:334:PRO:HG2	2:W:325:GLU:O	2.13	0.48
2:W:143:TRP:CD1	2:W:149:PRO:HD2	2.47	0.48
2:B:88:ARG:NH2	10:B:5913:HOH:O	2.43	0.48
3:C:305:LYS:HE2	8:C:401:HEM:C4A	2.47	0.48
1:D:166:ARG:HB2	1:D:166:ARG:NH1	2.29	0.48
1:D:200:ILE:HD13	1:D:237:ALA:HB3	1.94	0.48
1:D:311:ALA:HB3	1:D:316:LEU:HD11	1.95	0.48
2:E:651:PHE:HD2	2:E:653:ASN:O	1.97	0.48
2:E:658:ASN:OD1	2:E:1024:ILE:HG23	2.12	0.48
2:H:90:GLU:HG2	2:H:91:GLN:N	2.28	0.48
2:H:293:MET:HE1	2:H:313:LYS:HD2	1.94	0.48
1:J:24:HIS:HB2	1:J:271:PHE:HB3	1.95	0.48
2:K:983:ASP:OD2	2:K:1061:ARG:NE	2.45	0.48
2:K:1003:LEU:HD23	2:K:1003:LEU:H	1.78	0.48
3:O:301:ARG:CG	3:O:301:ARG:NH1	2.71	0.48
3:O:305:LYS:HE2	8:O:401:HEM:C1B	2.48	0.48
2:Q:150:GLU:H	2:Q:150:GLU:CD	2.20	0.48
3:R:81:LEU:HA	3:R:307:ILE:O	2.14	0.48
1:S:217:GLN:NE2	10:S:605:HOH:O	2.34	0.48
1:S:373:PHE:HE2	1:S:375:MET:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:983:ASP:HB3	2:T:984:ARG:CD	2.43	0.48
2:W:73:HIS:CG	2:W:315:PRO:HG2	2.48	0.48
2:B:661:LYS:NZ	2:B:1096:THR:OG1	2.33	0.48
1:G:149:ALA:O	2:H:1009:PRO:HG2	2.14	0.48
3:I:321:TRP:C	3:I:322:GLN:OXT	2.57	0.48
1:J:38:CYS:O	2:K:116:LEU:HD22	2.13	0.48
1:J:267:ARG:NH1	4:J:503:SF4:S1	2.86	0.48
2:K:948:ARG:NH1	2:K:1112:GLY:O	2.47	0.48
1:M:189:ARG:HH11	1:M:189:ARG:CG	2.25	0.48
2:N:822:TYR:HB3	2:N:1076:LYS:HB2	1.96	0.48
2:N:836:GLU:H	2:N:836:GLU:HG3	1.36	0.48
2:Q:451:GLU:O	2:Q:454:VAL:HG22	2.13	0.48
2:Q:814:GLN:HA	2:Q:819:LEU:HB2	1.95	0.48
2:Q:888:ARG:HG2	2:Q:888:ARG:HH21	1.79	0.48
1:S:292:PRO:HB2	1:S:301:PRO:HG2	1.94	0.48
2:T:377:VAL:O	2:T:381:THR:HB	2.13	0.48
1:V:65:THR:HG21	1:V:147:ASP:H	1.78	0.48
1:V:364:PHE:CZ	1:V:366:THR:HB	2.49	0.48
1:A:6:ASN:HD22	1:A:13:MET:HE1	1.78	0.48
1:A:211:TYR:CE2	3:C:302:ASN:HB3	2.49	0.48
1:A:246:ASP:OD1	2:B:59:TYR:OH	2.20	0.48
3:C:275:ASP:OD1	3:C:277:LEU:N	2.37	0.48
2:E:71:ASP:O	2:E:72:THR:CB	2.60	0.48
2:H:571:PHE:CE1	2:H:773:LEU:HB3	2.48	0.48
3:I:307:ILE:CD1	8:I:401:HEM:HAB	2.43	0.48
2:N:189:THR:O	2:N:218:GLY:HA3	2.13	0.48
2:N:462:LEU:N	2:N:462:LEU:HD23	2.28	0.48
2:N:928:VAL:HG11	2:N:1048:GLN:HB3	1.95	0.48
2:Q:1011:TYR:CE2	2:Q:1017:MET:HB2	2.47	0.48
2:T:588:ASP:OD2	2:T:591:LYS:N	2.46	0.48
2:T:915:THR:OG1	6:T:5801:MD1:N17	2.40	0.48
3:I:302:ASN:CG	8:I:401:HEM:CAA	2.72	0.48
1:M:62:ASN:HD22	1:M:71:PHE:HB3	1.78	0.48
2:N:760:PHE:HB2	2:N:769:TYR:CE2	2.49	0.48
1:P:397:GLU:OE2	2:Q:107:THR:OG1	2.24	0.48
2:Q:527:GLU:N	2:Q:527:GLU:OE1	2.46	0.48
2:Q:811:PHE:HA	2:Q:814:GLN:CG	2.42	0.48
2:Q:950:PRO:CD	2:Q:954:GLU:HB3	2.38	0.48
2:Q:957:ILE:HG23	2:Q:957:ILE:O	2.14	0.48
1:S:76:ASP:N	1:S:76:ASP:OD1	2.46	0.48
2:T:780:MET:HG3	2:T:801:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:351:ARG:O	2:W:354:THR:OG1	2.26	0.48
2:W:834:GLU:OE2	10:W:5903:HOH:O	2.20	0.48
2:B:784:THR:HG22	2:B:787:ASP:H	1.79	0.48
3:F:95:VAL:CG2	3:F:306:ASN:HD22	2.26	0.48
1:G:236:ILE:HB	1:G:239:TYR:CD1	2.49	0.48
3:I:241:PHE:CD1	3:I:241:PHE:N	2.82	0.48
2:K:388:ARG:HB3	2:K:390:ASP:OD1	2.13	0.48
2:K:803:PHE:CG	2:K:808:ARG:HG3	2.48	0.48
2:N:485:TYR:OH	2:N:830:ALA:O	2.22	0.48
2:N:991:PRO:HA	2:N:996:TYR:HD1	1.78	0.48
2:Q:543:TYR:O	2:Q:547:MET:HG3	2.13	0.48
1:S:65:THR:HG21	1:S:147:ASP:H	1.79	0.48
3:U:145:ILE:CG1	3:U:288:TYR:CE2	2.97	0.48
1:V:15:TYR:CZ	1:V:185:ALA:HB2	2.46	0.48
2:W:114:MET:HE2	2:W:119:TYR:CE1	2.48	0.48
2:W:937:ASN:OD1	2:W:953:GLY:HA3	2.13	0.48
1:D:44:ALA:HB2	2:E:119:TYR:HE2	1.79	0.48
1:D:292:PRO:O	1:D:320:PHE:HD1	1.97	0.48
2:H:379:LYS:HD3	2:H:450:GLY:HA2	1.96	0.48
1:J:267:ARG:HD2	4:J:503:SF4:S1	2.53	0.48
2:K:142:ARG:NH1	2:K:158:LYS:HE2	2.28	0.48
1:M:26:PHE:CE1	1:M:237:ALA:HB1	2.49	0.48
2:N:376:TYR:CD2	2:N:550:GLY:HA2	2.49	0.48
2:N:398:LYS:O	2:N:471:ILE:HD13	2.14	0.48
2:N:950:PRO:HD2	2:N:954:GLU:HB3	1.95	0.48
3:O:233:VAL:HG11	3:O:252:VAL:HG12	1.96	0.48
2:T:189:THR:O	2:T:193:SER:OG	2.23	0.48
2:T:273:HIS:HB3	6:T:5801:MD1:C13	2.44	0.48
2:T:1022:ALA:HB1	2:T:1050:SER:CB	2.41	0.48
2:W:115:CYS:HB2	2:W:314:MET:CE	2.44	0.48
2:W:521:VAL:H	2:W:551:ASN:ND2	2.12	0.48
2:W:531:HIS:HA	2:W:1097:VAL:HG12	1.96	0.48
3:X:228:PRO:O	3:X:228:PRO:HG2	2.14	0.48
1:D:258:CYS:CB	4:D:501:SF4:S2	3.02	0.48
1:D:264:GLY:O	1:D:266:ILE:N	2.43	0.48
2:E:322:GLU:HA	2:E:325:GLU:OE1	2.14	0.48
2:E:619:HIS:HD2	2:E:1062:ASP:OD2	1.97	0.48
2:E:671:ASN:N	2:E:672:PRO:HD2	2.28	0.48
2:H:376:TYR:CD2	2:H:550:GLY:HA2	2.48	0.48
2:H:382:ASP:HA	2:H:385:LEU:HD13	1.95	0.48
2:H:973:ASP:OD1	2:H:1111:GLY:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:706:PHE:CZ	2:K:722:LYS:HD2	2.49	0.48
2:K:1087:PHE:CD1	2:K:1093:CYS:HB3	2.47	0.48
1:M:266:ILE:HG13	1:M:267:ARG:HG3	1.94	0.48
3:O:152:SER:HB3	3:O:157:ASP:HB2	1.95	0.48
2:Q:577:SER:O	2:Q:776:GLY:HA2	2.14	0.48
2:Q:914:VAL:HG12	2:Q:1099:LYS:HD3	1.95	0.48
3:R:86:LYS:HE2	3:R:309:ILE:HD11	1.96	0.48
2:T:99:SER:HB3	2:T:105:LYS:HG3	1.95	0.48
2:W:893:SER:OG	2:W:896:GLU:HG3	2.14	0.48
1:D:135:GLU:HG3	3:F:128:GLN:OE1	2.13	0.47
2:E:92:ASN:HB3	2:E:94:ASP:OD1	2.14	0.47
2:H:76:ARG:HH12	2:H:720:TRP:HB3	1.79	0.47
3:I:154:ARG:NH1	10:I:501:HOH:O	2.47	0.47
1:J:255:GLU:OE1	1:J:346:ARG:NH2	2.47	0.47
2:K:98:TYR:CD1	2:K:798:VAL:HG21	2.49	0.47
1:M:127:GLN:OE1	3:O:89:PRO:HB3	2.14	0.47
2:N:388:ARG:NH2	2:N:390:ASP:OD2	2.45	0.47
2:N:893:SER:O	2:N:897:THR:N	2.42	0.47
2:N:925:GLN:HB2	2:N:926:TRP:CE3	2.49	0.47
2:N:1069:GLN:NE2	2:N:1094:ILE:HD11	2.28	0.47
2:Q:79:ALA:HA	2:Q:89:VAL:HG23	1.95	0.47
2:Q:641:HIS:CG	2:Q:1087:PHE:HB2	2.49	0.47
3:R:48:VAL:HG22	3:R:313:PRO:HB2	1.96	0.47
3:R:95:VAL:HG22	3:R:306:ASN:ND2	2.29	0.47
1:S:90:TRP:HE1	2:T:1144:ILE:HD11	1.79	0.47
1:S:257:ARG:HH22	2:T:90:GLU:HB2	1.79	0.47
1:V:209:ARG:HH12	3:X:234:GLU:CD	2.22	0.47
2:W:39:ASN:OD1	2:W:39:ASN:N	2.36	0.47
2:W:70:ASN:HD21	2:W:228:MET:HE3	1.79	0.47
2:B:531:HIS:CG	2:B:1098:PRO:HD2	2.49	0.47
3:C:302:ASN:O	3:C:305:LYS:HG3	2.14	0.47
2:E:617:TRP:O	2:E:666:MET:HE1	2.14	0.47
2:E:703:PHE:CB	2:E:722:LYS:H	2.27	0.47
3:F:37:VAL:HA	3:F:154:ARG:HH21	1.79	0.47
3:F:161:PRO:HG3	3:O:321:TRP:CD2	2.50	0.47
2:H:184:GLY:HA3	2:H:676:GLN:NE2	2.30	0.47
2:H:428:ILE:HD11	2:H:1074:PHE:CG	2.49	0.47
1:J:63:VAL:HG21	4:J:503:SF4:S4	2.53	0.47
2:K:1069:GLN:CD	2:K:1094:ILE:HD11	2.39	0.47
2:K:1119:TRP:CD2	2:K:1121:PRO:HD2	2.49	0.47
3:L:155:MET:CG	8:L:401:HEM:NC	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:89:ILE:HG12	2:N:1145:LYS:HB3	1.96	0.47
2:N:273:HIS:HB3	6:N:5801:MD1:S13	2.54	0.47
2:N:703:PHE:O	2:N:722:LYS:HA	2.14	0.47
2:Q:260:GLN:HA	2:Q:260:GLN:OE1	2.13	0.47
2:Q:631:TYR:OH	2:Q:871:ASP:OD2	2.26	0.47
2:Q:923:HIS:O	2:Q:1021:SER:HB3	2.14	0.47
2:Q:1020:HIS:CE1	6:Q:5801:MD1:C20	2.97	0.47
1:S:34:ARG:HB2	1:S:266:ILE:HG22	1.95	0.47
1:S:149:ALA:HA	1:S:168:PHE:HB3	1.95	0.47
2:T:533:PHE:HB2	2:T:1100:GLU:HG3	1.95	0.47
2:T:942:PRO:HA	2:T:952:VAL:HG12	1.95	0.47
1:V:66:LYS:HD2	1:V:66:LYS:HA	1.44	0.47
2:W:166:ASN:HD21	2:W:1027:ASP:HB3	1.78	0.47
2:B:355:ASP:H	2:B:538:MET:HE3	1.79	0.47
2:B:957:ILE:HB	2:B:1003:LEU:HD11	1.97	0.47
3:C:111:PHE:O	3:C:266:VAL:HA	2.14	0.47
3:F:95:VAL:HG23	3:F:306:ASN:HD22	1.79	0.47
3:F:128:GLN:H	3:F:128:GLN:HG2	1.38	0.47
2:H:130:ARG:NH1	2:H:702:GLU:OE2	2.44	0.47
2:K:115:CYS:SG	2:K:117:LYS:HB2	2.55	0.47
3:O:109:ILE:HB	3:O:271:LEU:CD1	2.44	0.47
3:O:165:TRP:CE2	3:O:252:VAL:HG21	2.49	0.47
2:Q:213:ARG:O	2:Q:220:ARG:NH2	2.47	0.47
2:Q:379:LYS:HB3	2:Q:450:GLY:HA2	1.96	0.47
2:Q:571:PHE:CD1	2:Q:780:MET:HE1	2.49	0.47
3:U:68:GLU:OE2	10:U:501:HOH:O	2.20	0.47
3:X:64:VAL:HG21	3:X:257:LYS:HB2	1.96	0.47
3:X:81:LEU:O	3:X:96:ASN:CA	2.60	0.47
1:D:44:ALA:HB3	1:D:258:CYS:HA	1.96	0.47
1:D:227:GLY:O	1:D:230:ARG:HD3	2.14	0.47
2:E:1119:TRP:CD2	2:E:1121:PRO:HD2	2.49	0.47
1:G:256:THR:OG1	1:G:259:MET:HG2	2.14	0.47
2:H:917:LYS:HD3	6:H:5802:MD1:H102	1.95	0.47
1:J:36:ILE:HG22	2:K:310:ILE:HG23	1.95	0.47
3:L:85:ASP:OD1	3:L:85:ASP:N	2.46	0.47
2:N:213:ARG:NH1	2:N:610:LEU:HD21	2.30	0.47
2:N:435:ASP:OD1	2:N:436:ALA:N	2.48	0.47
2:N:1124:THR:CG2	2:N:1126:TYR:CG	2.96	0.47
2:Q:466:PHE:O	2:Q:477:GLU:HG2	2.14	0.47
1:S:302:ASN:HA	1:S:304:TYR:CE1	2.50	0.47
2:T:409:ILE:CG2	2:T:445:THR:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:496:SER:O	2:T:500:MET:HG3	2.15	0.47
2:T:654:VAL:HG23	6:T:5801:MD1:O2B	2.15	0.47
1:V:76:ASP:OD1	1:V:76:ASP:N	2.46	0.47
2:W:69:PRO:HD2	2:W:71:ASP:HB2	1.96	0.47
2:W:100:ASP:OD2	2:W:104:ASN:HB2	2.15	0.47
2:W:274:GLY:O	2:W:527:GLU:HG3	2.14	0.47
2:W:393:LYS:HA	2:W:833:ASP:OD2	2.13	0.47
2:W:434:TRP:HB3	2:W:461:VAL:CG2	2.41	0.47
2:B:80:PHE:HE1	2:B:90:GLU:HB2	1.77	0.47
2:B:307:LYS:HD3	2:B:562:TRP:HB2	1.97	0.47
3:C:193:ASP:H	3:C:197:THR:HG1	1.58	0.47
1:D:192:ILE:HD11	1:D:214:CYS:SG	2.54	0.47
3:F:89:PRO:HD2	3:F:302:ASN:ND2	2.26	0.47
3:I:155:MET:HE1	3:I:241:PHE:HA	1.87	0.47
1:J:346:ARG:CZ	1:J:346:ARG:HA	2.44	0.47
2:K:31:LEU:HD11	3:R:107:ILE:CD1	2.37	0.47
2:N:977:VAL:CG1	2:N:1001:LEU:HD23	2.45	0.47
2:Q:68:SER:C	2:Q:231:LEU:HD12	2.40	0.47
2:Q:467:LYS:C	2:Q:468:LEU:HD23	2.39	0.47
2:Q:959:ILE:HG13	2:Q:960:HIS:N	2.29	0.47
1:S:65:THR:HG21	1:S:147:ASP:N	2.29	0.47
1:V:34:ARG:NH1	1:V:342:MET:HB3	2.29	0.47
1:V:137:LYS:HG2	2:W:945:MET:SD	2.54	0.47
1:V:241:ARG:HH12	1:V:257:ARG:HD2	1.60	0.47
2:W:115:CYS:HB2	2:W:314:MET:HE3	1.97	0.47
2:W:392:LEU:O	2:W:831:TYR:OH	2.20	0.47
2:W:857:LEU:CB	2:W:900:THR:CG2	2.81	0.47
2:E:278:PRO:HG2	2:E:535:ALA:HB3	1.96	0.47
1:G:238:CYS:SG	1:G:257:ARG:HB2	2.55	0.47
3:I:171:TRP:CG	3:I:229:ARG:NH1	2.83	0.47
2:K:917:LYS:HE2	2:K:923:HIS:HD2	1.79	0.47
2:K:1088:GLU:HB3	2:K:1091:ASN:HB3	1.96	0.47
2:Q:575:LYS:H	2:Q:575:LYS:CD	2.26	0.47
2:Q:668:LYS:HG2	2:Q:986:TYR:CD2	2.49	0.47
2:T:291:VAL:O	2:T:562:TRP:HH2	1.98	0.47
2:T:348:ILE:HG12	2:T:507:LEU:HB3	1.96	0.47
1:V:61:ASN:HD22	1:V:62:ASN:N	2.12	0.47
2:W:527:GLU:OE2	6:W:5802:MD1:H101	2.15	0.47
2:W:1065:MET:O	2:W:1069:GLN:HG3	2.15	0.47
3:X:84:GLN:HG2	3:X:86:LYS:H	1.78	0.47
1:A:150:LYS:HD2	1:A:167:TRP:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:LYS:HA	6:B:5802:MD1:H5'1	1.97	0.47
2:B:923:HIS:C	2:B:1021:SER:HB3	2.39	0.47
2:B:937:ASN:ND2	2:B:954:GLU:H	2.12	0.47
2:E:131:LEU:HD12	2:E:132:ARG:H	1.79	0.47
2:E:193:SER:O	2:E:217:ALA:O	2.31	0.47
2:E:650:TRP:HB3	2:E:678:MET:CB	2.45	0.47
2:E:849:GLU:O	2:E:859:ASN:N	2.48	0.47
3:F:131:ARG:CD	3:F:168:LYS:HG2	2.45	0.47
1:G:189:ARG:HD2	1:G:209:ARG:HD3	1.97	0.47
1:G:236:ILE:HB	1:G:239:TYR:HD1	1.79	0.47
2:H:950:PRO:HD2	2:H:954:GLU:HB3	1.97	0.47
2:H:971:ASP:HB2	2:H:1007:TYR:CD2	2.50	0.47
2:H:1037:PRO:HD3	2:Q:160:MET:HE3	1.96	0.47
2:K:914:VAL:HG11	6:K:5802:MD1:H8	1.96	0.47
1:M:141:SER:OG	2:N:938:ASN:O	2.23	0.47
2:N:116:LEU:HD21	2:N:919:ARG:O	2.14	0.47
2:N:824:PRO:HG3	2:N:1074:PHE:HB3	1.95	0.47
3:O:294:TRP:HE1	3:O:305:LYS:HB3	1.74	0.47
2:Q:238:GLY:C	2:Q:738:LEU:HD21	2.40	0.47
2:Q:267:TRP:CE3	2:Q:614:VAL:HG22	2.49	0.47
2:Q:301:LEU:HD23	2:Q:521:VAL:HG22	1.96	0.47
2:Q:338:SER:HB2	2:Q:339:PRO:CD	2.45	0.47
2:Q:379:LYS:O	2:Q:449:VAL:HG22	2.14	0.47
2:Q:923:HIS:CG	6:Q:5801:MD1:H102	2.49	0.47
2:Q:930:ASP:OD1	2:Q:931:TRP:N	2.44	0.47
2:Q:971:ASP:HB2	2:Q:1007:TYR:CD2	2.50	0.47
6:Q:5802:MD1:N15	6:Q:5802:MD1:O11	2.47	0.47
2:T:139:GLY:O	2:T:159:TYR:HB3	2.15	0.47
2:T:1131:GLU:HG2	2:T:1139:LEU:HD11	1.95	0.47
3:U:62:ILE:HD11	3:U:67:LEU:HD11	1.95	0.47
3:U:302:ASN:CG	3:U:303:GLY:N	2.71	0.47
1:V:65:THR:HG23	1:V:170:TYR:CE1	2.50	0.47
1:V:181:PRO:HG2	1:V:184:LEU:HB3	1.95	0.47
1:V:229:THR:O	1:V:231:VAL:HG23	2.13	0.47
2:W:293:MET:HE3	2:W:713:SER:HB2	1.97	0.47
2:W:545:PRO:O	2:W:549:THR:CG2	2.62	0.47
2:W:551:ASN:O	2:W:557:SER:CB	2.60	0.47
2:W:661:LYS:HE3	6:W:5801:MD1:N8	2.29	0.47
2:W:684:ILE:O	2:W:1023:TRP:CZ3	2.68	0.47
2:W:934:ILE:CD1	2:W:952:VAL:CG1	2.89	0.47
2:W:954:GLU:OE2	2:W:974:TYR:OH	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:1024:ILE:O	2:W:1047:TYR:OH	2.29	0.47
3:X:98:ALA:HB3	3:X:291:MET:CE	2.45	0.47
1:A:177:HIS:NE2	1:A:237:ALA:HB2	2.29	0.47
2:B:206:TYR:HE1	2:B:621:GLU:HG2	1.80	0.47
3:C:55:GLN:O	3:C:55:GLN:HG3	2.15	0.47
3:C:223:ASN:OD1	3:C:225:LEU:N	2.47	0.47
1:D:192:ILE:HA	1:D:202:LEU:O	2.15	0.47
2:H:611:ASP:HB3	2:H:1089:ALA:HB2	1.97	0.47
2:H:917:LYS:CE	6:H:5801:MD1:H15	2.27	0.47
2:K:70:ASN:OD1	2:K:923:HIS:HE1	1.98	0.47
2:K:408:ASP:OD2	2:K:410:SER:OG	2.32	0.47
2:K:689:GLU:OE2	2:K:1045:SER:OG	2.27	0.47
1:M:177:HIS:NE2	1:M:237:ALA:HB2	2.30	0.47
2:N:72:THR:HG21	2:N:313:LYS:HE3	1.95	0.47
2:N:115:CYS:SG	2:N:117:LYS:HB2	2.54	0.47
2:N:381:THR:HG23	2:N:547[B]:MET:HE2	1.96	0.47
2:N:404:TYR:C	2:N:405:LYS:HD2	2.40	0.47
2:N:763:GLU:HG2	2:N:765:ARG:HD2	1.97	0.47
2:N:985:PRO:HB2	2:N:999:SER:HB3	1.95	0.47
1:S:189:ARG:HD2	1:S:209:ARG:HD2	1.95	0.47
2:W:381:THR:CG2	2:W:382:ASP:N	2.76	0.47
2:W:900:THR:O	2:W:901:LYS:HD3	2.15	0.47
2:W:983:ASP:CG	2:W:984:ARG:HH21	2.23	0.47
2:B:79:ALA:HA	2:B:89:VAL:HA	1.97	0.47
1:D:166:ARG:HB2	1:D:166:ARG:CZ	2.44	0.47
1:D:259:MET:HE1	1:D:269:GLN:CB	2.45	0.47
1:D:331:PHE:HD2	1:D:332:MET:SD	2.38	0.47
2:E:272:TRP:HH2	2:E:618:ASN:ND2	2.13	0.47
1:G:45:CYS:HB2	4:G:501:SF4:S2	2.54	0.47
1:G:90:TRP:HB2	2:H:1146:VAL:HG22	1.97	0.47
1:G:207:ARG:HD3	2:H:44:TYR:OH	2.15	0.47
2:H:93:TYR:CE1	2:H:112:PRO:HB3	2.50	0.47
3:I:163:ASN:HD22	3:I:164:LEU:H	1.60	0.47
2:N:174:TRP:HE1	2:N:730:GLU:HG2	1.79	0.47
2:N:1119:TRP:CD2	2:N:1121:PRO:HD2	2.50	0.47
3:O:81:LEU:O	10:O:501:HOH:O	2.20	0.47
3:O:252:VAL:HG22	3:O:269:ARG:CG	2.45	0.47
3:R:140:LEU:HD11	3:R:237:ASN:HD21	1.79	0.47
1:V:275:ASN:O	1:V:281:THR:OG1	2.23	0.47
2:W:192:TYR:CE2	2:W:647:LYS:HE2	2.50	0.47
2:W:271:THR:HG23	2:W:1090:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:406:LEU:HD23	2:W:429:GLY:HA2	1.95	0.47
3:X:302:ASN:CG	3:X:303:GLY:N	2.73	0.47
1:D:188:PRO:HB3	3:F:302:ASN:ND2	2.30	0.47
2:E:157:THR:C	2:E:160:MET:H	2.23	0.47
2:E:194:GLY:O	2:E:195:PRO:C	2.58	0.47
2:E:857:LEU:CB	2:E:900:THR:HG21	2.45	0.47
3:F:244:LEU:HB2	8:F:401:HEM:O1A	2.15	0.47
1:G:25:GLN:CD	1:G:302:ASN:HD22	2.23	0.47
1:G:207:ARG:NH2	2:H:44:TYR:OH	2.40	0.47
2:K:89:VAL:HG12	2:K:114:MET:HE1	1.96	0.47
2:K:577:SER:O	2:K:776:GLY:HA2	2.15	0.47
2:N:336:GLU:OE2	6:N:5802:MD1:O2'	2.33	0.47
1:P:36:ILE:HD12	2:Q:310:ILE:HG23	1.96	0.47
2:Q:233:VAL:HB	2:Q:708:ILE:HG23	1.97	0.47
2:T:113:ARG:NH2	2:T:714:ASN:HD22	2.13	0.47
3:U:129:GLU:CD	3:U:187:ARG:NH1	2.73	0.47
2:W:361:GLY:HA3	2:W:497:VAL:HG11	1.97	0.47
2:W:864:THR:HG22	2:W:893:SER:HB3	1.96	0.47
2:W:974:TYR:O	2:W:1108:ALA:N	2.43	0.47
3:X:241:PHE:CD2	8:X:401:HEM:HMB3	2.50	0.47
1:A:16:PRO:HG2	1:A:185:ALA:HB1	1.97	0.46
2:B:527:GLU:OE1	6:B:5802:MD1:H101	2.15	0.46
2:E:141:LYS:O	2:E:145:ASP:N	2.43	0.46
2:H:91:GLN:HG2	2:H:112:PRO:HB2	1.96	0.46
2:H:350:ILE:HG13	2:H:501:THR:HB	1.97	0.46
2:H:388:ARG:HG3	2:H:395:VAL:HG12	1.97	0.46
2:H:1040:ARG:NE	2:H:1048:GLN:OE1	2.47	0.46
3:I:172:GLU:OE2	3:I:255:CYS:HA	2.15	0.46
1:J:149:ALA:O	2:K:1009:PRO:HG2	2.15	0.46
2:K:117:LYS:HB3	2:K:926:TRP:CE2	2.50	0.46
2:K:287:GLN:OE1	2:K:1078:LYS:HB2	2.14	0.46
2:K:594:LEU:HD22	2:K:759:LYS:HD2	1.98	0.46
1:M:190:LYS:HB3	2:N:37:VAL:CG1	2.45	0.46
2:N:61:ARG:HG3	2:N:61:ARG:NH1	2.31	0.46
1:P:256:THR:OG1	1:P:259:MET:HG2	2.14	0.46
1:S:175:CYS:HA	1:S:222:LYS:HG3	1.97	0.46
2:T:567:LYS:HB2	2:T:712:CYS:HB3	1.97	0.46
2:T:917:LYS:NZ	6:T:5801:MD1:O14	2.45	0.46
2:W:114:MET:HG2	4:W:5804:SF4:S1	2.54	0.46
2:W:265:ARG:HH21	2:W:612:GLU:HB2	1.80	0.46
2:W:709:THR:CG2	2:W:718:GLN:HB2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:1023:TRP:HE3	2:W:1047:TYR:CE1	2.33	0.46
1:A:408:ASN:OD1	2:B:803:PHE:HB3	2.14	0.46
2:E:320:VAL:O	2:E:323:VAL:HG22	2.15	0.46
2:H:414:SER:OG	2:H:447:ASP:OD1	2.31	0.46
1:J:39:GLN:NE2	1:J:63:VAL:HB	2.30	0.46
2:K:72:THR:HG21	2:K:313:LYS:NZ	2.30	0.46
2:K:397:PRO:HG2	2:K:430:ASP:HB2	1.97	0.46
3:L:137:MET:HG2	3:L:290:ASN:HB3	1.98	0.46
3:L:303:GLY:HA2	3:L:305:LYS:HD2	1.97	0.46
1:M:8:HIS:ND1	1:M:300:GLU:HA	2.30	0.46
1:M:126:ASN:CB	3:O:90:ASN:OD1	2.62	0.46
1:P:68:TYR:CE1	2:Q:1139:LEU:HD11	2.50	0.46
2:Q:228:MET:O	2:Q:231:LEU:HD23	2.15	0.46
2:Q:246:LEU:O	2:Q:249:VAL:HG22	2.15	0.46
1:S:249:THR:O	1:S:252:ARG:HG3	2.14	0.46
1:S:408:ASN:OD1	2:T:803:PHE:HB3	2.14	0.46
2:T:527:GLU:OE1	2:T:527:GLU:N	2.49	0.46
1:V:9:LEU:H	1:V:9:LEU:HD12	1.80	0.46
2:W:504:PRO:HG3	2:W:507:LEU:CD1	2.45	0.46
3:X:137:MET:HB3	3:X:164:LEU:HG	1.97	0.46
1:D:99:THR:HG21	1:D:286:HIS:HA	1.98	0.46
1:G:338:LEU:HG	1:G:342:MET:HE2	1.97	0.46
3:I:231:ARG:HH11	3:I:250:GLN:HB2	1.80	0.46
2:K:626:VAL:HG13	2:K:628:THR:HG23	1.97	0.46
1:M:30:PHE:CD2	1:M:172:GLN:HB2	2.50	0.46
1:M:115:THR:HG23	1:M:297:PHE:O	2.15	0.46
2:N:527:GLU:OE1	6:N:5802:MD1:H101	2.15	0.46
2:N:958:HIS:CD2	2:N:1006:LYS:HD3	2.51	0.46
1:P:257:ARG:HH11	2:Q:90:GLU:CG	2.28	0.46
2:Q:640:THR:HB	2:Q:1087:PHE:CB	2.39	0.46
1:S:262:CYS:HA	4:S:503:SF4:S3	2.55	0.46
1:V:249:THR:OG1	1:V:252:ARG:O	2.32	0.46
2:W:1023:TRP:N	2:W:1023:TRP:HD1	2.13	0.46
3:X:95:VAL:H	3:X:306:ASN:ND2	2.14	0.46
2:B:776:GLY:H	2:B:781:LYS:NZ	2.13	0.46
2:E:253:ASN:C	2:E:253:ASN:OD1	2.57	0.46
2:H:381:THR:O	2:H:827:ARG:HD3	2.15	0.46
2:H:760:PHE:HB2	2:H:769:TYR:CE2	2.50	0.46
2:H:930:ASP:OD1	2:H:931:TRP:N	2.49	0.46
3:I:137:MET:SD	3:I:155:MET:HA	2.55	0.46
1:J:150:LYS:HE2	2:K:1139:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:ILE:HD11	1:J:256:THR:HG22	1.97	0.46
2:N:468:LEU:O	2:N:476:ILE:N	2.48	0.46
2:Q:917:LYS:C	2:Q:1019:LYS:HZ2	2.20	0.46
1:V:216:GLU:HG2	1:V:217:GLN:HG3	1.97	0.46
2:W:309:LEU:HD12	2:W:313:LYS:HG3	1.98	0.46
2:W:554:TYR:O	2:W:557:SER:OG	2.27	0.46
3:X:41:GLU:O	3:X:310:GLN:HA	2.15	0.46
3:X:43:THR:HG22	3:X:147:PRO:HD3	1.97	0.46
3:X:117:ASP:HB3	3:X:263:TRP:CD1	2.47	0.46
3:X:154:ARG:HD3	3:X:241:PHE:HE2	1.79	0.46
1:A:146:GLU:O	2:B:1006:LYS:NZ	2.46	0.46
2:B:479:MET:HE1	2:B:867:TYR:CZ	2.51	0.46
2:B:554:TYR:O	2:B:557:SER:OG	2.32	0.46
2:B:930:ASP:OD1	2:B:931:TRP:N	2.47	0.46
2:B:1065:MET:O	2:B:1069:GLN:HG3	2.15	0.46
1:D:186:ALA:HB2	1:D:217:GLN:HB2	1.96	0.46
1:D:313:ARG:HH12	1:D:325:ASP:HA	1.80	0.46
2:E:582:TYR:HB3	2:E:586:ALA:HB3	1.96	0.46
2:E:664:TYR:CE1	2:E:999:SER:HA	2.51	0.46
3:F:51:VAL:HG12	3:F:102:ALA:C	2.41	0.46
2:H:123:ARG:HD2	3:I:194:ASP:HB2	1.97	0.46
2:H:466:PHE:HB2	2:H:478:VAL:HG22	1.98	0.46
1:J:189:ARG:CD	1:J:209:ARG:HG3	2.44	0.46
1:J:410:ILE:HB	2:K:572:GLN:HE21	1.80	0.46
2:K:185:ILE:HD12	2:K:741:MET:HE2	1.96	0.46
2:K:822:TYR:HB3	2:K:1076:LYS:HB2	1.97	0.46
2:K:971:ASP:HB2	2:K:1007:TYR:CD2	2.51	0.46
3:L:110:TYR:HD1	3:L:268:CYS:HB2	1.81	0.46
2:N:653:ASN:C	2:N:653:ASN:ND2	2.72	0.46
2:Q:546:VAL:HG12	2:Q:551:ASN:HB2	1.97	0.46
3:R:295:ASN:H	3:R:300:ASP:HB2	1.81	0.46
2:T:305:THR:HG23	2:T:525:TYR:HB3	1.97	0.46
2:T:355:ASP:OD2	2:T:542:TYR:OH	2.34	0.46
2:T:960:HIS:ND1	2:T:961:PRO:HD2	2.31	0.46
1:V:259:MET:O	1:V:346:ARG:NH2	2.48	0.46
1:V:331:PHE:C	1:V:331:PHE:CD2	2.93	0.46
2:W:431:PHE:CE2	2:W:825:THR:HA	2.50	0.46
2:W:930:ASP:O	2:W:934:ILE:HG12	2.16	0.46
1:A:402:ARG:HB3	1:A:406:HIS:HD2	1.80	0.46
2:B:350:ILE:HD12	2:B:358:LEU:HD22	1.98	0.46
3:C:143:ILE:HD13	3:C:151:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:617:TRP:O	2:E:666:MET:CE	2.63	0.46
3:F:95:VAL:CG2	3:F:306:ASN:ND2	2.79	0.46
1:J:2:THR:N	1:J:14:GLU:OE2	2.49	0.46
2:K:117:LYS:HB3	2:K:926:TRP:CD2	2.51	0.46
2:K:937:ASN:CB	2:K:954:GLU:O	2.63	0.46
1:M:36:ILE:HG22	2:N:310:ILE:HG23	1.97	0.46
1:P:192:ILE:CD1	1:P:203:ILE:HG12	2.46	0.46
1:P:282:TRP:HE3	1:P:283:LEU:HD12	1.80	0.46
2:Q:974:TYR:CE1	2:Q:1052:ARG:HD2	2.50	0.46
3:R:236:LEU:HB3	3:R:246:SER:HA	1.97	0.46
2:T:130:ARG:NH1	2:T:702:GLU:OE2	2.46	0.46
2:T:230:LEU:HD23	2:T:565:ASN:CG	2.40	0.46
2:T:291:VAL:CG1	2:T:295:ASP:HB3	2.46	0.46
1:V:31:ASN:ND2	1:V:34:ARG:HG3	2.31	0.46
2:W:538:MET:O	2:W:541:SER:HB3	2.15	0.46
3:X:137:MET:HE2	3:X:137:MET:HB2	1.77	0.46
2:B:421:LYS:HB2	2:B:424:GLN:HG3	1.96	0.46
2:B:441:PRO:HG3	2:B:468:LEU:HD11	1.97	0.46
2:B:446:ARG:NH1	2:B:446:ARG:CG	2.75	0.46
1:D:190:LYS:HD3	2:E:40:PRO:CG	2.46	0.46
2:E:619:HIS:ND1	2:E:619:HIS:O	2.49	0.46
2:E:729:TYR:OH	3:F:200:HIS:O	2.29	0.46
2:H:225:ARG:NH1	2:H:272:TRP:CD1	2.82	0.46
2:K:274:GLY:HA2	2:K:1095:ASN:OD1	2.16	0.46
2:K:314:MET:HE2	2:K:314:MET:HB3	1.86	0.46
3:L:237:ASN:OD1	3:L:247:GLN:NE2	2.49	0.46
2:N:234:ILE:N	2:N:707:GLU:OE2	2.49	0.46
2:N:381:THR:O	2:N:827:ARG:HD3	2.16	0.46
3:O:95:VAL:HG21	3:O:115:TRP:CD1	2.51	0.46
3:O:111:PHE:O	3:O:266:VAL:HA	2.16	0.46
1:P:13:MET:HE2	1:P:13:MET:HB3	1.64	0.46
1:P:229:THR:O	1:P:231:VAL:HG13	2.15	0.46
1:P:309:ARG:HG3	1:P:310:TRP:CE3	2.51	0.46
2:Q:384:PRO:HG2	2:Q:385:LEU:HD12	1.96	0.46
1:S:225:TYR:OH	3:U:124:ALA:O	2.28	0.46
1:S:399:ILE:HD11	2:T:298:PHE:CE2	2.51	0.46
2:T:77:ILE:HG22	2:T:89:VAL:HG22	1.98	0.46
1:V:115:THR:O	1:V:119:VAL:HG12	2.15	0.46
2:W:822:TYR:HB3	2:W:1076:LYS:HB2	1.98	0.46
2:E:925:GLN:O	2:E:926:TRP:HB2	2.15	0.46
2:E:979:ALA:HB1	2:E:1103:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:289:PHE:CD1	3:F:314:LEU:HB3	2.50	0.46
1:G:189:ARG:HG3	1:G:211:TYR:HE2	1.80	0.46
3:I:155:MET:HE2	3:I:155:MET:HB2	1.76	0.46
1:J:45:CYS:HB2	4:J:501:SF4:S2	2.55	0.46
1:J:211:TYR:O	3:L:301:ARG:NE	2.43	0.46
2:K:143:TRP:CD1	2:K:149:PRO:HD2	2.51	0.46
2:K:330:ILE:HB	2:K:344:ALA:HA	1.97	0.46
2:K:415:TYR:CE1	2:K:420:LEU:HD23	2.50	0.46
2:N:270:TYR:HB3	2:N:1090:ASP:HB3	1.97	0.46
3:O:235:ASP:CA	3:O:250:GLN:OE1	2.64	0.46
1:P:29:VAL:HG21	1:P:283:LEU:CD2	2.45	0.46
2:Q:117:LYS:HE2	2:Q:919:ARG:O	2.16	0.46
2:Q:132:ARG:NH2	2:Q:133:TYR:OH	2.46	0.46
2:Q:420:LEU:HD12	2:Q:424:GLN:OE1	2.16	0.46
1:S:42:THR:HA	1:S:61:ASN:HD22	1.81	0.46
2:T:124:ARG:HD2	2:T:926:TRP:CD1	2.51	0.46
2:T:658:ASN:OD1	2:T:1024:ILE:HG23	2.15	0.46
2:T:692:ASP:C	2:T:693:PHE:HD1	2.23	0.46
1:V:106:ALA:N	1:V:107:PRO:HD3	2.30	0.46
2:W:1029:THR:CB	2:W:1049:SER:OG	2.64	0.46
1:A:404:ASP:CA	2:B:804:ARG:NH2	2.78	0.46
2:B:236:LYS:HG2	2:B:653:ASN:HB2	1.98	0.46
2:B:760:PHE:HB2	2:B:769:TYR:CE2	2.51	0.46
3:C:130:PHE:CE2	3:C:299:GLU:HG2	2.51	0.46
3:F:269:ARG:NH2	3:F:279:VAL:O	2.44	0.46
2:H:425:ARG:NH2	2:H:430:ASP:OD1	2.43	0.46
1:J:256:THR:OG1	1:J:259:MET:HG2	2.16	0.46
2:K:70:ASN:HA	2:K:231:LEU:HD11	1.97	0.46
3:L:165:TRP:CZ2	3:L:269:ARG:HD3	2.51	0.46
2:N:379:LYS:HD3	2:N:450:GLY:HA2	1.98	0.46
2:N:434:TRP:HB3	2:N:461:VAL:HG23	1.98	0.46
1:P:14:GLU:HG2	1:P:121:LYS:HD2	1.97	0.46
1:P:147:ASP:HA	1:P:168:PHE:CE1	2.51	0.46
2:Q:888:ARG:HG2	2:Q:888:ARG:NH2	2.30	0.46
2:T:378:LYS:HG2	2:T:462:LEU:CD1	2.46	0.46
1:V:181:PRO:HG2	1:V:184:LEU:CB	2.46	0.46
2:W:373:ASP:N	2:W:548:LEU:O	2.46	0.46
1:A:123:LYS:HB2	1:A:125:ILE:HG22	1.98	0.46
3:C:305:LYS:O	3:C:307:ILE:HG23	2.16	0.46
1:D:35:CYS:HA	1:D:266:ILE:CD1	2.43	0.46
1:D:226:ARG:HH22	3:F:216:SER:CB	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:LYS:C	2:E:140:TRP:H	2.23	0.46
2:E:155:ASN:O	2:E:159:TYR:HB2	2.15	0.46
2:E:257:GLY:O	2:E:261:ALA:HB3	2.16	0.46
2:E:663:VAL:CA	2:E:664:TYR:N	2.70	0.46
2:H:824:PRO:HG3	2:H:1074:PHE:HB3	1.98	0.46
3:I:290:ASN:OD1	3:I:308:SER:OG	2.33	0.46
2:K:89:VAL:CG1	2:K:114:MET:HE1	2.46	0.46
2:K:138:LYS:HG3	2:K:170:LEU:CD1	2.44	0.46
3:O:271:LEU:HG	3:O:281:PHE:HB2	1.98	0.46
2:Q:467:LYS:O	2:Q:468:LEU:HD23	2.16	0.46
2:Q:759:LYS:O	2:Q:763:GLU:CG	2.54	0.46
2:T:294:ASN:HA	2:T:319:TRP:CD2	2.51	0.46
2:W:60:ASP:OD1	2:W:82:ARG:HA	2.16	0.46
2:W:676:GLN:NE2	2:W:678:MET:SD	2.87	0.46
2:W:937:ASN:CB	2:W:954:GLU:O	2.64	0.46
3:X:98:ALA:HB3	3:X:291:MET:HE1	1.98	0.46
1:A:410:ILE:HB	2:B:572:GLN:HE21	1.81	0.45
2:B:594:LEU:HD11	2:B:756:ASP:HB3	1.97	0.45
2:B:659:ASN:OD1	2:B:1021:SER:OG	2.34	0.45
2:E:663:VAL:O	2:E:666:MET:HB2	2.16	0.45
1:G:398:PRO:O	1:G:399:ILE:HD13	2.16	0.45
3:I:154:ARG:CD	8:I:401:HEM:HBB1	2.44	0.45
3:I:306:ASN:N	3:I:306:ASN:ND2	2.63	0.45
2:K:213:ARG:HD3	2:K:642:MET:HB3	1.97	0.45
1:M:126:ASN:HB3	3:O:90:ASN:OD1	2.17	0.45
1:M:181:PRO:HG2	1:M:184:LEU:HB3	1.98	0.45
2:N:61:ARG:NH1	10:N:5913:HOH:O	2.49	0.45
2:N:296:VAL:HG11	2:N:320:VAL:HG22	1.97	0.45
2:N:851:PRO:O	2:N:858:PRO:HB3	2.16	0.45
2:T:56:GLN:HG3	3:U:214:GLU:HA	1.98	0.45
2:T:97:ASN:O	2:T:794:GLY:HA3	2.16	0.45
2:T:722:LYS:NZ	10:T:5905:HOH:O	2.24	0.45
3:U:51:VAL:HG12	3:U:102:ALA:HB3	1.98	0.45
1:V:164:HIS:HB2	1:V:167:TRP:HB3	1.97	0.45
1:V:236:ILE:HB	1:V:239:TYR:CD2	2.51	0.45
2:W:318:HIS:HA	2:W:321:THR:OG1	2.15	0.45
2:W:1017:MET:SD	2:W:1019:LYS:HG2	2.56	0.45
2:W:1022:ALA:HB1	2:W:1050:SER:CB	2.46	0.45
3:X:109:ILE:C	3:X:110:TYR:HD1	2.19	0.45
1:A:13:MET:HG2	1:A:14:GLU:N	2.31	0.45
2:B:335:PRO:HG3	2:B:352:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1014:ASN:O	2:E:1015:CYS:HB2	2.15	0.45
2:E:1062:ASP:HA	2:E:1096:THR:HG22	1.95	0.45
3:F:95:VAL:H	3:F:306:ASN:HD21	1.63	0.45
2:H:485:TYR:HA	2:H:488:HIS:HB3	1.97	0.45
1:M:62:ASN:OD1	1:M:173:ARG:HB2	2.16	0.45
1:M:161:LEU:HA	1:M:161:LEU:HD23	1.75	0.45
1:M:276:PRO:HB3	1:M:286:HIS:NE2	2.31	0.45
2:N:82:ARG:HB2	2:N:87:MET:HG3	1.98	0.45
2:N:229:GLY:HA3	2:N:237:TYR:CD1	2.51	0.45
1:P:16:PRO:HG2	1:P:185:ALA:HB1	1.98	0.45
1:P:159:SER:HB2	2:Q:347:TRP:HB3	1.98	0.45
2:Q:307:LYS:HZ1	2:Q:313:LYS:NZ	2.13	0.45
2:Q:531:HIS:C	2:Q:1097:VAL:CG2	2.89	0.45
2:Q:613:GLU:HG3	2:Q:615:ALA:H	1.81	0.45
2:T:382:ASP:CG	2:T:829:GLN:HA	2.41	0.45
3:U:44:PRO:HG3	3:U:145:ILE:HB	1.98	0.45
3:U:54:MET:O	3:U:56:ILE:HG13	2.16	0.45
1:V:238:CYS:SG	1:V:256:THR:HG23	2.56	0.45
1:V:239:TYR:OH	2:W:53:TYR:HB2	2.17	0.45
1:V:379:THR:O	1:V:379:THR:HG22	2.14	0.45
2:W:69:PRO:HB2	2:W:922:VAL:HG11	1.98	0.45
2:W:210:MET:HE3	2:W:643:PRO:HG2	1.99	0.45
2:W:1124:THR:O	2:W:1126:TYR:CE2	2.68	0.45
3:X:51:VAL:HG23	3:X:103:ILE:N	2.31	0.45
1:A:377:ASN:ND2	1:A:377:ASN:O	2.49	0.45
2:B:379:LYS:HB3	2:B:450:GLY:HA2	1.98	0.45
2:B:410:SER:HA	2:B:415:TYR:CD2	2.51	0.45
2:B:606:LYS:HD3	2:B:608:ARG:HH21	1.81	0.45
2:B:1088:GLU:CB	2:B:1091:ASN:HB3	2.46	0.45
1:D:52:ASN:HD21	3:F:215:LEU:HA	1.81	0.45
1:D:135:GLU:HG3	1:D:136:ASP:N	2.32	0.45
1:G:65:THR:HG21	1:G:147:ASP:N	2.31	0.45
1:G:256:THR:HG23	1:G:269:GLN:OE1	2.16	0.45
2:H:213:ARG:CZ	2:H:610:LEU:HD21	2.47	0.45
2:H:504:PRO:HG2	2:H:507:LEU:HD12	1.97	0.45
3:I:305:LYS:C	3:I:306:ASN:HD22	2.25	0.45
1:J:208:CYS:SG	1:J:231:VAL:HB	2.57	0.45
2:K:31:LEU:HD13	2:K:31:LEU:H	1.75	0.45
2:K:321:THR:HG22	2:K:343:LYS:HG2	1.99	0.45
2:K:384:PRO:O	2:K:433:VAL:HG23	2.17	0.45
2:N:91:GLN:NE2	2:N:114:MET:HB2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:173:SER:OG	2:N:176:GLU:HG2	2.16	0.45
1:P:408:ASN:OD1	2:Q:803:PHE:HB3	2.16	0.45
2:Q:543:TYR:CE1	2:Q:559:SER:HB3	2.52	0.45
1:V:368:ILE:HG12	1:V:369:HIS:ND1	2.31	0.45
2:W:225:ARG:NE	2:W:269:ASN:OD1	2.35	0.45
2:W:336:GLU:OE2	6:W:5802:MD1:O3'	2.25	0.45
2:W:1023:TRP:CE3	2:W:1047:TYR:CE1	3.04	0.45
1:A:239:TYR:N	1:A:240:PRO:HD2	2.31	0.45
2:B:382:ASP:HA	2:B:385:LEU:HD13	1.99	0.45
2:E:37:VAL:HG12	2:E:45:PRO:HD3	1.98	0.45
2:E:658:ASN:ND2	2:E:1023:TRP:HA	2.29	0.45
2:E:690:TYR:OH	2:E:1027:ASP:OD2	2.32	0.45
3:F:104:HIS:O	3:F:104:HIS:CD2	2.70	0.45
3:F:305:LYS:HE2	8:F:401:HEM:C1D	2.52	0.45
2:H:759:LYS:O	2:H:763:GLU:CG	2.64	0.45
2:H:923:HIS:CG	6:H:5801:MD1:H102	2.51	0.45
1:J:293:LEU:HB2	1:J:305:TYR:CE2	2.51	0.45
2:K:313:LYS:HE3	2:K:562:TRP:HB3	1.98	0.45
2:K:527:GLU:O	2:K:1099:LYS:HE3	2.17	0.45
2:K:546:VAL:HG12	2:K:552:VAL:HG23	1.98	0.45
2:K:865:ASN:HB3	2:K:868:ILE:HG12	1.98	0.45
2:K:921:THR:HG21	2:K:1021:SER:HB3	1.99	0.45
1:M:149:ALA:O	2:N:1009:PRO:HG2	2.16	0.45
2:N:722:LYS:NZ	10:N:5915:HOH:O	2.45	0.45
3:O:241:PHE:HB2	8:O:401:HEM:HMA3	1.98	0.45
1:P:16:PRO:HG3	1:P:128:TRP:CE3	2.50	0.45
2:Q:225:ARG:HB2	2:Q:267:TRP:CB	2.45	0.45
2:Q:305:THR:O	2:Q:333:ILE:O	2.35	0.45
2:Q:488:HIS:CE1	2:Q:868:ILE:HD11	2.51	0.45
2:Q:616:TYR:CD2	2:Q:623:PRO:HA	2.52	0.45
2:Q:963:ALA:HA	2:Q:1013:TYR:CE1	2.52	0.45
2:T:82:ARG:HB3	2:T:87:MET:HG3	1.97	0.45
2:T:505:LYS:O	2:T:509:GLU:HG3	2.17	0.45
1:V:170:TYR:OH	2:W:339:PRO:HB3	2.16	0.45
2:W:372:TYR:HB3	2:W:548:LEU:HB3	1.98	0.45
2:W:415:TYR:CD1	2:W:420:LEU:HB3	2.50	0.45
2:W:848:ARG:NH1	2:W:889:ASN:OD1	2.44	0.45
3:X:291:MET:C	8:X:401:HEM:HAC	2.42	0.45
1:A:29:VAL:O	1:A:267:ARG:HA	2.17	0.45
2:B:618:ASN:ND2	2:B:661:LYS:O	2.45	0.45
2:B:823:THR:HG21	2:B:829:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:287:THR:HG22	3:C:314:LEU:HD23	1.99	0.45
1:D:296:GLN:H	1:D:296:GLN:HG3	1.54	0.45
2:E:182:SER:HA	2:E:185:ILE:HG22	1.97	0.45
2:H:689:GLU:OE2	2:H:1045:SER:OG	2.31	0.45
1:M:209:ARG:HH11	3:O:234:GLU:CD	2.23	0.45
2:N:123:ARG:HH12	3:O:193:ASP:CG	2.24	0.45
2:Q:553:GLY:H	2:Q:809:HIS:HE1	1.64	0.45
2:Q:618:ASN:HD21	2:Q:661:LYS:HB2	1.82	0.45
3:R:86:LYS:HE2	3:R:309:ILE:HD13	1.98	0.45
1:S:256:THR:OG1	1:S:259:MET:HG2	2.16	0.45
1:V:92:THR:HG22	2:W:1147:ASP:O	2.16	0.45
1:V:215:VAL:HG22	1:V:223:PRO:O	2.15	0.45
1:V:346:ARG:HB3	2:W:112:PRO:HD3	1.99	0.45
2:W:239:MET:HE1	2:W:650:TRP:CE2	2.52	0.45
2:W:273:HIS:HB3	6:W:5801:MD1:C13	2.47	0.45
2:W:282:PHE:CE1	2:W:837:ILE:HD11	2.50	0.45
2:W:532:TYR:HB2	2:W:538:MET:HE1	1.98	0.45
2:W:717:ILE:O	2:W:798:VAL:HG23	2.17	0.45
2:W:1057:GLN:HE22	6:W:5801:MD1:C17	2.29	0.45
2:W:1064:SER:OG	2:W:1069:GLN:NE2	2.47	0.45
2:B:1057:GLN:OE1	2:B:1060:THR:HG21	2.16	0.45
2:E:385:LEU:HA	2:E:433:VAL:CG1	2.42	0.45
2:E:1042:LEU:HD23	2:E:1043:SER:O	2.17	0.45
2:H:217:ALA:HB2	2:H:262:LEU:HD12	1.98	0.45
2:H:531:HIS:CG	2:H:1098:PRO:HD2	2.52	0.45
2:H:1057:GLN:OE1	2:H:1060:THR:HG21	2.15	0.45
1:J:257:ARG:NH1	2:K:119:TYR:HE2	2.13	0.45
2:K:91:GLN:HG3	2:K:114:MET:SD	2.57	0.45
2:K:334:THR:HG22	2:K:336:GLU:N	2.29	0.45
1:M:63:VAL:HG21	4:M:503:SF4:S4	2.56	0.45
1:M:190:LYS:CB	2:N:37:VAL:CG1	2.94	0.45
1:M:194:LYS:HG3	1:M:201:VAL:CG2	2.42	0.45
2:N:350:ILE:HD12	2:N:358:LEU:HD22	1.98	0.45
2:N:447:ASP:O	2:N:449:VAL:HG22	2.16	0.45
2:N:722:LYS:HB2	2:Q:83:ASN:HA	1.99	0.45
2:Q:164:ARG:NH2	2:Q:674:ILE:O	2.48	0.45
2:Q:232:GLY:O	2:Q:236:LYS:HB2	2.17	0.45
2:Q:371:TRP:HB3	2:Q:516:ALA:HB1	1.97	0.45
3:R:94:SER:HB2	3:R:298:ARG:HG3	1.99	0.45
3:R:143:ILE:C	3:R:143:ILE:CD1	2.89	0.45
2:T:811:PHE:O	2:T:815:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:939:PHE:CZ	2:T:1004:ARG:HD2	2.52	0.45
3:U:294:TRP:CZ2	3:U:305:LYS:HE3	2.52	0.45
1:V:173:ARG:NH2	1:V:220:TYR:O	2.47	0.45
1:V:282:TRP:CE3	1:V:283:LEU:HD12	2.51	0.45
2:W:37:VAL:HG22	2:W:45:PRO:CD	2.47	0.45
2:W:116:LEU:HD21	2:W:919:ARG:O	2.17	0.45
2:W:265:ARG:NE	2:W:612:GLU:HB2	2.30	0.45
1:D:65:THR:HG23	1:D:170:TYR:HE1	1.81	0.45
2:E:916:PRO:O	2:E:1019:LYS:HA	2.17	0.45
2:E:1020:HIS:HD2	6:E:5801:MD1:C16	2.30	0.45
2:H:468:LEU:HD12	2:H:478:VAL:HG21	1.98	0.45
2:H:515:ILE:HG23	2:H:521:VAL:HG11	1.99	0.45
2:H:861:ILE:HB	2:H:891:LYS:HA	1.99	0.45
1:J:181:PRO:HG2	1:J:184:LEU:HB3	1.98	0.45
2:K:141:LYS:HE2	2:K:180:TYR:HE2	1.82	0.45
6:K:5801:MD1:H7	6:K:5801:MD1:H11	1.98	0.45
1:M:276:PRO:HB3	1:M:286:HIS:CE1	2.52	0.45
1:M:302:ASN:HA	1:M:304:TYR:CE1	2.52	0.45
3:O:51:VAL:HG12	3:O:104:HIS:CD2	2.52	0.45
1:P:314:ALA:HA	1:P:317:ARG:HG3	1.99	0.45
2:Q:338:SER:HB2	2:Q:339:PRO:HD2	1.98	0.45
1:S:90:TRP:NE1	2:T:1144:ILE:HD11	2.32	0.45
2:T:571:PHE:HB2	2:T:581:PHE:HB2	1.98	0.45
2:W:705:GLU:HG3	2:W:706:PHE:N	2.31	0.45
1:A:181:PRO:HG2	1:A:184:LEU:HB3	1.98	0.45
2:B:656:LEU:O	2:B:660:ALA:HB2	2.16	0.45
2:B:662:HIS:H	2:B:1060:THR:CG2	2.29	0.45
1:D:202:LEU:HD21	1:D:236:ILE:CB	2.47	0.45
2:E:377:VAL:HG22	2:E:547:MET:O	2.17	0.45
2:E:679:SER:O	2:E:694:ALA:HA	2.17	0.45
2:E:1020:HIS:ND1	2:E:1020:HIS:C	2.71	0.45
2:E:1033:HIS:CE1	2:E:1052:ARG:CG	2.99	0.45
2:H:276:GLN:O	2:H:278:PRO:HD3	2.17	0.45
2:H:293:MET:HE2	2:H:713:SER:HB2	1.99	0.45
3:I:321:TRP:CE2	3:X:161:PRO:CG	2.99	0.45
2:K:814:GLN:HA	2:K:819:LEU:HB2	1.98	0.45
1:M:173:ARG:NH2	1:M:220:TYR:O	2.50	0.45
2:N:531:HIS:O	2:N:1099:LYS:HB2	2.16	0.45
2:N:971:ASP:HB2	2:N:1007:TYR:CD2	2.51	0.45
2:Q:872:ASP:OD2	2:Q:890:ILE:HG12	2.16	0.45
3:U:46:LYS:N	3:U:46:LYS:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:364:PHE:CZ	2:W:300:LYS:HD2	2.52	0.45
1:V:367:GLU:OE1	1:V:372:LYS:HD3	2.17	0.45
2:W:210:MET:SD	2:W:623:PRO:HD3	2.57	0.45
2:W:301:LEU:HB3	2:W:521:VAL:HG22	1.99	0.45
2:W:1124:THR:HG22	2:W:1126:TYR:H	1.82	0.45
2:B:596:PRO:HG3	2:B:760:PHE:HE1	1.82	0.45
3:C:168:LYS:HD2	3:C:171:TRP:CE2	2.51	0.45
1:D:64:GLU:HG2	1:D:70:GLY:HA2	1.98	0.45
1:D:64:GLU:OE2	1:D:75:TRP:NE1	2.50	0.45
3:F:280:GLN:HB2	3:O:282:VAL:CG1	2.46	0.45
3:I:171:TRP:HH2	3:I:234:GLU:HG3	1.81	0.45
2:K:537:LEU:HD22	2:K:846:VAL:H	1.82	0.45
2:K:543:TYR:CE1	2:K:559:SER:HB3	2.51	0.45
2:K:893:SER:O	2:K:897:THR:OG1	2.29	0.45
3:L:131:ARG:NH1	3:L:170:ASP:OD2	2.50	0.45
1:M:408:ASN:OD1	2:N:803:PHE:HB3	2.17	0.45
2:N:124:ARG:CD	2:N:929:THR:HG21	2.47	0.45
3:O:87:ALA:HB2	3:O:241:PHE:HE1	1.82	0.45
3:O:231:ARG:HB2	3:O:231:ARG:CZ	2.47	0.45
1:P:32:ILE:HG21	1:P:308:PRO:HG3	1.97	0.45
2:Q:69:PRO:O	2:Q:922:VAL:CG1	2.54	0.45
2:Q:1059:ILE:HD12	2:Q:1060:THR:HG23	1.99	0.45
2:T:813:GLU:H	2:T:813:GLU:HG3	1.38	0.45
1:V:187:CYS:HA	1:V:188:PRO:HD2	1.82	0.45
2:W:974:TYR:CD1	2:W:1002:MET:SD	3.06	0.45
3:C:137:MET:HE3	3:C:311:TRP:CH2	2.51	0.45
2:E:223:LYS:O	2:E:649:LEU:HA	2.16	0.45
3:F:137:MET:HB2	3:F:137:MET:HE3	1.58	0.45
2:H:308:ASN:HD21	2:H:339:PRO:HD2	1.82	0.45
2:H:380:PHE:CZ	2:H:815:VAL:HA	2.52	0.45
2:K:271:THR:HG21	2:K:1093:CYS:SG	2.57	0.45
2:N:400:ILE:HG13	2:N:401:ILE:HG13	1.99	0.45
3:O:172:GLU:OE2	3:O:232:ALA:HB1	2.17	0.45
2:Q:388:ARG:O	2:Q:392:LEU:HA	2.16	0.45
2:Q:930:ASP:O	2:Q:934:ILE:HG13	2.17	0.45
2:T:223:LYS:HG2	2:T:267:TRP:NE1	2.31	0.45
2:T:648:VAL:HG13	2:T:676:GLN:HB2	1.98	0.45
1:V:9:LEU:HD12	1:V:9:LEU:N	2.32	0.45
2:W:116:LEU:CD2	2:W:314:MET:HE1	2.47	0.45
3:X:168:LYS:NZ	3:X:234:GLU:OE1	2.47	0.45
2:B:218:GLY:O	2:B:221:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:655:ASN:HD22	2:B:924:SER:CB	2.28	0.44
2:B:917:LYS:NZ	6:B:5801:MD1:S13	2.85	0.44
2:E:126:TYR:O	3:F:195:PHE:CE1	2.70	0.44
2:E:849:GLU:O	2:E:860:ALA:N	2.49	0.44
2:H:284:HIS:ND1	2:H:286:LEU:HB3	2.32	0.44
2:H:361:GLY:HA3	2:H:497:VAL:HG21	1.97	0.44
1:J:23:LYS:HE3	1:J:24:HIS:NE2	2.32	0.44
1:J:189:ARG:HD2	1:J:209:ARG:HG3	2.00	0.44
3:L:242:GLY:H	8:L:401:HEM:HBA1	1.82	0.44
2:N:80:PHE:CE1	2:N:90:GLU:HB2	2.50	0.44
2:N:469:LYS:HA	2:N:475:GLU:HA	1.99	0.44
2:N:705:GLU:OE2	2:N:766:ALA:HB2	2.17	0.44
6:N:5801:MD1:H11	6:N:5801:MD1:H7	1.98	0.44
3:O:35:LYS:O	3:O:154:ARG:NH1	2.42	0.44
3:O:164:LEU:HD11	3:O:238:ALA:CB	2.47	0.44
1:P:338:LEU:O	1:P:341:VAL:HG12	2.16	0.44
1:P:377:ASN:OD1	1:P:394:THR:OG1	2.34	0.44
2:Q:527:GLU:HA	2:Q:530:ASN:HB2	1.98	0.44
2:Q:774:LEU:HA	2:Q:780:MET:HE3	1.98	0.44
3:R:309:ILE:HD12	3:R:309:ILE:HA	1.74	0.44
2:T:413:PRO:HD2	2:T:447:ASP:OD2	2.18	0.44
1:V:64:GLU:OE1	1:V:173:ARG:NH1	2.33	0.44
2:W:37:VAL:HG22	2:W:45:PRO:HD3	1.99	0.44
2:W:272:TRP:CZ3	2:W:618:ASN:HB2	2.51	0.44
2:W:396:SER:O	2:W:399:ASP:HB2	2.17	0.44
2:W:998:VAL:HG12	2:W:1030:VAL:HG21	1.99	0.44
1:A:211:TYR:O	3:C:301:ARG:NE	2.49	0.44
1:A:410:ILE:HD11	2:B:803:PHE:HE1	1.81	0.44
2:B:139:GLY:O	2:B:159:TYR:HB3	2.17	0.44
2:B:386:LEU:HD13	2:B:478:VAL:HG23	1.98	0.44
1:D:294:TYR:CE1	1:D:319:MET:HG3	2.53	0.44
2:E:413:PRO:HB2	2:E:820:PRO:HD2	1.99	0.44
2:E:664:TYR:N	2:E:664:TYR:CD2	2.84	0.44
3:F:215:LEU:HD13	3:F:219:TYR:HE1	1.82	0.44
1:G:58:MET:HE1	1:G:233:GLU:HG3	1.98	0.44
2:H:390:ASP:OD1	2:H:390:ASP:N	2.47	0.44
2:H:434:TRP:HB3	2:H:461:VAL:HG22	1.98	0.44
2:H:922:VAL:CG2	2:H:926:TRP:HZ3	2.30	0.44
1:J:189:ARG:CZ	1:J:209:ARG:HD2	2.47	0.44
2:K:804:ARG:NH2	2:K:817:GLU:OE2	2.46	0.44
2:K:937:ASN:HB3	2:K:954:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:THR:O	1:M:3:LEU:HD23	2.18	0.44
2:N:124:ARG:NH2	2:N:925:GLN:OE1	2.42	0.44
3:O:258:PHE:HB2	3:O:263:TRP:CD2	2.52	0.44
2:Q:70:ASN:ND2	6:Q:5801:MD1:S12	2.90	0.44
1:S:6:ASN:OD1	1:S:8:HIS:N	2.50	0.44
1:S:41:CYS:SG	1:S:61:ASN:ND2	2.82	0.44
2:T:151:LEU:HA	2:T:151:LEU:HD23	1.75	0.44
2:T:861:ILE:HB	2:T:891:LYS:HA	1.99	0.44
2:T:909:TYR:HE2	2:T:980:ASN:HA	1.82	0.44
1:V:77:VAL:HG22	2:W:1138:PHE:HE1	1.82	0.44
1:V:116:ILE:HA	1:V:119:VAL:CG1	2.47	0.44
1:A:256:THR:HG22	1:A:259:MET:HG2	1.98	0.44
2:B:970:GLU:HG2	2:B:1118:VAL:CG2	2.47	0.44
1:D:65:THR:HG23	1:D:170:TYR:CE1	2.51	0.44
2:H:498:VAL:HG21	2:H:505:LYS:HB2	1.99	0.44
2:H:533:PHE:HB2	2:H:1100:GLU:HG3	1.98	0.44
2:H:648:VAL:HG13	2:H:676:GLN:HB2	1.98	0.44
2:H:661:LYS:HA	2:H:1057:GLN:OE1	2.17	0.44
2:H:813:GLU:O	2:H:819:LEU:HG	2.18	0.44
1:J:141:SER:HB3	2:K:938:ASN:O	2.16	0.44
2:N:89:VAL:CG1	2:N:119:TYR:HA	2.47	0.44
2:N:398:LYS:O	2:N:471:ILE:CD1	2.66	0.44
2:N:712:CYS:O	2:N:808:ARG:NH2	2.49	0.44
2:N:825:THR:OG1	2:N:829:GLN:NE2	2.45	0.44
1:P:284:ILE:HD13	1:P:304:TYR:CD2	2.52	0.44
2:Q:351:ARG:O	2:Q:354:THR:OG1	2.29	0.44
2:T:284:HIS:CE1	2:T:286:LEU:HB3	2.53	0.44
2:T:300:LYS:NZ	2:T:326:ARG:O	2.50	0.44
1:V:13:MET:HE3	1:V:13:MET:HB3	1.65	0.44
1:V:262:CYS:HB3	1:V:346:ARG:HD2	1.99	0.44
1:V:263:VAL:HG21	2:W:315:PRO:HA	1.99	0.44
2:W:121:PHE:HZ	2:W:699:SER:HB2	1.82	0.44
2:W:381:THR:HG21	2:W:383:PHE:CD2	2.52	0.44
2:W:500:MET:HA	2:W:894:TRP:CZ2	2.52	0.44
2:W:995:PHE:O	2:W:998:VAL:HG22	2.17	0.44
1:A:175:CYS:HA	1:A:222:LYS:HG3	1.99	0.44
2:B:309:LEU:HD12	2:B:309:LEU:HA	1.81	0.44
1:D:8:HIS:CD2	1:D:292:PRO:CG	3.01	0.44
1:D:270:GLY:C	1:D:271:PHE:HD1	2.26	0.44
2:E:927:ALA:O	2:E:933:PHE:CD1	2.71	0.44
2:H:117:LYS:HB3	2:H:926:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1057:GLN:OE1	6:H:5801:MD1:N16	2.46	0.44
3:I:84:GLN:HE21	3:I:84:GLN:HB3	1.64	0.44
1:J:239:TYR:N	1:J:240:PRO:HD2	2.33	0.44
2:K:814:GLN:HB3	2:K:821:PHE:HE1	1.83	0.44
2:K:949:MET:HG2	2:K:954:GLU:OE1	2.18	0.44
3:L:164:LEU:O	3:L:236:LEU:HD23	2.18	0.44
1:M:222:LYS:HD3	1:M:222:LYS:HA	1.76	0.44
2:N:74:ALA:O	10:N:5902:HOH:O	2.21	0.44
2:N:91:GLN:OE1	2:N:119:TYR:OH	2.35	0.44
2:N:301:LEU:HD23	2:N:521:VAL:HG22	1.99	0.44
2:Q:642:MET:SD	2:Q:643:PRO:HD2	2.58	0.44
2:Q:803:PHE:CE1	2:Q:808:ARG:HD3	2.53	0.44
2:Q:943:TYR:HB3	3:R:188:TYR:HB3	1.98	0.44
1:S:373:PHE:CE2	1:S:375:MET:HB2	2.53	0.44
2:T:164:ARG:NH2	2:T:674:ILE:O	2.49	0.44
3:U:236:LEU:N	3:U:236:LEU:CD2	2.80	0.44
1:V:29:VAL:HA	1:V:304:TYR:O	2.17	0.44
2:W:914:VAL:O	2:W:1017:MET:HA	2.18	0.44
2:W:1119:TRP:CD2	2:W:1121:PRO:HD2	2.52	0.44
2:B:133:TYR:CD2	2:B:171:ARG:HG3	2.52	0.44
2:B:393:LYS:HA	2:B:833:ASP:HB2	2.00	0.44
3:F:171:TRP:O	3:F:174:ASP:HB2	2.18	0.44
2:H:1056:GLN:HG2	2:H:1057:GLN:HG2	1.98	0.44
1:J:175:CYS:HA	1:J:222:LYS:HG3	2.00	0.44
2:K:70:ASN:OD1	2:K:923:HIS:CE1	2.70	0.44
3:L:303:GLY:CA	3:L:305:LYS:HD2	2.47	0.44
1:M:313:ARG:HA	1:M:313:ARG:HD3	1.87	0.44
1:P:356:LYS:C	1:P:357:ILE:HD12	2.43	0.44
2:Q:229:GLY:HA3	2:Q:237:TYR:CG	2.52	0.44
3:R:111:PHE:O	3:R:266:VAL:HA	2.18	0.44
2:T:382:ASP:HB3	2:T:481:LEU:HD23	2.00	0.44
2:W:70:ASN:ND2	2:W:228:MET:HG3	2.33	0.44
2:W:91:GLN:HG2	2:W:112:PRO:O	2.16	0.44
2:E:126:TYR:HB3	3:F:205:HIS:HD2	1.82	0.44
2:E:1020:HIS:O	2:E:1020:HIS:CG	2.68	0.44
3:F:51:VAL:HG12	3:F:102:ALA:HB3	1.99	0.44
3:F:67:LEU:HD11	3:F:110:TYR:CE1	2.52	0.44
2:H:964:ALA:HB1	2:H:969:ILE:HB	1.99	0.44
3:I:51:VAL:HB	3:I:315:SER:O	2.17	0.44
1:J:33:ASN:OD1	1:J:308:PRO:HA	2.18	0.44
1:J:271:PHE:O	1:J:278:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:983:ASP:CG	2:K:1061:ARG:HE	2.26	0.44
2:K:1024:ILE:O	2:K:1047:TYR:OH	2.22	0.44
2:N:123:ARG:NH1	2:N:930:ASP:OD1	2.51	0.44
1:P:90:TRP:CG	1:P:322:PRO:HG3	2.53	0.44
1:P:92:THR:O	1:P:95:LYS:HG2	2.17	0.44
1:P:239:TYR:N	1:P:240:PRO:HD2	2.33	0.44
2:Q:923:HIS:C	2:Q:1021:SER:HB3	2.43	0.44
3:R:130:PHE:CE2	3:R:299:GLU:HG2	2.53	0.44
1:V:289:ILE:HG12	1:V:306:ILE:HG12	2.00	0.44
2:W:70:ASN:HA	2:W:231:LEU:HD21	1.99	0.44
2:W:372:TYR:CB	2:W:548:LEU:HB3	2.47	0.44
3:X:63:THR:HG23	3:X:66:ALA:H	1.82	0.44
2:B:834:GLU:HB2	2:B:837:ILE:HD12	1.99	0.44
1:D:56:GLU:H	1:D:56:GLU:CD	2.25	0.44
1:D:134:PRO:HB2	1:D:139:TRP:NE1	2.33	0.44
1:D:190:LYS:HD3	2:E:40:PRO:HG3	1.98	0.44
2:E:995:PHE:HD2	2:E:999:SER:OG	2.01	0.44
3:F:305:LYS:NZ	8:F:401:HEM:C4B	2.86	0.44
1:G:34:ARG:CB	1:G:266:ILE:HG22	2.47	0.44
1:G:173:ARG:HH21	1:G:220:TYR:HB3	1.82	0.44
1:J:85:SER:O	10:J:601:HOH:O	2.21	0.44
1:J:212:ARG:HD2	1:J:225:TYR:CD1	2.53	0.44
1:J:266:ILE:HG13	1:J:267:ARG:HG3	2.00	0.44
2:K:484:MET:HE2	2:K:844:PHE:HZ	1.83	0.44
1:M:229:THR:O	1:M:231:VAL:HG23	2.18	0.44
2:N:917:LYS:NZ	2:N:1020:HIS:ND1	2.65	0.44
2:Q:475:GLU:O	2:Q:475:GLU:HG2	2.18	0.44
3:R:155:MET:HE3	3:R:241:PHE:HA	2.00	0.44
2:T:479:MET:HE1	2:T:487:ILE:HD12	2.00	0.44
2:W:1069:GLN:HE21	2:W:1094:ILE:HG12	1.82	0.44
1:A:276:PRO:HB3	1:A:286:HIS:CE1	2.52	0.44
1:D:45:CYS:SG	1:D:60:TRP:HB2	2.58	0.44
2:H:271:THR:OG1	2:H:1093:CYS:SG	2.74	0.44
2:H:330:ILE:HB	2:H:344:ALA:HA	1.99	0.44
2:H:1135:MET:HE3	2:H:1139:LEU:HD21	1.99	0.44
2:K:301:LEU:HD23	2:K:521:VAL:HG22	1.98	0.44
2:K:641:HIS:CE1	2:K:1087:PHE:HB2	2.53	0.44
2:K:851:PRO:O	2:K:858:PRO:HB3	2.18	0.44
1:M:9:LEU:HD22	1:M:111:TYR:CD2	2.53	0.44
1:M:208:CYS:SG	1:M:231:VAL:HG13	2.57	0.44
2:Q:359:PHE:HB2	2:Q:541:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:34:ARG:HB3	1:S:266:ILE:HG22	2.00	0.44
2:T:181:ALA:HB2	2:T:693:PHE:CE2	2.52	0.44
2:T:1036:ARG:NH2	2:T:1040:ARG:HB3	2.33	0.44
3:U:84:GLN:NE2	3:U:89:PRO:O	2.51	0.44
1:V:16:PRO:HG2	1:V:128:TRP:CD1	2.38	0.44
2:W:44:TYR:CD1	2:W:45:PRO:HD2	2.52	0.44
2:W:69:PRO:HG2	2:W:71:ASP:HB2	2.00	0.44
2:B:189:THR:O	2:B:218:GLY:HA3	2.18	0.44
2:B:449:VAL:HG23	10:B:5919:HOH:O	2.18	0.44
1:D:230:ARG:NH1	3:F:182:GLU:O	2.51	0.44
1:D:382:GLY:C	1:D:383:PHE:HD1	2.26	0.44
2:E:995:PHE:CD2	2:E:999:SER:OG	2.71	0.44
3:F:137:MET:HG2	3:F:290:ASN:O	2.18	0.44
2:H:113:ARG:CG	2:H:315:PRO:HB2	2.48	0.44
3:I:51:VAL:HG11	3:I:316:LEU:HD22	2.00	0.44
1:J:150:LYS:HD3	1:J:167:TRP:HE1	1.83	0.44
2:K:69:PRO:O	2:K:70:ASN:HB3	2.18	0.44
2:K:270:TYR:HE2	2:K:276:GLN:HG3	1.82	0.44
2:K:397:PRO:HB3	2:K:404:TYR:CE1	2.53	0.44
2:N:67:CYS:HB2	2:N:77:ILE:HD12	1.99	0.44
2:N:525:TYR:CE2	2:N:561:THR:HB	2.53	0.44
2:N:613:GLU:HG3	2:N:615:ALA:H	1.82	0.44
1:P:150:LYS:HD3	2:Q:1139:LEU:HD13	2.00	0.44
2:Q:273:HIS:HB3	6:Q:5801:MD1:C13	2.48	0.44
1:S:36:ILE:CD1	2:T:317:ALA:HB3	2.46	0.44
2:T:271:THR:HG23	2:T:1090:ASP:HA	1.99	0.44
2:T:414:SER:OG	2:T:447:ASP:OD1	2.31	0.44
2:W:711:SER:HB3	2:W:714:ASN:OD1	2.17	0.44
2:W:882:TRP:HD1	2:W:883:GLU:OE2	2.01	0.44
3:X:123:GLN:HG2	3:X:125:ILE:HG13	2.00	0.44
3:X:162:VAL:HG12	3:X:238:ALA:O	2.18	0.44
1:A:123:LYS:HB2	1:A:125:ILE:CG2	2.48	0.43
1:A:365:GLU:HB2	1:A:374:THR:HG22	2.00	0.43
2:B:189:THR:O	2:B:193:SER:HB3	2.18	0.43
2:B:973:ASP:OD1	2:B:1111:GLY:N	2.44	0.43
2:B:1057:GLN:OE1	6:B:5801:MD1:N16	2.45	0.43
1:D:52:ASN:HD22	3:F:215:LEU:C	2.24	0.43
1:D:294:TYR:HE1	1:D:319:MET:HE2	1.83	0.43
3:F:136:LEU:HD12	3:F:267:PHE:CD2	2.52	0.43
3:I:154:ARG:CD	8:I:401:HEM:HBB2	2.46	0.43
3:I:171:TRP:CH2	3:I:234:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:VAL:HG13	2:K:315:PRO:HA	2.00	0.43
2:K:117:LYS:HZ2	2:K:922:VAL:HG22	1.83	0.43
2:K:297:ARG:HA	2:K:323:VAL:HG12	2.00	0.43
2:K:334:THR:HB	2:K:347:TRP:HE1	1.83	0.43
3:L:163:ASN:OD1	3:L:278:ASP:HA	2.18	0.43
3:L:302:ASN:O	3:L:305:LYS:CE	2.55	0.43
3:O:241:PHE:CD2	3:O:241:PHE:O	2.70	0.43
3:O:303:GLY:CA	3:O:305:LYS:HD3	2.46	0.43
2:Q:97:ASN:O	2:Q:794:GLY:HA3	2.18	0.43
1:S:317:ARG:NH1	1:S:325:ASP:OD2	2.51	0.43
2:T:332:VAL:HG23	2:T:344:ALA:HB2	1.98	0.43
2:T:841:GLY:HA3	2:T:870:PRO:HB3	1.99	0.43
2:T:868:ILE:HG22	2:T:870:PRO:HD3	2.00	0.43
1:V:5:HIS:O	1:V:180:TYR:OH	2.22	0.43
1:V:100:SER:OG	1:V:104:THR:CG2	2.64	0.43
1:A:255:GLU:HG2	1:A:351:ILE:HG12	1.99	0.43
1:A:410:ILE:HB	2:B:572:GLN:NE2	2.33	0.43
2:B:69:PRO:O	2:B:922:VAL:HG11	2.19	0.43
2:B:484:MET:HE2	2:B:867:TYR:CD2	2.52	0.43
3:F:115:TRP:CD1	3:F:293:VAL:HG11	2.52	0.43
3:F:166:HIS:CD2	8:F:401:HEM:HMD3	2.53	0.43
3:F:269:ARG:HG2	3:F:270:SER:N	2.33	0.43
2:H:351:ARG:O	2:H:354:THR:OG1	2.34	0.43
1:J:209:ARG:NH1	3:L:234:GLU:OE1	2.51	0.43
2:K:110:TRP:CZ3	2:K:316:GLU:OE1	2.62	0.43
2:K:225:ARG:NE	2:K:269:ASN:OD1	2.52	0.43
2:K:290:ASP:OD2	2:K:712:CYS:HB2	2.17	0.43
2:K:314:MET:HE1	2:K:919:ARG:CB	2.48	0.43
1:M:4:VAL:HG21	1:M:180:TYR:CE1	2.53	0.43
2:N:803:PHE:CG	2:N:808:ARG:HG3	2.53	0.43
2:N:1057:GLN:HE22	6:N:5801:MD1:C17	2.31	0.43
1:P:149:ALA:O	2:Q:1009:PRO:HG2	2.18	0.43
2:Q:355:ASP:OD2	2:Q:542:TYR:OH	2.31	0.43
2:Q:445:THR:HG22	2:Q:448:ASP:CG	2.39	0.43
2:Q:469:LYS:HA	2:Q:475:GLU:HA	2.01	0.43
2:T:190:LYS:HA	2:T:193:SER:OG	2.17	0.43
2:T:977:VAL:HG12	2:T:1059:ILE:HG21	2.00	0.43
2:T:1065:MET:SD	2:T:1065:MET:N	2.91	0.43
3:U:51:VAL:HG21	3:U:316:LEU:HG	1.99	0.43
2:W:132:ARG:NH2	3:X:200:HIS:CE1	2.86	0.43
2:W:872:ASP:O	2:W:875:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:HG3	1:A:194:LYS:HE3	2.00	0.43
2:B:674:ILE:HB	2:B:677:ILE:HD11	2.00	0.43
1:D:342:MET:HE2	1:D:342:MET:HB3	1.87	0.43
2:E:914:VAL:O	2:E:1017:MET:HA	2.18	0.43
3:I:53:TYR:HE1	3:I:319:ILE:HA	1.71	0.43
3:I:84:GLN:NE2	3:I:89:PRO:O	2.50	0.43
1:J:262:CYS:HA	4:J:503:SF4:S3	2.58	0.43
2:K:824:PRO:HG3	2:K:1074:PHE:HB3	2.00	0.43
1:M:8:HIS:CE1	1:M:300:GLU:HG2	2.53	0.43
2:N:272:TRP:O	2:N:1096:THR:OG1	2.32	0.43
3:O:241:PHE:HB2	8:O:401:HEM:CMA	2.48	0.43
1:P:334:PRO:HG2	2:Q:325:GLU:O	2.18	0.43
2:Q:230:LEU:HD11	2:Q:710:ASN:OD1	2.18	0.43
3:R:63:THR:HG23	3:R:66:ALA:H	1.83	0.43
1:S:39:GLN:NE2	1:S:63:VAL:HB	2.32	0.43
1:V:283:LEU:HD11	1:V:341:VAL:HG11	1.99	0.43
1:V:402:ARG:HD2	2:W:803:PHE:O	2.16	0.43
2:W:1023:TRP:HE3	2:W:1047:TYR:CD1	2.36	0.43
1:A:21:ARG:HE	1:A:179:THR:HG21	1.83	0.43
2:B:213:ARG:NH1	2:B:610:LEU:HD21	2.34	0.43
2:B:311:GLU:HG2	2:B:919:ARG:NH2	2.33	0.43
2:B:856:TYR:HB3	2:B:900:THR:OG1	2.17	0.43
1:D:225:TYR:HA	1:D:232:SER:HA	2.00	0.43
2:E:49:TRP:O	2:E:52:VAL:HG22	2.18	0.43
2:E:959:ILE:HD13	2:E:1016:THR:CG2	2.45	0.43
2:E:1014:ASN:ND2	2:E:1014:ASN:N	2.64	0.43
2:H:915:THR:HA	2:H:1018:MET:O	2.19	0.43
3:I:53:TYR:HE1	3:I:319:ILE:CG2	2.26	0.43
1:J:263:VAL:HG21	2:K:114:MET:O	2.19	0.43
2:K:261:ALA:O	2:K:608:ARG:HD3	2.18	0.43
2:K:273:HIS:HB3	6:K:5801:MD1:S13	2.59	0.43
2:K:303:ILE:HB	2:K:523:ILE:HD13	2.01	0.43
3:L:199:PRO:CB	2:N:632:GLY:HA3	2.48	0.43
2:N:139:GLY:O	2:N:159:TYR:HB3	2.18	0.43
1:P:190:LYS:HB3	2:Q:40:PRO:HG3	2.01	0.43
2:Q:542:TYR:N	2:Q:542:TYR:CD2	2.85	0.43
1:S:149:ALA:O	2:T:1009:PRO:HG2	2.19	0.43
1:S:239:TYR:N	1:S:240:PRO:HD2	2.34	0.43
2:T:143:TRP:CD1	2:T:149:PRO:HD2	2.54	0.43
2:T:753:ARG:HA	2:T:756:ASP:CB	2.47	0.43
2:T:1074:PHE:HB2	2:T:1085:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:213:LYS:CD	3:X:301:ARG:HH21	2.27	0.43
1:V:272:LEU:HD23	1:V:272:LEU:HA	1.93	0.43
1:V:310:TRP:CE2	2:W:342:GLN:HG3	2.54	0.43
1:V:353:TYR:HD2	1:V:384:GLY:HA2	1.83	0.43
2:W:113:ARG:O	2:W:113:ARG:HG2	2.19	0.43
2:W:300:LYS:CG	2:W:520:PRO:HD3	2.48	0.43
2:W:386:LEU:HD22	2:W:478:VAL:HG23	2.00	0.43
2:W:937:ASN:HB3	2:W:954:GLU:O	2.19	0.43
1:A:277:LYS:HB3	1:A:354:GLU:HG3	1.99	0.43
2:B:984:ARG:NH1	2:B:1061:ARG:HB3	2.33	0.43
1:D:66:LYS:O	1:D:168:PHE:HB2	2.19	0.43
2:E:182:SER:O	2:E:185:ILE:HG22	2.18	0.43
2:E:920:HIS:N	2:E:920:HIS:ND1	2.66	0.43
2:E:995:PHE:O	2:E:999:SER:OG	2.36	0.43
1:G:2:THR:HG21	1:G:18:PHE:CD2	2.53	0.43
1:J:331:PHE:HE2	2:K:324:MET:HE2	1.83	0.43
2:K:121:PHE:HZ	2:K:699:SER:HB2	1.83	0.43
2:K:616:TYR:CG	2:K:643:PRO:HG3	2.53	0.43
2:K:917:LYS:HE2	2:K:923:HIS:CD2	2.53	0.43
3:L:58:VAL:HG21	3:L:62:ILE:HG23	2.00	0.43
1:M:178:CYS:HB3	1:M:299:THR:O	2.19	0.43
2:N:386:LEU:HD12	2:N:432:VAL:HG12	2.01	0.43
2:N:706:PHE:CD1	2:N:721:GLY:HA3	2.53	0.43
2:Q:225:ARG:HE	2:Q:227:GLY:HA2	1.84	0.43
3:U:31:ALA:HB3	3:U:34:VAL:HG22	2.00	0.43
1:V:9:LEU:HD11	1:V:298:GLY:HA2	2.00	0.43
2:W:91:GLN:HG3	2:W:114:MET:SD	2.59	0.43
2:W:834:GLU:H	2:W:834:GLU:CD	2.27	0.43
3:X:49:LEU:HD13	3:X:77:VAL:HG13	2.00	0.43
3:X:56:ILE:HD12	3:X:105:ASP:HB3	2.00	0.43
1:A:149:ALA:O	2:B:1009:PRO:HG2	2.17	0.43
2:B:861:ILE:HB	2:B:891:LYS:HA	2.00	0.43
1:D:71:PHE:HB2	1:D:142:PRO:HA	2.01	0.43
1:D:377:ASN:O	1:D:377:ASN:ND2	2.51	0.43
2:E:577:SER:O	2:E:776:GLY:HA2	2.18	0.43
2:E:1013:TYR:CD2	2:E:1013:TYR:C	2.97	0.43
2:H:297:ARG:HA	2:H:323:VAL:HG12	1.99	0.43
2:K:355:ASP:OD2	6:K:5802:MD1:N2	2.51	0.43
2:N:95:HIS:NE2	2:N:113:ARG:HD3	2.34	0.43
2:N:232:GLY:O	2:N:236:LYS:HB2	2.18	0.43
2:N:837:ILE:HG13	2:N:1070:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:983:ASP:HB3	2:N:984:ARG:HD3	2.01	0.43
3:O:110:TYR:HA	3:O:267:PHE:O	2.18	0.43
1:P:24:HIS:HB2	1:P:271:PHE:HB3	2.01	0.43
1:P:34:ARG:NH1	1:P:342:MET:HB3	2.34	0.43
1:P:107:PRO:CG	1:P:285:ARG:HH11	2.25	0.43
2:Q:284:HIS:CE1	2:Q:286:LEU:HB3	2.54	0.43
2:Q:425:ARG:NH2	2:Q:430:ASP:OD1	2.52	0.43
2:Q:723:THR:O	2:Q:723:THR:OG1	2.29	0.43
3:R:136:LEU:HG	3:R:267:PHE:CE2	2.54	0.43
2:T:223:LYS:HG2	2:T:267:TRP:CE2	2.53	0.43
3:U:231:ARG:NH2	3:U:250:GLN:HB2	2.34	0.43
3:U:236:LEU:HA	3:U:247:GLN:HG3	2.00	0.43
1:V:366:THR:HG23	1:V:367:GLU:N	2.34	0.43
1:A:6:ASN:HB2	1:A:13:MET:HE3	2.00	0.43
2:B:554:TYR:O	2:B:809:HIS:NE2	2.52	0.43
2:B:923:HIS:O	2:B:1021:SER:CB	2.59	0.43
2:B:1022:ALA:HB3	2:B:1051:PHE:CZ	2.53	0.43
3:C:137:MET:HG2	3:C:290:ASN:HB3	1.99	0.43
1:D:115:THR:HB	1:D:297:PHE:O	2.19	0.43
1:D:211:TYR:O	3:F:301:ARG:NE	2.48	0.43
2:E:63:PHE:CD2	2:E:724:GLY:HA2	2.54	0.43
2:E:272:TRP:CD1	2:E:273:HIS:HD1	2.36	0.43
2:E:664:TYR:CZ	2:E:1054:GLY:O	2.71	0.43
2:E:849:GLU:O	2:E:859:ASN:CA	2.66	0.43
1:G:9:LEU:HD22	1:G:111:TYR:CD2	2.54	0.43
1:G:410:ILE:HB	2:H:572:GLN:HE21	1.82	0.43
3:I:168:LYS:HD2	3:I:171:TRP:CE2	2.54	0.43
2:K:492:TYR:OH	2:K:847:HIS:HB3	2.19	0.43
2:N:121:PHE:HZ	2:N:699:SER:HB2	1.83	0.43
2:N:579:PRO:HB3	2:N:605:ILE:HG13	2.01	0.43
3:O:168:LYS:HD2	3:O:171:TRP:CE2	2.53	0.43
1:P:348:THR:OG1	1:P:349:GLN:N	2.51	0.43
1:P:364:PHE:CZ	2:Q:300:LYS:HD2	2.54	0.43
2:Q:143:TRP:CE2	2:Q:151:LEU:HD11	2.54	0.43
2:Q:271:THR:HB	2:Q:1094:ILE:O	2.19	0.43
2:Q:376:TYR:CD2	2:Q:550:GLY:HA2	2.53	0.43
2:Q:388:ARG:CG	2:Q:476:ILE:HD12	2.48	0.43
2:Q:616:TYR:CZ	2:Q:1094:ILE:HD11	2.53	0.43
1:S:346:ARG:HA	1:S:346:ARG:NE	2.34	0.43
2:T:252:HIS:NE2	2:T:751:ASP:OD1	2.41	0.43
3:U:41:GLU:O	10:U:502:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:393:THR:OG1	2:W:109:ASN:OD1	2.27	0.43
2:W:36:VAL:HG11	3:X:158:ARG:HE	1.82	0.43
2:W:265:ARG:NH1	2:W:610:LEU:HD23	2.33	0.43
3:X:130:PHE:HE1	3:X:301:ARG:HD3	1.82	0.43
3:X:155:MET:HG2	8:X:401:HEM:NC	2.34	0.43
2:B:680:THR:HG22	6:B:5801:MD1:N2	2.34	0.43
2:B:1021:SER:H	2:B:1056:GLN:NE2	2.17	0.43
2:E:75:CYS:SG	2:E:114:MET:HA	2.59	0.43
2:E:479:MET:C	2:E:484:MET:HE1	2.44	0.43
2:E:964:ALA:HB3	2:E:1007:TYR:CE1	2.51	0.43
2:E:1063:TRP:N	2:E:1096:THR:CG2	2.74	0.43
2:H:91:GLN:NE2	2:H:114:MET:HB2	2.33	0.43
2:H:252:HIS:NE2	2:H:751:ASP:OD1	2.38	0.43
2:H:321:THR:O	2:H:324:MET:HG2	2.19	0.43
2:H:661:LYS:HD3	2:H:661:LYS:N	2.34	0.43
2:H:948:ARG:NH1	2:H:1112:GLY:O	2.52	0.43
2:K:116:LEU:HG	2:K:117:LYS:N	2.33	0.43
2:K:476:ILE:HD13	2:K:478:VAL:HG23	2.00	0.43
2:N:365:ILE:HD11	2:N:494:ILE:HD13	2.00	0.43
1:P:408:ASN:OD1	2:Q:804:ARG:N	2.48	0.43
2:Q:332:VAL:HG21	2:Q:341:ALA:HA	2.00	0.43
1:S:196:LYS:HB2	1:S:196:LYS:HE3	1.77	0.43
1:S:409:SER:O	1:S:409:SER:OG	2.31	0.43
2:T:230:LEU:HD11	2:T:710:ASN:OD1	2.18	0.43
3:U:287:THR:CG2	3:U:314:LEU:HD23	2.49	0.43
1:V:8:HIS:HE1	1:V:301:PRO:O	2.01	0.43
1:V:11:ARG:NH2	1:V:113:GLY:O	2.52	0.43
1:V:77:VAL:HG21	2:W:1126:TYR:CD1	2.53	0.43
1:V:78:LYS:HD3	1:V:132:TYR:CZ	2.54	0.43
2:W:397:PRO:HB2	2:W:404:TYR:CD2	2.53	0.43
3:X:95:VAL:HG22	3:X:306:ASN:ND2	2.34	0.43
2:E:957:ILE:CB	2:E:1003:LEU:HD11	2.49	0.43
3:F:71:PHE:CE2	3:F:112:GLN:HB2	2.53	0.43
3:F:119:THR:HG21	3:F:297:ASP:CG	2.43	0.43
1:G:9:LEU:HD22	1:G:111:TYR:HB3	2.00	0.43
1:G:149:ALA:HA	1:G:168:PHE:HB3	2.01	0.43
1:G:302:ASN:HA	1:G:304:TYR:CE1	2.54	0.43
2:H:125:VAL:HG21	2:H:701:VAL:HG21	2.01	0.43
2:H:223:LYS:HG2	2:H:267:TRP:CE2	2.54	0.43
2:H:430:ASP:HB3	2:H:444:ILE:O	2.19	0.43
3:I:49:LEU:HD13	3:I:77:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:36:ILE:HD12	2:N:314:MET:HB2	2.01	0.43
1:M:212:ARG:CZ	3:O:130:PHE:CE2	3.02	0.43
1:M:263:VAL:HG21	2:N:114:MET:O	2.18	0.43
2:N:120:THR:HG22	2:N:931:TRP:CE3	2.49	0.43
2:N:425:ARG:HG2	2:N:425:ARG:HH11	1.83	0.43
2:N:434:TRP:HD1	2:N:461:VAL:HG21	1.83	0.43
2:N:814:GLN:H	2:N:814:GLN:HG2	1.48	0.43
1:P:309:ARG:NH1	2:Q:324:MET:HB2	2.34	0.43
2:Q:513:LYS:O	2:Q:517:THR:OG1	2.35	0.43
3:R:140:LEU:HD21	3:R:278:ASP:C	2.44	0.43
1:S:37:ALA:HB3	2:T:919:ARG:NH2	2.34	0.43
2:T:47:ARG:HE	2:T:47:ARG:HB3	1.52	0.43
1:V:36:ILE:CG1	2:W:310:ILE:HG23	2.44	0.43
1:V:82:LEU:HB3	1:V:130:VAL:HG21	2.00	0.43
1:V:208:CYS:HB3	1:V:231:VAL:HG13	2.01	0.43
2:W:276:GLN:O	2:W:1095:ASN:ND2	2.52	0.43
2:B:379:LYS:HD3	2:B:450:GLY:C	2.44	0.43
2:B:716:PHE:N	2:B:716:PHE:CD1	2.85	0.43
2:B:788:ILE:HG12	2:B:799:ALA:HB2	2.01	0.43
2:B:977:VAL:HG23	2:B:1001:LEU:HG	1.99	0.43
1:D:226:ARG:NH1	3:F:216:SER:OG	2.52	0.43
2:E:67:CYS:HB2	2:E:77:ILE:HD11	2.01	0.43
2:E:272:TRP:HH2	2:E:618:ASN:HB2	1.80	0.43
3:F:201:SER:HB2	3:F:206:LYS:HE3	2.01	0.43
2:H:525:TYR:CE2	2:H:561:THR:HB	2.54	0.43
2:H:709:THR:CG2	2:H:718:GLN:HB2	2.41	0.43
2:H:893:SER:O	2:H:897:THR:OG1	2.33	0.43
1:M:132:TYR:O	1:M:221:LYS:HE3	2.19	0.43
1:M:149:ALA:HB2	1:M:168:PHE:CD2	2.42	0.43
1:M:151:SER:OG	1:M:157:GLU:OE1	2.35	0.43
2:N:113:ARG:NH1	2:N:714:ASN:ND2	2.66	0.43
2:N:268:SER:OG	2:N:613:GLU:OE1	2.32	0.43
2:N:305:THR:O	6:N:5802:MD1:N2	2.50	0.43
1:P:410:ILE:HA	2:Q:1076:LYS:NZ	2.34	0.43
2:Q:72:THR:CG2	2:Q:713:SER:CB	2.97	0.43
2:Q:929:THR:O	2:Q:933:PHE:N	2.48	0.43
2:Q:951:GLY:CA	2:Q:1048:GLN:NE2	2.82	0.43
3:R:165:TRP:HE3	3:R:267:PHE:HD2	1.67	0.43
1:S:63:VAL:HG21	4:S:503:SF4:S4	2.59	0.43
2:T:100:ASP:OD1	2:T:104:ASN:N	2.51	0.43
2:T:333:ILE:O	6:T:5802:MD1:N2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1132:ASN:H	2:T:1135:MET:HB3	1.83	0.43
1:V:149:ALA:CB	1:V:168:PHE:HD2	2.16	0.43
1:V:347:MET:HE1	2:W:109:ASN:HA	2.00	0.43
2:W:232:GLY:O	2:W:236:LYS:HB2	2.19	0.43
2:W:1076:LYS:NZ	2:W:1080:GLY:O	2.52	0.43
3:X:302:ASN:CG	3:X:303:GLY:H	2.27	0.43
1:A:245:ARG:C	2:H:790:ASN:HD21	2.25	0.42
2:B:449:VAL:HA	10:B:5919:HOH:O	2.18	0.42
2:B:462:LEU:HB3	2:B:482:LEU:HD13	2.01	0.42
2:B:894:TRP:HA	2:B:897:THR:OG1	2.19	0.42
3:C:48:VAL:HG22	3:C:313:PRO:HB2	1.99	0.42
1:G:239:TYR:N	1:G:240:PRO:HD2	2.34	0.42
2:H:760:PHE:HB3	2:H:765:ARG:O	2.19	0.42
2:H:882:TRP:CD1	2:H:1061:ARG:NH2	2.87	0.42
2:K:360:LEU:HD13	2:K:492:TYR:CE1	2.54	0.42
6:K:5802:MD1:N15	6:K:5802:MD1:O11	2.52	0.42
1:M:52:ASN:ND2	3:O:215:LEU:HA	2.34	0.42
1:M:356:LYS:HD3	1:M:383:PHE:CZ	2.54	0.42
2:N:625:ILE:HG12	2:N:635:VAL:HG22	2.00	0.42
3:O:33:GLY:O	3:O:88:PHE:N	2.52	0.42
1:P:48:THR:OG1	1:P:257:ARG:NH2	2.51	0.42
1:P:148:THR:HA	2:Q:1008:ASN:OD1	2.19	0.42
2:Q:91:GLN:HG2	2:Q:113:ARG:O	2.19	0.42
2:Q:361:GLY:HA3	2:Q:497:VAL:HG11	2.01	0.42
2:Q:404:TYR:CE2	2:Q:406:LEU:HD23	2.49	0.42
3:R:155:MET:HE1	8:R:401:HEM:C1A	2.54	0.42
1:S:30:PHE:HB2	1:S:305:TYR:CD2	2.54	0.42
1:V:252:ARG:NH2	1:V:386:ASP:OD1	2.49	0.42
2:W:282:PHE:HB3	2:W:832:ASN:ND2	2.34	0.42
2:W:699:SER:O	2:W:703:PHE:CD1	2.71	0.42
1:A:11:ARG:NH2	1:A:113:GLY:O	2.52	0.42
2:B:71:ASP:OD2	2:B:73:HIS:HD2	2.02	0.42
1:D:222:LYS:HB2	4:D:502:SF4:S2	2.59	0.42
2:E:55:ASP:O	2:E:58:GLN:NE2	2.49	0.42
3:F:155:MET:CG	8:F:401:HEM:C1C	3.02	0.42
3:F:302:ASN:OD1	3:F:302:ASN:C	2.63	0.42
1:G:80:LEU:HD11	1:G:294:TYR:CE1	2.54	0.42
2:H:901:LYS:HD2	2:H:906:GLU:OE2	2.18	0.42
3:I:237:ASN:HD22	3:I:237:ASN:HA	1.55	0.42
1:J:337:GLU:OE2	1:J:355:TYR:OH	2.30	0.42
2:K:307:LYS:NZ	2:K:313:LYS:HE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:903:PHE:CE2	2:K:904:LEU:HG	2.54	0.42
2:N:480:THR:HG23	2:N:483:GLU:H	1.83	0.42
2:N:848:ARG:NH1	2:N:859:ASN:OD1	2.52	0.42
1:P:170:TYR:OH	2:Q:339:PRO:HB3	2.19	0.42
2:Q:962:GLN:N	2:Q:965:ARG:HH11	2.17	0.42
3:R:91:GLY:HA3	3:R:304:GLN:HA	2.00	0.42
2:T:152:THR:HG23	2:T:153:PRO:HD2	2.01	0.42
2:T:657:ILE:O	2:T:663:VAL:HG23	2.19	0.42
3:U:193:ASP:H	3:U:197:THR:HB	1.84	0.42
1:V:35:CYS:C	1:V:36:ILE:HD12	2.43	0.42
2:W:301:LEU:HD23	2:W:521:VAL:HG22	2.02	0.42
1:A:410:ILE:HD11	2:B:803:PHE:CE1	2.53	0.42
2:B:249:VAL:HG13	2:B:749:LEU:HD11	2.01	0.42
2:B:446:ARG:HH11	2:B:446:ARG:HG2	1.84	0.42
2:B:717:ILE:HD11	2:B:801:LEU:HB3	2.01	0.42
2:E:123:ARG:HD2	2:E:931:TRP:CD2	2.54	0.42
1:G:65:THR:HG21	1:G:147:ASP:H	1.83	0.42
1:G:408:ASN:OD1	2:H:803:PHE:HB3	2.20	0.42
2:H:293:MET:HE1	2:H:313:LYS:HB3	2.01	0.42
3:I:285:GLU:CD	3:X:142:LYS:HG2	2.43	0.42
1:J:51:PHE:C	1:J:51:PHE:CD1	2.98	0.42
2:K:296:VAL:HG11	2:K:320:VAL:HG22	2.00	0.42
2:N:301:LEU:HB3	2:N:521:VAL:HG22	2.01	0.42
2:T:225:ARG:NH1	2:T:656:LEU:HD12	2.34	0.42
2:T:228:MET:HB3	2:T:231:LEU:HD23	2.02	0.42
2:T:710:ASN:HB2	2:T:801:LEU:HD11	2.01	0.42
1:V:30:PHE:CE1	1:V:267:ARG:HG2	2.55	0.42
2:W:986:TYR:CE2	2:W:989:TRP:HA	2.55	0.42
1:A:190:LYS:HB3	2:B:40:PRO:HG3	2.00	0.42
2:B:121:PHE:O	2:B:125:VAL:HG23	2.19	0.42
2:B:445:THR:HG23	2:B:447:ASP:H	1.83	0.42
2:B:661:LYS:HE2	6:B:5801:MD1:N8	2.34	0.42
2:B:912:TYR:HA	2:B:1102:LEU:HD23	2.00	0.42
2:B:963:ALA:O	2:B:967:LEU:HD12	2.19	0.42
1:D:188:PRO:HG2	1:D:189:ARG:H	1.84	0.42
1:D:258:CYS:HB3	4:D:501:SF4:S2	2.59	0.42
2:E:177:ALA:HB1	2:E:695:PHE:CE2	2.53	0.42
2:E:958:HIS:O	2:E:1016:THR:HA	2.19	0.42
2:E:1033:HIS:CE1	2:E:1052:ARG:CD	3.02	0.42
2:E:1087:PHE:HA	2:E:1092:HIS:O	2.20	0.42
2:H:117:LYS:HZ2	2:H:921:THR:C	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:923:HIS:O	2:H:1021:SER:HA	2.20	0.42
2:K:34:ALA:HB1	3:L:243:THR:HG22	2.01	0.42
2:K:99:SER:HB3	2:K:105:LYS:HG2	2.01	0.42
2:K:231:LEU:HD22	2:K:653:ASN:ND2	2.34	0.42
1:M:179:THR:HA	1:M:194:LYS:HZ1	1.85	0.42
2:N:229:GLY:HA3	2:N:237:TYR:CG	2.54	0.42
2:N:852:GLU:OE2	2:N:984:ARG:NH1	2.51	0.42
2:Q:707:GLU:O	2:Q:719:ILE:HA	2.20	0.42
2:T:94:ASP:OD2	2:T:94:ASP:N	2.47	0.42
2:T:229:GLY:HA3	2:T:237:TYR:CG	2.55	0.42
2:W:35:VAL:HG22	3:X:245:THR:CG2	2.49	0.42
2:W:92:ASN:HD22	2:W:92:ASN:C	2.18	0.42
2:W:359:PHE:HA	2:W:362:ILE:CG2	2.48	0.42
2:B:115:CYS:SG	2:B:117:LYS:HE2	2.60	0.42
2:B:278:PRO:HD2	2:B:539:ASN:OD1	2.19	0.42
2:B:425:ARG:HH21	2:B:425:ARG:HD2	1.67	0.42
2:B:979:ALA:O	2:B:980:ASN:C	2.62	0.42
1:D:7:TRP:CD1	1:D:103:GLY:HA2	2.54	0.42
1:D:331:PHE:CZ	2:E:324:MET:HG3	2.54	0.42
2:E:979:ALA:CB	2:E:1103:VAL:HA	2.50	0.42
2:H:36:VAL:CG1	3:I:243:THR:HG21	2.40	0.42
2:H:449:VAL:HG21	2:H:820:PRO:HA	2.01	0.42
2:K:232:GLY:O	2:K:236:LYS:HB2	2.19	0.42
1:M:268:LEU:HD22	1:M:345:PHE:CE1	2.55	0.42
2:N:230:LEU:O	2:N:709:THR:OG1	2.36	0.42
2:N:309:LEU:HD23	2:N:320:VAL:HG21	2.02	0.42
2:Q:61:ARG:HB3	2:Q:81:VAL:HB	2.01	0.42
2:Q:505:LYS:HA	2:Q:508:ILE:HG12	2.01	0.42
3:U:35:LYS:HD3	3:U:85:ASP:O	2.19	0.42
3:X:95:VAL:HG12	3:X:116:ASP:O	2.20	0.42
2:B:543:TYR:HA	2:B:546:VAL:HG12	2.00	0.42
2:B:923:HIS:NE2	6:B:5802:MD1:S13	2.91	0.42
2:B:983:ASP:HB3	2:B:984:ARG:CD	2.45	0.42
2:B:984:ARG:NH1	2:B:1061:ARG:CB	2.83	0.42
1:D:65:THR:HB	1:D:145:GLY:O	2.20	0.42
1:D:346:ARG:CZ	1:D:346:ARG:HA	2.49	0.42
2:E:140:TRP:CZ3	2:E:693:PHE:CD1	3.08	0.42
2:E:353:ASN:HD22	2:E:353:ASN:HA	1.66	0.42
2:E:527:GLU:OE2	2:E:527:GLU:N	2.53	0.42
2:E:838:ILE:C	2:E:841:GLY:H	2.28	0.42
3:F:51:VAL:HG12	3:F:102:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:VAL:HG11	3:F:115:TRP:HD1	1.85	0.42
3:F:275:ASP:HB3	3:F:278:ASP:OD2	2.19	0.42
1:G:315:TYR:O	1:G:318:GLN:HG2	2.20	0.42
2:H:284:HIS:CE1	2:H:286:LEU:HB3	2.55	0.42
2:H:351:ARG:CZ	2:H:354:THR:HG21	2.50	0.42
2:H:974:TYR:CE1	2:H:1004:ARG:HD3	2.55	0.42
3:I:218:GLY:O	3:I:223:ASN:N	2.45	0.42
2:K:87:MET:HE1	3:L:209:ILE:HD13	2.02	0.42
2:K:91:GLN:HG2	2:K:112:PRO:HB2	2.01	0.42
2:K:814:GLN:NE2	10:K:5918:HOH:O	2.52	0.42
2:N:930:ASP:OD2	2:N:931:TRP:N	2.52	0.42
2:N:937:ASN:ND2	2:N:954:GLU:H	2.18	0.42
3:O:51:VAL:HG12	3:O:104:HIS:HD2	1.83	0.42
1:P:364:PHE:HB3	1:P:375:MET:HE2	2.01	0.42
2:Q:77:ILE:HG23	2:Q:114:MET:CE	2.50	0.42
2:Q:309:LEU:HD13	2:Q:320:VAL:HG21	2.01	0.42
2:Q:357:ALA:HB1	2:Q:500:MET:SD	2.59	0.42
2:Q:430:ASP:HB3	2:Q:444:ILE:O	2.18	0.42
2:Q:821:PHE:N	2:Q:821:PHE:CD1	2.87	0.42
3:R:300:ASP:HA	3:R:304:GLN:HB3	2.01	0.42
2:T:173:SER:OG	2:T:176:GLU:HB2	2.20	0.42
2:T:759:LYS:O	2:T:763:GLU:HG3	2.19	0.42
2:T:979:ALA:O	2:T:980:ASN:C	2.62	0.42
2:T:1119:TRP:CD2	2:T:1121:PRO:HD2	2.55	0.42
1:V:65:THR:HG21	1:V:147:ASP:HA	2.02	0.42
2:W:332:VAL:HG21	2:W:341:ALA:HA	2.01	0.42
2:W:415:TYR:HD1	2:W:420:LEU:HB3	1.85	0.42
2:B:73:HIS:CG	2:B:315:PRO:HG2	2.55	0.42
2:B:662:HIS:CE1	2:B:665:GLN:HB2	2.54	0.42
2:B:882:TRP:CD1	2:B:1061:ARG:NH2	2.88	0.42
2:E:349:PRO:C	2:E:350:ILE:HG13	2.45	0.42
2:E:917:LYS:CE	2:E:923:HIS:HD2	2.33	0.42
2:H:190:LYS:HA	2:H:193:SER:HB2	2.02	0.42
2:H:654:VAL:HG23	6:H:5801:MD1:O2B	2.19	0.42
3:I:53:TYR:HE1	3:I:319:ILE:CB	2.33	0.42
1:J:238:CYS:HB3	1:J:241:ARG:HD3	2.01	0.42
2:K:980:ASN:CB	2:K:984:ARG:HH21	2.32	0.42
3:L:168:LYS:HD2	3:L:171:TRP:CE2	2.54	0.42
2:N:503:SER:HB2	2:N:508:ILE:HD11	2.01	0.42
1:P:189:ARG:HH21	1:P:207:ARG:HB3	1.84	0.42
1:P:373:PHE:CZ	1:P:375:MET:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:866:PRO:O	2:Q:869:ARG:HD2	2.19	0.42
2:Q:897:THR:C	2:Q:900:THR:HG1	2.26	0.42
2:T:278:PRO:HD2	2:T:539:ASN:OD1	2.19	0.42
2:T:301:LEU:HB3	2:T:521:VAL:HG22	2.01	0.42
2:T:423:GLU:H	2:T:423:GLU:HG3	1.60	0.42
3:U:142:LYS:NZ	10:U:507:HOH:O	2.52	0.42
3:U:301:ARG:HH21	3:U:301:ARG:CG	2.32	0.42
1:V:121:LYS:O	1:V:124:ASN:OD1	2.38	0.42
1:V:261:ALA:O	1:V:262:CYS:C	2.61	0.42
2:W:803:PHE:CD2	2:W:808:ARG:HB2	2.55	0.42
2:B:34:ALA:HB1	3:C:243:THR:HG22	2.02	0.42
2:B:789:LEU:HD23	2:B:789:LEU:HA	1.91	0.42
3:C:120:ASP:OD2	3:C:120:ASP:N	2.45	0.42
1:D:13:MET:HE3	1:D:13:MET:HB2	1.80	0.42
2:E:663:VAL:O	2:E:664:TYR:HA	2.19	0.42
2:E:956:GLN:C	2:E:1003:LEU:CD1	2.92	0.42
3:F:71:PHE:HE2	3:F:266:VAL:HG11	1.84	0.42
3:F:162:VAL:HG22	3:F:238:ALA:O	2.20	0.42
3:F:241:PHE:HB2	8:F:401:HEM:HMA2	2.01	0.42
2:H:537:LEU:HD13	2:H:846:VAL:O	2.19	0.42
2:K:229:GLY:HA3	2:K:237:TYR:CD1	2.55	0.42
2:K:811:PHE:HA	2:K:814:GLN:OE1	2.19	0.42
2:K:814:GLN:HB3	2:K:821:PHE:CE1	2.55	0.42
2:K:964:ALA:HB1	2:K:969:ILE:HB	2.01	0.42
1:M:53:LYS:O	1:M:226:ARG:NH2	2.39	0.42
1:M:76:ASP:OD1	1:M:76:ASP:N	2.53	0.42
1:M:395:VAL:O	2:N:326:ARG:NH2	2.49	0.42
2:N:752:LYS:HE3	2:N:756:ASP:OD2	2.19	0.42
2:N:923:HIS:NE2	6:N:5801:MD1:S12	2.93	0.42
3:O:305:LYS:HE3	8:O:401:HEM:NB	2.27	0.42
1:P:63:VAL:HG21	4:P:503:SF4:S4	2.59	0.42
2:Q:209:GLU:OE2	2:Q:633:ARG:NH1	2.52	0.42
2:Q:1065:MET:SD	2:Q:1065:MET:N	2.93	0.42
1:S:315:TYR:O	1:S:318:GLN:HG2	2.19	0.42
1:V:11:ARG:NH2	1:V:118:GLU:OE2	2.53	0.42
1:V:65:THR:HG23	1:V:170:TYR:HE1	1.85	0.42
1:V:260:SER:HA	1:V:346:ARG:CZ	2.50	0.42
2:W:286:LEU:HD23	2:W:287:GLN:H	1.83	0.42
2:W:811:PHE:HA	2:W:814:GLN:OE1	2.19	0.42
3:X:117:ASP:O	3:X:261:LYS:O	2.37	0.42
1:A:245:ARG:CD	2:B:54:ARG:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:MET:SD	2:B:623:PRO:HD3	2.60	0.42
2:B:286:LEU:HD23	2:B:287:GLN:N	2.35	0.42
2:B:717:ILE:O	2:B:798:VAL:HA	2.20	0.42
2:B:913:CYS:HB2	2:B:1103:VAL:HG23	2.01	0.42
2:B:913:CYS:CB	2:B:1103:VAL:CG2	2.97	0.42
2:B:967:LEU:HD22	2:B:1105:ILE:O	2.19	0.42
2:B:1070:LEU:HB2	2:B:1092:HIS:NE2	2.34	0.42
1:D:175:CYS:HA	1:D:222:LYS:HG3	2.01	0.42
1:G:32:ILE:HG21	1:G:308:PRO:HG3	2.02	0.42
2:H:811:PHE:HA	2:H:814:GLN:OE1	2.20	0.42
3:I:64:VAL:HG22	3:I:266:VAL:HG13	2.01	0.42
1:J:13:MET:HE2	1:J:13:MET:HB3	1.95	0.42
1:J:30:PHE:CD1	1:J:267:ARG:HG2	2.55	0.42
1:M:236:ILE:HG13	1:M:238:CYS:H	1.85	0.42
2:N:547[A]:MET:HG2	2:N:828:LEU:HD13	2.01	0.42
3:O:170:ASP:OD1	3:O:170:ASP:N	2.52	0.42
1:P:37:ALA:HA	1:P:63:VAL:HG11	2.01	0.42
2:Q:294:ASN:HA	2:Q:319:TRP:CD2	2.55	0.42
2:Q:358:LEU:CD1	2:Q:508:ILE:HD12	2.50	0.42
2:Q:445:THR:HG23	2:Q:447:ASP:H	1.84	0.42
2:Q:628:THR:N	2:Q:632:GLY:O	2.53	0.42
2:Q:641:HIS:CD2	2:Q:1069:GLN:HA	2.55	0.42
2:Q:912:TYR:HD2	2:Q:1014:ASN:O	2.02	0.42
1:S:239:TYR:OH	2:T:53:TYR:HB2	2.20	0.42
1:S:271:PHE:O	1:S:278:ASN:ND2	2.53	0.42
2:T:400:ILE:HG13	2:T:401:ILE:HG13	2.00	0.42
2:W:333:ILE:HG12	2:W:348:ILE:HB	2.01	0.42
2:W:546:VAL:HG12	2:W:551:ASN:HB2	2.01	0.42
2:B:611:ASP:HB3	2:B:1089:ALA:HB2	2.01	0.42
2:B:903:PHE:CE2	2:B:904:LEU:HG	2.55	0.42
2:E:187:HIS:O	2:E:191:LYS:N	2.53	0.42
3:F:71:PHE:HE1	3:F:102:ALA:CA	2.32	0.42
1:G:296:GLN:HG2	2:H:1144:ILE:HD11	2.01	0.42
2:H:56:GLN:HG3	3:I:214:GLU:HA	2.00	0.42
2:H:121:PHE:HZ	2:H:699:SER:HB2	1.85	0.42
2:H:375:ASP:O	2:H:379:LYS:HG2	2.20	0.42
2:H:483:GLU:O	2:H:486:LYS:HB2	2.20	0.42
2:H:571:PHE:CD1	2:H:780:MET:HE1	2.55	0.42
1:J:212:ARG:HD2	1:J:225:TYR:CG	2.54	0.42
2:K:973:ASP:OD1	2:K:1111:GLY:N	2.51	0.42
1:M:23:LYS:HE3	1:M:24:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:265:ARG:HH11	2:N:644:SER:N	2.18	0.42
2:N:784:THR:OG1	2:N:787:ASP:HB2	2.20	0.42
2:T:152:THR:HG22	2:T:154:GLU:H	1.85	0.42
3:U:49:LEU:HD23	3:U:314:LEU:HD13	2.01	0.42
1:V:46:LYS:NZ	1:V:55:GLN:O	2.53	0.42
2:W:974:TYR:OH	2:W:1052:ARG:HD2	2.20	0.42
2:W:1075:HIS:HE1	2:W:1086:GLY:O	2.03	0.42
3:X:99:GLU:O	3:X:113:VAL:HA	2.20	0.42
2:B:446:ARG:NH1	2:B:446:ARG:HG2	2.34	0.41
2:B:661:LYS:HZ3	2:B:1098:PRO:HG3	1.85	0.41
3:C:67:LEU:HD12	3:C:266:VAL:HG21	2.01	0.41
1:D:22:PRO:HG2	1:D:25:GLN:HB2	2.02	0.41
1:D:204:ASP:O	1:D:208:CYS:N	2.49	0.41
2:E:148:PHE:CD1	2:E:148:PHE:N	2.88	0.41
2:E:293:MET:HE3	2:E:713:SER:CB	2.50	0.41
2:E:414:SER:HB3	2:E:420:LEU:HG	2.02	0.41
2:E:677:ILE:O	2:E:692:ASP:N	2.39	0.41
2:E:856:TYR:CE2	2:E:894:TRP:CH2	3.08	0.41
2:E:928:VAL:O	2:E:928:VAL:HG12	2.20	0.41
3:F:235:ASP:N	3:F:250:GLN:OE1	2.48	0.41
2:H:662:HIS:O	2:H:666:MET:HG2	2.20	0.41
2:H:666:MET:HA	2:H:670:VAL:HB	2.01	0.41
3:I:146:SER:O	3:I:149:GLU:N	2.49	0.41
1:J:62:ASN:ND2	1:J:71:PHE:HB3	2.28	0.41
3:L:222:HIS:HA	3:L:227:LEU:HD11	2.02	0.41
3:L:247:GLN:OE1	3:L:278:ASP:OD2	2.38	0.41
2:N:641:HIS:CG	2:N:1087:PHE:HB2	2.55	0.41
2:N:661:LYS:HD2	6:N:5801:MD1:N8	2.35	0.41
2:Q:201:LEU:HD13	2:Q:645:PRO:HG2	2.01	0.41
2:Q:803:PHE:CD1	2:Q:808:ARG:HD3	2.55	0.41
2:Q:821:PHE:N	2:Q:821:PHE:HD1	2.17	0.41
2:Q:957:ILE:HG22	2:Q:1004:ARG:O	2.20	0.41
2:T:220:ARG:HG3	2:T:265:ARG:HD3	2.02	0.41
2:T:760:PHE:HB2	2:T:769:TYR:CE2	2.55	0.41
2:W:222:PHE:CD2	2:W:246:LEU:HD11	2.54	0.41
2:W:1061:ARG:HH11	2:W:1061:ARG:HG3	1.85	0.41
3:X:269:ARG:NH1	3:X:279:VAL:O	2.53	0.41
3:X:301:ARG:H	3:X:304:GLN:HB2	1.85	0.41
1:A:34:ARG:CB	1:A:266:ILE:HG22	2.50	0.41
2:B:229:GLY:HA3	2:B:237:TYR:CD1	2.55	0.41
2:B:1001:LEU:HA	2:B:1054:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:CYS:HB3	1:D:218:CYS:HB2	2.01	0.41
2:E:195:PRO:O	2:E:199:GLN:N	2.48	0.41
1:G:246:ASP:OD1	2:H:59:TYR:OH	2.29	0.41
2:H:151:LEU:HD23	2:H:151:LEU:HA	1.68	0.41
2:H:543:TYR:CE1	2:H:559:SER:HB3	2.55	0.41
1:J:257:ARG:NH1	2:K:119:TYR:CE2	2.88	0.41
2:K:220:ARG:CZ	2:K:610:LEU:HD22	2.50	0.41
2:K:392:LEU:HD21	2:K:869:ARG:NH1	2.34	0.41
2:K:882:TRP:CD1	2:K:883:GLU:HG2	2.55	0.41
2:N:983:ASP:HB3	2:N:984:ARG:NE	2.35	0.41
2:Q:73:HIS:ND1	2:Q:315:PRO:CG	2.83	0.41
2:Q:133:TYR:CD2	2:Q:171:ARG:HG3	2.55	0.41
3:R:229:ARG:N	3:R:229:ARG:HD2	2.34	0.41
2:T:900:THR:O	2:T:901:LYS:HG2	2.20	0.41
2:T:939:PHE:CE1	2:T:1004:ARG:HD2	2.55	0.41
3:U:236:LEU:HD23	3:U:236:LEU:H	1.84	0.41
1:V:181:PRO:HB3	4:V:502:SF4:S1	2.60	0.41
2:W:230:LEU:HD21	2:W:710:ASN:HB2	2.02	0.41
2:W:282:PHE:HB3	2:W:832:ASN:HD21	1.85	0.41
2:W:629:PRO:HG2	2:W:874:GLY:O	2.20	0.41
3:X:137:MET:HE1	3:X:155:MET:HA	2.02	0.41
3:X:225:LEU:HA	10:X:501:HOH:O	2.20	0.41
2:B:70:ASN:N	2:B:231:LEU:HD21	2.35	0.41
2:B:914:VAL:HG23	2:B:1017:MET:HG2	2.03	0.41
2:E:126:TYR:CG	3:F:205:HIS:CD2	3.08	0.41
2:E:915:THR:OG1	6:E:5801:MD1:N16	2.54	0.41
3:F:305:LYS:HE2	8:F:401:HEM:ND	1.94	0.41
3:F:305:LYS:HD3	8:F:401:HEM:NA	2.35	0.41
1:G:16:PRO:HG2	1:G:185:ALA:HB1	2.02	0.41
2:H:613:GLU:OE1	2:H:614:VAL:N	2.52	0.41
2:H:1040:ARG:HH21	2:H:1042:LEU:HD22	1.84	0.41
2:K:301:LEU:HB3	2:K:521:VAL:HG22	2.02	0.41
2:K:358:LEU:HB2	2:K:501:THR:HG21	2.01	0.41
3:L:67:LEU:HD13	3:L:266:VAL:HG11	2.01	0.41
3:L:203:ASN:ND2	2:N:207:PRO:HA	2.35	0.41
1:M:333:VAL:HG13	1:M:373:PHE:HB2	2.02	0.41
2:N:515:ILE:HG22	2:N:549:THR:HG21	2.01	0.41
2:N:1040:ARG:NH1	2:N:1048:GLN:OE1	2.53	0.41
3:O:110:TYR:HD1	3:O:268:CYS:HB2	1.77	0.41
3:O:241:PHE:HB2	8:O:401:HEM:C4A	2.56	0.41
2:Q:124:ARG:HD3	2:Q:926:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:296:VAL:HG11	2:Q:320:VAL:HG22	2.01	0.41
2:T:89:VAL:HG11	2:T:119:TYR:HA	2.01	0.41
2:T:94:ASP:OD1	2:T:98:TYR:OH	2.28	0.41
2:T:355:ASP:HB2	2:T:538:MET:HE3	2.01	0.41
2:T:434:TRP:HB3	2:T:461:VAL:CG2	2.50	0.41
2:T:760:PHE:HB3	2:T:765:ARG:O	2.20	0.41
2:T:768:VAL:O	2:T:772:ARG:HG3	2.19	0.41
1:V:189:ARG:HH21	1:V:207:ARG:NH1	2.18	0.41
2:W:35:VAL:H	3:X:245:THR:CG2	2.31	0.41
3:X:192:HIS:CD2	3:X:192:HIS:C	2.97	0.41
2:B:359:PHE:HB2	2:B:541:SER:OG	2.20	0.41
2:B:862:VAL:HG22	2:B:897:THR:HG21	2.03	0.41
2:B:1064:SER:OG	2:B:1069:GLN:NE2	2.47	0.41
2:E:666:MET:HA	2:E:670:VAL:HG23	2.02	0.41
2:E:939:PHE:HD2	2:E:954:GLU:HG3	1.86	0.41
2:E:959:ILE:HD11	2:E:963:ALA:HB3	2.03	0.41
1:G:181:PRO:HG2	1:G:184:LEU:HB3	2.01	0.41
1:G:346:ARG:CZ	1:G:346:ARG:HA	2.50	0.41
3:I:284:GLY:C	3:X:142:LYS:HB3	2.44	0.41
2:K:93:TYR:O	2:K:96:GLN:NE2	2.53	0.41
2:K:359:PHE:HB2	2:K:541:SER:OG	2.21	0.41
3:L:145:ILE:HG12	3:L:151:PHE:HB3	2.03	0.41
2:N:425:ARG:HG2	2:N:425:ARG:NH1	2.35	0.41
3:O:155:MET:HE3	3:O:155:MET:HB2	1.77	0.41
3:O:168:LYS:HB3	3:O:170:ASP:OD1	2.20	0.41
1:P:132:TYR:O	1:P:221:LYS:NZ	2.35	0.41
2:Q:628:THR:HG21	2:Q:873:TYR:HB3	2.03	0.41
2:Q:916:PRO:O	2:Q:1020:HIS:N	2.52	0.41
1:S:152:SER:OG	1:S:157:GLU:OE1	2.25	0.41
2:T:909:TYR:CD1	2:T:909:TYR:N	2.87	0.41
1:V:32:ILE:HG13	1:V:306:ILE:O	2.20	0.41
1:V:189:ARG:NH1	1:V:209:ARG:CB	2.60	0.41
1:V:257:ARG:CD	2:W:90:GLU:OE1	2.64	0.41
2:W:648:VAL:HG23	2:W:676:GLN:CB	2.46	0.41
2:W:663:VAL:HG21	2:W:1024:ILE:HD13	2.03	0.41
2:W:795:GLU:HA	2:W:796:PRO:HD3	1.93	0.41
2:W:1061:ARG:HG3	2:W:1061:ARG:NH1	2.36	0.41
1:A:198:ASP:OD1	1:A:198:ASP:N	2.50	0.41
1:D:15:TYR:HE1	1:D:180:TYR:CA	2.32	0.41
2:E:51:SER:O	2:E:52:VAL:C	2.63	0.41
3:F:302:ASN:OD1	8:F:401:HEM:HAA1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:331:PHE:CE2	2:K:324:MET:HE2	2.56	0.41
2:K:179:THR:HG22	2:K:744:LYS:HD2	2.02	0.41
1:M:22:PRO:HA	1:M:196:LYS:O	2.21	0.41
1:M:164:HIS:HB2	1:M:167:TRP:HB3	2.01	0.41
1:M:213:LYS:HB2	5:M:504:F3S:S2	2.60	0.41
2:N:290:ASP:O	2:N:808:ARG:NH1	2.54	0.41
2:N:294:ASN:OD1	2:N:807:PRO:HB3	2.20	0.41
2:N:543:TYR:CE1	2:N:559:SER:HB3	2.55	0.41
2:N:1003:LEU:HD23	2:N:1003:LEU:H	1.86	0.41
3:O:303:GLY:C	3:O:305:LYS:N	2.78	0.41
1:P:29:VAL:HA	1:P:304:TYR:O	2.20	0.41
2:Q:393:LYS:HA	2:Q:833:ASP:HB2	2.03	0.41
2:Q:864:THR:CG2	2:Q:893:SER:HB2	2.50	0.41
1:S:239:TYR:OH	2:T:50:GLU:O	2.30	0.41
1:S:402:ARG:HD2	2:T:803:PHE:O	2.21	0.41
2:T:70:ASN:ND2	2:T:228:MET:HG3	2.35	0.41
2:T:293:MET:HE1	2:T:313:LYS:HB3	2.02	0.41
2:T:882:TRP:CD1	2:T:883:GLU:HG2	2.56	0.41
1:V:111:TYR:CZ	1:V:113:GLY:HA3	2.56	0.41
2:W:181:ALA:CB	2:W:741:MET:HE1	2.51	0.41
2:W:531:HIS:O	2:W:1097:VAL:HB	2.21	0.41
2:W:663:VAL:O	2:W:667:LEU:HG	2.20	0.41
2:W:923:HIS:ND1	6:W:5801:MD1:H102	2.35	0.41
3:X:54:MET:O	3:X:56:ILE:HG13	2.20	0.41
1:A:8:HIS:HE1	1:A:301:PRO:O	2.03	0.41
1:A:107:PRO:HG3	1:A:285:ARG:NH2	2.35	0.41
2:B:295:ASP:OD1	2:B:556:GLY:N	2.53	0.41
3:C:301:ARG:CG	3:C:301:ARG:NH2	2.72	0.41
1:G:128:TRP:CE2	3:I:88:PHE:HD2	2.38	0.41
2:H:71:ASP:OD2	2:H:73:HIS:HB2	2.21	0.41
2:H:286:LEU:HD12	2:H:287:GLN:H	1.85	0.41
3:I:280:GLN:OE1	3:X:272:ASN:OD1	2.38	0.41
1:J:9:LEU:HD22	1:J:111:TYR:HB3	2.02	0.41
2:K:116:LEU:HD12	2:K:932:ASN:ND2	2.35	0.41
2:K:117:LYS:HE2	2:K:919:ARG:O	2.20	0.41
2:K:881:TYR:O	2:K:885:ARG:HG3	2.21	0.41
2:K:1094:ILE:H	2:K:1094:ILE:HD12	1.86	0.41
1:M:320:PHE:HB2	1:M:324:VAL:HG12	2.02	0.41
2:N:67:CYS:O	2:N:74:ALA:HA	2.21	0.41
2:N:116:LEU:HG	2:N:117:LYS:N	2.36	0.41
2:N:141:LYS:HE2	2:N:180:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:689:GLU:OE2	2:N:1045:SER:OG	2.36	0.41
2:N:705:GLU:HG3	2:N:706:PHE:H	1.85	0.41
3:O:151:PHE:CE1	3:O:160:LYS:HB3	2.56	0.41
1:P:181:PRO:HG2	1:P:184:LEU:HB3	2.02	0.41
1:S:291:LEU:HB2	1:S:320:PHE:HB3	2.02	0.41
2:T:1121:PRO:O	2:T:1124:THR:OG1	2.28	0.41
1:V:150:LYS:HD3	1:V:167:TRP:HE1	1.86	0.41
2:W:117:LYS:HE2	2:W:921:THR:O	2.20	0.41
2:W:468:LEU:HD12	2:W:468:LEU:HA	1.64	0.41
2:W:618:ASN:OD1	2:W:661:LYS:HB2	2.20	0.41
1:A:309:ARG:NH1	2:B:343:LYS:O	2.52	0.41
2:B:87:MET:HE3	2:B:87:MET:HB3	1.70	0.41
2:B:533:PHE:HB2	2:B:1100:GLU:HG3	2.03	0.41
2:B:801:LEU:HD12	2:B:801:LEU:O	2.21	0.41
1:D:289:ILE:HG12	1:D:306:ILE:CG2	2.50	0.41
2:E:666:MET:CE	2:E:670:VAL:HG21	2.50	0.41
2:E:856:TYR:HE2	2:E:894:TRP:CH2	2.38	0.41
1:G:6:ASN:OD1	1:G:8:HIS:N	2.53	0.41
2:H:844:PHE:O	2:H:846:VAL:HG23	2.20	0.41
1:J:276:PRO:HB3	1:J:286:HIS:NE2	2.36	0.41
2:K:712:CYS:O	2:K:808:ARG:NH2	2.53	0.41
1:M:212:ARG:NH1	3:O:129:GLU:O	2.28	0.41
1:M:263:VAL:CG1	2:N:315:PRO:HA	2.50	0.41
2:N:348:ILE:HG12	2:N:507:LEU:HB3	2.02	0.41
2:N:397:PRO:HB2	2:N:404:TYR:CE2	2.56	0.41
1:P:410:ILE:HB	2:Q:572:GLN:OE1	2.21	0.41
2:T:77:ILE:CG2	2:T:89:VAL:HG22	2.51	0.41
2:T:302:LEU:HD23	2:T:320:VAL:HG13	2.01	0.41
2:T:547:MET:HG2	2:T:828:LEU:HD13	2.01	0.41
2:T:1024:ILE:HG22	2:T:1055:SER:HB2	2.01	0.41
3:U:163:ASN:HD22	3:U:164:LEU:H	1.68	0.41
1:V:42:THR:HG21	2:W:935:TRP:CZ2	2.56	0.41
2:W:192:TYR:HB3	2:W:201:LEU:HD21	2.03	0.41
2:W:567:LYS:HG2	2:W:570:ASN:CG	2.46	0.41
3:X:172:GLU:O	3:X:176:LEU:HD12	2.20	0.41
2:B:626:VAL:HG11	2:B:887:VAL:HG21	2.03	0.41
3:C:105:ASP:HB2	3:C:108:THR:H	1.86	0.41
2:E:281:PRO:HA	2:E:285:GLY:HA2	2.01	0.41
2:E:497:VAL:O	2:E:501:THR:HG22	2.21	0.41
2:E:928:VAL:HG21	2:E:1023:TRP:CE3	2.55	0.41
2:E:1033:HIS:NE2	2:E:1052:ARG:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:914:VAL:HG12	2:H:916:PRO:HD3	2.03	0.41
2:K:133:TYR:CD2	2:K:171:ARG:HB2	2.56	0.41
1:M:314:ALA:C	2:N:1141:GLY:HA3	2.45	0.41
1:M:410:ILE:HB	2:N:572:GLN:NE2	2.35	0.41
2:N:47:ARG:HG3	2:N:47:ARG:NH2	2.36	0.41
3:O:272:ASN:HD22	3:O:280:GLN:HB3	1.86	0.41
1:P:225:TYR:OH	3:R:124:ALA:O	2.31	0.41
1:P:346:ARG:HA	1:P:346:ARG:CZ	2.51	0.41
1:P:408:ASN:ND2	2:Q:805:THR:OG1	2.31	0.41
2:Q:72:THR:HG23	2:Q:711:SER:OG	2.20	0.41
2:Q:116:LEU:HD21	2:Q:919:ARG:O	2.21	0.41
2:Q:171:ARG:HG2	2:Q:172:ALA:N	2.35	0.41
2:Q:278:PRO:O	2:Q:281:PRO:HD2	2.21	0.41
3:R:295:ASN:H	3:R:300:ASP:CB	2.34	0.41
2:T:470:THR:HG23	2:T:474:LYS:O	2.21	0.41
2:T:923:HIS:CG	6:T:5801:MD1:H102	2.55	0.41
1:V:343:SER:OG	1:V:395:VAL:HG13	2.21	0.41
2:W:395:VAL:HG13	2:W:432:VAL:CG2	2.50	0.41
2:W:666:MET:HA	2:W:670:VAL:HB	2.02	0.41
3:X:51:VAL:HG13	3:X:316:LEU:HA	2.02	0.41
1:A:6:ASN:HD22	1:A:13:MET:CE	2.33	0.41
1:A:9:LEU:O	1:A:110:THR:HA	2.21	0.41
1:A:211:TYR:O	3:C:301:ARG:CD	2.69	0.41
2:B:305:THR:O	6:B:5802:MD1:N2	2.53	0.41
2:B:712:CYS:O	2:B:808:ARG:NH2	2.54	0.41
2:B:914:VAL:C	2:B:916:PRO:HD3	2.46	0.41
2:B:980:ASN:OD1	2:B:981:PRO:HD2	2.21	0.41
2:B:1074:PHE:HB2	2:B:1085:PHE:HE1	1.86	0.41
2:B:1087:PHE:CD2	2:B:1093:CYS:HB3	2.56	0.41
1:D:140:ARG:H	1:D:140:ARG:HG3	1.76	0.41
1:G:399:ILE:HD11	2:H:298:PHE:HE2	1.85	0.41
2:H:271:THR:HB	2:H:1094:ILE:O	2.21	0.41
2:H:1017:MET:SD	2:H:1019:LYS:HD3	2.61	0.41
3:I:63:THR:HG23	3:I:66:ALA:H	1.85	0.41
3:I:193:ASP:HB3	3:I:196:SER:OG	2.21	0.41
3:I:256:SER:HB2	3:I:265:VAL:HG12	2.03	0.41
1:J:402:ARG:HD2	2:K:803:PHE:O	2.21	0.41
2:K:72:THR:O	2:K:711:SER:OG	2.29	0.41
2:K:94:ASP:OD1	2:K:94:ASP:N	2.54	0.41
2:K:151:LEU:HD23	2:K:151:LEU:HA	1.77	0.41
2:K:348:ILE:HG12	2:K:507:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:428:ILE:HD13	2:K:428:ILE:HA	1.91	0.41
2:K:462:LEU:HD23	2:K:462:LEU:HA	1.92	0.41
2:K:944:ARG:HA	2:K:949:MET:CE	2.51	0.41
2:K:984:ARG:HH11	2:K:1061:ARG:HB3	1.86	0.41
3:L:237:ASN:CG	3:L:247:GLN:HE21	2.29	0.41
2:N:91:GLN:HG2	2:N:112:PRO:HB2	2.02	0.41
2:N:515:ILE:HG23	2:N:521:VAL:HG11	2.03	0.41
2:N:903:PHE:CE2	2:N:904:LEU:HG	2.56	0.41
2:N:923:HIS:CG	6:N:5801:MD1:H102	2.56	0.41
3:O:237:ASN:OD1	10:O:502:HOH:O	2.22	0.41
3:O:269:ARG:NH1	3:O:278:ASP:HB3	2.36	0.41
3:O:303:GLY:HA2	3:O:305:LYS:HE2	2.02	0.41
3:O:321:TRP:HA	3:O:321:TRP:CE3	2.56	0.41
1:P:36:ILE:O	2:Q:919:ARG:NH2	2.54	0.41
1:P:393:THR:OG1	2:Q:109:ASN:OD1	2.37	0.41
2:Q:234:ILE:N	2:Q:707:GLU:OE2	2.52	0.41
2:Q:363:THR:HG23	2:Q:548:LEU:HD11	2.03	0.41
2:Q:616:TYR:CG	2:Q:643:PRO:HG3	2.55	0.41
2:Q:625:ILE:HD11	2:Q:633:ARG:CG	2.50	0.41
2:Q:625:ILE:HB	2:Q:635:VAL:HG12	2.02	0.41
2:Q:1040:ARG:NE	2:Q:1048:GLN:OE1	2.46	0.41
1:S:2:THR:HG21	1:S:18:PHE:CD1	2.56	0.41
2:T:225:ARG:HB2	2:T:267:TRP:HB2	2.02	0.41
2:T:307:LYS:HE2	2:T:309:LEU:HD13	2.03	0.41
2:T:717:ILE:O	2:T:798:VAL:HA	2.20	0.41
3:U:53:TYR:CZ	3:U:319:ILE:HG23	2.56	0.41
1:V:174:ILE:C	1:V:222:LYS:HD2	2.46	0.41
1:V:211:TYR:CD1	3:X:302:ASN:HB3	2.56	0.41
2:W:77:ILE:CG2	2:W:89:VAL:HG21	2.51	0.41
2:W:155:ASN:O	2:W:159:TYR:HD1	2.04	0.41
2:W:229:GLY:HA3	2:W:237:TYR:CG	2.55	0.41
2:W:364:LYS:HA	2:W:489:LEU:HD13	2.03	0.41
2:W:389:THR:HG23	2:W:867:TYR:CE1	2.54	0.41
2:W:958:HIS:HB2	2:W:1017:MET:HB3	2.03	0.41
3:X:131:ARG:HE	3:X:170:ASP:CG	2.29	0.41
3:X:241:PHE:CE2	8:X:401:HEM:HMB3	2.56	0.41
1:A:181:PRO:HG2	1:A:184:LEU:CB	2.51	0.41
2:B:285:GLY:HA3	2:B:822:TYR:O	2.20	0.41
2:B:356:THR:HG23	2:B:541:SER:HB2	2.03	0.41
2:B:431:PHE:CE2	2:B:825:THR:HA	2.56	0.41
1:D:402:ARG:HB2	2:E:804:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:ASP:CG	2:E:168:GLU:H	2.29	0.41
2:E:566:TYR:O	2:E:568:ALA:N	2.50	0.41
3:F:51:VAL:CG1	3:F:102:ALA:HB3	2.51	0.41
2:H:554:TYR:CZ	2:H:815:VAL:HG11	2.56	0.41
2:H:581:PHE:HB3	2:H:1079:ILE:HG23	2.03	0.41
3:I:234:GLU:OE2	3:I:246:SER:OG	2.32	0.41
1:J:33:ASN:O	2:K:343:LYS:NZ	2.50	0.41
1:J:181:PRO:HG2	1:J:184:LEU:CB	2.51	0.41
2:K:284:HIS:CE1	2:K:286:LEU:HB3	2.56	0.41
2:K:917:LYS:NZ	6:K:5801:MD1:N15	2.56	0.41
3:O:140:LEU:CG	3:O:161:PRO:HG2	2.51	0.41
1:P:311:ALA:HB3	1:P:316:LEU:HD11	2.02	0.41
2:Q:139:GLY:O	2:Q:159:TYR:HB3	2.22	0.41
2:Q:310:ILE:HG13	2:Q:340:SER:HA	2.02	0.41
2:Q:497:VAL:HA	2:Q:500:MET:CG	2.48	0.41
2:Q:1137:LYS:HE2	2:Q:1143:LEU:HD13	2.02	0.41
1:S:64:GLU:OE1	1:S:70:GLY:HA2	2.21	0.41
1:S:397:GLU:OE1	2:T:806:TYR:OH	2.26	0.41
1:V:102:TYR:CD1	1:V:102:TYR:C	2.99	0.41
1:V:309:ARG:NH2	2:W:324:MET:HB2	2.35	0.41
2:W:192:TYR:OH	2:W:675:GLU:OE2	2.20	0.41
2:W:658:ASN:HD21	2:W:1024:ILE:HG23	1.84	0.41
2:W:952:VAL:CG1	2:W:952:VAL:O	2.69	0.41
2:B:380:PHE:CZ	2:B:815:VAL:HA	2.56	0.40
2:B:397:PRO:HB2	2:B:404:TYR:CE2	2.56	0.40
2:B:849:GLU:O	2:B:859:ASN:HA	2.21	0.40
2:B:977:VAL:HG12	2:B:1103:VAL:CG1	2.42	0.40
1:D:334:PRO:HG2	2:E:325:GLU:O	2.22	0.40
2:E:657:ILE:HD12	2:E:657:ILE:N	2.35	0.40
3:F:207:GLY:HA2	2:Q:208:LYS:HD2	2.03	0.40
1:G:291:LEU:HB2	1:G:320:PHE:HB3	2.03	0.40
2:H:261:ALA:O	2:H:608:ARG:HD3	2.20	0.40
2:H:424:GLN:HG2	2:H:1085:PHE:HE2	1.85	0.40
2:H:945:MET:HE2	3:I:188:TYR:CE1	2.56	0.40
2:H:974:TYR:CE1	2:H:1052:ARG:HD2	2.55	0.40
3:I:54:MET:HB2	3:I:54:MET:HE3	1.88	0.40
3:I:160:LYS:HB3	3:I:160:LYS:HE3	1.74	0.40
3:I:281:PHE:HB3	3:I:316:LEU:HD11	2.03	0.40
3:I:285:GLU:OE1	3:X:285:GLU:CD	2.64	0.40
1:J:410:ILE:HB	2:K:572:GLN:NE2	2.36	0.40
2:K:227:GLY:O	2:K:228:MET:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:868:ILE:HG22	2:K:870:PRO:HD3	2.04	0.40
2:K:1121:PRO:O	2:K:1124:THR:OG1	2.29	0.40
1:M:189:ARG:HD2	1:M:209:ARG:HG3	2.03	0.40
2:N:390:ASP:OD1	2:N:391:THR:N	2.53	0.40
3:O:39:GLU:O	3:O:43:THR:N	2.52	0.40
2:Q:275:ASP:HB3	2:Q:563:ALA:CB	2.45	0.40
2:Q:417:ILE:O	2:Q:575:LYS:NZ	2.54	0.40
2:T:415:TYR:HE1	2:T:422:ASP:OD1	2.04	0.40
2:T:1137:LYS:HG2	2:T:1142:GLU:HB2	2.03	0.40
1:V:46:LYS:O	1:V:51:PHE:HB3	2.22	0.40
2:W:1059:ILE:H	2:W:1059:ILE:HG13	1.81	0.40
2:B:383:PHE:N	2:B:384:PRO:HD2	2.37	0.40
2:B:481:LEU:O	2:B:485:TYR:N	2.45	0.40
2:B:806:TYR:HB3	2:B:807:PRO:HD3	2.04	0.40
2:B:909:TYR:CD2	2:B:909:TYR:N	2.90	0.40
1:D:41:CYS:SG	1:D:61:ASN:ND2	2.88	0.40
1:D:136:ASP:CG	2:E:945:MET:HE1	2.46	0.40
2:E:531:HIS:HE1	6:E:5801:MD1:N15	2.19	0.40
2:E:586:ALA:O	2:E:606:LYS:C	2.64	0.40
2:E:998:VAL:O	2:E:1054:GLY:N	2.54	0.40
6:E:5801:MD1:O11	6:E:5801:MD1:C7	2.70	0.40
1:G:62:ASN:ND2	1:G:71:PHE:HB3	2.29	0.40
3:I:151:PHE:HA	3:I:160:LYS:HE2	2.04	0.40
2:K:640:THR:HG22	2:K:1087:PHE:HB3	2.02	0.40
2:N:248:ILE:HB	2:N:754:PHE:CZ	2.56	0.40
2:N:500:MET:HG2	2:N:894:TRP:CE2	2.56	0.40
1:P:318:GLN:OE1	2:Q:1141:GLY:HA2	2.21	0.40
1:P:362:LYS:HE3	1:P:374:THR:CG2	2.51	0.40
2:Q:719:ILE:HG22	2:Q:789:LEU:HD21	2.04	0.40
1:S:181:PRO:HG2	1:S:184:LEU:HB3	2.03	0.40
1:S:259:MET:SD	1:S:267:ARG:HD3	2.61	0.40
1:S:368:ILE:HG12	1:S:369:HIS:CE1	2.56	0.40
2:T:301:LEU:HD23	2:T:521:VAL:HG22	2.03	0.40
1:V:34:ARG:NH1	1:V:342:MET:O	2.45	0.40
1:V:77:VAL:HG22	2:W:1138:PHE:CE1	2.55	0.40
1:V:211:TYR:HD1	1:V:211:TYR:HA	1.80	0.40
2:W:641:HIS:HE1	2:W:1092:HIS:O	2.03	0.40
2:W:976:TYR:CE1	2:W:1000:ARG:CZ	3.04	0.40
2:B:276:GLN:HE22	2:B:1092:HIS:N	2.05	0.40
2:B:977:VAL:HG21	2:B:1001:LEU:HD23	2.03	0.40
2:E:922:VAL:O	2:E:922:VAL:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:ILE:HD12	2:H:807:PRO:HD3	2.03	0.40
2:H:201:LEU:HD13	2:H:645:PRO:HG2	2.03	0.40
2:H:577:SER:O	2:H:776:GLY:HA2	2.22	0.40
2:K:225:ARG:NH1	2:K:654:VAL:HG11	2.37	0.40
1:M:337:GLU:O	1:M:341:VAL:HG23	2.21	0.40
3:O:59:PRO:HD3	3:O:66:ALA:HB1	2.03	0.40
2:Q:527:GLU:OE1	6:Q:5802:MD1:H101	2.20	0.40
1:V:26:PHE:HA	1:V:271:PHE:CD2	2.56	0.40
1:V:33:ASN:ND2	1:V:331:PHE:CD2	2.89	0.40
1:V:61:ASN:HB2	4:V:501:SF4:S4	2.62	0.40
1:V:187:CYS:HB2	1:V:192:ILE:HG13	2.03	0.40
1:V:211:TYR:CZ	3:X:302:ASN:HB3	2.56	0.40
2:W:1023:TRP:CE3	2:W:1047:TYR:CD1	3.09	0.40
3:X:109:ILE:HD12	3:X:316:LEU:HD21	2.03	0.40
1:A:6:ASN:OD1	1:A:6:ASN:C	2.65	0.40
2:B:332:VAL:HG23	2:B:344:ALA:HB2	2.03	0.40
2:B:624:LEU:HB2	2:B:1064:SER:OG	2.21	0.40
2:B:842:GLU:OE1	2:B:848:ARG:NH2	2.55	0.40
2:B:925:GLN:CD	6:B:5801:MD1:H2'	2.47	0.40
2:B:1061:ARG:CG	2:B:1062:ASP:N	2.85	0.40
3:C:131:ARG:HE	3:C:170:ASP:CG	2.29	0.40
3:C:305:LYS:HD3	3:C:307:ILE:CG2	2.52	0.40
1:D:136:ASP:OD2	2:E:945:MET:HE1	2.21	0.40
1:D:220:TYR:OH	1:D:294:TYR:O	2.39	0.40
2:E:413:PRO:HB2	2:E:820:PRO:CD	2.51	0.40
3:F:171:TRP:HZ3	3:F:233:VAL:O	2.04	0.40
3:F:256:SER:CB	3:F:265:VAL:HG12	2.52	0.40
1:G:184:LEU:HD21	2:H:40:PRO:HB2	2.03	0.40
2:H:271:THR:HA	2:H:1095:ASN:OD1	2.22	0.40
3:I:305:LYS:NZ	8:I:401:HEM:NC	2.69	0.40
1:J:372:LYS:HZ3	1:J:372:LYS:HG3	1.50	0.40
2:K:641:HIS:CG	2:K:1087:PHE:HB2	2.56	0.40
2:N:409:ILE:HG13	2:N:415:TYR:HE2	1.86	0.40
2:N:834:GLU:HB2	2:N:837:ILE:HD12	2.03	0.40
2:N:973:ASP:OD1	2:N:1111:GLY:N	2.47	0.40
2:Q:307:LYS:HZ3	2:Q:313:LYS:NZ	2.19	0.40
2:Q:497:VAL:CA	2:Q:500:MET:HG3	2.49	0.40
2:Q:717:ILE:O	2:Q:798:VAL:HA	2.21	0.40
3:R:145:ILE:HD11	3:R:151:PHE:HD2	1.87	0.40
1:S:140:ARG:HD3	2:T:945:MET:CE	2.51	0.40
2:T:278:PRO:O	2:T:281:PRO:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:379:LYS:HD2	2:T:450:GLY:C	2.46	0.40
2:T:436:ALA:HB3	2:T:459:ASP:OD2	2.22	0.40
2:T:462:LEU:HA	2:T:462:LEU:HD12	1.75	0.40
1:V:36:ILE:HG13	2:W:310:ILE:HD12	2.02	0.40
1:V:237:ALA:HA	4:V:501:SF4:S1	2.61	0.40
2:W:181:ALA:HB3	2:W:741:MET:HE1	2.03	0.40
2:W:413:PRO:HD2	2:W:447:ASP:CG	2.46	0.40
2:W:760:PHE:HB3	2:W:765:ARG:O	2.22	0.40
3:X:237:ASN:OD1	3:X:247:GLN:NE2	2.51	0.40
1:A:404:ASP:HA	2:B:804:ARG:HH21	1.82	0.40
2:B:506:ASP:OD2	2:B:506:ASP:N	2.53	0.40
2:B:801:LEU:HD11	2:B:803:PHE:CE2	2.56	0.40
1:D:34:ARG:NH2	2:E:318:HIS:ND1	2.70	0.40
1:D:55:GLN:NE2	1:D:233:GLU:OE1	2.54	0.40
3:F:153:PRO:HB3	3:F:311:TRP:CD1	2.56	0.40
2:H:160:MET:O	2:H:164:ARG:HG2	2.21	0.40
2:H:848:ARG:NH1	2:H:859:ASN:OD1	2.55	0.40
1:J:8:HIS:CD2	1:J:300:GLU:HA	2.56	0.40
2:K:417:ILE:HD13	2:K:417:ILE:HA	1.91	0.40
3:L:280:GLN:HB2	3:R:282:VAL:HG22	2.04	0.40
2:N:751:ASP:OD1	2:N:753:ARG:NH2	2.55	0.40
2:N:892:LYS:HG2	2:N:896:GLU:HB3	2.04	0.40
3:O:67:LEU:HD13	3:O:266:VAL:HG21	2.04	0.40
2:Q:250:ASP:CG	2:Q:254:ARG:HH21	2.30	0.40
2:Q:456:LYS:HB2	2:Q:458:ILE:HD12	2.04	0.40
2:Q:970:GLU:HA	2:Q:1007:TYR:OH	2.21	0.40
1:S:32:ILE:HG21	1:S:308:PRO:HG3	2.03	0.40
2:T:920:HIS:CD2	2:T:936:ASN:HA	2.56	0.40
1:V:259:MET:CE	1:V:269:GLN:CG	2.83	0.40
3:X:108:THR:OG1	3:X:110:TYR:CE1	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	D	406/410 (99%)	388 (96%)	18 (4%)	0	100	100
1	G	407/410 (99%)	399 (98%)	8 (2%)	0	100	100
1	J	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	M	407/410 (99%)	401 (98%)	6 (2%)	0	100	100
1	P	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	S	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	V	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
2	B	1119/1148 (98%)	1078 (96%)	41 (4%)	0	100	100
2	E	1104/1148 (96%)	1034 (94%)	68 (6%)	2 (0%)	43	73
2	H	1117/1148 (97%)	1073 (96%)	43 (4%)	1 (0%)	48	78
2	K	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	N	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	Q	1113/1148 (97%)	1071 (96%)	39 (4%)	3 (0%)	36	67
2	T	1117/1148 (97%)	1079 (97%)	38 (3%)	0	100	100
2	W	1117/1148 (97%)	1072 (96%)	44 (4%)	1 (0%)	48	78
3	C	291/322 (90%)	282 (97%)	9 (3%)	0	100	100
3	F	290/322 (90%)	278 (96%)	12 (4%)	0	100	100
3	I	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
3	L	291/322 (90%)	288 (99%)	3 (1%)	0	100	100
3	O	289/322 (90%)	280 (97%)	9 (3%)	0	100	100
3	R	289/322 (90%)	279 (96%)	10 (4%)	0	100	100
3	U	290/322 (90%)	284 (98%)	6 (2%)	0	100	100
3	X	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
All	All	14498/15040 (96%)	13995 (96%)	496 (3%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	520	PRO
2	H	1021	SER
2	Q	69	PRO

