



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:22 PM EDT

PDB ID : 3L71 / pdb_00003l71
Title : Cytochrome BC1 complex from chicken with azoxystrobin bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 2.84 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

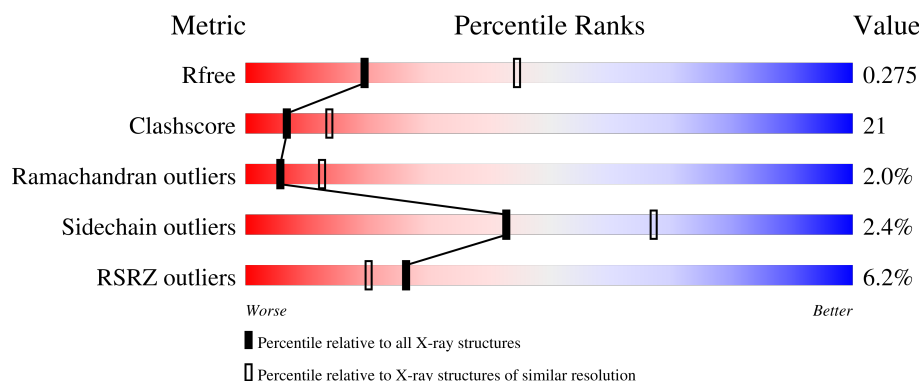
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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.



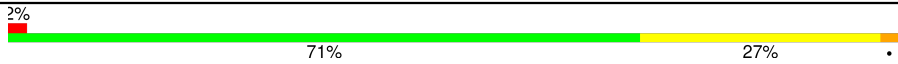
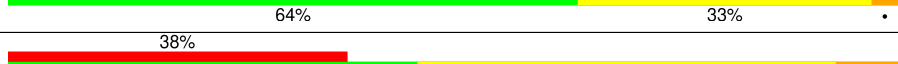
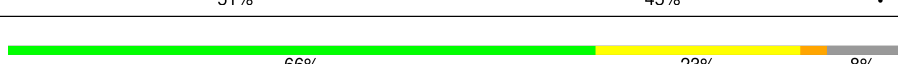
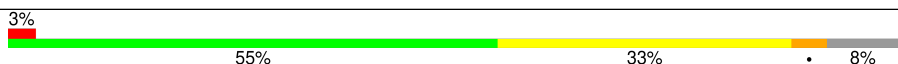
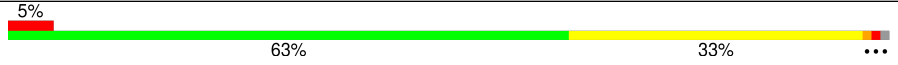
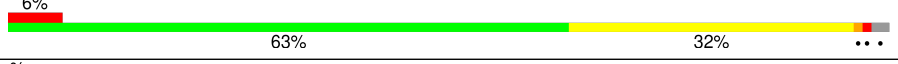
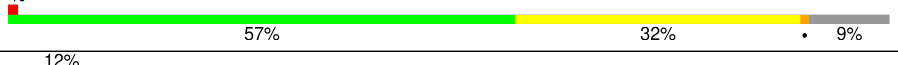
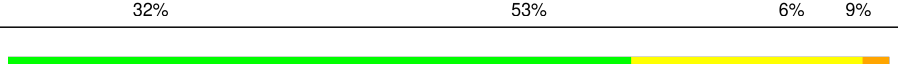
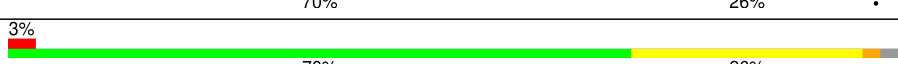
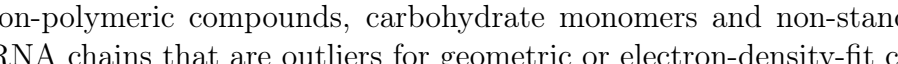
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	446	3% 60% 36% .
1	N	446	4% 57% 38% ..
2	B	441	4% 50% 40% 5% 5%
2	O	441	5% 52% 38% 5% .
3	C	380	3% 73% 24% .

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Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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
11	PEE	N	3008	-	X	-	-
16	HEC	D	501	X	-	-	-
16	HEC	Q	501	X	-	-	-
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32655 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	28	UNK	-	insertion	UNP Q5ZLR5

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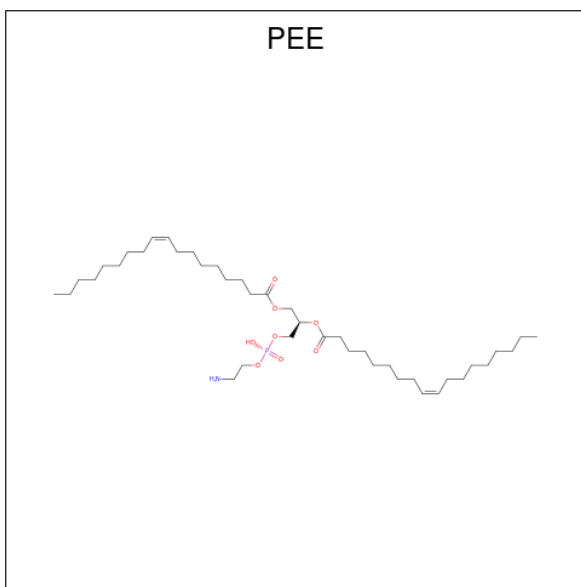
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Chain	Residue	Modelled	Actual	Comment	Reference
I	29	UNK	-	insertion	UNP Q5ZLR5
I	30	UNK	-	insertion	UNP Q5ZLR5
I	31	UNK	-	insertion	UNP Q5ZLR5
I	32	UNK	-	insertion	UNP Q5ZLR5
I	33	UNK	-	insertion	UNP Q5ZLR5
I	34	UNK	-	insertion	UNP Q5ZLR5
I	35	UNK	-	insertion	UNP Q5ZLR5
I	36	UNK	-	insertion	UNP Q5ZLR5
I	37	UNK	-	insertion	UNP Q5ZLR5
I	38	UNK	-	insertion	UNP Q5ZLR5
I	39	UNK	-	insertion	UNP Q5ZLR5
I	40	UNK	-	insertion	UNP Q5ZLR5
I	41	UNK	-	insertion	UNP Q5ZLR5
I	42	UNK	-	insertion	UNP Q5ZLR5
V	25	UNK	-	insertion	UNP Q5ZLR5
V	26	UNK	-	insertion	UNP Q5ZLR5
V	27	UNK	-	insertion	UNP Q5ZLR5
V	28	UNK	-	insertion	UNP Q5ZLR5
V	29	UNK	-	insertion	UNP Q5ZLR5
V	30	UNK	-	insertion	UNP Q5ZLR5
V	31	UNK	-	insertion	UNP Q5ZLR5
V	32	UNK	-	insertion	UNP Q5ZLR5
V	33	UNK	-	insertion	UNP Q5ZLR5
V	35	UNK	-	insertion	UNP Q5ZLR5
V	36	UNK	-	insertion	UNP Q5ZLR5
V	37	UNK	-	insertion	UNP Q5ZLR5
V	38	UNK	-	insertion	UNP Q5ZLR5
V	39	UNK	-	insertion	UNP Q5ZLR5
V	40	UNK	-	insertion	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