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Mol	Chain	Res	Type
2	Q	113	ARG
2	Q	1021	SER
2	W	72	THR
2	E	72	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/365 (98%)	355 (99%)	4 (1%)	65	82
1	D	229/365 (63%)	228 (100%)	1 (0%)	84	90
1	G	356/365 (98%)	355 (100%)	1 (0%)	86	91
1	J	362/365 (99%)	360 (99%)	2 (1%)	78	88
1	M	348/365 (95%)	342 (98%)	6 (2%)	53	77
1	P	350/365 (96%)	340 (97%)	10 (3%)	37	68
1	S	355/365 (97%)	355 (100%)	0	100	100
1	V	324/365 (89%)	300 (93%)	24 (7%)	13	40
2	B	943/991 (95%)	914 (97%)	29 (3%)	35	66
2	E	373/991 (38%)	357 (96%)	16 (4%)	26	58
2	H	952/991 (96%)	943 (99%)	9 (1%)	70	85
2	K	956/991 (96%)	941 (98%)	15 (2%)	55	78
2	N	959/991 (97%)	945 (98%)	14 (2%)	57	79
2	Q	913/991 (92%)	879 (96%)	34 (4%)	30	62
2	T	953/991 (96%)	934 (98%)	19 (2%)	48	75
2	W	918/991 (93%)	884 (96%)	34 (4%)	30	62
3	C	238/265 (90%)	233 (98%)	5 (2%)	47	74
3	F	175/265 (66%)	168 (96%)	7 (4%)	28	60
3	I	220/265 (83%)	209 (95%)	11 (5%)	22	54
3	L	236/265 (89%)	228 (97%)	8 (3%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	196/265 (74%)	180 (92%)	16 (8%)	10	35
3	R	235/265 (89%)	228 (97%)	7 (3%)	36	67
3	U	235/265 (89%)	227 (97%)	8 (3%)	32	64
3	X	223/265 (84%)	205 (92%)	18 (8%)	11	36
All	All	11408/12968 (88%)	11110 (97%)	298 (3%)	40	70

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	101	GLN
1	A	123	LYS
1	A	125	ILE
2	B	58	GLN
2	B	89	VAL
2	B	142[A]	ARG
2	B	142[B]	ARG
2	B	228	MET
2	B	262	LEU
2	B	276	GLN
2	B	307	LYS
2	B	309	LEU
2	B	310	ILE
2	B	370	LYS
2	B	387	ILE
2	B	425	ARG
2	B	445	THR
2	B	446	ARG
2	B	486	LYS
2	B	628	THR
2	B	653	ASN
2	B	654	VAL
2	B	656	LEU
2	B	804	ARG
2	B	924	SER
2	B	977	VAL
2	B	983	ASP
2	B	984	ARG
2	B	1048	GLN
2	B	1087	PHE
2	B	1088	GLU

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Mol	Chain	Res	Type
2	B	1105	ILE
3	C	123	GLN
3	C	197	THR
3	C	216	SER
3	C	301	ARG
3	C	305	LYS
1	D	235	CYS
2	E	73	HIS
2	E	110	TRP
2	E	353	ASN
2	E	420	LEU
2	E	651	PHE
2	E	666	MET
2	E	670	VAL
2	E	700	TRP
2	E	872	ASP
2	E	957	ILE
2	E	1003	LEU
2	E	1014	ASN
2	E	1020	HIS
2	E	1057	GLN
2	E	1094	ILE
2	E	1096	THR
3	F	84	GLN
3	F	172	GLU
3	F	229	ARG
3	F	233	VAL
3	F	251	ASP
3	F	291	MET
3	F	305	LYS
1	G	98	GLU
2	H	152	THR
2	H	154	GLU
2	H	228	MET
2	H	723	THR
2	H	751	ASP
2	H	823	THR
2	H	895	GLU
2	H	922	VAL
2	H	955	HIS
3	I	32	GLU
3	I	48	VAL

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Mol	Chain	Res	Type
3	I	51	VAL
3	I	155	MET
3	I	237	ASN
3	I	241	PHE
3	I	243	THR
3	I	291	MET
3	I	299	GLU
3	I	305	LYS
3	I	321	TRP
1	J	11	ARG
1	J	141	SER
2	K	31	LEU
2	K	32	LYS
2	K	36	VAL
2	K	241	ARG
2	K	401	ILE
2	K	405	LYS
2	K	421	LYS
2	K	425	ARG
2	K	449	VAL
2	K	647	LYS
2	K	648	VAL
2	K	649	LEU
2	K	765	ARG
2	K	917	LYS
2	K	984	ARG
3	L	216	SER
3	L	268	CYS
3	L	270	SER
3	L	271	LEU
3	L	291	MET
3	L	301	ARG
3	L	302	ASN
3	L	305	LYS
1	M	20	SER
1	M	21	ARG
1	M	125	ILE
1	M	189	ARG
1	M	209	ARG
1	M	359	GLU
2	N	461	VAL
2	N	469	LYS

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Mol	Chain	Res	Type
2	N	471	ILE
2	N	475	GLU
2	N	476	ILE
2	N	511	LEU
2	N	654	VAL
2	N	722	LYS
2	N	752	LYS
2	N	800	MET
2	N	814	GLN
2	N	897	THR
2	N	1035	THR
2	N	1122	VAL
3	O	48	VAL
3	O	142	LYS
3	O	208	VAL
3	O	209	ILE
3	O	210	GLN
3	O	215	LEU
3	O	241	PHE
3	O	246	SER
3	O	250	GLN
3	O	251	ASP
3	O	268	CYS
3	O	269	ARG
3	O	282	VAL
3	O	286	SER
3	O	301	ARG
3	O	305	LYS
1	P	11	ARG
1	P	12	ARG
1	P	151	SER
1	P	257	ARG
1	P	283	LEU
1	P	284	ILE
1	P	285	ARG
1	P	309	ARG
1	P	346	ARG
1	P	405	LYS
2	Q	69	PRO
2	Q	96	GLN
2	Q	99	SER
2	Q	196	GLU

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Mol	Chain	Res	Type
2	Q	302	LEU
2	Q	304	GLN
2	Q	331	VAL
2	Q	382	ASP
2	Q	394	ARG
2	Q	395	VAL
2	Q	425	ARG
2	Q	445	THR
2	Q	446	ARG
2	Q	449	VAL
2	Q	465	SER
2	Q	469	LYS
2	Q	479	MET
2	Q	482	LEU
2	Q	483	GLU
2	Q	484	MET
2	Q	625	ILE
2	Q	640	THR
2	Q	661	LYS
2	Q	819	LEU
2	Q	821	PHE
2	Q	827	ARG
2	Q	829	GLN
2	Q	861	ILE
2	Q	888	ARG
2	Q	897	THR
2	Q	901	LYS
2	Q	937	ASN
2	Q	959	ILE
2	Q	1021	SER
3	R	51	VAL
3	R	216	SER
3	R	229	ARG
3	R	236	LEU
3	R	314	LEU
3	R	315	SER
3	R	316	LEU
2	T	96	GLN
2	T	220	ARG
2	T	293	MET
2	T	316	GLU
2	T	445	THR

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Mol	Chain	Res	Type
2	T	476	ILE
2	T	653	ASN
2	T	661	LYS
2	T	676	GLN
2	T	713	SER
2	T	718	GLN
2	T	813	GLU
2	T	823	THR
2	T	922	VAL
2	T	924	SER
2	T	954	GLU
2	T	983	ASP
2	T	984	ARG
2	T	1061	ARG
3	U	142	LYS
3	U	143	ILE
3	U	144	THR
3	U	145	ILE
3	U	236	LEU
3	U	269	ARG
3	U	301	ARG
3	U	305	LYS
1	V	13	MET
1	V	32	ILE
1	V	61	ASN
1	V	64	GLU
1	V	66	LYS
1	V	67	PRO
1	V	76	ASP
1	V	116	ILE
1	V	126	ASN
1	V	146	GLU
1	V	150	LYS
1	V	161	LEU
1	V	189	ARG
1	V	192	ILE
1	V	207	ARG
1	V	212	ARG
1	V	241	ARG
1	V	259	MET
1	V	366	THR
1	V	371	LYS

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Mol	Chain	Res	Type
1	V	375	MET
1	V	379	THR
1	V	386	ASP
1	V	392	ARG
2	W	35	VAL
2	W	36	VAL
2	W	39	ASN
2	W	41	LEU
2	W	72	THR
2	W	89	VAL
2	W	157	THR
2	W	220	ARG
2	W	313	LYS
2	W	342	GLN
2	W	352	ASN
2	W	379	LYS
2	W	381	THR
2	W	433	VAL
2	W	438	SER
2	W	468	LEU
2	W	470	THR
2	W	479	MET
2	W	496	SER
2	W	500	MET
2	W	552	VAL
2	W	654	VAL
2	W	767	SER
2	W	892	LYS
2	W	924	SER
2	W	952	VAL
2	W	955	HIS
2	W	967	LEU
2	W	1000	ARG
2	W	1001	LEU
2	W	1049	SER
2	W	1118	VAL
2	W	1122	VAL
2	W	1124	THR
3	X	39	GLU
3	X	41	GLU
3	X	77	VAL
3	X	79	VAL

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Mol	Chain	Res	Type
3	X	80	LYS
3	X	137	MET
3	X	142	LYS
3	X	154	ARG
3	X	227	LEU
3	X	229	ARG
3	X	259	GLU
3	X	269	ARG
3	X	277	LEU
3	X	278	ASP
3	X	279	VAL
3	X	305	LYS
3	X	308	SER
3	X	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
2	B	58	GLN
2	B	276	GLN
2	B	488	HIS
2	B	551	ASN
2	B	572	GLN
2	B	655	ASN
2	B	790	ASN
2	B	958	HIS
2	B	962	GLN
2	B	1008	ASN
2	B	1130	ASN
3	C	50	ASN
3	C	61	HIS
3	C	78	GLN
3	C	304	GLN
1	D	8	HIS
1	D	31	ASN
1	D	143	ASN
1	D	302	ASN
2	E	39	ASN
2	E	58	GLN
2	E	70	ASN
2	E	671	ASN

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Mol	Chain	Res	Type
2	E	932	ASN
2	E	1014	ASN
2	E	1020	HIS
3	F	90	ASN
3	F	121	ASN
3	F	163	ASN
3	F	302	ASN
3	F	306	ASN
1	G	302	ASN
2	H	84	ASN
2	H	308	ASN
2	H	572	GLN
2	H	627	ASN
2	H	809	HIS
2	H	955	HIS
2	H	1069	GLN
2	H	1130	ASN
3	I	104	HIS
3	I	200	HIS
3	I	302	ASN
1	J	8	HIS
1	J	205	GLN
2	K	352	ASN
2	K	369	ASN
2	K	424	GLN
2	K	539	ASN
2	K	551	ASN
2	K	572	GLN
2	K	653	ASN
2	K	676	GLN
2	K	790	ASN
2	K	923	HIS
2	K	932	ASN
2	K	962	GLN
2	K	1095	ASN
3	L	90	ASN
3	L	200	HIS
3	L	205	HIS
1	M	88	ASN
1	M	176	ASN
1	M	217	GLN
1	M	296	GLN

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Mol	Chain	Res	Type
2	N	104	ASN
2	N	308	ASN
2	N	312	ASN
2	N	757	ASN
2	N	1020	HIS
2	N	1057	GLN
3	O	159	GLN
3	O	190	ASN
3	O	272	ASN
1	P	302	ASN
2	Q	199	GLN
2	Q	342	GLN
2	Q	502	ASN
2	Q	539	ASN
2	Q	618	ASN
2	Q	662	HIS
2	Q	814	GLN
2	Q	829	GLN
2	Q	937	ASN
2	Q	962	GLN
2	Q	1057	GLN
2	Q	1130	ASN
3	R	205	HIS
3	R	249	HIS
3	R	302	ASN
1	S	5	HIS
1	S	302	ASN
2	T	312	ASN
2	T	676	GLN
2	T	962	GLN
3	U	159	GLN
1	V	31	ASN
1	V	153	ASN
1	V	176	ASN
2	W	56	GLN
2	W	244	ASN
2	W	308	ASN
2	W	572	GLN
2	W	662	HIS
2	W	704	GLN
2	W	829	GLN
2	W	832	ASN

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Mol	Chain	Res	Type
2	W	1069	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	P	502	1	0,12,12	-	-	-		
5	F3S	J	504	1	0,9,9	-	-	-		
6	MD1	W	5802	7	47,51,51	5.86	29 (61%)	56,78,78	1.86	16 (28%)
6	MD1	W	5801	7	47,51,51	5.73	29 (61%)	56,78,78	1.83	13 (23%)
6	MD1	N	5802	7	47,51,51	5.84	29 (61%)	56,78,78	1.86	17 (30%)
4	SF4	H	5804	2	0,12,12	-	-	-		
8	HEM	O	401	3	50,50,50	1.65	8 (16%)	67,82,82	1.16	5 (7%)
8	HEM	C	401	3	50,50,50	1.85	8 (16%)	67,82,82	1.28	7 (10%)
4	SF4	M	501	1	0,12,12	-	-	-		
8	HEM	L	401	3	50,50,50	1.57	8 (16%)	67,82,82	1.22	5 (7%)
5	F3S	S	504	1	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	D	502	1	0,12,12	-	-	-		
6	MD1	B	5802	7	47,51,51	5.85	29 (61%)	56,78,78	1.87	17 (30%)
4	SF4	N	5804	2	0,12,12	-	-	-		
4	SF4	G	502	1	0,12,12	-	-	-		
6	MD1	N	5801	7	47,51,51	5.72	29 (61%)	56,78,78	1.83	15 (26%)
6	MD1	Q	5801	7	47,51,51	5.69	29 (61%)	56,78,78	1.90	16 (28%)
4	SF4	M	502	1	0,12,12	-	-	-		
4	SF4	A	501	1	0,12,12	-	-	-		
4	SF4	S	503	1	0,12,12	-	-	-		
6	MD1	E	5801	6,7	47,51,51	5.55	31 (65%)	56,78,78	1.80	16 (28%)
5	F3S	G	504	1	0,9,9	-	-	-		
6	MD1	K	5801	7	47,51,51	5.75	29 (61%)	56,78,78	1.82	14 (25%)
8	HEM	I	401	3	50,50,50	2.35	22 (44%)	67,82,82	1.82	20 (29%)
6	MD1	H	5802	7	47,51,51	5.84	29 (61%)	56,78,78	1.83	16 (28%)
6	MD1	E	5802	6,7	47,51,51	5.86	29 (61%)	56,78,78	1.85	14 (25%)
6	MD1	H	5801	7	47,51,51	5.77	29 (61%)	56,78,78	1.82	14 (25%)
4	SF4	A	503	1	0,12,12	-	-	-		
4	SF4	P	501	1	0,12,12	-	-	-		
4	SF4	V	501	1	0,12,12	-	-	-		
8	HEM	X	401	3	50,50,50	1.60	7 (14%)	67,82,82	1.28	6 (8%)
5	F3S	A	504	1	0,9,9	-	-	-		
6	MD1	Q	5802	7	47,51,51	5.83	29 (61%)	56,78,78	1.89	16 (28%)
4	SF4	S	502	1	0,12,12	-	-	-		
6	MD1	T	5801	7	47,51,51	5.77	29 (61%)	56,78,78	1.82	13 (23%)
4	SF4	V	502	1	0,12,12	-	-	-		
5	F3S	D	504	1	0,9,9	-	-	-		
4	SF4	J	501	1	0,12,12	-	-	-		
6	MD1	T	5802	7	47,51,51	5.86	29 (61%)	56,78,78	1.88	17 (30%)
8	HEM	F	401	-	50,50,50	1.56	5 (10%)	67,82,82	1.26	10 (14%)
4	SF4	Q	5804	2	0,12,12	-	-	-		
4	SF4	B	5804	2	0,12,12	-	-	-		
4	SF4	J	502	1	0,12,12	-	-	-		
8	HEM	U	401	3	50,50,50	1.51	8 (16%)	67,82,82	1.13	5 (7%)
4	SF4	G	503	1	0,12,12	-	-	-		
5	F3S	P	504	1	0,9,9	-	-	-		
4	SF4	P	503	1	0,12,12	-	-	-		
4	SF4	T	5804	2	0,12,12	-	-	-		
4	SF4	D	501	1	0,12,12	-	-	-		
4	SF4	V	503	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MD1	K	5802	7	47,51,51	5.84	29 (61%)	56,78,78	1.88	17 (30%)
4	SF4	M	503	1	0,12,12	-	-	-		
4	SF4	G	501	1	0,12,12	-	-	-		
5	F3S	V	504	1	0,9,9	-	-	-		
4	SF4	K	5804	2	0,12,12	-	-	-		
4	SF4	S	501	1	0,12,12	-	-	-		
6	MD1	B	5801	7	47,51,51	5.75	30 (63%)	56,78,78	1.82	14 (25%)
4	SF4	W	5804	2	0,12,12	-	-	-		
4	SF4	A	502	1	0,12,12	-	-	-		
5	F3S	M	504	1	0,9,9	-	-	-		
4	SF4	J	503	1	0,12,12	-	-	-		
4	SF4	D	503	1	0,12,12	-	-	-		
4	SF4	E	5804	2	0,12,12	-	-	-		
8	HEM	R	401	3	50,50,50	1.63	9 (18%)	67,82,82	1.17	4 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	P	502	1	-	-	0/6/5/5
5	F3S	J	504	1	-	-	0/3/3/3
4	SF4	D	503	1	-	-	0/6/5/5
6	MD1	W	5801	7	-	10/22/59/59	0/5/5/5
6	MD1	N	5802	7	-	5/22/59/59	0/5/5/5
4	SF4	H	5804	2	-	-	0/6/5/5
8	HEM	O	401	3	-	4/14/54/54	-
8	HEM	C	401	3	-	5/14/54/54	-
8	HEM	L	401	3	-	3/14/54/54	-
4	SF4	M	501	1	-	-	0/6/5/5
5	F3S	S	504	1	-	-	0/3/3/3
6	MD1	B	5802	7	-	5/22/59/59	0/5/5/5
6	MD1	N	5801	7	-	12/22/59/59	0/5/5/5
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	G	502	1	-	-	0/6/5/5
4	SF4	N	5804	2	-	-	0/6/5/5
6	MD1	Q	5801	7	-	10/22/59/59	0/5/5/5
4	SF4	M	502	1	-	-	0/6/5/5
4	SF4	A	501	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	S	503	1	-	-	0/6/5/5
6	MD1	E	5801	6,7	1/1/10/12	8/22/59/59	0/5/5/5
5	F3S	G	504	1	-	-	0/3/3/3
6	MD1	K	5801	7	-	10/22/59/59	0/5/5/5
8	HEM	I	401	3	-	7/14/54/54	-
6	MD1	E	5802	6,7	-	5/22/59/59	0/5/5/5
6	MD1	H	5801	7	-	11/22/59/59	0/5/5/5
4	SF4	A	503	1	-	-	0/6/5/5
4	SF4	P	501	1	-	-	0/6/5/5
8	HEM	X	401	3	-	4/14/54/54	-
4	SF4	V	501	1	-	-	0/6/5/5
5	F3S	A	504	1	-	-	0/3/3/3
6	MD1	Q	5802	7	-	9/22/59/59	0/5/5/5
4	SF4	S	502	1	-	-	0/6/5/5
6	MD1	T	5801	7	-	10/22/59/59	0/5/5/5
4	SF4	V	502	1	-	-	0/6/5/5
5	F3S	D	504	1	-	-	0/3/3/3
4	SF4	J	501	1	-	-	0/6/5/5
6	MD1	T	5802	7	-	4/22/59/59	0/5/5/5
8	HEM	F	401	-	-	6/14/54/54	-
4	SF4	Q	5804	2	-	-	0/6/5/5
4	SF4	B	5804	2	-	-	0/6/5/5
4	SF4	J	502	1	-	-	0/6/5/5
8	HEM	U	401	3	-	5/14/54/54	-
4	SF4	G	503	1	-	-	0/6/5/5
5	F3S	P	504	1	-	-	0/3/3/3
4	SF4	P	503	1	-	-	0/6/5/5
4	SF4	T	5804	2	-	-	0/6/5/5
4	SF4	D	501	1	-	-	0/6/5/5
4	SF4	V	503	1	-	-	0/6/5/5
6	MD1	K	5802	7	-	5/22/59/59	0/5/5/5
4	SF4	M	503	1	-	-	0/6/5/5
4	SF4	A	502	1	-	-	0/6/5/5
4	SF4	G	501	1	-	-	0/6/5/5
5	F3S	V	504	1	-	-	0/3/3/3
4	SF4	K	5804	2	-	-	0/6/5/5
4	SF4	S	501	1	-	-	0/6/5/5
6	MD1	B	5801	7	-	11/22/59/59	0/5/5/5
4	SF4	W	5804	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MD1	H	5802	7	-	5/22/59/59	0/5/5/5
5	F3S	M	504	1	-	-	0/3/3/3
4	SF4	J	503	1	-	-	0/6/5/5
6	MD1	W	5802	7	-	7/22/59/59	0/5/5/5
4	SF4	E	5804	2	-	-	0/6/5/5
8	HEM	R	401	3	-	5/14/54/54	-

All (542) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5802	MD1	C7-N8	26.31	1.61	1.28
6	T	5802	MD1	C7-N8	26.03	1.61	1.28
6	K	5802	MD1	C7-N8	26.00	1.61	1.28
6	W	5802	MD1	C7-N8	25.87	1.61	1.28
6	N	5802	MD1	C7-N8	25.85	1.61	1.28
6	B	5802	MD1	C7-N8	25.77	1.61	1.28
6	Q	5802	MD1	C7-N8	25.74	1.60	1.28
6	H	5802	MD1	C7-N8	25.71	1.60	1.28
6	H	5801	MD1	C7-N8	25.46	1.60	1.28
6	T	5801	MD1	C7-N8	25.45	1.60	1.28
6	K	5801	MD1	C7-N8	25.34	1.60	1.28
6	W	5801	MD1	C7-N8	25.31	1.60	1.28
6	B	5801	MD1	C7-N8	25.27	1.60	1.28
6	N	5801	MD1	C7-N8	25.08	1.60	1.28
6	Q	5801	MD1	C7-N8	23.89	1.58	1.28
6	E	5801	MD1	C7-N8	23.11	1.57	1.28
6	E	5801	MD1	C3'-C4'	-9.89	1.27	1.53
6	W	5802	MD1	C3'-C4'	-9.77	1.28	1.53
6	H	5801	MD1	C3'-C4'	-9.76	1.28	1.53
6	Q	5801	MD1	C3'-C4'	-9.76	1.28	1.53
6	B	5801	MD1	C3'-C4'	-9.73	1.28	1.53
6	E	5802	MD1	C3'-C4'	-9.73	1.28	1.53
6	T	5801	MD1	C3'-C4'	-9.69	1.28	1.53
6	N	5802	MD1	C3'-C4'	-9.69	1.28	1.53
6	B	5802	MD1	C3'-C4'	-9.66	1.28	1.53
6	H	5802	MD1	C3'-C4'	-9.63	1.28	1.53
6	K	5801	MD1	C3'-C4'	-9.63	1.28	1.53
6	T	5802	MD1	C3'-C4'	-9.62	1.28	1.53
6	N	5801	MD1	C3'-C4'	-9.62	1.28	1.53
6	W	5801	MD1	C3'-C4'	-9.61	1.28	1.53
6	Q	5802	MD1	C3'-C4'	-9.61	1.28	1.53
6	K	5802	MD1	C3'-C4'	-9.60	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5801	MD1	C16-C20	8.75	1.62	1.39
6	K	5801	MD1	C16-C20	8.60	1.61	1.39
6	N	5801	MD1	C16-C20	8.58	1.61	1.39
6	E	5801	MD1	O11-C11	8.56	1.61	1.42
6	B	5801	MD1	C16-C20	8.55	1.61	1.39
6	T	5801	MD1	C16-C20	8.49	1.61	1.39
6	W	5801	MD1	C16-C20	8.46	1.61	1.39
6	H	5801	MD1	C16-C20	8.44	1.61	1.39
6	Q	5801	MD1	O11-C11	8.39	1.61	1.42
6	Q	5801	MD1	C16-C20	8.39	1.61	1.39
6	B	5801	MD1	O11-C11	8.33	1.61	1.42
6	W	5802	MD1	C2'-C1'	-8.30	1.27	1.53
6	W	5802	MD1	O11-C11	8.30	1.61	1.42
6	Q	5802	MD1	C2'-C1'	-8.30	1.27	1.53
6	E	5802	MD1	O11-C11	8.29	1.61	1.42
6	W	5801	MD1	O11-C11	8.29	1.61	1.42
6	T	5801	MD1	O11-C11	8.29	1.61	1.42
6	K	5802	MD1	O11-C11	8.28	1.61	1.42
6	N	5802	MD1	C2'-C1'	-8.26	1.27	1.53
6	H	5801	MD1	O11-C11	8.26	1.61	1.42
6	K	5802	MD1	C2'-C1'	-8.26	1.27	1.53
6	K	5801	MD1	O11-C11	8.25	1.61	1.42
6	N	5801	MD1	O11-C11	8.25	1.61	1.42
6	T	5802	MD1	C2'-C1'	-8.24	1.27	1.53
6	B	5802	MD1	C2'-C1'	-8.24	1.27	1.53
6	H	5802	MD1	O11-C11	8.24	1.60	1.42
6	H	5802	MD1	C2'-C1'	-8.22	1.27	1.53
6	N	5802	MD1	O11-C11	8.22	1.60	1.42
6	B	5802	MD1	O11-C11	8.21	1.60	1.42
6	T	5802	MD1	O11-C11	8.20	1.60	1.42
6	Q	5802	MD1	O11-C11	8.20	1.60	1.42
6	E	5802	MD1	C2'-C1'	-8.19	1.27	1.53
6	B	5801	MD1	C2'-C1'	-8.18	1.27	1.53
6	E	5801	MD1	C2'-C1'	-8.18	1.27	1.53
6	T	5802	MD1	C16-C20	8.17	1.60	1.39
6	W	5802	MD1	C16-C20	8.17	1.60	1.39
6	W	5801	MD1	C2'-C1'	-8.16	1.27	1.53
6	H	5802	MD1	C16-C20	8.16	1.60	1.39
6	Q	5802	MD1	C16-C20	8.16	1.60	1.39
6	K	5801	MD1	C2'-C1'	-8.14	1.27	1.53
6	K	5802	MD1	C16-C20	8.14	1.60	1.39
6	N	5801	MD1	C2'-C1'	-8.13	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	5801	MD1	C2'-C1'	-8.13	1.27	1.53
6	E	5802	MD1	C16-C20	8.12	1.60	1.39
6	N	5802	MD1	C16-C20	8.12	1.60	1.39
6	H	5801	MD1	C2'-C1'	-8.11	1.28	1.53
6	Q	5801	MD1	C2'-C1'	-8.11	1.28	1.53
6	B	5802	MD1	C16-C20	8.08	1.60	1.39
6	Q	5801	MD1	C14-N15	7.86	1.61	1.46
6	E	5802	MD1	C17-N18	7.80	1.52	1.33
6	K	5801	MD1	C17-N18	7.76	1.52	1.33
6	T	5802	MD1	C17-N18	7.74	1.51	1.33
6	W	5802	MD1	C17-N18	7.67	1.51	1.33
6	N	5802	MD1	C17-N18	7.61	1.51	1.33
6	W	5801	MD1	C17-N18	7.60	1.51	1.33
6	N	5801	MD1	C17-N18	7.59	1.51	1.33
6	B	5802	MD1	C17-N18	7.58	1.51	1.33
6	T	5801	MD1	C17-N18	7.58	1.51	1.33
6	H	5802	MD1	C17-N18	7.54	1.51	1.33
6	H	5801	MD1	C17-N18	7.52	1.51	1.33
6	B	5802	MD1	C14-N15	7.50	1.60	1.46
6	B	5801	MD1	C17-N18	7.48	1.51	1.33
6	Q	5802	MD1	C17-N18	7.46	1.51	1.33
6	E	5802	MD1	C14-N15	7.44	1.60	1.46
6	Q	5801	MD1	C12-C13	7.43	1.57	1.34
8	C	401	HEM	FE-NC	7.42	2.19	1.95
6	K	5802	MD1	C17-N18	7.40	1.51	1.33
6	T	5802	MD1	C14-N15	7.39	1.60	1.46
6	H	5801	MD1	C14-N15	7.39	1.60	1.46
6	W	5802	MD1	C14-N15	7.39	1.60	1.46
6	H	5802	MD1	C14-C13	-7.39	1.43	1.51
6	B	5801	MD1	C14-N15	7.38	1.60	1.46
6	H	5802	MD1	C14-N15	7.37	1.60	1.46
6	E	5801	MD1	C17-N18	7.27	1.50	1.33
6	K	5802	MD1	C17-N17	7.26	1.55	1.37
6	N	5802	MD1	C14-N15	7.25	1.60	1.46
6	W	5801	MD1	C14-N15	7.24	1.60	1.46
6	Q	5802	MD1	C14-C13	-7.22	1.43	1.51
6	Q	5802	MD1	C14-N15	7.22	1.60	1.46
6	B	5802	MD1	C17-N17	7.19	1.55	1.37
6	W	5802	MD1	C17-N17	7.19	1.55	1.37
6	Q	5802	MD1	C17-N17	7.19	1.55	1.37
6	H	5802	MD1	C17-N17	7.18	1.55	1.37
6	Q	5801	MD1	C17-N17	7.17	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	401	HEM	FE-ND	7.17	2.17	1.94
6	N	5802	MD1	C17-N17	7.17	1.55	1.37
6	N	5802	MD1	C14-C13	-7.17	1.44	1.51
6	E	5801	MD1	C17-N17	7.15	1.55	1.37
6	N	5801	MD1	C14-N15	7.15	1.60	1.46
6	T	5802	MD1	C17-N17	7.14	1.55	1.37
6	E	5802	MD1	C17-N17	7.12	1.54	1.37
6	E	5801	MD1	C12-C13	7.12	1.56	1.34
6	Q	5801	MD1	C17-N18	7.12	1.50	1.33
6	E	5801	MD1	C14-N15	7.09	1.60	1.46
6	N	5801	MD1	C12-C13	7.09	1.56	1.34
6	T	5801	MD1	C17-N17	7.06	1.54	1.37
6	K	5801	MD1	C14-N15	7.06	1.60	1.46
6	W	5801	MD1	C12-C13	7.06	1.56	1.34
6	H	5801	MD1	C17-N17	7.05	1.54	1.37
6	B	5801	MD1	C17-N17	7.05	1.54	1.37
6	K	5802	MD1	C14-C13	-7.04	1.44	1.51
6	T	5801	MD1	C14-N15	7.03	1.59	1.46
6	N	5801	MD1	C17-N17	7.01	1.54	1.37
6	K	5802	MD1	C14-N15	6.99	1.59	1.46
6	B	5801	MD1	C12-C13	6.99	1.56	1.34
6	T	5801	MD1	C12-C13	6.98	1.56	1.34
6	B	5802	MD1	C14-C13	-6.94	1.44	1.51
6	K	5801	MD1	C12-C13	6.93	1.56	1.34
6	E	5801	MD1	C14-C13	-6.91	1.44	1.51
6	Q	5802	MD1	C12-C13	6.87	1.55	1.34
6	W	5801	MD1	C17-N17	6.85	1.54	1.37
6	H	5801	MD1	C12-C13	6.85	1.55	1.34
6	N	5802	MD1	C12-C13	6.83	1.55	1.34
6	B	5802	MD1	C12-C13	6.82	1.55	1.34
6	K	5802	MD1	C12-C13	6.82	1.55	1.34
6	W	5802	MD1	C14-C13	-6.81	1.44	1.51
6	E	5802	MD1	C4-N3	6.81	1.49	1.34
6	K	5801	MD1	C17-N17	6.80	1.54	1.37
6	W	5802	MD1	C4-N3	6.77	1.49	1.34
6	T	5802	MD1	C14-C13	-6.77	1.44	1.51
6	T	5802	MD1	C12-C13	6.77	1.55	1.34
8	O	401	HEM	FE-ND	6.75	2.15	1.94
6	W	5801	MD1	C4-N3	6.75	1.49	1.34
6	H	5802	MD1	C12-C13	6.75	1.55	1.34
6	T	5802	MD1	C4-N3	6.74	1.49	1.34
6	Q	5801	MD1	C4-N3	6.73	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	5802	MD1	C4-N3	6.72	1.49	1.34
6	H	5801	MD1	C4-N3	6.71	1.49	1.34
6	W	5802	MD1	C12-C13	6.71	1.55	1.34
6	H	5802	MD1	C4-N3	6.70	1.49	1.34
6	N	5801	MD1	C4-N3	6.69	1.49	1.34
6	B	5802	MD1	C4-N3	6.69	1.49	1.34
6	T	5801	MD1	C4-N3	6.69	1.49	1.34
6	N	5802	MD1	C4-N3	6.68	1.49	1.34
6	K	5802	MD1	C4-N3	6.68	1.49	1.34
6	K	5801	MD1	C4-N3	6.67	1.49	1.34
6	E	5802	MD1	C12-C13	6.61	1.55	1.34
6	E	5801	MD1	C4-N3	6.49	1.49	1.34
6	B	5801	MD1	C4-N3	6.44	1.49	1.34
6	E	5802	MD1	C14-C13	-6.31	1.44	1.51
6	T	5801	MD1	O4'-C1'	6.21	1.56	1.42
6	B	5801	MD1	O4'-C1'	6.20	1.56	1.42
6	Q	5801	MD1	O4'-C1'	6.16	1.56	1.42
6	W	5801	MD1	O4'-C1'	6.15	1.56	1.42
6	K	5801	MD1	O4'-C1'	6.13	1.56	1.42
6	N	5801	MD1	O4'-C1'	6.11	1.56	1.42
6	E	5801	MD1	O4'-C1'	6.08	1.56	1.42
6	W	5802	MD1	O4'-C1'	6.06	1.56	1.42
6	H	5801	MD1	O4'-C1'	6.06	1.56	1.42
6	E	5802	MD1	O4'-C1'	6.00	1.55	1.42
6	N	5802	MD1	O4'-C1'	6.00	1.55	1.42
6	Q	5801	MD1	C14-C13	-5.99	1.45	1.51
6	H	5802	MD1	O4'-C1'	5.99	1.55	1.42
6	B	5802	MD1	O4'-C1'	5.99	1.55	1.42
6	Q	5801	MD1	C15-N17	5.98	1.50	1.38
6	K	5802	MD1	O4'-C1'	5.97	1.55	1.42
6	T	5802	MD1	O4'-C1'	5.95	1.55	1.42
6	Q	5802	MD1	O4'-C1'	5.93	1.55	1.42
6	Q	5801	MD1	PA-O3B	5.79	1.65	1.59
6	E	5802	MD1	C2-N3	5.66	1.46	1.33
6	B	5801	MD1	PA-O3B	5.59	1.65	1.59
6	W	5802	MD1	C2-N3	5.59	1.46	1.33
6	B	5802	MD1	C15-N17	5.57	1.49	1.38
6	Q	5801	MD1	C2-N3	5.56	1.46	1.33
6	K	5802	MD1	C2-N3	5.56	1.46	1.33
6	N	5802	MD1	C2-N3	5.55	1.46	1.33
6	T	5802	MD1	C2-N3	5.55	1.46	1.33
6	W	5801	MD1	C2-N3	5.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5802	MD1	C2-N3	5.54	1.46	1.33
6	K	5801	MD1	C2-N3	5.53	1.46	1.33
6	H	5802	MD1	C2-N3	5.53	1.46	1.33
6	W	5802	MD1	C15-N17	5.51	1.49	1.38
6	E	5801	MD1	C15-N17	5.51	1.49	1.38
6	T	5801	MD1	C2-N3	5.50	1.46	1.33
6	B	5801	MD1	C15-N17	5.50	1.49	1.38
6	N	5801	MD1	C2-N3	5.50	1.46	1.33
6	Q	5802	MD1	C2-N3	5.50	1.46	1.33
6	H	5802	MD1	PA-O3B	5.49	1.65	1.59
6	Q	5802	MD1	C15-N17	5.49	1.49	1.38
6	H	5801	MD1	C2-N3	5.48	1.46	1.33
6	T	5802	MD1	C15-N17	5.48	1.49	1.38
8	F	401	HEM	FE-ND	5.46	2.11	1.94
6	K	5802	MD1	C15-N17	5.45	1.49	1.38
6	Q	5801	MD1	PB-O3B	5.45	1.65	1.59
6	H	5801	MD1	C14-C13	-5.44	1.45	1.51
6	N	5802	MD1	C15-N17	5.44	1.49	1.38
6	E	5802	MD1	C15-N17	5.44	1.49	1.38
6	T	5802	MD1	PA-O3B	5.43	1.65	1.59
6	B	5802	MD1	PA-O3B	5.42	1.65	1.59
6	N	5801	MD1	C15-N17	5.41	1.49	1.38
6	H	5802	MD1	PB-O3B	5.40	1.65	1.59
6	H	5801	MD1	C15-N17	5.39	1.48	1.38
6	H	5802	MD1	C15-N17	5.38	1.48	1.38
6	K	5802	MD1	PA-O3B	5.37	1.65	1.59
6	N	5801	MD1	C14-C13	-5.36	1.45	1.51
6	T	5801	MD1	C15-N17	5.35	1.48	1.38
6	T	5801	MD1	C14-C13	-5.34	1.45	1.51
6	B	5801	MD1	C2-N3	5.34	1.46	1.33
6	H	5801	MD1	PA-O3B	5.33	1.65	1.59
6	T	5801	MD1	PA-O3B	5.30	1.65	1.59
6	W	5802	MD1	O4'-C4'	5.28	1.56	1.45
6	W	5801	MD1	C15-N17	5.26	1.48	1.38
6	W	5802	MD1	PB-O3B	5.25	1.65	1.59
6	K	5802	MD1	PB-O3B	5.24	1.65	1.59
6	B	5802	MD1	PB-O3B	5.23	1.65	1.59
6	K	5802	MD1	O4'-C4'	5.22	1.56	1.45
6	B	5802	MD1	O4'-C4'	5.21	1.56	1.45
6	W	5802	MD1	PA-O3B	5.20	1.65	1.59
6	Q	5802	MD1	PA-O3B	5.20	1.65	1.59
6	E	5802	MD1	O4'-C4'	5.20	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	5802	MD1	PB-O3B	5.20	1.65	1.59
6	K	5801	MD1	PA-O3B	5.19	1.65	1.59
6	Q	5802	MD1	O4'-C4'	5.19	1.56	1.45
6	T	5802	MD1	O4'-C4'	5.18	1.56	1.45
6	K	5801	MD1	C14-C13	-5.18	1.46	1.51
6	Q	5802	MD1	PB-O3B	5.18	1.65	1.59
6	N	5802	MD1	PA-O3B	5.17	1.65	1.59
6	B	5801	MD1	C14-C13	-5.17	1.46	1.51
6	N	5802	MD1	O4'-C4'	5.17	1.56	1.45
6	H	5802	MD1	O4'-C4'	5.14	1.56	1.45
6	K	5801	MD1	C15-N17	5.13	1.48	1.38
8	I	401	HEM	C1B-NB	-5.10	1.31	1.40
8	O	401	HEM	FE-NC	5.10	2.12	1.95
8	F	401	HEM	FE-NC	5.09	2.12	1.95
6	Q	5801	MD1	O4'-C4'	5.08	1.56	1.45
6	T	5801	MD1	O4'-C4'	5.08	1.56	1.45
6	E	5801	MD1	C2-N3	5.08	1.45	1.33
6	H	5801	MD1	PB-O3B	5.06	1.65	1.59
8	X	401	HEM	FE-ND	5.05	2.10	1.94
6	H	5801	MD1	O4'-C4'	5.05	1.56	1.45
6	B	5801	MD1	PB-O3B	5.02	1.64	1.59
6	K	5801	MD1	O4'-C4'	5.01	1.56	1.45
6	N	5801	MD1	O4'-C4'	5.01	1.56	1.45
6	W	5801	MD1	PA-O3B	4.99	1.64	1.59
6	N	5802	MD1	PB-O3B	4.97	1.64	1.59
6	W	5801	MD1	O4'-C4'	4.95	1.56	1.45
6	B	5801	MD1	O4'-C4'	4.95	1.56	1.45
6	N	5801	MD1	PA-O3B	4.94	1.64	1.59
6	E	5802	MD1	C2-N2	4.90	1.45	1.34
6	W	5802	MD1	C2-N2	4.90	1.45	1.34
6	Q	5802	MD1	C2-N2	4.90	1.45	1.34
6	N	5802	MD1	C2-N2	4.89	1.45	1.34
6	T	5802	MD1	C2-N2	4.89	1.45	1.34
6	B	5802	MD1	C2-N2	4.89	1.45	1.34
6	K	5801	MD1	PB-O3B	4.89	1.64	1.59
6	H	5802	MD1	C2-N2	4.88	1.45	1.34
6	N	5801	MD1	C17-N16	4.87	1.45	1.34
6	H	5801	MD1	C2-N2	4.87	1.45	1.34
6	T	5802	MD1	C17-N16	4.87	1.45	1.34
6	K	5801	MD1	C2-N2	4.87	1.45	1.34
6	W	5802	MD1	C17-N16	4.87	1.45	1.34
6	Q	5801	MD1	C2-N2	4.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5801	MD1	C17-N16	4.86	1.45	1.34
6	N	5802	MD1	C17-N16	4.86	1.45	1.34
6	W	5801	MD1	C2-N2	4.86	1.45	1.34
6	B	5801	MD1	C17-N16	4.85	1.45	1.34
6	K	5802	MD1	C2-N2	4.85	1.45	1.34
6	H	5801	MD1	C17-N16	4.85	1.45	1.34
6	W	5801	MD1	C17-N16	4.84	1.45	1.34
6	K	5801	MD1	C17-N16	4.84	1.45	1.34
6	E	5802	MD1	C17-N16	4.84	1.45	1.34
6	T	5801	MD1	PB-O3B	4.84	1.64	1.59
6	B	5802	MD1	C17-N16	4.84	1.45	1.34
6	B	5802	MD1	C3'-C2'	4.83	1.66	1.53
8	I	401	HEM	FE-ND	-4.82	1.80	1.94
6	T	5801	MD1	C2-N2	4.82	1.45	1.34
6	Q	5801	MD1	C3'-C2'	4.81	1.66	1.53
6	H	5802	MD1	C3'-C2'	4.81	1.66	1.53
6	T	5802	MD1	C3'-C2'	4.80	1.66	1.53
6	N	5801	MD1	C2-N2	4.80	1.45	1.34
6	W	5801	MD1	C3'-C2'	4.79	1.66	1.53
6	E	5801	MD1	O4'-C4'	4.79	1.55	1.45
6	K	5802	MD1	C3'-C2'	4.79	1.66	1.53
6	N	5801	MD1	C3'-C2'	4.79	1.66	1.53
6	H	5801	MD1	C3'-C2'	4.78	1.66	1.53
6	T	5801	MD1	C3'-C2'	4.78	1.66	1.53
6	Q	5802	MD1	C3'-C2'	4.77	1.66	1.53
6	N	5802	MD1	C3'-C2'	4.77	1.66	1.53
6	T	5801	MD1	C17-N16	4.76	1.45	1.34
6	K	5801	MD1	C3'-C2'	4.76	1.66	1.53
6	W	5801	MD1	C14-C13	-4.73	1.46	1.51
6	H	5802	MD1	C17-N16	4.72	1.45	1.34
6	B	5801	MD1	C3'-C2'	4.71	1.66	1.53
6	E	5802	MD1	PB-O3B	4.71	1.64	1.59
8	L	401	HEM	FE-NB	4.71	2.09	1.94
6	W	5802	MD1	C3'-C2'	4.70	1.66	1.53
6	Q	5802	MD1	C17-N16	4.70	1.45	1.34
6	E	5802	MD1	C3'-C2'	4.69	1.66	1.53
6	E	5802	MD1	PA-O3B	4.65	1.64	1.59
6	E	5801	MD1	C3'-C2'	4.65	1.66	1.53
6	Q	5801	MD1	C17-N16	4.64	1.45	1.34
6	B	5801	MD1	C2-N2	4.61	1.45	1.34
6	E	5801	MD1	PA-O3B	4.53	1.64	1.59
8	I	401	HEM	C4D-ND	-4.52	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	401	HEM	FE-ND	4.51	2.08	1.94
8	R	401	HEM	FE-NC	4.51	2.10	1.95
6	W	5801	MD1	PB-O3B	4.51	1.64	1.59
6	K	5802	MD1	C17-N16	4.50	1.44	1.34
6	E	5801	MD1	PB-O3B	4.43	1.64	1.59
8	U	401	HEM	FE-NA	4.35	2.09	1.95
8	R	401	HEM	FE-NA	4.29	2.09	1.95
6	N	5801	MD1	PB-O3B	4.26	1.64	1.59
8	I	401	HEM	C1D-ND	-4.22	1.30	1.38
8	I	401	HEM	C1C-C2C	-4.21	1.37	1.45
8	U	401	HEM	FE-ND	4.14	2.07	1.94
8	L	401	HEM	FE-NA	3.99	2.08	1.95
8	X	401	HEM	FE-NB	3.91	2.06	1.94
8	I	401	HEM	FE-NB	3.83	2.06	1.94
6	E	5801	MD1	C2-N2	3.81	1.43	1.34
8	R	401	HEM	FE-NB	3.67	2.06	1.94
8	X	401	HEM	FE-NC	3.67	2.07	1.95
8	U	401	HEM	FE-NB	3.59	2.06	1.94
6	K	5801	MD1	C20-N18	3.56	1.44	1.36
8	L	401	HEM	FE-NC	3.53	2.06	1.95
6	W	5802	MD1	C20-N18	3.48	1.44	1.36
6	E	5802	MD1	C20-N18	3.47	1.44	1.36
8	F	401	HEM	CAC-C3C	3.47	1.56	1.47
6	T	5802	MD1	C20-N18	3.47	1.44	1.36
8	L	401	HEM	FE-ND	3.46	2.05	1.94
6	N	5801	MD1	C20-N18	3.45	1.44	1.36
6	W	5801	MD1	C20-N18	3.45	1.44	1.36
6	T	5801	MD1	C20-N18	3.43	1.44	1.36
8	I	401	HEM	C1A-C2A	-3.41	1.37	1.44
6	B	5802	MD1	C20-N18	3.40	1.44	1.36
6	H	5802	MD1	C20-N18	3.38	1.44	1.36
8	I	401	HEM	C4B-NB	-3.38	1.32	1.38
6	N	5802	MD1	C20-N18	3.37	1.44	1.36
6	H	5801	MD1	C20-N18	3.36	1.44	1.36
6	B	5801	MD1	C20-N18	3.36	1.44	1.36
6	E	5802	MD1	C20-N8	3.28	1.41	1.36
8	I	401	HEM	C3C-C4C	-3.24	1.40	1.46
8	X	401	HEM	FE-NA	3.24	2.05	1.95
6	Q	5802	MD1	C20-N18	3.23	1.44	1.36
6	E	5801	MD1	C20-N18	3.20	1.44	1.36
6	K	5802	MD1	C20-N8	3.20	1.41	1.36
8	I	401	HEM	C4A-C3A	-3.13	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	5802	MD1	C20-N18	3.12	1.43	1.36
8	U	401	HEM	CAB-C3B	3.12	1.55	1.47
8	O	401	HEM	CAB-C3B	3.09	1.55	1.47
8	C	401	HEM	CAB-C3B	3.09	1.55	1.47
8	R	401	HEM	CAB-C3B	3.08	1.55	1.47
8	O	401	HEM	CAC-C3C	3.06	1.55	1.47
8	L	401	HEM	CAB-C3B	3.05	1.55	1.47
6	T	5802	MD1	C20-N8	3.04	1.41	1.36
6	N	5802	MD1	C20-N8	3.03	1.41	1.36
6	T	5801	MD1	C20-N8	3.02	1.41	1.36
8	I	401	HEM	C1B-C2B	-2.98	1.38	1.44
8	R	401	HEM	CAC-C3C	2.96	1.55	1.47
6	K	5801	MD1	C20-N8	2.96	1.41	1.36
8	X	401	HEM	CAC-C3C	2.96	1.55	1.47
6	Q	5802	MD1	C20-N8	2.95	1.41	1.36
8	I	401	HEM	C4C-NC	-2.95	1.34	1.39
8	X	401	HEM	CAB-C3B	2.95	1.55	1.47
6	W	5802	MD1	C20-N8	2.94	1.41	1.36
6	Q	5801	MD1	C20-N18	2.94	1.43	1.36
8	I	401	HEM	C2A-C3A	-2.93	1.31	1.38
6	B	5802	MD1	C2-N1	2.93	1.44	1.37
8	L	401	HEM	CAC-C3C	2.93	1.55	1.47
6	W	5801	MD1	C2-N1	2.93	1.44	1.37
6	B	5802	MD1	C20-N8	2.92	1.41	1.36
6	H	5802	MD1	C20-N8	2.91	1.41	1.36
6	T	5802	MD1	C2-N1	2.91	1.44	1.37
8	I	401	HEM	O2D-CGD	-2.90	1.21	1.30
6	N	5801	MD1	C2-N1	2.90	1.44	1.37
6	K	5801	MD1	C2-N1	2.89	1.44	1.37
6	H	5801	MD1	C20-N8	2.89	1.41	1.36
6	Q	5802	MD1	C2-N1	2.88	1.44	1.37
6	Q	5801	MD1	C2-N1	2.88	1.44	1.37
6	B	5801	MD1	C5-N7	-2.87	1.33	1.39
8	C	401	HEM	CAC-C3C	2.87	1.55	1.47
6	K	5802	MD1	C2-N1	2.87	1.44	1.37
6	N	5801	MD1	C20-N8	2.87	1.41	1.36
6	H	5802	MD1	C2-N1	2.86	1.44	1.37
6	T	5801	MD1	C2-N1	2.86	1.44	1.37
6	T	5802	MD1	C5-N7	-2.85	1.33	1.39
6	Q	5801	MD1	C5-N7	-2.85	1.33	1.39
6	N	5802	MD1	C2-N1	2.84	1.44	1.37
6	N	5801	MD1	C5-N7	-2.83	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	5802	MD1	C5-N7	-2.82	1.33	1.39
6	B	5801	MD1	C2-N1	2.82	1.44	1.37
6	Q	5801	MD1	C16-C15	2.82	1.50	1.41
6	Q	5802	MD1	C5-N7	-2.82	1.33	1.39
8	U	401	HEM	CAC-C3C	2.81	1.54	1.47
6	H	5801	MD1	C2-N1	2.81	1.44	1.37
6	H	5802	MD1	C5-N7	-2.81	1.33	1.39
6	E	5802	MD1	C2-N1	2.81	1.44	1.37
6	H	5801	MD1	C5-N7	-2.80	1.33	1.39
6	T	5801	MD1	C5-N7	-2.80	1.33	1.39
6	K	5801	MD1	C5-N7	-2.80	1.33	1.39
6	W	5801	MD1	C5-N7	-2.80	1.33	1.39
8	I	401	HEM	C4A-NA	-2.80	1.34	1.39
8	I	401	HEM	O2A-CGA	-2.80	1.21	1.30
6	B	5802	MD1	C5-N7	-2.80	1.33	1.39
6	W	5802	MD1	C2-N1	2.79	1.44	1.37
6	N	5802	MD1	C5-N7	-2.79	1.33	1.39
6	K	5802	MD1	C5-N7	-2.78	1.33	1.39
6	E	5802	MD1	C5-N7	-2.78	1.33	1.39
8	I	401	HEM	C1C-NC	-2.78	1.34	1.39
6	W	5802	MD1	O6-C6	-2.71	1.18	1.23
6	E	5801	MD1	C5-N7	-2.71	1.33	1.39
6	W	5801	MD1	C20-N8	2.70	1.40	1.36
8	F	401	HEM	CAB-C3B	2.67	1.54	1.47
8	I	401	HEM	CHD-C4C	-2.66	1.33	1.38
6	B	5801	MD1	C20-N8	2.60	1.40	1.36
6	E	5801	MD1	O6-C6	-2.60	1.18	1.23
6	E	5801	MD1	C2-N1	2.58	1.43	1.37
8	I	401	HEM	C1A-NA	-2.56	1.34	1.39
6	B	5801	MD1	C5-C6	2.56	1.53	1.44
6	K	5801	MD1	C5-C6	2.55	1.53	1.44
6	K	5802	MD1	C5-C6	2.55	1.53	1.44
6	W	5801	MD1	C16-C15	2.54	1.49	1.41
6	W	5801	MD1	C6-N1	2.54	1.43	1.38
6	K	5801	MD1	O14-C15	-2.54	1.18	1.23
6	N	5802	MD1	C5-C6	2.54	1.53	1.44
6	W	5801	MD1	C5-C6	2.54	1.53	1.44
6	E	5802	MD1	C5-C6	2.53	1.53	1.44
6	E	5802	MD1	O6-C6	-2.53	1.18	1.23
6	N	5801	MD1	C5-C6	2.53	1.53	1.44
6	Q	5802	MD1	C6-N1	2.53	1.43	1.38
6	H	5802	MD1	C5-C6	2.53	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	5801	MD1	C5-C6	2.53	1.53	1.44
6	T	5802	MD1	C5-C6	2.53	1.53	1.44
6	B	5802	MD1	C5-C6	2.52	1.53	1.44
6	B	5802	MD1	O6-C6	-2.52	1.18	1.23
6	Q	5801	MD1	O6-C6	-2.52	1.18	1.23
6	W	5801	MD1	O6-C6	-2.52	1.18	1.23
6	Q	5802	MD1	C5-C6	2.51	1.53	1.44
6	N	5801	MD1	C6-N1	2.51	1.43	1.38
6	N	5802	MD1	O6-C6	-2.51	1.18	1.23
6	W	5801	MD1	O14-C15	-2.51	1.18	1.23
6	E	5801	MD1	C5-C6	2.51	1.53	1.44
6	K	5802	MD1	C6-N1	2.51	1.43	1.38
6	T	5801	MD1	C6-N1	2.50	1.43	1.38
6	E	5801	MD1	C16-C15	2.50	1.49	1.41
6	B	5802	MD1	C6-N1	2.50	1.43	1.38
6	T	5801	MD1	C5-C6	2.49	1.53	1.44
6	W	5802	MD1	C5-C6	2.49	1.53	1.44
6	H	5801	MD1	C5-C6	2.48	1.53	1.44
6	N	5801	MD1	O6-C6	-2.48	1.18	1.23
6	Q	5802	MD1	O6-C6	-2.48	1.18	1.23
6	H	5802	MD1	O6-C6	-2.47	1.18	1.23
6	B	5801	MD1	O6-C6	-2.47	1.18	1.23
6	N	5802	MD1	C6-N1	2.47	1.43	1.38
6	T	5801	MD1	C16-C15	2.47	1.49	1.41
6	T	5802	MD1	O6-C6	-2.47	1.18	1.23
6	K	5802	MD1	O6-C6	-2.47	1.18	1.23
6	N	5801	MD1	O14-C15	-2.47	1.18	1.23
6	T	5801	MD1	O6-C6	-2.47	1.18	1.23
6	H	5801	MD1	C16-C15	2.47	1.49	1.41
6	T	5801	MD1	O14-C15	-2.46	1.18	1.23
6	T	5802	MD1	C6-N1	2.46	1.43	1.38
6	K	5801	MD1	O6-C6	-2.46	1.18	1.23
6	K	5801	MD1	C6-N1	2.45	1.43	1.38
6	B	5801	MD1	O14-C15	-2.45	1.18	1.23
6	H	5801	MD1	C6-N1	2.45	1.43	1.38
6	H	5801	MD1	O14-C15	-2.45	1.18	1.23
6	B	5801	MD1	C16-C15	2.45	1.49	1.41
6	H	5801	MD1	O6-C6	-2.45	1.18	1.23
6	H	5802	MD1	C6-N1	2.44	1.43	1.38
6	B	5802	MD1	C16-C15	2.44	1.49	1.41
6	B	5802	MD1	O14-C15	-2.43	1.19	1.23
6	T	5802	MD1	O14-C15	-2.42	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	5802	MD1	O14-C15	-2.42	1.19	1.23
6	N	5801	MD1	C16-C15	2.42	1.49	1.41
6	Q	5801	MD1	C6-N1	2.42	1.43	1.38
6	N	5802	MD1	O14-C15	-2.42	1.19	1.23
6	E	5802	MD1	C16-C15	2.41	1.49	1.41
6	T	5802	MD1	C16-C15	2.41	1.49	1.41
6	E	5802	MD1	O14-C15	-2.41	1.19	1.23
6	K	5801	MD1	C16-C15	2.41	1.49	1.41
6	H	5802	MD1	O14-C15	-2.40	1.19	1.23
6	E	5801	MD1	O14-C15	-2.38	1.19	1.23
6	Q	5801	MD1	O14-C15	-2.38	1.19	1.23
6	B	5801	MD1	C6-N1	2.38	1.43	1.38
6	W	5802	MD1	C16-C15	2.38	1.49	1.41
6	K	5802	MD1	C16-C15	2.37	1.49	1.41
6	E	5801	MD1	C6-N1	2.37	1.43	1.38
6	E	5802	MD1	C6-N1	2.36	1.43	1.38
6	Q	5802	MD1	O14-C15	-2.36	1.19	1.23
6	Q	5802	MD1	C16-C15	2.36	1.48	1.41
6	N	5802	MD1	C16-C15	2.35	1.48	1.41
6	W	5802	MD1	C6-N1	2.31	1.43	1.38
8	I	401	HEM	C3B-C2B	-2.29	1.32	1.37
6	K	5802	MD1	O14-C15	-2.29	1.19	1.23
8	U	401	HEM	FE-NC	2.28	2.02	1.95
6	H	5802	MD1	C16-C15	2.27	1.48	1.41
8	O	401	HEM	CMC-C2C	2.27	1.55	1.50
6	Q	5801	MD1	C20-N8	2.23	1.40	1.36
8	F	401	HEM	CMB-C2B	2.20	1.55	1.50
6	E	5801	MD1	C20-N8	2.19	1.40	1.36
6	E	5801	MD1	C4-N9	-2.17	1.32	1.38
8	L	401	HEM	CMB-C2B	2.17	1.55	1.50
8	I	401	HEM	C3D-C2D	-2.16	1.32	1.36
8	I	401	HEM	CHB-C4A	-2.15	1.34	1.39
8	C	401	HEM	FE-NB	2.14	2.01	1.94
8	L	401	HEM	CMA-C3A	2.13	1.55	1.50
8	U	401	HEM	CMB-C2B	2.13	1.55	1.50
8	X	401	HEM	CMA-C3A	2.12	1.55	1.50
8	U	401	HEM	CMA-C3A	2.12	1.55	1.50
8	R	401	HEM	CMA-C3A	2.12	1.55	1.50
8	O	401	HEM	CMB-C2B	2.12	1.55	1.50
6	B	5801	MD1	C4-N9	-2.11	1.32	1.38
8	O	401	HEM	CMA-C3A	2.09	1.55	1.50
8	R	401	HEM	CMB-C2B	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	401	HEM	CMC-C2C	2.07	1.55	1.50
8	C	401	HEM	CMA-C3A	2.05	1.55	1.50
8	O	401	HEM	CMD-C2D	2.05	1.55	1.50
8	C	401	HEM	CMB-C2B	2.02	1.54	1.50
6	E	5801	MD1	C14-C7	2.01	1.55	1.50
8	R	401	HEM	CMD-C2D	2.01	1.54	1.50

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5802	MD1	C5-C4-N3	-5.33	119.90	128.39
6	Q	5801	MD1	C5-C4-N3	-5.23	120.07	128.39
6	W	5802	MD1	C5-C4-N3	-5.19	120.13	128.39
6	N	5802	MD1	C5-C4-N3	-5.18	120.15	128.39
6	T	5802	MD1	C5-C4-N3	-5.16	120.18	128.39
6	T	5801	MD1	C5-C4-N3	-5.14	120.21	128.39
6	K	5802	MD1	C5-C4-N3	-5.11	120.26	128.39
6	K	5801	MD1	C5-C4-N3	-5.09	120.29	128.39
6	Q	5802	MD1	C5-C4-N3	-5.07	120.33	128.39
6	W	5801	MD1	C5-C4-N3	-5.04	120.38	128.39
6	B	5802	MD1	C5-C4-N3	-5.03	120.38	128.39
6	H	5801	MD1	C5-C4-N3	-5.03	120.39	128.39
6	H	5802	MD1	C5-C4-N3	-5.02	120.40	128.39
6	N	5801	MD1	C5-C4-N3	-5.02	120.40	128.39
6	B	5801	MD1	C5-C4-N3	-5.01	120.42	128.39
6	Q	5801	MD1	C17-N18-C20	4.83	120.89	114.20
8	I	401	HEM	CHD-C1D-ND	4.80	129.58	124.42
6	E	5801	MD1	C5-C4-N3	-4.72	120.87	128.39
6	H	5801	MD1	C17-N18-C20	4.62	120.60	114.20
6	B	5801	MD1	C17-N18-C20	4.58	120.54	114.20
6	Q	5801	MD1	C2-N3-C4	4.54	120.12	112.30
6	N	5802	MD1	C2-N3-C4	4.53	120.10	112.30
6	T	5802	MD1	C2-N3-C4	4.53	120.10	112.30
6	W	5801	MD1	C2-N3-C4	4.50	120.06	112.30
6	W	5802	MD1	C2-N3-C4	4.50	120.05	112.30
6	K	5801	MD1	C2-N3-C4	4.50	120.04	112.30
6	K	5802	MD1	C2-N3-C4	4.50	120.04	112.30
6	B	5802	MD1	C2-N3-C4	4.49	120.04	112.30
6	Q	5802	MD1	C2-N3-C4	4.49	120.04	112.30
6	E	5802	MD1	C2-N3-C4	4.49	120.03	112.30
6	N	5801	MD1	C2-N3-C4	4.47	120.00	112.30
6	H	5801	MD1	C2-N3-C4	4.47	120.00	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	5801	MD1	C2-N3-C4	4.46	119.98	112.30
6	H	5802	MD1	C2-N3-C4	4.44	119.95	112.30
6	W	5801	MD1	C17-N18-C20	4.41	120.31	114.20
6	T	5801	MD1	C17-N18-C20	4.41	120.31	114.20
6	N	5801	MD1	C17-N18-C20	4.32	120.18	114.20
6	K	5801	MD1	C17-N18-C20	4.31	120.17	114.20
6	B	5801	MD1	C2-N3-C4	4.19	119.52	112.30
6	E	5802	MD1	C17-N18-C20	4.16	119.97	114.20
6	B	5802	MD1	C17-N18-C20	4.09	119.86	114.20
6	N	5802	MD1	C17-N18-C20	4.07	119.83	114.20
6	Q	5802	MD1	C17-N18-C20	3.97	119.70	114.20
6	T	5802	MD1	C17-N18-C20	3.96	119.69	114.20
6	W	5802	MD1	C17-N18-C20	3.94	119.66	114.20
6	E	5801	MD1	C2-N3-C4	3.89	119.01	112.30
8	I	401	HEM	CHD-C1D-C2D	-3.83	118.98	125.03
6	K	5802	MD1	C17-N18-C20	3.76	119.41	114.20
8	I	401	HEM	CHB-C1B-NB	3.73	128.98	124.37
6	E	5801	MD1	C17-N18-C20	3.70	119.33	114.20
6	H	5802	MD1	C17-N18-C20	3.67	119.28	114.20
6	Q	5802	MD1	C4'-O4'-C1'	-3.59	101.55	109.47
6	E	5801	MD1	C2-N1-C6	-3.46	118.84	125.11
6	E	5801	MD1	N9-C8-N7	-3.36	107.17	113.40
6	E	5802	MD1	N9-C4-N3	3.36	132.67	125.95
6	T	5802	MD1	C4'-O4'-C1'	-3.32	102.14	109.47
6	K	5802	MD1	C17-N17-C15	-3.28	119.16	125.11
6	W	5802	MD1	N9-C4-N3	3.27	132.49	125.95
6	B	5801	MD1	C2-N1-C6	-3.25	119.21	125.11
6	K	5802	MD1	C4'-O4'-C1'	-3.24	102.31	109.47
6	Q	5801	MD1	N9-C4-N3	3.20	132.35	125.95
8	O	401	HEM	C1B-NB-C4B	3.20	108.99	105.21
6	Q	5802	MD1	N9-C8-N7	-3.19	107.49	113.40
8	I	401	HEM	C4C-CHD-C1D	-3.18	119.25	126.02
6	W	5802	MD1	N9-C8-N7	-3.16	107.55	113.40
8	I	401	HEM	CHC-C4B-NB	3.15	127.81	124.42
6	H	5802	MD1	C4'-O4'-C1'	-3.15	102.51	109.47
6	B	5801	MD1	O14-C15-C16	-3.15	119.67	127.26
8	I	401	HEM	C4A-CHB-C1B	-3.15	118.85	126.25
6	W	5801	MD1	N9-C8-N7	-3.15	107.57	113.40
6	B	5802	MD1	N9-C8-N7	-3.14	107.57	113.40
6	K	5802	MD1	N9-C8-N7	-3.14	107.58	113.40
6	T	5802	MD1	N9-C8-N7	-3.14	107.58	113.40
6	T	5802	MD1	N9-C4-N3	3.12	132.19	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	5802	MD1	N9-C4-N3	3.12	132.19	125.95
6	K	5801	MD1	N9-C8-N7	-3.12	107.62	113.40
6	H	5802	MD1	N9-C8-N7	-3.11	107.63	113.40
6	E	5802	MD1	N9-C8-N7	-3.11	107.64	113.40
6	N	5801	MD1	N9-C8-N7	-3.10	107.66	113.40
6	T	5801	MD1	N9-C4-N3	3.10	132.15	125.95
6	B	5801	MD1	N9-C8-N7	-3.10	107.66	113.40
6	E	5802	MD1	C2-N1-C6	-3.08	119.53	125.11
6	T	5801	MD1	N9-C8-N7	-3.07	107.70	113.40
6	N	5801	MD1	O14-C15-C16	-3.07	119.86	127.26
8	I	401	HEM	C1A-CHA-C4D	-3.07	119.04	126.25
6	N	5802	MD1	N9-C8-N7	-3.07	107.71	113.40
6	Q	5801	MD1	N9-C8-N7	-3.05	107.75	113.40
6	H	5801	MD1	O14-C15-C16	-3.03	119.94	127.26
6	K	5802	MD1	C2-N1-C6	-3.03	119.62	125.11
6	K	5801	MD1	C2-N1-C6	-3.03	119.62	125.11
6	H	5801	MD1	N9-C4-N3	3.03	132.01	125.95
6	T	5801	MD1	C2-N1-C6	-3.03	119.62	125.11
6	B	5802	MD1	C2-N1-C6	-3.02	119.63	125.11
6	N	5802	MD1	C2-N1-C6	-3.02	119.63	125.11
6	K	5801	MD1	N9-C4-N3	3.02	132.00	125.95
6	Q	5801	MD1	C2-N1-C6	-3.02	119.63	125.11
6	B	5802	MD1	N9-C4-N3	3.02	131.99	125.95
6	W	5802	MD1	C2-N1-C6	-3.01	119.66	125.11
8	C	401	HEM	C1B-NB-C4B	3.00	108.76	105.21
6	N	5801	MD1	C2-N1-C6	-3.00	119.67	125.11
6	H	5801	MD1	N9-C8-N7	-3.00	107.84	113.40
6	K	5802	MD1	N9-C4-N3	3.00	131.95	125.95
6	K	5802	MD1	O14-C15-C16	-3.00	120.03	127.26
6	W	5801	MD1	N9-C4-N3	2.99	131.94	125.95
6	Q	5802	MD1	N9-C4-N3	2.99	131.94	125.95
6	B	5802	MD1	C4'-O4'-C1'	-2.99	102.86	109.47
6	T	5802	MD1	C2-N1-C6	-2.99	119.69	125.11
6	T	5801	MD1	C17-N17-C15	-2.98	119.71	125.11
6	Q	5802	MD1	C2-N1-C6	-2.98	119.72	125.11
6	H	5802	MD1	N9-C4-N3	2.97	131.90	125.95
6	W	5801	MD1	C2-N1-C6	-2.97	119.72	125.11
6	H	5802	MD1	C2-N1-C6	-2.96	119.75	125.11
6	T	5801	MD1	O14-C15-C16	-2.96	120.13	127.26
8	X	401	HEM	C3B-C2B-C1B	2.95	108.63	106.41
6	E	5801	MD1	C1'-N9-C4	-2.93	117.82	126.49
6	N	5801	MD1	N9-C4-N3	2.93	131.82	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	5802	MD1	O14-C15-C16	-2.92	120.21	127.26
6	Q	5801	MD1	C17-N17-C15	-2.92	119.81	125.11
8	I	401	HEM	CHA-C4D-ND	2.92	127.97	124.37
6	W	5801	MD1	C16-C15-N17	2.91	120.13	112.13
6	Q	5802	MD1	O14-C15-C16	-2.90	120.26	127.26
6	W	5802	MD1	O14-C15-C16	-2.90	120.26	127.26
6	K	5801	MD1	C16-C15-N17	2.90	120.10	112.13
6	B	5801	MD1	C16-C15-N17	2.90	120.09	112.13
6	E	5802	MD1	C17-N17-C15	-2.90	119.86	125.11
6	N	5802	MD1	C4'-O4'-C1'	-2.89	103.08	109.47
6	B	5802	MD1	O14-C15-C16	-2.89	120.29	127.26
6	N	5802	MD1	O14-C15-C16	-2.89	120.30	127.26
6	H	5802	MD1	O14-C15-C16	-2.87	120.33	127.26
6	Q	5802	MD1	C17-N17-C15	-2.87	119.90	125.11
6	Q	5801	MD1	O14-C15-C16	-2.87	120.34	127.26
8	X	401	HEM	C3B-C4B-NB	-2.87	107.41	109.47
6	W	5802	MD1	C4'-O4'-C1'	-2.86	103.14	109.47
8	F	401	HEM	C3C-C2C-C1C	2.86	109.75	107.05
8	I	401	HEM	CHC-C1C-NC	2.86	127.56	124.45
6	K	5801	MD1	O14-C15-C16	-2.85	120.38	127.26
6	H	5801	MD1	C16-C15-N17	2.85	119.95	112.13
6	E	5802	MD1	O14-C15-C16	-2.85	120.40	127.26
6	N	5801	MD1	C16-C15-N17	2.84	119.94	112.13
6	Q	5801	MD1	C16-C15-N17	2.84	119.92	112.13
8	L	401	HEM	C4D-ND-C1D	2.84	108.56	105.21
6	H	5801	MD1	C17-N17-C15	-2.83	119.98	125.11
6	N	5801	MD1	C17-N17-C15	-2.81	120.02	125.11
6	H	5801	MD1	C2-N1-C6	-2.80	120.03	125.11
6	T	5801	MD1	C16-C15-N17	2.80	119.81	112.13
6	W	5801	MD1	C17-N17-C15	-2.79	120.06	125.11
6	E	5801	MD1	O14-C15-C16	-2.78	120.55	127.26
6	N	5802	MD1	C17-N17-C15	-2.76	120.10	125.11
6	K	5801	MD1	C17-N17-C15	-2.76	120.10	125.11
8	I	401	HEM	CBD-CAD-C3D	-2.76	104.89	112.53
6	B	5801	MD1	C17-N17-C15	-2.75	120.11	125.11
6	W	5802	MD1	C5-C6-N1	2.72	120.17	113.25
8	X	401	HEM	C1B-NB-C4B	2.71	108.42	105.21
6	E	5801	MD1	N9-C4-N3	2.71	131.37	125.95
8	O	401	HEM	C3B-C4B-NB	-2.71	107.53	109.47
8	I	401	HEM	CHB-C1B-C2B	-2.70	119.28	126.95
6	T	5802	MD1	C17-N17-C15	-2.68	120.25	125.11
6	E	5801	MD1	C5-C6-N1	2.68	120.08	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5802	MD1	C5-C6-N1	2.67	120.06	113.25
6	W	5801	MD1	O14-C15-C16	-2.67	120.82	127.26
6	B	5802	MD1	C5-C6-N1	2.67	120.04	113.25
6	K	5801	MD1	C5-C6-N1	2.66	120.01	113.25
6	E	5801	MD1	C16-C15-N17	2.65	119.42	112.13
8	F	401	HEM	O1A-CGA-CBA	-2.65	114.68	123.09
6	W	5802	MD1	C17-N17-C15	-2.65	120.30	125.11
6	B	5801	MD1	N9-C4-N3	2.65	131.26	125.95
8	U	401	HEM	CAA-CBA-CGA	-2.65	106.63	113.67
6	W	5801	MD1	C5-C6-N1	2.65	119.99	113.25
6	Q	5801	MD1	C5-C6-N1	2.65	119.99	113.25
6	N	5801	MD1	C5-C6-N1	2.64	119.98	113.25
6	B	5802	MD1	C17-N17-C15	-2.64	120.32	125.11
6	N	5802	MD1	C5-C6-N1	2.64	119.98	113.25
6	Q	5801	MD1	N16-C17-N17	2.64	122.34	116.76
6	K	5802	MD1	C5-C6-N1	2.64	119.97	113.25
8	F	401	HEM	CBD-CAD-C3D	-2.64	105.24	112.53
6	T	5802	MD1	C5-C6-N1	2.63	119.95	113.25
6	H	5802	MD1	C5-C6-N1	2.63	119.95	113.25
6	Q	5802	MD1	C5-C6-N1	2.62	119.92	113.25
6	T	5801	MD1	C5-C6-N1	2.62	119.92	113.25
6	B	5801	MD1	C1'-N9-C4	-2.61	118.78	126.49
6	H	5802	MD1	C17-N17-C15	-2.59	120.41	125.11
8	C	401	HEM	C2A-C1A-NA	-2.58	107.29	110.15
6	Q	5802	MD1	O4'-C1'-C2'	-2.57	101.11	106.62
8	O	401	HEM	CAA-CBA-CGA	-2.57	106.85	113.67
6	B	5802	MD1	C16-C15-N17	2.57	119.19	112.13
6	H	5801	MD1	C5-C6-N1	2.57	119.79	113.25
6	B	5801	MD1	C5-C6-N1	2.55	119.75	113.25
6	Q	5801	MD1	C3'-C2'-C1'	2.55	106.29	101.46
6	W	5802	MD1	C16-C15-N17	2.55	119.12	112.13
6	E	5802	MD1	C4'-O4'-C1'	-2.55	103.85	109.47
6	E	5801	MD1	O3A-C10-C11	-2.54	100.82	107.96
6	T	5802	MD1	C16-C15-N17	2.52	119.06	112.13
6	N	5802	MD1	C16-C15-N17	2.50	118.99	112.13
6	Q	5801	MD1	O6-C6-C5	-2.50	119.94	126.53
6	W	5802	MD1	O4'-C1'-C2'	-2.50	101.28	106.62
6	B	5802	MD1	O6-C6-C5	-2.49	119.95	126.53
6	E	5801	MD1	O6-C6-C5	-2.49	119.95	126.53
6	W	5801	MD1	O6-C6-C5	-2.49	119.95	126.53
8	L	401	HEM	C3D-C4D-ND	-2.49	107.44	110.17
6	E	5802	MD1	C16-C15-N17	2.48	118.94	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	5801	MD1	O6-C6-C5	-2.47	120.00	126.53
6	E	5801	MD1	C17-N17-C15	-2.47	120.63	125.11
6	N	5802	MD1	O6-C6-C5	-2.46	120.04	126.53
6	K	5801	MD1	O6-C6-C5	-2.45	120.06	126.53
6	N	5801	MD1	O6-C6-C5	-2.45	120.06	126.53
6	K	5802	MD1	O4'-C1'-C2'	-2.44	101.40	106.62
6	E	5802	MD1	O6-C6-C5	-2.43	120.11	126.53
6	T	5802	MD1	O6-C6-C5	-2.42	120.14	126.53
6	H	5801	MD1	C3'-C2'-C1'	2.42	106.04	101.46
8	F	401	HEM	CAA-CBA-CGA	-2.42	107.25	113.67
6	H	5801	MD1	O6-C6-C5	-2.42	120.15	126.53
6	Q	5802	MD1	O6-C6-C5	-2.41	120.18	126.53
6	Q	5802	MD1	C16-C15-N17	2.41	118.74	112.13
6	W	5802	MD1	O6-C6-C5	-2.40	120.20	126.53
6	H	5802	MD1	C16-C15-N17	2.40	118.71	112.13
8	C	401	HEM	C3B-C2B-C1B	2.39	108.21	106.41
6	K	5802	MD1	O6-C6-C5	-2.39	120.22	126.53
6	H	5802	MD1	O6-C6-C5	-2.39	120.23	126.53
8	C	401	HEM	C3B-C4B-NB	-2.38	107.76	109.47
8	R	401	HEM	C4D-ND-C1D	2.37	108.01	105.21
6	N	5801	MD1	C1'-N9-C4	-2.36	119.51	126.49
8	U	401	HEM	C1B-NB-C4B	2.36	108.00	105.21
6	W	5801	MD1	C1'-N9-C4	-2.36	119.53	126.49
6	T	5802	MD1	N8-C20-N18	2.34	122.36	117.75
6	Q	5802	MD1	C8-N7-C5	2.34	108.42	104.26
8	L	401	HEM	C1B-NB-C4B	2.34	107.97	105.21
6	E	5801	MD1	C4'-O4'-C1'	-2.33	104.31	109.47
6	B	5802	MD1	O4'-C1'-C2'	-2.33	101.63	106.62
6	K	5802	MD1	C16-C15-N17	2.33	118.53	112.13
6	H	5802	MD1	C1'-N9-C4	-2.33	119.61	126.49
6	K	5802	MD1	C8-N7-C5	2.32	108.39	104.26
6	E	5802	MD1	N8-C20-N18	2.31	122.32	117.75
6	Q	5802	MD1	C1'-N9-C4	-2.31	119.65	126.49
8	F	401	HEM	C3A-C4A-NA	-2.30	106.45	110.14
6	B	5802	MD1	C1'-N9-C4	-2.30	119.70	126.49
6	T	5802	MD1	O4'-C1'-C2'	-2.29	101.71	106.62
8	R	401	HEM	CHC-C1C-NC	2.29	126.95	124.45
8	F	401	HEM	C4A-C3A-C2A	2.29	109.44	106.82
6	T	5802	MD1	C8-N7-C5	2.29	108.34	104.26
6	W	5802	MD1	N8-C20-N18	2.28	122.25	117.75
6	W	5802	MD1	C8-N7-C5	2.27	108.31	104.26
8	I	401	HEM	CHA-C4D-C3D	-2.27	121.04	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	5801	MD1	C1'-N9-C8	2.27	133.17	126.73
6	K	5801	MD1	C1'-N9-C4	-2.26	119.80	126.49
8	I	401	HEM	C4B-C3B-C2B	-2.26	105.20	107.28
6	Q	5802	MD1	O4'-C1'-N9	2.26	113.48	108.36
6	E	5801	MD1	C8-N7-C5	2.25	108.27	104.26
6	B	5801	MD1	C8-N7-C5	2.25	108.26	104.26
6	B	5802	MD1	C8-N7-C5	2.25	108.26	104.26
6	K	5801	MD1	C8-N7-C5	2.24	108.25	104.26
6	K	5802	MD1	C1'-N9-C4	-2.24	119.87	126.49
6	B	5802	MD1	N8-C20-N18	2.23	122.16	117.75
6	B	5802	MD1	C15-C16-N15	2.23	122.35	116.27
6	E	5802	MD1	C8-N7-C5	2.23	108.23	104.26
6	H	5802	MD1	O4'-C1'-C2'	-2.23	101.85	106.62
6	W	5801	MD1	C8-N7-C5	2.22	108.22	104.26
6	N	5802	MD1	C8-N7-C5	2.22	108.21	104.26
8	R	401	HEM	C3D-C4D-ND	-2.21	107.75	110.17
8	F	401	HEM	CMA-C3A-C4A	-2.21	122.06	125.42
6	B	5801	MD1	O6-C6-C5	-2.20	120.71	126.53
6	B	5801	MD1	C1'-N9-C8	2.20	132.98	126.73
8	L	401	HEM	C2D-C1D-ND	-2.20	107.36	109.90
6	T	5801	MD1	C1'-N9-C4	-2.20	120.00	126.49
6	N	5801	MD1	C8-N7-C5	2.19	108.17	104.26
8	O	401	HEM	C3B-C2B-C1B	2.19	108.06	106.41
8	I	401	HEM	CHB-C4A-C3A	-2.19	121.06	127.43
6	N	5802	MD1	C2'-C3'-C4'	2.19	106.84	102.61
6	H	5802	MD1	C8-N7-C5	2.19	108.16	104.26
6	T	5801	MD1	C8-N7-C5	2.19	108.16	104.26
6	H	5801	MD1	C1'-N9-C4	-2.18	120.03	126.49
8	C	401	HEM	C4D-ND-C1D	2.18	107.78	105.21
8	U	401	HEM	C4D-ND-C1D	2.17	107.78	105.21
8	X	401	HEM	CBD-CAD-C3D	-2.16	106.55	112.53
8	U	401	HEM	C3D-C4D-ND	-2.16	107.80	110.17
6	Q	5801	MD1	C8-N7-C5	2.16	108.10	104.26
8	I	401	HEM	O2D-CGD-CBD	2.15	120.80	114.00
6	T	5802	MD1	C1'-N9-C4	-2.14	120.15	126.49
6	H	5801	MD1	C8-N7-C5	2.12	108.04	104.26
8	I	401	HEM	CHB-C4A-NA	2.12	127.70	123.86
8	X	401	HEM	CAA-CBA-CGA	-2.12	108.05	113.67
6	N	5802	MD1	C1'-N9-C4	-2.12	120.23	126.49
6	N	5801	MD1	C3'-C2'-C1'	2.11	105.45	101.46
8	I	401	HEM	CBA-CAA-C2A	-2.10	106.73	112.53
6	N	5802	MD1	O4'-C1'-C2'	-2.10	102.13	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	401	HEM	C3B-C2B-C1B	2.09	107.98	106.41
8	I	401	HEM	C1C-CHC-C4B	-2.09	121.59	126.02
8	F	401	HEM	CHC-C4B-NB	2.08	126.67	124.42
8	R	401	HEM	C1B-NB-C4B	2.07	107.66	105.21
8	L	401	HEM	C3C-C2C-C1C	2.07	109.00	107.05
8	X	401	HEM	C4D-ND-C1D	2.06	107.64	105.21
6	K	5802	MD1	O4'-C1'-N9	2.06	113.02	108.36
6	K	5802	MD1	C2'-C3'-C4'	2.05	106.57	102.61
6	N	5801	MD1	C2'-C3'-C4'	2.05	106.56	102.61
6	T	5802	MD1	C2'-C3'-C4'	2.04	106.56	102.61
8	I	401	HEM	CBB-CAB-C3B	-2.04	117.31	127.53
8	C	401	HEM	C3D-C4D-ND	-2.04	107.94	110.17
6	Q	5801	MD1	C15-C16-N15	2.03	121.81	116.27
6	H	5802	MD1	C2'-C3'-C4'	2.03	106.54	102.61
8	F	401	HEM	C2A-C1A-NA	-2.03	107.90	110.15
8	I	401	HEM	C4C-C3C-C2C	-2.03	105.06	106.81
8	F	401	HEM	CHA-C1A-NA	2.03	127.54	123.86
6	Q	5801	MD1	C1'-N9-C4	-2.02	120.51	126.49
8	O	401	HEM	C2B-C1B-NB	-2.02	107.51	109.84
6	W	5802	MD1	C1'-N9-C4	-2.02	120.51	126.49
6	K	5801	MD1	C3'-C2'-C1'	2.02	105.28	101.46
8	C	401	HEM	C4A-NA-C1A	2.01	109.10	105.82
6	N	5802	MD1	C15-C16-N15	2.01	121.75	116.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	5801	MD1	C14

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5801	MD1	O3A-C10-C11-O11
6	B	5801	MD1	O3A-C10-C11-C12
6	E	5801	MD1	O3A-C10-C11-O11
6	E	5801	MD1	O3A-C10-C11-C12
6	E	5801	MD1	C5'-O5'-PA-O3B
6	E	5802	MD1	O3A-C10-C11-C12
6	H	5801	MD1	C10-O3A-PB-O3B
6	H	5801	MD1	C10-O3A-PB-O2B
6	H	5801	MD1	O3A-C10-C11-O11
6	H	5801	MD1	O3A-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	H	5801	MD1	C5'-O5'-PA-O3B
6	H	5801	MD1	C5'-O5'-PA-O2A
6	K	5801	MD1	O3A-C10-C11-O11
6	K	5801	MD1	O3A-C10-C11-C12
6	K	5801	MD1	C5'-O5'-PA-O2A
6	N	5801	MD1	O3A-C10-C11-O11
6	N	5801	MD1	O3A-C10-C11-C12
6	N	5801	MD1	C5'-O5'-PA-O3B
6	N	5801	MD1	C5'-O5'-PA-O2A
6	N	5801	MD1	O4'-C4'-C5'-O5'
6	Q	5801	MD1	C10-O3A-PB-O2B
6	Q	5801	MD1	O3A-C10-C11-C12
6	Q	5801	MD1	C5'-O5'-PA-O3B
6	Q	5801	MD1	C5'-O5'-PA-O2A
6	Q	5802	MD1	C5'-O5'-PA-O3B
6	Q	5802	MD1	C5'-O5'-PA-O2A
6	T	5801	MD1	O3A-C10-C11-O11
6	T	5801	MD1	O3A-C10-C11-C12
6	T	5801	MD1	C5'-O5'-PA-O2A
6	T	5801	MD1	O4'-C4'-C5'-O5'
6	T	5801	MD1	C3'-C4'-C5'-O5'
6	W	5801	MD1	O3A-C10-C11-O11
6	W	5801	MD1	O3A-C10-C11-C12
6	W	5801	MD1	C5'-O5'-PA-O2A
6	W	5801	MD1	O4'-C4'-C5'-O5'
6	W	5802	MD1	O3A-C10-C11-O11
6	W	5802	MD1	O3A-C10-C11-C12
8	I	401	HEM	C1A-C2A-CAA-CBA
8	I	401	HEM	C2B-C3B-CAB-CBB
6	B	5801	MD1	O4'-C4'-C5'-O5'
6	B	5801	MD1	C3'-C4'-C5'-O5'
6	H	5801	MD1	O4'-C4'-C5'-O5'
6	K	5801	MD1	O4'-C4'-C5'-O5'
6	K	5801	MD1	C3'-C4'-C5'-O5'
6	N	5801	MD1	C3'-C4'-C5'-O5'
6	W	5801	MD1	C3'-C4'-C5'-O5'
6	E	5801	MD1	O4'-C4'-C5'-O5'
6	E	5801	MD1	C3'-C4'-C5'-O5'
6	H	5801	MD1	C3'-C4'-C5'-O5'
6	Q	5801	MD1	O4'-C4'-C5'-O5'
6	Q	5801	MD1	C3'-C4'-C5'-O5'
6	Q	5802	MD1	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	I	401	HEM	C3A-C2A-CAA-CBA
8	I	401	HEM	C2A-CAA-CBA-CGA
8	I	401	HEM	C4B-C3B-CAB-CBB
6	B	5802	MD1	O3A-C10-C11-O11
6	E	5802	MD1	O3A-C10-C11-O11
6	H	5802	MD1	O3A-C10-C11-O11
6	K	5802	MD1	O3A-C10-C11-O11
6	N	5802	MD1	O3A-C10-C11-O11
6	Q	5802	MD1	O3A-C10-C11-O11
6	T	5802	MD1	O3A-C10-C11-O11
6	Q	5802	MD1	O3A-C10-C11-C12
6	Q	5802	MD1	C3'-C4'-C5'-O5'
6	B	5801	MD1	PB-O3B-PA-O5'
6	E	5801	MD1	PB-O3B-PA-O5'
6	H	5801	MD1	PB-O3B-PA-O5'
6	K	5801	MD1	PB-O3B-PA-O5'
6	N	5801	MD1	PB-O3B-PA-O5'
6	T	5801	MD1	PB-O3B-PA-O5'
6	W	5801	MD1	PB-O3B-PA-O5'
8	C	401	HEM	C2C-C3C-CAC-CBC
8	U	401	HEM	C2C-C3C-CAC-CBC
8	C	401	HEM	C4C-C3C-CAC-CBC
8	R	401	HEM	C4C-C3C-CAC-CBC
8	U	401	HEM	C4C-C3C-CAC-CBC
8	X	401	HEM	C4B-C3B-CAB-CBB
6	B	5801	MD1	C4'-C5'-O5'-PA
6	K	5801	MD1	C4'-C5'-O5'-PA
6	Q	5801	MD1	C4'-C5'-O5'-PA
6	T	5801	MD1	C4'-C5'-O5'-PA
6	B	5801	MD1	C10-O3A-PB-O3B
6	B	5801	MD1	C10-O3A-PB-O1B
6	B	5801	MD1	C10-O3A-PB-O2B
6	B	5801	MD1	C5'-O5'-PA-O2A
6	E	5801	MD1	C5'-O5'-PA-O2A
6	H	5801	MD1	C10-O3A-PB-O1B
6	K	5801	MD1	C10-O3A-PB-O3B
6	K	5801	MD1	C10-O3A-PB-O1B
6	K	5801	MD1	C10-O3A-PB-O2B
6	N	5801	MD1	C10-O3A-PB-O3B
6	N	5801	MD1	C10-O3A-PB-O1B
6	N	5801	MD1	C10-O3A-PB-O2B
6	Q	5801	MD1	C10-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
6	Q	5802	MD1	C5'-O5'-PA-O1A
6	T	5801	MD1	C10-O3A-PB-O3B
6	T	5801	MD1	C10-O3A-PB-O1B
6	T	5801	MD1	C10-O3A-PB-O2B
6	W	5801	MD1	C10-O3A-PB-O3B
6	W	5801	MD1	C10-O3A-PB-O1B
6	W	5801	MD1	C10-O3A-PB-O2B
6	W	5802	MD1	C10-O3A-PB-O1B
6	E	5801	MD1	C4'-C5'-O5'-PA
6	H	5801	MD1	C4'-C5'-O5'-PA
6	N	5801	MD1	C4'-C5'-O5'-PA
6	W	5801	MD1	C4'-C5'-O5'-PA
8	C	401	HEM	C2A-CAA-CBA-CGA
8	R	401	HEM	C2A-CAA-CBA-CGA
8	U	401	HEM	C2A-CAA-CBA-CGA
6	N	5802	MD1	C2'-C1'-N9-C8
6	B	5802	MD1	PA-O3B-PB-O1B
6	E	5802	MD1	PA-O3B-PB-O1B
6	H	5802	MD1	PA-O3B-PB-O1B
6	K	5802	MD1	PA-O3B-PB-O1B
6	N	5802	MD1	PA-O3B-PB-O1B
6	Q	5802	MD1	PA-O3B-PB-O1B
6	T	5802	MD1	PA-O3B-PB-O1B
6	W	5802	MD1	PA-O3B-PB-O1B
6	B	5802	MD1	C2'-C1'-N9-C8
6	K	5802	MD1	C2'-C1'-N9-C8
6	W	5802	MD1	C2'-C1'-N9-C8
8	O	401	HEM	C2A-CAA-CBA-CGA
6	K	5802	MD1	C2'-C1'-N9-C4
6	W	5802	MD1	C2'-C1'-N9-C4
8	L	401	HEM	C2A-CAA-CBA-CGA
6	H	5802	MD1	C2'-C1'-N9-C8
8	F	401	HEM	C3A-C2A-CAA-CBA
6	Q	5801	MD1	PB-O3B-PA-O5'
6	H	5802	MD1	C2'-C1'-N9-C4
6	N	5802	MD1	C2'-C1'-N9-C4
6	Q	5801	MD1	C2'-C1'-N9-C8
6	B	5802	MD1	C2'-C1'-N9-C4
6	B	5801	MD1	C2'-C1'-N9-C8
6	E	5802	MD1	C2'-C1'-N9-C8
6	T	5802	MD1	C2'-C1'-N9-C8
6	B	5802	MD1	PA-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
6	E	5802	MD1	PA-O3B-PB-O2B
6	H	5802	MD1	PA-O3B-PB-O2B
6	K	5802	MD1	PA-O3B-PB-O2B
6	N	5802	MD1	PA-O3B-PB-O2B
6	Q	5802	MD1	PA-O3B-PB-O2B
6	T	5802	MD1	PA-O3B-PB-O2B
6	W	5802	MD1	PA-O3B-PB-O2B
6	N	5801	MD1	C2'-C1'-N9-C8
8	F	401	HEM	CAA-CBA-CGA-O1A
8	X	401	HEM	CAD-CBD-CGD-O2D
8	O	401	HEM	CAA-CBA-CGA-O1A
8	I	401	HEM	CAD-CBD-CGD-O2D
8	F	401	HEM	C2A-CAA-CBA-CGA
8	F	401	HEM	CAD-CBD-CGD-O2D
8	R	401	HEM	CAD-CBD-CGD-O2D
8	O	401	HEM	CAA-CBA-CGA-O2A
8	F	401	HEM	CAA-CBA-CGA-O2A
8	R	401	HEM	CAA-CBA-CGA-O1A
8	I	401	HEM	CAD-CBD-CGD-O1D
8	U	401	HEM	CAD-CBD-CGD-O2D
8	C	401	HEM	CAA-CBA-CGA-O1A
8	U	401	HEM	CAA-CBA-CGA-O1A
8	L	401	HEM	CAA-CBA-CGA-O1A
8	X	401	HEM	CAD-CBD-CGD-O1D
8	C	401	HEM	CAD-CBD-CGD-O2D
8	F	401	HEM	CAD-CBD-CGD-O1D
8	R	401	HEM	CAD-CBD-CGD-O1D
8	X	401	HEM	C2A-CAA-CBA-CGA
8	L	401	HEM	CAA-CBA-CGA-O2A
8	O	401	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

48 monomers are involved in 294 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	5802	MD1	8	0
6	W	5801	MD1	13	0
6	N	5802	MD1	9	0
8	O	401	HEM	11	0
8	C	401	HEM	8	0
4	M	501	SF4	1	0
8	L	401	HEM	7	0

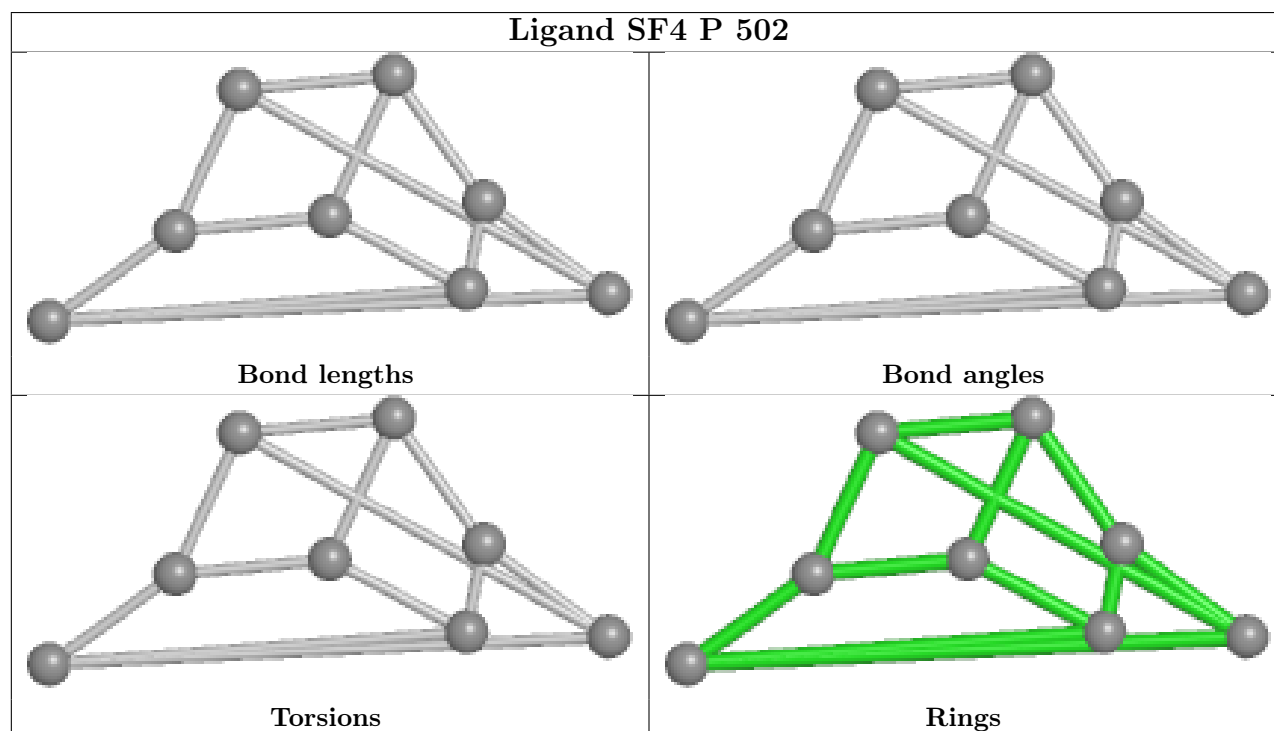
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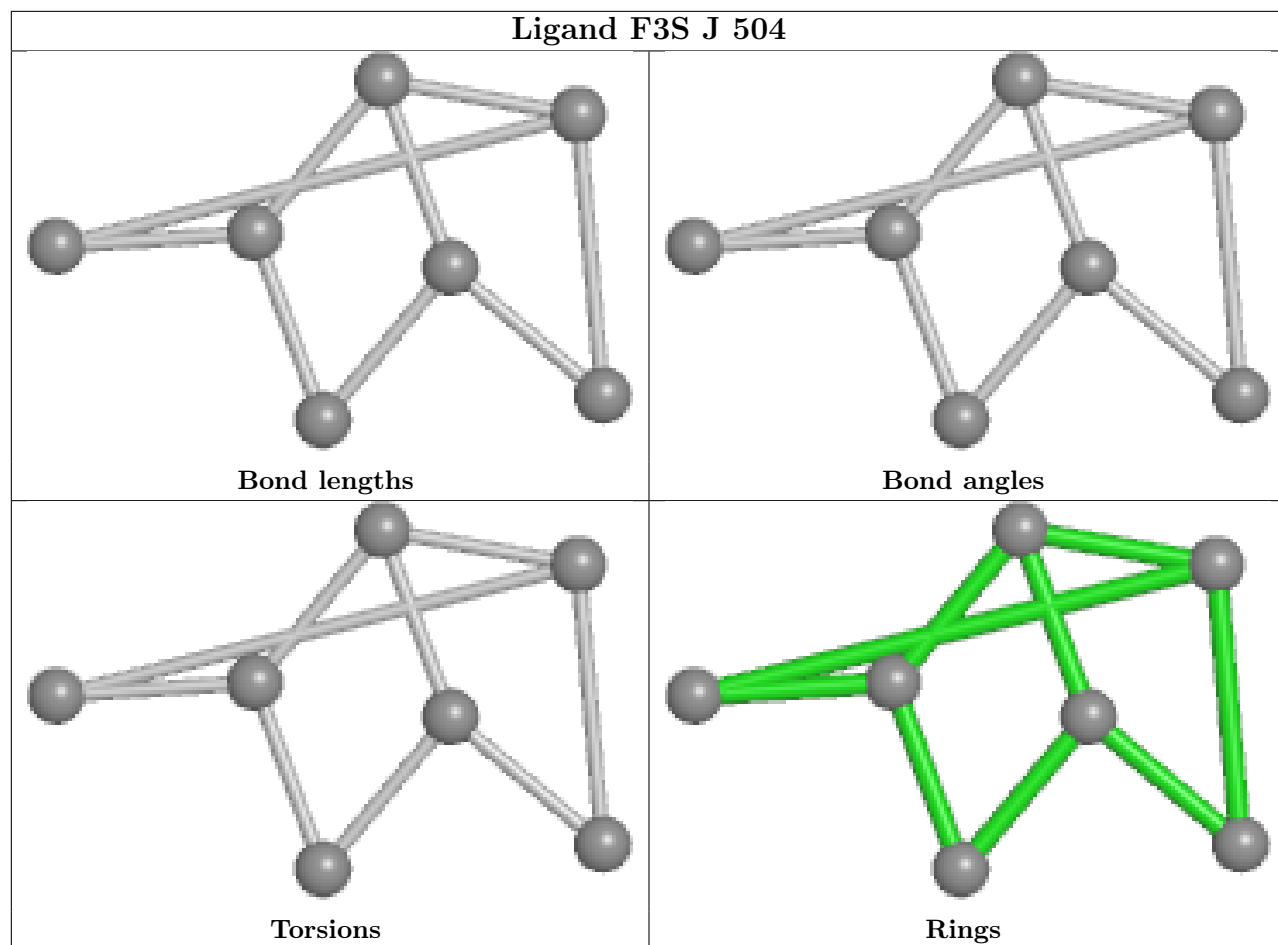
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	502	SF4	2	0
6	B	5802	MD1	6	0
4	N	5804	SF4	3	0
6	N	5801	MD1	10	0
6	Q	5801	MD1	12	0
4	S	503	SF4	2	0
6	E	5801	MD1	14	0
6	K	5801	MD1	11	0
8	I	401	HEM	29	0
6	H	5802	MD1	8	0
6	E	5802	MD1	5	0
6	H	5801	MD1	6	0
4	A	503	SF4	1	0
4	V	501	SF4	2	0
8	X	401	HEM	15	0
6	Q	5802	MD1	7	0
6	T	5801	MD1	8	0
4	V	502	SF4	1	0
5	D	504	F3S	3	0
4	J	501	SF4	1	0
6	T	5802	MD1	5	0
8	F	401	HEM	25	0
4	Q	5804	SF4	3	0
8	U	401	HEM	4	0
4	G	503	SF4	2	0
4	P	503	SF4	3	0
4	T	5804	SF4	3	0
4	D	501	SF4	4	0
4	V	503	SF4	3	0
6	K	5802	MD1	7	0
4	M	503	SF4	2	0
4	G	501	SF4	1	0
5	V	504	F3S	5	0
4	K	5804	SF4	1	0
4	S	501	SF4	1	0
6	B	5801	MD1	8	0
4	W	5804	SF4	2	0
5	M	504	F3S	2	0
4	J	503	SF4	4	0
4	D	503	SF4	1	0
8	R	401	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

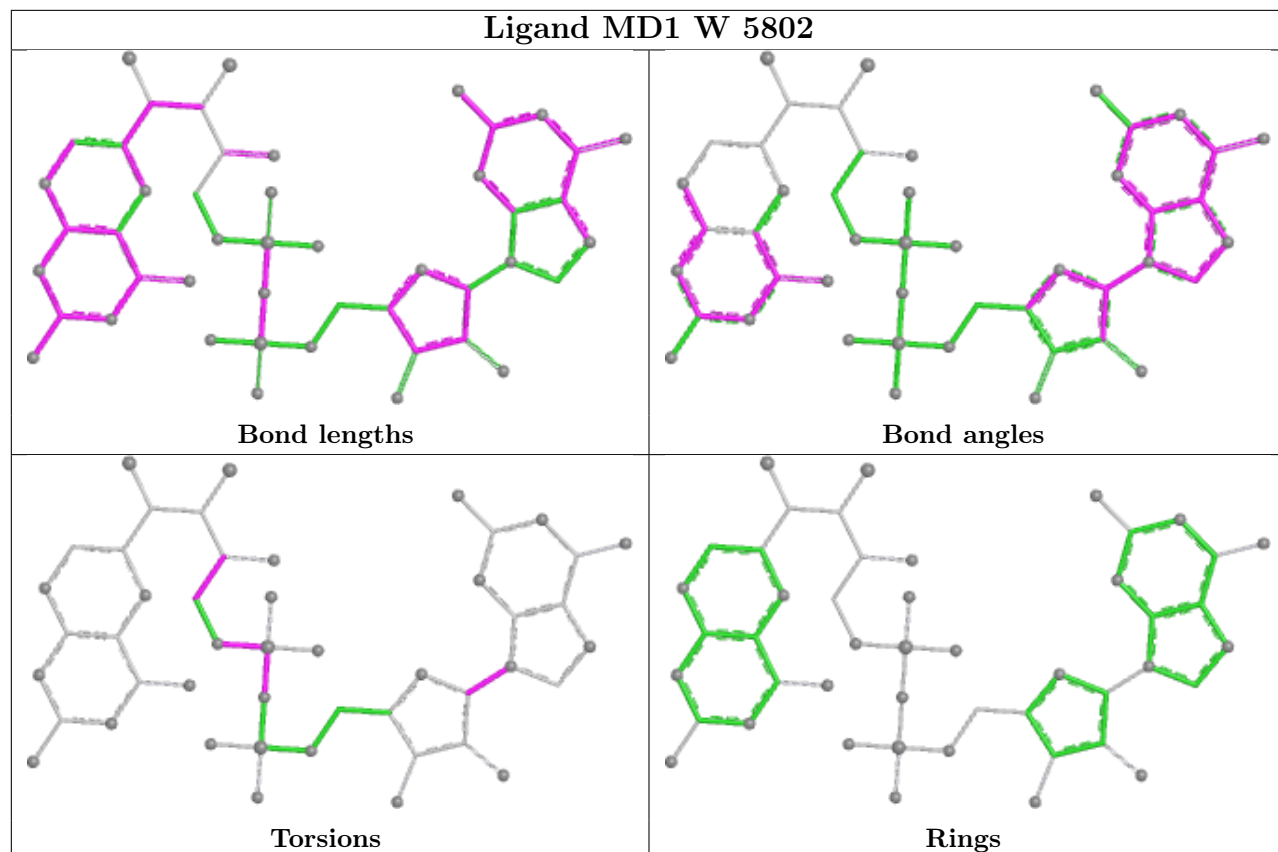
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



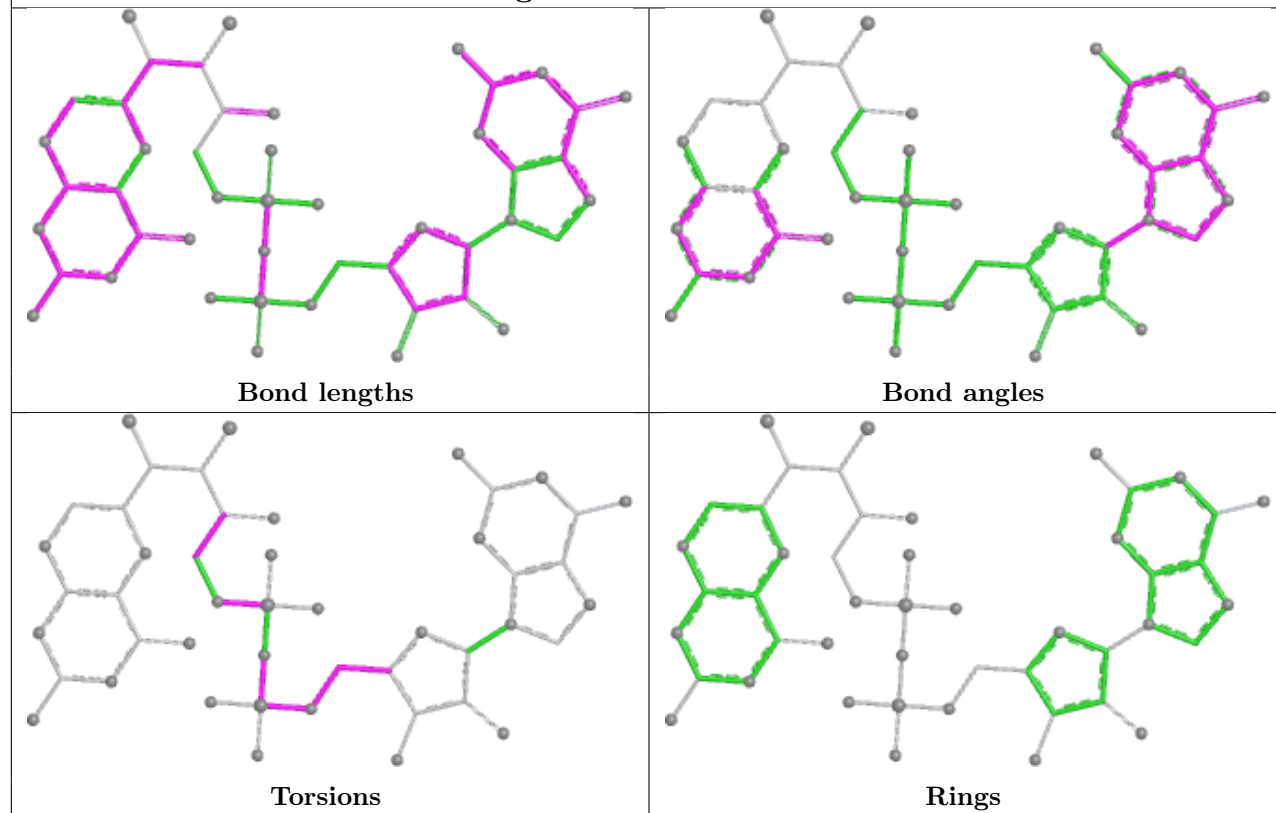
Ligand F3S J 504



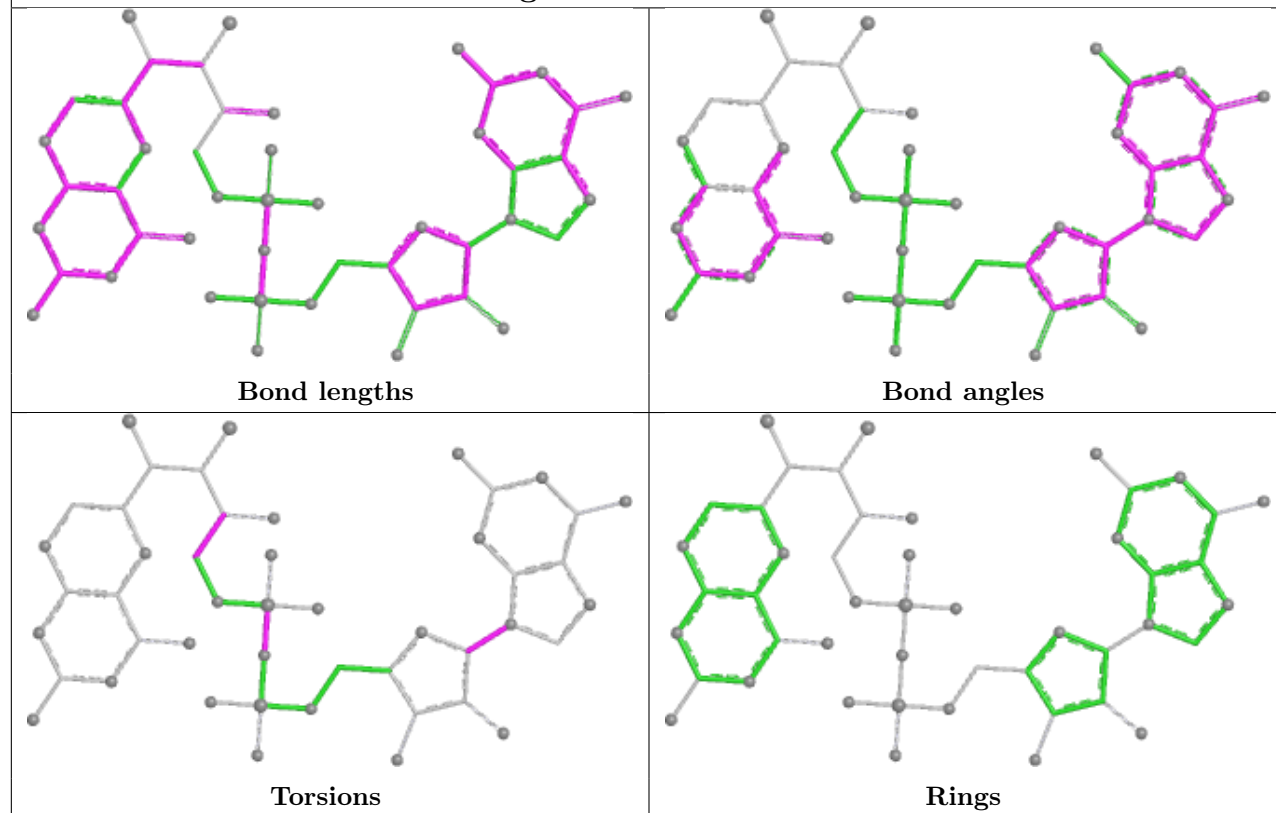
Ligand MD1 W 5802

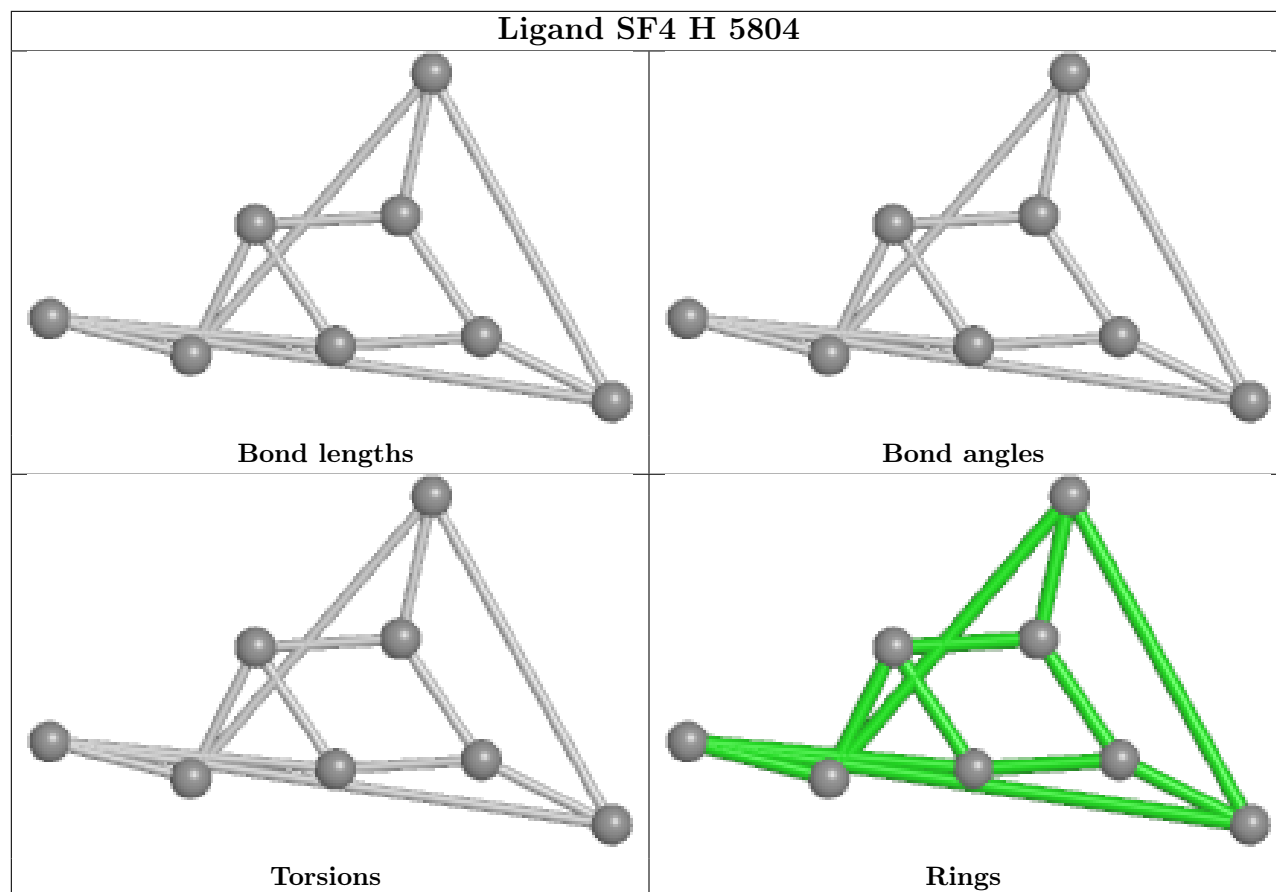


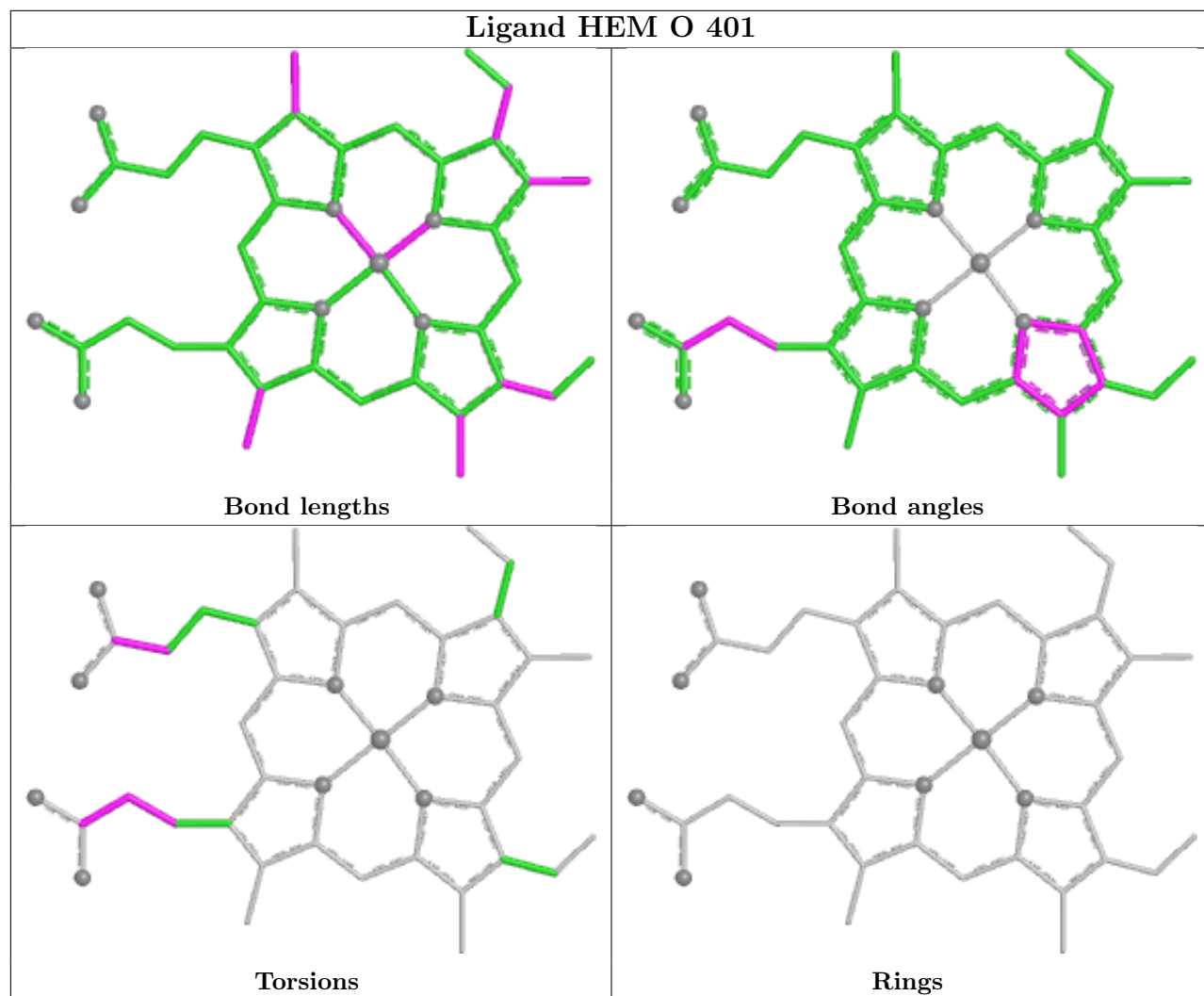
Ligand MD1 W 5801

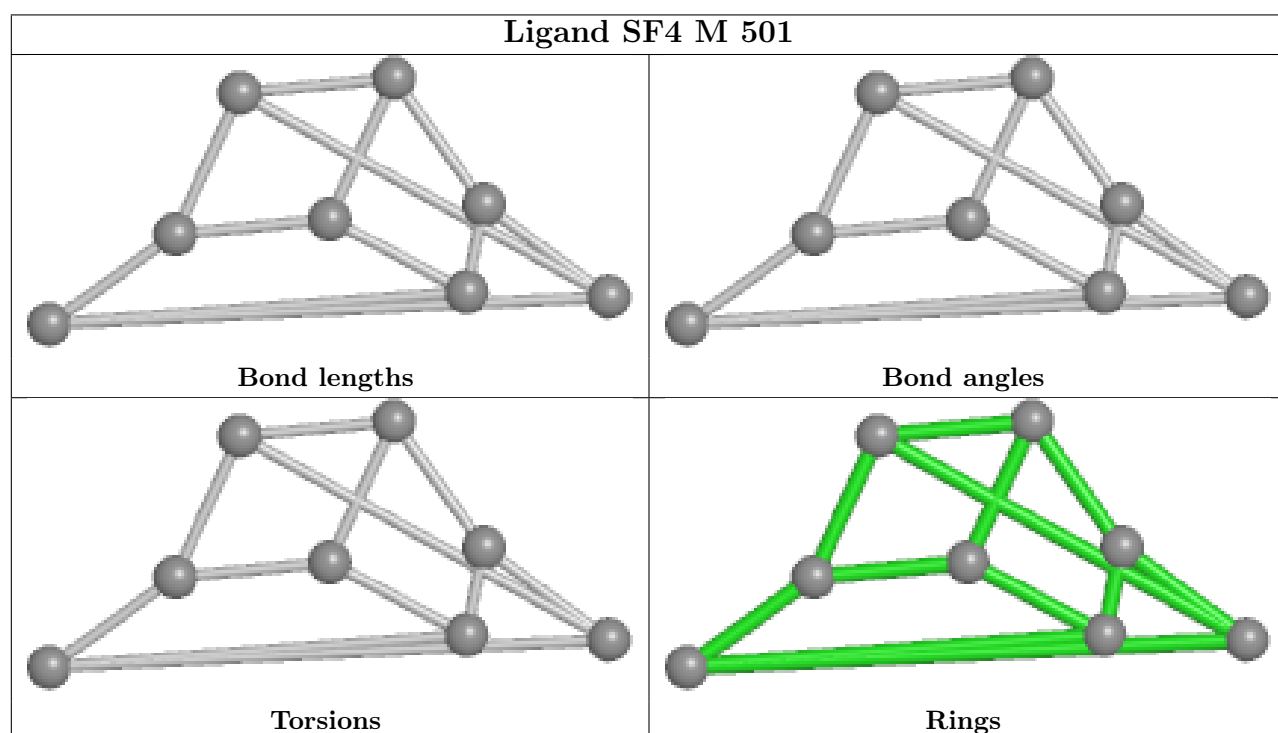
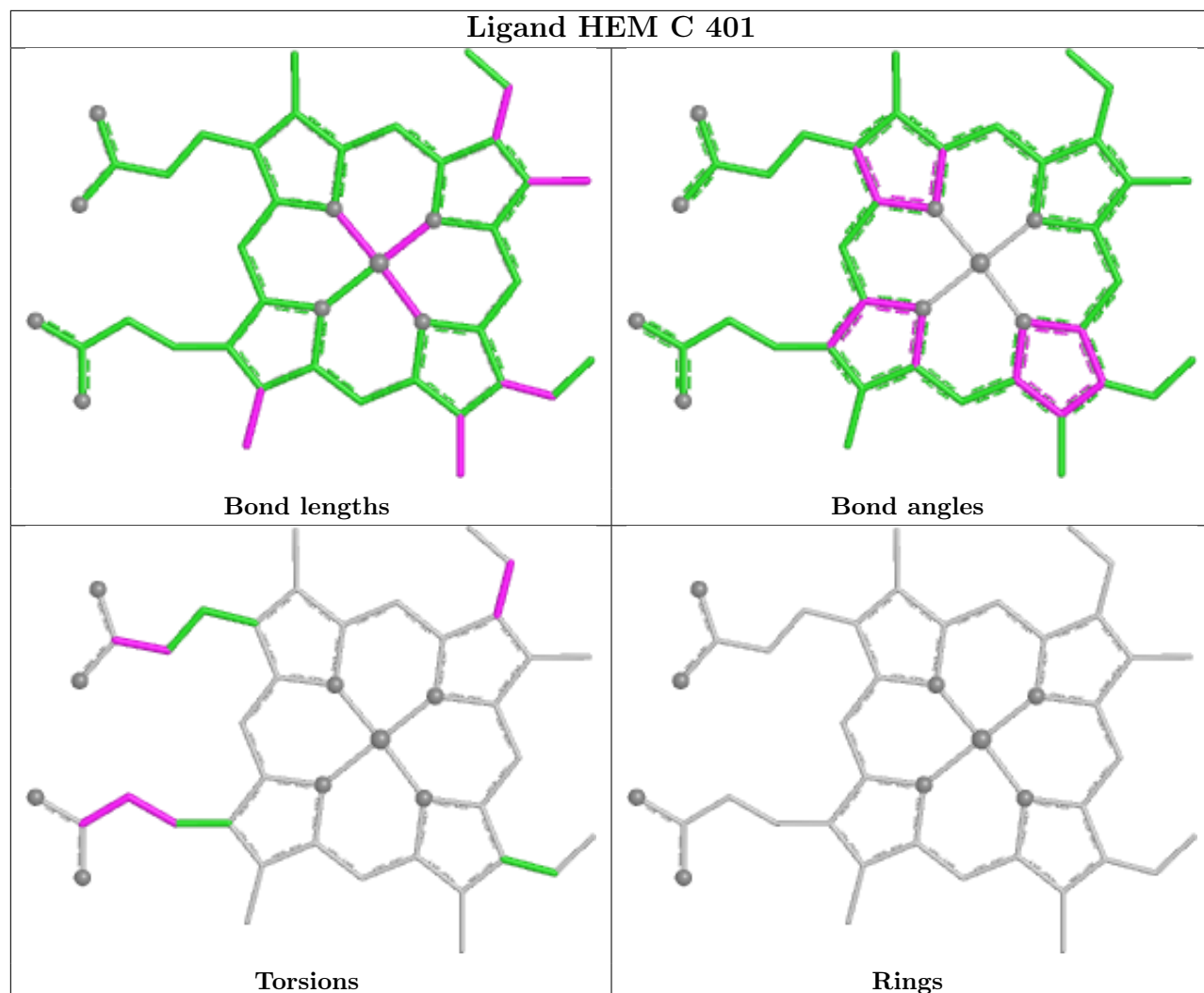