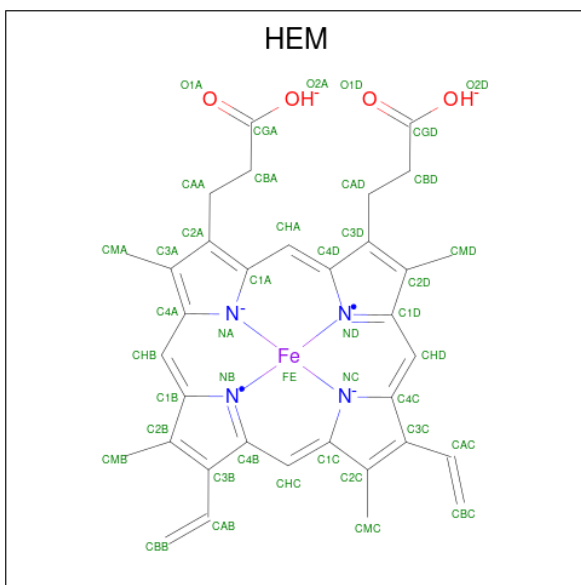
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



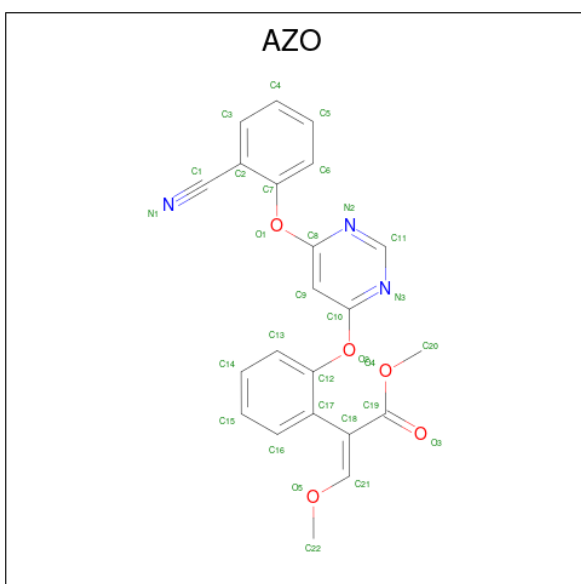
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	A	1	Total	C	O	P		0	0
			21	12	8	1			
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



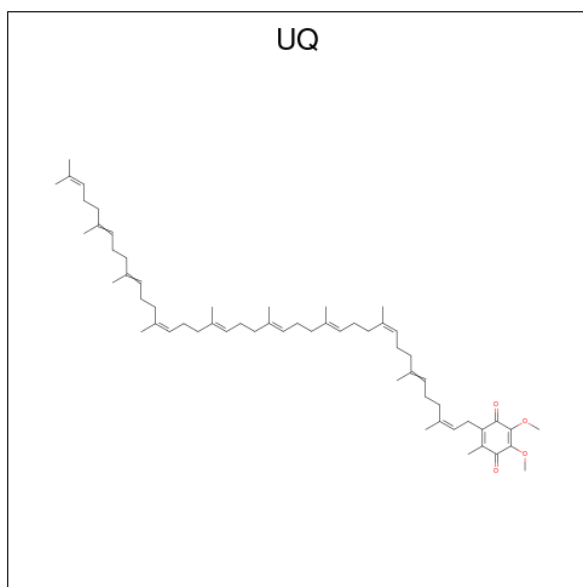
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (CCD ID: AZO) (formula: $C_{22}H_{17}N_3O_5$).



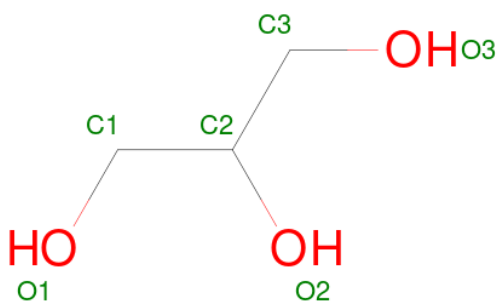
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			30	22	3	5		
13	P	1	Total	C	N	O	0	0
			30	22	3	5		

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



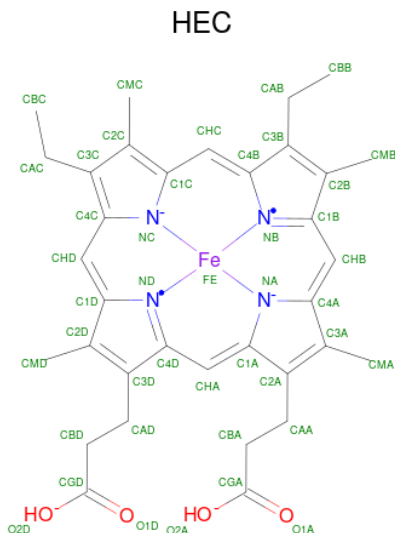
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



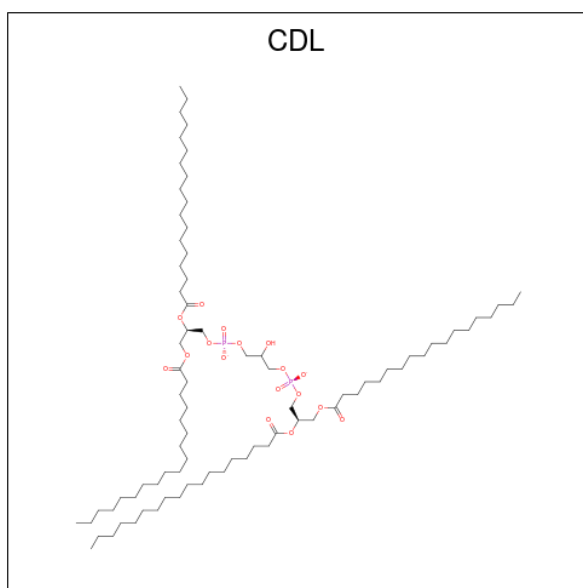
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total 6	C 3	O 3	0	0
15	P	1	Total 6	C 3	O 3	0	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