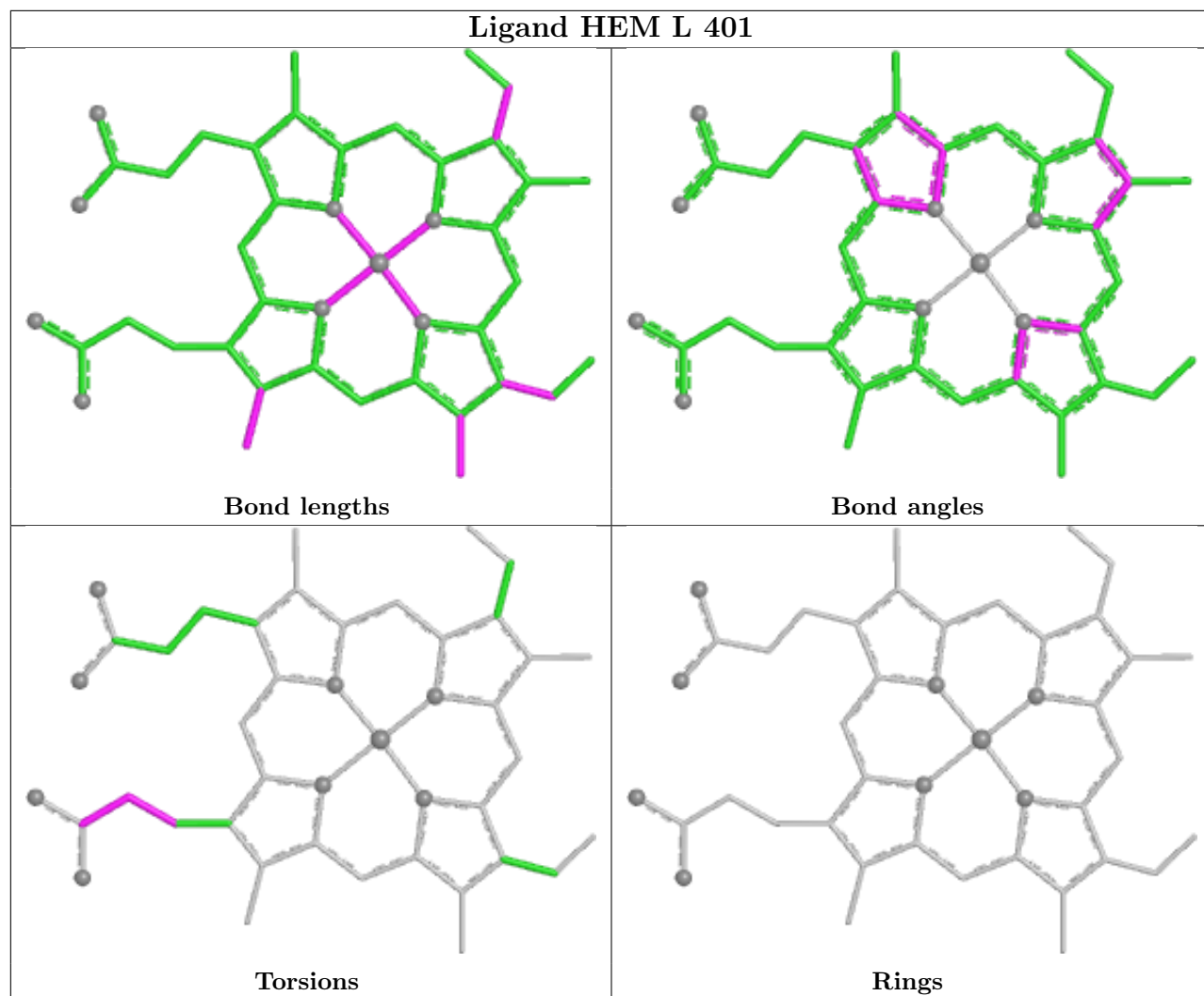
Ligand MD1 N 5802



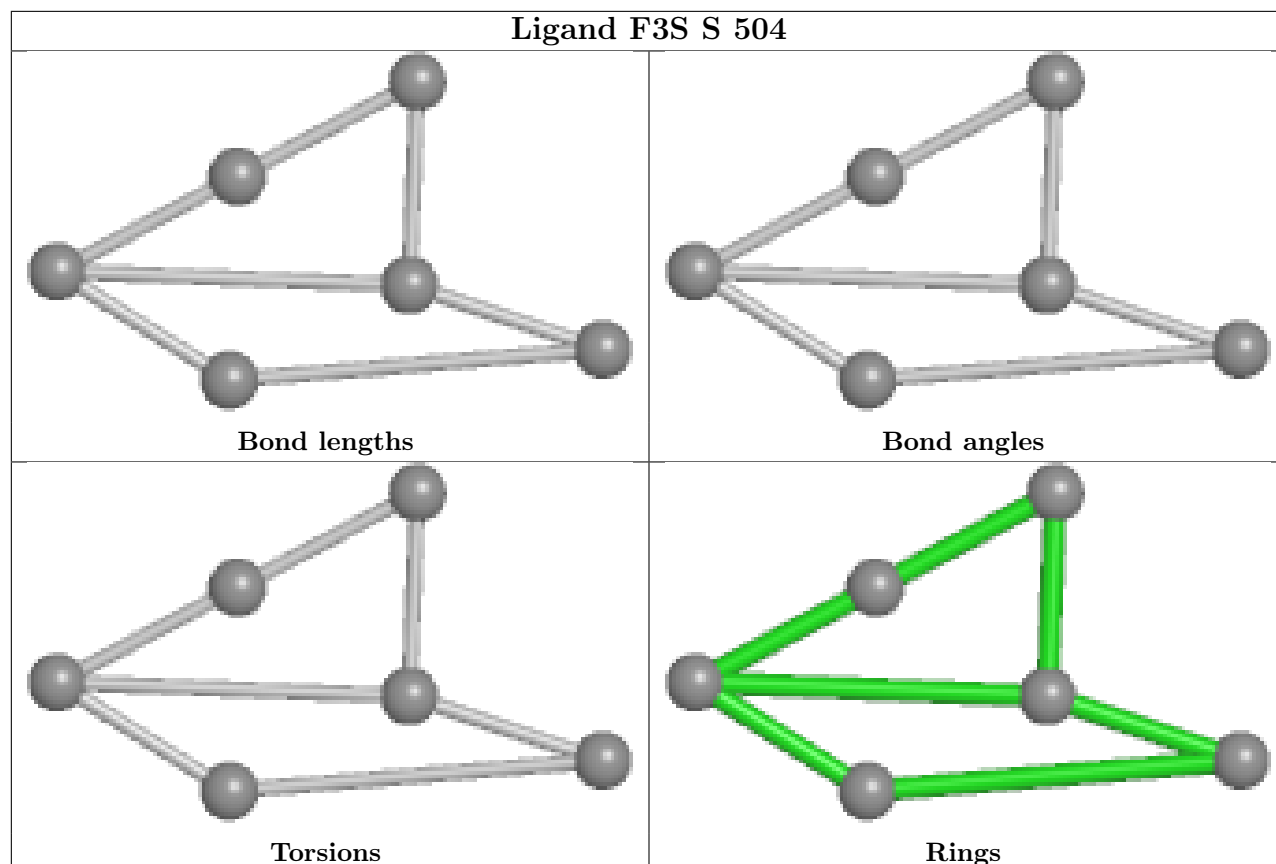




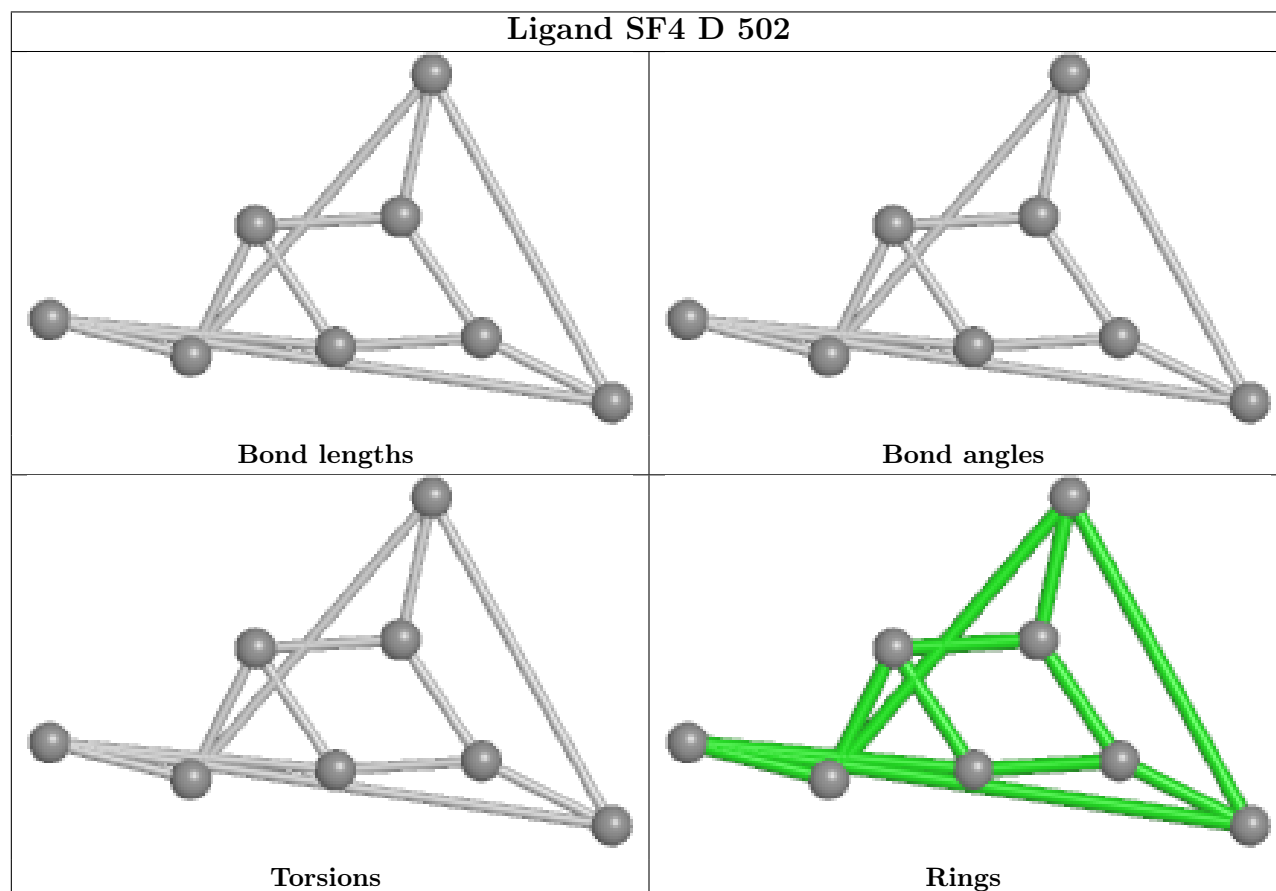




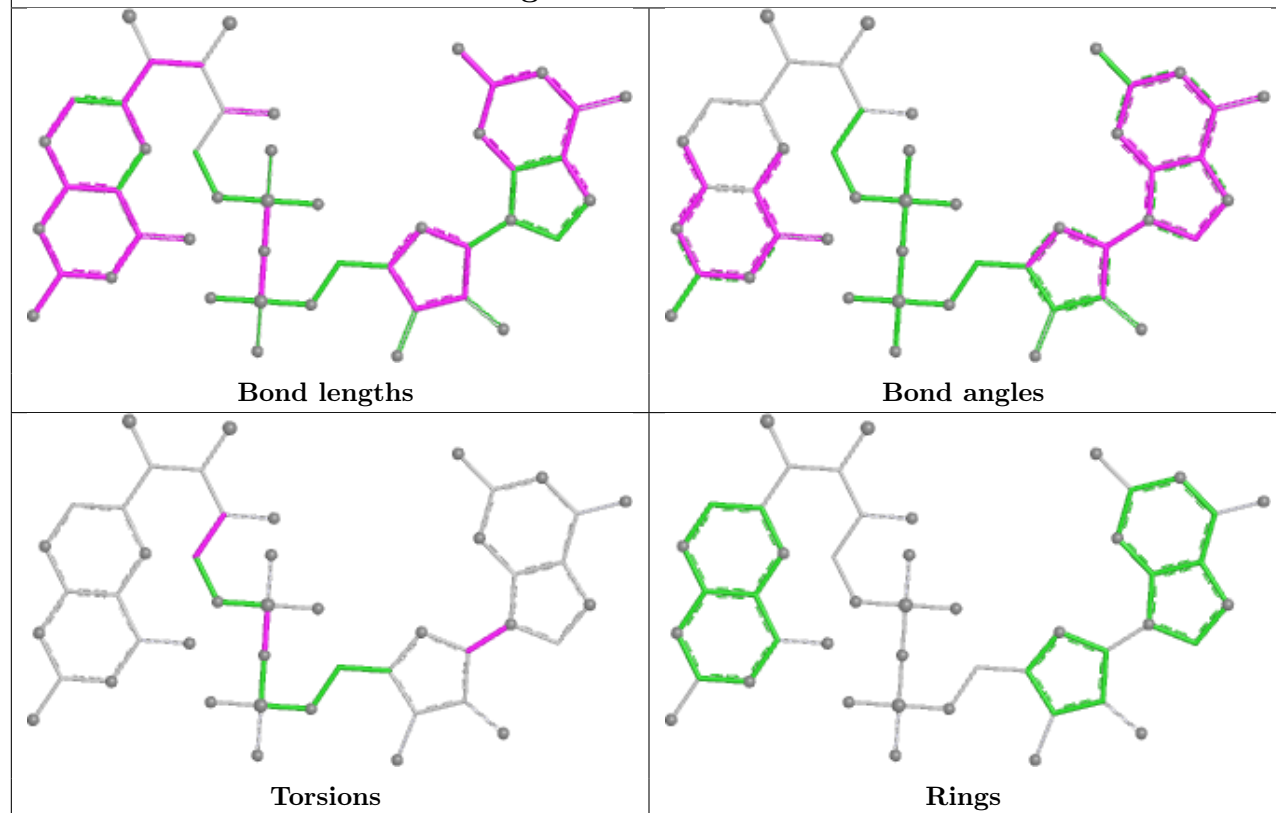
Ligand F3S S 504



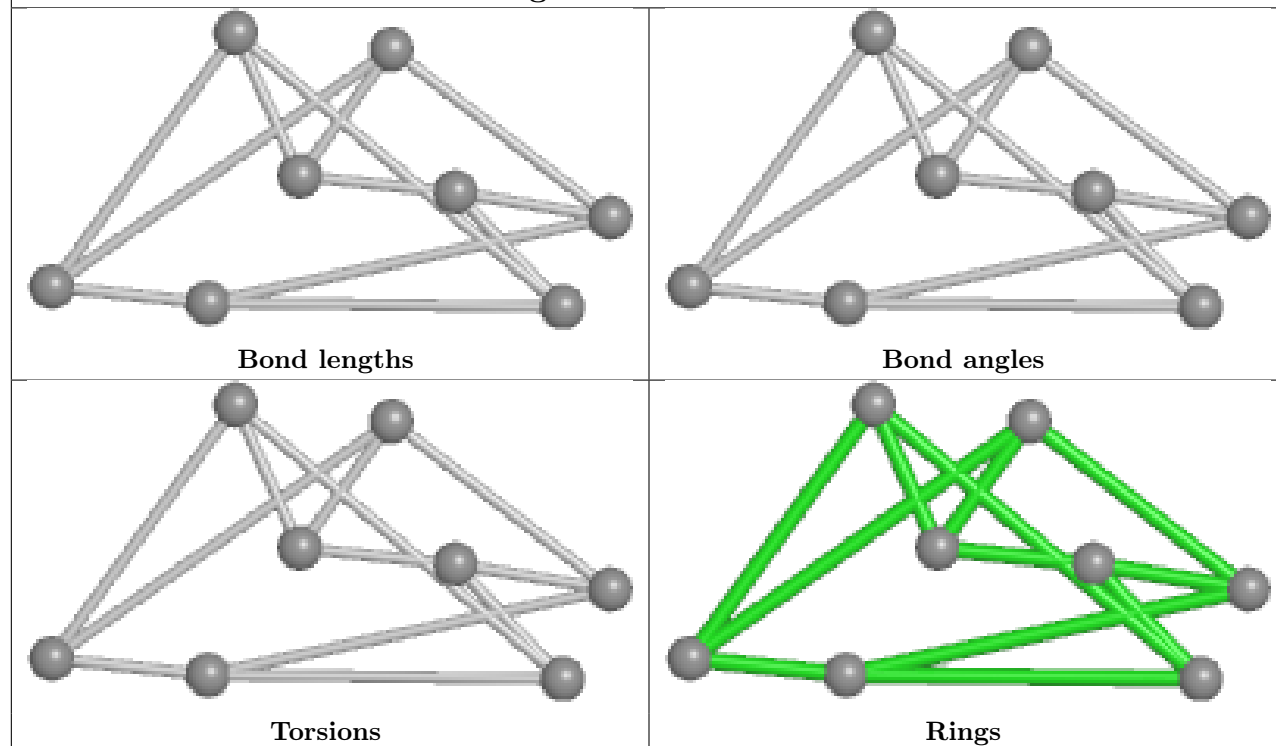
Ligand SF4 D 502

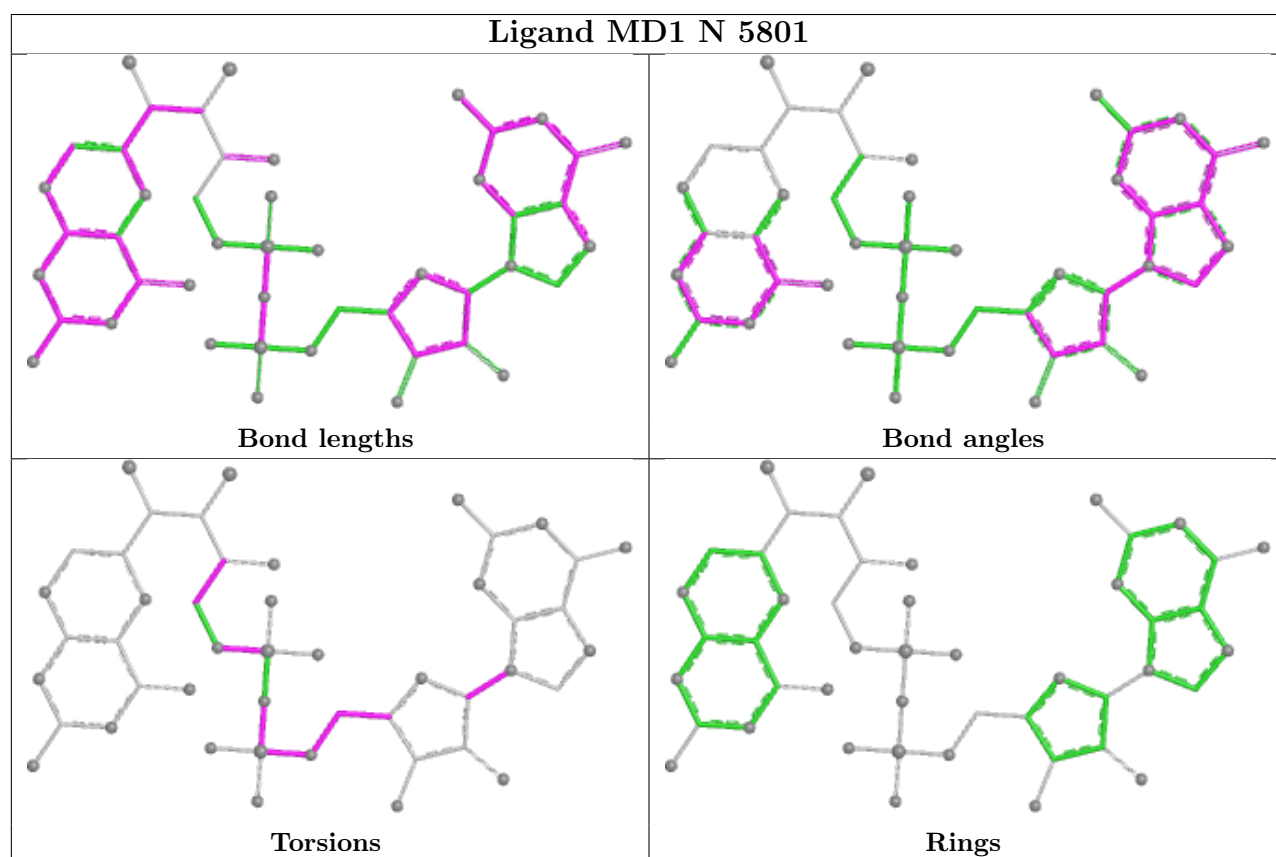
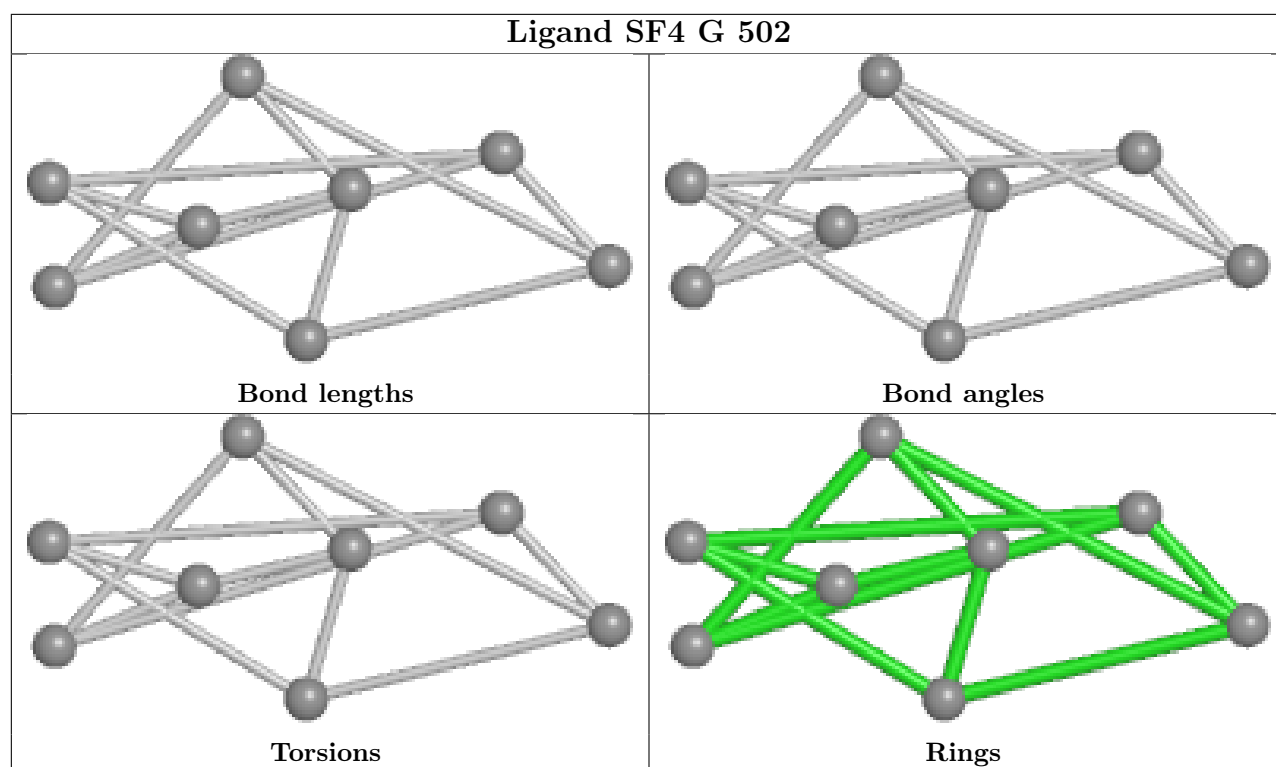


Ligand MD1 B 5802

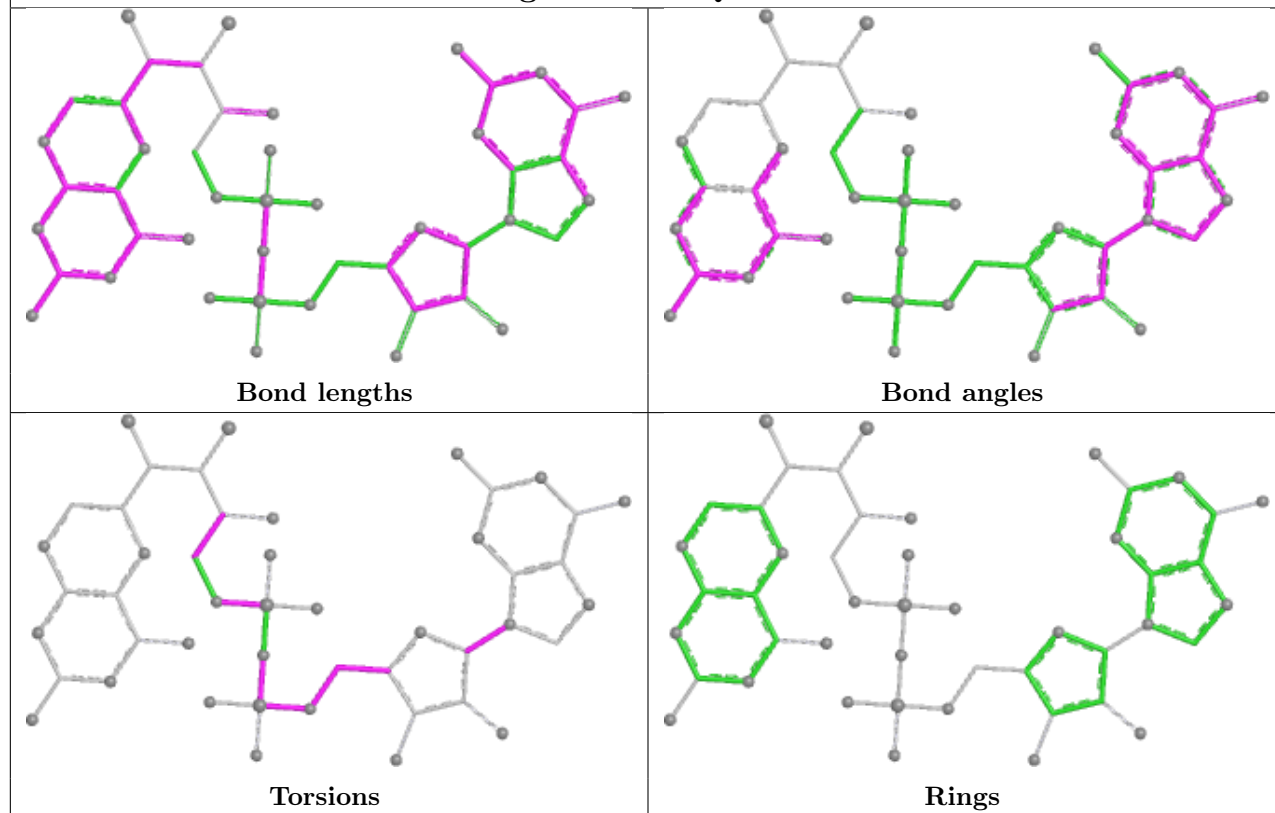


Ligand SF4 N 5804

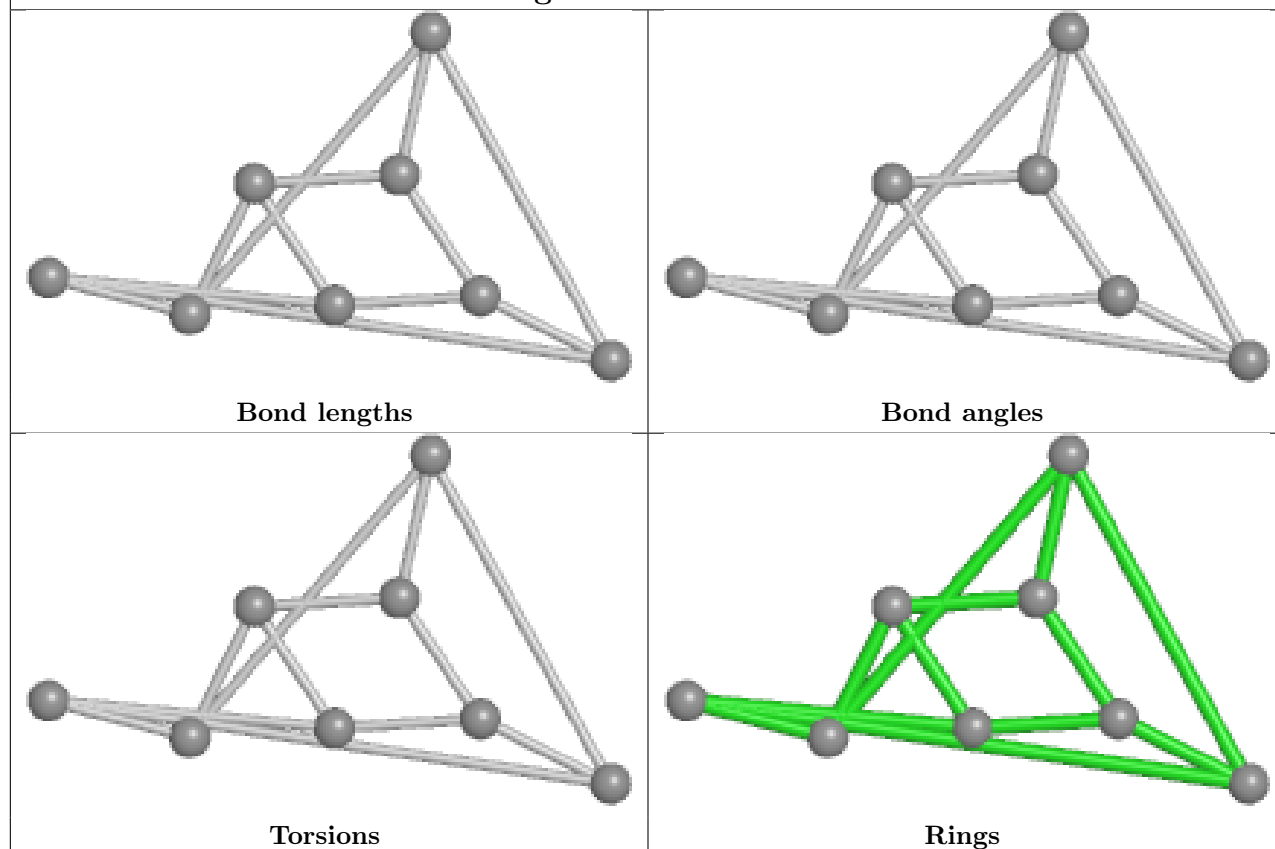




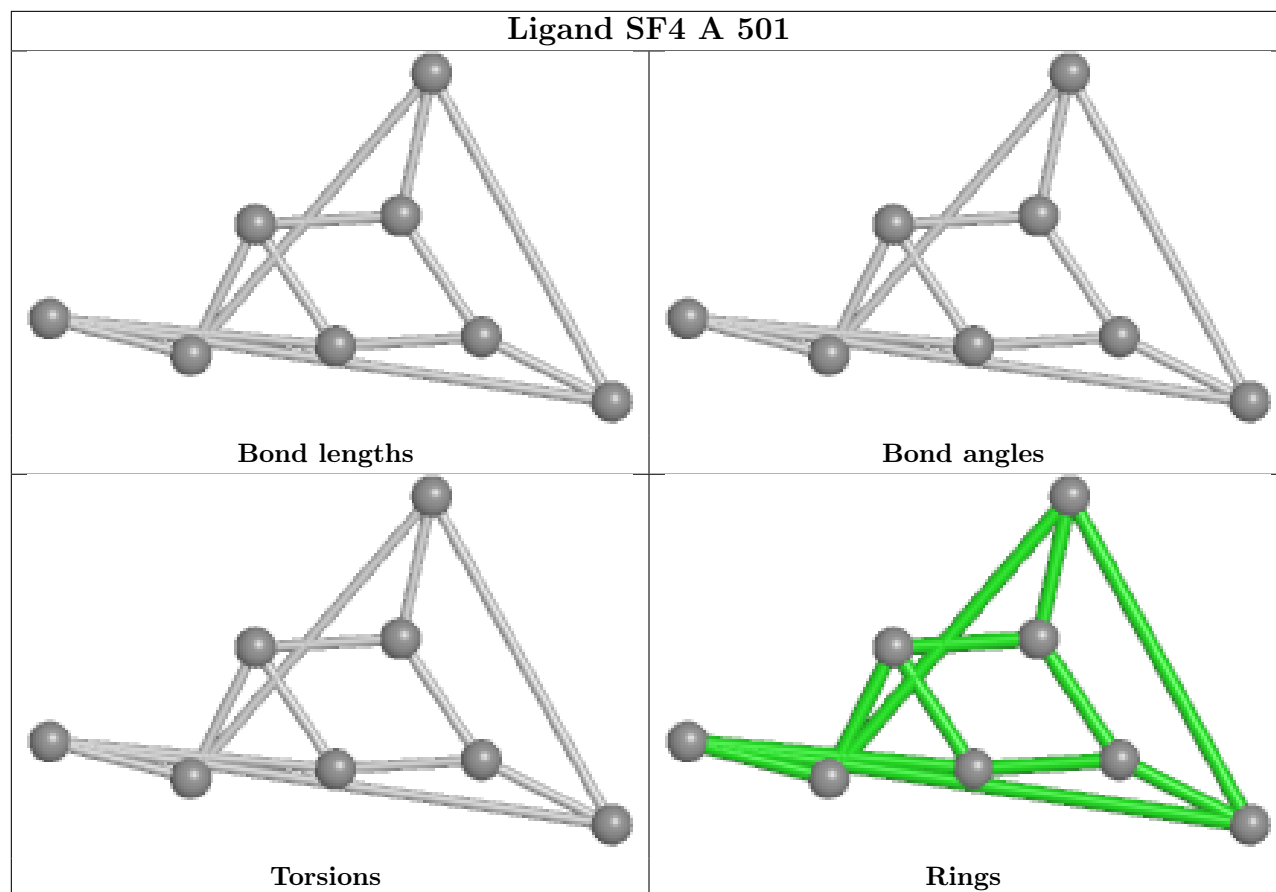
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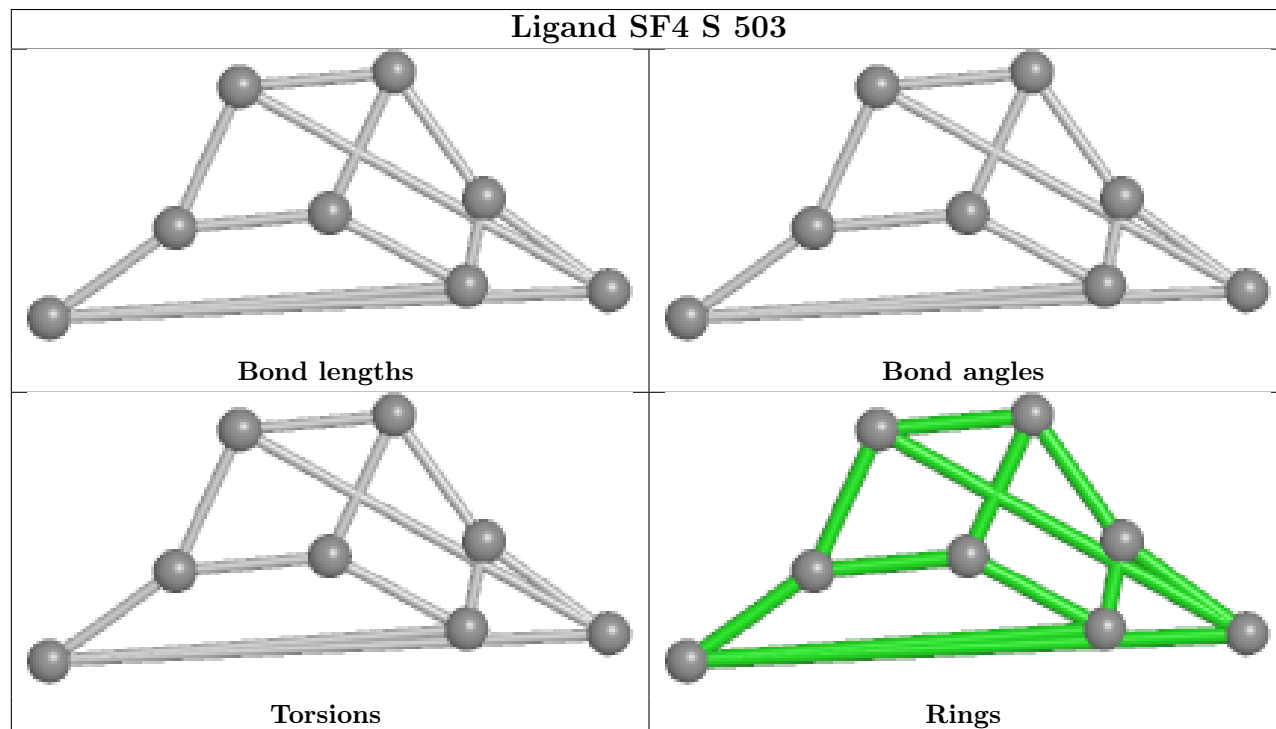
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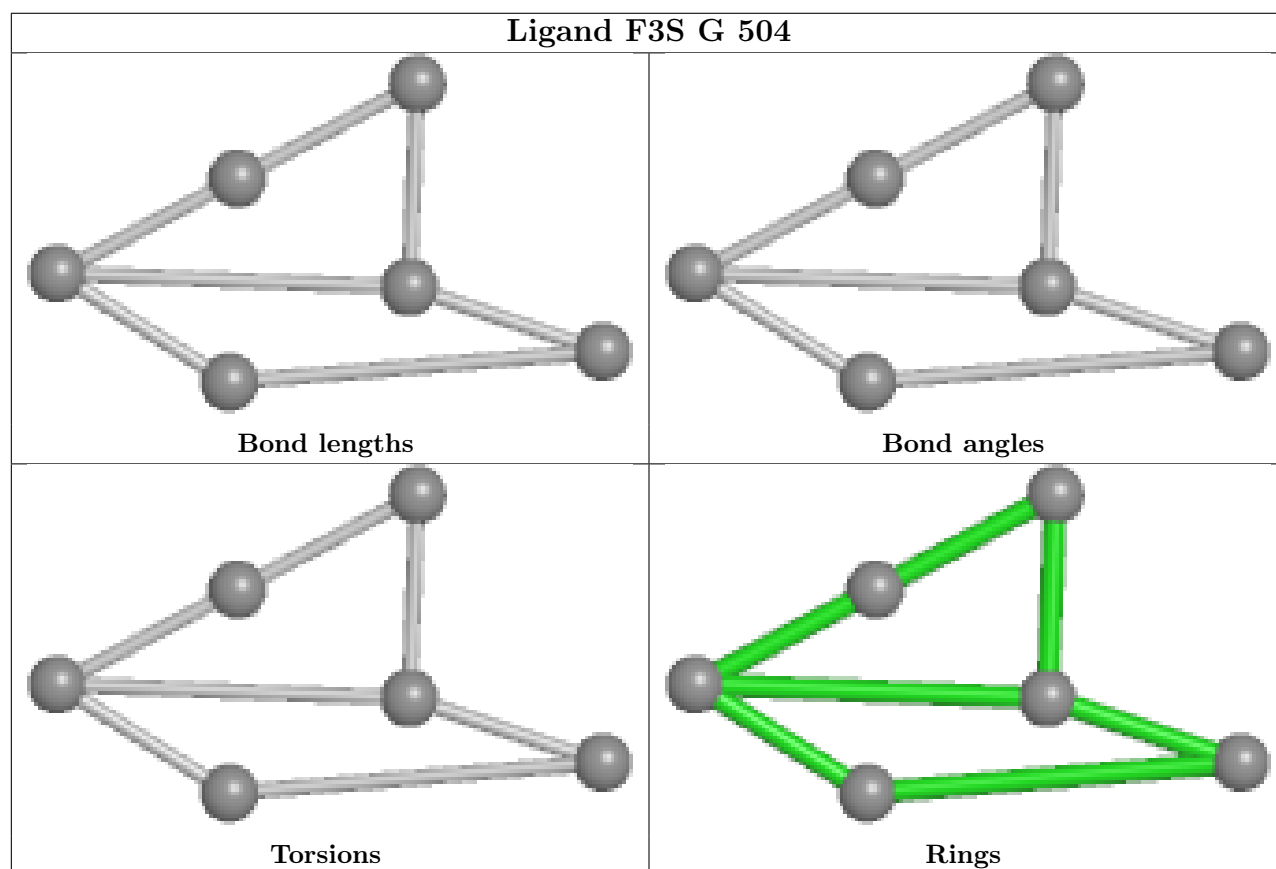
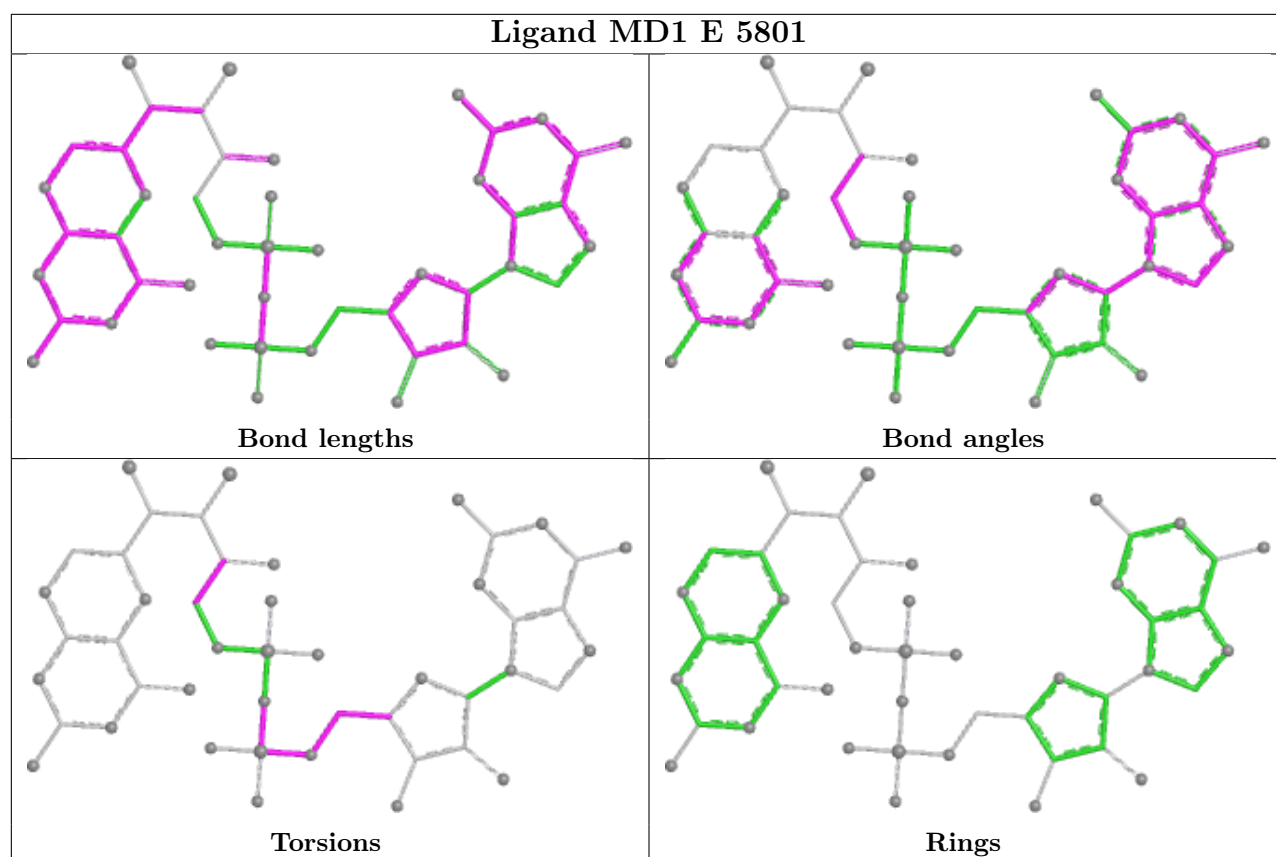


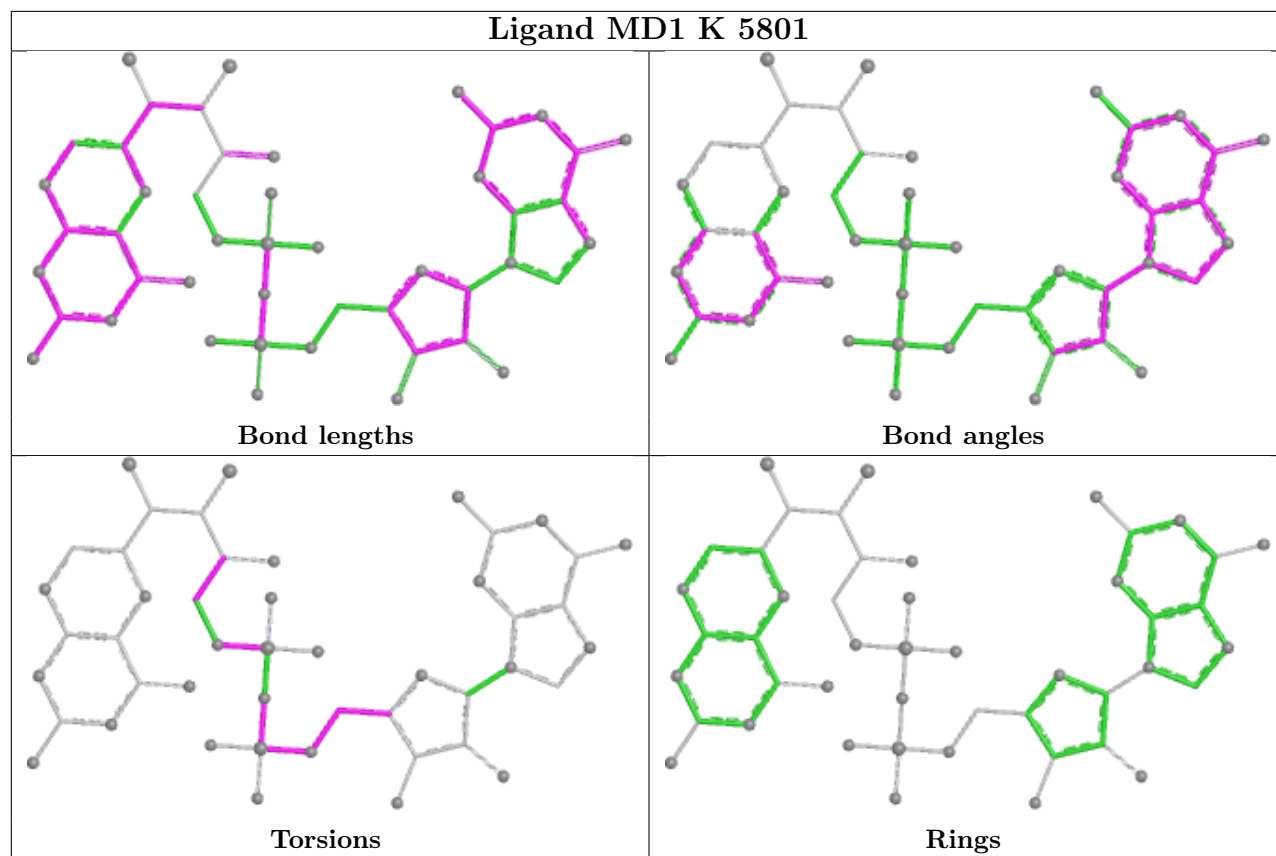
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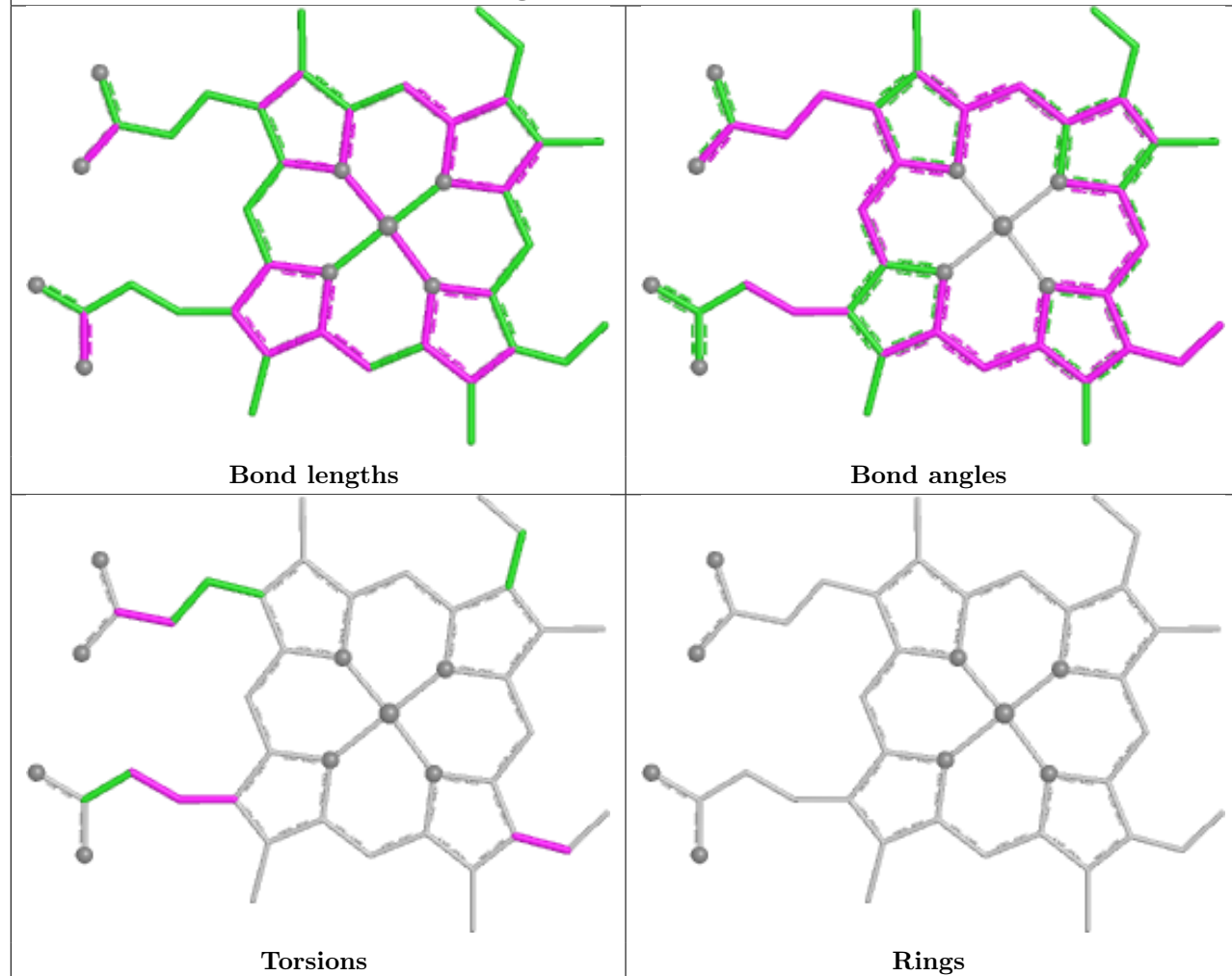
Ligand SF4 S 503



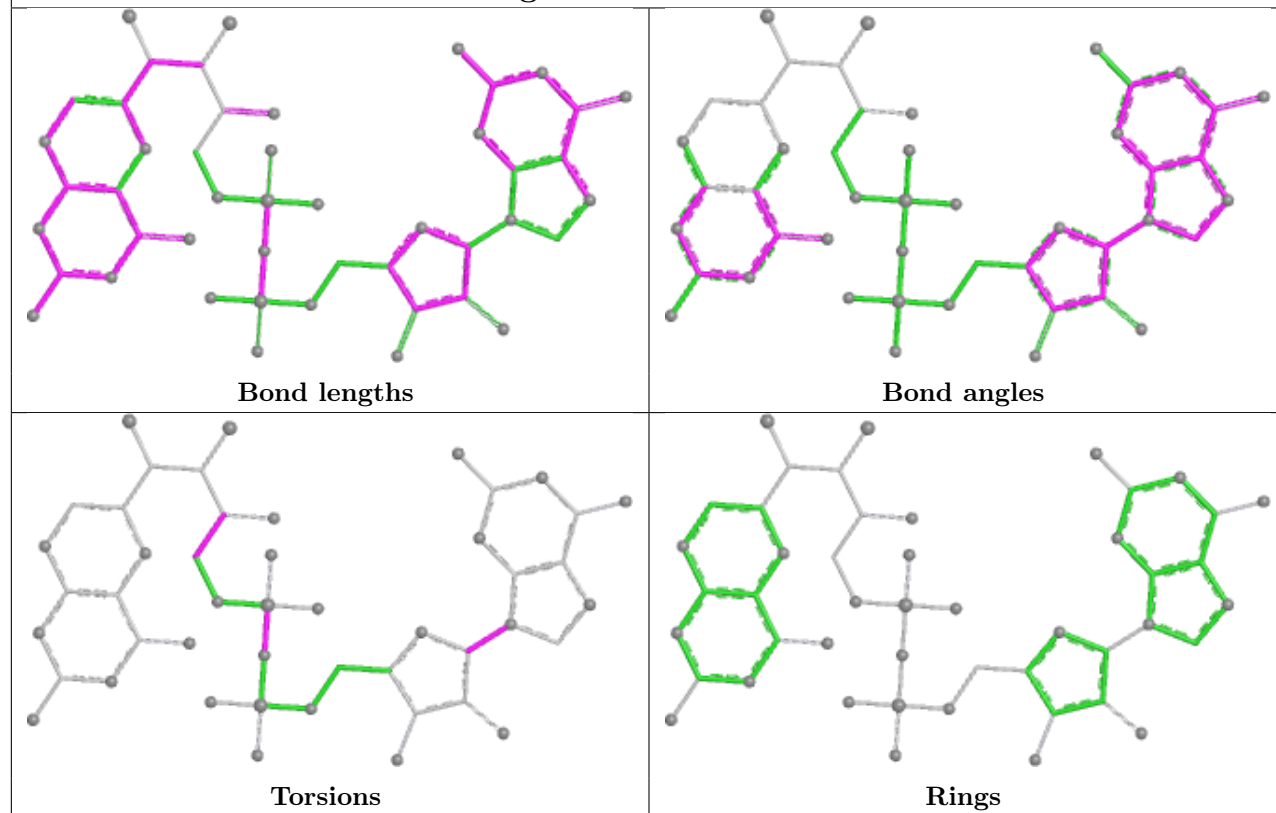




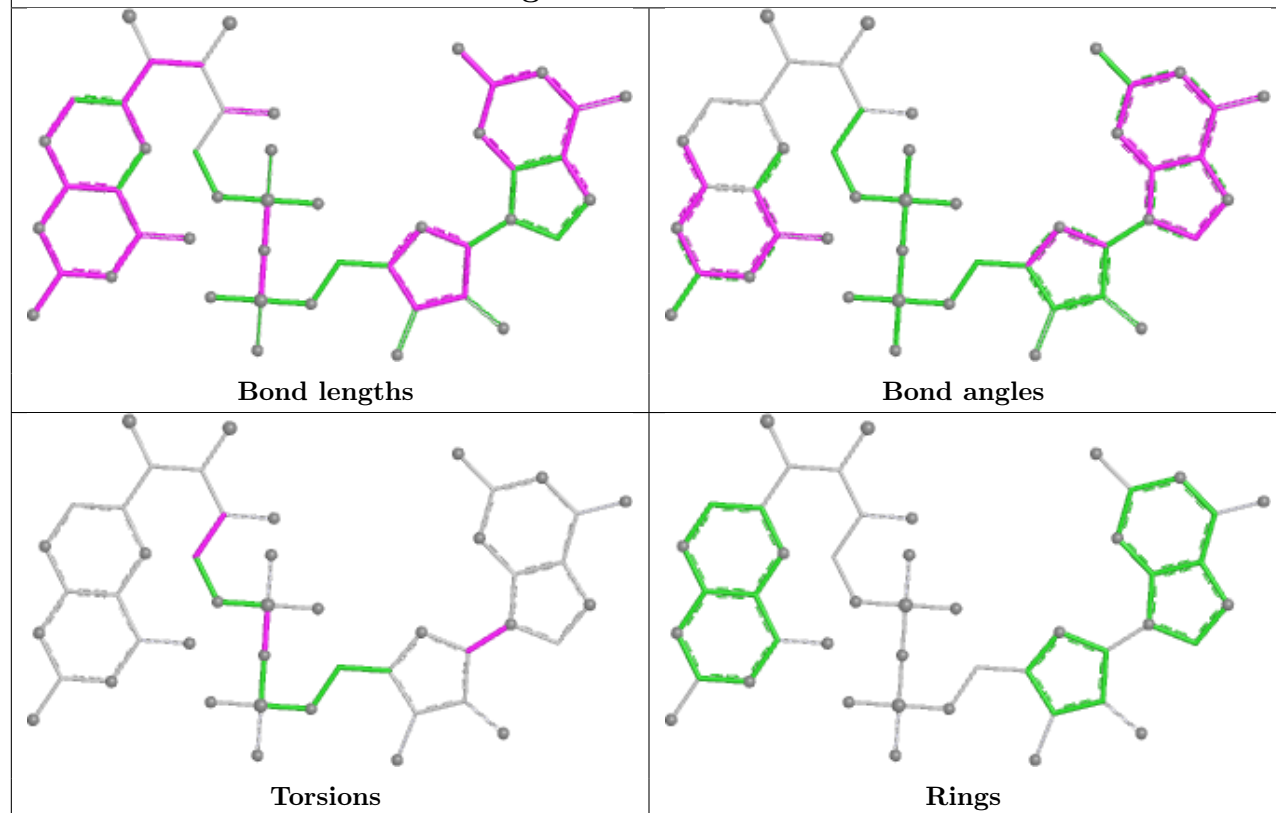
Ligand HEM I 401



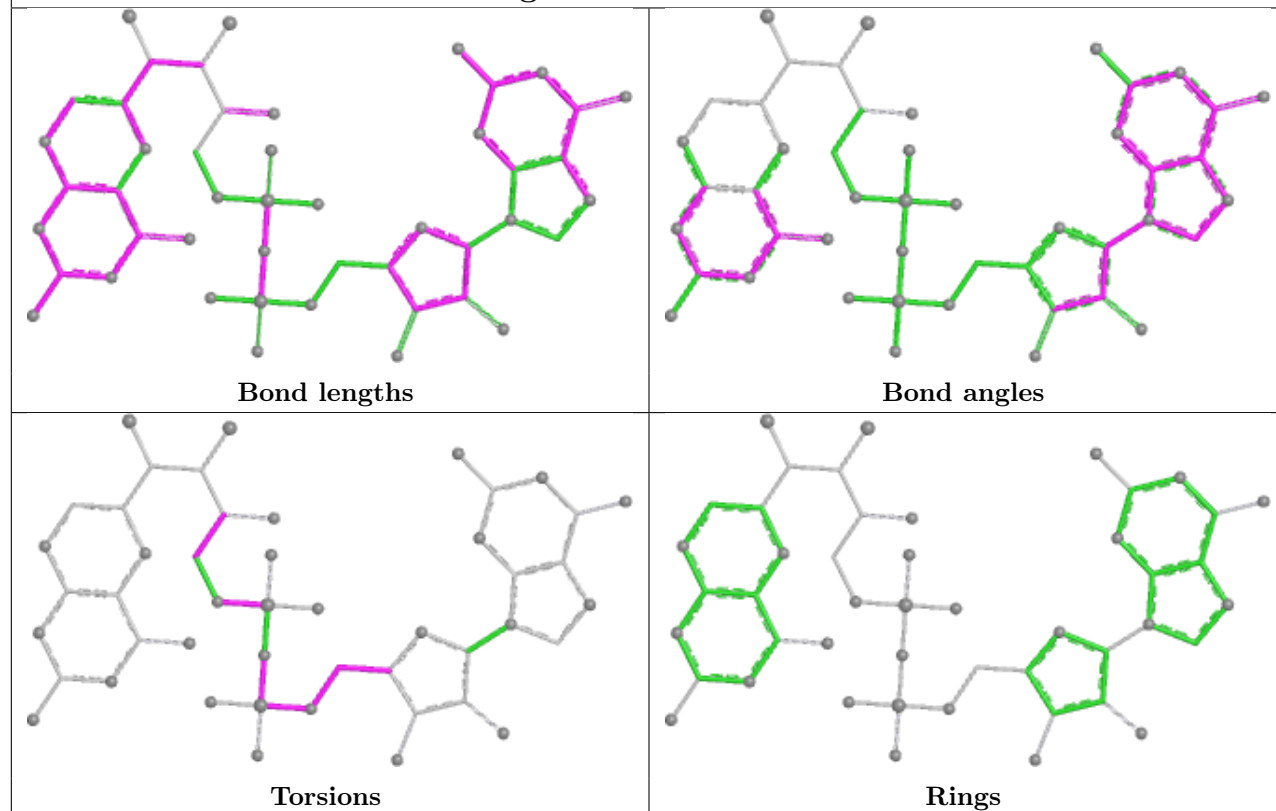
Ligand MD1 H 5802



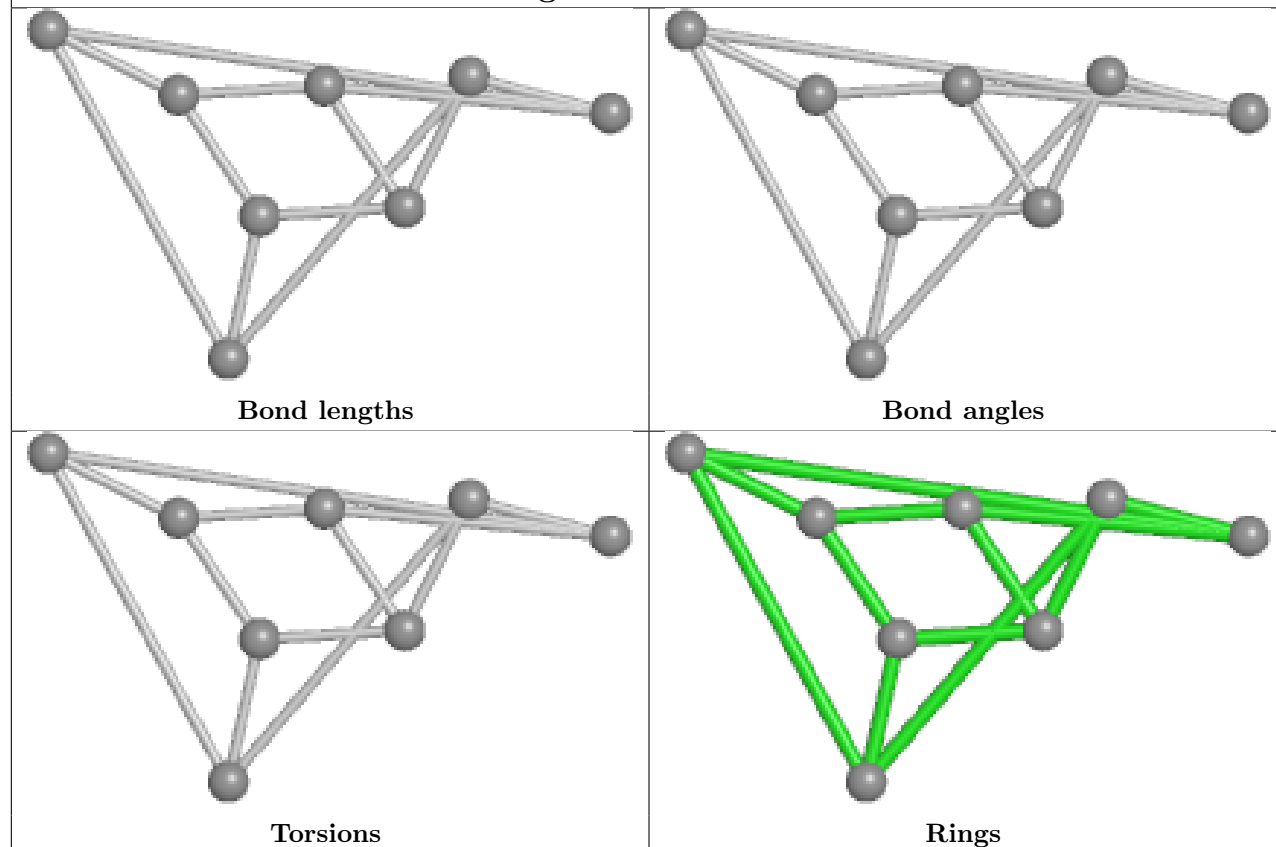
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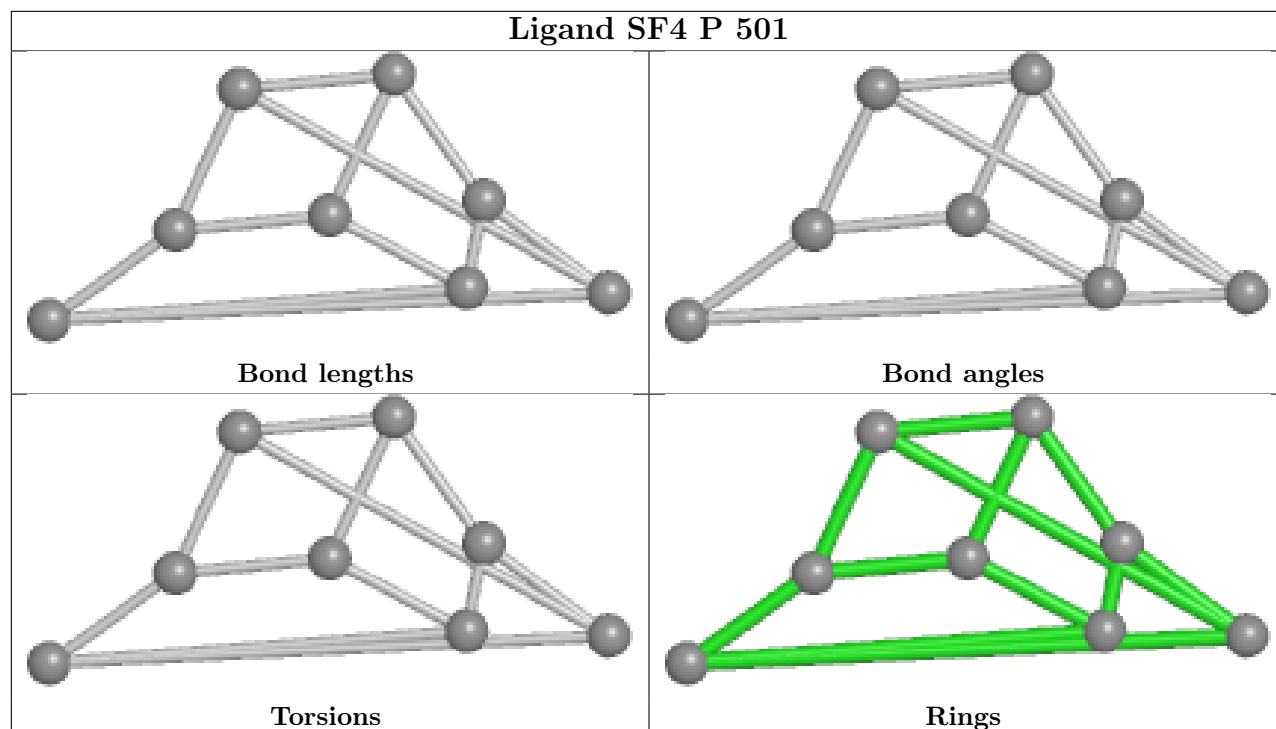
Ligand MD1 H 5801



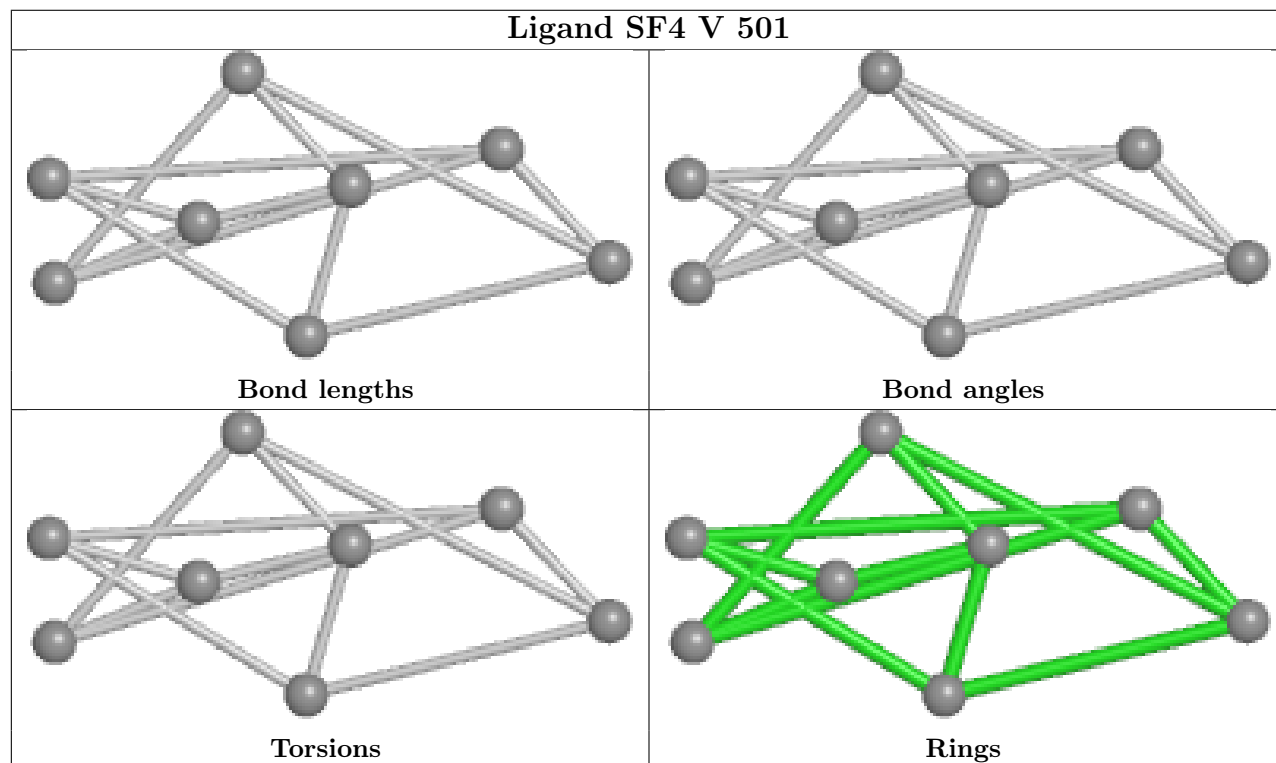
Ligand SF4 A 503

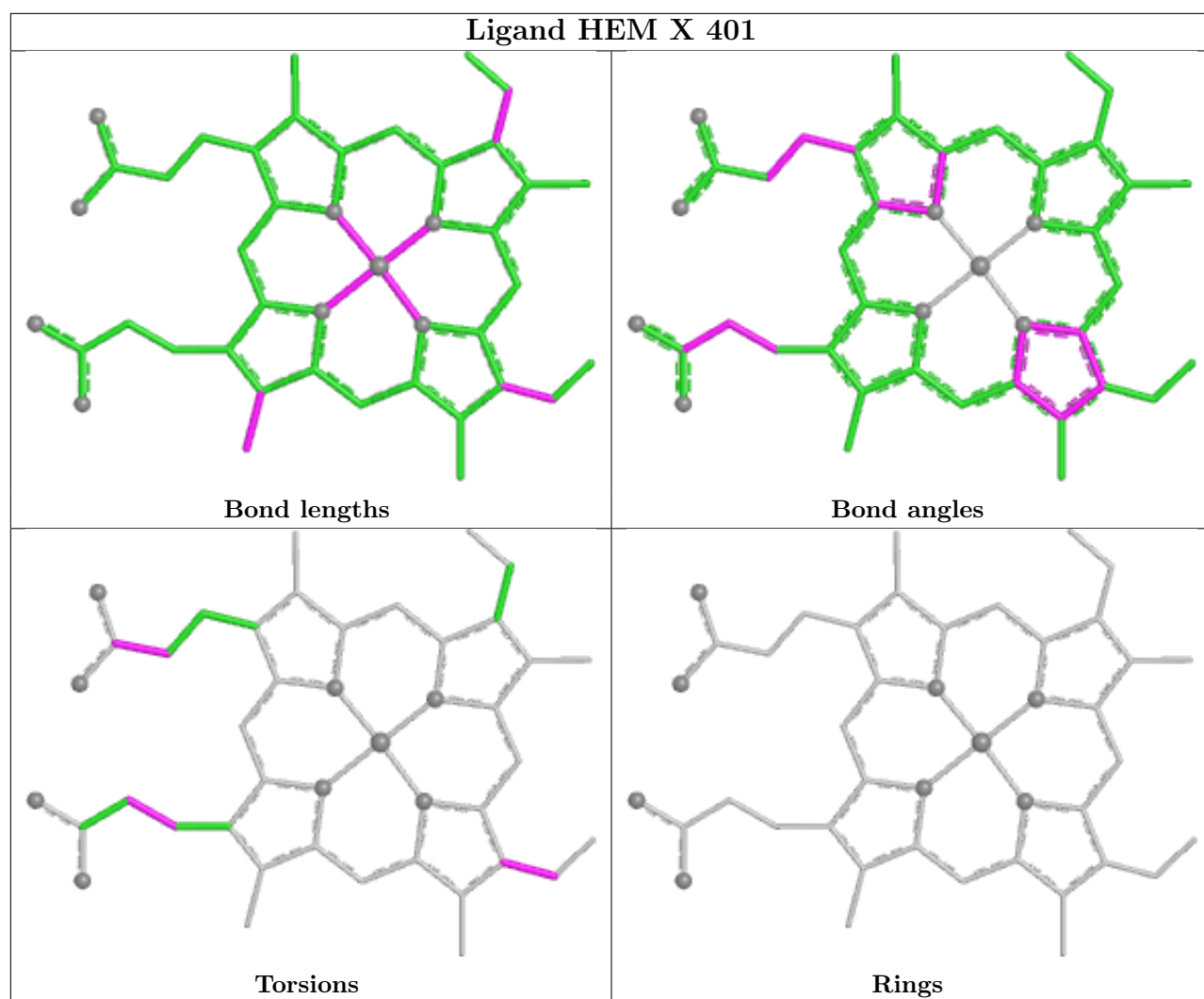


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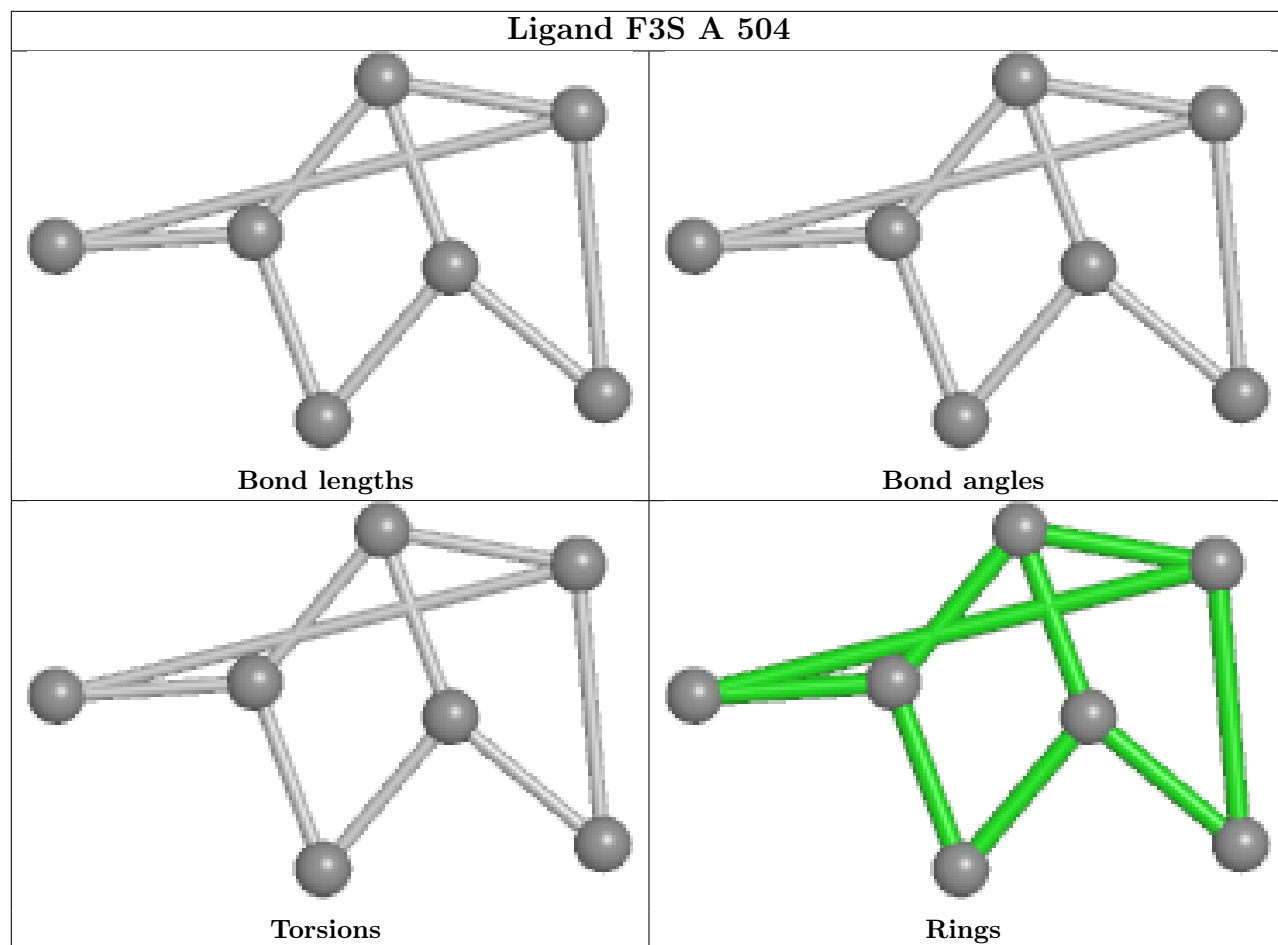


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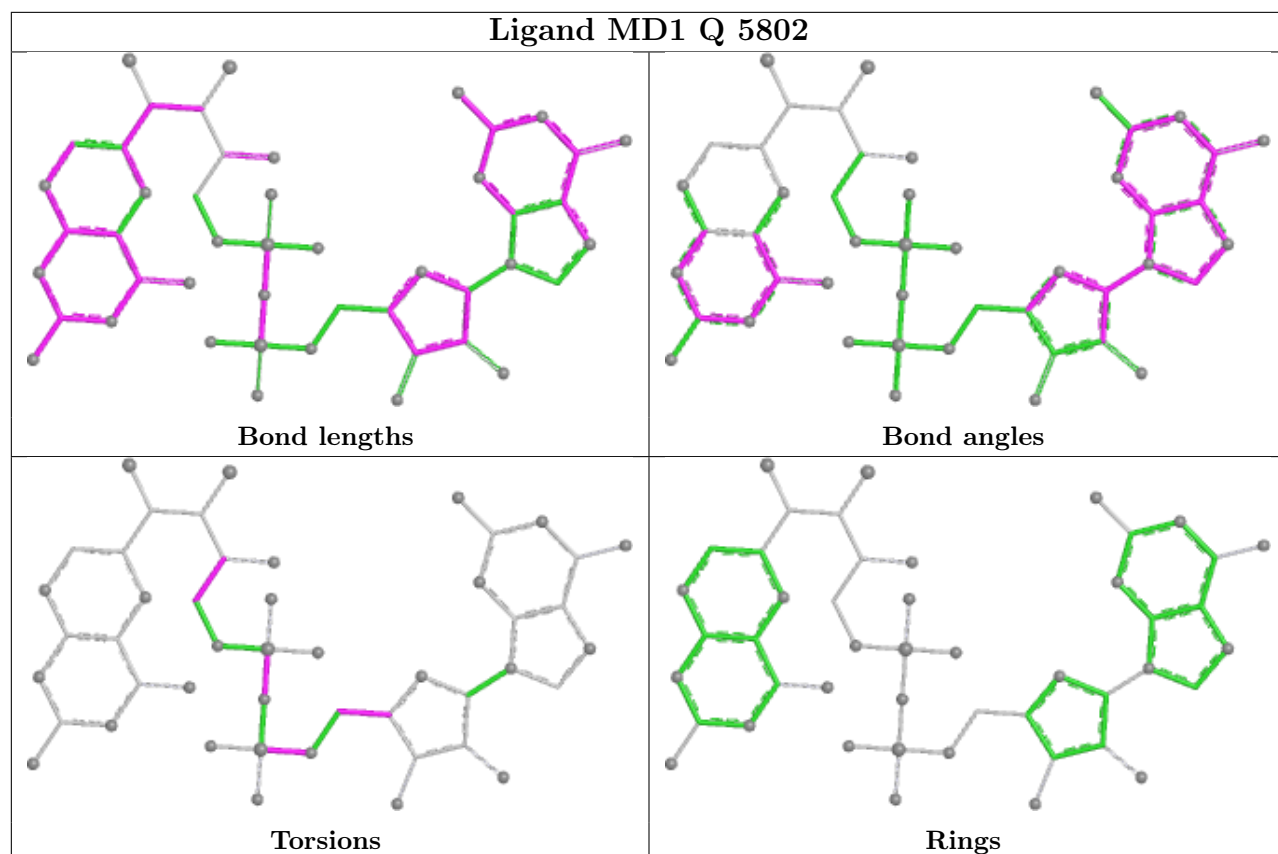




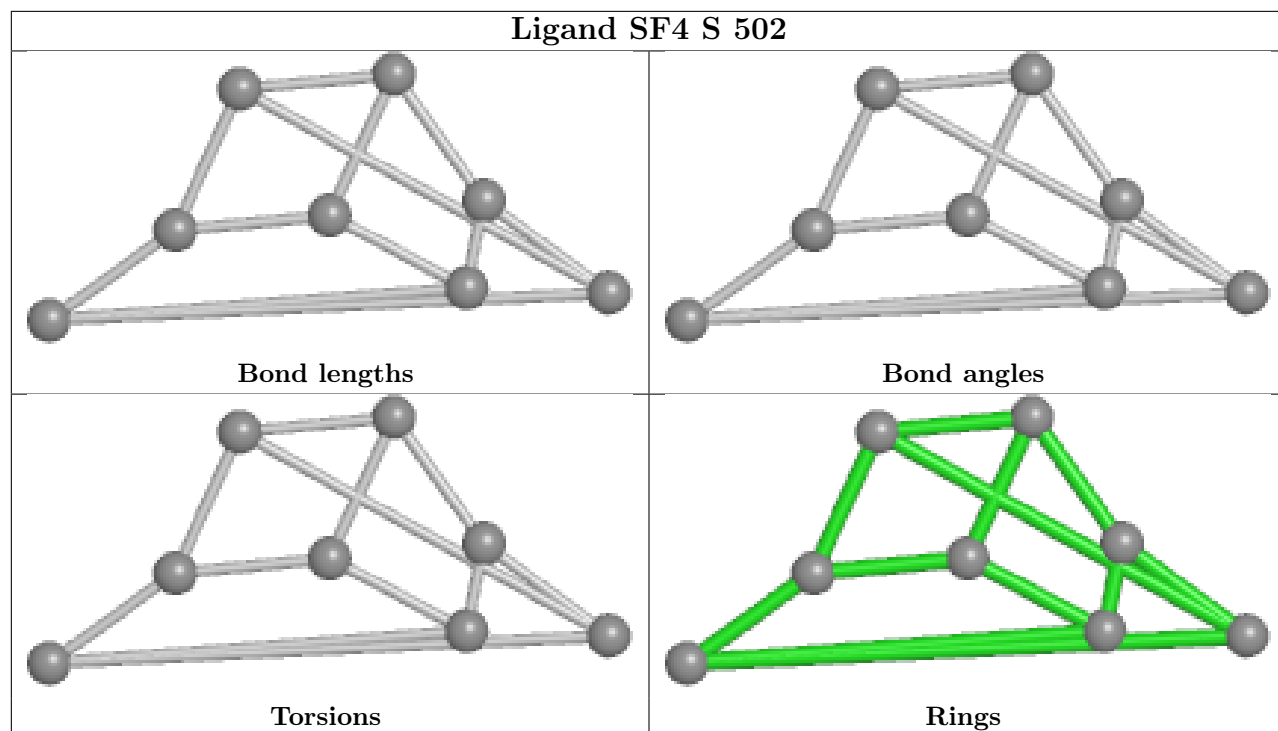
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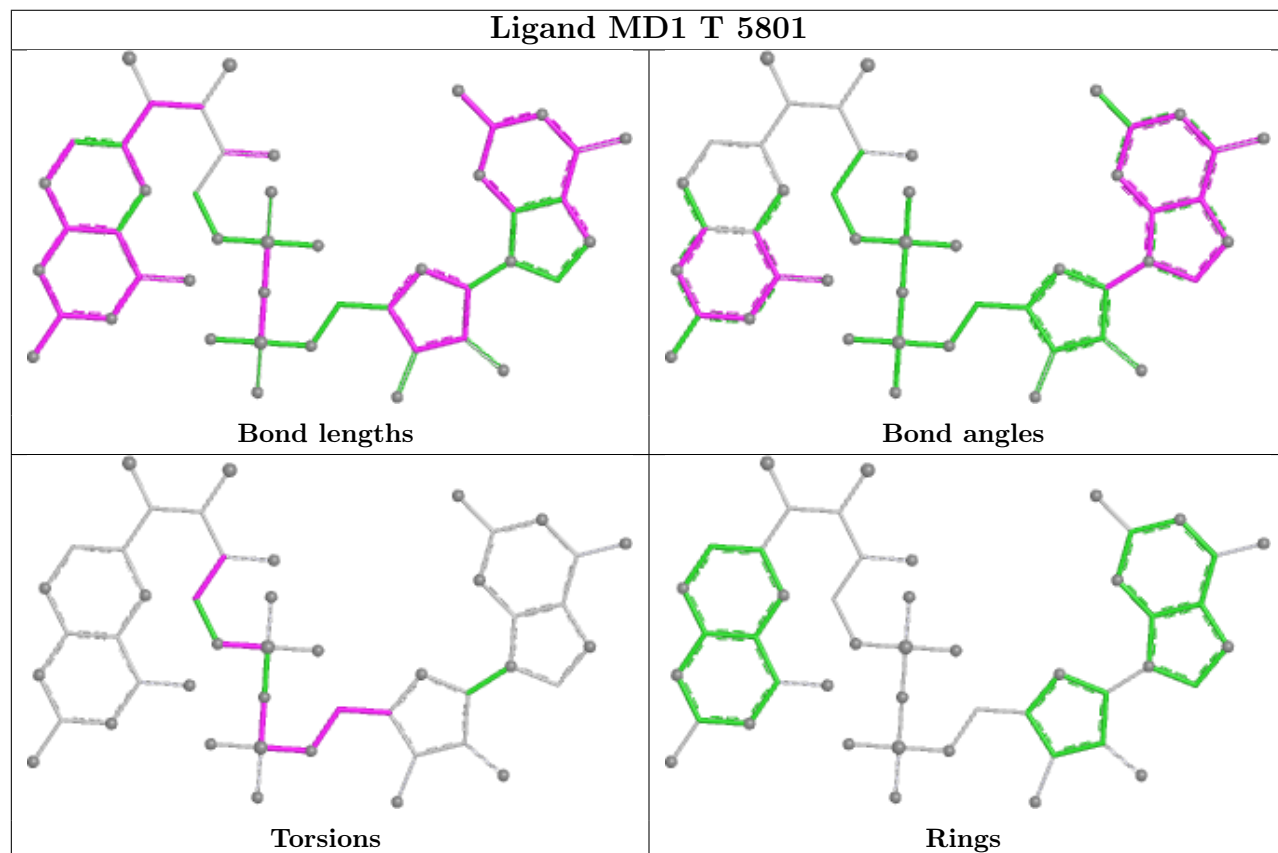
Ligand MD1 Q 5802