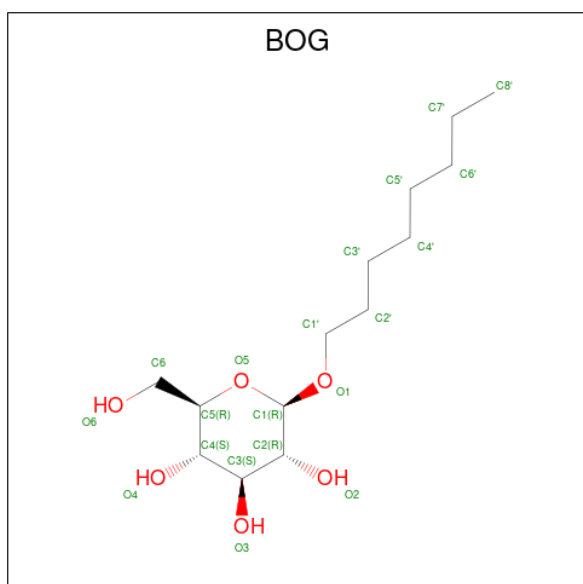
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



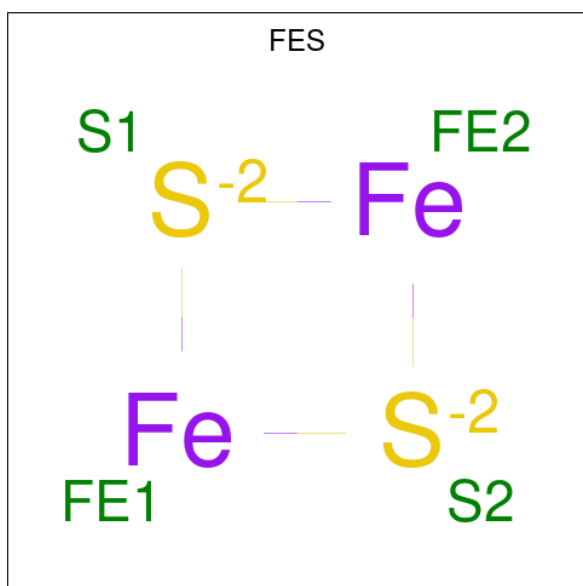
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 18 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	C	O	0	0
			20	14	6		
18	D	1	Total	C	O	0	0
			13	7	6		
18	P	1	Total	C	O	0	0
			12	6	6		
18	Q	1	Total	C	O	0	0
			20	14	6		
18	Q	1	Total	C	O	0	0
			13	7	6		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	E	1	Total	Fe	S	0	0
			4	2	2		
19	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	8	Total	O	0	0
			8	8		
20	E	1	Total	O	0	0
			1	1		
20	P	9	Total	O	0	0
			9	9		

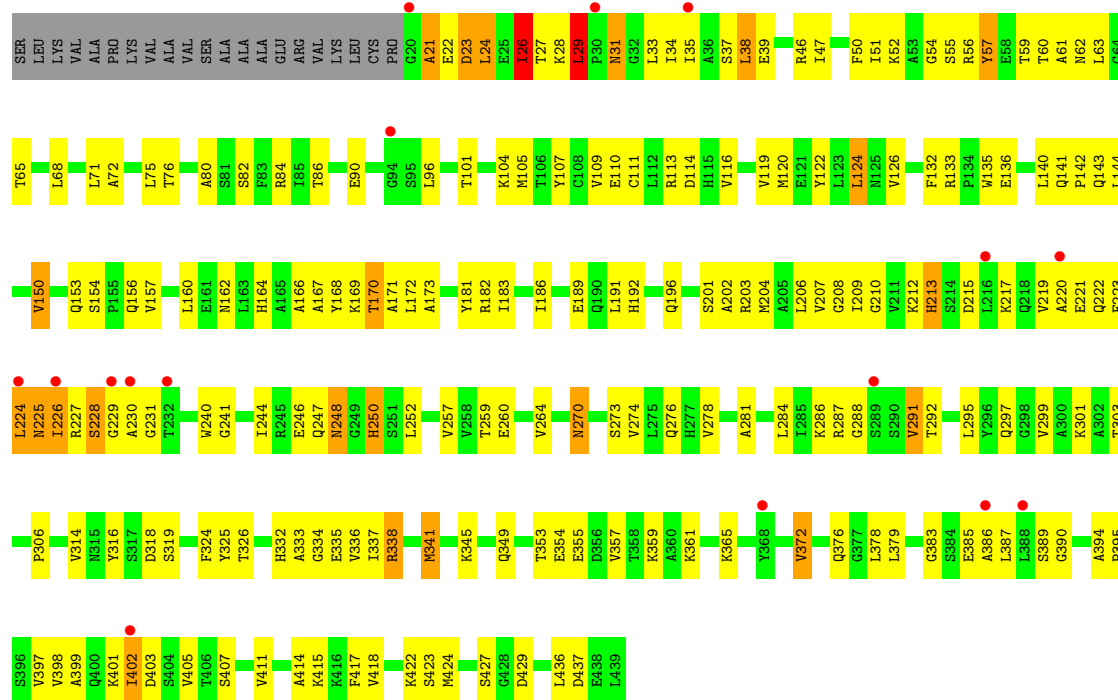
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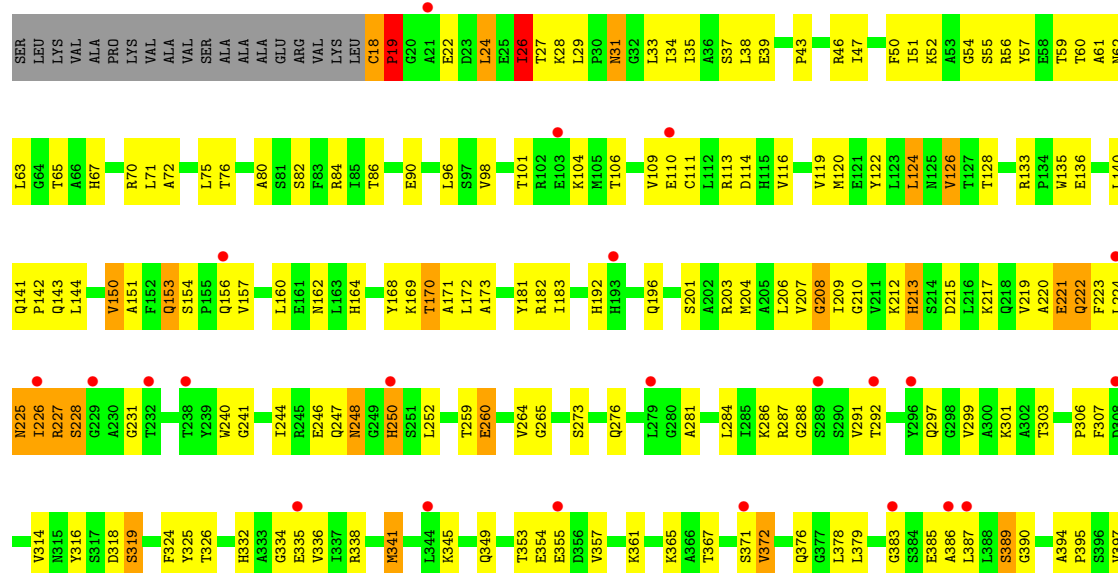
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	R	1	Total	O	0	0
			1	1		



- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

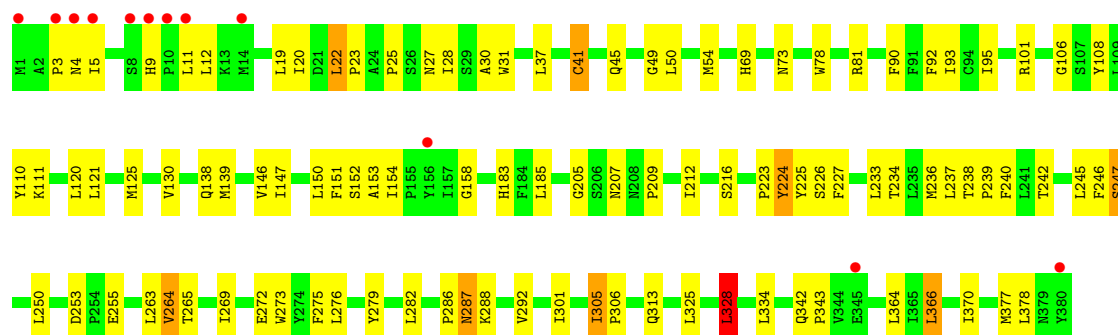
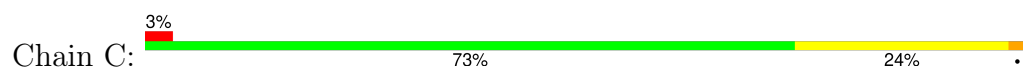


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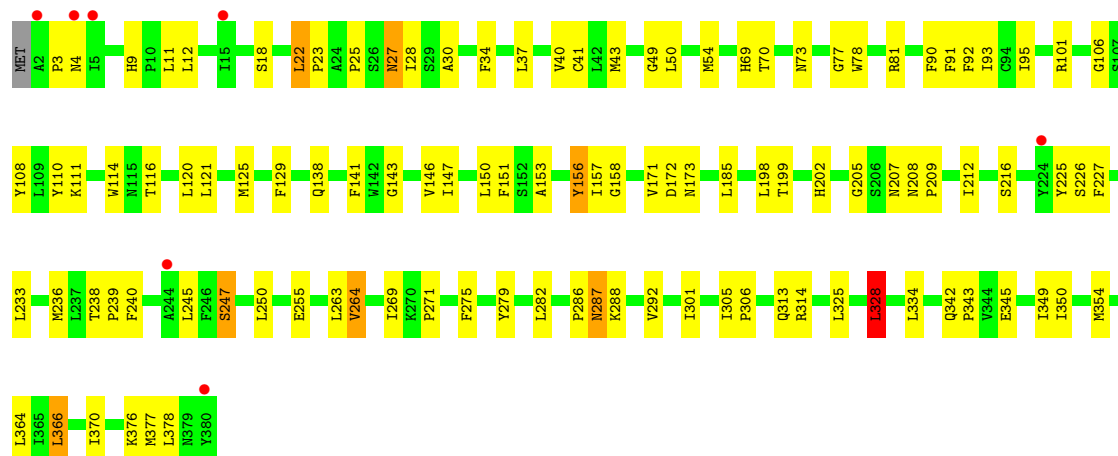




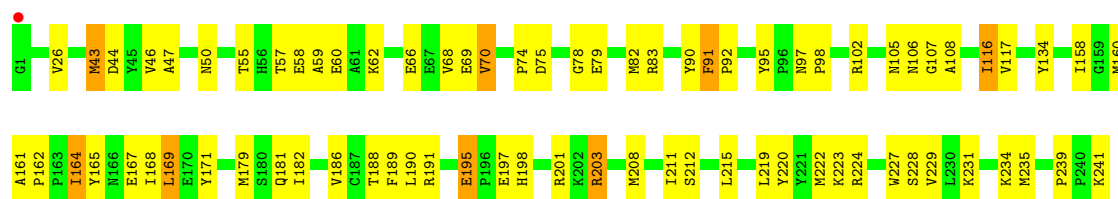
• Molecule 3: Cytochrome b



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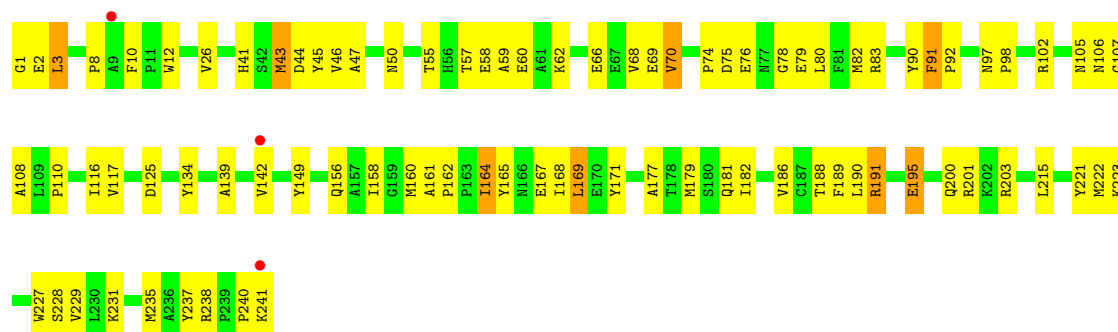