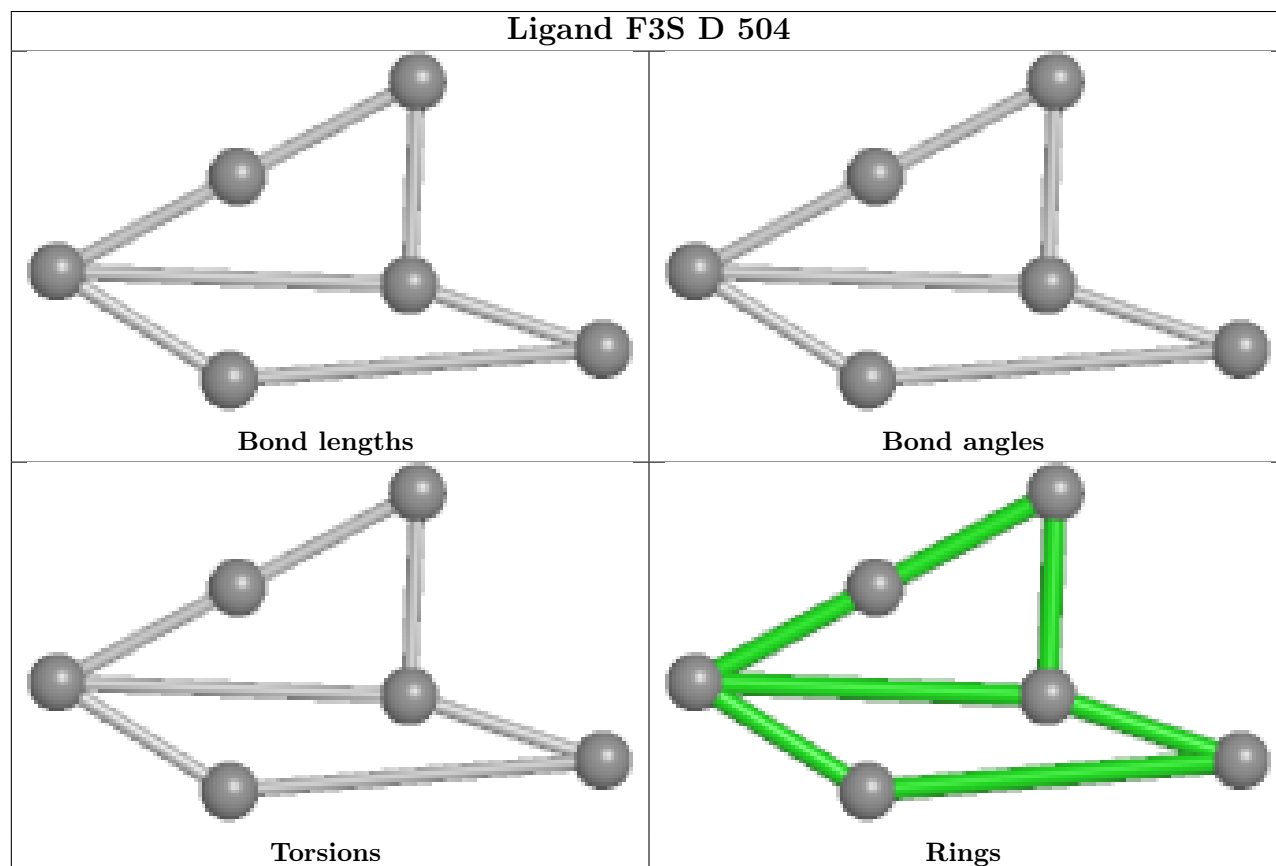
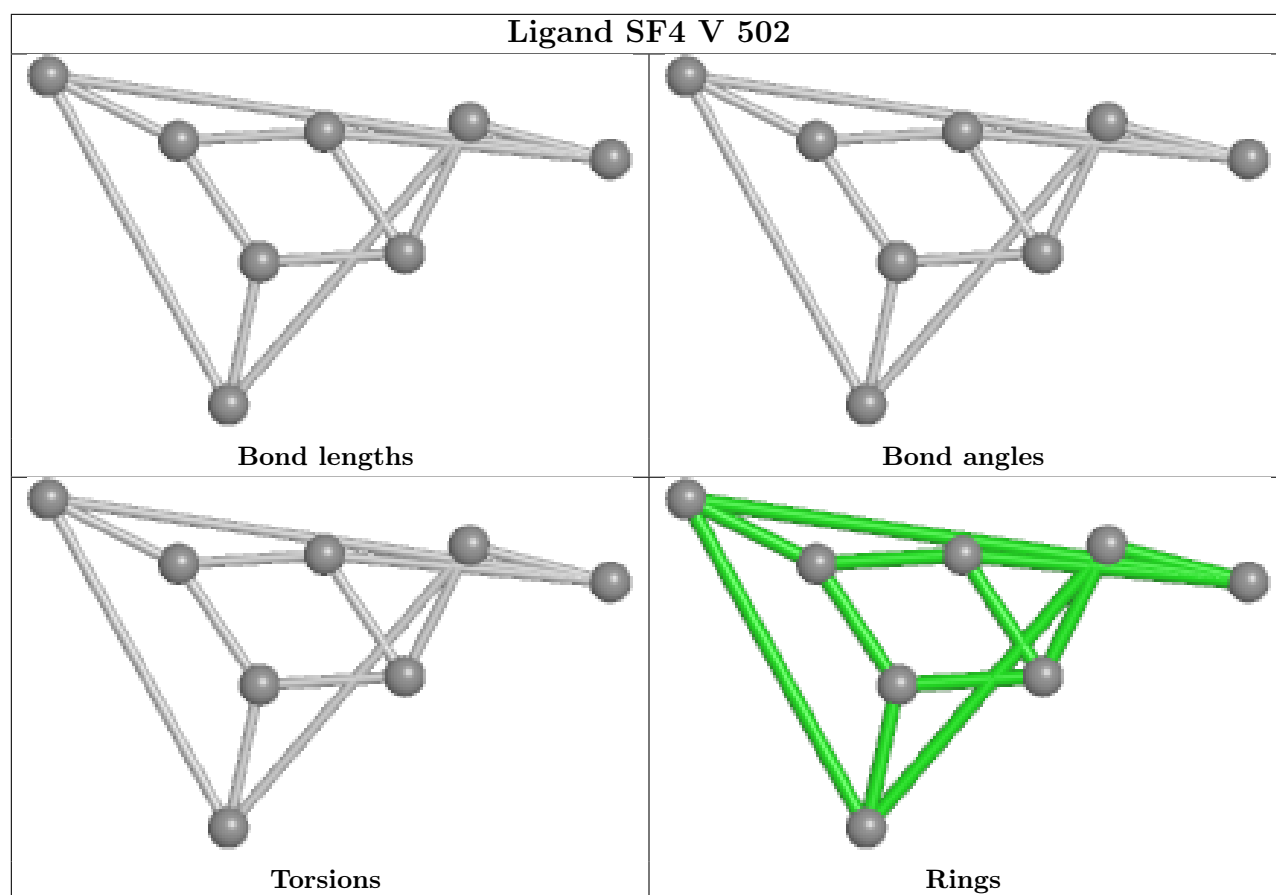


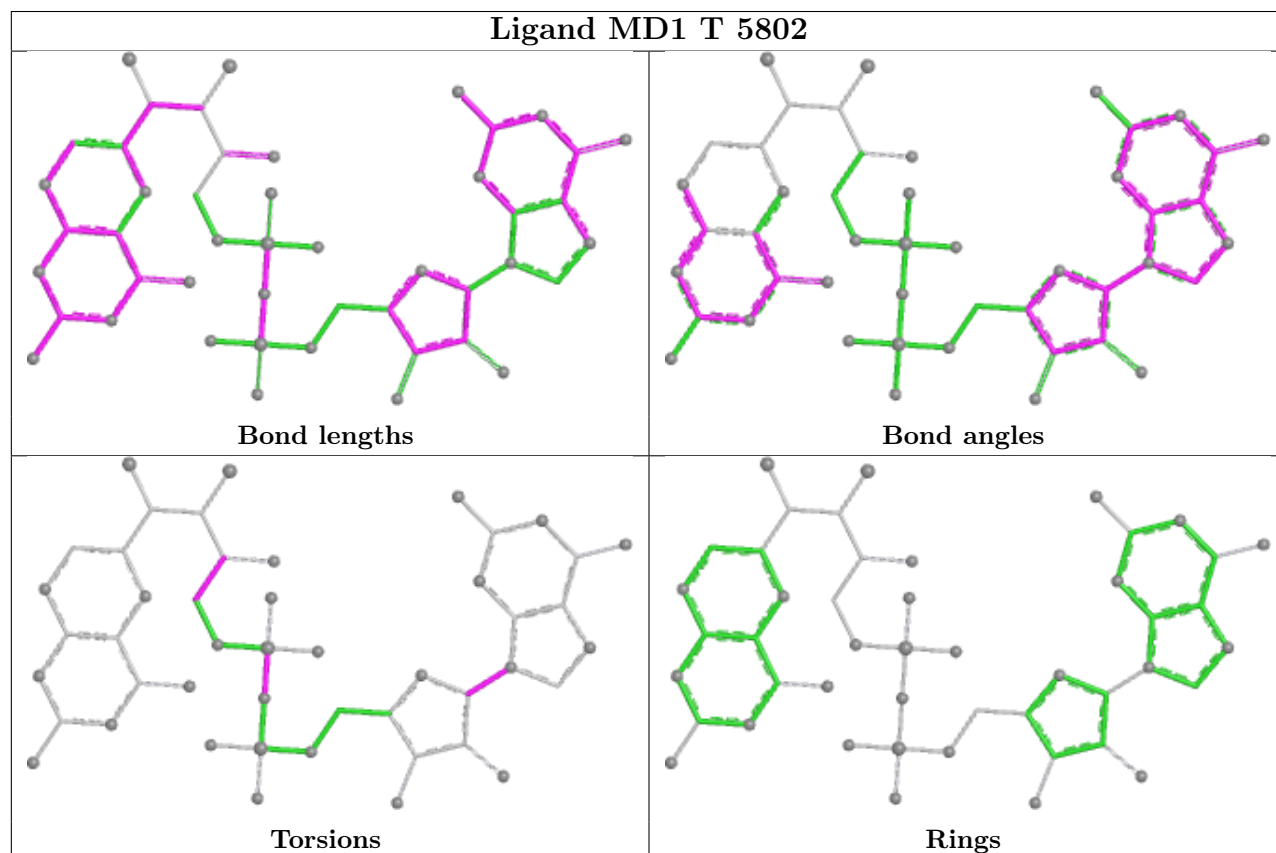
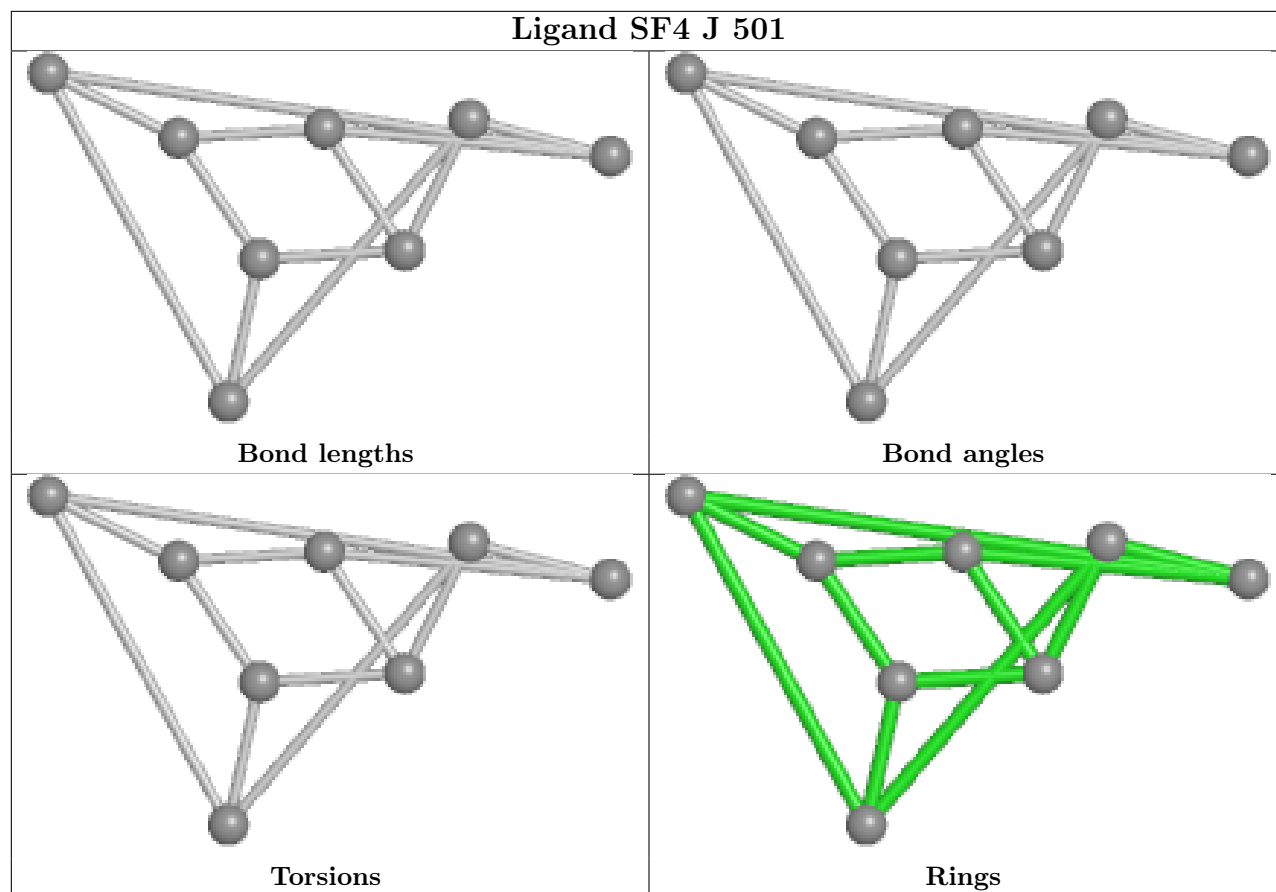
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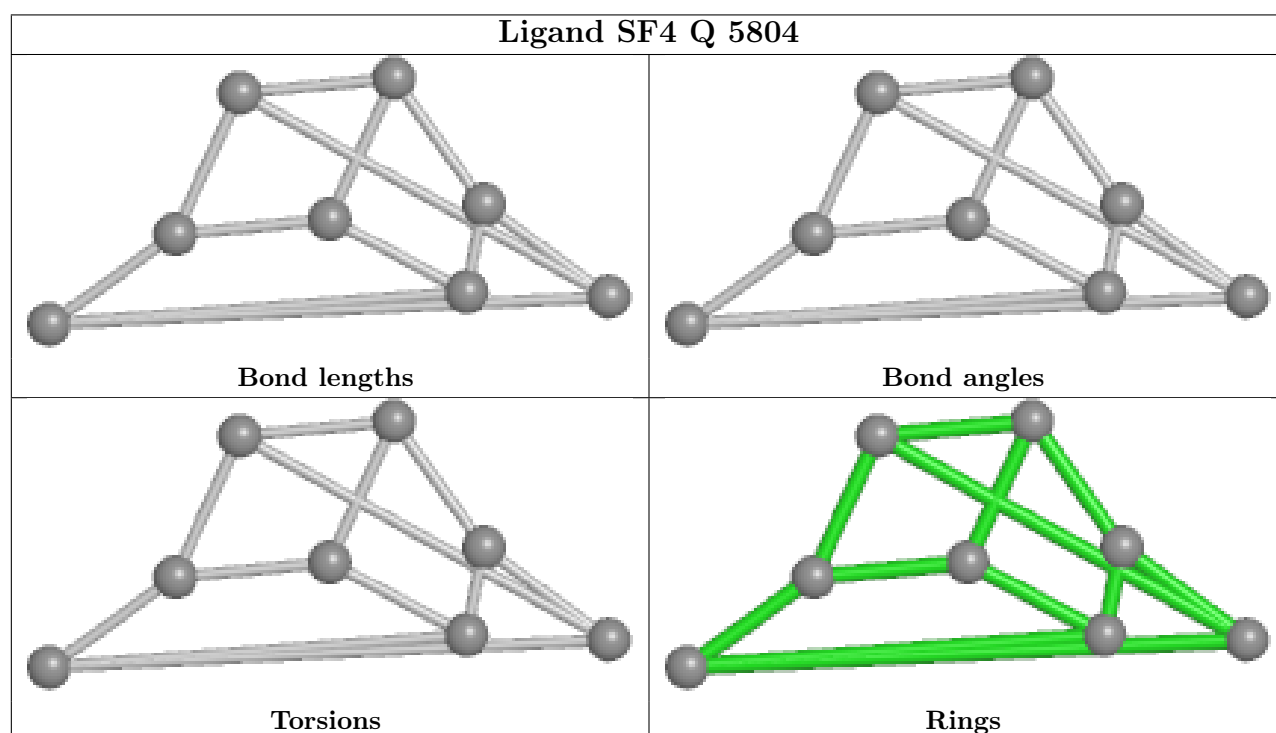
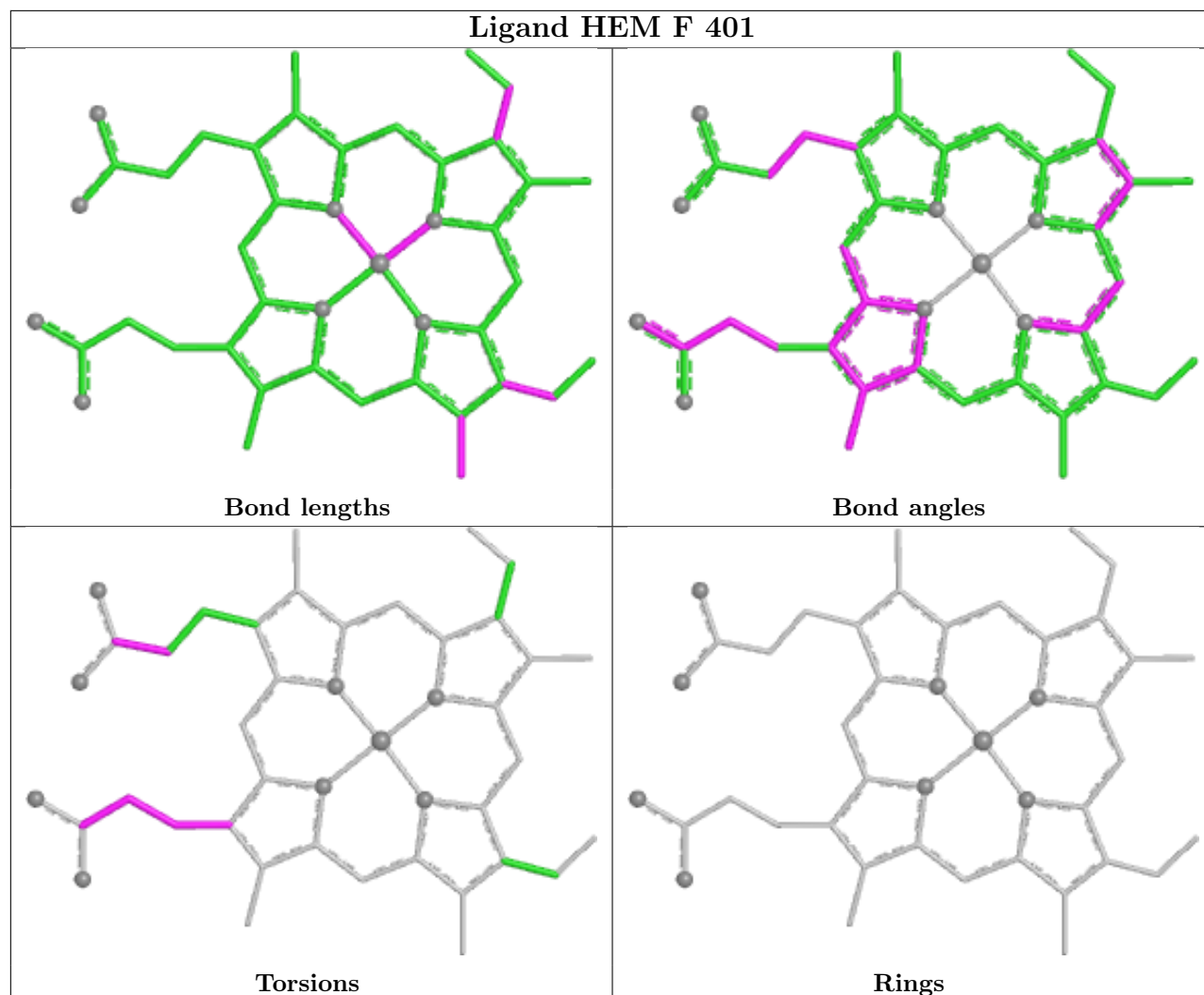


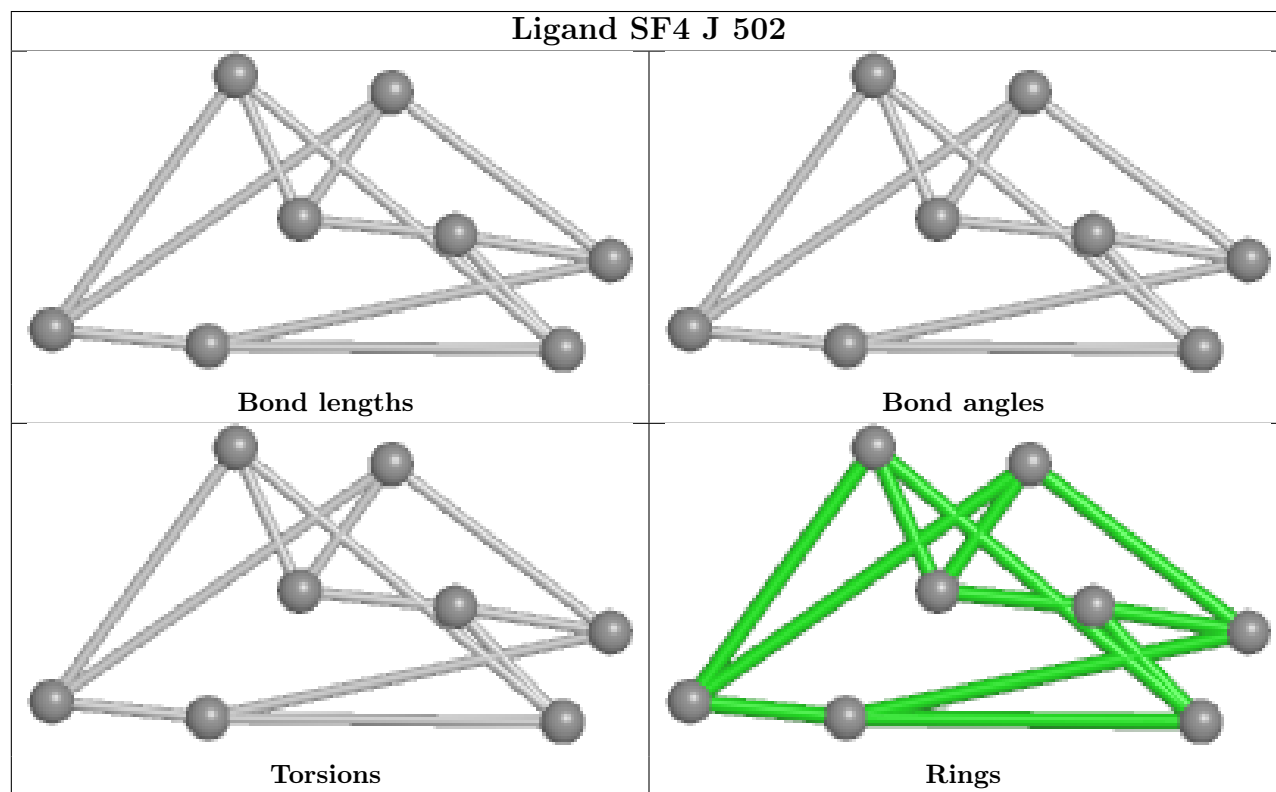
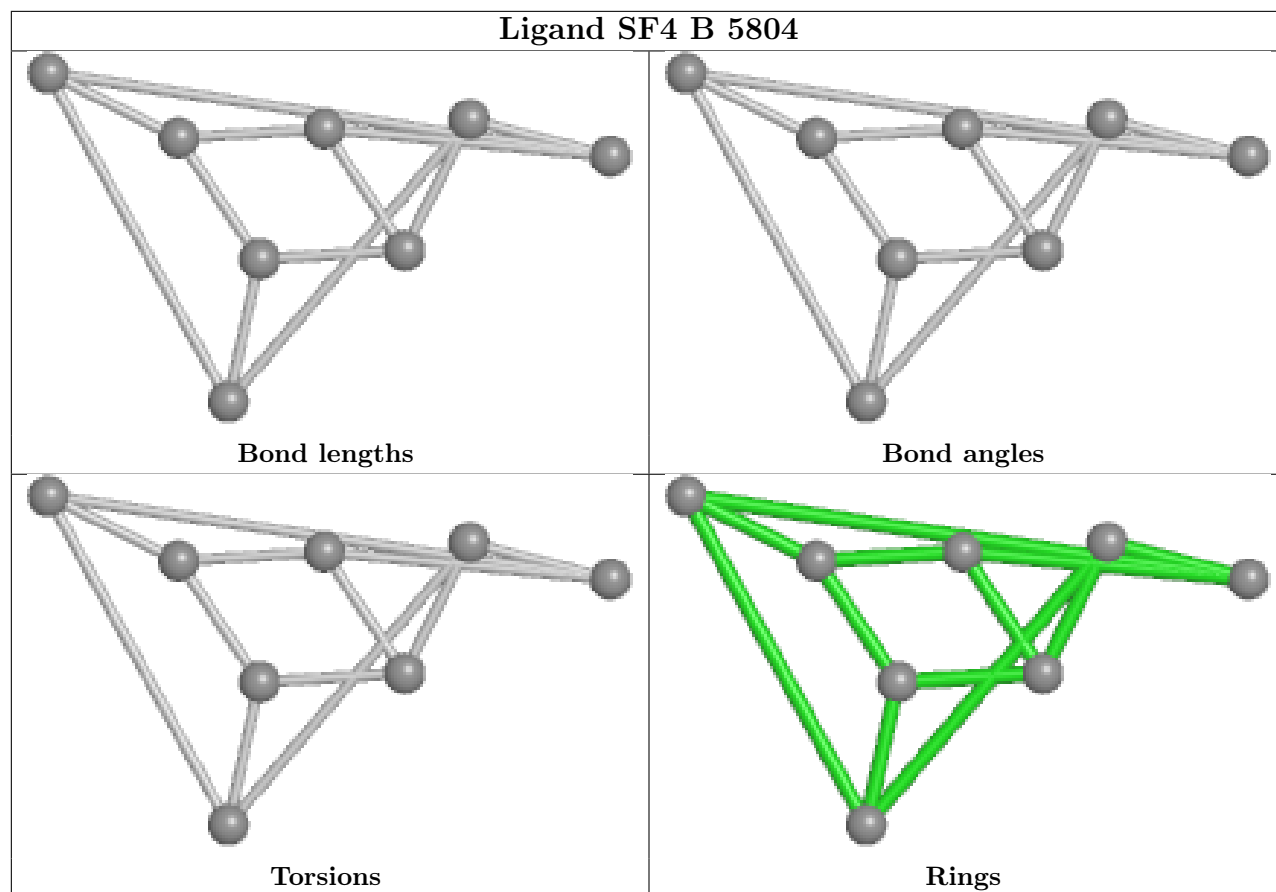
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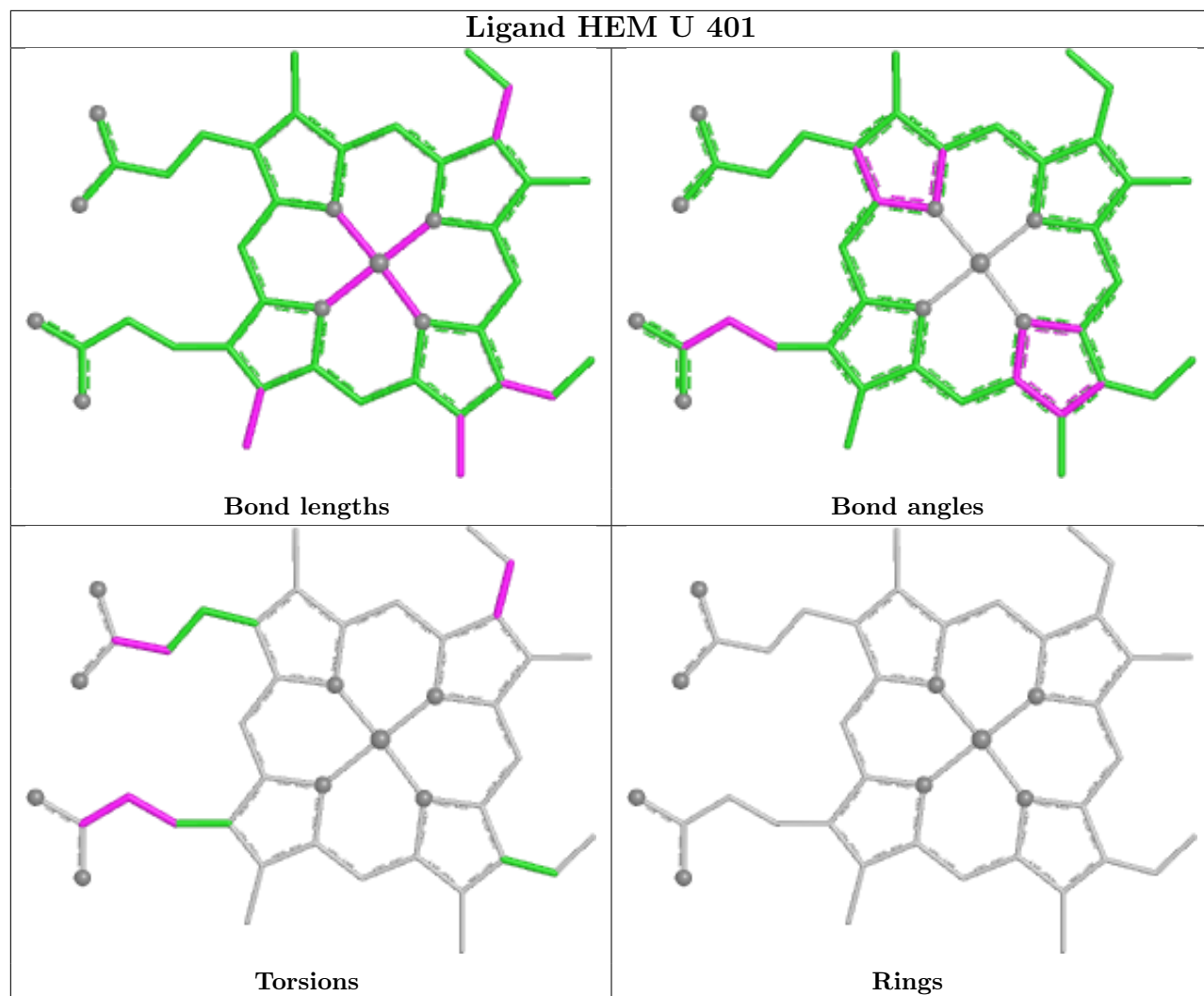




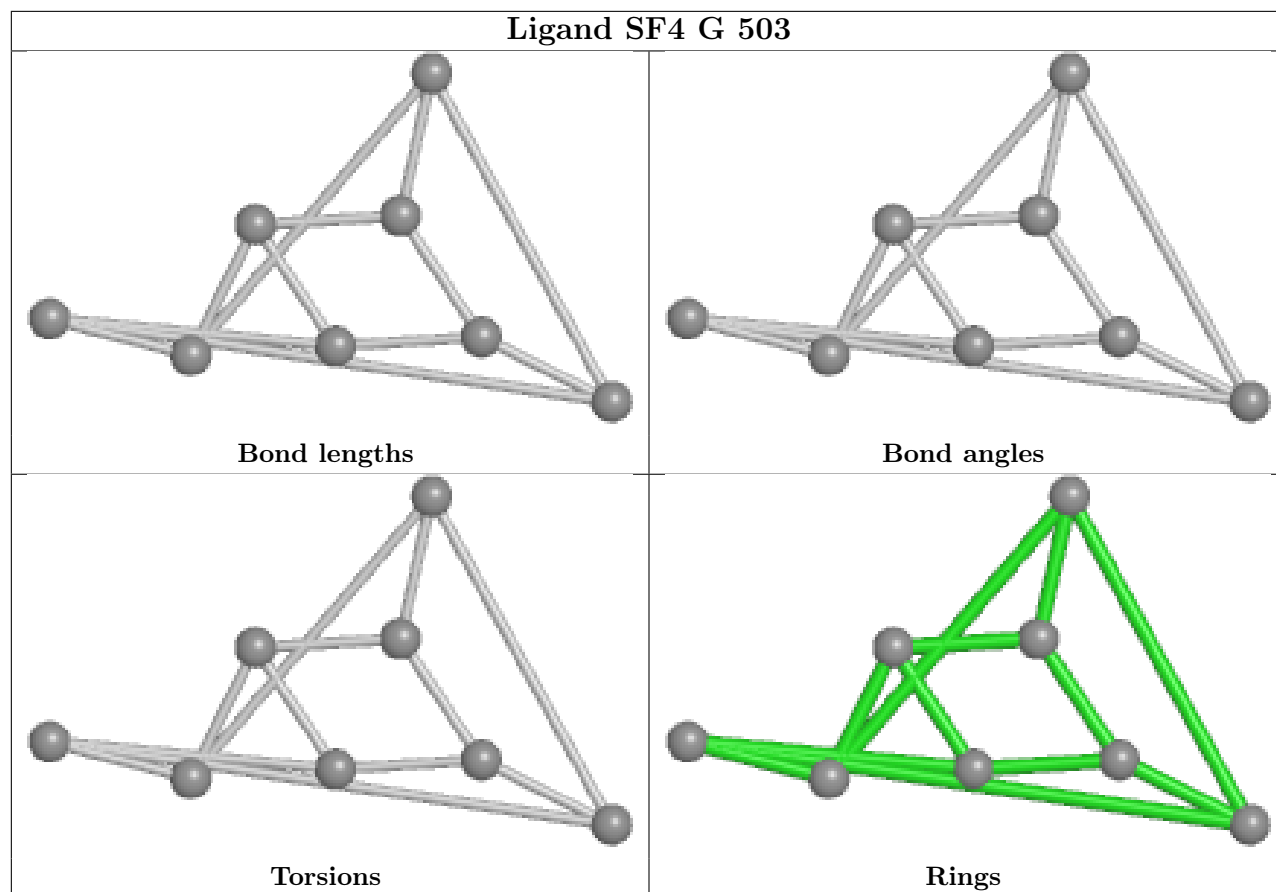




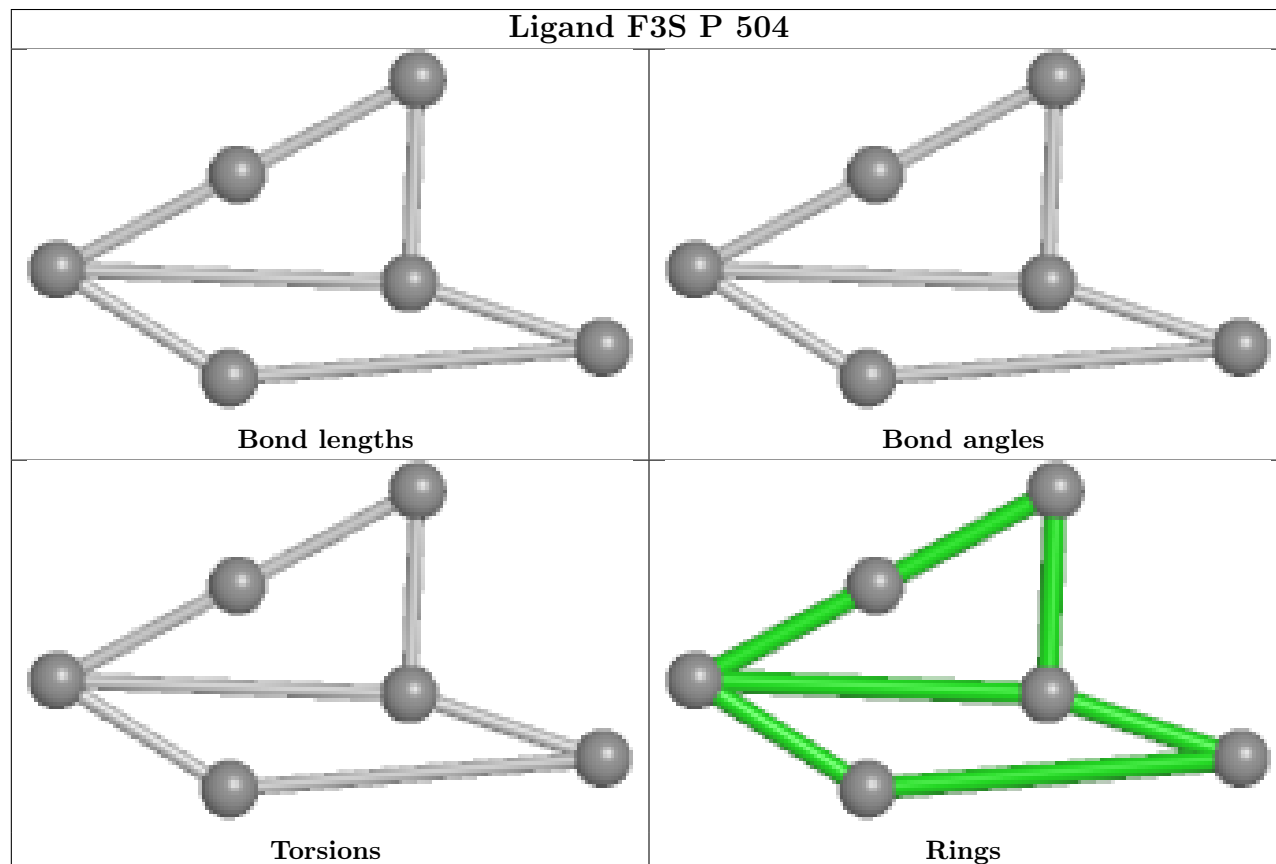




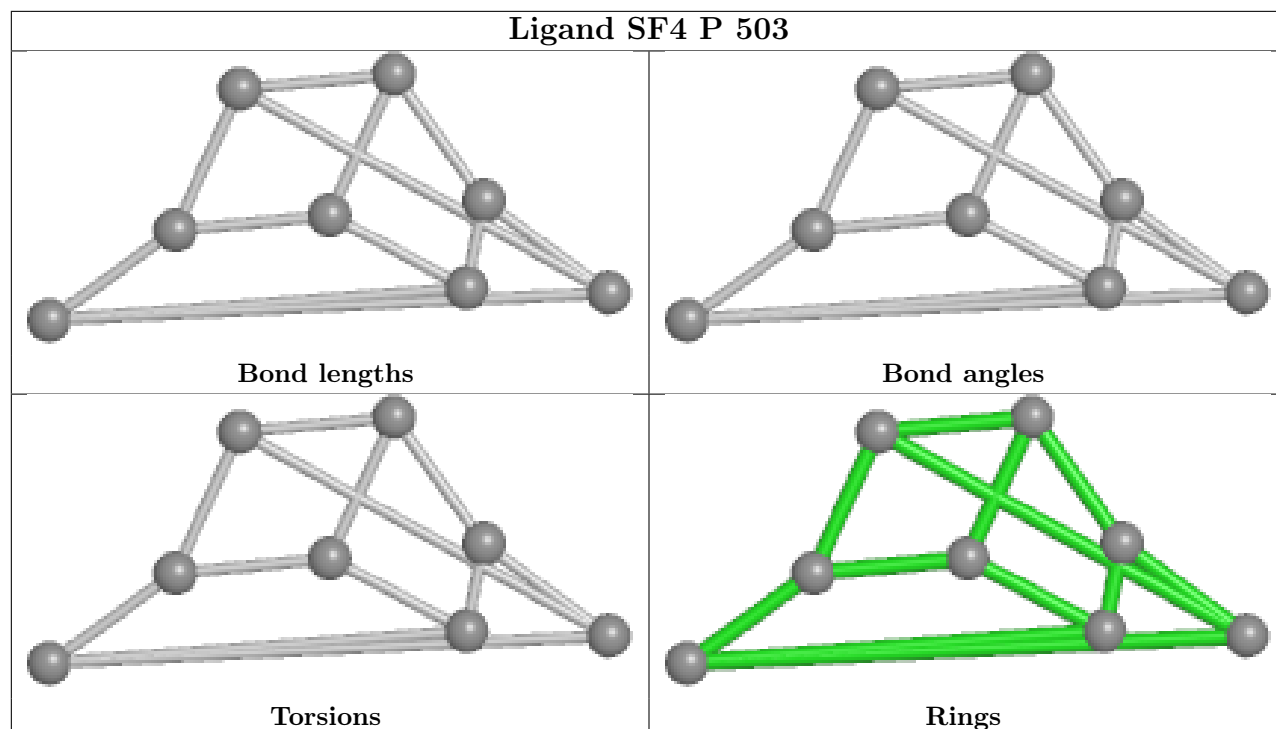
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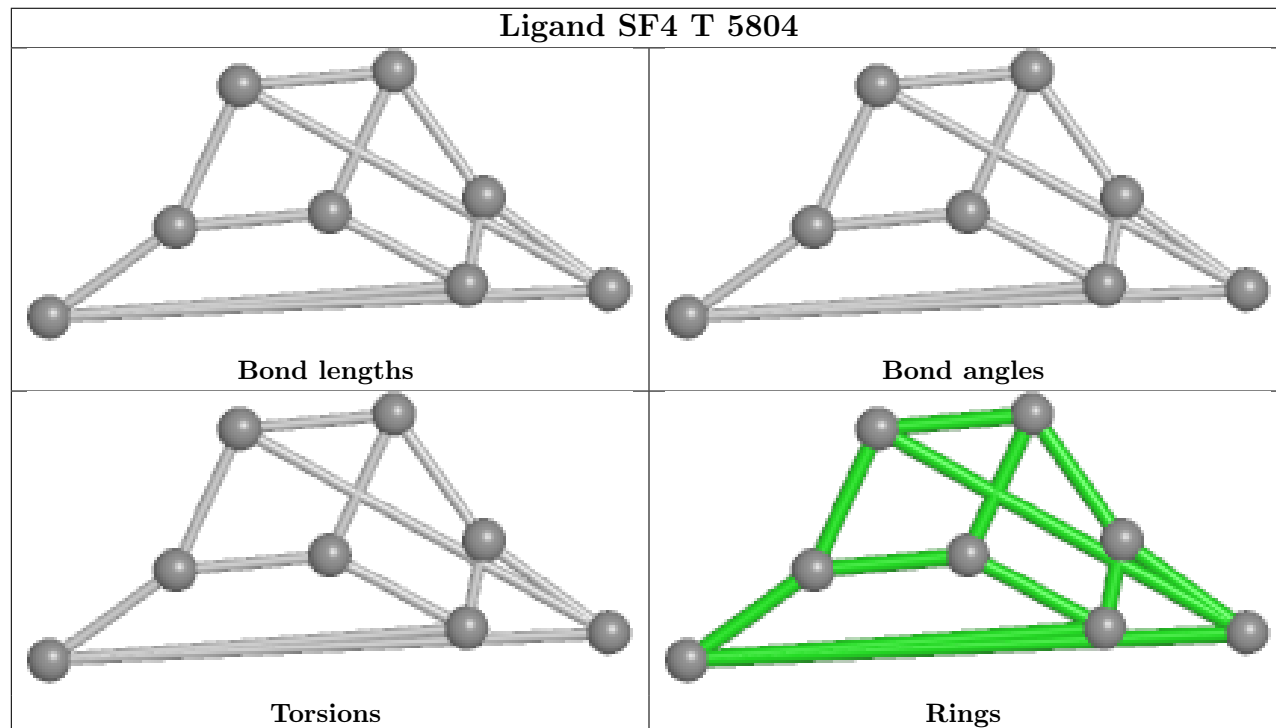
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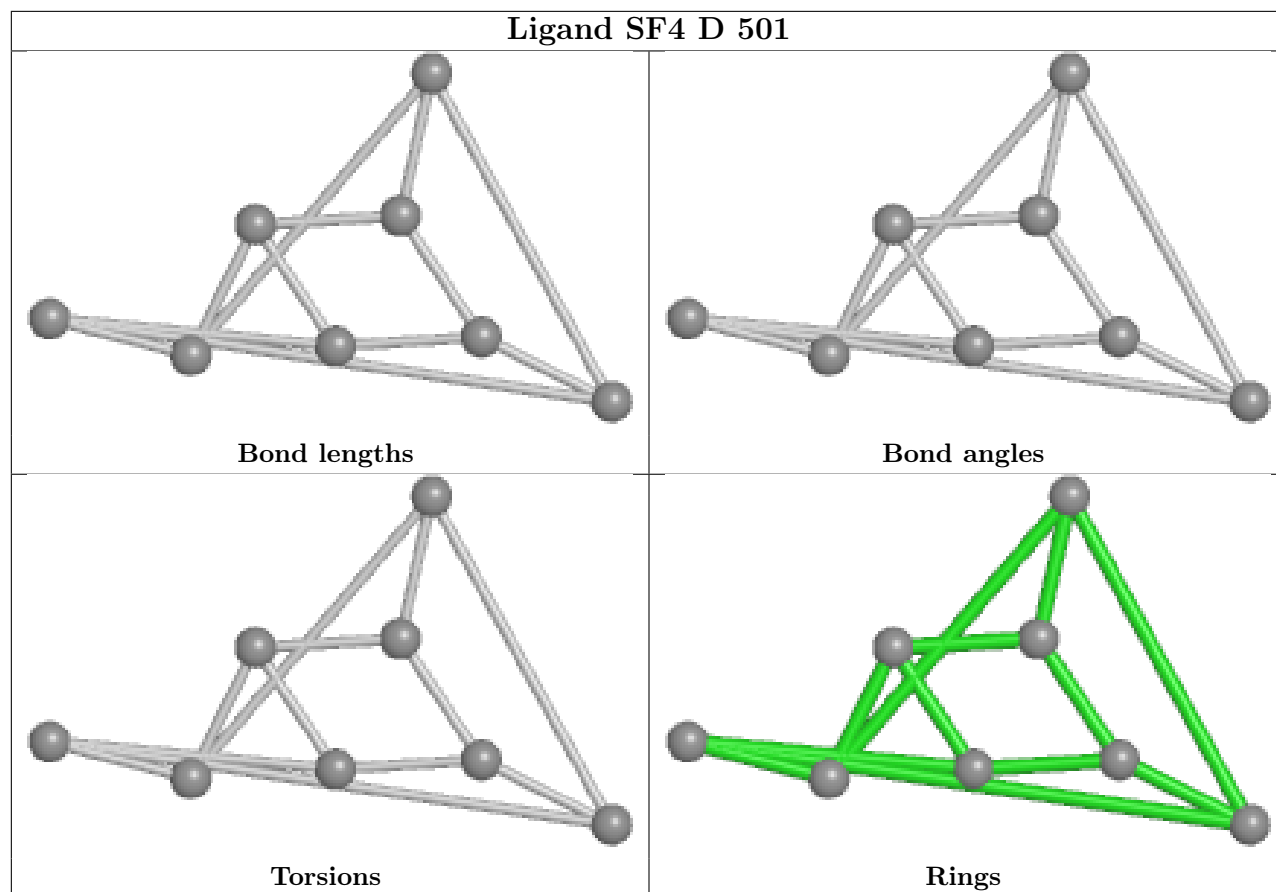
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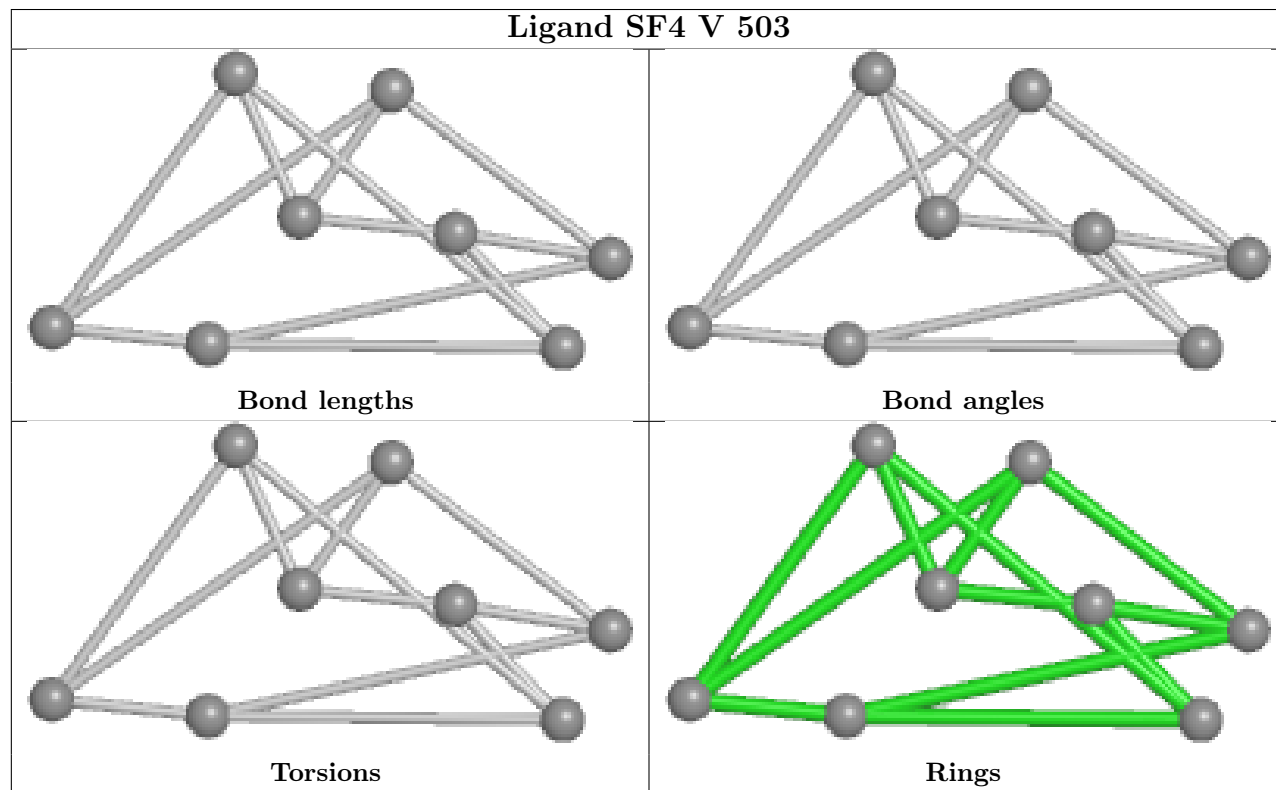
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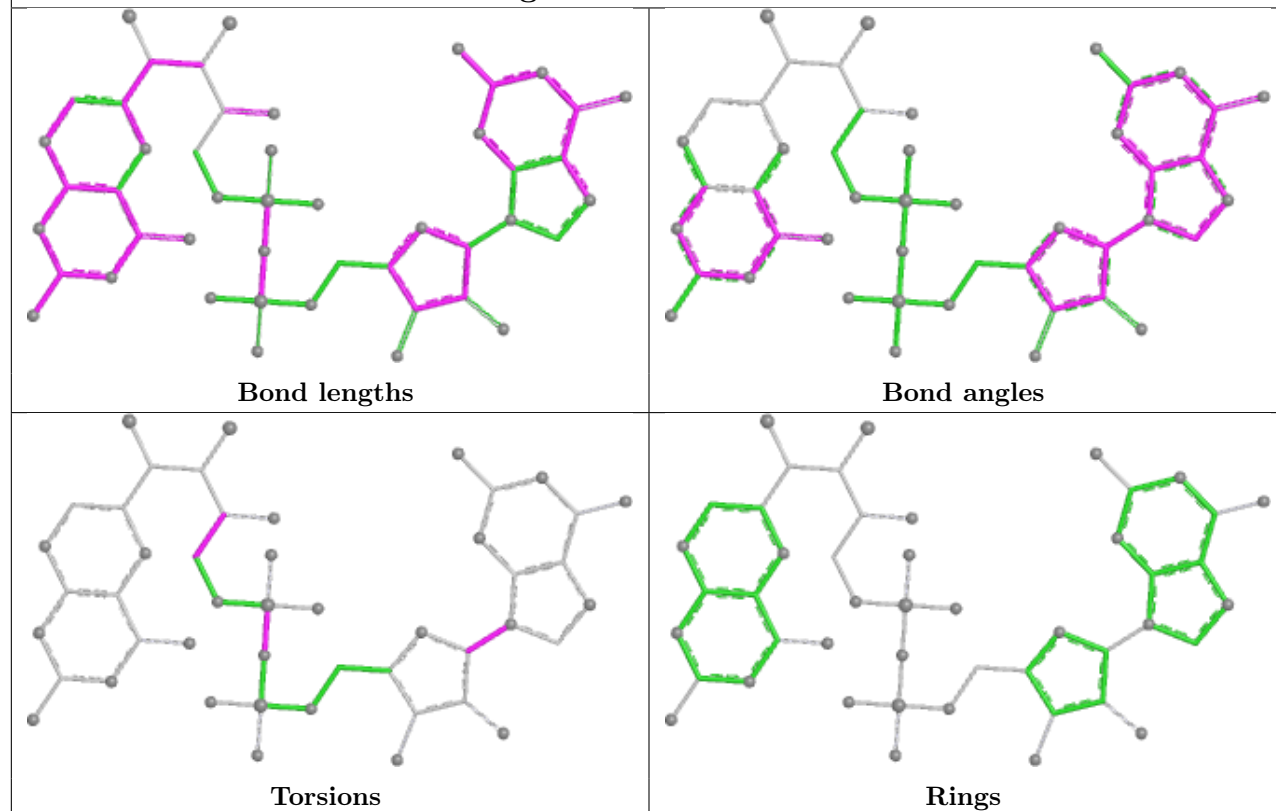
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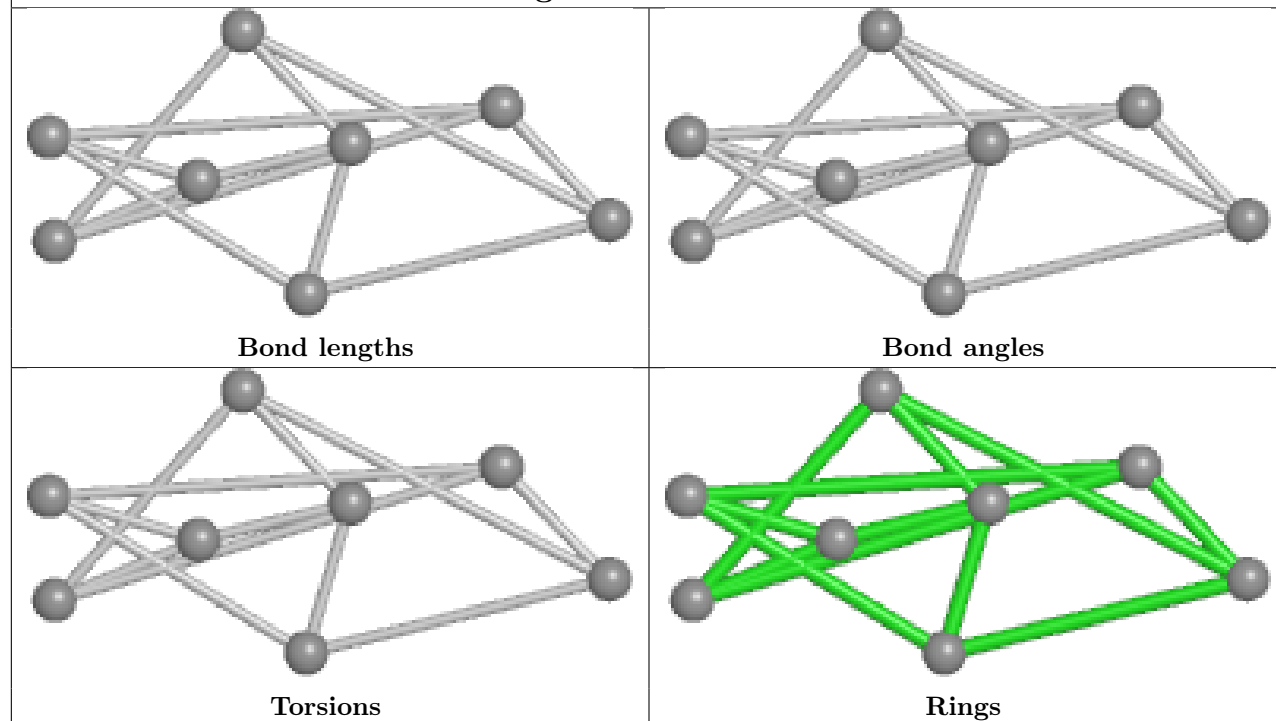
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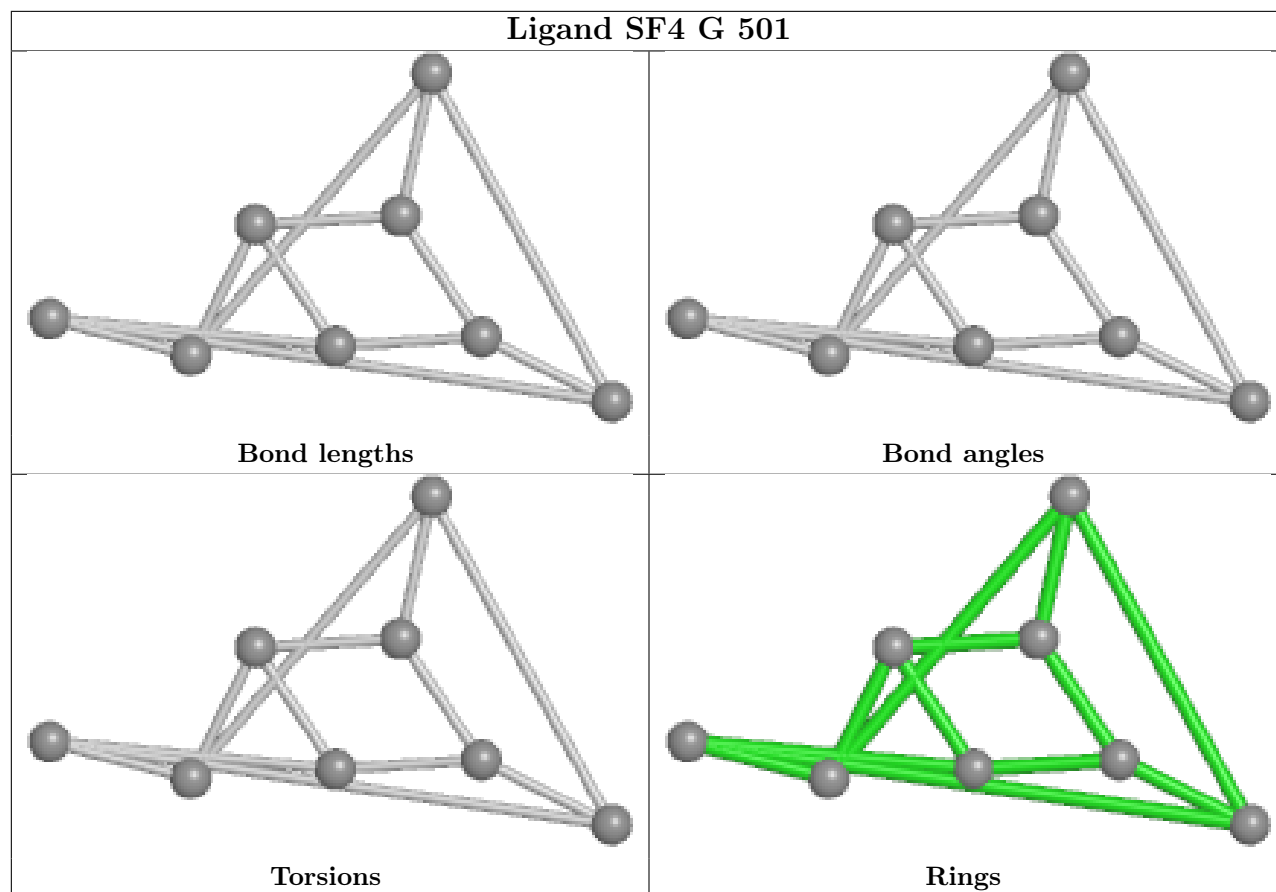


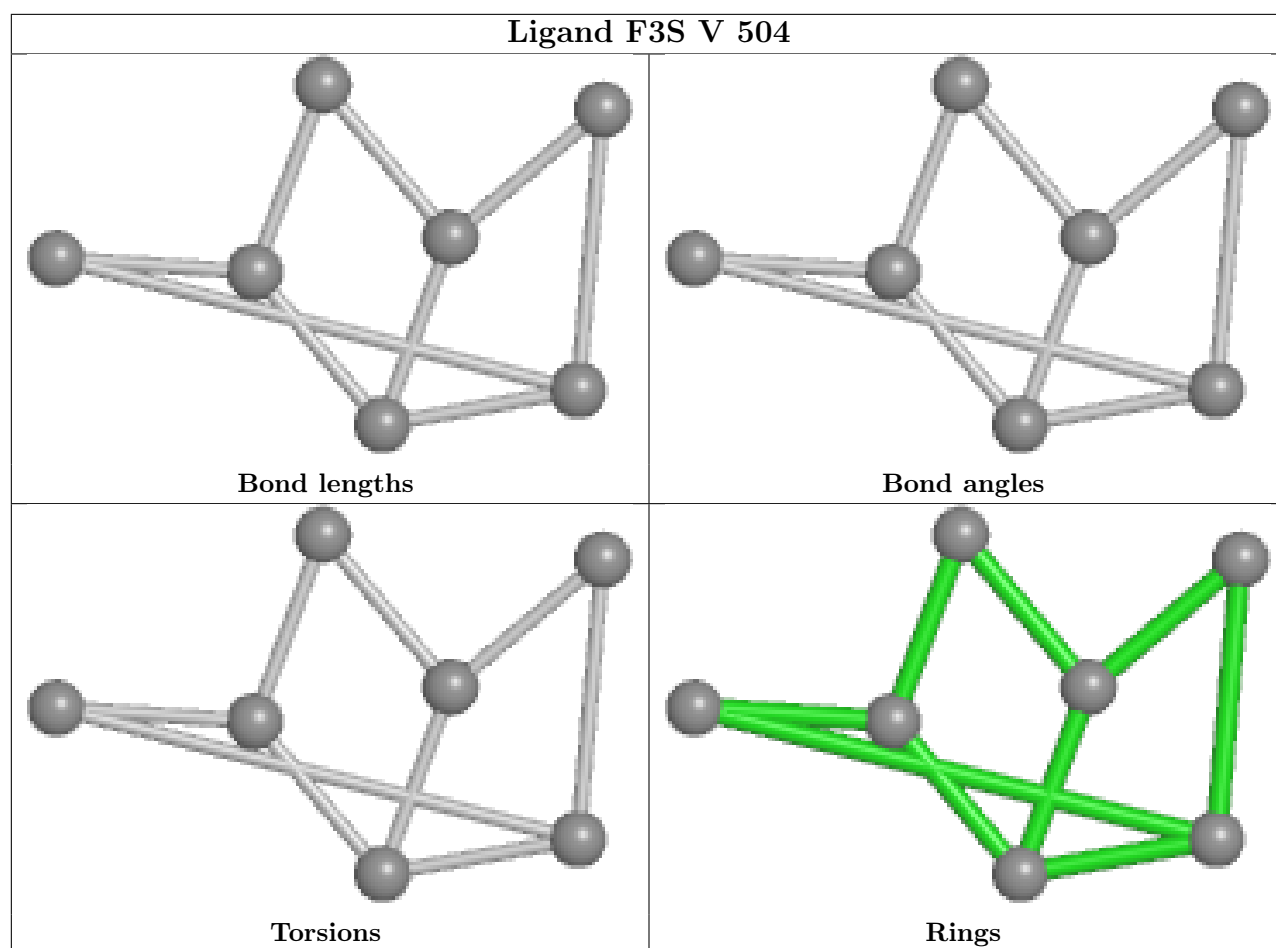
Ligand MD1 K 5802

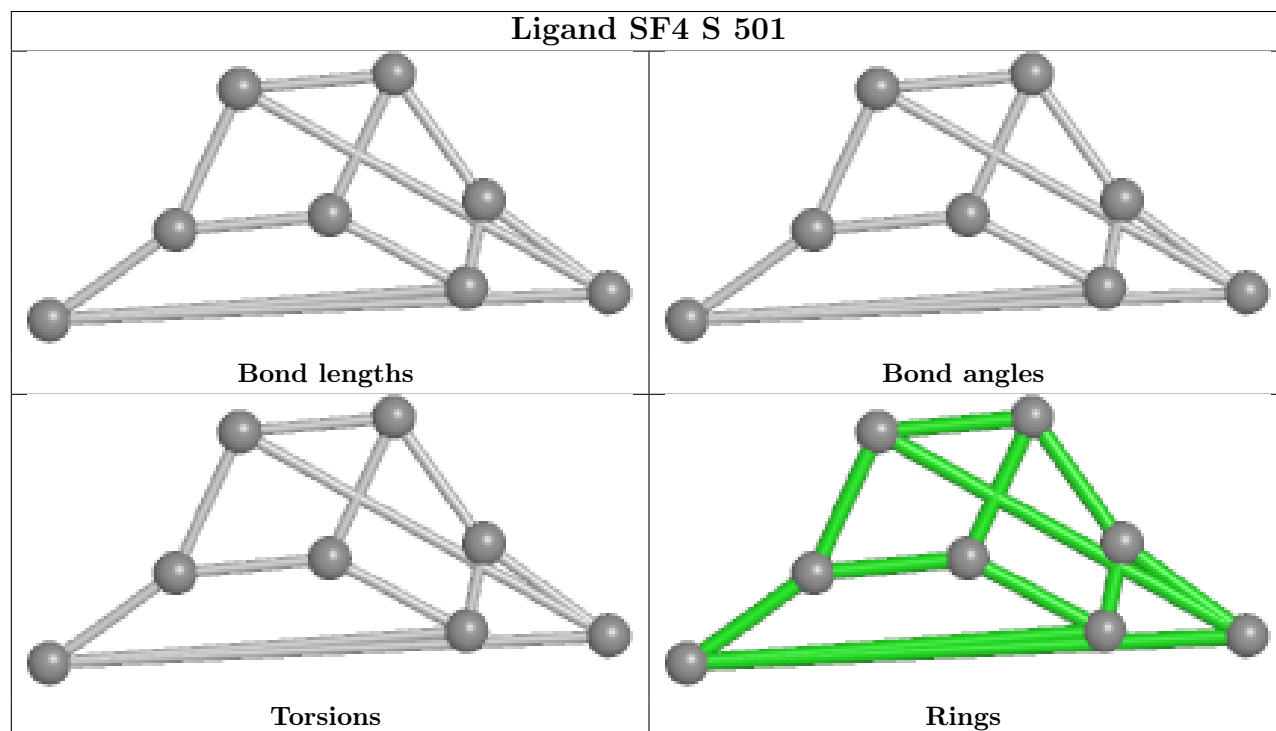
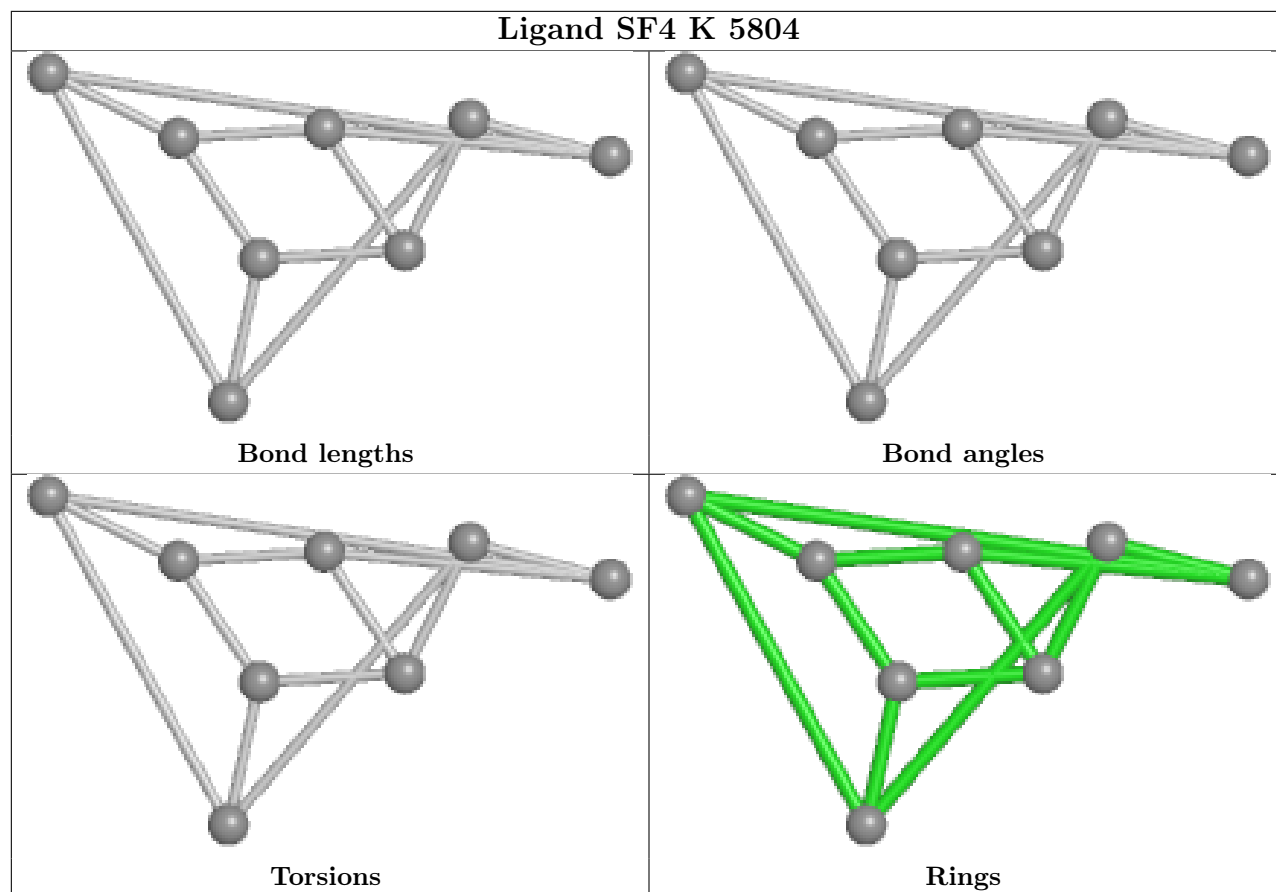


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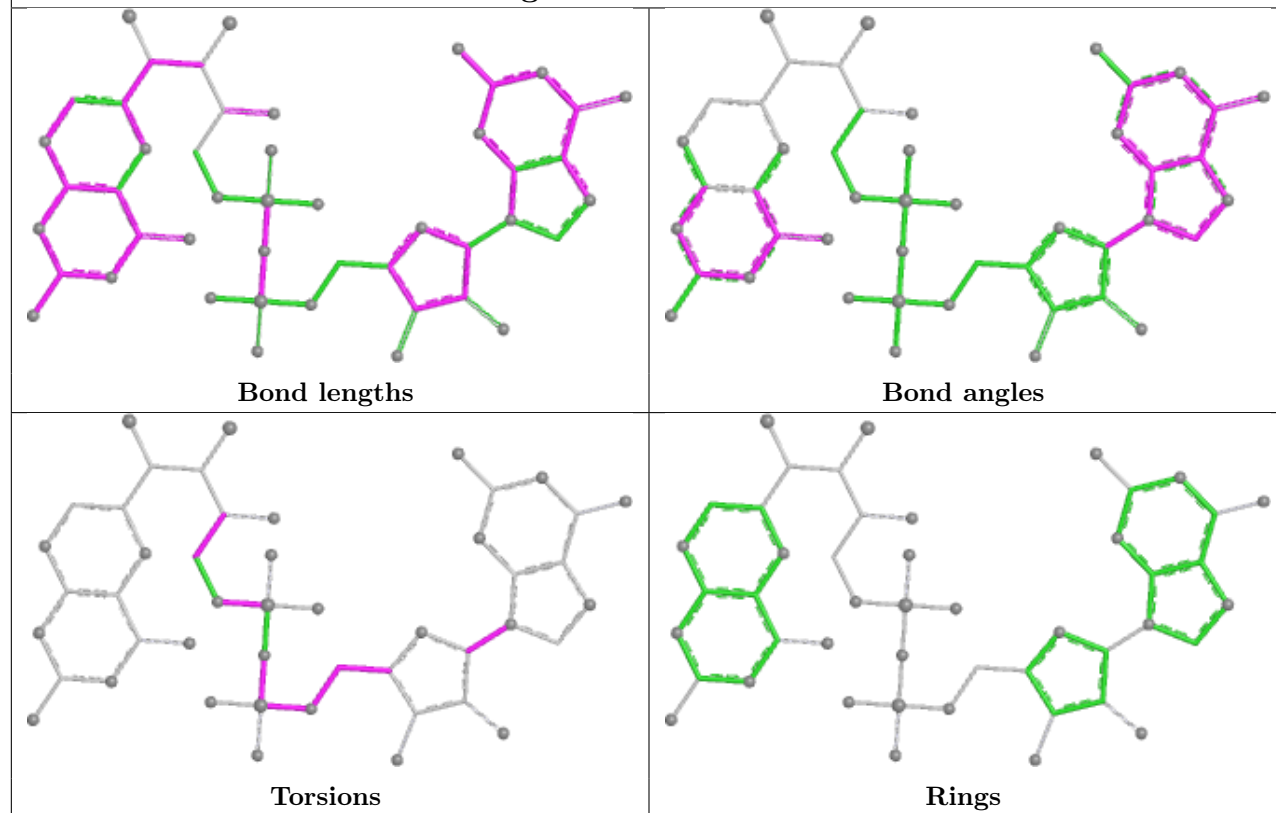




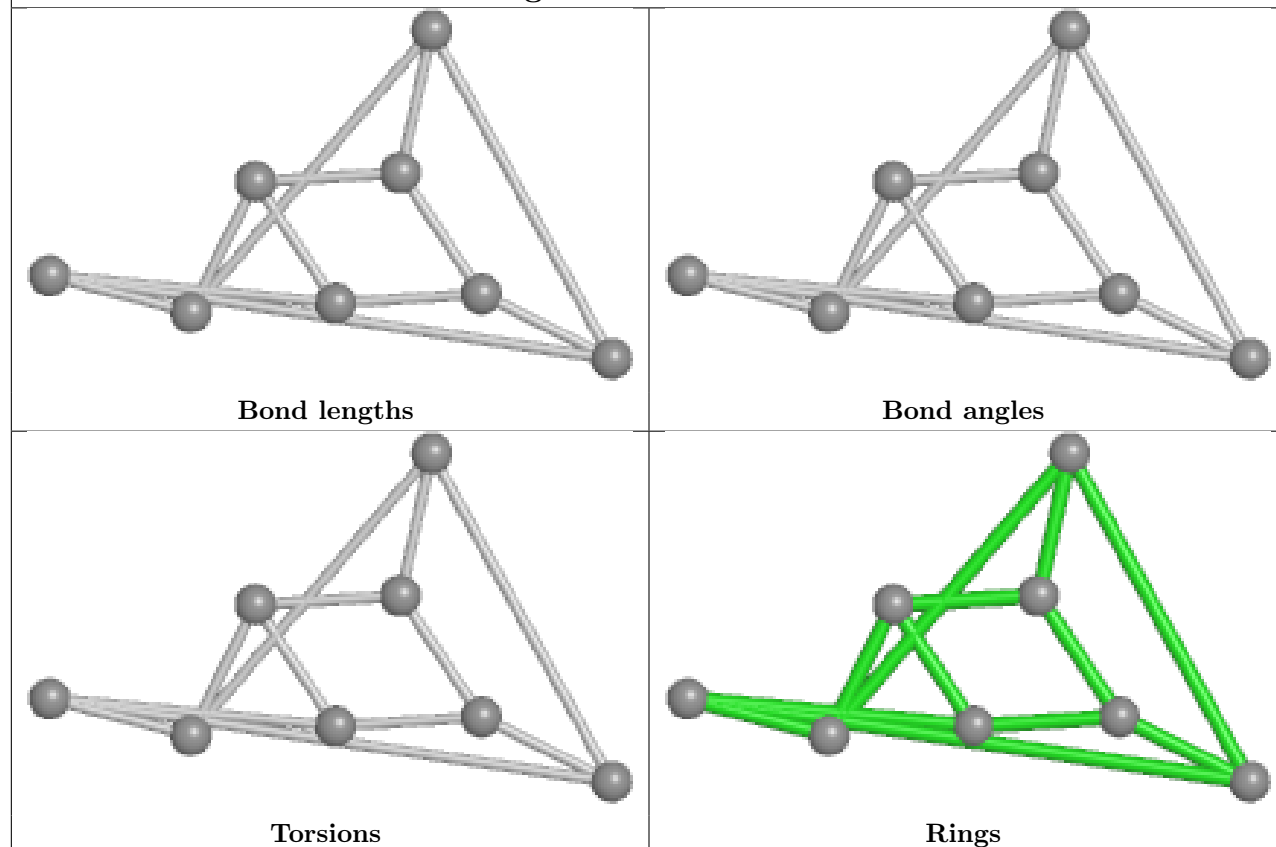




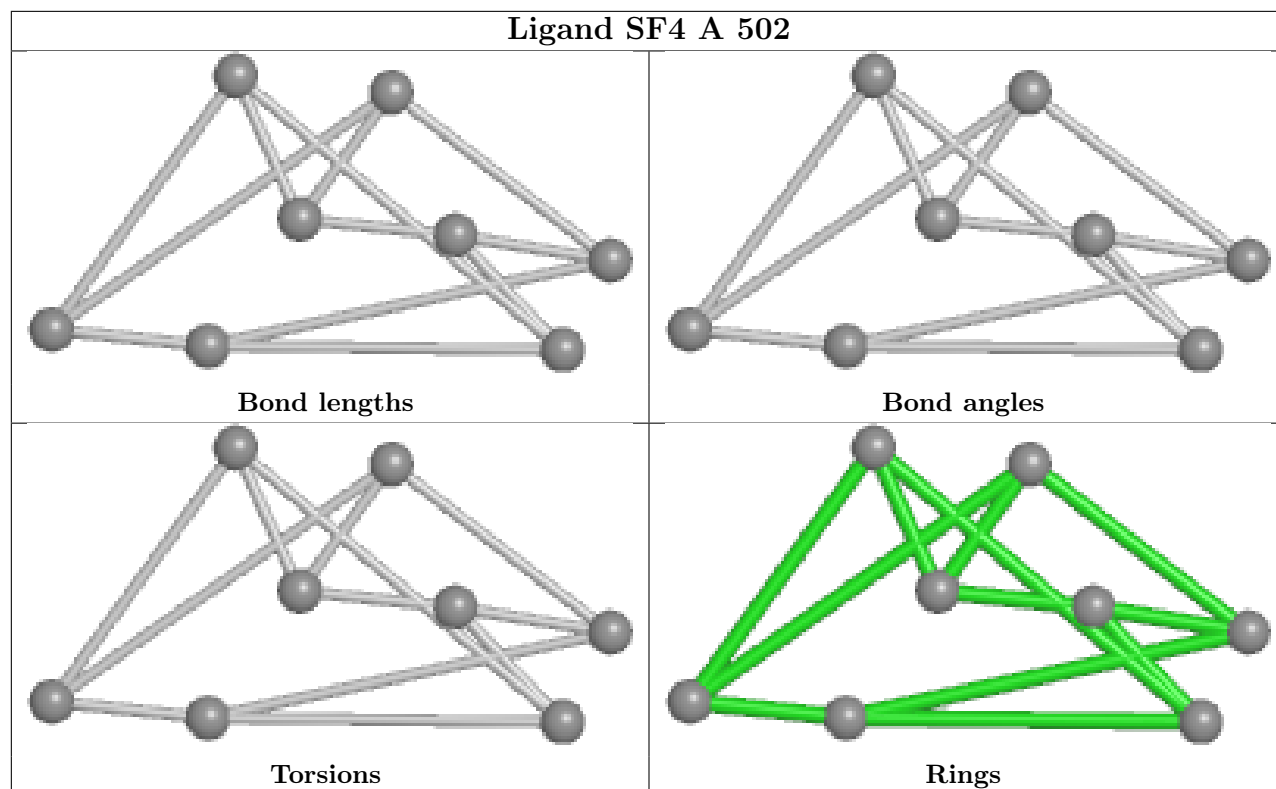
Ligand MD1 B 5801



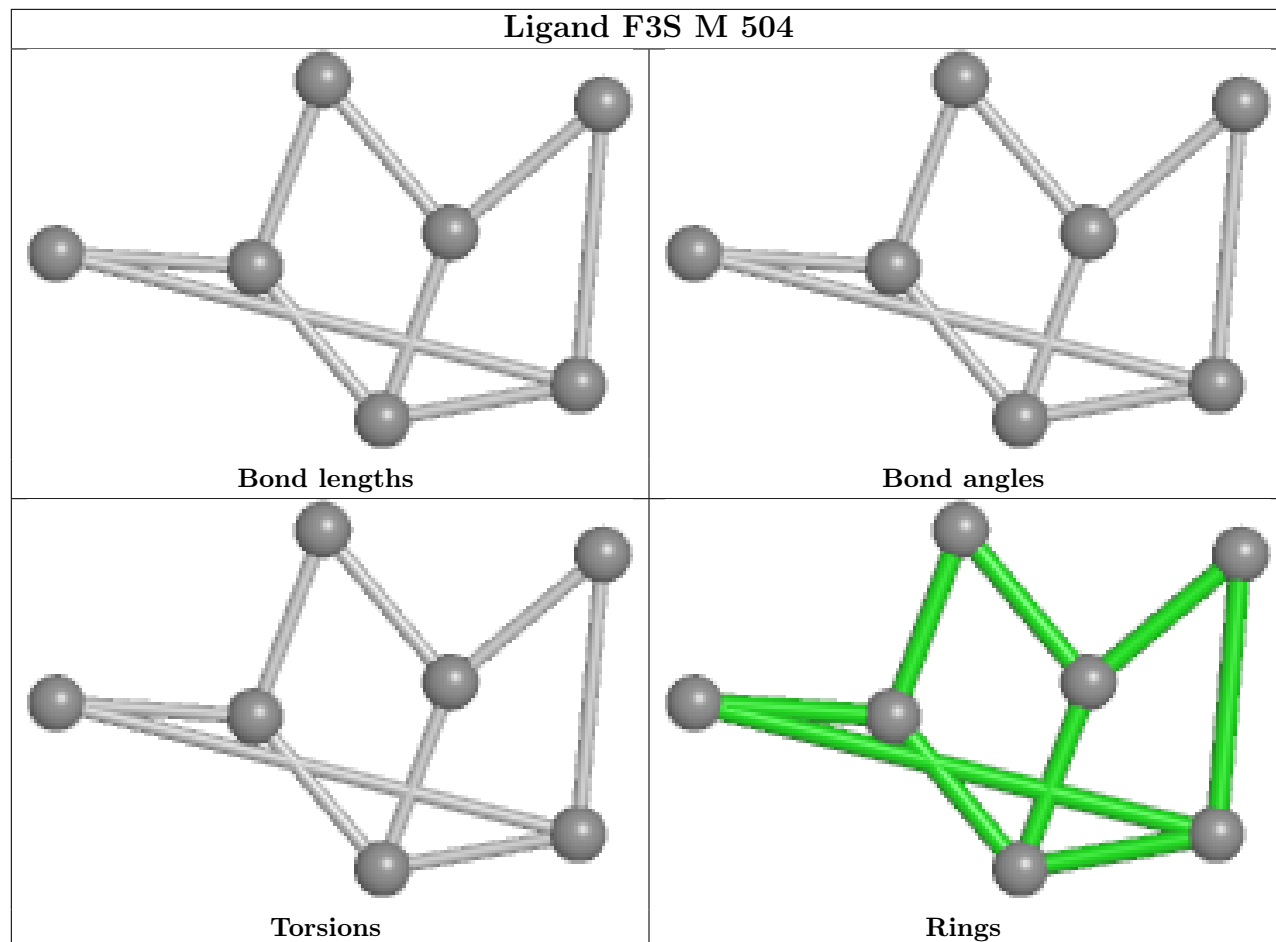
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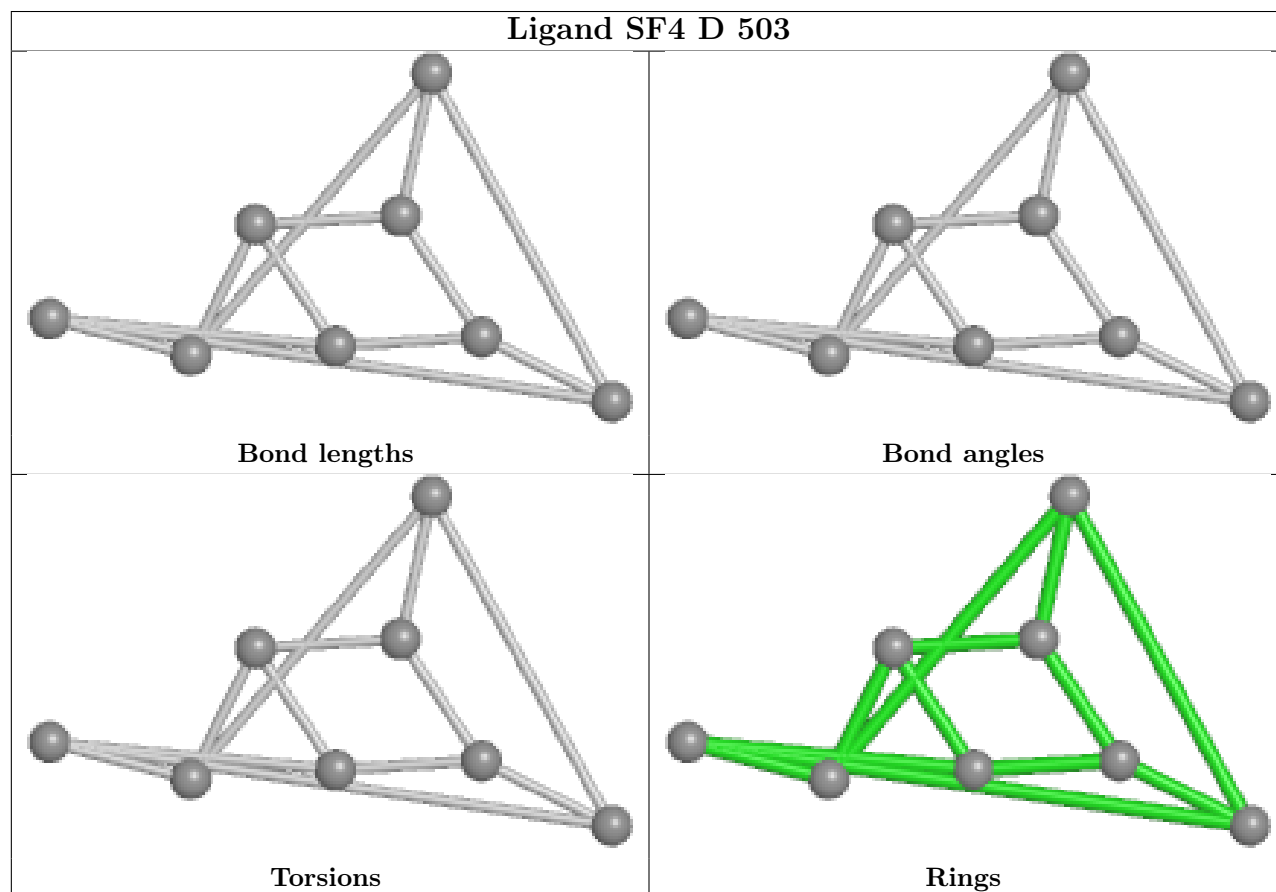
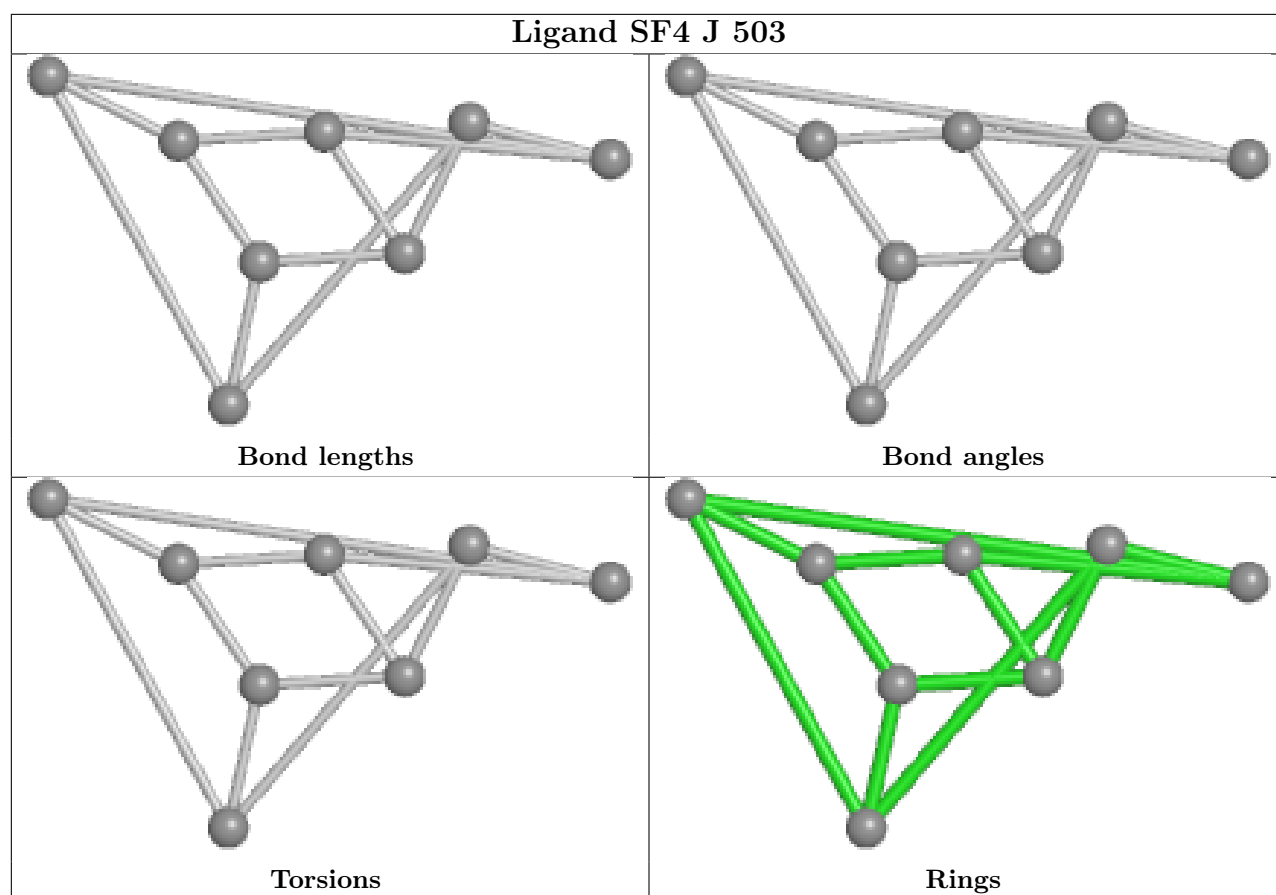