• Molecule 4: Mitochondrial cytochrome c1, heme protein

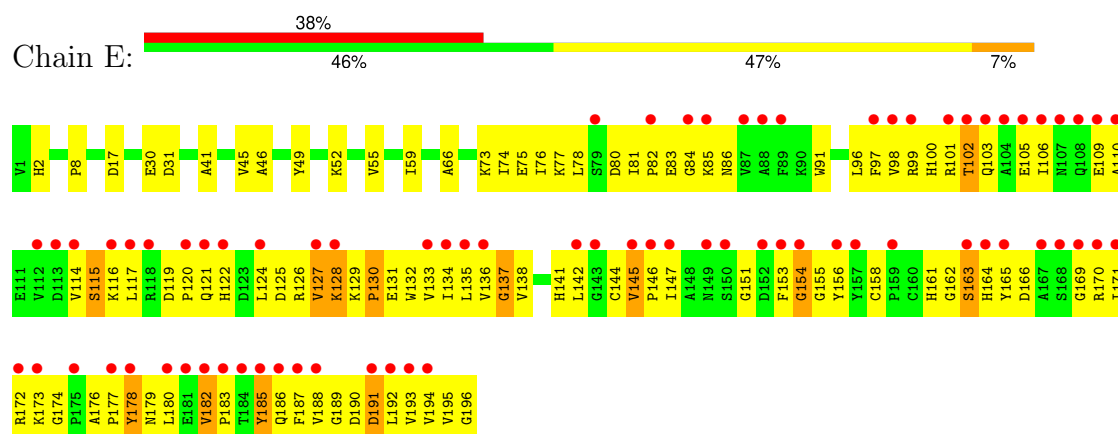


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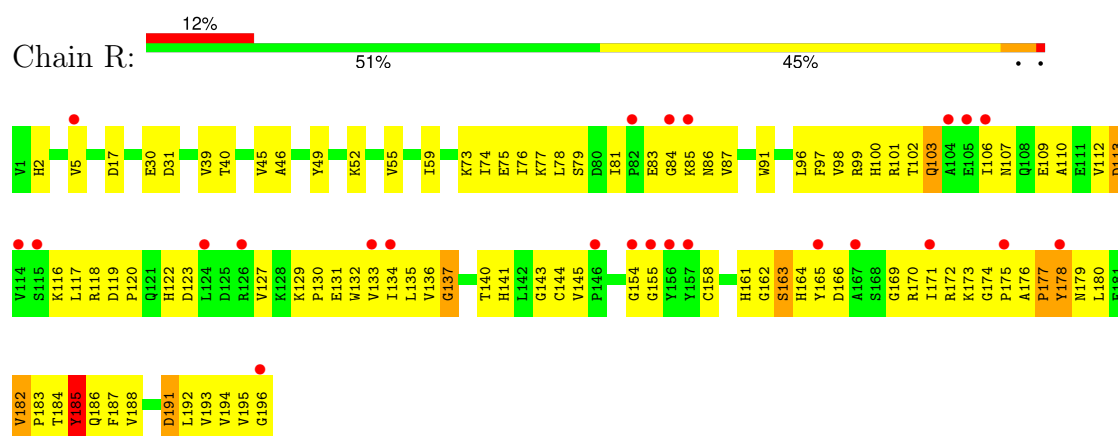




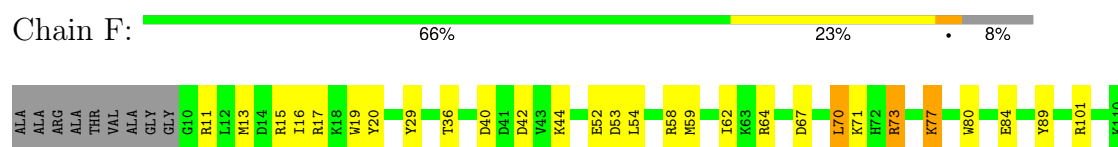
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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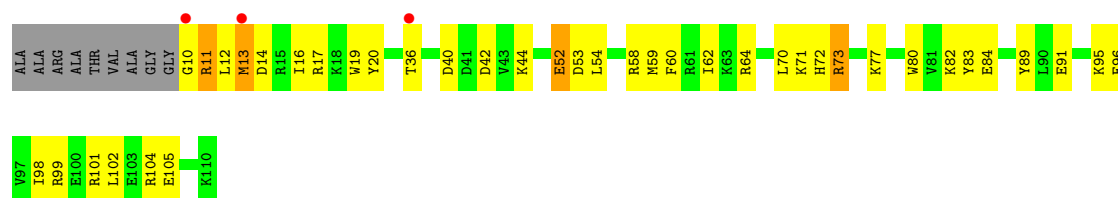


• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

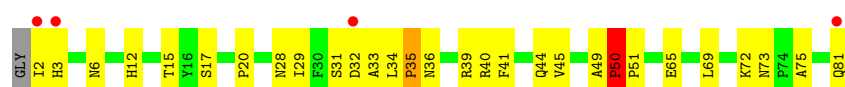


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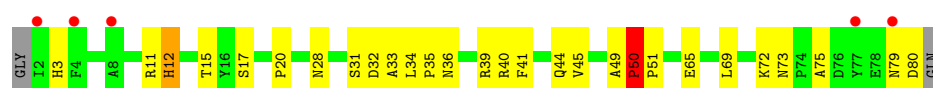




- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



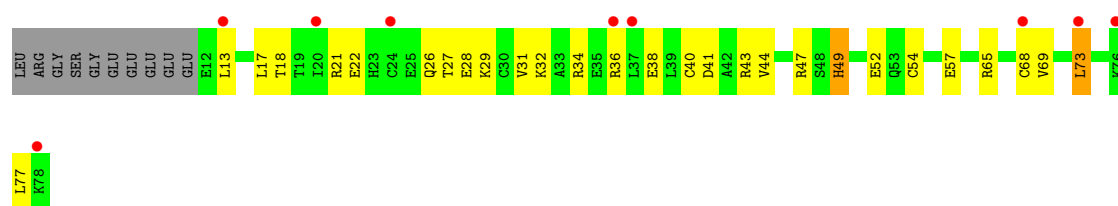
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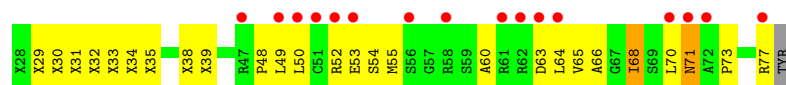
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



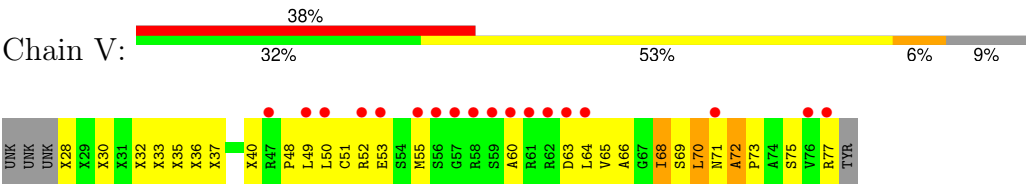
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



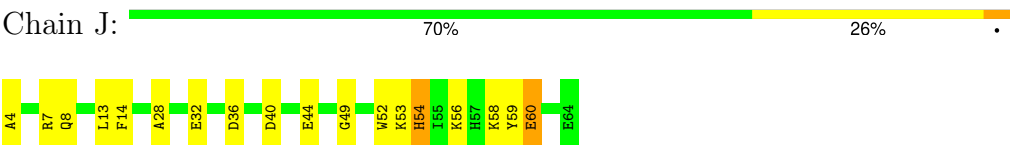
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



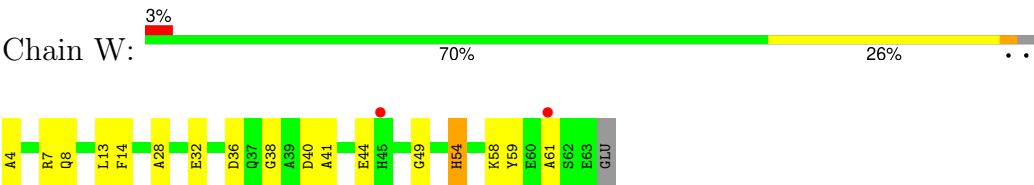
● Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.15Å 181.31Å 240.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.84 24.94 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.94-2.84) 94.3 (24.94-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.281 0.245 , 0.275	Depositor DCC
R_{free} test set	3351 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32655	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: BOG, HEC, AZO, FES, CDL, PEE, GOL, HEM, UQ

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	0.54	0/3518	1.01	22/4767 (0.5%)
1	N	0.49	0/3508	1.00	19/4753 (0.4%)
2	B	0.47	0/3187	0.96	6/4321 (0.1%)
2	O	0.49	0/3202	0.97	8/4343 (0.2%)
3	C	0.65	0/3119	1.03	21/4270 (0.5%)
3	P	0.55	0/3114	1.02	17/4263 (0.4%)
4	D	0.59	0/1956	1.04	9/2658 (0.3%)
4	Q	0.48	0/1956	1.00	10/2658 (0.4%)
5	E	0.47	0/1547	0.91	5/2103 (0.2%)
5	R	0.45	0/1543	0.96	5/2098 (0.2%)
6	F	0.60	0/911	0.92	0/1219
6	S	0.48	0/911	0.90	0/1219
7	G	0.55	0/694	1.00	2/941 (0.2%)
7	T	0.44	0/684	0.97	2/929 (0.2%)
8	H	0.49	0/582	0.94	1/779 (0.1%)
8	U	0.39	0/561	0.91	1/751 (0.1%)
9	I	0.58	0/218	0.96	0/293
9	V	0.56	0/218	1.04	3/293 (1.0%)
10	J	0.51	0/508	0.93	3/682 (0.4%)
10	W	0.47	0/490	0.92	3/660 (0.5%)
All	All	0.52	0/32427	0.99	137/44000 (0.3%)

There are no bond length outliers.