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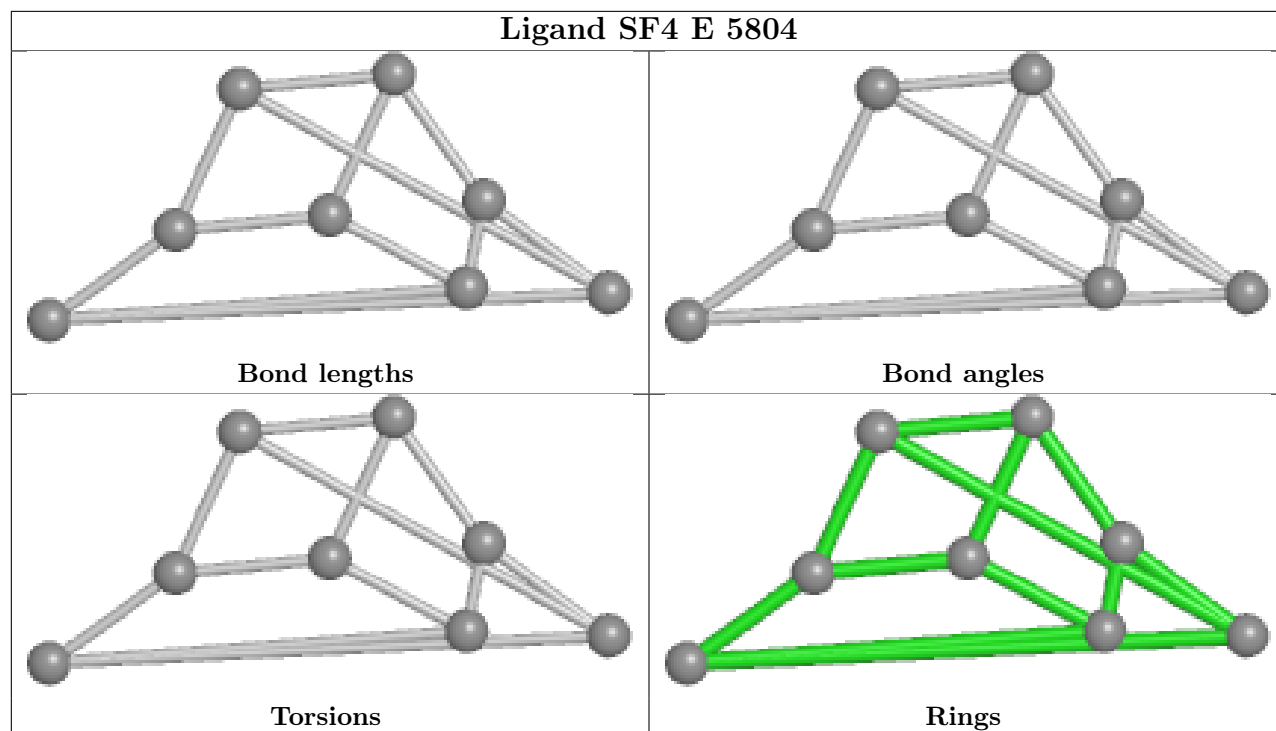


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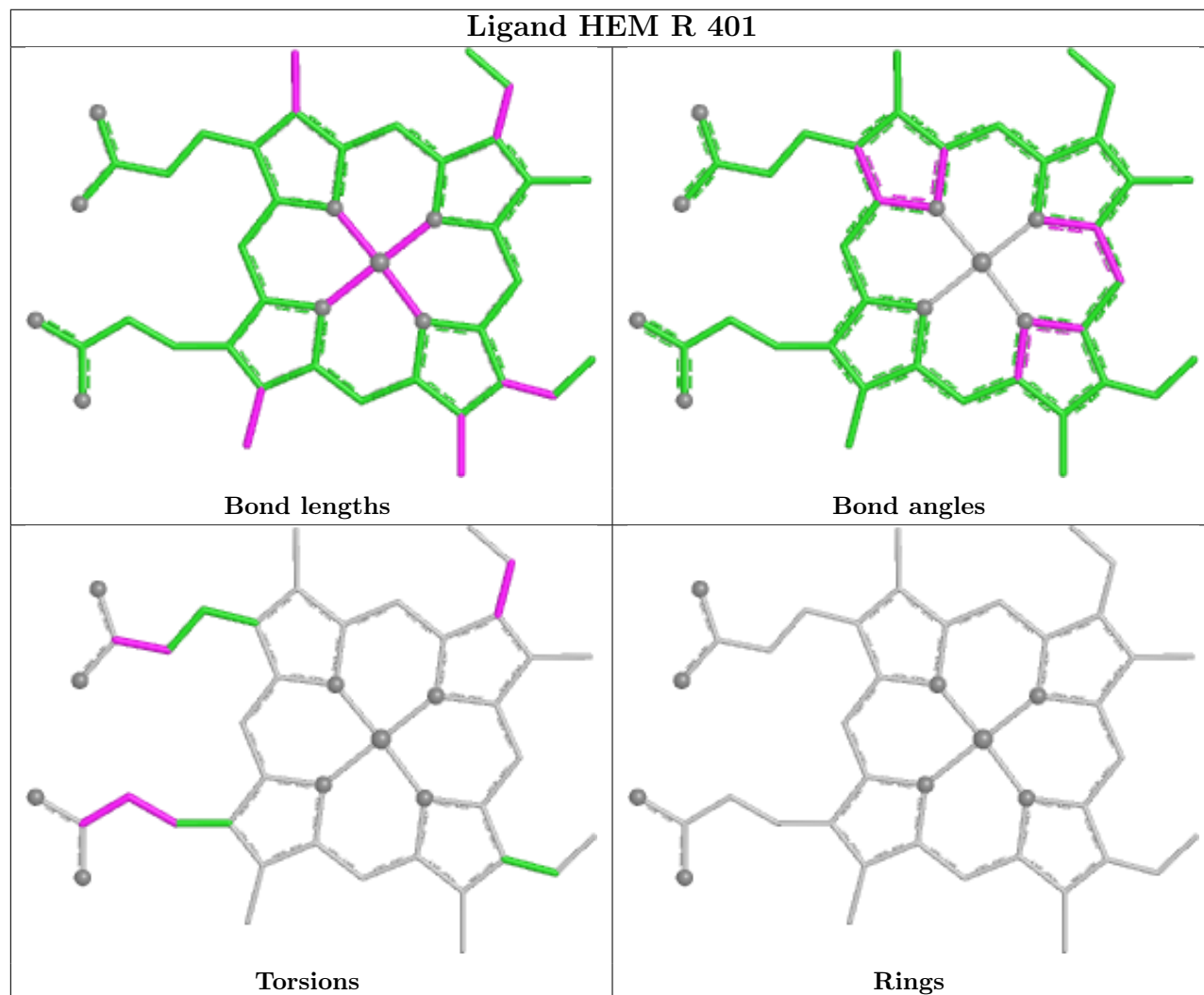




Ligand SF4 E 5804



Ligand HEM R 401



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	663:VAL	C	664:TYR	N	1.68

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/410 (99%)	0.17	1 (0%) 91 85	22, 37, 53, 68	2 (0%)
1	D	408/410 (99%)	2.34	239 (58%) 0 0	66, 97, 117, 133	0
1	G	409/410 (99%)	0.13	6 (1%) 72 53	21, 32, 45, 93	0
1	J	409/410 (99%)	-0.14	1 (0%) 91 85	18, 25, 37, 58	0
1	M	409/410 (99%)	0.53	7 (1%) 69 50	27, 48, 65, 79	0
1	P	409/410 (99%)	0.65	18 (4%) 39 24	26, 46, 64, 77	3 (0%)
1	S	409/410 (99%)	0.22	0 100 100	21, 33, 47, 61	1 (0%)
1	V	409/410 (99%)	1.35	87 (21%) 2 2	43, 61, 79, 86	1 (0%)
2	B	1120/1148 (97%)	0.52	29 (2%) 57 38	19, 41, 62, 92	2 (0%)
2	E	1111/1148 (96%)	3.26	902 (81%) 0 0	61, 117, 155, 175	1 (0%)
2	H	1118/1148 (97%)	0.15	13 (1%) 76 59	16, 29, 45, 85	3 (0%)
2	K	1119/1148 (97%)	0.15	8 (0%) 84 70	17, 32, 47, 76	2 (0%)
2	N	1117/1148 (97%)	0.19	6 (0%) 87 75	18, 33, 54, 85	4 (0%)
2	Q	1116/1148 (97%)	0.65	41 (3%) 45 28	21, 47, 70, 92	6 (0%)
2	T	1119/1148 (97%)	0.32	12 (1%) 78 61	21, 37, 57, 88	2 (0%)
2	W	1118/1148 (97%)	0.83	59 (5%) 32 19	29, 49, 66, 95	5 (0%)
3	C	292/322 (90%)	0.17	7 (2%) 59 40	18, 31, 49, 72	1 (0%)
3	F	292/322 (90%)	1.40	54 (18%) 3 2	57, 83, 104, 121	0
3	I	292/322 (90%)	0.88	25 (8%) 16 10	25, 50, 69, 83	0
3	L	292/322 (90%)	0.20	3 (1%) 79 63	19, 31, 47, 70	1 (0%)
3	O	291/322 (90%)	1.21	54 (18%) 3 2	35, 69, 89, 102	0
3	R	291/322 (90%)	0.19	2 (0%) 84 70	23, 34, 51, 72	1 (0%)
3	U	292/322 (90%)	0.18	5 (1%) 69 50	23, 34, 51, 70	1 (0%)
3	X	292/322 (90%)	1.23	42 (14%) 6 4	30, 62, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	14543/15040 (96%)	0.72	1621 (11%) 10 7	16, 41, 109, 175	36 (0%)

All (1621) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	710	ASN	9.7
2	E	112	PRO	8.8
2	E	713	SER	8.8
2	E	91	GLN	8.6
2	E	283	SER	8.5
2	E	309	LEU	8.2
2	E	525	TYR	8.1
2	E	266	ASN	7.6
2	E	694	ALA	7.4
2	E	637	THR	7.3
2	E	1090	ASP	7.1
2	E	784	THR	7.1
2	E	434	TRP	7.0
2	E	569	GLY	6.9
2	E	317	ALA	6.8
2	E	568	ALA	6.8
2	E	314	MET	6.7
2	E	801	LEU	6.6
2	E	769	TYR	6.5
2	E	533	PHE	6.4
2	E	701	VAL	6.4
2	E	716	PHE	6.4
2	E	295	ASP	6.3
2	E	717	ILE	6.3
2	E	74	ALA	6.3
2	E	565	ASN	6.3
2	E	236	LYS	6.3
2	E	564	GLY	6.2
2	E	355	ASP	6.2
2	E	1071	ASP	6.2
2	E	712	CYS	6.2
2	E	567	LYS	6.2
2	E	529	VAL	6.2
2	E	230	LEU	6.1
2	E	80	PHE	6.1
2	E	687	SER	6.1
2	E	832	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
2	E	566	TYR	6.0
2	E	597	TYR	6.0
2	E	308	ASN	6.0
2	E	1069	GLN	6.0
2	E	269	ASN	6.0
2	E	756	ASP	6.0
2	E	799	ALA	6.0
2	E	584	TRP	6.0
2	E	1094	ILE	6.0
2	E	598	ALA	6.0
2	E	1087	PHE	6.0
2	E	809	HIS	5.9
2	E	806	TYR	5.9
1	D	307	PRO	5.9
2	E	270	TYR	5.9
2	E	120	THR	5.9
2	E	68	SER	5.9
2	E	840	TYR	5.8
2	E	465	SER	5.8
2	E	720	TRP	5.8
2	E	282	PHE	5.8
2	E	646	THR	5.8
2	E	919	ARG	5.8
2	E	570	ASN	5.8
2	E	620	SER	5.7
2	E	233	VAL	5.7
2	E	1067	MET	5.7
2	E	851	PRO	5.7
2	E	316	GLU	5.7
2	E	813	GLU	5.7
1	D	348	THR	5.7
2	E	797	GLY	5.7
2	E	524	HIS	5.7
2	E	552	VAL	5.7
2	E	95	HIS	5.6
2	E	542	TYR	5.6
2	E	75	CYS	5.6
2	E	551	ASN	5.6
2	E	290	ASP	5.6
2	E	641	HIS	5.6
2	E	231	LEU	5.6
2	E	690	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
2	E	310	ILE	5.5
2	E	101	LEU	5.5
2	E	169	LEU	5.5
2	E	477	GLU	5.5
2	E	66	CYS	5.5
2	E	545	PRO	5.5
2	E	448	ASP	5.4
2	E	268	SER	5.4
2	E	679	SER	5.4
2	E	862	VAL	5.4
2	E	492	TYR	5.4
2	E	463	GLU	5.4
2	E	709	THR	5.4
2	E	543	TYR	5.4
1	D	49	TRP	5.3
2	E	561	THR	5.3
1	D	68	TYR	5.3
1	D	172	GLN	5.3
2	E	313	LYS	5.3
2	E	36	VAL	5.3
2	E	549	THR	5.3
2	E	100	ASP	5.3
2	E	276	GLN	5.3
2	E	240	TYR	5.3
2	E	783	TYR	5.3
2	B	28	PHE	5.3
2	E	321	THR	5.2
2	E	685	THR	5.2
2	E	715	PRO	5.2
2	E	96	GLN	5.2
2	E	267	TRP	5.2
2	E	839	GLU	5.2
2	E	599	SER	5.2
2	E	264	GLY	5.2
2	E	389	THR	5.2
2	E	617	TRP	5.2
2	E	485	TYR	5.2
2	E	235	GLY	5.2
2	E	234	ILE	5.2
2	E	739	ALA	5.2
2	E	1068	HIS	5.2
2	E	281	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
2	E	886	THR	5.1
2	E	466	PHE	5.1
2	E	688	ILE	5.1
2	E	452	THR	5.1
2	E	625	ILE	5.1
2	E	885	ARG	5.1
2	E	589	VAL	5.1
2	E	1095	ASN	5.1
3	O	322	GLN	5.1
2	E	444	ILE	5.1
2	E	46	ASP	5.1
2	E	563	ALA	5.1
2	E	643	PRO	5.1
2	E	76	ARG	5.1
2	E	265	ARG	5.1
2	E	821	PHE	5.1
2	E	238	GLY	5.1
2	E	322	GLU	5.1
2	E	284	HIS	5.0
2	E	409	ILE	5.0
2	E	1046	GLY	5.0
1	G	97	LYS	5.0
1	D	344	LEU	5.0
2	E	785	CYS	5.0
2	E	834	GLU	5.0
2	E	1022	ALA	5.0
2	E	611	ASP	5.0
2	E	585	VAL	5.0
2	E	1064	SER	5.0
2	E	740	GLY	5.0
2	E	562	TRP	5.0
2	E	63	PHE	4.9
2	E	496	SER	4.9
2	E	98	TYR	4.9
2	E	417	ILE	4.9
1	D	345	PHE	4.9
2	E	780	MET	4.9
2	E	844	PHE	4.9
2	E	559	SER	4.9
2	E	1021	SER	4.9
2	E	118	GLY	4.9
2	E	294	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
2	E	422	ASP	4.9
2	E	742	ALA	4.9
1	D	62	ASN	4.9
2	E	827	ARG	4.9
2	E	287	GLN	4.9
2	E	339	PRO	4.9
2	E	111	ASN	4.9
2	E	358	LEU	4.9
2	E	1091	ASN	4.9
1	D	409	SER	4.8
2	E	185	ILE	4.8
2	E	681	ASP	4.8
2	E	734	ASP	4.8
2	E	523	ILE	4.8
2	E	318	HIS	4.8
2	E	655	ASN	4.8
2	E	286	LEU	4.8
2	E	340	SER	4.8
2	E	395	VAL	4.8
2	E	811	PHE	4.8
1	D	375	MET	4.8
2	E	764	GLY	4.8
2	E	812	TRP	4.8
2	E	106	ALA	4.8
2	E	652	THR	4.7
2	E	770	ILE	4.7
2	E	1061	ARG	4.7
3	U	302	ASN	4.7
2	E	867	TYR	4.7
2	E	833	ASP	4.7
2	E	636	PHE	4.7
2	E	530	ASN	4.7
2	E	572	GLN	4.7
2	E	344	ALA	4.7
2	E	1070	LEU	4.7
2	E	849	GLU	4.7
2	E	102	TYR	4.7
2	E	581	PHE	4.7
2	E	87	MET	4.7
2	E	623	PRO	4.7
2	E	89	VAL	4.7
2	E	626	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	E	684	ILE	4.6
2	E	938	ASN	4.6
2	E	846	VAL	4.6
2	E	430	ASP	4.6
2	E	678	MET	4.6
2	E	289	SER	4.6
2	E	1023	TRP	4.6
2	E	129	TYR	4.6
2	E	1011	TYR	4.6
2	E	413	PRO	4.6
2	E	1100	GLU	4.6
2	E	539	ASN	4.6
2	E	778	THR	4.6
2	E	831	TYR	4.6
2	E	610	LEU	4.6
2	E	349	PRO	4.6
2	E	354	THR	4.5
2	E	544	LEU	4.5
2	E	1066	PRO	4.5
2	E	836	GLU	4.5
2	E	391	THR	4.5
2	E	640	THR	4.5
2	E	251	ALA	4.5
2	E	1098	PRO	4.5
2	E	447	ASP	4.5
2	E	495	ASP	4.5
2	E	296	VAL	4.5
2	E	658	ASN	4.5
2	E	110	TRP	4.5
2	E	854	THR	4.5
2	E	493	ASP	4.5
2	E	883	GLU	4.5
2	E	305	THR	4.5
2	E	882	TRP	4.5
2	E	1063	TRP	4.5
1	D	355	TYR	4.5
2	E	345	ASP	4.5
2	E	359	PHE	4.5
1	D	261	ALA	4.4
2	E	825	THR	4.4
2	E	181	ALA	4.4
2	E	824	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	1074	PHE	4.4
2	E	708	ILE	4.4
1	D	343	SER	4.4
2	E	92	ASN	4.4
2	E	97	ASN	4.4
2	E	443	ALA	4.4
2	E	807	PRO	4.4
2	W	563	ALA	4.4
2	E	479	MET	4.4
1	D	169	PHE	4.4
1	D	239	TYR	4.4
2	E	237	TYR	4.4
2	E	113	ARG	4.4
2	E	838	ILE	4.4
2	E	397	PRO	4.4
2	E	221	THR	4.3
2	E	600	ALA	4.3
2	E	645	PRO	4.3
2	E	334	THR	4.3
2	E	453	LEU	4.3
2	E	380	PHE	4.3
2	E	680	THR	4.3
2	E	1088	GLU	4.3
3	F	40	GLU	4.3
2	E	57	TYR	4.3
2	E	392	LEU	4.3
2	E	721	GLY	4.3
2	E	790	ASN	4.3
2	E	488	HIS	4.3
2	E	271	THR	4.2
3	C	302	ASN	4.2
2	E	188	ILE	4.2
2	E	554	TYR	4.2
2	E	259	ASP	4.2
2	E	808	ARG	4.2
1	D	338	LEU	4.2
2	E	390	ASP	4.2
2	E	288	THR	4.2
2	E	362	ILE	4.2
2	E	829	GLN	4.2
2	E	70	ASN	4.2
2	E	206	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	E	863	SER	4.2
2	E	918	SER	4.2
2	E	1082	LYS	4.2
1	D	341	VAL	4.2
1	D	36	ILE	4.2
1	D	351	ILE	4.2
2	E	367	ILE	4.2
2	E	476	ILE	4.2
2	E	280	HIS	4.2
1	D	308	PRO	4.2
2	E	860	ALA	4.2
2	E	695	PHE	4.2
2	E	73	HIS	4.1
2	E	35	VAL	4.1
2	E	782	GLY	4.1
3	F	159	GLN	4.1
2	E	241	ARG	4.1
2	E	360	LEU	4.1
2	H	30	LEU	4.1
2	E	893	SER	4.1
1	D	221	LYS	4.1
2	E	212	ASP	4.1
2	E	382	ASP	4.1
2	E	104	ASN	4.1
2	E	441	PRO	4.1
2	E	198	ALA	4.1
2	E	609	ALA	4.1
2	E	830	ALA	4.1
2	E	1093	CYS	4.1
2	E	815	VAL	4.1
2	E	119	TYR	4.1
2	E	401	ILE	4.1
2	B	1021	SER	4.1
2	E	704	GLN	4.1
2	E	789	LEU	4.0
2	E	1073	LEU	4.0
2	E	1092	HIS	4.0
1	D	244	GLY	4.0
2	E	890	ILE	4.0
1	D	243	GLU	4.0
2	E	683	GLU	4.0
2	E	842	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	366	LEU	4.0
1	D	240	PRO	4.0
1	D	253	PRO	4.0
2	E	894	TRP	4.0
2	E	483	GLU	4.0
2	E	873	TYR	4.0
2	E	99	SER	4.0
2	E	718	GLN	4.0
1	D	4	VAL	4.0
1	D	394	THR	4.0
2	E	892	LYS	4.0
2	E	547	MET	4.0
2	E	583	GLY	4.0
2	E	220	ARG	4.0
2	E	388	ARG	4.0
2	E	843	ASN	4.0
2	E	346	TYR	4.0
2	E	759	LYS	4.0
2	E	868	ILE	4.0
2	E	650	TRP	4.0
2	E	180	TYR	4.0
2	E	293	MET	4.0
2	E	357	ALA	3.9
2	Q	142[A]	ARG	3.9
1	D	182	GLY	3.9
2	E	550	GLY	3.9
1	D	71	PHE	3.9
2	E	109	ASN	3.9
2	E	143	TRP	3.9
1	D	260	SER	3.9
2	E	635	VAL	3.9
2	E	1075	HIS	3.9
2	N	382	ASP	3.9
2	E	802	LEU	3.9
1	D	263	VAL	3.9
2	E	433	VAL	3.9
2	E	384	PRO	3.9
1	D	339	LEU	3.9
2	E	93	TYR	3.9
2	E	616	TYR	3.9
2	E	534	HIS	3.9
2	E	541	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	1072	SER	3.9
1	D	79	THR	3.9
1	D	202	LEU	3.9
2	E	781	LYS	3.9
2	E	94	ASP	3.9
2	E	210	MET	3.9
2	E	771	ASN	3.9
2	E	204	GLN	3.9
2	E	404	TYR	3.9
2	E	596	PRO	3.9
2	E	682	ILE	3.9
2	E	421	LYS	3.8
1	D	273	ASP	3.8
2	E	250	ASP	3.8
2	E	787	ASP	3.8
1	D	352	VAL	3.8
3	F	212	ALA	3.8
2	E	711	SER	3.8
2	E	420	LEU	3.8
2	E	450	GLY	3.8
2	E	774	LEU	3.8
1	V	271	PHE	3.8
2	E	706	PHE	3.8
1	D	35	CYS	3.8
2	E	588	ASP	3.8
1	D	63	VAL	3.8
2	E	85	VAL	3.8
2	E	211	VAL	3.8
2	E	312	ASN	3.8
2	E	315	PRO	3.8
3	O	45	ALA	3.8
2	K	1021	SER	3.8
2	Q	438	SER	3.8
2	E	613	GLU	3.8
2	E	411	ASP	3.8
2	E	432	VAL	3.8
2	E	614	VAL	3.8
3	F	157	ASP	3.8
1	D	101	GLN	3.8
2	E	335	PRO	3.8
1	D	193	TYR	3.8
2	E	697	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	E	482	LEU	3.8
2	E	773	LEU	3.8
1	V	384	GLY	3.8
2	E	1101	THR	3.8
1	D	364	PHE	3.8
2	E	383	PHE	3.8
2	E	426	GLU	3.8
2	E	394	ARG	3.8
2	E	408	ASP	3.8
2	E	195	PRO	3.8
2	E	810	PRO	3.8
2	E	955	HIS	3.8
2	E	319	TRP	3.8
2	B	1022	ALA	3.8
2	E	192	TYR	3.8
2	E	229	GLY	3.8
2	E	521	VAL	3.7
1	V	284	ILE	3.7
2	E	77	ILE	3.7
3	L	61	HIS	3.7
2	E	177	ALA	3.7
2	E	879	ALA	3.7
2	E	822	TYR	3.7
2	E	484	MET	3.7
2	E	777	SER	3.7
2	E	167	ASP	3.7
2	E	1089	ALA	3.7
2	E	865	ASN	3.7
2	E	555	PHE	3.7
2	E	88	ARG	3.7
2	E	331	VAL	3.7
2	E	442	LYS	3.7
2	E	792	LYS	3.7
1	D	219	PRO	3.7
2	E	642	MET	3.7
1	D	108	TYR	3.7
1	D	321	GLY	3.7
2	E	419	GLY	3.7
2	E	841	GLY	3.7
1	P	410	ILE	3.7
2	E	377	VAL	3.7
2	E	962	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	1056	GLN	3.7
2	E	700	TRP	3.7
2	E	67	CYS	3.7
2	E	311	GLU	3.7
1	D	24	HIS	3.6
3	F	146	SER	3.6
1	D	378	ASP	3.6
2	E	224	GLY	3.6
2	E	647	LYS	3.6
2	E	115	CYS	3.6
2	E	451	GLU	3.6
3	O	73	ASN	3.6
2	E	546	VAL	3.6
2	E	735	VAL	3.6
2	E	356	THR	3.6
2	E	904	LEU	3.6
2	E	553	GLY	3.6
2	E	692	ASP	3.6
1	V	108	TYR	3.6
2	E	353	ASN	3.6
2	E	673	ASN	3.6
2	E	837	ILE	3.6
2	E	189	THR	3.6
1	D	188	PRO	3.6
2	E	1081	MET	3.6
1	D	165	SER	3.6
2	E	108	ARG	3.6
2	E	845	ILE	3.6
2	E	931	TRP	3.6
2	E	798	VAL	3.6
2	E	53	TYR	3.6
2	E	698	ASN	3.6
2	E	757	ASN	3.6
2	E	62	THR	3.6
2	E	624	LEU	3.6
2	E	891	LYS	3.6
2	E	136	ILE	3.6
2	E	186	ILE	3.6
2	E	458	ILE	3.6
3	O	47	GLU	3.6
2	E	272	TRP	3.6
2	E	859	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	881	TYR	3.6
1	A	2	THR	3.6
1	V	272	LEU	3.6
2	E	500	MET	3.6
3	F	237	ASN	3.6
2	E	958	HIS	3.5
1	D	245	ARG	3.5
1	G	100	SER	3.5
2	E	972	GLY	3.5
2	E	612	GLU	3.5
2	E	627	ASN	3.5
1	D	137	LYS	3.5
2	E	779	THR	3.5
2	E	888	ARG	3.5
2	E	920	HIS	3.5
2	E	242	PHE	3.5
2	E	387	ILE	3.5
2	E	887	VAL	3.5
2	E	1122	VAL	3.5
2	E	292	ASP	3.5
2	E	307	LYS	3.5
1	D	158	TYR	3.5
2	E	402	PRO	3.5
2	E	796	PRO	3.5
2	E	912	TYR	3.5
1	D	256	THR	3.5
2	E	107	THR	3.5
2	E	714	ASN	3.5
2	E	726	THR	3.5
2	E	878	ASN	3.5
2	E	540	ARG	3.5
1	D	237	ALA	3.5
2	E	277	ALA	3.5
2	E	298	PHE	3.5
3	F	148	GLU	3.5
2	E	116	LEU	3.5
1	M	93	ASP	3.5
2	E	140	TRP	3.5
2	E	856	TYR	3.5
2	E	964	ALA	3.5
2	E	571	PHE	3.5
2	E	328	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	1141	GLY	3.5
3	O	296	GLY	3.5
2	E	291	VAL	3.5
2	E	385	LEU	3.5
2	E	1142	GLU	3.5
1	D	159	SER	3.5
2	E	608	ARG	3.5
2	E	65	TYR	3.5
3	O	267	PHE	3.4
3	F	274	GLY	3.4
2	E	967	LEU	3.4
2	E	644	SER	3.4
2	E	573	ALA	3.4
2	E	662	HIS	3.4
3	U	203	ASN	3.4
2	E	248	ILE	3.4
2	E	957	ILE	3.4
2	E	1079	ILE	3.4
2	E	1083	PHE	3.4
2	E	214	MET	3.4
2	E	765	ARG	3.4
2	E	869	ARG	3.4
1	D	404	ASP	3.4
1	D	376	TYR	3.4
2	E	653	ASN	3.4
3	X	306	ASN	3.4
2	E	228	MET	3.4
2	E	478	VAL	3.4
2	E	621	GLU	3.4
2	E	705	GLU	3.4
1	D	189	ARG	3.4
2	E	985	PRO	3.4
2	E	1084	ILE	3.4
2	E	424	GLN	3.4
2	E	693	PHE	3.4
2	E	659	ASN	3.4
2	E	461	VAL	3.4
3	O	40	GLU	3.4
2	E	876	PRO	3.4
2	E	374	ALA	3.4
2	E	1128	ALA	3.4
3	O	102	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	105	LYS	3.4
1	D	374	THR	3.4
2	E	347	TRP	3.4
2	E	925	GLN	3.4
2	E	1106	THR	3.4
1	D	325	ASP	3.4
1	G	96	ASP	3.4
1	D	291	LEU	3.3
2	E	386	LEU	3.3
1	D	395	VAL	3.3
2	E	258	PRO	3.3
2	W	796	PRO	3.3
3	O	147	PRO	3.3
1	D	238	CYS	3.3
1	D	59	TRP	3.3
1	G	99	THR	3.3
2	B	68	SER	3.3
1	D	15	TYR	3.3
1	D	363	VAL	3.3
1	G	93	ASP	3.3
2	E	1133	ASP	3.3
2	E	297	ARG	3.3
1	D	322	PRO	3.3
1	D	196	LYS	3.3
2	E	853	ALA	3.3
1	D	38	CYS	3.3
2	E	131	LEU	3.3
2	E	182	SER	3.3
2	E	1119	TRP	3.3
1	V	273	ASP	3.3
2	E	133	TYR	3.3
2	E	361	GLY	3.3
2	E	506	ASP	3.3
2	E	971	ASP	3.3
2	Q	806	TYR	3.3
2	E	352	ASN	3.3
3	F	39	GLU	3.3
1	D	401	ILE	3.3
2	E	1144	ILE	3.3
2	E	416	HIS	3.3
3	F	60	ALA	3.3
1	D	320	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	29	ARG	3.3
2	E	445	THR	3.3
2	E	723	THR	3.3
2	E	864	THR	3.3
3	O	265	VAL	3.3
2	E	576	TRP	3.3
2	E	327	GLY	3.3
2	E	968	GLY	3.3
3	I	76	GLY	3.3
2	E	983	ASP	3.3
3	C	120	ASP	3.3
2	E	702	GLU	3.3
2	E	786	GLU	3.3
2	E	835	PRO	3.3
2	E	861	ILE	3.3
2	E	761	ALA	3.3
2	E	201	LEU	3.3
2	E	468	LEU	3.3
2	E	656	LEU	3.3
1	D	12	ARG	3.3
2	E	848	ARG	3.3
1	D	350	THR	3.3
2	B	652	THR	3.3
2	E	363	THR	3.3
2	E	913	CYS	3.3
2	E	338	SER	3.3
2	T	1021	SER	3.3
3	F	149	GLU	3.2
1	D	408	ASN	3.2
2	E	800	MET	3.2
1	D	27	ALA	3.2
2	E	164	ARG	3.2
2	E	956	GLN	3.2
2	E	59	TYR	3.2
1	D	250	ASP	3.2
2	E	602	ASP	3.2
2	W	290	ASP	3.2
2	E	719	ILE	3.2
2	E	762	ILE	3.2
3	F	320	ALA	3.2
1	D	383	PHE	3.2
2	E	805	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	396	GLU	3.2
2	E	793	TYR	3.2
3	F	246	SER	3.2
1	D	236	ILE	3.2
2	E	217	ALA	3.2
2	E	766	ALA	3.2
1	V	24	HIS	3.2
2	E	847	HIS	3.2
2	E	256	VAL	3.2
2	E	722	LYS	3.2
1	V	145	GLY	3.2
2	E	139	GLY	3.2
2	E	423	GLU	3.2
1	V	128	TRP	3.2
1	D	242	ILE	3.2
1	D	303	ILE	3.2
2	E	351	ARG	3.2
2	W	937	ASN	3.2
2	E	522	ALA	3.2
2	E	982	ALA	3.2
2	E	161	PHE	3.2
2	E	329	LYS	3.2
1	D	318	GLN	3.2
2	W	564	GLY	3.2
1	D	342	MET	3.2
2	E	64	THR	3.2
1	D	98	GLU	3.2
2	E	196	GLU	3.2
1	D	203	ILE	3.2
2	E	33	PRO	3.2
3	F	145	ILE	3.2
1	D	171	LEU	3.1
1	D	285	ARG	3.1
2	E	489	LEU	3.1
2	E	749	LEU	3.1
2	H	597	TYR	3.1
1	D	311	ALA	3.1
1	V	191	ALA	3.1
2	E	691	ALA	3.1
2	E	638	GLY	3.1
2	E	536	THR	3.1
2	E	427	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	820	PRO	3.1
1	D	80	LEU	3.1
2	E	49	TRP	3.1
2	E	245	CYS	3.1
2	E	630	LYS	3.1
2	E	1050	SER	3.1
3	X	31	ALA	3.1
1	V	18	PHE	3.1
2	E	889	ASN	3.1
3	O	111	PHE	3.1
2	E	497	VAL	3.1
1	D	69	GLY	3.1
2	E	127	GLY	3.1
1	D	32	ILE	3.1
2	E	605	ILE	3.1
2	E	696	PRO	3.1
3	F	147	PRO	3.1
3	F	42	LEU	3.1
2	E	32	LYS	3.1
2	E	634	LYS	3.1
3	F	61	HIS	3.1
1	D	45	CYS	3.1
2	E	249	VAL	3.1
2	E	320	VAL	3.1
2	E	939	PHE	3.1
2	E	618	ASN	3.1
3	I	57	ASP	3.1
1	D	43	MET	3.1
2	E	538	MET	3.1
3	X	78	GLN	3.1
2	E	285	GLY	3.1
2	E	460	PRO	3.1
2	E	738	LEU	3.1
2	E	916	PRO	3.1
2	E	921	THR	3.1
2	E	343	LYS	3.1
2	E	905	TRP	3.1
2	E	178	PHE	3.1
2	E	410	SER	3.1
2	E	992	ASN	3.1
1	D	265	GLN	3.1
2	E	215	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	407	GLN	3.1
2	E	826	GLY	3.1
3	O	141	GLY	3.1
2	E	515	ILE	3.1
2	E	633	ARG	3.1
2	E	591	LYS	3.1
3	X	42	LEU	3.1
1	D	299	THR	3.1
3	X	320	ALA	3.0
1	D	373	PHE	3.0
2	E	376	TYR	3.0
2	E	454	VAL	3.0
1	M	87	ASP	3.0
2	Q	686	GLY	3.0
3	F	93	GLY	3.0
2	E	446	ARG	3.0
2	E	674	ILE	3.0
3	C	318[A]	ARG	3.0
2	E	795	GLU	3.0
1	D	380	VAL	3.0
1	V	345	PHE	3.0
2	E	396	SER	3.0
2	E	994	SER	3.0
2	E	814	GLN	3.0
2	Q	29	ARG	3.0
2	W	264	GLY	3.0
1	D	398	PRO	3.0
2	E	520	PRO	3.0
1	D	104	THR	3.0
3	U	178	THR	3.0
2	E	114	MET	3.0
2	E	760	PHE	3.0
2	W	1092	HIS	3.0
2	E	372	TYR	3.0
2	E	82	ARG	3.0
1	D	274	ASP	3.0
2	E	103	GLY	3.0
2	E	455	LYS	3.0
2	E	469	LYS	3.0
2	E	471	ILE	3.0
3	L	318[A]	ARG	3.0
2	W	710	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	X	296	GLY	3.0
3	X	304	GLN	3.0
2	K	31	LEU	3.0
2	E	628	THR	3.0
2	E	823	THR	3.0
2	E	1060	THR	3.0
2	E	1124	THR	3.0
2	E	586	ALA	3.0
2	E	121	PHE	3.0
2	E	252	HIS	3.0
2	E	989	TRP	3.0
2	E	365	ILE	3.0
2	Q	708	ILE	3.0
2	W	934	ILE	3.0
2	E	794	GLY	3.0
2	E	299	SER	3.0
2	W	938	ASN	3.0
1	G	98	GLU	3.0
2	E	69	PRO	3.0
2	E	336	GLU	3.0
2	E	587	GLU	3.0
1	D	324	VAL	3.0
2	E	222	PHE	3.0
2	E	654	VAL	3.0
3	O	282	VAL	3.0
2	E	467	LYS	2.9
2	E	828	LEU	2.9
2	E	1013	TYR	2.9
2	E	429	GLY	2.9
2	E	763	GLU	2.9
2	E	1062	ASP	2.9
3	X	302	ASN	2.9
2	E	1077	ALA	2.9
3	F	213	ALA	2.9
3	O	38	ALA	2.9
2	E	1134	PHE	2.9
2	E	330	ILE	2.9
2	E	494	ILE	2.9
2	E	508	ILE	2.9
1	V	304	TYR	2.9
2	E	686	GLY	2.9
2	E	729	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	579	PRO	2.9
2	E	1140	ASN	2.9
3	X	260	ASN	2.9
2	E	767	SER	2.9
2	E	768	VAL	2.9
3	F	241	PHE	2.9
3	X	268	CYS	2.9
2	E	213	ARG	2.9
1	D	316	LEU	2.9
2	E	594	LEU	2.9
1	V	10	GLY	2.9
2	E	415	TYR	2.9
1	D	292	PRO	2.9
2	E	504	PRO	2.9
1	D	259	MET	2.9
1	V	14	GLU	2.9
2	E	671	ASN	2.9
2	E	902	ASN	2.9
2	E	937	ASN	2.9
2	Q	403	ASN	2.9
2	E	247	ALA	2.9
2	E	449	VAL	2.9
2	E	431	PHE	2.9
2	E	772	ARG	2.9
2	W	685	THR	2.9
2	E	940	GLY	2.9
3	I	284	GLY	2.9
2	E	126	TYR	2.9
2	E	90	GLU	2.9
2	E	736	LYS	2.9
2	E	1099	LYS	2.9
1	D	77	VAL	2.9
2	Q	563	ALA	2.9
2	Q	1147	ASP	2.9
3	F	45	ALA	2.9
3	O	57	ASP	2.9
2	E	619	HIS	2.9
3	F	43	THR	2.9
3	F	144	THR	2.9
2	E	151	LEU	2.9
1	D	199	GLY	2.8
2	E	850	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	V	353	TYR	2.8
2	E	456	LYS	2.8
2	E	896	GLU	2.8
1	D	267	ARG	2.8
1	D	87	ASP	2.8
2	E	173	SER	2.8
2	N	1021	SER	2.8
1	D	92	THR	2.8
1	D	110	THR	2.8
2	E	302	LEU	2.8
3	I	42	LEU	2.8
1	D	279	PRO	2.8
2	K	474	LYS	2.8
1	D	397	GLU	2.8
2	E	209	GLU	2.8
3	O	321	TRP	2.8
1	D	290	ALA	2.8
1	D	402	ARG	2.8
2	E	81	VAL	2.8
3	O	320	ALA	2.8
2	E	903	PHE	2.8
3	R	302	ASN	2.8
2	E	511	LEU	2.8
2	E	1059	ILE	2.8
3	F	277	LEU	2.8
2	T	305	THR	2.8
3	X	308	SER	2.8
1	D	70	GLY	2.8
1	D	39	GLN	2.8
2	E	278	PRO	2.8
2	E	629	PRO	2.8
3	F	150	PRO	2.8
3	U	147	PRO	2.8
3	F	47	GLU	2.8
2	E	61	ARG	2.8
2	E	728	VAL	2.8
2	W	570	ASN	2.8
1	D	347	MET	2.8
2	E	324	MET	2.8
2	E	1076	LYS	2.8
2	Q	402	PRO	2.8
3	I	268	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	157	GLU	2.8
1	D	163	GLU	2.8
2	E	37	VAL	2.8
1	D	17	TYR	2.8
1	D	149	ALA	2.8
1	V	132	TYR	2.8
2	E	341	ALA	2.8
2	E	512	ALA	2.8
2	E	1085	PHE	2.8
2	E	677	ILE	2.8
2	E	122	HIS	2.8
2	E	1078	LYS	2.8
2	Q	260	GLN	2.7
1	D	252	ARG	2.7
1	D	359	GLU	2.7
3	X	293	VAL	2.7
2	E	371	TRP	2.7
3	X	263	TRP	2.7
1	D	26	PHE	2.7
1	D	271	PHE	2.7
2	E	590	PHE	2.7
1	D	9	LEU	2.7
2	E	44	TYR	2.7
2	E	487	ILE	2.7
2	E	1047	TYR	2.7
2	Q	372	TYR	2.7
2	W	684	ILE	2.7
2	E	816	HIS	2.7
2	E	505	LYS	2.7
2	E	243	ASN	2.7
2	W	1014	ASN	2.7
2	E	1096	THR	2.7
2	E	306	GLY	2.7
1	D	155	PRO	2.7
2	E	858	PRO	2.7
1	D	367	GLU	2.7
1	D	340	ALA	2.7
1	V	7	TRP	2.7
2	E	428	ILE	2.7
2	E	1051	PHE	2.7
2	E	560	HIS	2.7
2	W	974	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	393	LYS	2.7
2	W	547	MET	2.7
2	E	776	GLY	2.7
2	W	472	ASP	2.7
2	E	207	PRO	2.7
1	D	268	LEU	2.7
2	E	208	LYS	2.7
2	E	1137	LYS	2.7
1	D	91	TYR	2.7
2	H	790	ASN	2.7
1	D	270	GLY	2.7
2	E	227	GLY	2.7
2	E	279	GLY	2.7
2	E	607	GLY	2.7
2	E	622	ARG	2.7
2	E	804	ARG	2.7
2	W	1117	GLY	2.7
3	F	85	ASP	2.7
3	F	89	PRO	2.7
3	O	69	GLY	2.7
2	E	459	ASP	2.7
2	W	1062	ASP	2.7
1	D	349	GLN	2.7
2	E	325	GLU	2.7
2	E	475	GLU	2.7
2	E	689	GLU	2.7
3	O	68	GLU	2.7
2	E	406	LEU	2.7
1	D	327	ALA	2.7
1	V	37	ALA	2.7
2	E	703	PHE	2.7
2	E	1105	ILE	2.7
3	I	31	ALA	2.7
2	E	174	TRP	2.7
2	E	758	TRP	2.7
2	E	1015	CYS	2.7
1	D	403	PRO	2.7
2	E	274	GLY	2.7
2	E	724	GLY	2.7
2	E	1080	GLY	2.7
1	D	233	GLU	2.7
2	E	877	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	977	VAL	2.7
2	E	987	GLU	2.7
1	D	289	ILE	2.6
2	E	262	LEU	2.7
3	I	152	SER	2.7
1	V	106	ALA	2.6
2	E	935	TRP	2.6
2	E	532	TYR	2.6
1	D	281	THR	2.6
1	V	256	THR	2.6
2	E	170	LEU	2.6
2	E	200	LYS	2.6
2	E	400	ILE	2.6
2	E	439	LYS	2.6
2	W	35	VAL	2.6
3	F	32	GLU	2.6
2	E	875	ILE	2.6
1	V	85	SER	2.6
2	H	563	ALA	2.6
3	I	111	PHE	2.6
1	D	346	ARG	2.6
2	Q	1080	GLY	2.6
1	D	160	THR	2.6
1	D	222	LYS	2.6
1	M	95	LYS	2.6
2	E	379	LYS	2.6
2	E	897	THR	2.6
1	D	184	LEU	2.6
1	V	62	ASN	2.6
1	V	82	LEU	2.6
2	W	1118	VAL	2.6
3	X	96	ASN	2.6
1	D	133	ILE	2.6
1	D	389	GLU	2.6
1	V	233	GLU	2.6
2	E	934	ILE	2.6
1	V	94	ASP	2.6
3	X	116	ASP	2.6
1	D	168	PHE	2.6
2	E	1032	ALA	2.6
3	F	151	PHE	2.6
3	O	204	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	174	ILE	2.6
1	D	333	VAL	2.6
2	E	788	ILE	2.6
3	O	75	GLU	2.6
3	O	109	ILE	2.6
2	Q	352	ASN	2.6
1	D	57	PHE	2.6
2	E	911	PHE	2.6
2	B	472	ASP	2.6
2	E	326	ARG	2.6
1	D	220	TYR	2.6
2	E	1019	LYS	2.6
1	D	384	GLY	2.6
1	V	264	GLY	2.6
2	E	556	GLY	2.6
2	E	1003	LEU	2.6
1	D	83	ILE	2.6
1	D	214	CYS	2.6
2	E	725	ILE	2.6
2	E	1017	MET	2.6
2	E	83	ASN	2.6
2	E	932	ASN	2.6
2	E	1014	ASN	2.6
2	E	1132	ASN	2.6
3	F	267	PHE	2.6
3	C	248	ASP	2.6
1	D	257	ARG	2.5
2	E	425	ARG	2.5
1	D	247	SER	2.5
2	W	307	LYS	2.5
1	D	353	TYR	2.5
1	V	3	LEU	2.5
2	E	537	LEU	2.5
2	E	914	VAL	2.5
1	D	28	ALA	2.5
2	E	79	ALA	2.5
3	X	130	PHE	2.5
2	B	710	ASN	2.5
3	O	260	ASN	2.5
2	E	48	ARG	2.5
1	D	152	SER	2.5
3	O	46	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	V	323	GLY	2.5
2	E	246	LEU	2.5
3	O	303	GLY	2.5
1	D	116	ILE	2.5
1	D	254	MET	2.5
2	E	741	MET	2.5
2	E	159	TYR	2.5
2	E	631	TYR	2.5
2	E	1126	TYR	2.5
2	E	50	GLU	2.5
2	E	755	GLU	2.5
1	D	18	PHE	2.5
1	D	205	GLN	2.5
2	E	260	GLN	2.5
2	E	535	ALA	2.5
2	W	927	ALA	2.5
1	V	12	ARG	2.5
2	E	155	ASN	2.5
2	E	171	ARG	2.5
1	D	85	SER	2.5
1	D	86	PRO	2.5
2	T	69	PRO	2.5
3	X	215	LEU	2.5
1	V	270	GLY	2.5
2	W	303	ILE	2.5
1	V	193	TYR	2.5
1	D	326	GLU	2.5
1	V	2	THR	2.5
2	E	179	THR	2.5
2	E	219	THR	2.5
2	E	132	ARG	2.5
1	V	88	ASN	2.5
2	Q	530	ASN	2.5
3	I	73	ASN	2.5
3	O	61	HIS	2.5
1	V	198	ASP	2.5
2	E	1065	MET	2.5
3	F	244	LEU	2.5
1	D	131	GLY	2.5
2	E	499	SER	2.5
2	E	1044	PRO	2.5
2	E	874	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	119	VAL	2.5
1	D	7	TRP	2.5
1	V	15	TYR	2.5
2	E	664	TYR	2.5
2	W	65	TYR	2.5
1	V	269	GLN	2.5
3	F	74	ALA	2.5
2	E	593	ASN	2.5
1	D	76	ASP	2.4
1	D	96	ASP	2.4
1	D	161	LEU	2.4
2	H	472	ASP	2.4
2	B	476	ILE	2.4
3	O	145	ILE	2.4
1	V	103	GLY	2.4
2	E	791	GLY	2.4
2	E	1086	GLY	2.4
1	V	47	SER	2.4
2	E	414	SER	2.4
2	E	743	SER	2.4
1	D	297	PHE	2.4
2	E	651	PHE	2.4
2	E	906	GLU	2.4
1	V	220	TYR	2.4
3	X	322	GLN	2.4
2	B	305	THR	2.4
2	B	389	THR	2.4
2	E	470	THR	2.4
1	D	400	HIS	2.4
2	E	819	LEU	2.4
2	N	115	CYS	2.4
2	Q	30	LEU	2.4
2	T	31	LEU	2.4
1	V	86	PRO	2.4
2	E	45	PRO	2.4
2	E	737	ILE	2.4
2	E	973	ASP	2.4
1	V	4	VAL	2.4
2	E	216	GLY	2.4
2	Q	457	GLY	2.4
1	D	11	ARG	2.4
1	D	117	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	154	GLU	2.4
1	D	180	TYR	2.4
2	K	597	TYR	2.4
2	Q	912	TYR	2.4
2	W	58	GLN	2.4
3	I	178	THR	2.4
1	V	400	HIS	2.4
2	E	273	HIS	2.4
2	K	662	HIS	2.4
1	D	283	LEU	2.4
2	E	135	LEU	2.4
2	E	603	LEU	2.4
2	E	667	LEU	2.4
2	E	1102	LEU	2.4
2	Q	544	LEU	2.4
3	F	96	ASN	2.4
1	D	72	PRO	2.4
1	D	357	ILE	2.4
2	E	134	PRO	2.4
2	E	961	PRO	2.4
1	D	264	GLY	2.4
2	B	473	GLY	2.4
2	E	145	ASP	2.4
2	E	218	GLY	2.4
2	E	498	VAL	2.4
2	N	1141	GLY	2.4
1	D	151	SER	2.4
2	B	924	SER	2.4
2	Q	683	GLU	2.4
2	Q	1064	SER	2.4
2	T	1072	SER	2.4
2	Q	434	TRP	2.4
2	W	573	ALA	2.4
1	D	170	TYR	2.4
2	T	806	TYR	2.4
3	F	219	TYR	2.4
1	V	344	LEU	2.4
2	H	31	LEU	2.4
2	E	244	ASN	2.4
2	E	870	PRO	2.4
2	E	942	PRO	2.4
2	E	980	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	W	70	ASN	2.4
2	E	663	VAL	2.4
1	D	262	CYS	2.4
1	M	76	ASP	2.4
2	E	364	LYS	2.4
2	W	686	GLY	2.4
3	X	303	GLY	2.4
2	E	368	ASP	2.4
1	D	365	GLU	2.4
2	E	675	GLU	2.4
2	E	852	GLU	2.4
3	I	148	GLU	2.4
3	F	38	ALA	2.4
3	F	315	SER	2.4
1	D	379	THR	2.4
2	W	57	TYR	2.4
2	W	356	THR	2.4
2	E	1139	LEU	2.4
1	D	67	PRO	2.4
2	E	1009	PRO	2.4
1	V	190	LYS	2.3
3	X	51	VAL	2.3
2	E	457	GLY	2.3
3	O	65	GLY	2.3
1	D	208	CYS	2.3
1	V	30	PHE	2.3
1	V	185	ALA	2.3
3	F	31	ALA	2.3
3	I	259	GLU	2.3
1	J	247	SER	2.3
2	Q	371	TRP	2.3
3	X	216	SER	2.3
1	D	148	THR	2.3
1	D	305	TYR	2.3
1	D	315	TYR	2.3
1	D	369	HIS	2.3
1	P	2	THR	2.3
2	E	72	THR	2.3
2	E	517	THR	2.3
2	Q	542	TYR	2.3
1	D	280	ILE	2.3
2	E	657	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	1024	ILE	2.3
1	D	142	PRO	2.3
2	E	899	LYS	2.3
3	F	86	LYS	2.3
3	X	44	PRO	2.3
2	E	254	ARG	2.3
2	E	1004	ARG	2.3
1	V	109	GLY	2.3
2	K	710	ASN	2.3
1	V	112	GLU	2.3
2	E	144	ALA	2.3
2	W	341	ALA	2.3
2	E	1048	GLN	2.3
1	D	89	ILE	2.3
2	E	337	TYR	2.3
2	E	986	TYR	2.3
2	E	1016	THR	2.3
2	H	631	TYR	2.3
2	W	305	THR	2.3
2	W	1124	THR	2.3
1	D	390	VAL	2.3
1	V	130	VAL	2.3
2	E	125	VAL	2.3
2	E	440	GLY	2.3
1	D	31	ASN	2.3
3	O	302	ASN	2.3
3	F	111	PHE	2.3
1	D	216	GLU	2.3
2	E	168	GLU	2.3
3	C	31	ALA	2.3
3	F	292	ALA	2.3
2	E	1120	ASP	2.3
1	D	183	CYS	2.3
2	E	857	LEU	2.3
1	D	90	TRP	2.3
1	D	206	LYS	2.3
2	B	1020	HIS	2.3
2	H	1021	SER	2.3
2	Q	401	ILE	2.3
2	W	487	ILE	2.3
3	O	103	ILE	2.3
1	D	249	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	249	THR	2.3
1	P	158	TYR	2.3
2	E	52	VAL	2.3
2	E	672	PRO	2.3
2	E	1103	VAL	2.3
1	D	109	GLY	2.3
3	F	217	GLY	2.3
3	X	133	GLY	2.3
1	V	13	MET	2.3
2	T	443	ALA	2.3
1	D	217	GLN	2.3
2	E	41	LEU	2.3
2	E	1001	LEU	2.3
2	E	1143	LEU	2.3
2	Q	756	ASP	2.3
3	O	140	LEU	2.3
3	X	82	GLN	2.3
1	V	23	LYS	2.3
2	E	639	LYS	2.3
1	D	317	ARG	2.3
3	X	321	TRP	2.3
1	P	335	SER	2.3
2	E	574	SER	2.3
1	D	102	TYR	2.3
2	Q	629	PRO	2.3
2	Q	1146	VAL	2.3
2	W	147	GLY	2.3
3	I	217	GLY	2.3
1	V	26	PHE	2.2
2	E	754	PHE	2.2
1	D	33	ASN	2.2
2	E	84	ASN	2.2
2	E	954	GLU	2.2
2	E	1130	ASN	2.2
3	L	60	ALA	2.2
3	X	292	ALA	2.2
2	B	30	LEU	2.2
1	D	194	LYS	2.2
2	W	718	GLN	2.2
3	F	46	LYS	2.2
2	Q	355	ASP	2.2
2	Q	472	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	Q	1144	ILE	2.2
1	V	8	HIS	2.2
2	E	47	ARG	2.2
2	E	490	ARG	2.2
1	V	299	THR	2.2
2	E	501	THR	2.2
2	E	1127	THR	2.2
2	H	796	PRO	2.2
2	Q	807	PRO	2.2
2	W	1096	THR	2.2
3	X	178	THR	2.2
1	D	29	VAL	2.2
2	E	670	VAL	2.2
1	V	211	TYR	2.2
2	E	699	SER	2.2
2	W	1064	SER	2.2
1	V	168	PHE	2.2
2	Q	1065	MET	2.2
1	D	186	ALA	2.2
1	D	197	GLU	2.2
1	V	202	LEU	2.2
2	B	477	GLU	2.2
2	E	747	GLU	2.2
3	F	75	GLU	2.2
3	O	259	GLU	2.2
2	E	606	LYS	2.2
3	O	306	ASN	2.2
1	D	313	ARG	2.2
1	D	336	ARG	2.2
2	E	78	ARG	2.2
2	H	71	ASP	2.2
2	W	1147	ASP	2.2
1	D	48	THR	2.2
1	P	90	TRP	2.2
2	B	784	THR	2.2
2	E	866	PRO	2.2
2	E	1118	VAL	2.2
3	O	64	VAL	2.2
2	B	119	TYR	2.2
2	T	597	TYR	2.2
2	T	924	SER	2.2
3	X	110	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	2.2
1	V	105	GLY	2.2
2	E	165	GLY	2.2
2	E	197	GLY	2.2
2	E	412	GLY	2.2
1	D	30	PHE	2.2
2	W	359	PHE	2.2
2	B	469	LYS	2.2
1	D	112	GLU	2.2
2	E	462	LEU	2.2
2	E	615	ALA	2.2
2	E	744	LYS	2.2
2	E	748	LEU	2.2
2	T	30	LEU	2.2
2	W	801	LEU	2.2
3	O	41	GLU	2.2
1	D	368	ILE	2.2
1	V	125	ILE	2.2
2	E	665	GLN	2.2
3	F	158	ARG	2.2
3	X	145	ILE	2.2
2	E	491	ASP	2.2
2	E	775	ASP	2.2
3	R	116	ASP	2.2
1	P	361	PRO	2.2
3	O	79	VAL	2.2
2	Q	72	THR	2.2
1	D	298	GLY	2.2
2	Q	500	MET	2.2
2	E	141	LYS	2.2
3	O	72	LYS	2.2
3	O	42	LEU	2.2
1	P	98	GLU	2.2
2	E	707	GLU	2.2
2	N	563	ALA	2.2
3	O	317	GLU	2.2
3	X	301	ARG	2.2
1	V	61	ASN	2.2
2	W	269	ASN	2.2
1	D	130	VAL	2.2
1	M	273	ASP	2.2
2	B	629	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	981	PRO	2.2
2	N	449	VAL	2.2
1	P	92	THR	2.2
1	D	190	LYS	2.2
1	V	78	LYS	2.2
2	B	474	LYS	2.2
2	E	473	GLY	2.2
1	V	305	TYR	2.2
2	B	346	TYR	2.2
2	W	1126	TYR	2.2
3	O	288	TYR	2.2
2	E	548	LEU	2.2
1	D	138	GLU	2.2
1	D	329	GLU	2.2
1	M	106	ALA	2.2
1	V	197	GLU	2.2
2	W	830	ALA	2.2
3	I	40	GLU	2.2
3	O	118	ALA	2.2
3	F	318	ARG	2.1
3	I	100	ILE	2.1
2	W	276	GLN	2.1
2	E	166	ASN	2.1
2	E	253	ASN	2.1
2	E	128	PRO	2.1
3	X	34	VAL	2.1
1	D	147	ASP	2.1
2	B	71	ASP	2.1
2	E	373	ASP	2.1
2	E	966	ASP	2.1
1	D	277	LYS	2.1
2	E	300	LYS	2.1
2	E	147	GLY	2.1
2	E	194	GLY	2.1
3	F	243	THR	2.1
1	V	117	PHE	2.1
1	V	291	LEU	2.1
2	W	571	PHE	2.1
3	O	71	PHE	2.1
2	W	1055	SER	2.1
3	I	216	SER	2.1
3	O	126	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	X	97	SER	2.1
1	D	306	ILE	2.1
1	D	399	ILE	2.1
3	X	62	ILE	2.1
3	I	310	GLN	2.1
1	D	286	HIS	2.1
2	E	923	HIS	2.1
3	C	61	HIS	2.1
3	F	73	ASN	2.1
3	I	260	ASN	2.1
2	W	89	VAL	2.1
2	E	86	MET	2.1
3	X	89	PRO	2.1
1	D	234	LYS	2.1
2	E	474	LYS	2.1
2	E	901	LYS	2.1
2	E	990	LYS	2.1
2	E	38	ASP	2.1
2	E	1125	GLY	2.1
2	W	709	THR	2.1
1	V	9	LEU	2.1
3	X	151	PHE	2.1
2	B	563	ALA	2.1
2	W	912	TYR	2.1
3	X	135	ALA	2.1
1	P	36	ILE	2.1
1	V	98	GLU	2.1
3	C	148	GLU	2.1
1	D	287	GLN	2.1
1	M	217	GLN	2.1
1	V	217	GLN	2.1
1	V	318	GLN	2.1
2	E	342	GLN	2.1
2	W	122	HIS	2.1
1	D	334	PRO	2.1
1	P	95	LYS	2.1
2	E	648	VAL	2.1
2	E	936	ASN	2.1
3	F	37	VAL	2.1
3	O	48	VAL	2.1
1	D	42	THR	2.1
1	P	273	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	114	ASP	2.1
2	E	203	ASP	2.1
2	E	632	GLY	2.1
3	O	284	GLY	2.1
2	Q	389	THR	2.1
2	W	121	PHE	2.1
3	X	157	ASP	2.1
2	E	124	ARG	2.1
2	E	926	TRP	2.1
3	O	115	TRP	2.1
1	D	132	TYR	2.1
1	D	284	ILE	2.1
1	P	112	GLU	2.1
1	V	36	ILE	2.1
2	E	1049	SER	2.1
3	I	196	SER	2.1
3	X	94	SER	2.1
1	V	222	LYS	2.1
2	E	323	VAL	2.1
2	E	378	LYS	2.1
2	Q	835	PRO	2.1
3	F	276	PRO	2.1
2	H	710	ASN	2.1
1	V	283	LEU	2.1
2	W	1073	LEU	2.1
3	X	140	LEU	2.1
1	P	168	PHE	2.1
1	V	320	PHE	2.1
2	B	306	GLY	2.1
2	E	526	GLY	2.1
2	W	569	GLY	2.1
3	F	195	PHE	2.1
3	I	230	GLY	2.1
1	D	166	ARG	2.1
2	B	1127	THR	2.1
2	E	71	ASP	2.1
2	E	137	ARG	2.1
2	Q	1062	ASP	2.1
1	D	129	ALA	2.1
1	V	192	ILE	2.1
2	E	172	ALA	2.1
2	E	927	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	Q	387	ILE	2.1
2	W	106	ALA	2.1
3	O	309	ILE	2.1
1	D	358	GLU	2.1
2	E	509	GLU	2.1
3	F	214	GLU	2.1
3	I	219	TYR	2.1
3	X	288	TYR	2.1
2	E	531	HIS	2.0
1	V	77	VAL	2.0
2	E	1097	VAL	2.0
3	O	266	VAL	2.0
3	O	283	PRO	2.0
1	D	61	ASN	2.0
1	V	6	ASN	2.0
2	E	369	ASN	2.0
2	E	507	LEU	2.0
2	E	1008	ASN	2.0
2	W	31	LEU	2.0
1	P	264	GLY	2.0
2	B	1129	GLY	2.0
2	E	184	GLY	2.0
2	H	473	GLY	2.0
2	T	412	GLY	2.0
3	O	151	PHE	2.0
3	O	281	PHE	2.0
1	D	50	THR	2.0
1	P	65	THR	2.0
1	P	399	ILE	2.0
1	V	83	ILE	2.0
1	V	280	ILE	2.0
2	E	381	THR	2.0
2	Q	202	ILE	2.0
2	E	34	ALA	2.0
2	T	60	ASP	2.0
2	Q	1063	TRP	2.0
2	W	935	TRP	2.0
3	O	165	TRP	2.0
2	E	156	LYS	2.0
2	W	102	TYR	2.0
3	F	110	TYR	2.0
3	I	53	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	V	224	MET	2.0
3	O	54	MET	2.0
2	B	51	SER	2.0
2	B	1031	GLN	2.0
2	E	58	GLN	2.0
2	E	922	VAL	2.0
2	H	711	SER	2.0
2	K	1072	SER	2.0
1	V	107	PRO	2.0
2	K	30	LEU	2.0
1	D	52	ASN	2.0
1	V	176	ASN	2.0
1	P	105	GLY	2.0
1	P	113	GLY	2.0
2	E	263	GLY	2.0
1	V	92	THR	2.0
2	E	261	ALA	2.0
3	I	238	ALA	2.0
3	O	134	ALA	2.0
3	I	85	ASP	2.0
3	U	85	ASP	2.0
1	D	405	LYS	2.0
2	E	158	LYS	2.0
3	X	148	GLU	2.0
3	F	294	TRP	2.0
3	X	294	TRP	2.0
1	V	180	TYR	2.0
3	I	110	TYR	2.0
1	D	391	VAL	2.0
1	V	119	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MD1	E	5801	47/47	0.60	0.19	75,111,136,150	0
6	MD1	E	5802	47/47	0.70	0.17	80,117,133,137	0
8	HEM	F	401	43/43	0.81	0.18	77,97,112,116	0
4	SF4	D	503	8/8	0.83	0.11	107,133,158,166	0
9	CA	F	403	1/1	0.83	0.11	104,104,104,104	0
4	SF4	D	501	8/8	0.85	0.18	91,115,146,160	0
5	F3S	V	504	7/7	0.87	0.14	65,87,97,112	0
8	HEM	X	401	43/43	0.88	0.17	59,75,81,89	0
4	SF4	E	5804	8/8	0.88	0.12	119,125,139,167	0
5	F3S	D	504	7/7	0.89	0.10	99,113,128,134	0
9	CA	F	402	1/1	0.90	0.11	76,76,76,76	0
8	HEM	O	401	43/43	0.90	0.15	57,69,75,84	0
6	MD1	Q	5802	47/47	0.91	0.13	30,43,56,59	0
4	SF4	D	502	8/8	0.91	0.09	112,118,142,149	0
9	CA	U	403	1/1	0.91	0.07	29,29,29,29	0
8	HEM	I	401	43/43	0.92	0.12	38,55,65,66	0
6	MD1	W	5802	47/47	0.92	0.12	28,47,62,72	0
6	MD1	Q	5801	47/47	0.92	0.11	21,34,44,54	0
4	SF4	V	501	8/8	0.93	0.10	43,63,75,78	0
6	MD1	W	5801	47/47	0.93	0.12	31,46,57,69	0
6	MD1	N	5802	47/47	0.94	0.11	26,34,44,46	0
6	MD1	B	5801	47/47	0.94	0.12	24,34,40,41	0
9	CA	L	403	1/1	0.94	0.08	29,29,29,29	0
6	MD1	B	5802	47/47	0.94	0.11	28,42,50,56	0
9	CA	X	403	1/1	0.94	0.07	71,71,71,71	0
4	SF4	W	5804	8/8	0.95	0.10	40,57,63,72	0
6	MD1	H	5801	47/47	0.95	0.09	16,24,36,38	0
6	MD1	H	5802	47/47	0.95	0.10	15,30,36,47	0
9	CA	C	403	1/1	0.95	0.06	35,35,35,35	0
6	MD1	T	5802	47/47	0.95	0.10	22,31,41,45	0
6	MD1	K	5801	47/47	0.95	0.09	20,25,33,37	0
9	CA	I	403	1/1	0.95	0.07	69,69,69,69	0
6	MD1	K	5802	47/47	0.95	0.10	15,29,38,45	0
8	HEM	C	401	43/43	0.95	0.12	19,27,32,49	0
6	MD1	N	5801	47/47	0.95	0.10	21,28,34,48	0
8	HEM	L	401	43/43	0.96	0.10	17,24,30,33	0
4	SF4	K	5804	8/8	0.96	0.09	18,32,40,42	0

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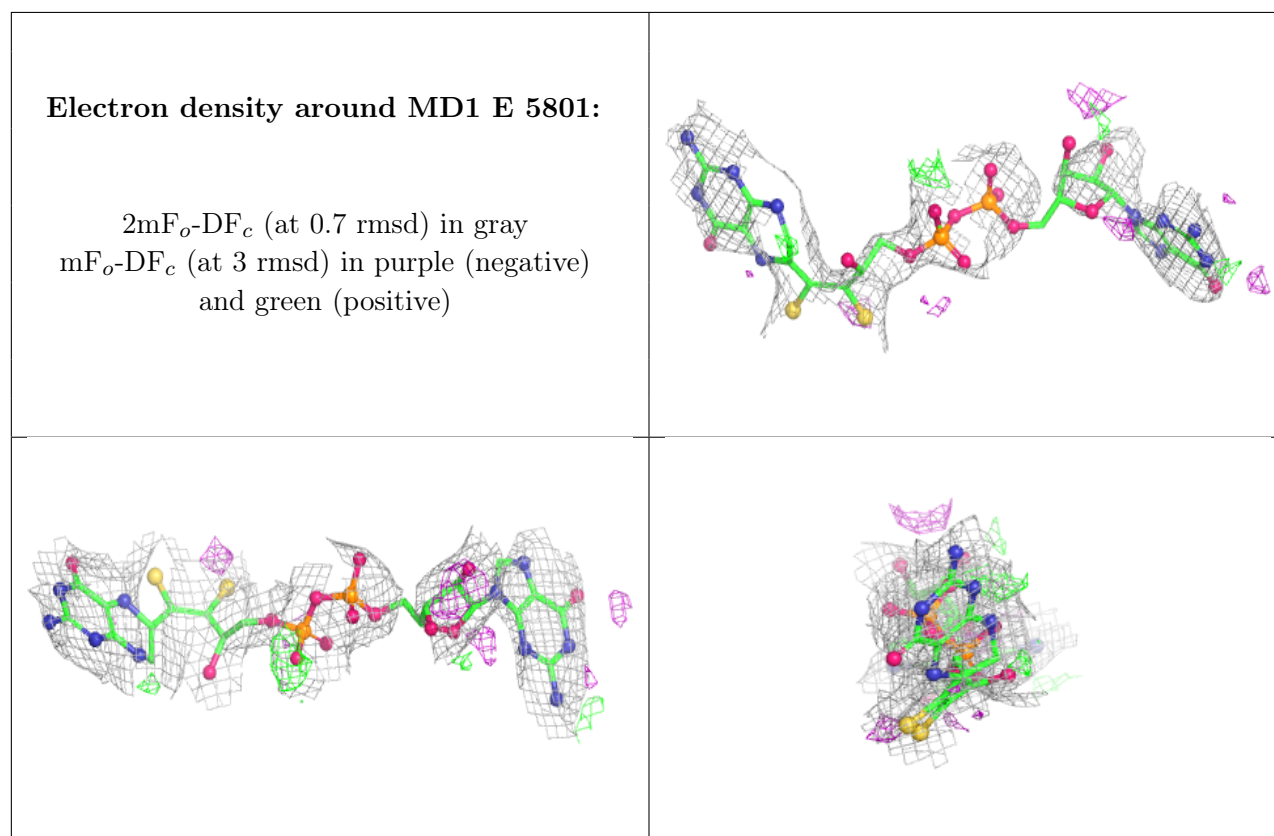
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	HEM	R	401	43/43	0.96	0.10	23,33,40,46	0
8	HEM	U	401	43/43	0.96	0.10	23,30,34,43	0
6	MD1	T	5801	47/47	0.96	0.09	23,29,35,38	0
5	F3S	M	504	7/7	0.96	0.08	46,67,69,70	0
4	SF4	N	5804	8/8	0.96	0.10	40,42,48,51	0
4	SF4	Q	5804	8/8	0.96	0.09	26,43,57,67	0
7	MO	E	5803	1/1	0.96	0.06	139,139,139,139	0
9	CA	L	402	1/1	0.96	0.05	27,27,27,27	0
4	SF4	B	5804	8/8	0.96	0.10	22,38,47,49	0
9	CA	O	402	1/1	0.96	0.05	61,61,61,61	0
9	CA	O	403	1/1	0.96	0.06	73,73,73,73	0
4	SF4	V	502	8/8	0.96	0.08	62,72,89,95	0
9	CA	X	402	1/1	0.96	0.05	56,56,56,56	0
4	SF4	H	5804	8/8	0.96	0.09	15,35,41,43	0
4	SF4	V	503	8/8	0.97	0.09	50,65,72,83	0
9	CA	C	402	1/1	0.97	0.04	33,33,33,33	0
4	SF4	M	502	8/8	0.97	0.07	58,64,82,84	0
5	F3S	A	504	7/7	0.97	0.07	24,32,43,44	0
7	MO	Q	5803	1/1	0.97	0.04	46,46,46,46	0
7	MO	T	5803	1/1	0.97	0.04	37,37,37,37	0
4	SF4	J	501	8/8	0.97	0.07	16,26,33,33	0
4	SF4	P	503	8/8	0.97	0.07	30,39,51,60	0
4	SF4	J	502	8/8	0.97	0.07	24,36,52,52	0
4	SF4	S	501	8/8	0.97	0.09	21,32,42,43	0
9	CA	R	403	1/1	0.97	0.04	35,35,35,35	0
4	SF4	T	5804	8/8	0.97	0.09	27,42,48,57	0
4	SF4	A	501	8/8	0.97	0.08	26,27,41,46	0
4	SF4	M	501	8/8	0.97	0.08	35,47,52,54	0
5	F3S	G	504	7/7	0.98	0.08	26,42,51,52	0
5	F3S	J	504	7/7	0.98	0.07	14,25,31,32	0
4	SF4	G	501	8/8	0.98	0.08	24,29,42,43	0
9	CA	I	402	1/1	0.98	0.04	46,46,46,46	0
5	F3S	P	504	7/7	0.98	0.07	24,34,45,47	0
5	F3S	S	504	7/7	0.98	0.06	19,29,43,43	0
4	SF4	P	501	8/8	0.98	0.08	30,35,42,42	0
4	SF4	P	502	8/8	0.98	0.08	37,47,60,63	0
4	SF4	G	502	8/8	0.98	0.07	30,38,54,60	0
9	CA	R	402	1/1	0.98	0.03	31,31,31,31	0
4	SF4	G	503	8/8	0.98	0.07	17,27,33,35	0
9	CA	U	402	1/1	0.98	0.06	32,32,32,32	0
4	SF4	M	503	8/8	0.98	0.06	32,44,56,57	0
4	SF4	S	502	8/8	0.98	0.08	29,39,52,53	0

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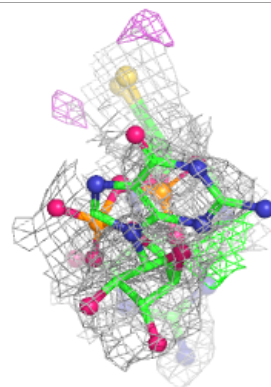
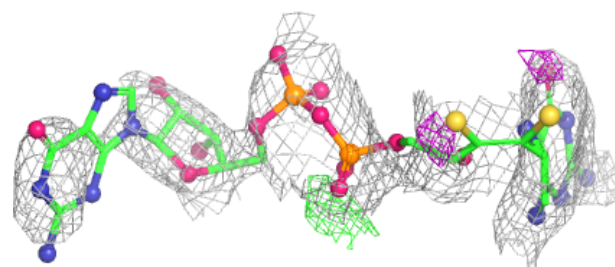
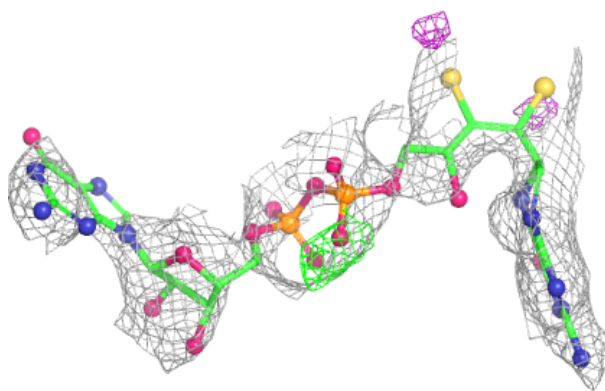
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MO	B	5803	1/1	0.98	0.04	45,45,45,45	0
4	SF4	A	503	8/8	0.99	0.07	27,34,49,51	0
4	SF4	A	502	8/8	0.99	0.05	27,43,54,56	0
7	MO	H	5803	1/1	0.99	0.04	38,38,38,38	0
7	MO	K	5803	1/1	0.99	0.03	36,36,36,36	0
7	MO	N	5803	1/1	0.99	0.03	30,30,30,30	0
4	SF4	S	503	8/8	0.99	0.05	28,33,41,47	0
4	SF4	J	503	8/8	0.99	0.05	25,29,37,38	0
7	MO	W	5803	1/1	0.99	0.04	61,61,61,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



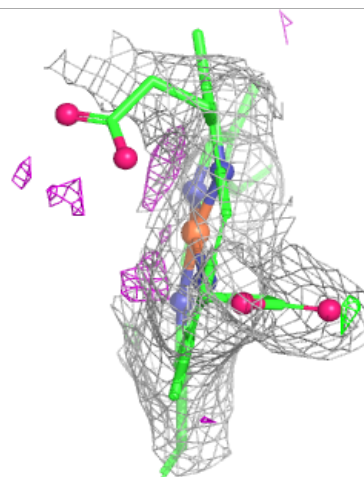
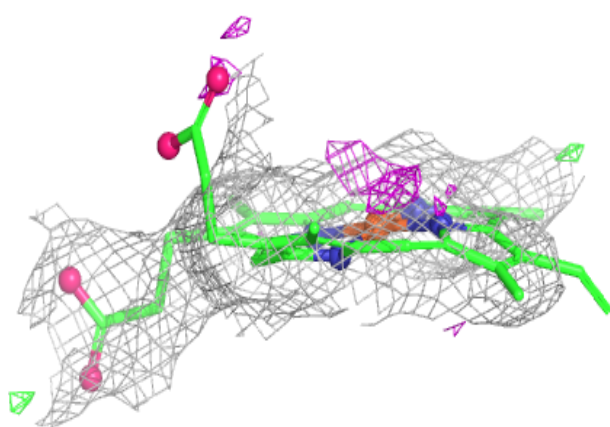
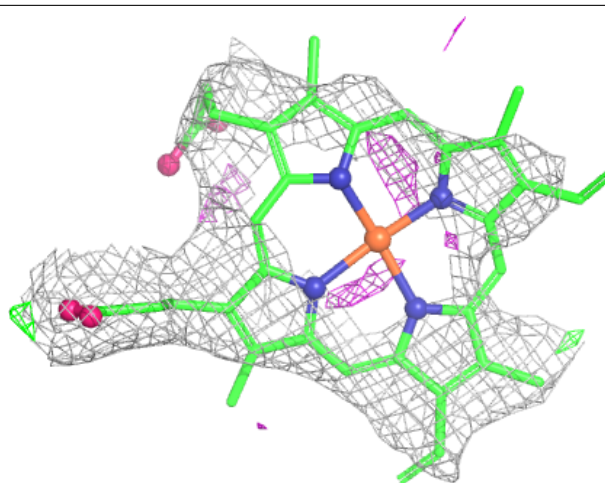
Electron density around MD1 E 5802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



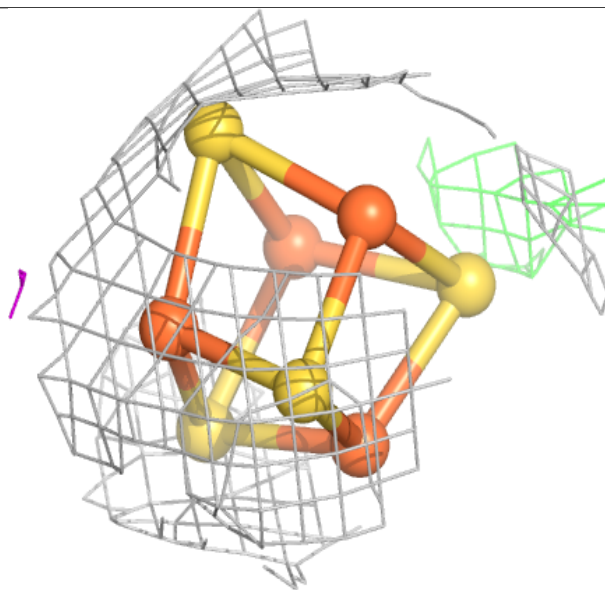
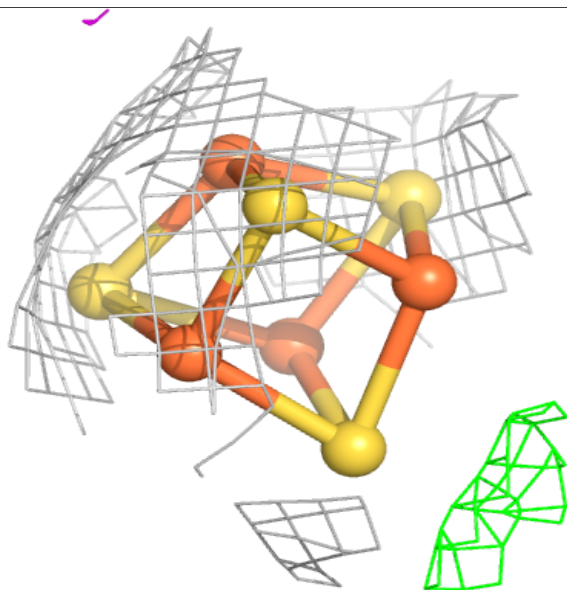
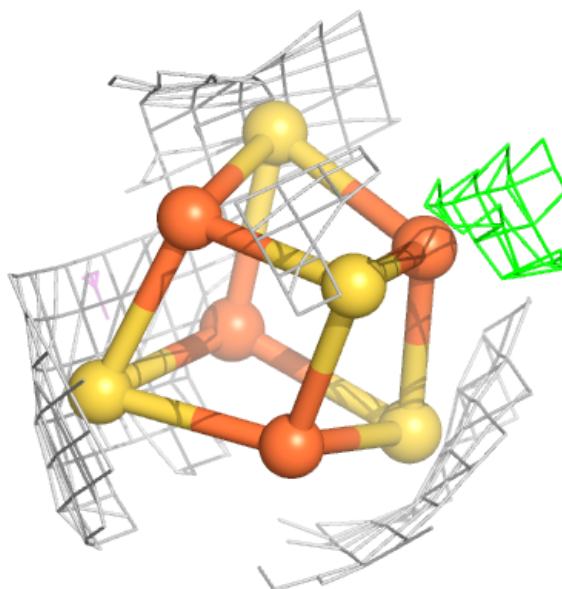
Electron density around HEM F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



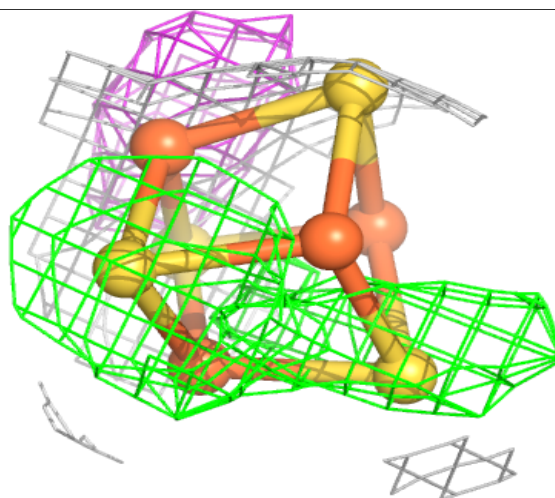
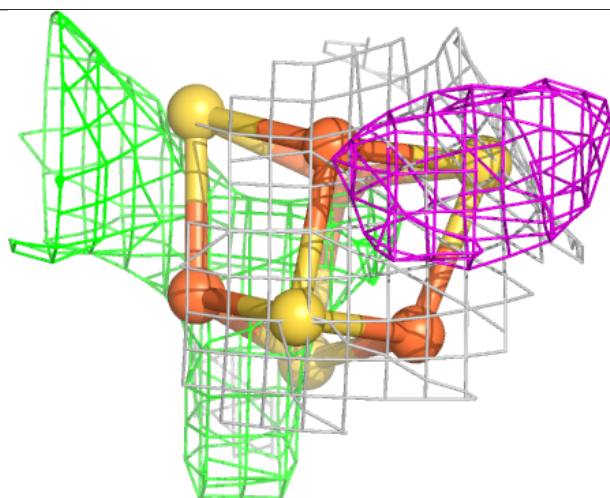
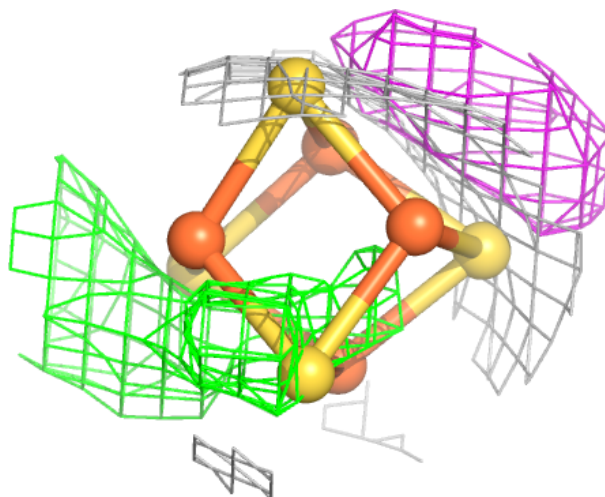
Electron density around SF4 D 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



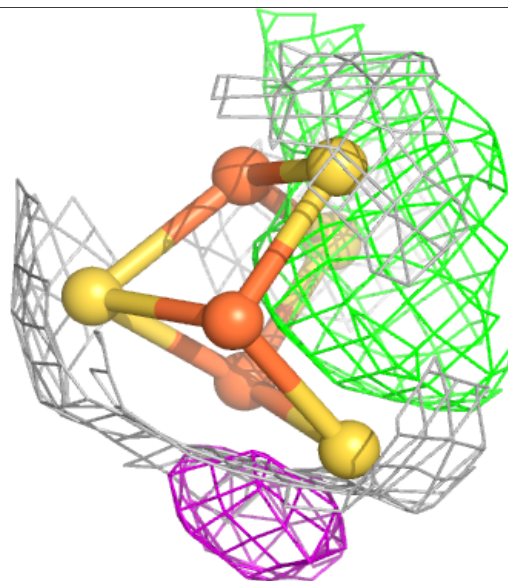
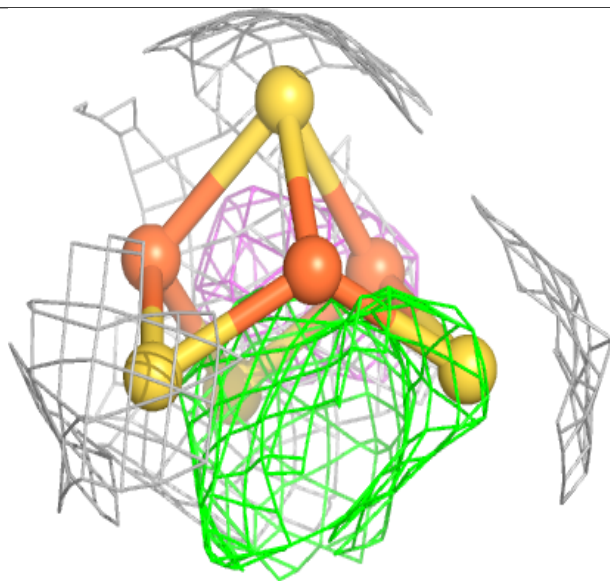
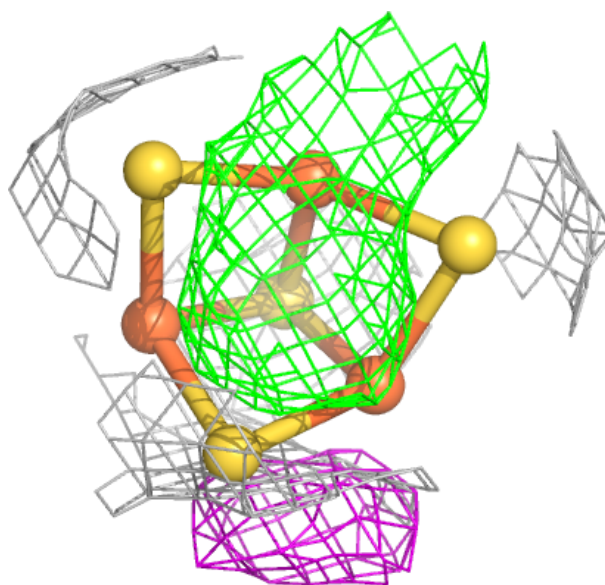
Electron density around SF4 D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



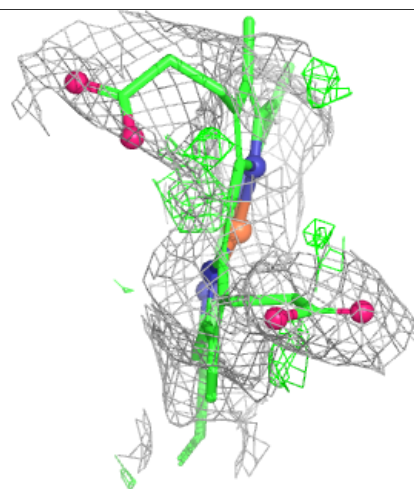
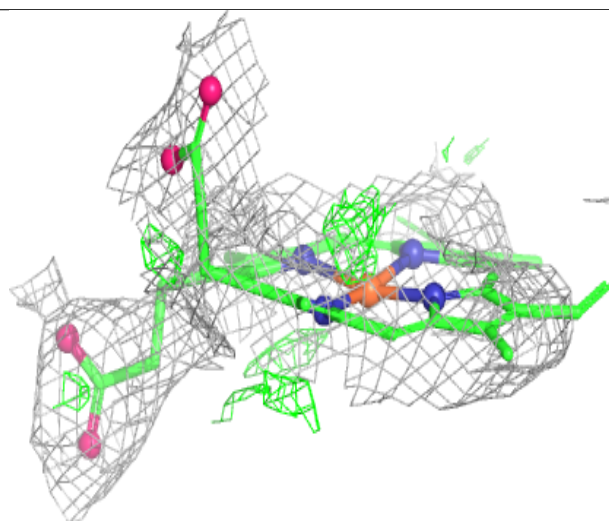
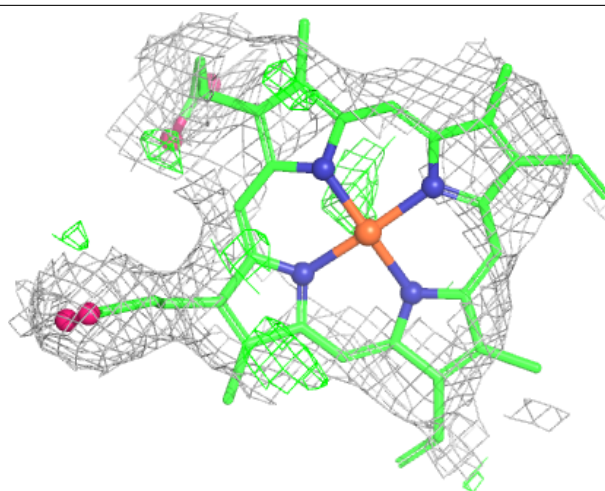
Electron density around F3S V 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



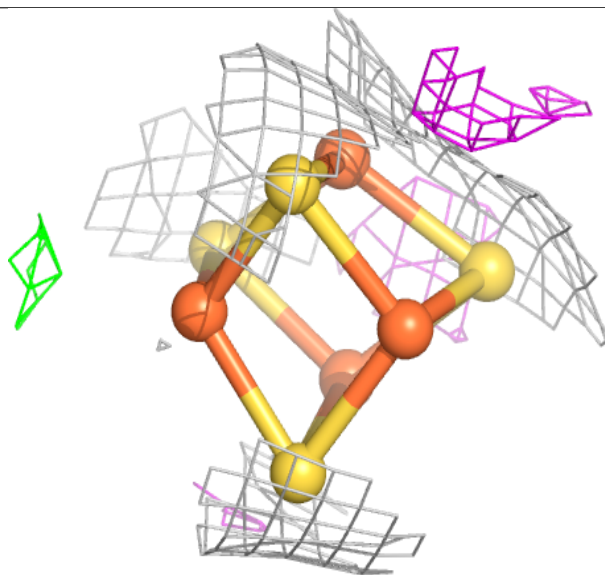
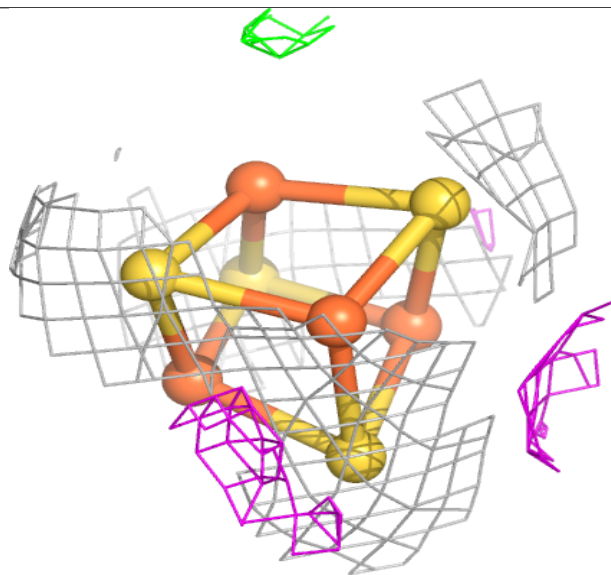
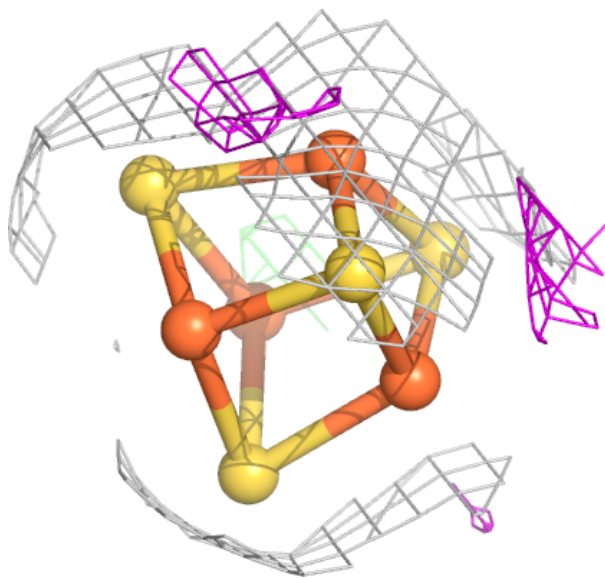
Electron density around HEM X 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