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	8.41	119.03	108.19
5	R	143	GLY	N-CA-C	8.23	127.15	115.30
1	A	32	GLN	CA-C-N	8.19	127.92	119.56
1	A	32	GLN	C-N-CA	8.19	127.92	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	32	GLN	CA-C-N	8.08	127.74	119.82
1	N	32	GLN	C-N-CA	8.08	127.74	119.82
4	D	44	ASP	N-CA-C	7.40	121.22	111.75
3	C	207	ASN	N-CA-C	-7.08	100.32	110.59
8	U	73	LEU	N-CA-C	7.04	119.61	111.02
4	D	91	PHE	CA-C-N	7.01	126.98	119.76
4	D	91	PHE	C-N-CA	7.01	126.98	119.76
3	P	247	SER	CA-C-N	7.01	127.31	119.32
3	P	247	SER	C-N-CA	7.01	127.31	119.32
3	P	147	ILE	N-CA-C	6.99	117.12	110.42
3	P	185	LEU	N-CA-C	6.99	118.78	111.03
1	N	415	ILE	N-CA-C	6.88	117.48	111.56
3	C	247	SER	CA-C-N	6.84	127.12	119.32
3	C	247	SER	C-N-CA	6.84	127.12	119.32
1	N	348	SER	N-CA-C	6.80	119.11	110.61
2	O	326	THR	N-CA-C	6.68	119.35	108.26
3	C	185	LEU	N-CA-C	6.65	118.42	111.03
1	N	347	THR	N-CA-C	6.63	121.50	113.41
4	Q	44	ASP	N-CA-C	6.59	120.18	111.75
2	O	226	ILE	N-CA-C	-6.56	100.07	108.93
1	N	189	HIS	N-CA-C	6.56	121.32	113.12
8	H	73	LEU	N-CA-C	6.54	118.95	111.11
1	A	189	HIS	N-CA-C	6.50	121.25	113.12
3	C	226	SER	N-CA-C	-6.47	104.31	111.36
3	P	226	SER	N-CA-C	-6.47	104.31	111.36
3	P	205	GLY	N-CA-C	-6.45	103.14	112.17
2	B	230	ALA	N-CA-C	-6.38	104.94	114.64
3	C	93	ILE	N-CA-C	-6.38	104.11	110.30
1	A	248	LEU	CA-C-N	6.37	126.12	119.05
1	A	248	LEU	C-N-CA	6.37	126.12	119.05
4	Q	195	GLU	CA-C-N	6.27	125.96	119.56
4	Q	195	GLU	C-N-CA	6.27	125.96	119.56
3	C	205	GLY	N-CA-C	-6.26	103.40	112.17
4	D	164	ILE	N-CA-C	6.26	117.78	108.46
2	B	326	THR	N-CA-C	6.25	118.64	108.26
3	P	207	ASN	N-CA-C	-6.23	101.56	110.59
10	J	13	LEU	N-CA-C	6.21	120.72	111.96
1	A	331	ILE	CB-CA-C	-6.20	104.04	111.97
4	D	95	TYR	CA-C-N	6.19	125.60	118.85
4	D	95	TYR	C-N-CA	6.19	125.60	118.85
10	J	14	PHE	N-CA-C	6.18	120.66	113.18
1	N	32	GLN	N-CA-C	6.17	118.56	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ILE	N-CA-C	6.15	116.82	110.36
4	Q	191	ARG	N-CA-C	-6.12	104.53	111.14
5	E	145	VAL	N-CA-C	6.12	113.61	107.55
1	A	348	SER	N-CA-C	6.11	118.79	110.06
1	A	432	LEU	N-CA-C	6.10	118.12	108.79
4	Q	164	ILE	N-CA-C	6.10	117.55	108.46
3	P	328	LEU	N-CA-C	-6.09	104.56	111.14
3	C	328	LEU	N-CA-C	-6.05	104.60	111.14
1	A	415	ILE	N-CA-C	6.03	116.75	111.56
10	J	54	HIS	N-CA-C	5.91	117.52	111.14
10	W	13	LEU	N-CA-C	5.90	120.53	112.68
4	D	195	GLU	CA-C-N	5.88	125.75	119.28
4	D	195	GLU	C-N-CA	5.88	125.75	119.28
4	D	116	ILE	N-CA-C	5.88	117.32	110.62
1	A	119	ASN	N-CA-C	5.85	120.12	111.87
10	W	14	PHE	N-CA-C	5.83	120.24	113.18
5	E	17	ASP	N-CA-C	5.77	119.93	113.01
3	C	366	LEU	N-CA-C	5.75	117.22	111.07
3	C	209	PRO	N-CA-C	5.74	121.30	113.84
2	B	213	HIS	N-CA-C	5.74	117.53	111.28
1	N	432	LEU	N-CA-C	5.73	117.55	108.79
5	E	182	VAL	CA-C-N	5.71	125.68	120.03
5	E	182	VAL	C-N-CA	5.71	125.68	120.03
7	T	12	HIS	N-CA-C	5.71	119.55	112.24
1	A	329	LEU	N-CA-C	5.69	119.92	113.15
1	N	331	ILE	CB-CA-C	-5.69	104.69	111.97
3	C	111	LYS	N-CA-C	5.68	120.75	111.37
1	N	329	LEU	N-CA-C	5.68	119.83	113.02
2	O	213	HIS	N-CA-C	5.66	117.45	111.28
1	A	303	LEU	N-CA-C	5.66	119.36	112.23
4	Q	91	PHE	CA-C-N	5.66	125.59	119.76
4	Q	91	PHE	C-N-CA	5.66	125.59	119.76
3	P	366	LEU	N-CA-C	5.63	117.09	111.07
3	P	110	TYR	N-CA-C	-5.61	101.21	109.62
3	P	111	LYS	N-CA-C	5.59	120.60	111.37
1	A	32	GLN	N-CA-C	5.59	117.72	109.62
4	Q	116	ILE	N-CA-C	5.55	116.95	110.62
1	N	119	ASN	N-CA-C	5.55	119.69	111.87
9	V	72	ALA	CA-C-N	5.54	125.82	119.83
9	V	72	ALA	C-N-CA	5.54	125.82	119.83
2	O	170	THR	N-CA-C	5.53	115.54	108.24
1	A	347	THR	N-CA-C	5.53	120.68	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	378	LEU	N-CA-C	-5.53	105.90	113.30
1	A	278	GLY	N-CA-C	5.51	120.95	111.47
3	P	143	GLY	N-CA-C	-5.50	106.12	112.50
1	A	66	GLY	N-CA-C	5.49	119.12	112.48
2	O	225	ASN	N-CA-C	5.48	119.74	112.72
3	C	154	ILE	N-CA-C	-5.45	103.95	109.02
3	P	314	ARG	N-CA-C	5.45	117.08	111.03
1	N	263	ALA	N-CA-C	5.43	118.70	111.75
3	C	110	TYR	N-CA-C	-5.41	101.51	109.62
1	N	264	ASP	N-CA-C	5.39	117.43	109.50
2	B	170	THR	N-CA-C	5.37	115.33	108.24
9	V	70	LEU	N-CA-C	-5.37	106.57	113.23
2	O	126	VAL	N-CA-C	5.35	115.55	110.42
3	C	27	ASN	N-CA-C	5.34	119.11	112.59
2	B	29	LEU	CA-C-N	5.28	125.34	119.32
2	B	29	LEU	C-N-CA	5.28	125.34	119.32
1	N	260	PRO	N-CA-C	5.26	120.46	113.57
1	A	440	GLY	N-CA-C	-5.25	107.38	115.73
1	N	278	GLY	N-CA-C	5.24	120.62	111.50
1	N	303	LEU	N-CA-C	5.24	118.83	112.23
3	C	265	THR	CA-C-N	-5.22	115.90	119.66
3	C	265	THR	C-N-CA	-5.22	115.90	119.66
3	P	116	THR	N-CA-C	-5.21	105.72	111.71
3	C	224	TYR	N-CA-C	5.20	117.37	111.02
3	C	378	LEU	N-CA-C	-5.18	106.35	113.30
7	G	50	PRO	N-CA-C	5.18	117.02	110.70
7	G	12	HIS	N-CA-C	5.17	118.88	112.58
4	Q	45	TYR	N-CA-C	5.16	119.56	113.16
1	N	66	GLY	N-CA-C	5.16	118.72	112.48
1	N	415	ILE	CB-CA-C	-5.15	106.54	111.44
1	A	263	ALA	N-CA-C	5.15	118.67	112.38
3	C	305	ILE	CB-CA-C	-5.15	108.81	113.70
3	P	27	ASN	N-CA-C	5.15	118.87	112.59
1	A	428	ILE	N-CA-C	5.13	120.00	109.34
3	P	93	ILE	N-CA-C	-5.12	104.91	110.23
7	T	50	PRO	N-CA-C	5.12	116.94	110.70
1	A	416	TYR	N-CA-C	5.11	117.97	110.30
5	R	182	VAL	CA-C-N	5.09	125.07	120.03
5	R	182	VAL	C-N-CA	5.09	125.07	120.03
4	Q	80	LEU	N-CA-C	-5.06	103.72	110.55
10	W	54	HIS	N-CA-C	5.04	116.58	111.14
5	R	17	ASP	N-CA-C	5.03	119.05	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ILE	CB-CA-C	-5.03	106.66	111.44
5	E	66	ALA	N-CA-C	5.02	117.41	111.33
5	R	103	GLN	N-CA-C	-5.02	106.25	112.38
3	C	152	SER	N-CA-C	-5.02	107.22	113.19
2	O	153	GLN	N-CA-C	-5.02	106.67	112.89
1	N	416	TYR	N-CA-C	5.01	117.82	110.30
1	A	238	GLY	N-CA-C	-5.00	103.17	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3447	0	3362	138	0
1	N	3437	0	3349	156	0
2	B	3133	0	3130	201	0
2	O	3147	0	3146	201	0
3	C	3017	0	3063	80	0
3	P	3012	0	3058	97	0
4	D	1898	0	1846	64	0
4	Q	1898	0	1846	79	0
5	E	1513	0	1478	117	0
5	R	1509	0	1474	102	0
6	F	891	0	893	27	0
6	S	891	0	893	38	0
7	G	672	0	653	30	0
7	T	662	0	645	35	0
8	H	574	0	548	21	0
8	U	553	0	535	27	0
9	I	287	0	250	39	0
9	V	277	0	249	39	0
10	J	497	0	490	17	0
10	W	479	0	478	16	0
11	A	71	0	90	0	0
11	C	49	0	72	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	5	0	0	0	0
11	P	99	0	149	3	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	30	0	17	0	0
13	P	30	0	17	2	0
14	C	19	0	17	2	0
14	P	19	0	17	3	0
15	C	6	0	8	1	0
15	P	6	0	8	0	0
16	D	43	0	30	1	0
16	Q	43	0	30	1	0
17	D	42	0	28	4	0
17	G	40	0	24	4	0
17	Q	42	0	28	3	0
17	T	40	0	24	3	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	0	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32655	0	32154	1386	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 21.