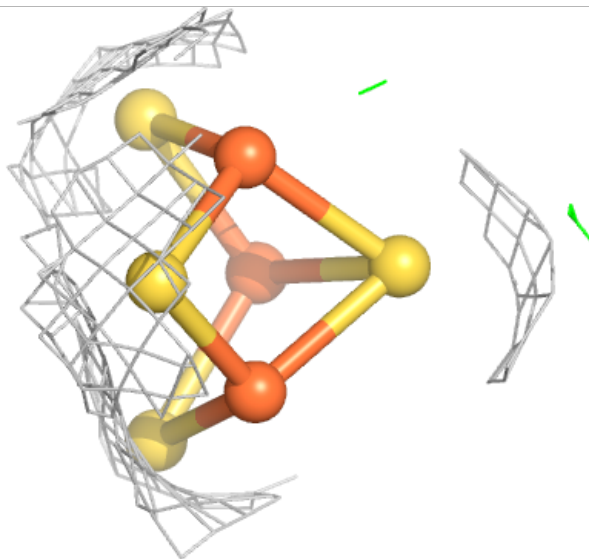
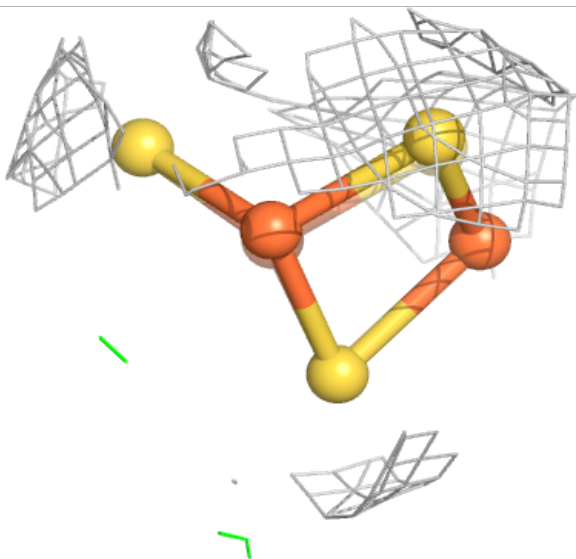
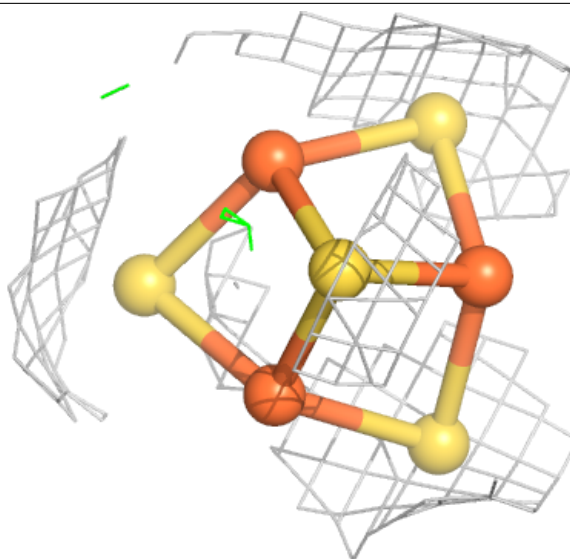
Electron density around SF4 E 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



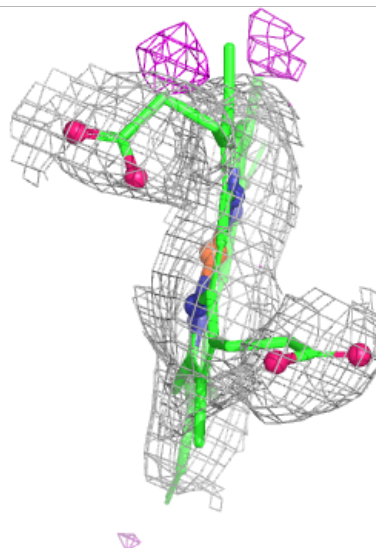
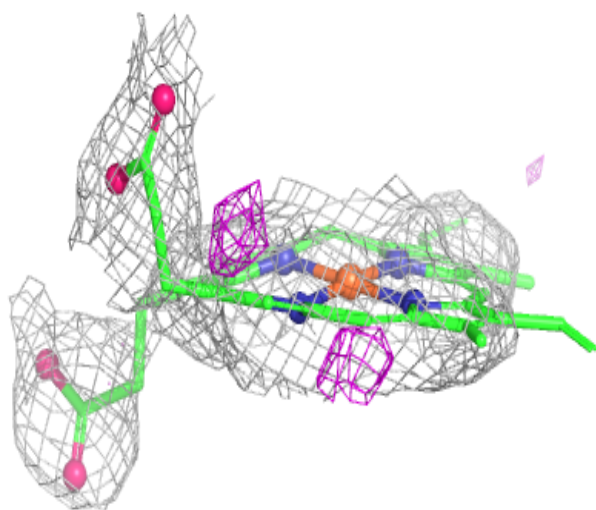
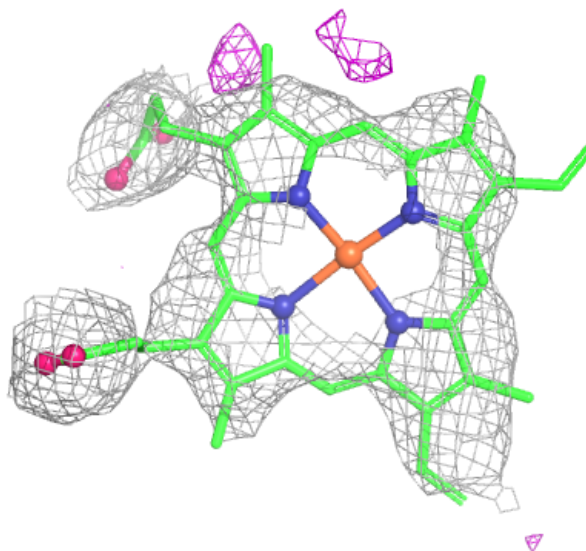
Electron density around F3S D 504:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



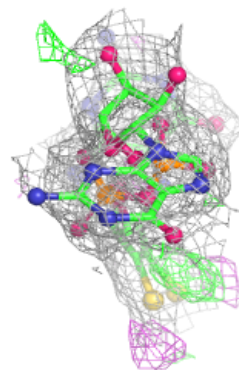
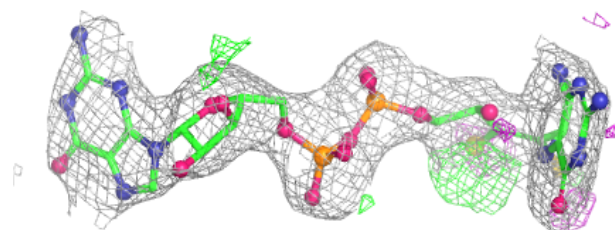
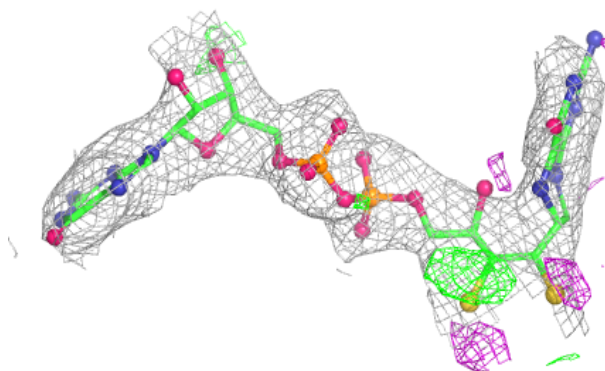
Electron density around HEM O 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



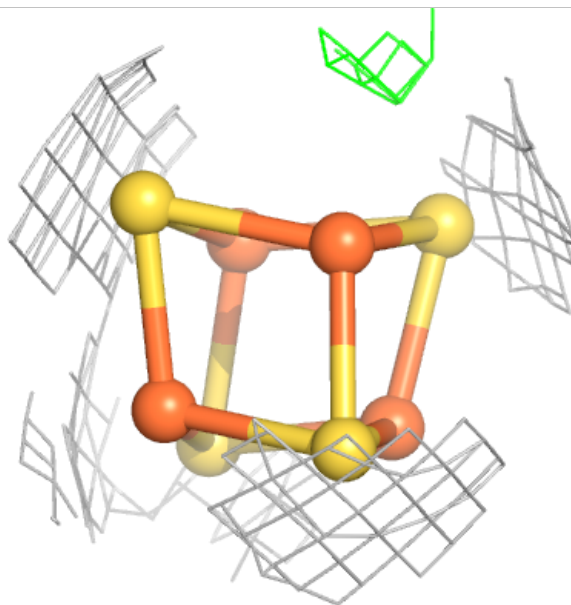
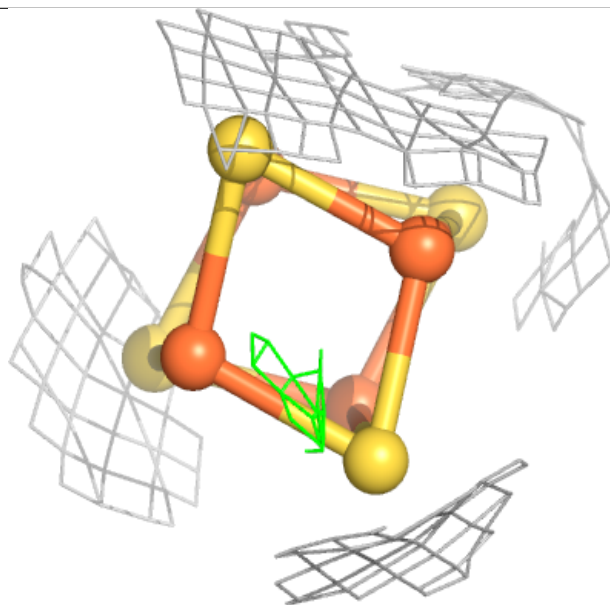
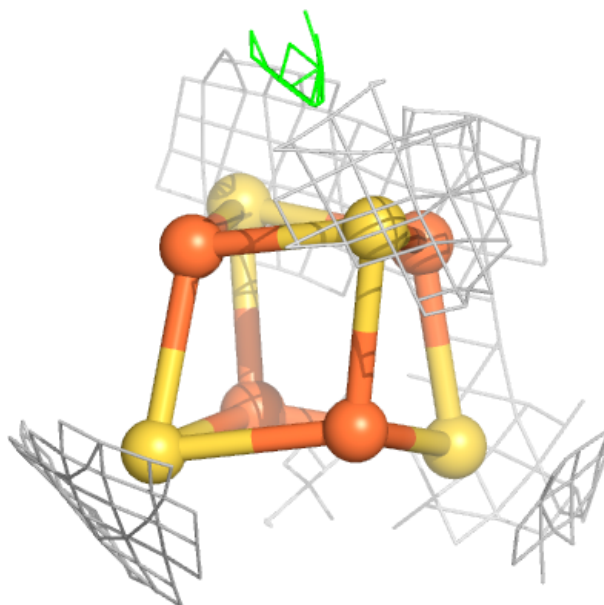
Electron density around MD1 Q 5802:

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and green (positive)



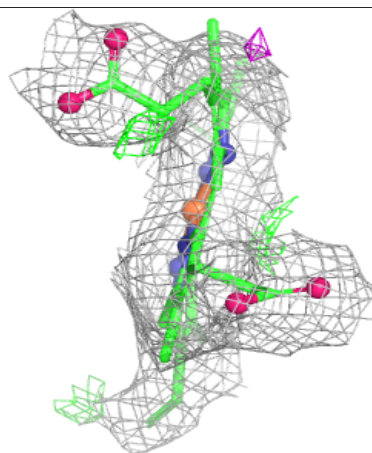
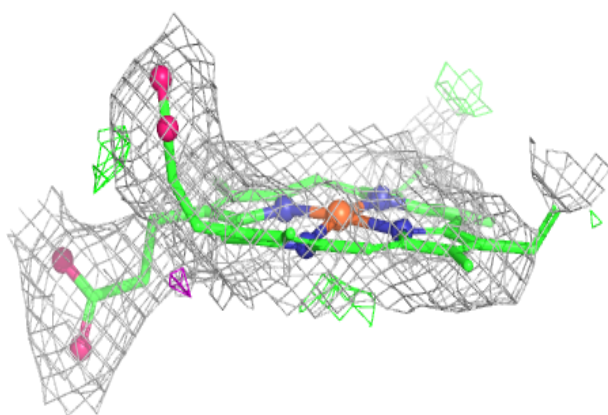
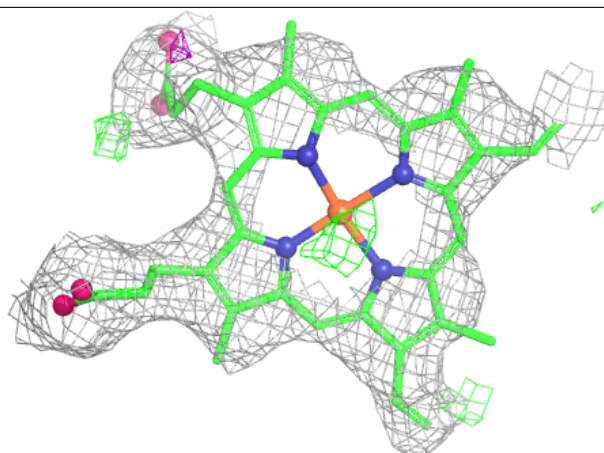
Electron density around SF4 D 502:

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and green (positive)

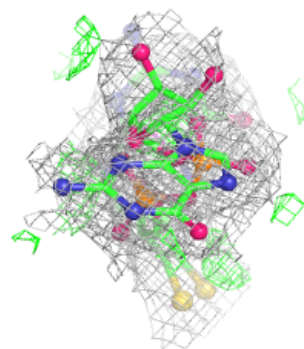
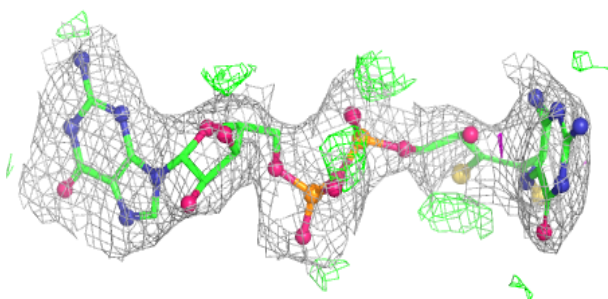
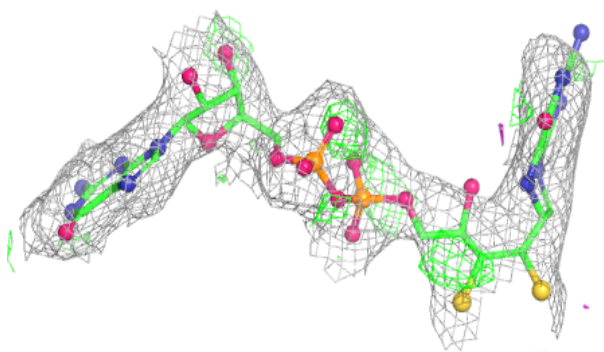


Electron density around HEM I 401:

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and green (positive)

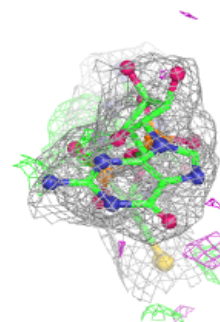
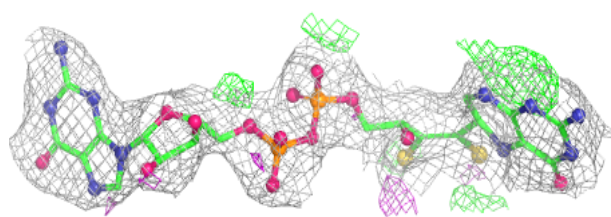
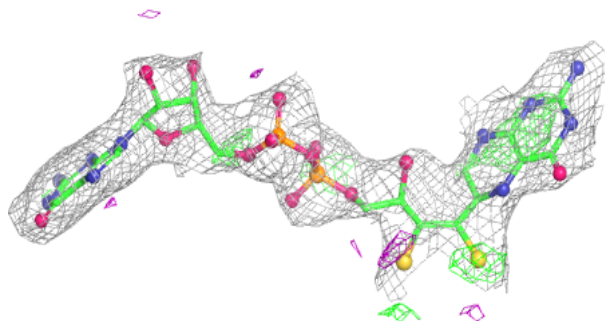
**Electron density around MD1 W 5802:**

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and green (positive)



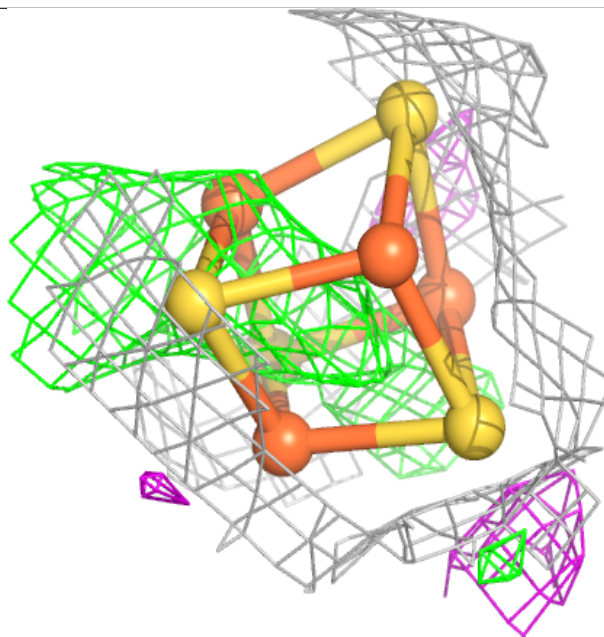
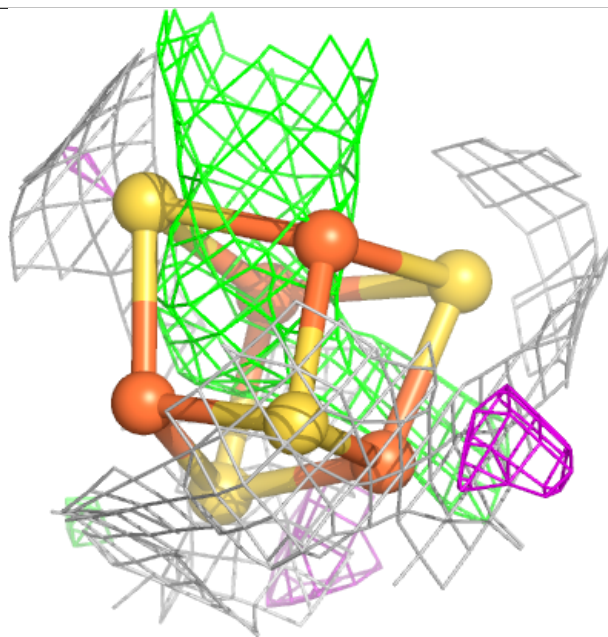
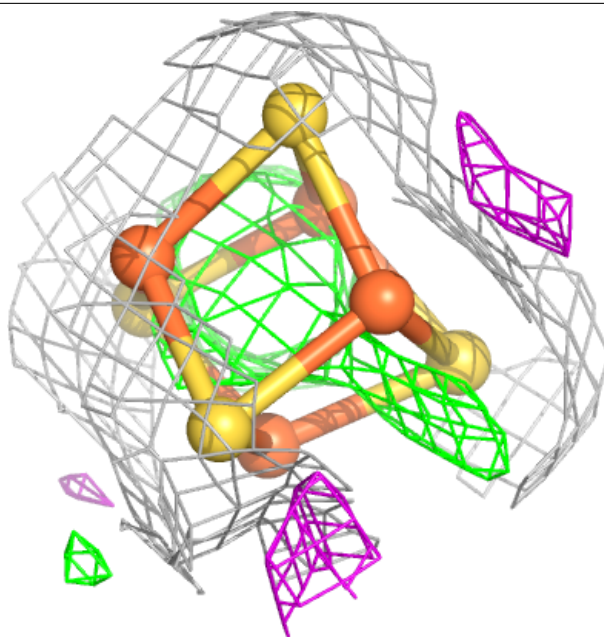
Electron density around MD1 Q 5801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



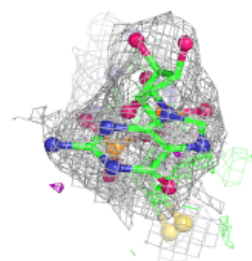
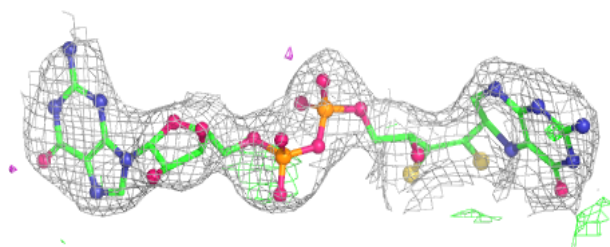
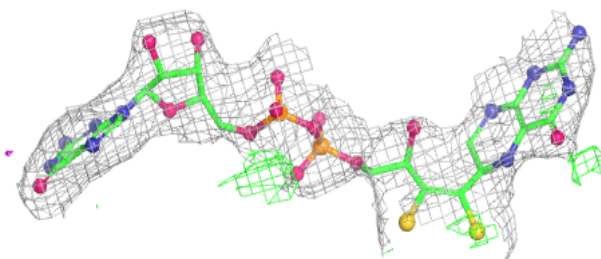
Electron density around SF4 V 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

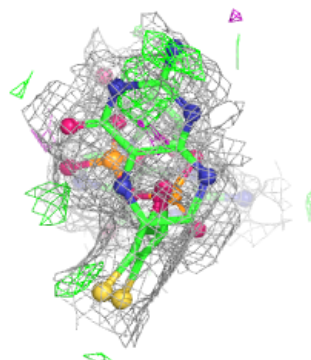
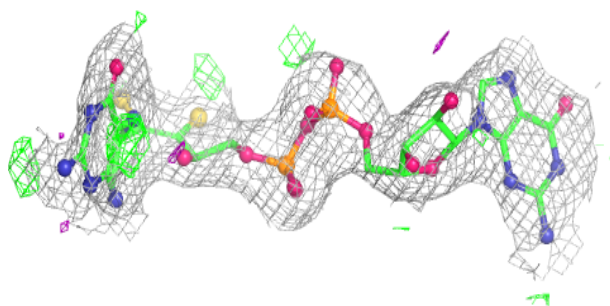
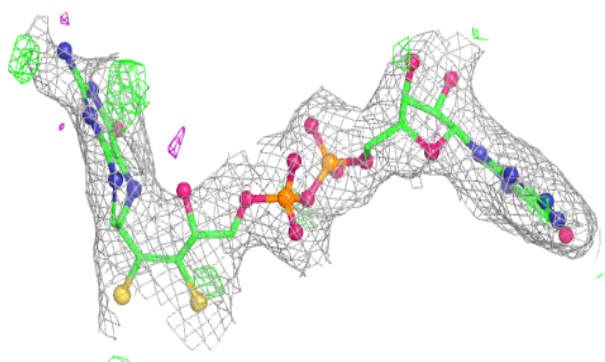


Electron density around MD1 W 5801:

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and green (positive)

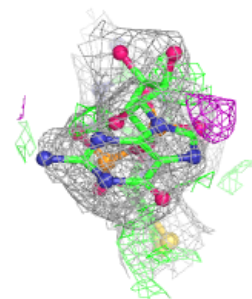
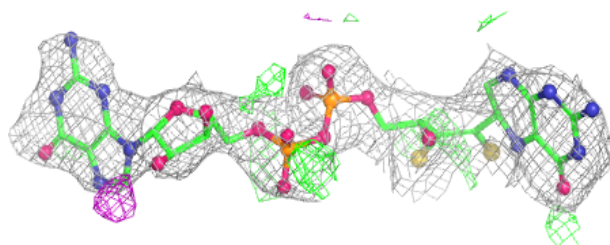
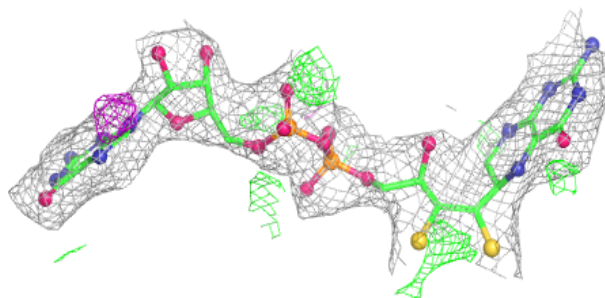
**Electron density around MD1 N 5802:**

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and green (positive)

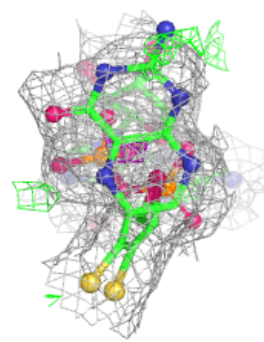
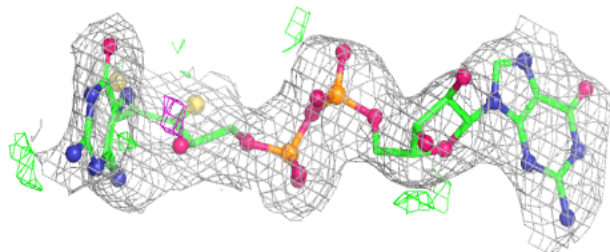
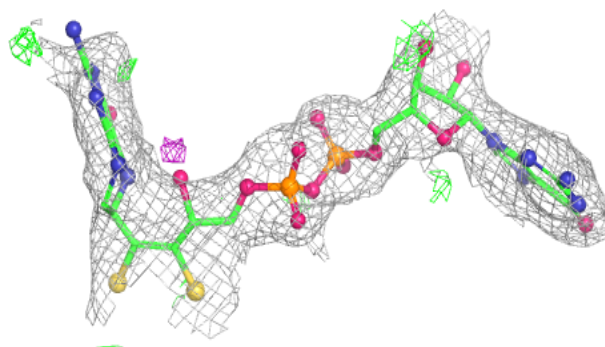


Electron density around MD1 B 5801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

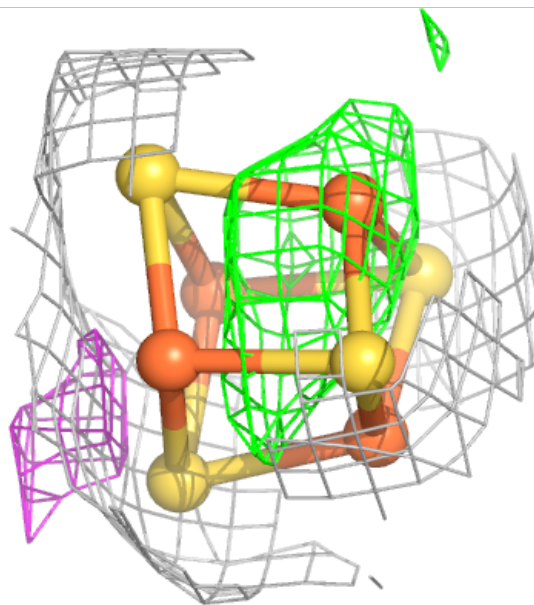
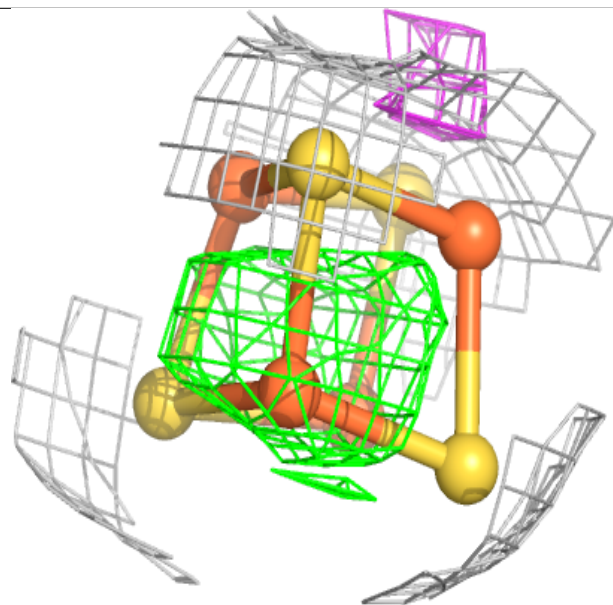
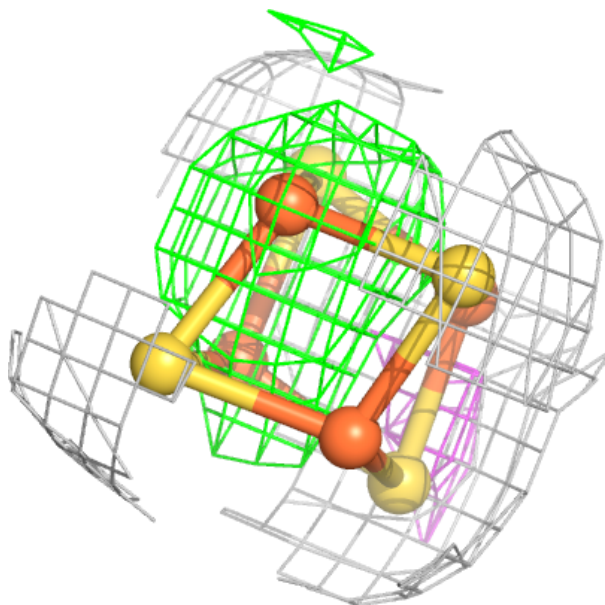
**Electron density around MD1 B 5802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



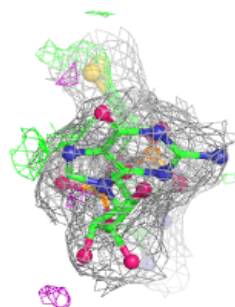
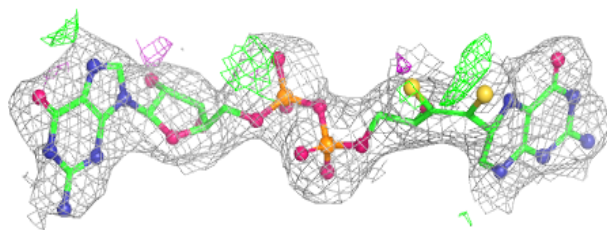
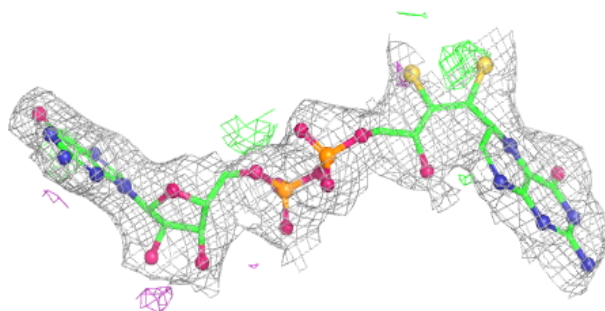
Electron density around SF4 W 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

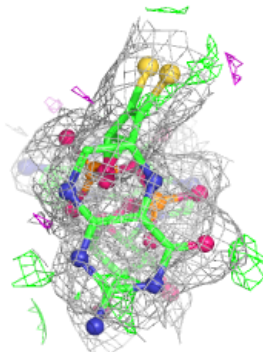
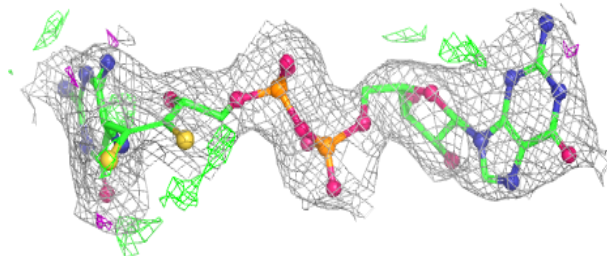
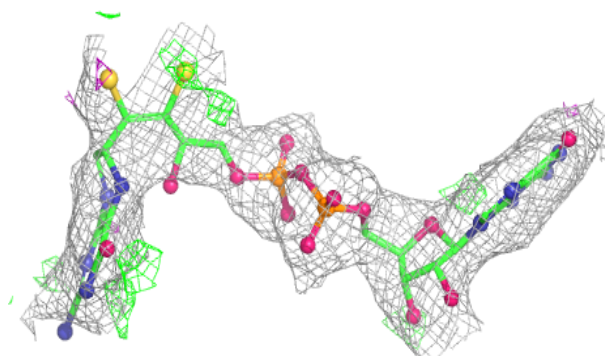


Electron density around MD1 H 5801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

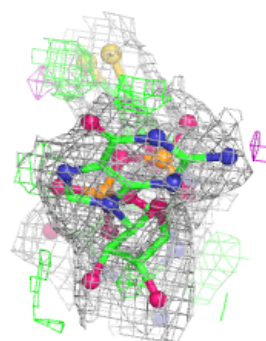
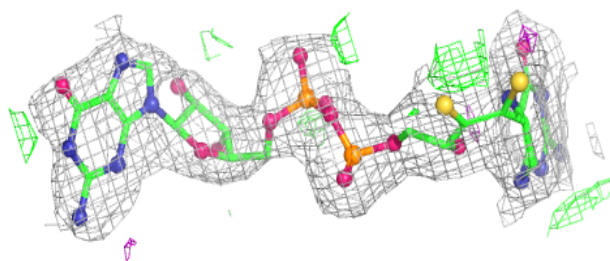
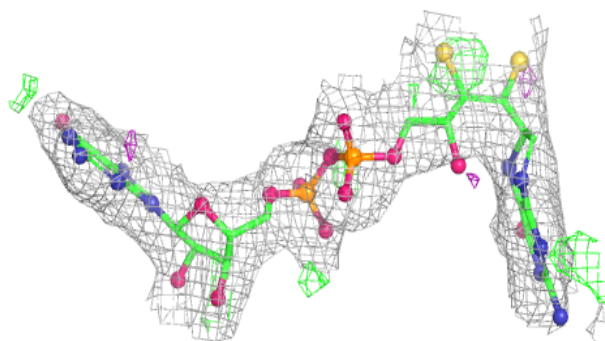
**Electron density around MD1 H 5802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

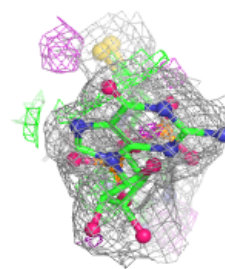
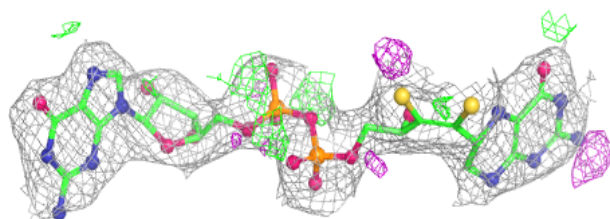
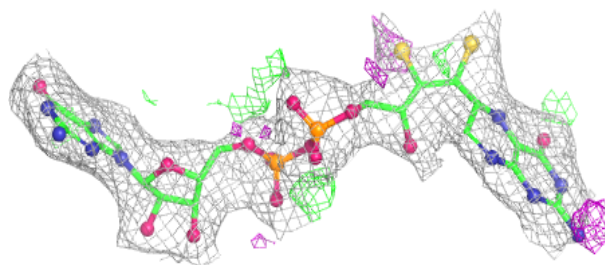


Electron density around MD1 T 5802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

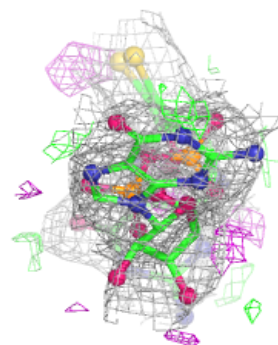
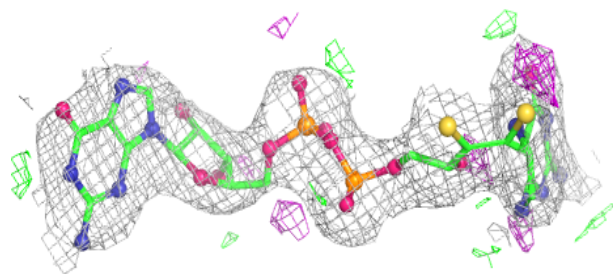
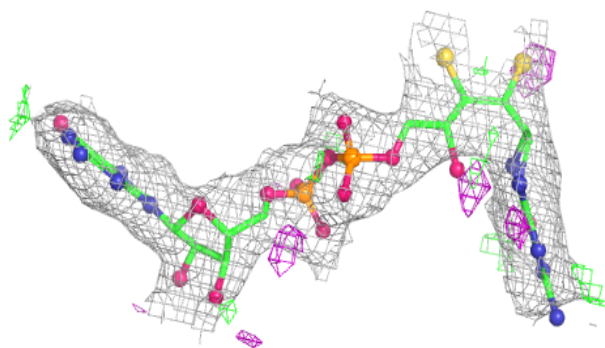
**Electron density around MD1 K 5801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



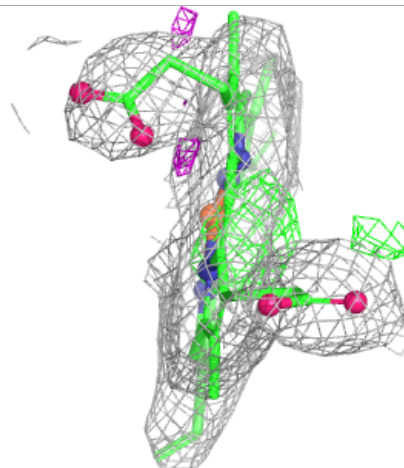
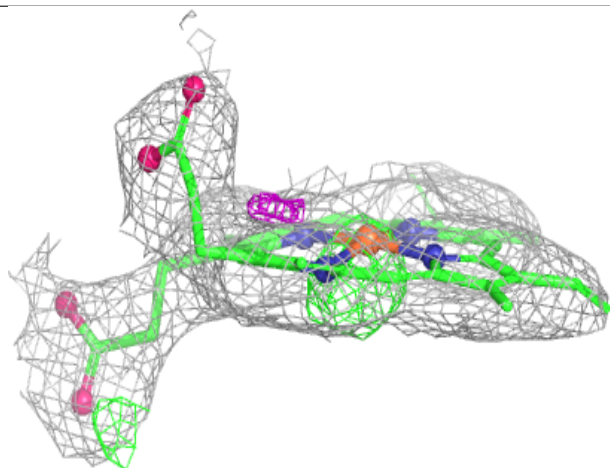
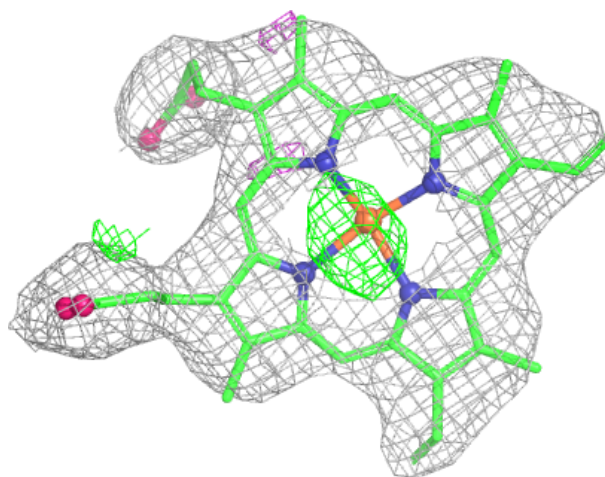
Electron density around MD1 K 5802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



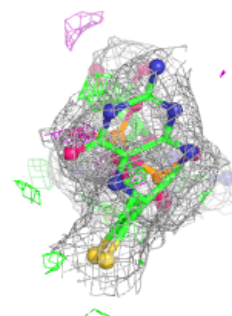
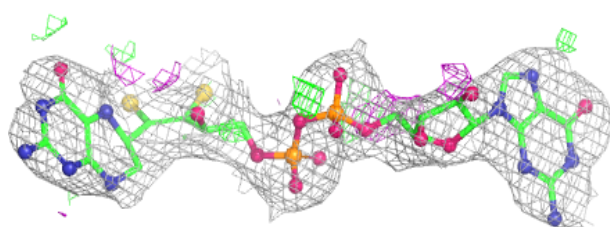
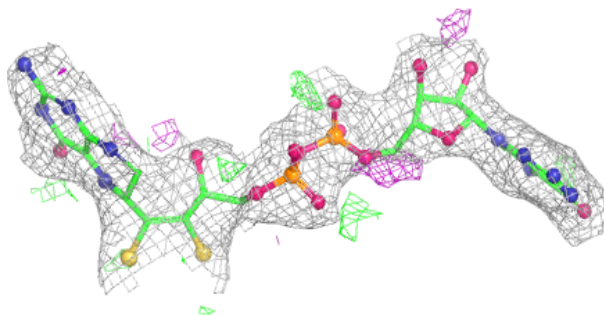
Electron density around HEM C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

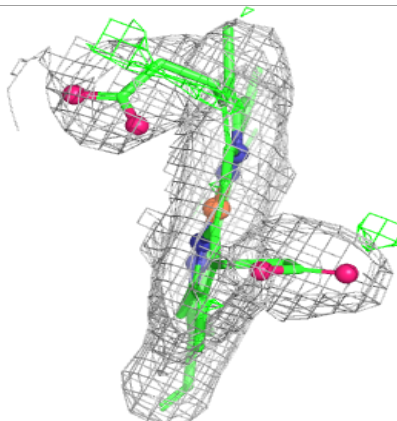
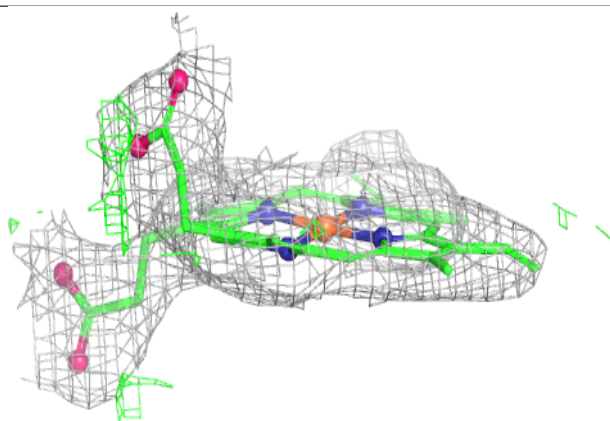
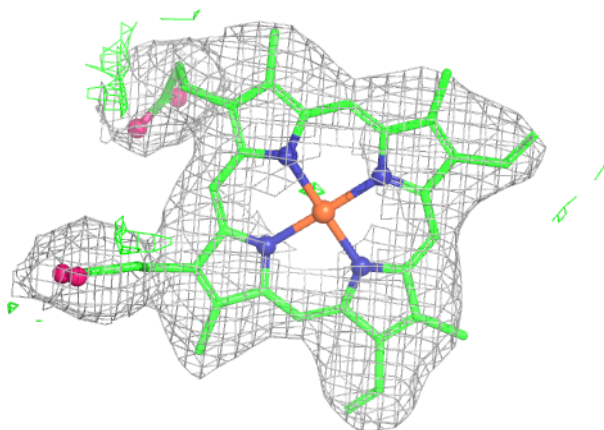


Electron density around MD1 N 5801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

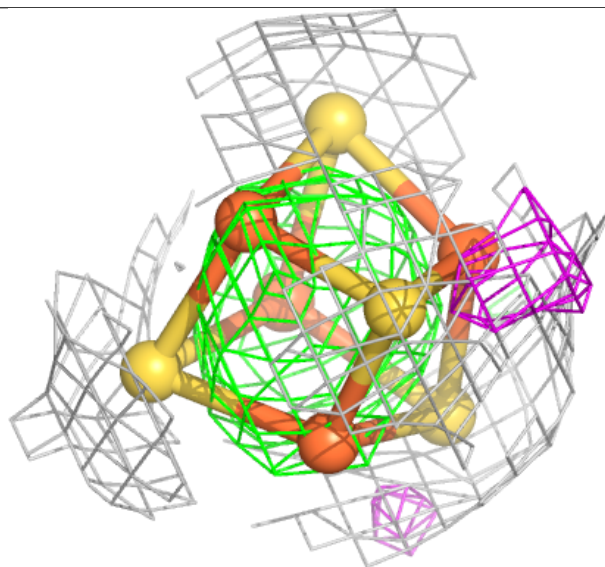
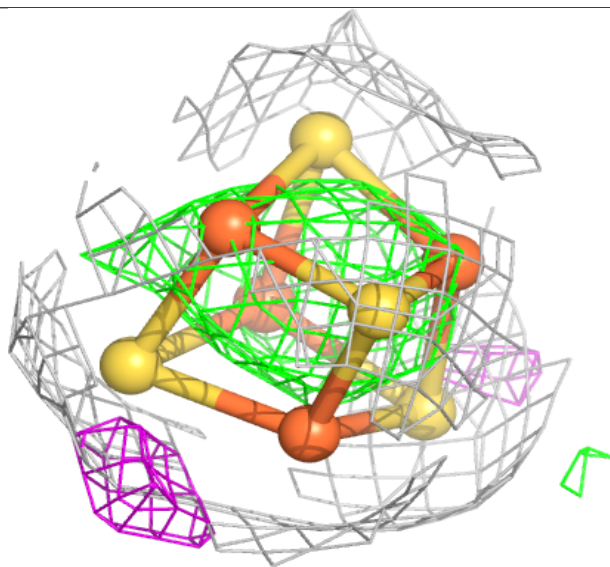
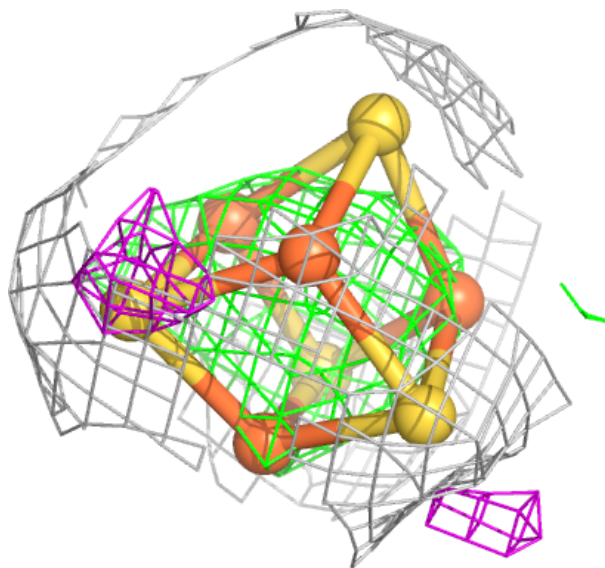
**Electron density around HEM L 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



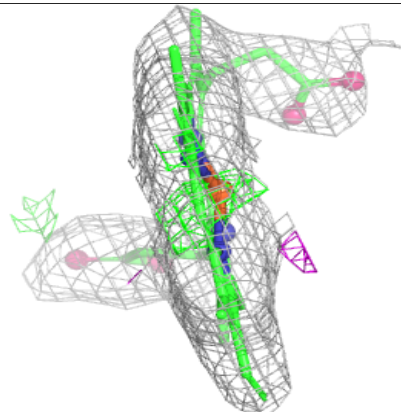
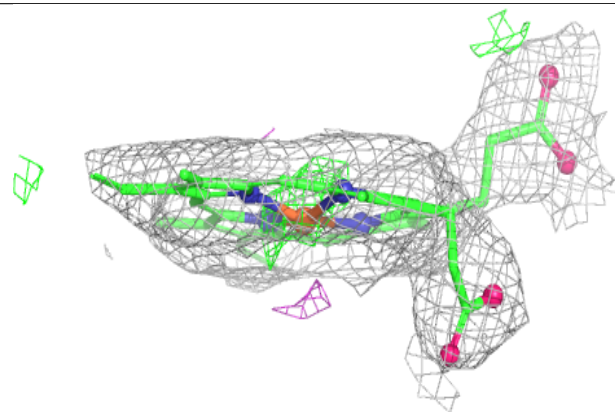
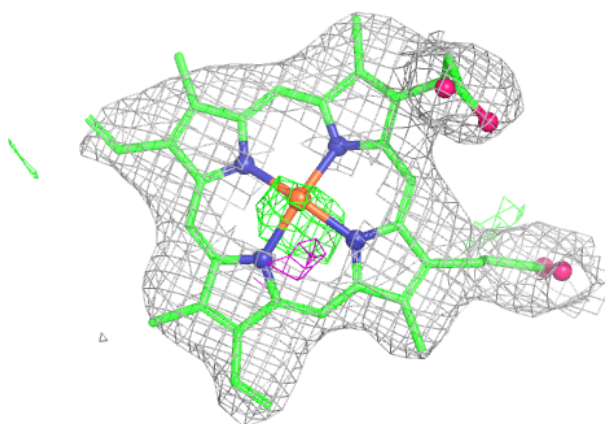
Electron density around SF4 K 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



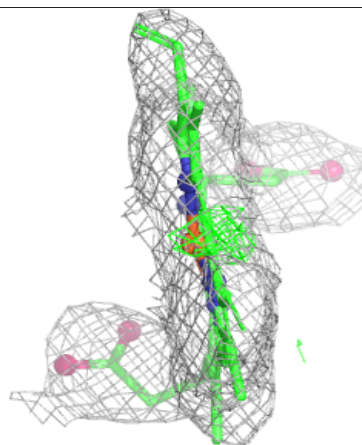
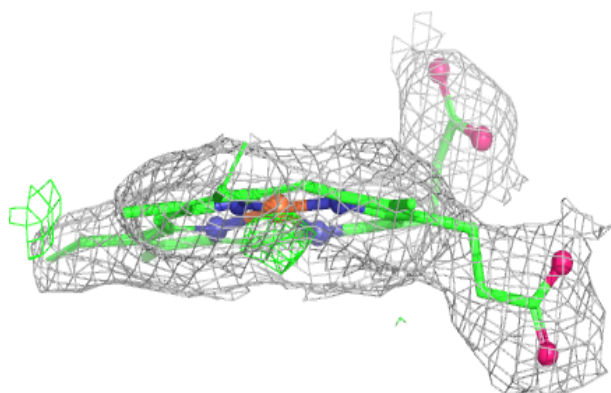
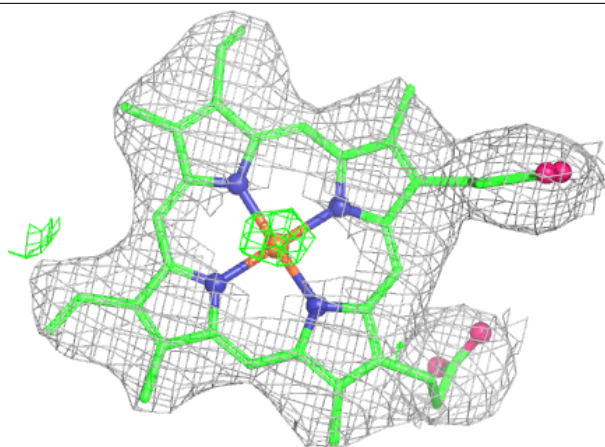
Electron density around HEM R 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

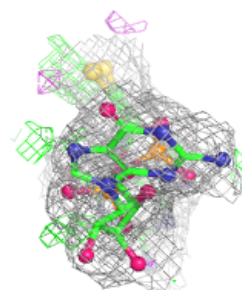
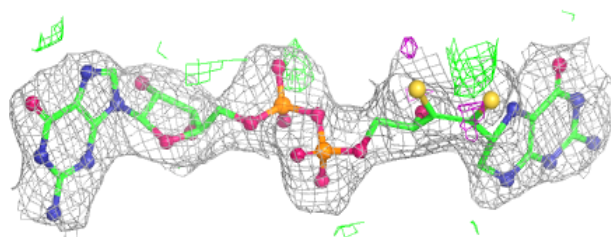
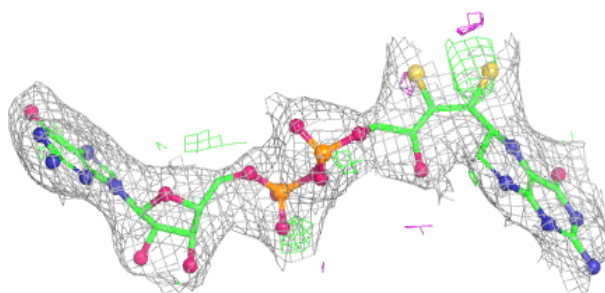


Electron density around HEM U 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

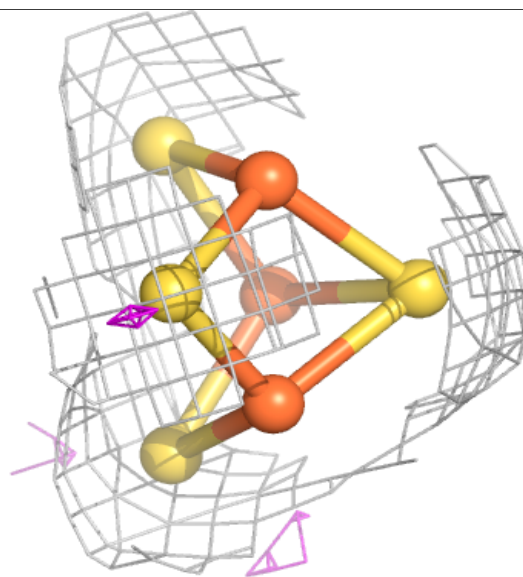
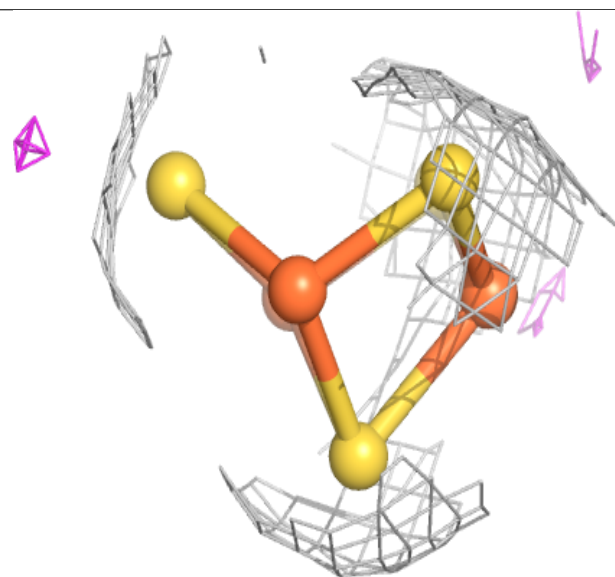
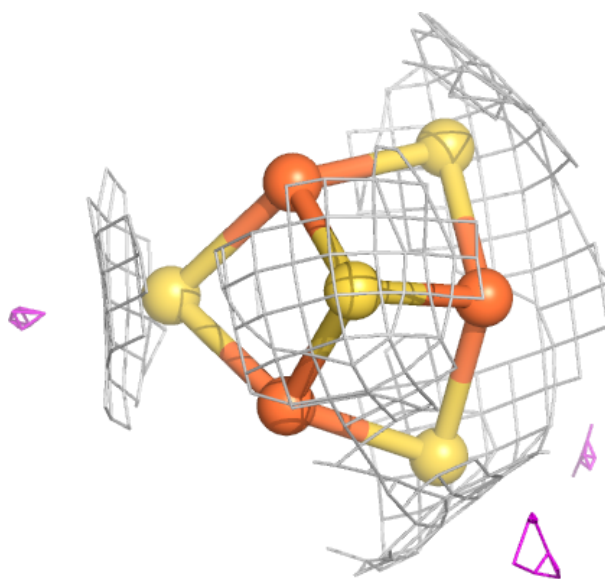
**Electron density around MD1 T 5801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



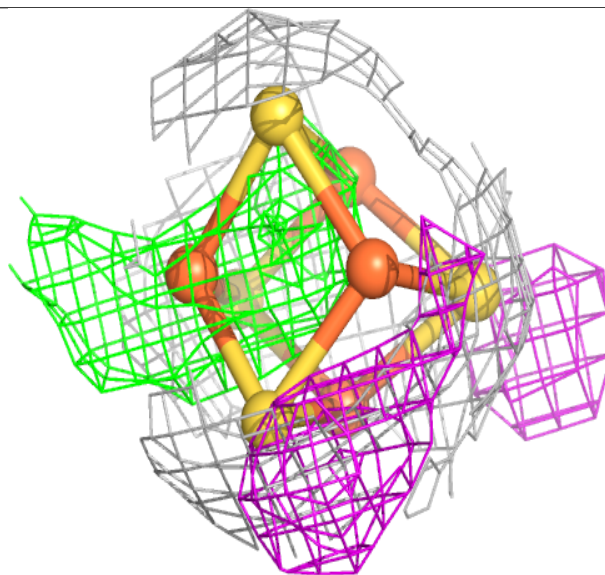
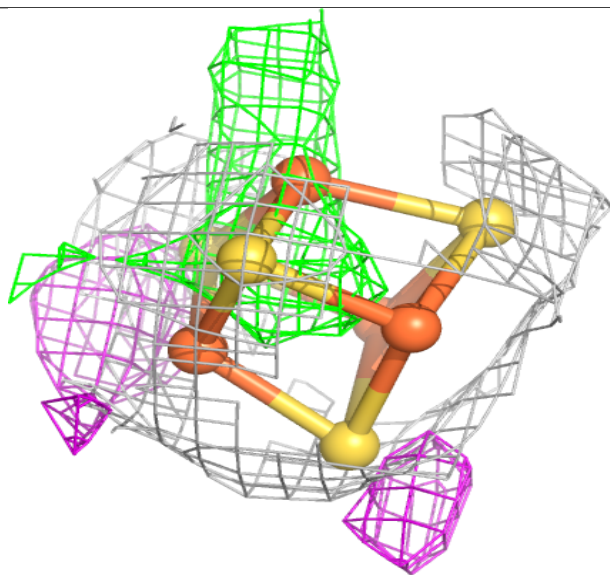
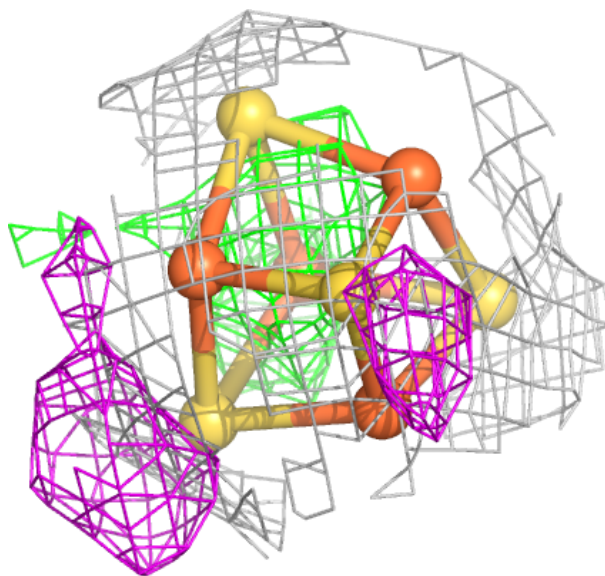
Electron density around F3S M 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



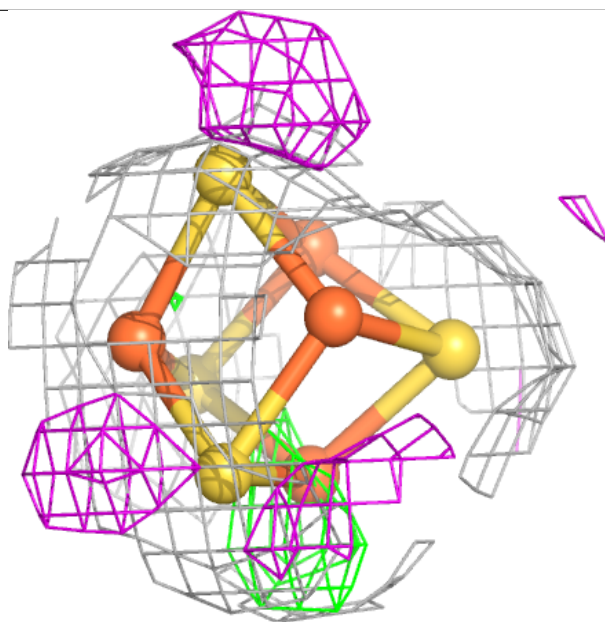
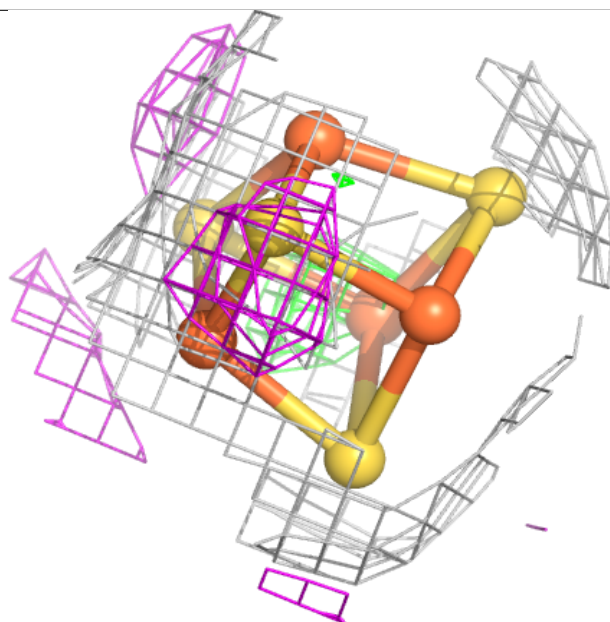
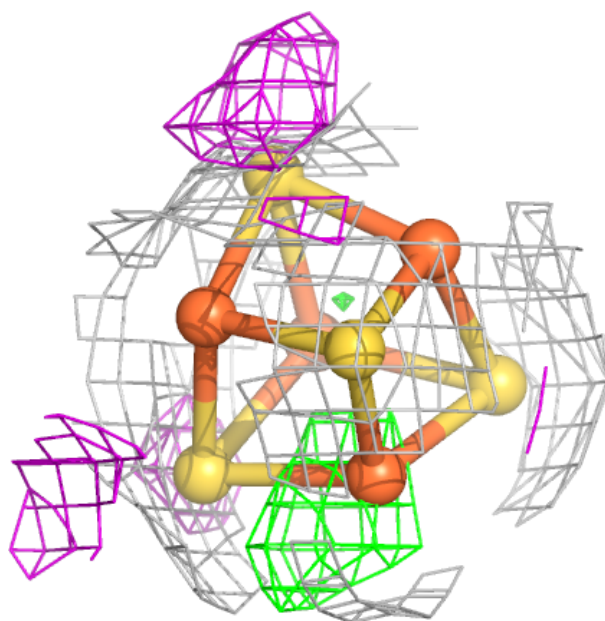
Electron density around SF4 N 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



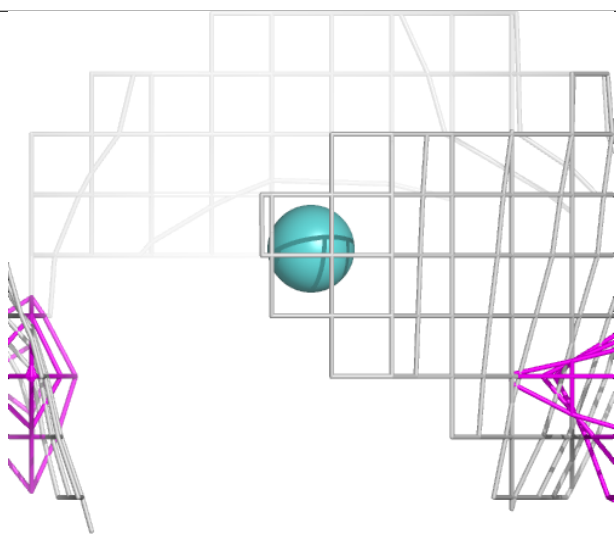
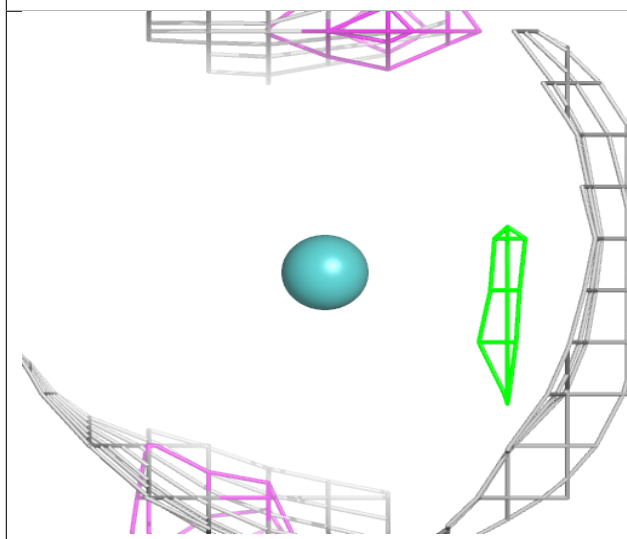
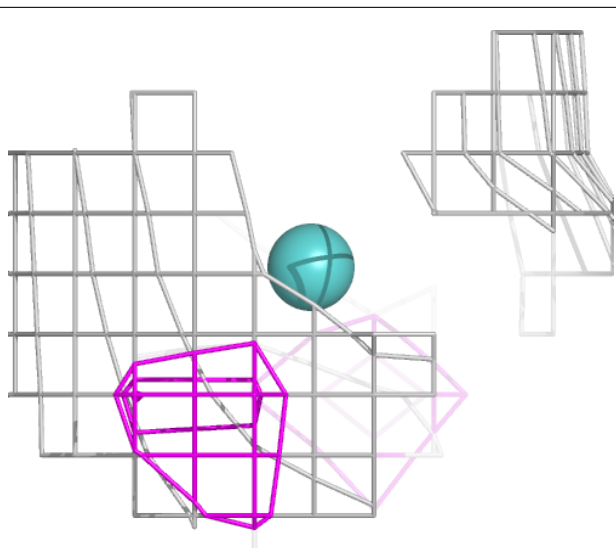
Electron density around SF4 Q 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



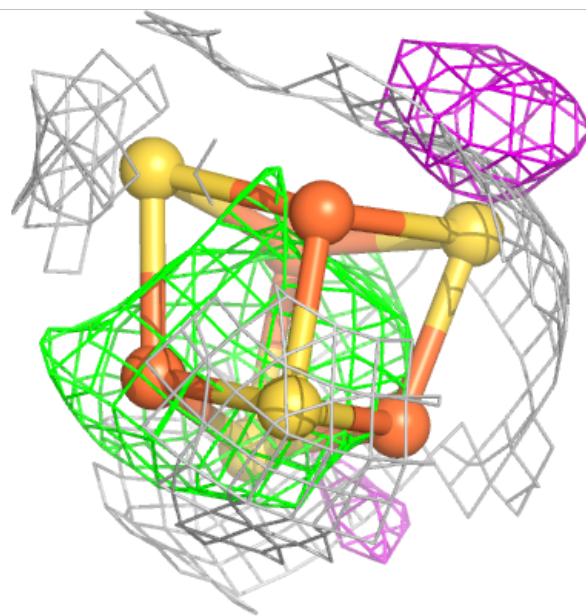
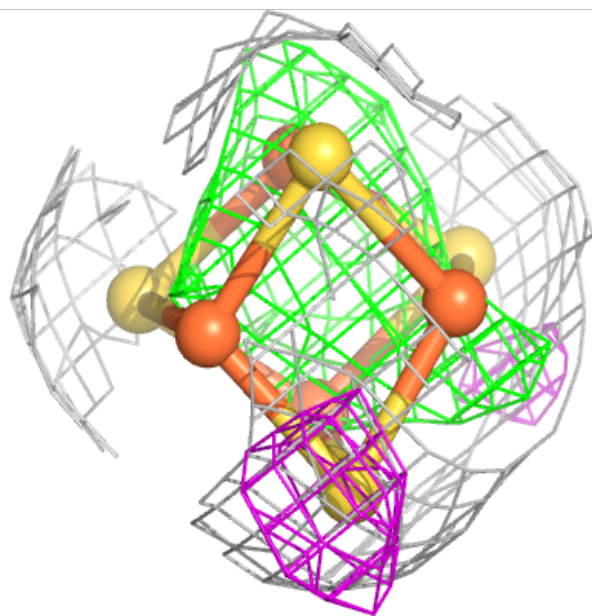
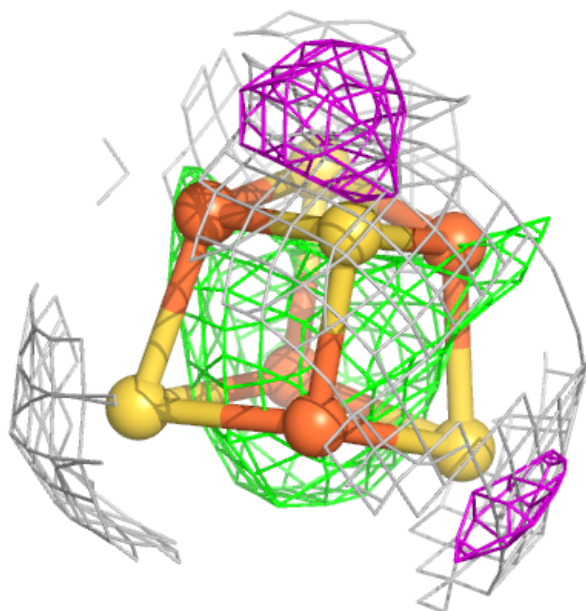
Electron density around MO E 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



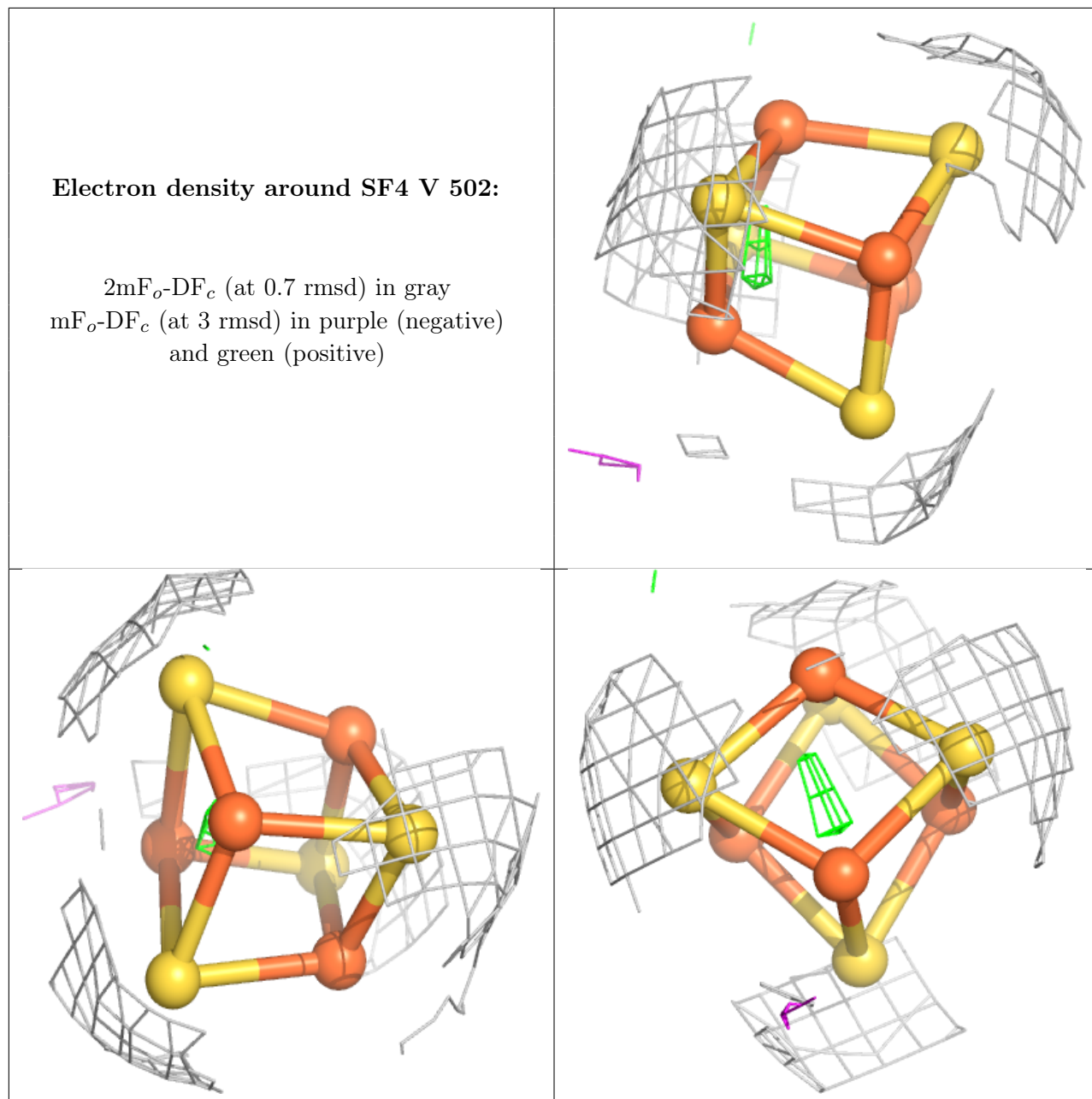
Electron density around SF4 B 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



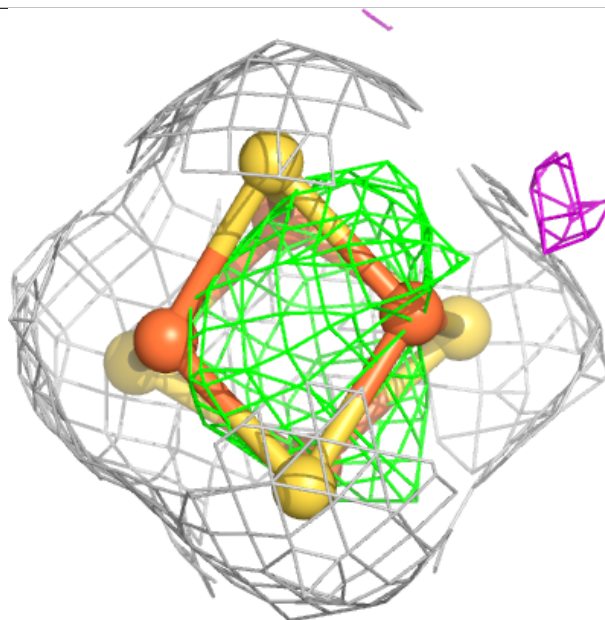
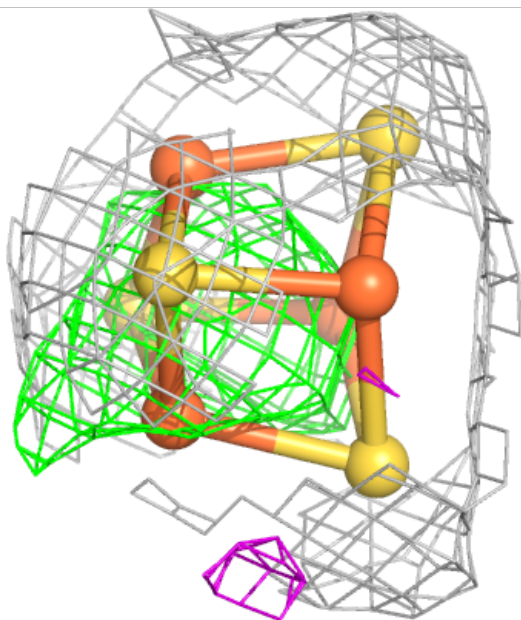
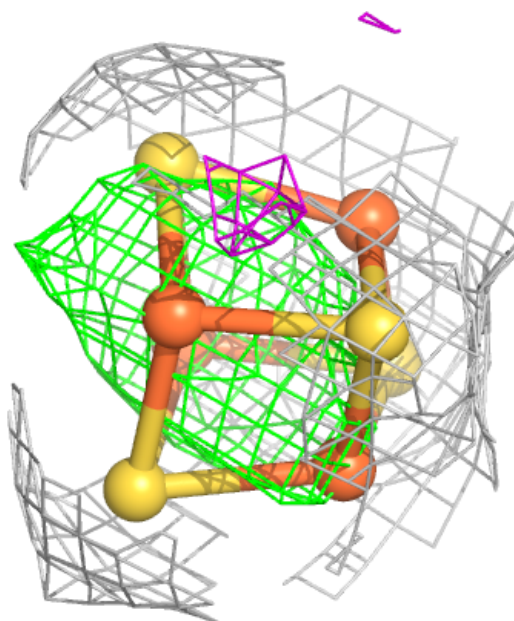
Electron density around SF4 V 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



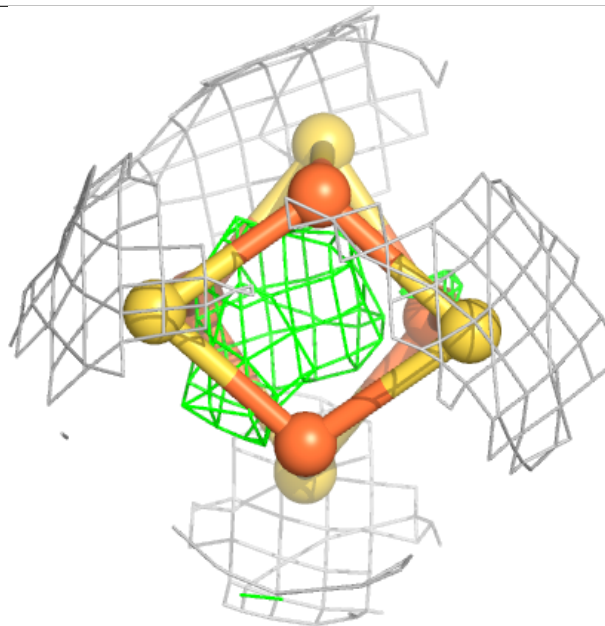
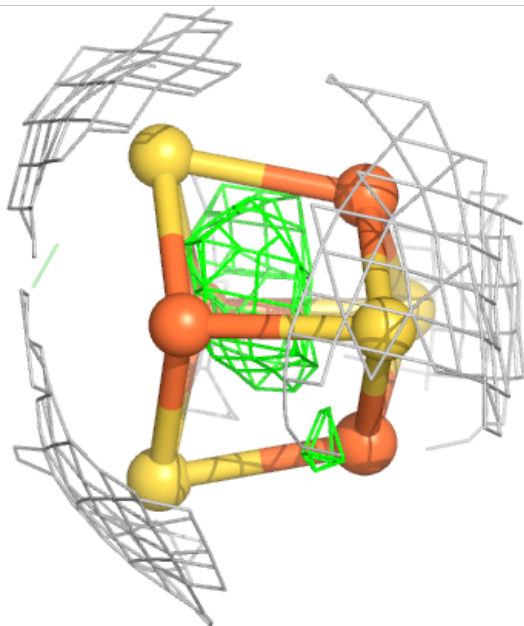
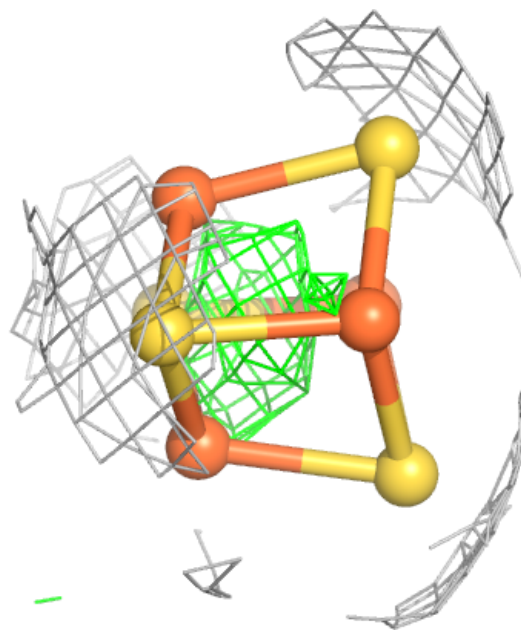
Electron density around SF4 H 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



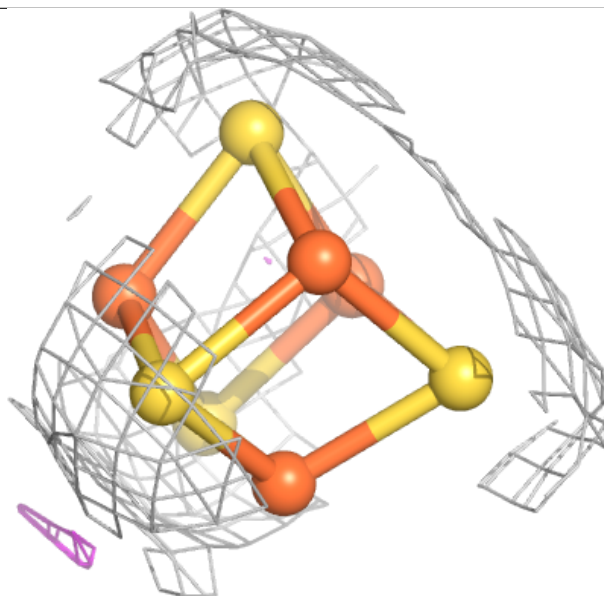
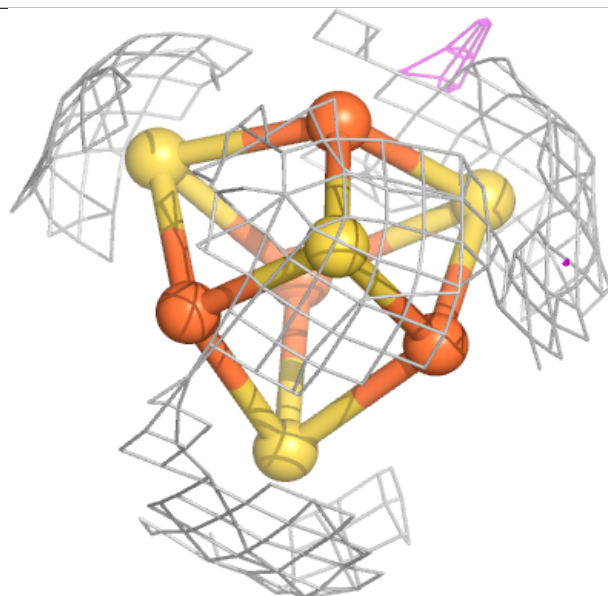
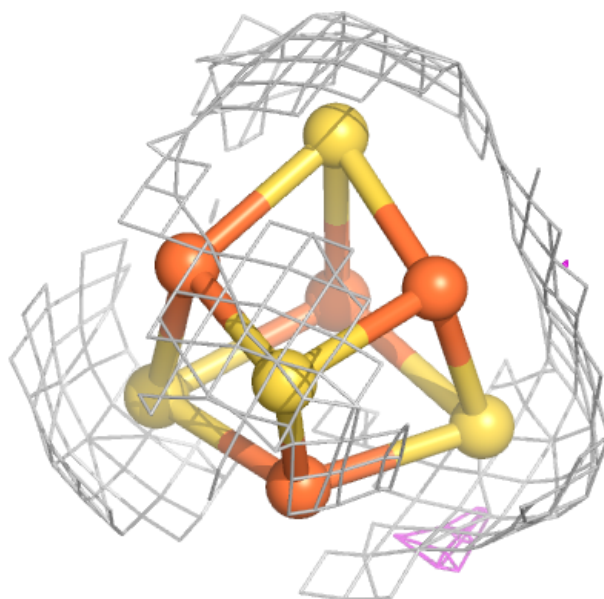
Electron density around SF4 V 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



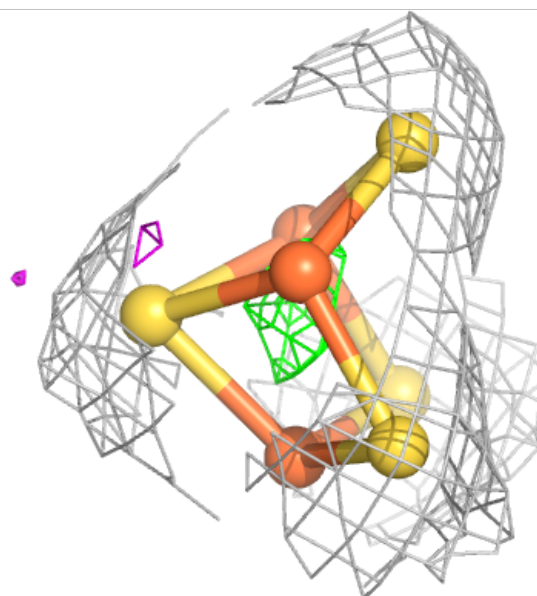
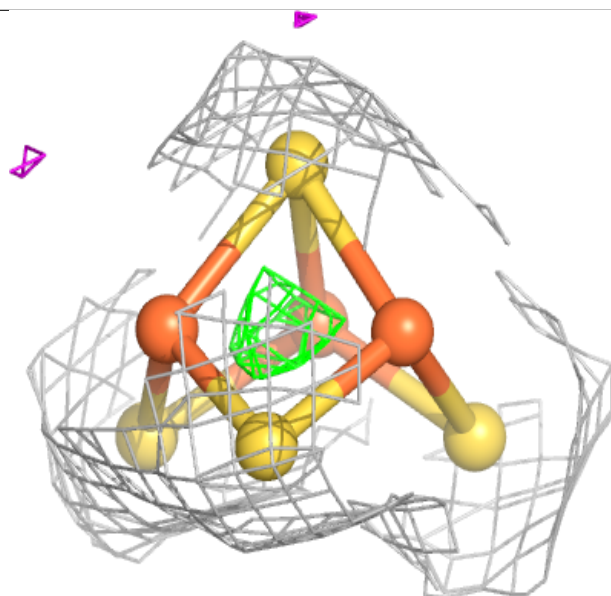
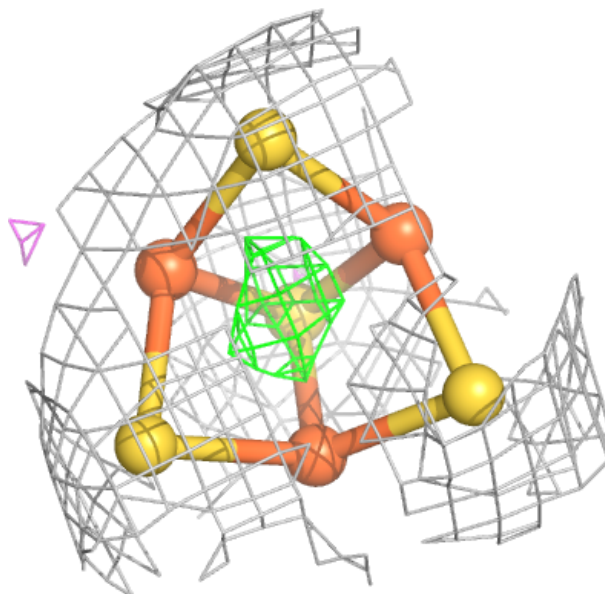
Electron density around SF4 M 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



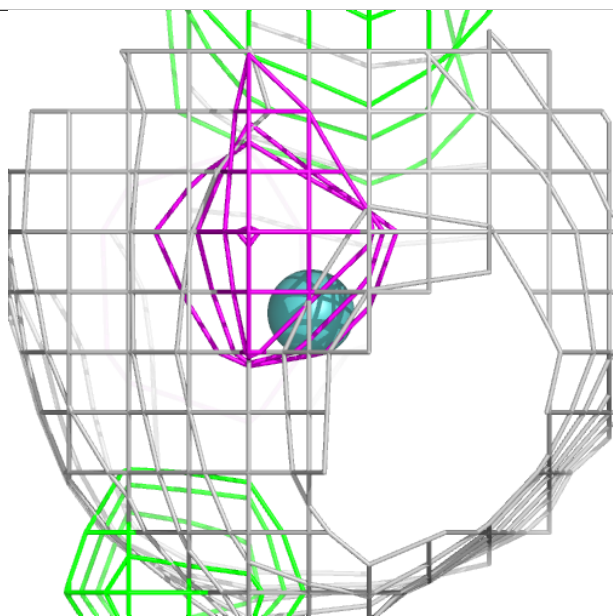
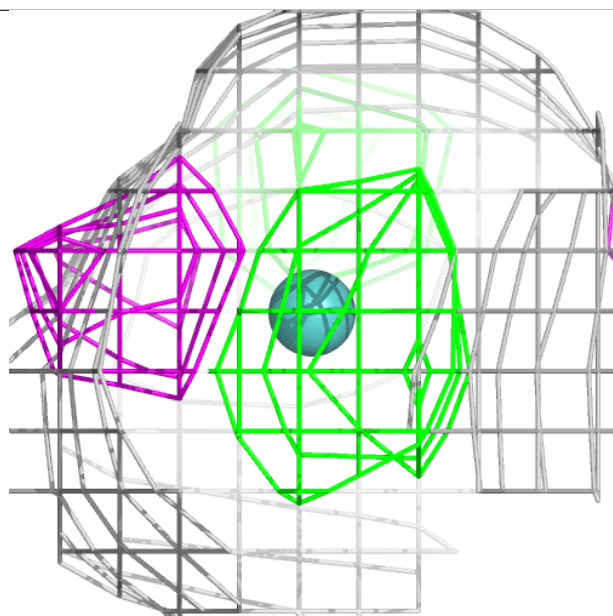
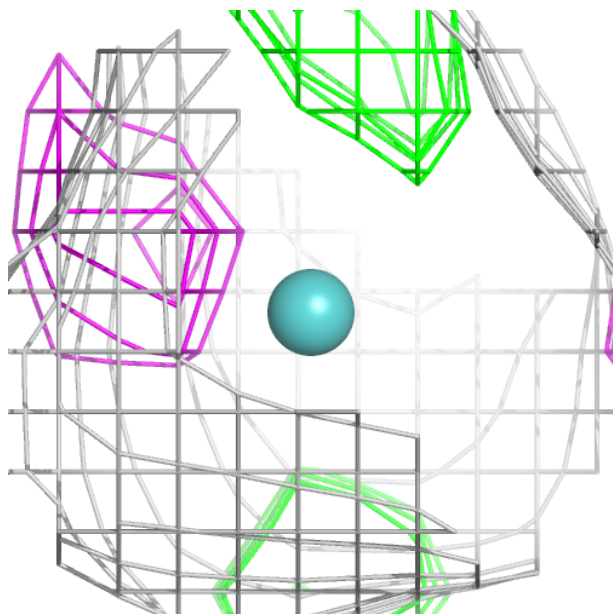
Electron density around F3S A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



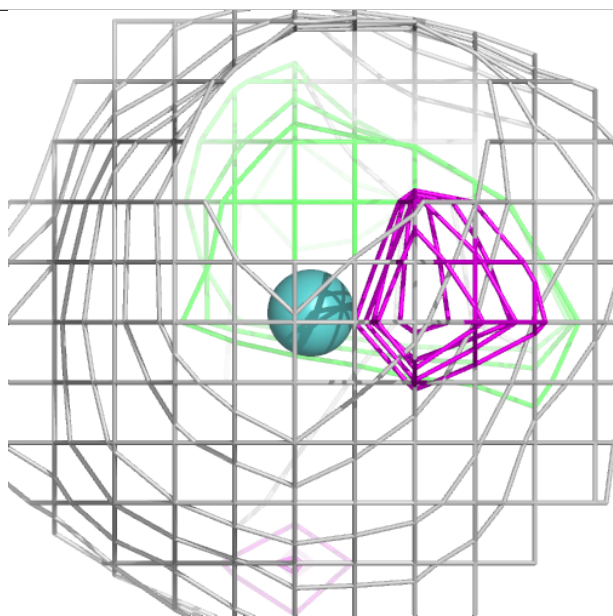
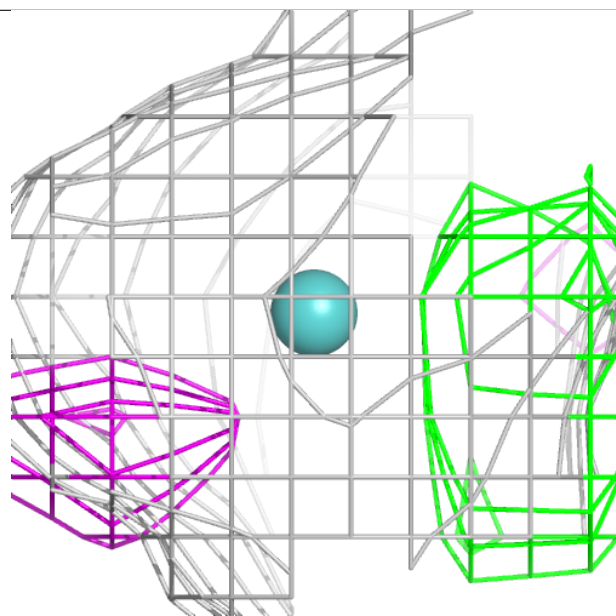
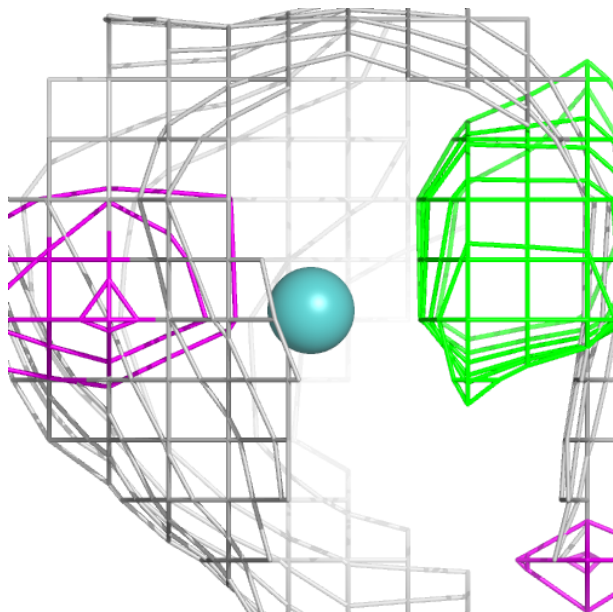
Electron density around MO Q 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



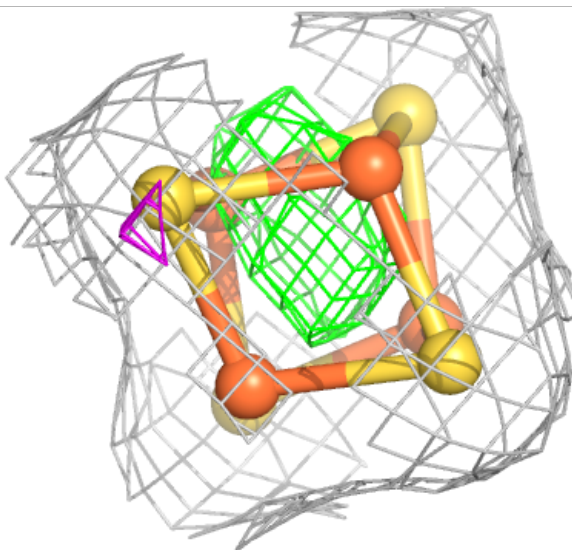
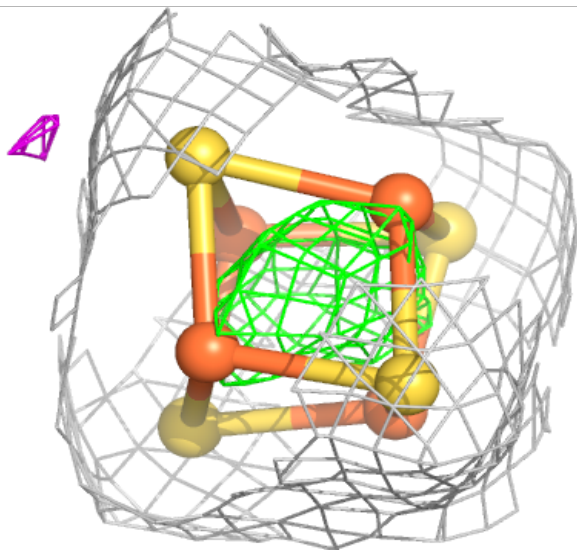
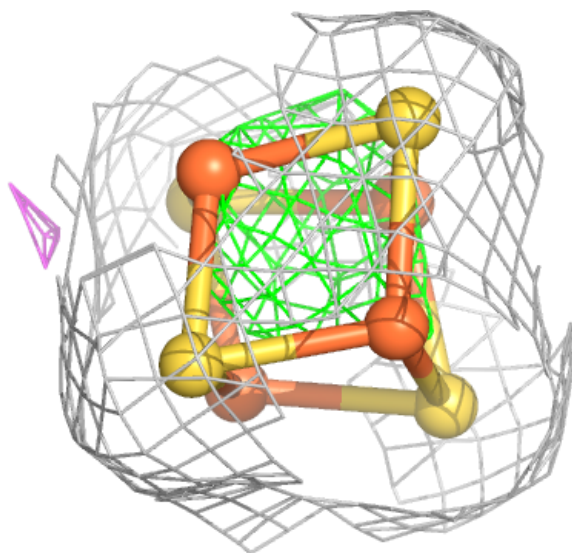
Electron density around MO T 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



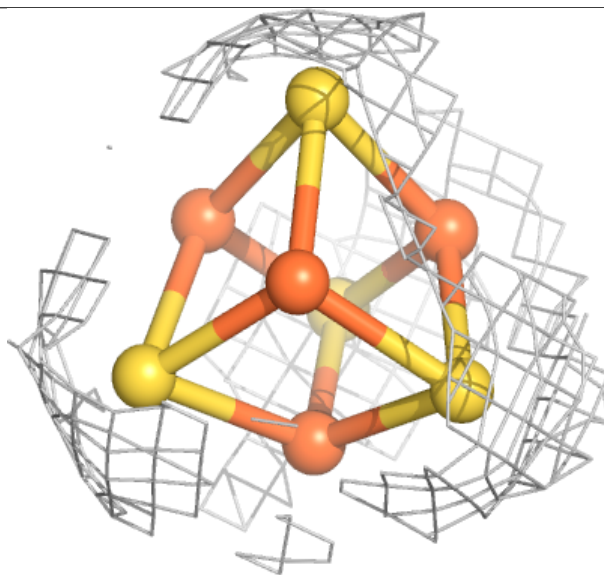
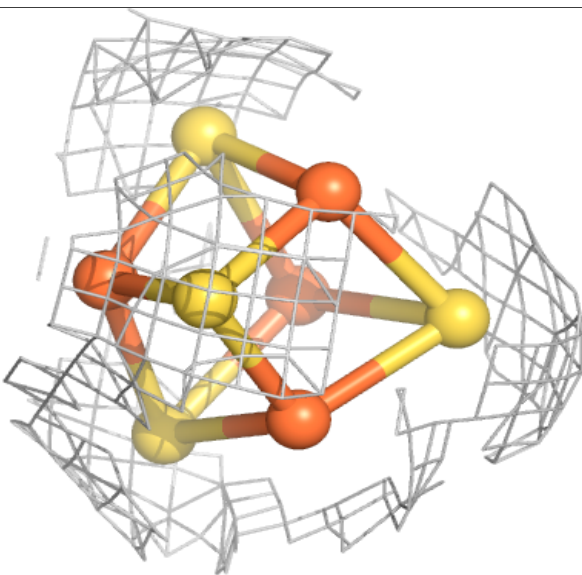
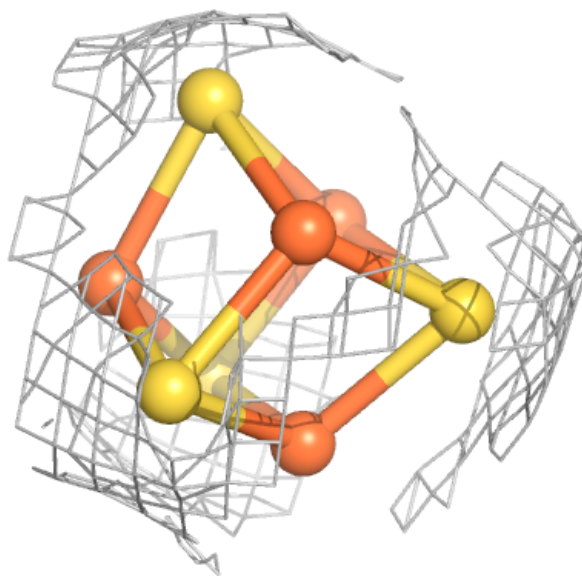
Electron density around SF4 J 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



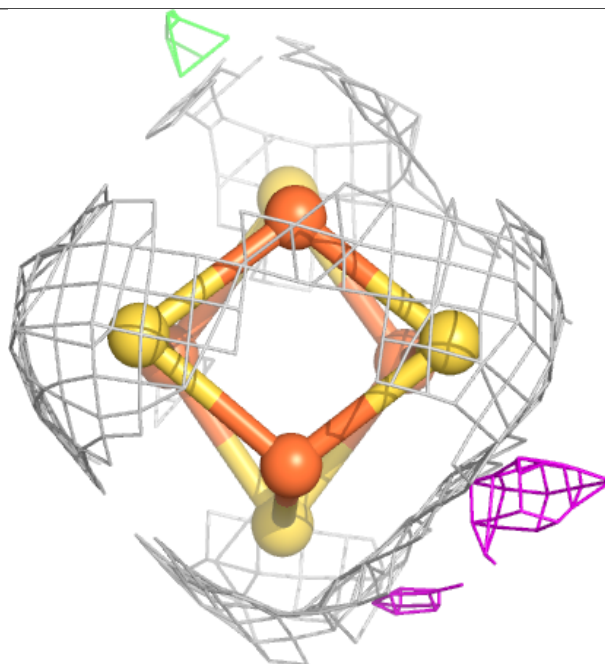
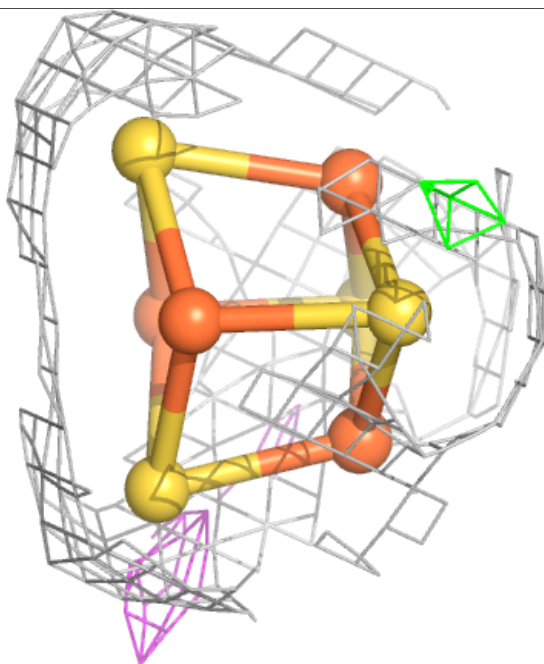
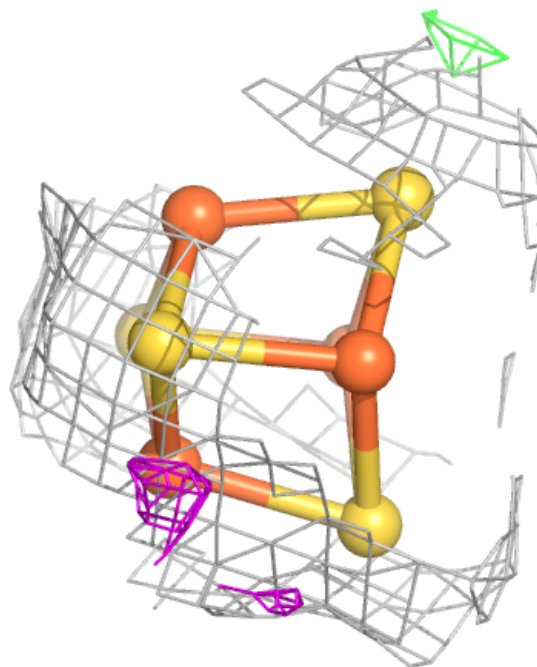
Electron density around SF4 P 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



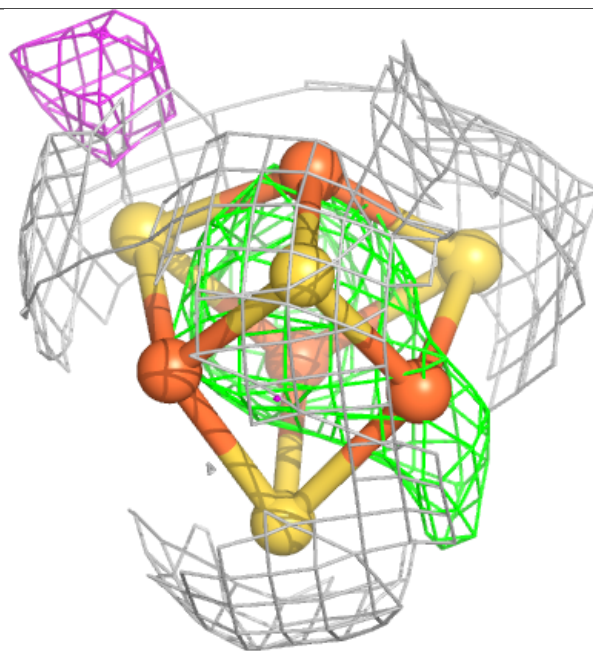
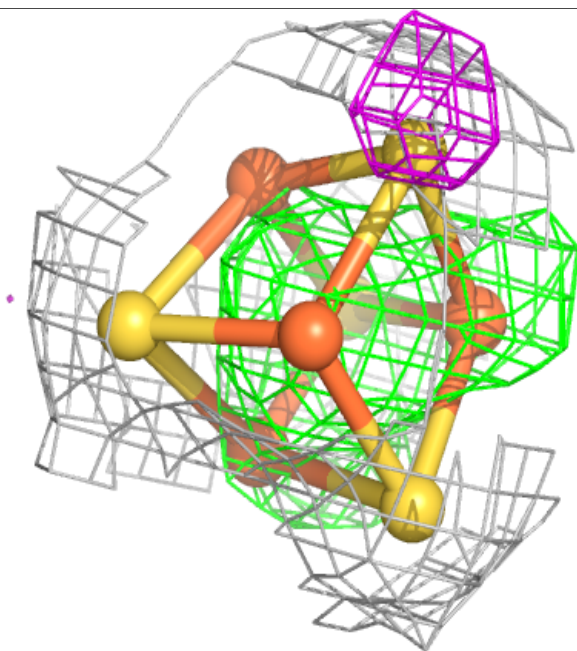
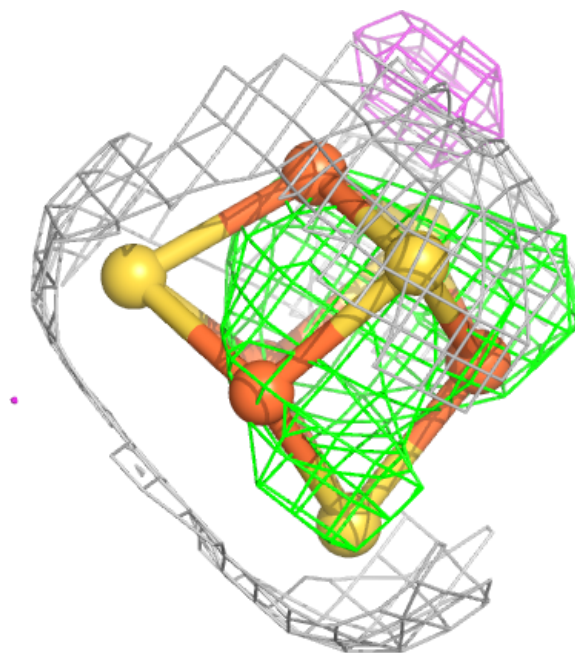
Electron density around SF4 J 502:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



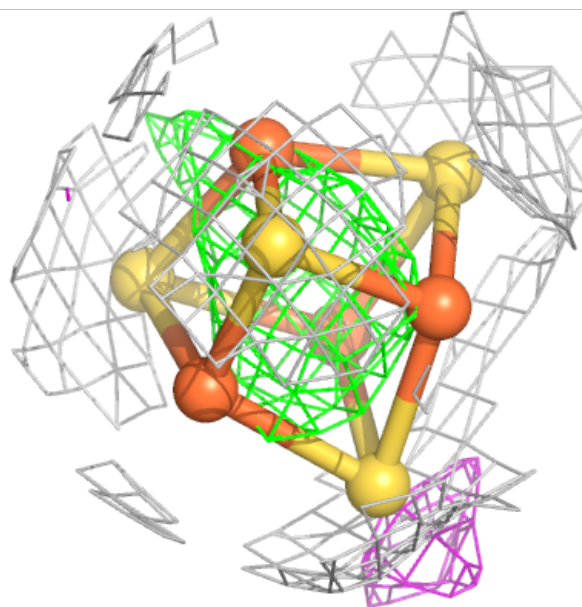
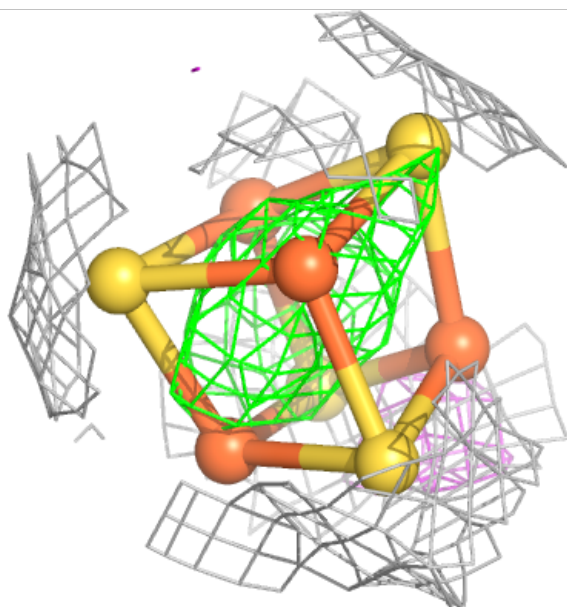
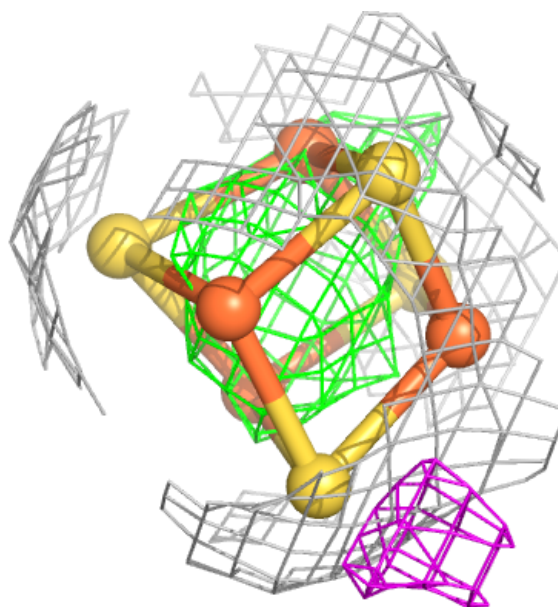
Electron density around SF4 S 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



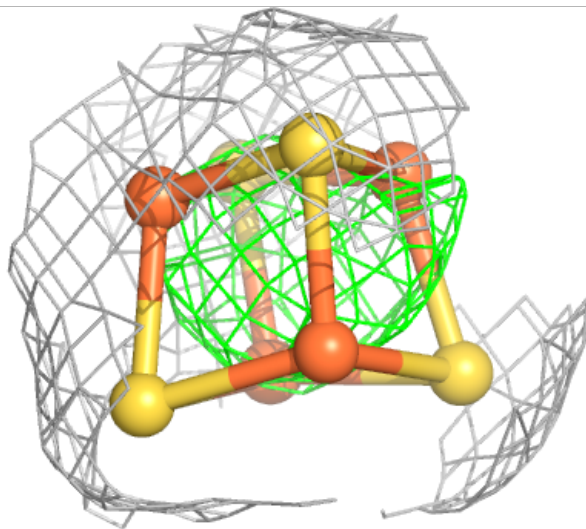
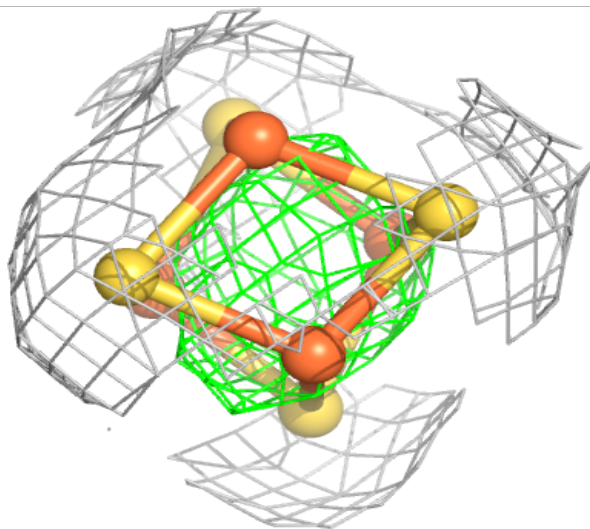
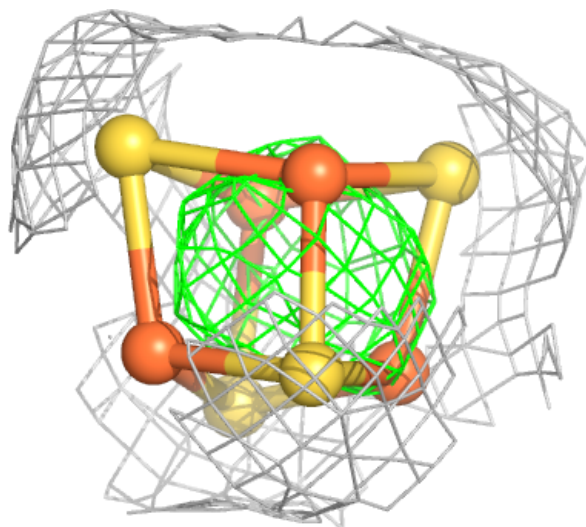
Electron density around SF4 T 5804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



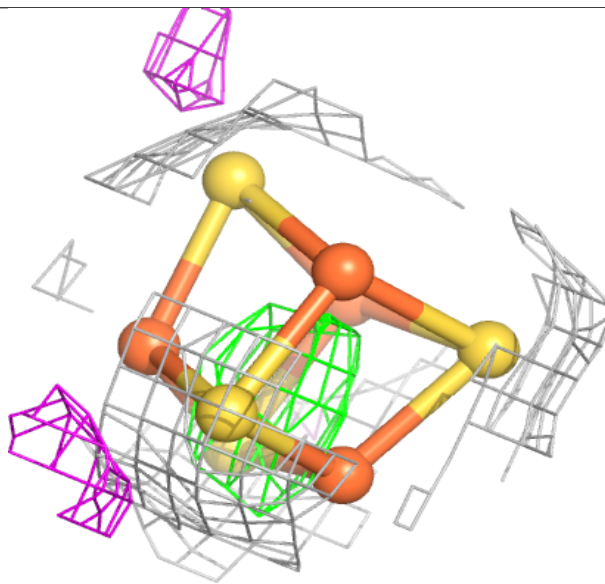
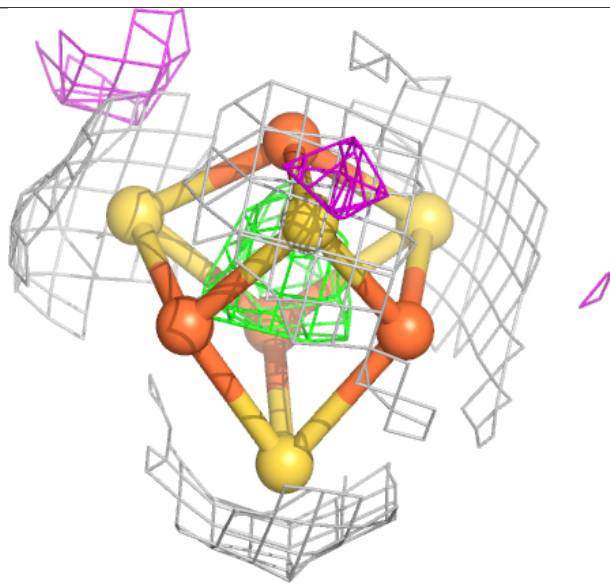
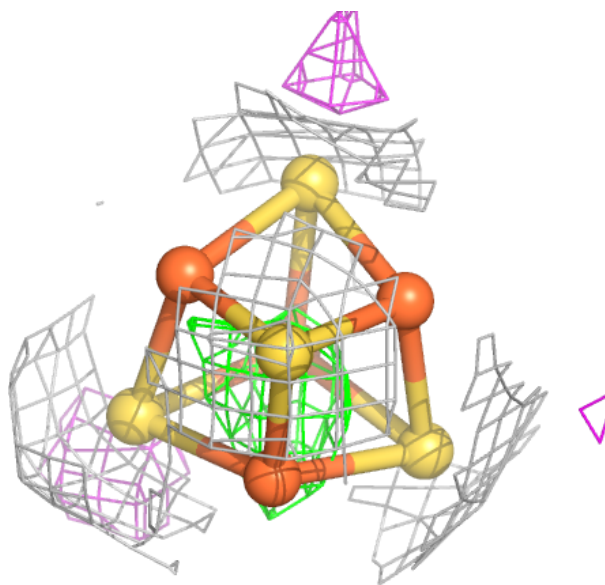
Electron density around SF4 A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



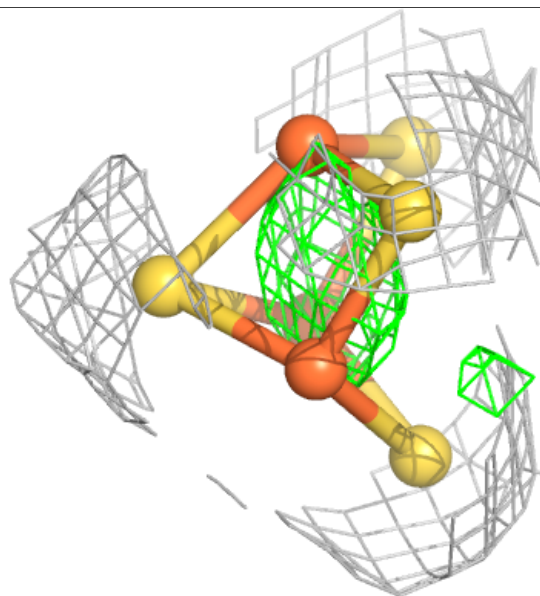
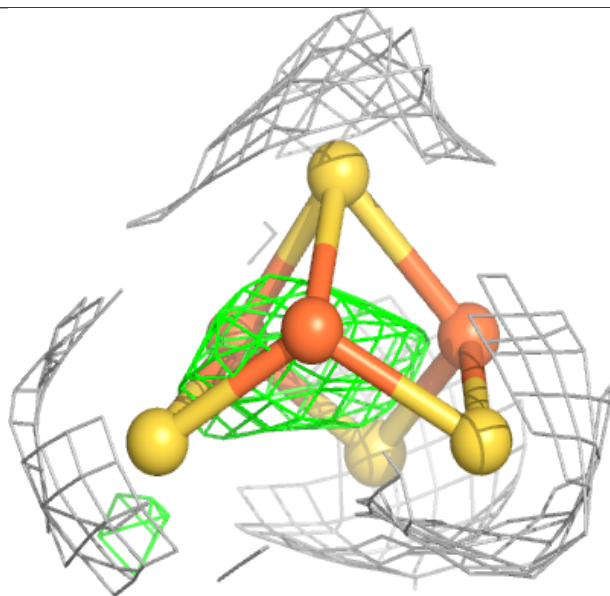
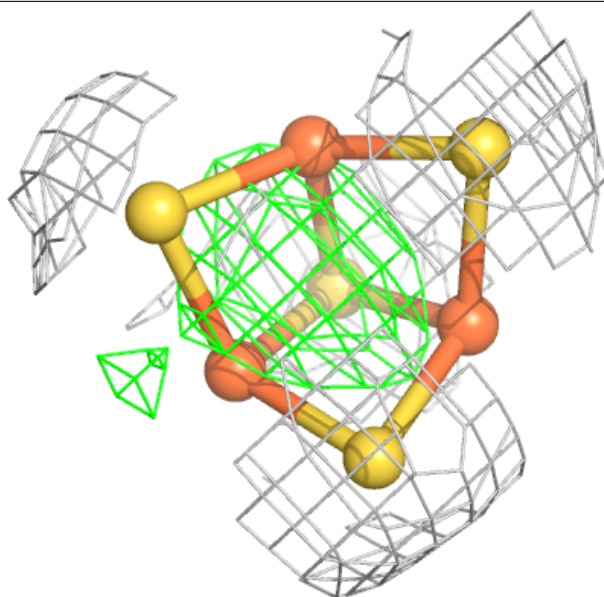
Electron density around SF4 M 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



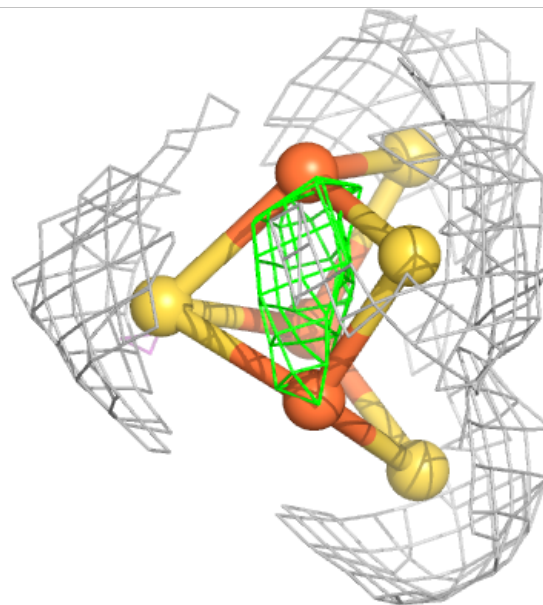
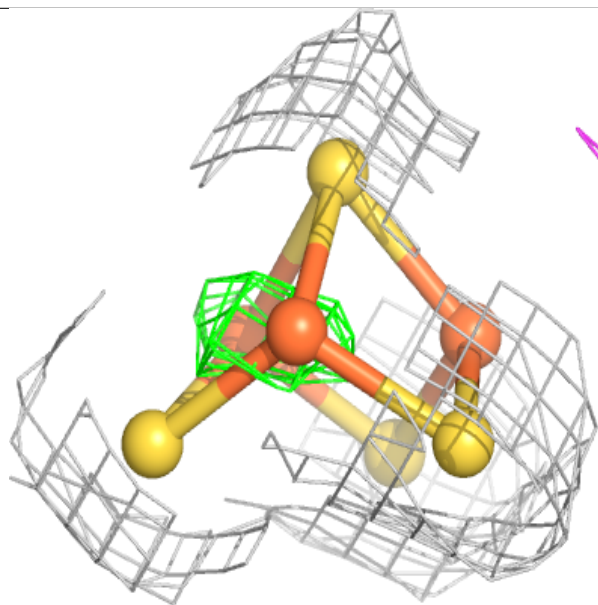
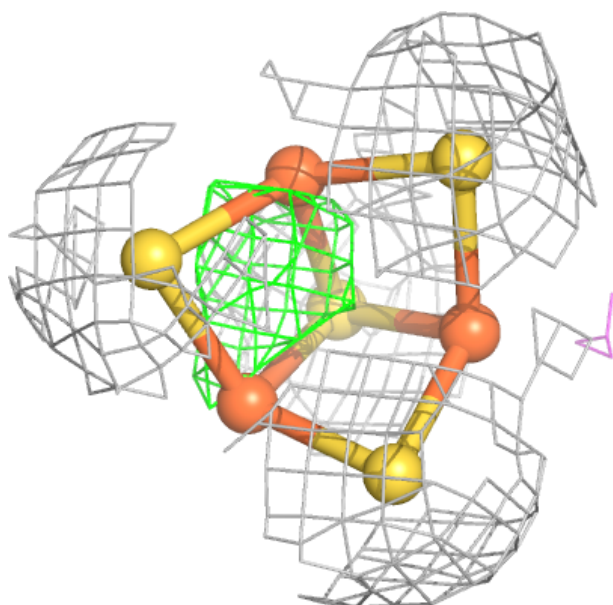
Electron density around F3S G 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



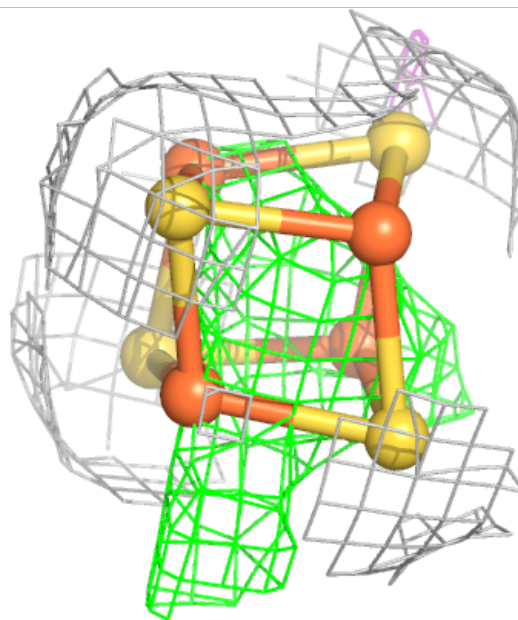
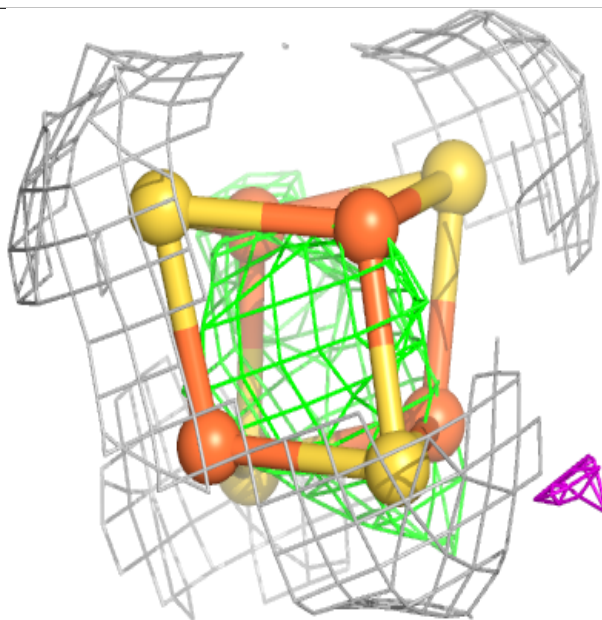
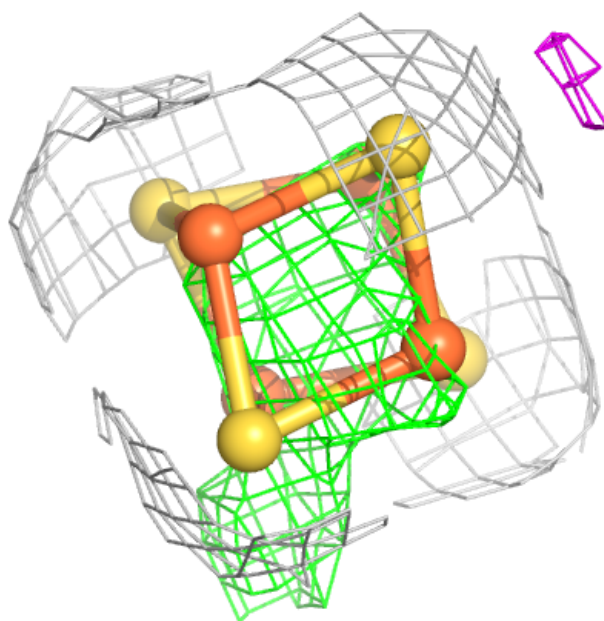
Electron density around F3S J 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



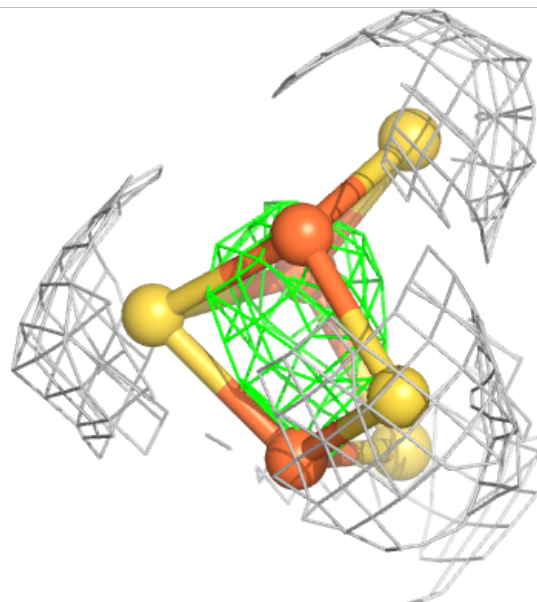
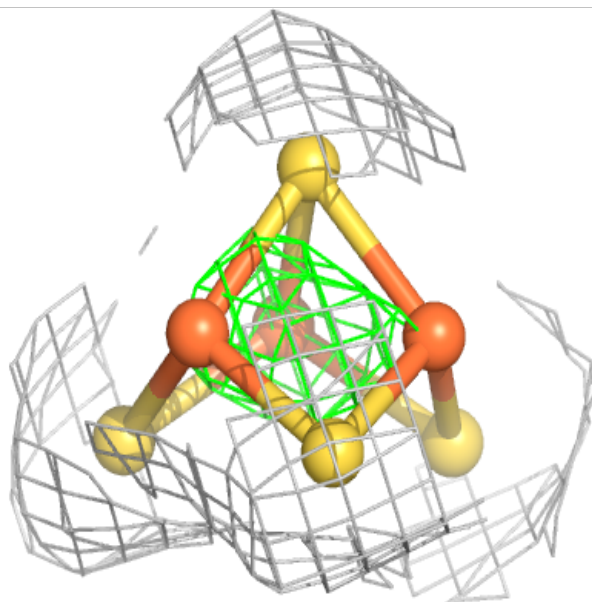
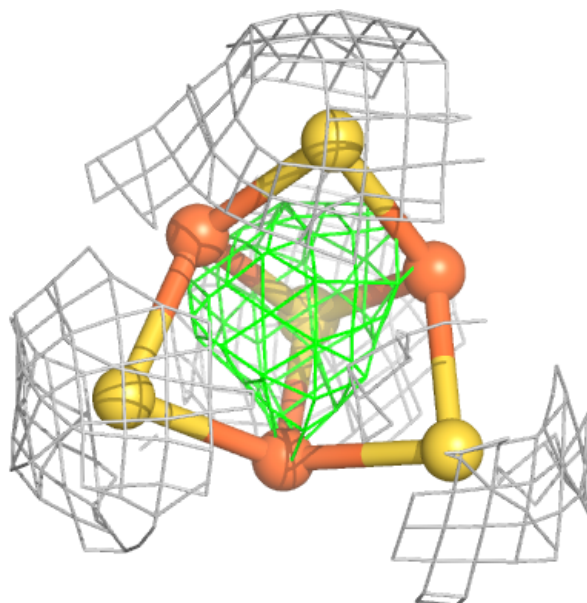
Electron density around SF4 G 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



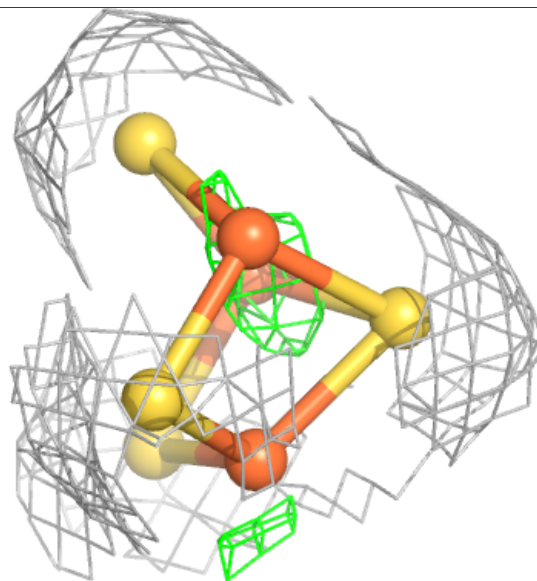
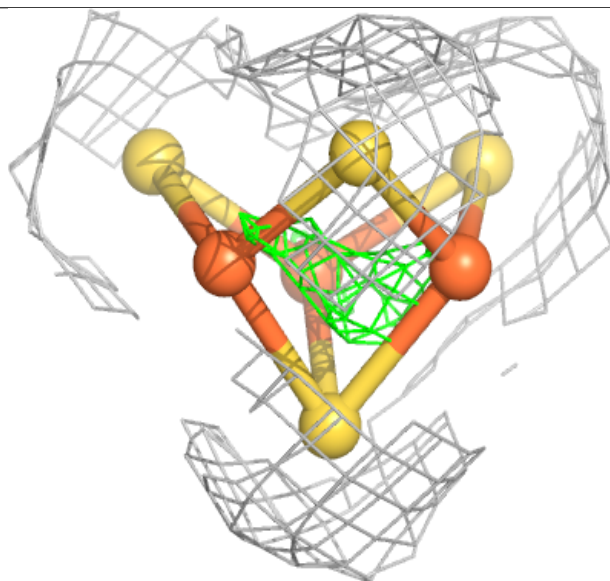
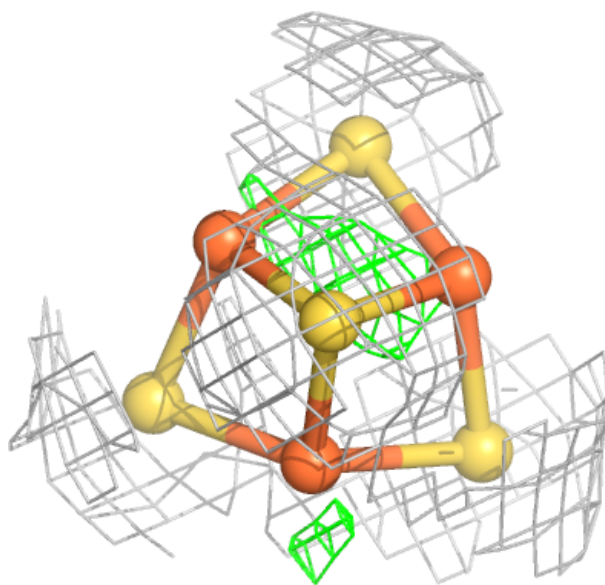
Electron density around F3S P 504:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



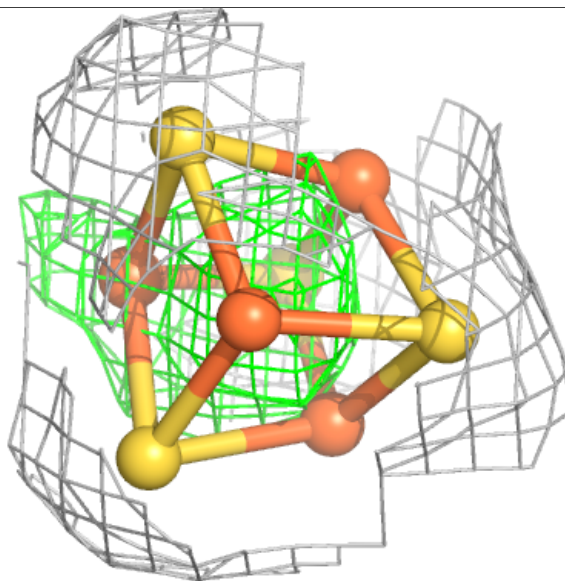
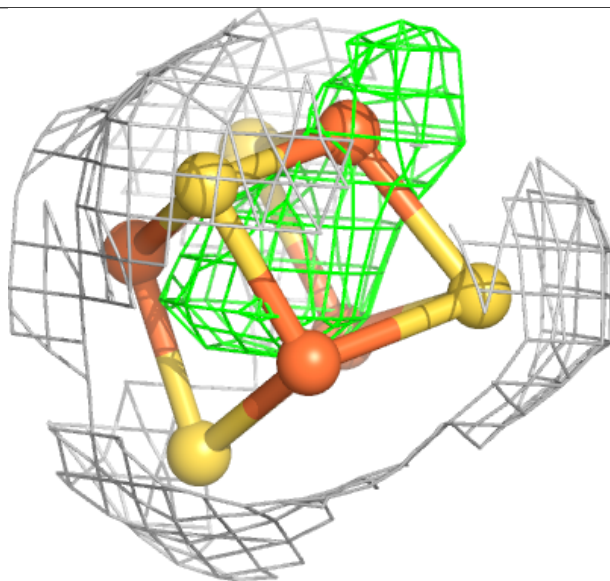
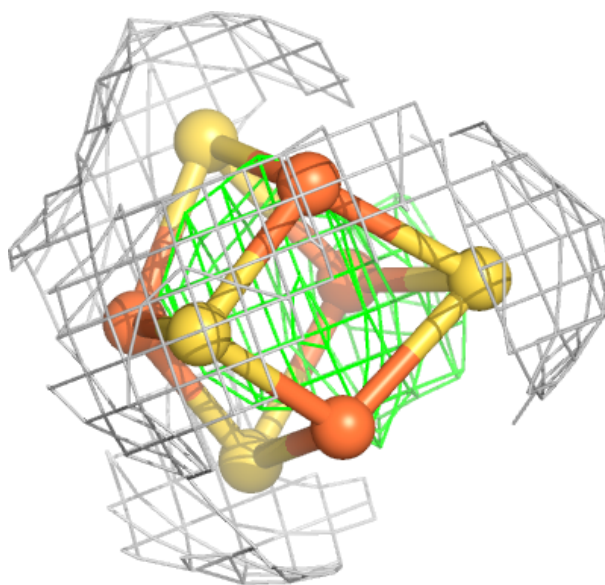
Electron density around F3S S 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



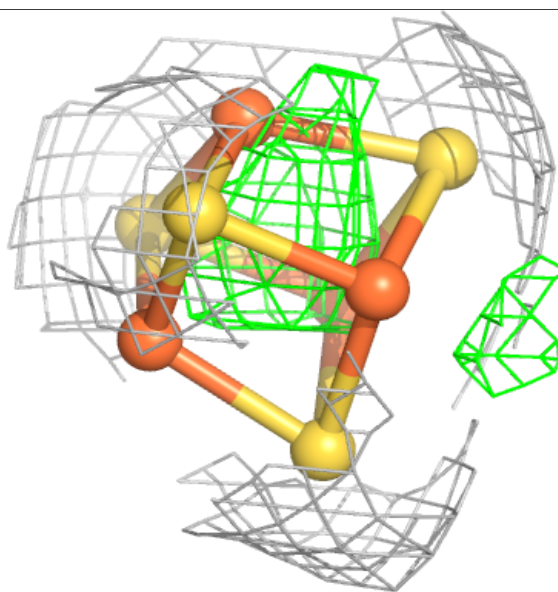
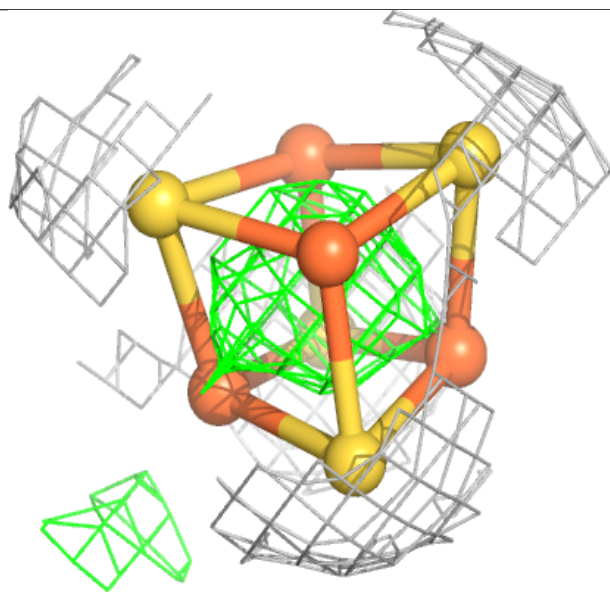
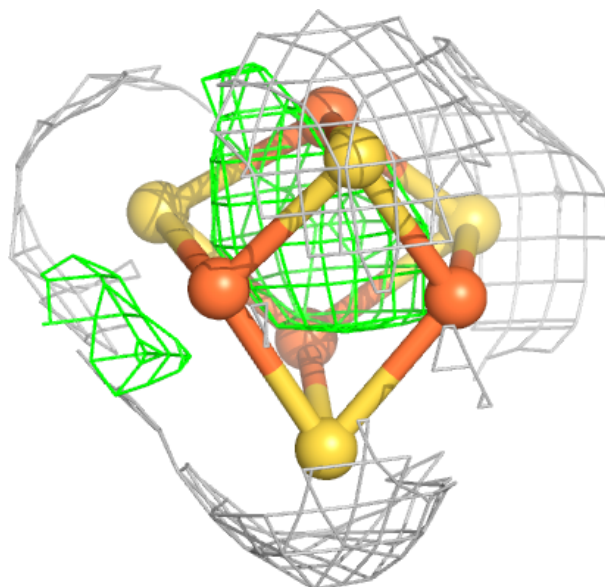
Electron density around SF4 P 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



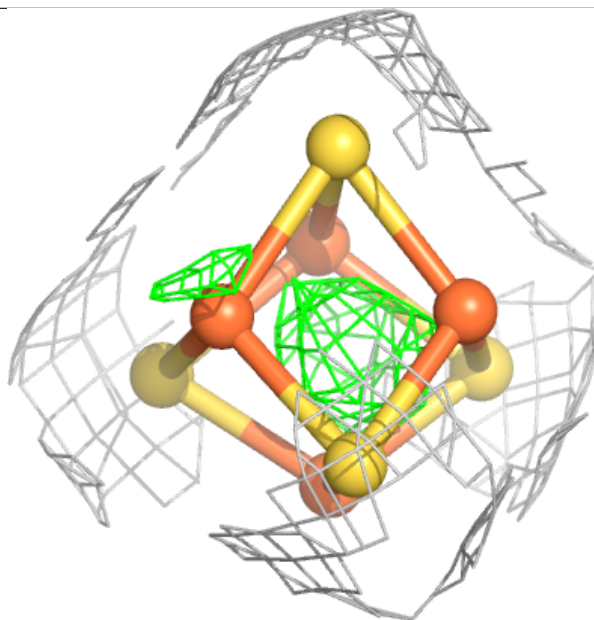
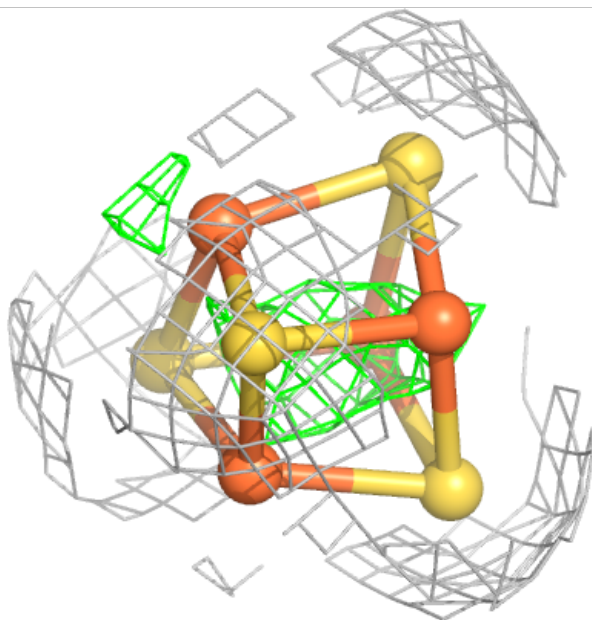
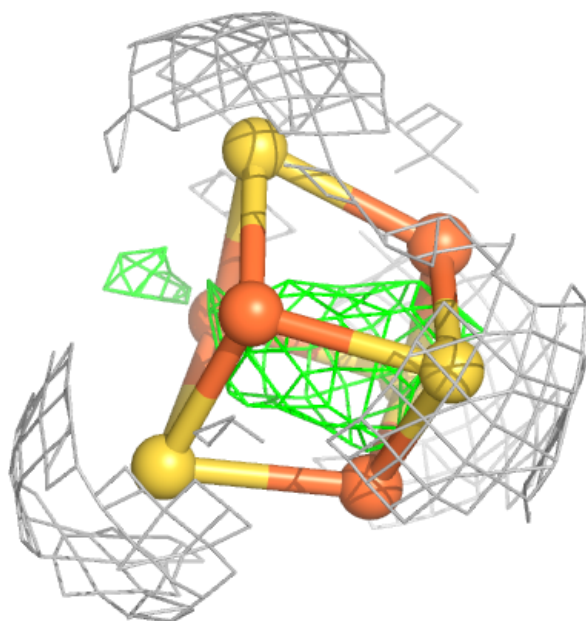
Electron density around SF4 P 502:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



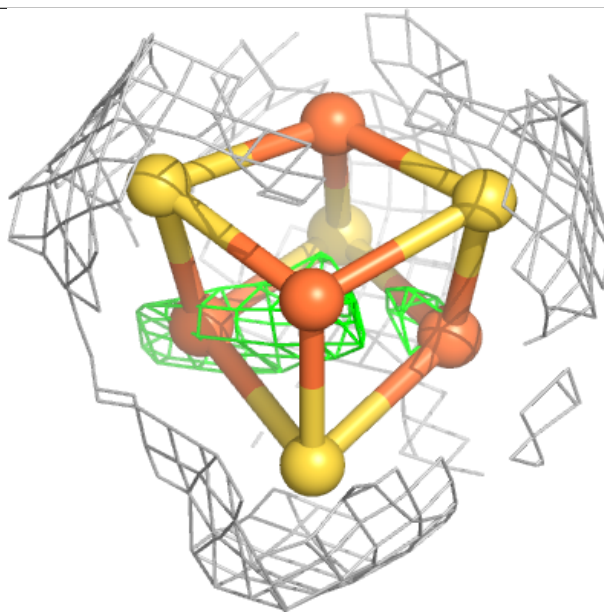
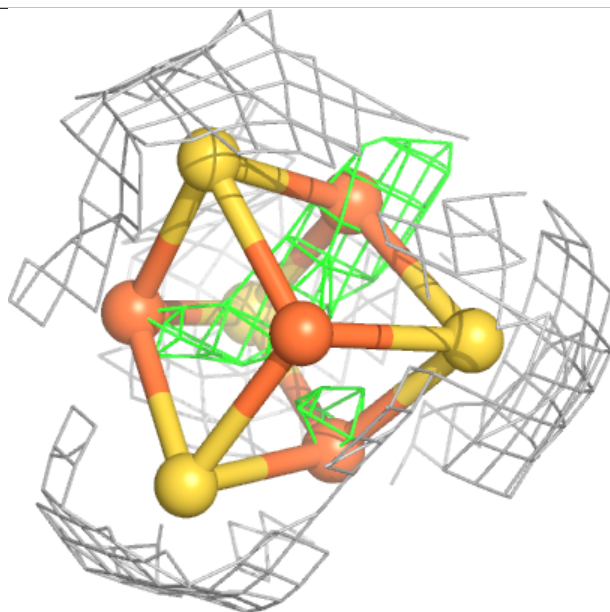
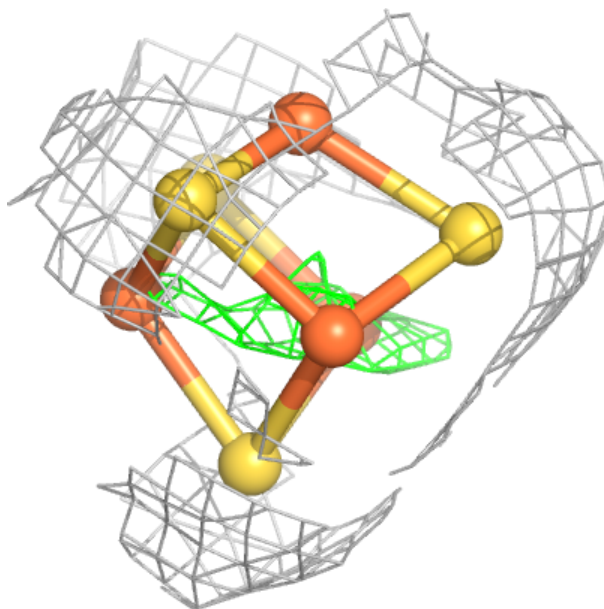
Electron density around SF4 G 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



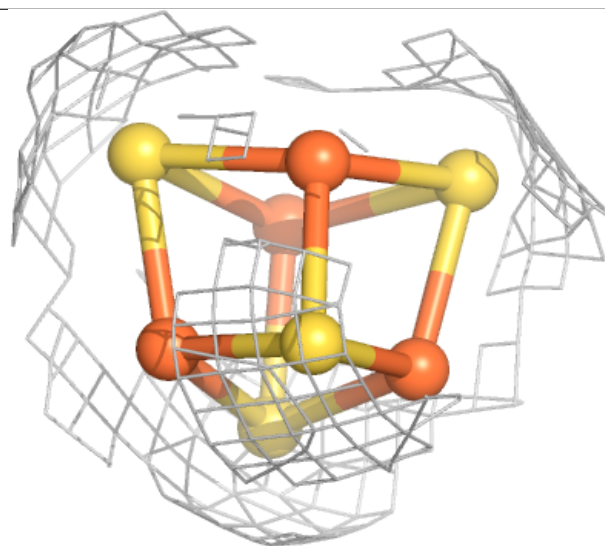
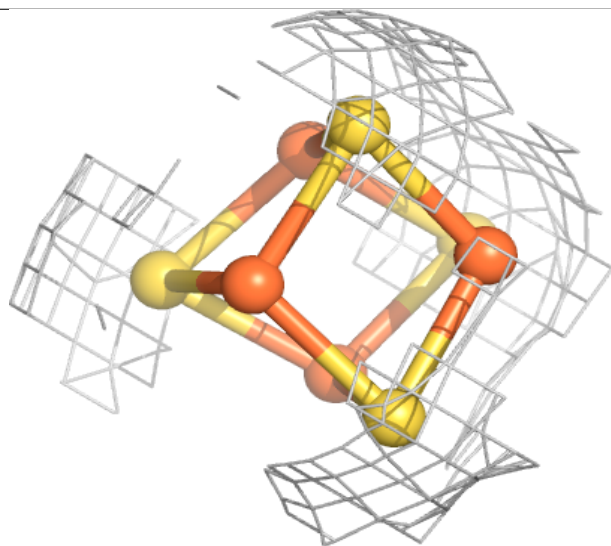
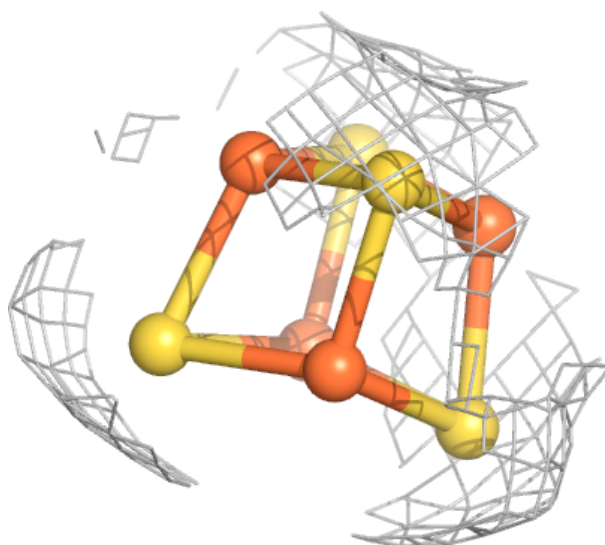
Electron density around SF4 G 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



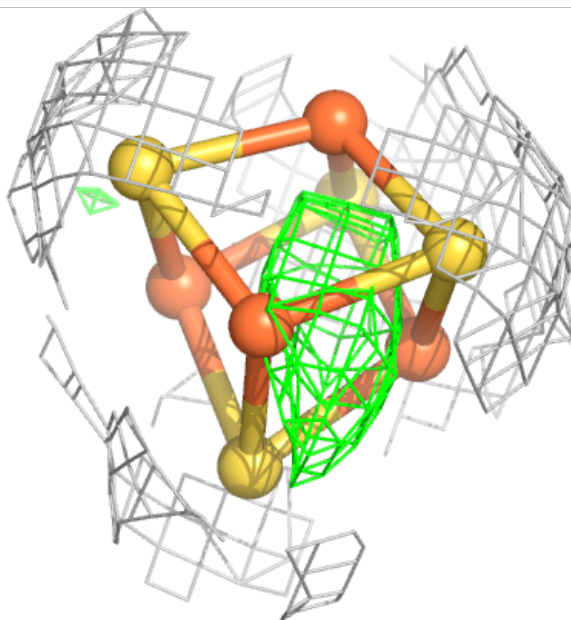
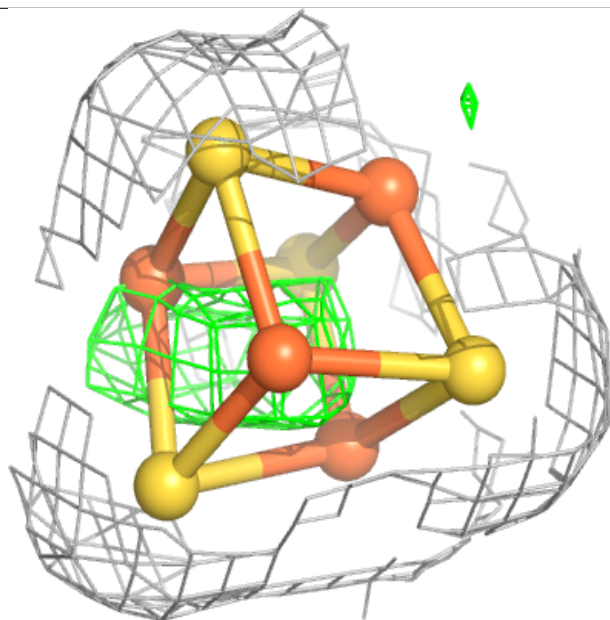
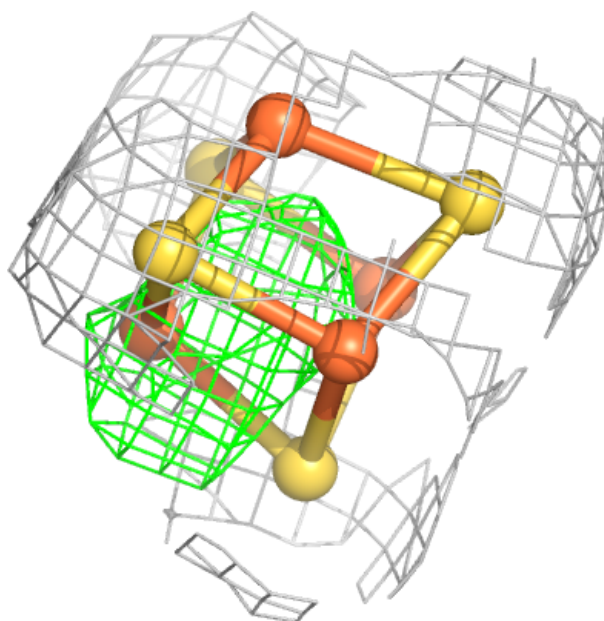
Electron density around SF4 M 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



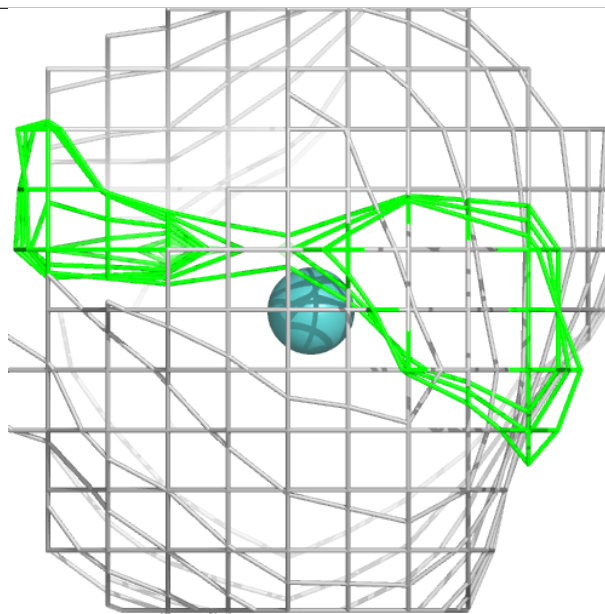
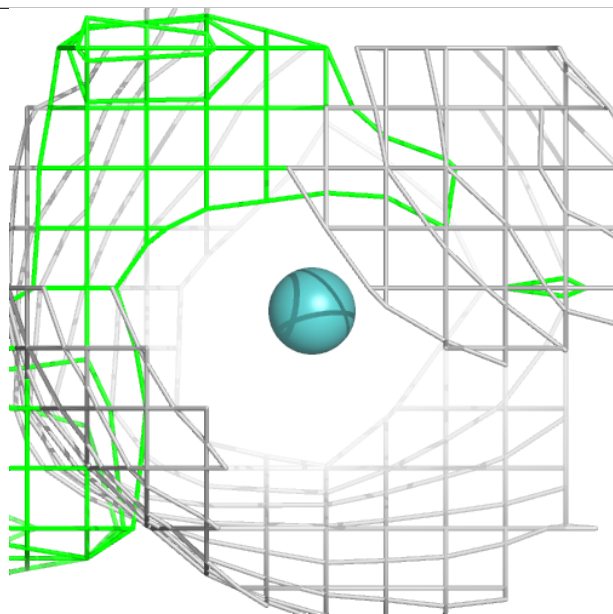
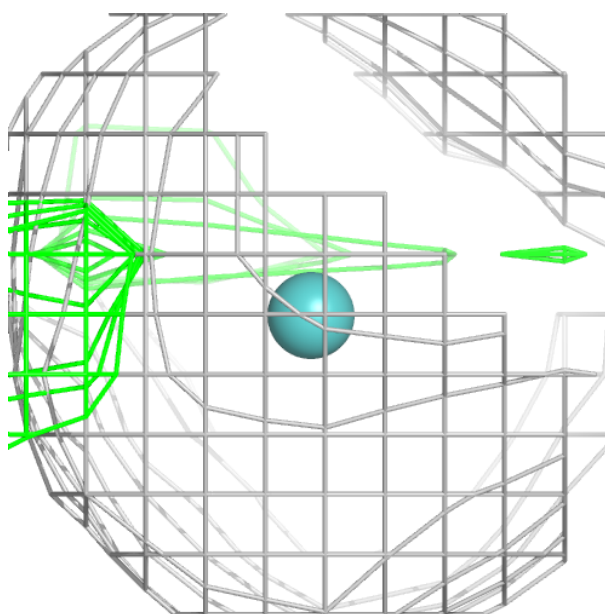
Electron density around SF4 S 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



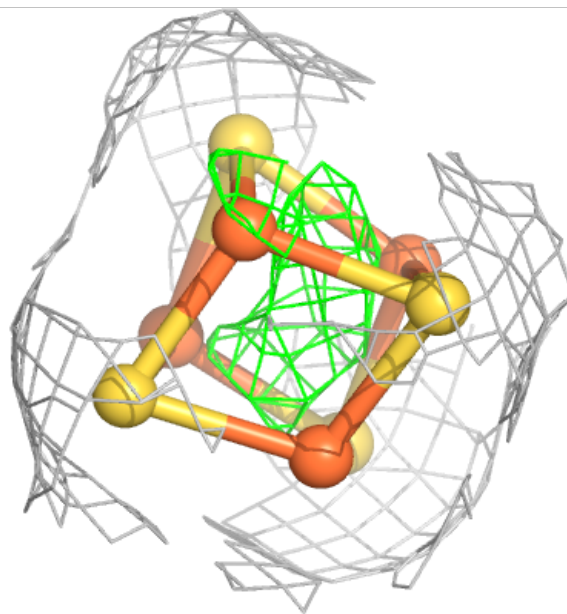
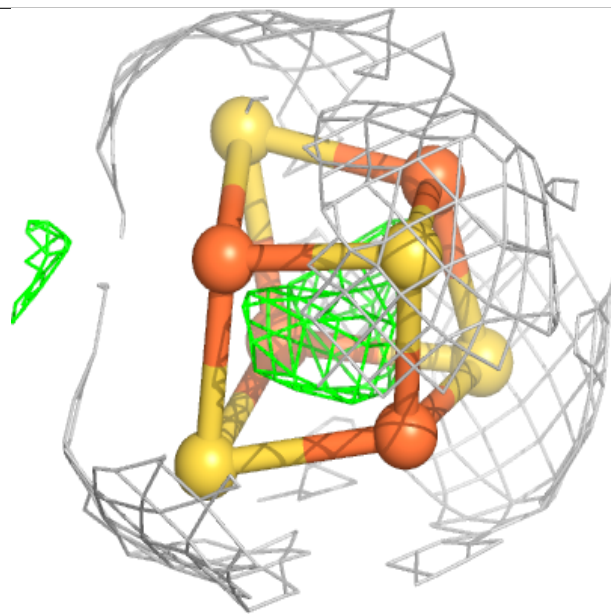
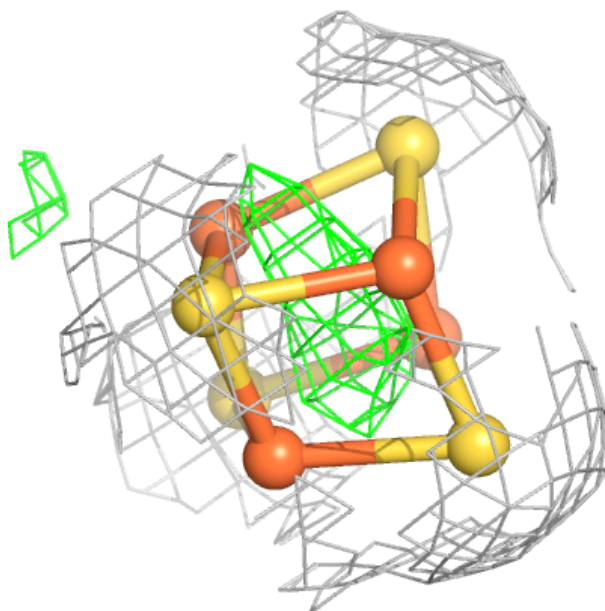
Electron density around MO B 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



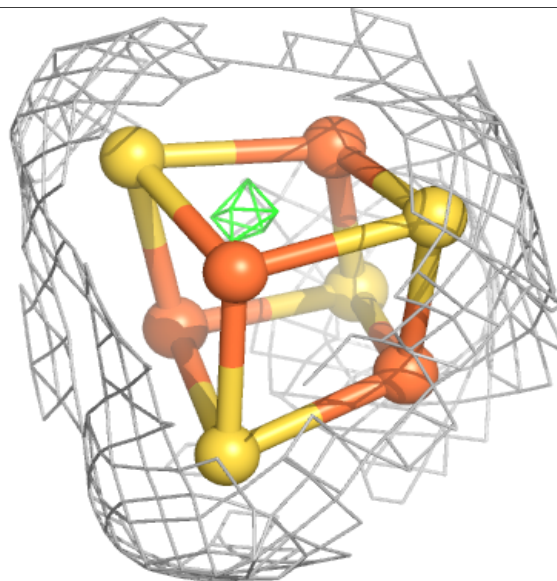
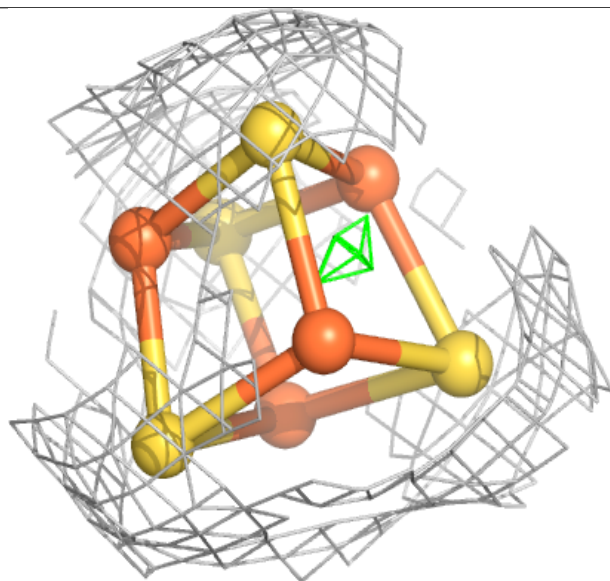
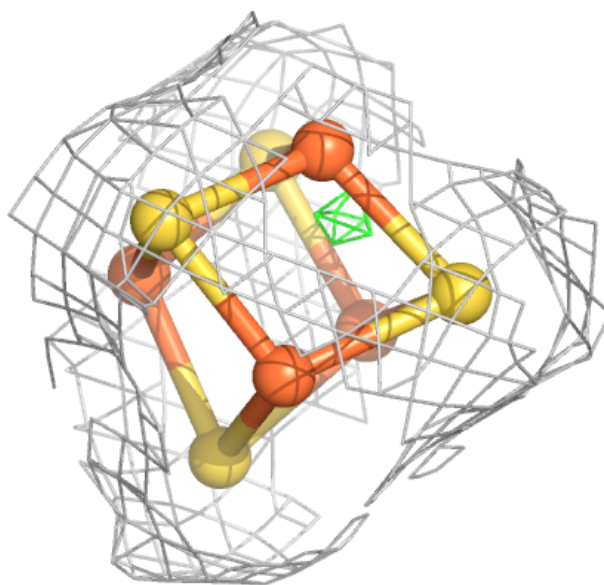
Electron density around SF4 A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



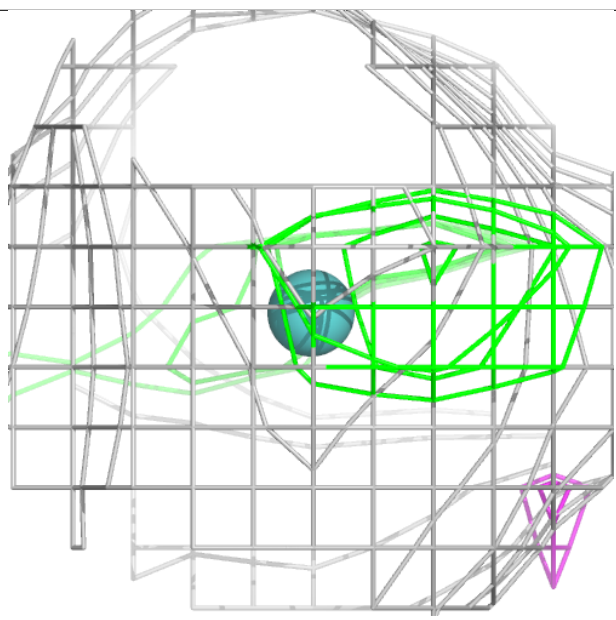
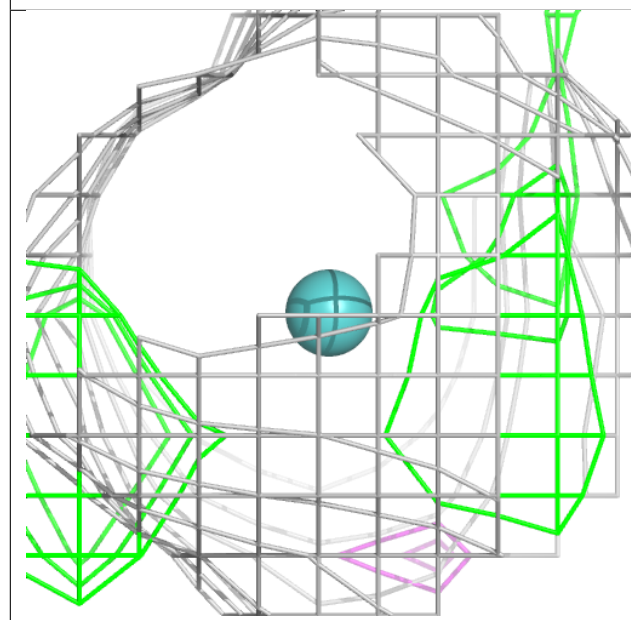
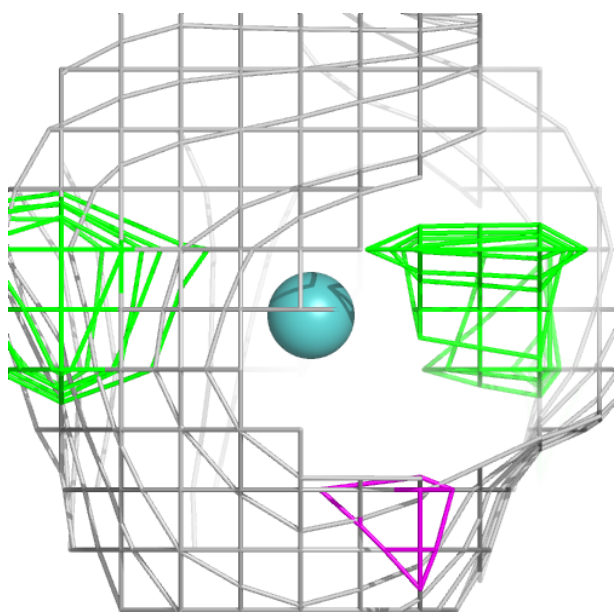
Electron density around SF4 A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



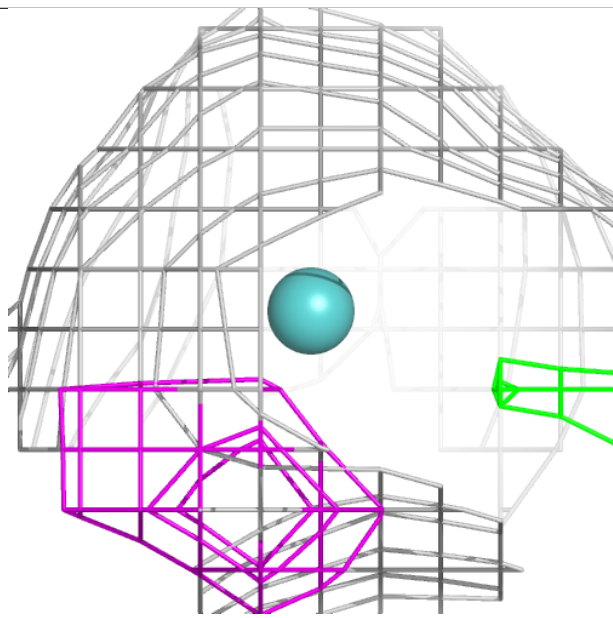
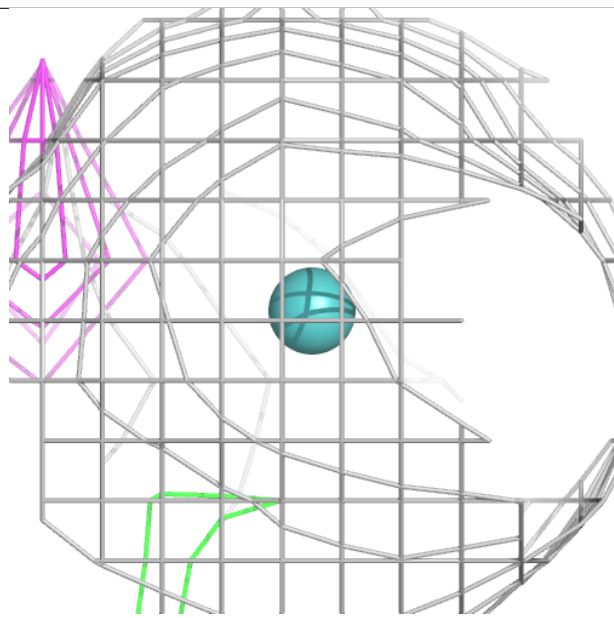
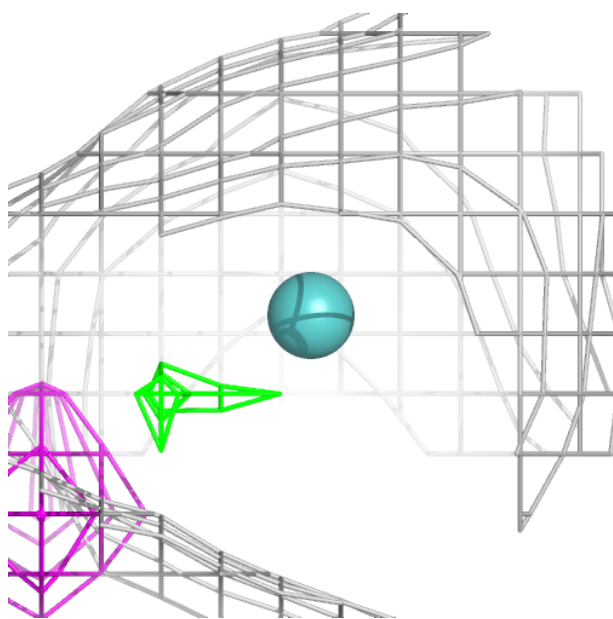
Electron density around MO H 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



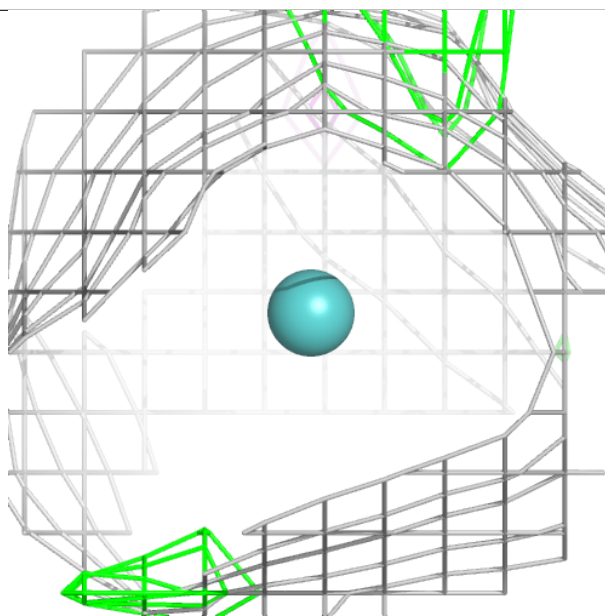
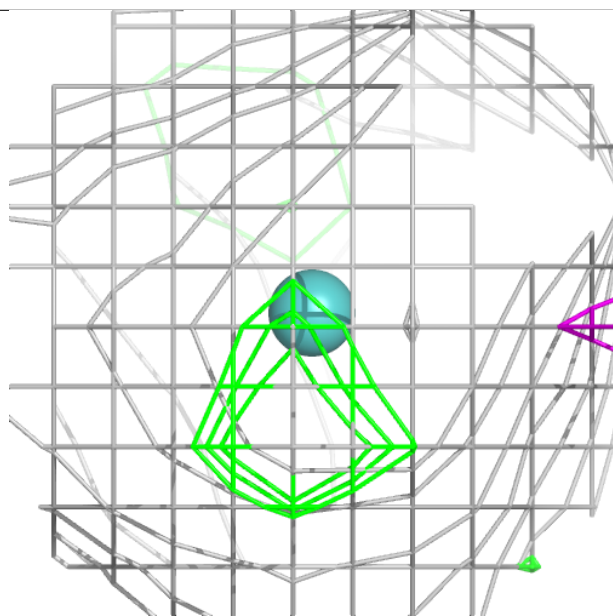
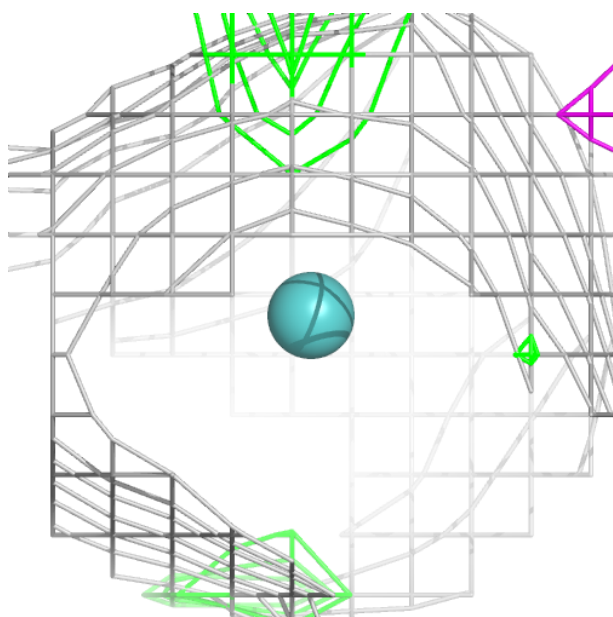
Electron density around MO K 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



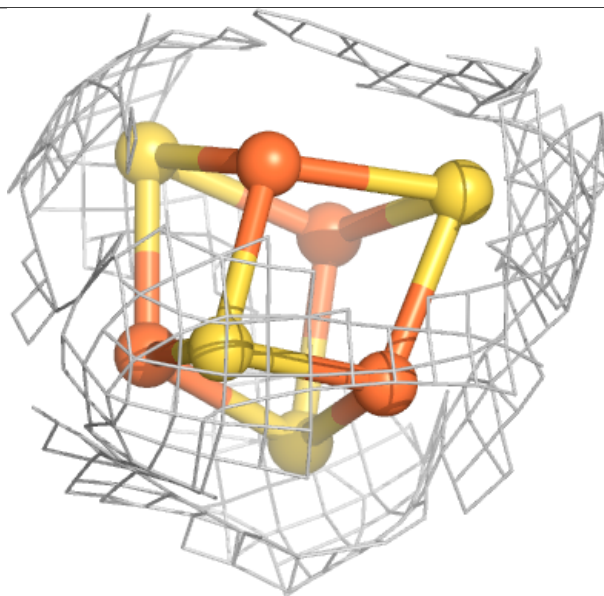
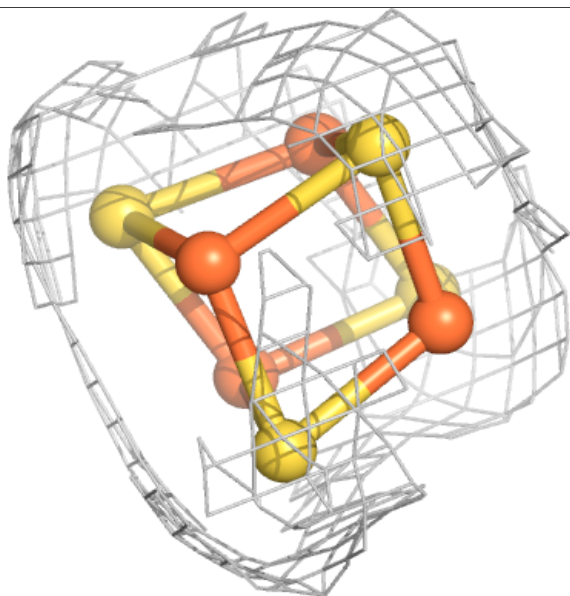
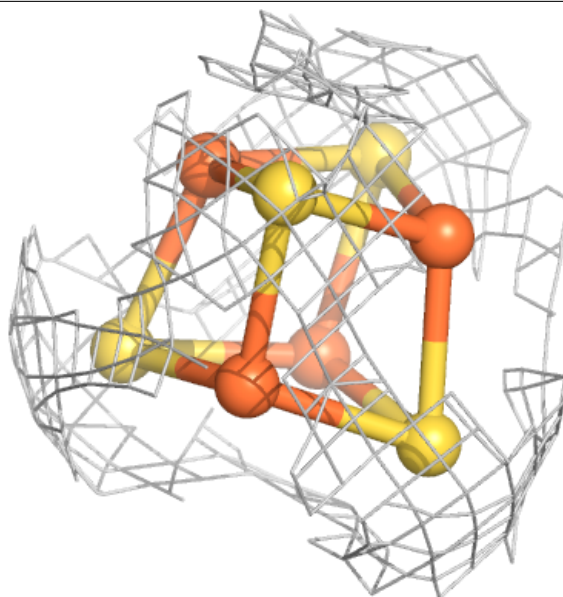
Electron density around MO N 5803:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



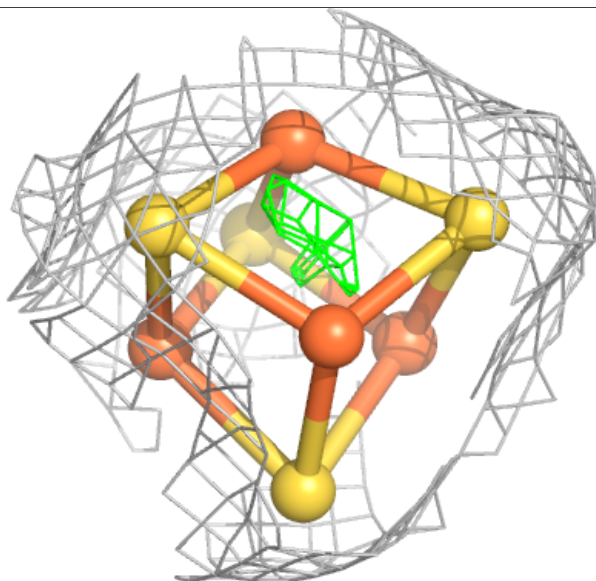
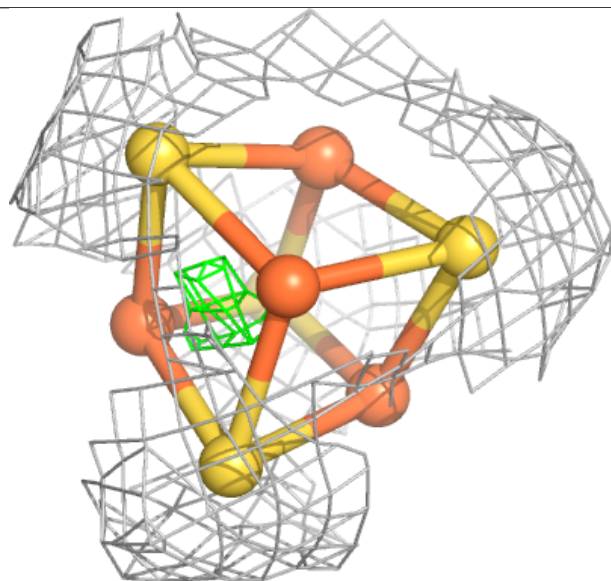
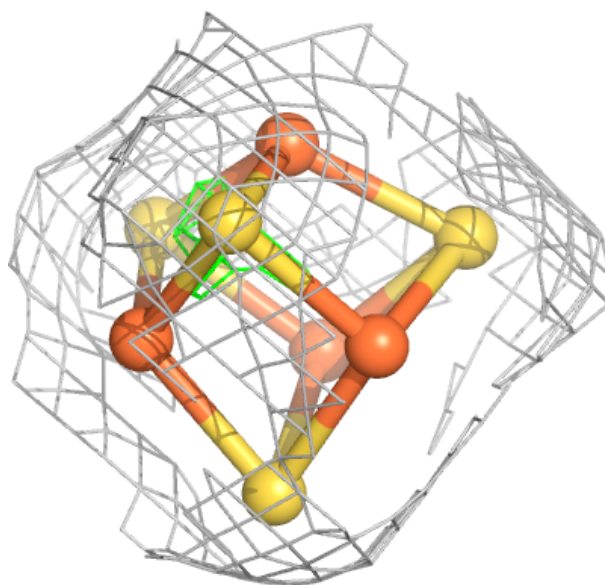
Electron density around SF4 S 503:

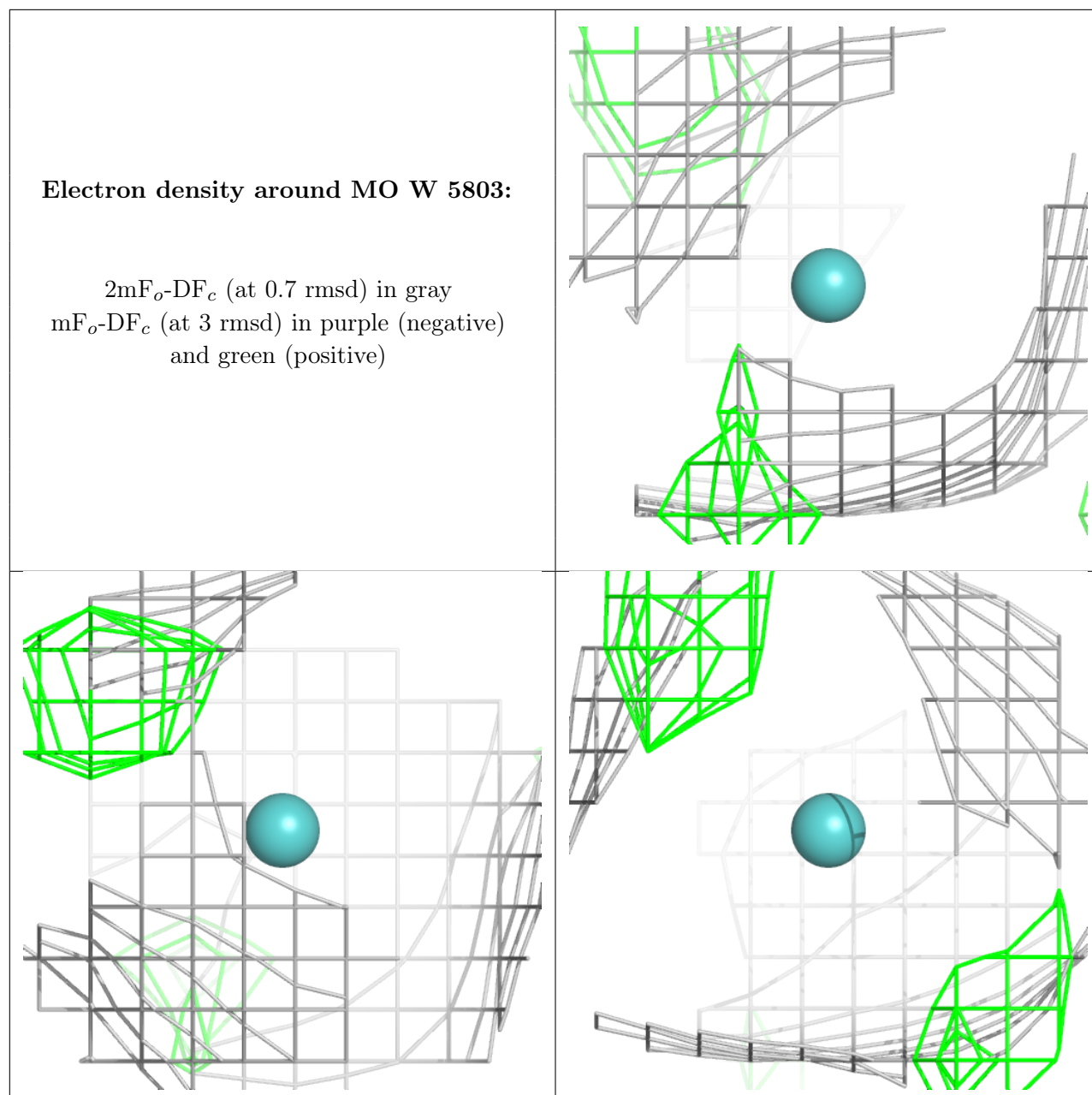
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SF4 J 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.