All (1386) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.14	1.11
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.12	1.09
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:O:353:THR:HG22	2:O:355:GLU:H	1.14	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.17	1.07
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.37	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.24	0.97
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.26	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.96
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.45	0.96
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.49	0.95
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.47	0.95
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.81	0.94
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.49	0.94
4:D:57:THR:HG22	4:D:59:ALA:H	1.32	0.93
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.51	0.92
4:D:47:ALA:H	4:D:50:ASN:HD22	1.05	0.92
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.50	0.92
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.32	0.92
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.51	0.91
2:O:27:THR:HG22	2:O:28:LYS:H	1.33	0.90
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.00	0.89
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.37	0.89
2:O:248:ASN:HD22	2:O:248:ASN:C	1.81	0.88
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.39	0.86
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.91	0.86
9:V:64:LEU:HD12	9:V:77:ARG:O	1.75	0.86
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.85
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
5:E:127:VAL:HG12	5:E:128:LYS:H	1.40	0.85
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.57	0.85
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.58	0.84
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.42	0.84
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.60	0.84
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.43	0.84
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.60	0.84
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.05	0.83
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.78	0.82
3:P:238:THR:HB	3:P:239:PRO:HD3	1.61	0.82
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.62	0.82
2:B:248:ASN:C	2:B:248:ASN:HD22	1.85	0.82
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.82
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.62	0.81
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:HIS:HD2	3:C:12:LEU:H	1.26	0.81
2:B:27:THR:HG22	2:B:28:LYS:H	1.43	0.81
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.81
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.63	0.80
2:O:338:ARG:HG3	2:O:338:ARG:NH1	1.95	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.63	0.80
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.17	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	1.99	0.79
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.63	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79
2:B:338:ARG:HG3	2:B:338:ARG:NH1	1.98	0.78
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.48	0.78
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.98	0.78
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.66	0.78
1:N:10:ASN:HD21	2:O:18:CYS:N	1.81	0.78
1:A:178:THR:HB	1:A:181:ASP:OD1	1.83	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.66	0.78
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.66	0.77
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.66	0.77
1:N:143:ASN:HD22	9:V:48:PRO:HD3	1.50	0.77
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.66	0.77
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.67	0.77
2:B:31:ASN:H	2:B:31:ASN:ND2	1.83	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.82	0.77
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.48	0.77
2:B:76:THR:HG22	2:B:82:SER:N	1.99	0.76
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.76
3:P:216:SER:HB3	6:S:59:MET:HE2	1.66	0.76
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.65	0.76
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.19	0.76
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.67	0.76
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.67	0.76
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.21	0.76
2:O:76:THR:HG22	2:O:82:SER:N	1.99	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.66	0.75
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.51	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.68	0.74
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.52	0.74
2:O:399:ALA:O	2:O:402:ILE:HG22	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.68	0.74
9:V:35:UNK:HG3	9:V:36:UNK:N	2.01	0.74
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.69	0.74
5:E:84:GLY:N	5:E:102:THR:HG23	2.02	0.74
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.70	0.74
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.74
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.23	0.74
9:I:34:UNK:HG3	9:I:35:UNK:N	2.03	0.74
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.13	0.74
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.87	0.74
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.86	0.74
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.52	0.73
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.88	0.73
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.53	0.73
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.53	0.73
1:A:281:ASP:OD2	9:I:33:UNK:HB2	1.88	0.73
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.68	0.73
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.20	0.73
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.69	0.73
1:N:105:ASP:O	1:N:109:VAL:HG23	1.88	0.73
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.19	0.73
3:C:216:SER:HB3	6:F:59:MET:HE2	1.69	0.73
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.72	0.72
1:A:343:MET:HB3	1:A:444:ILE:HA	1.72	0.72
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.72	0.72
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.54	0.72
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.72
4:D:57:THR:HG22	4:D:59:ALA:N	2.04	0.72
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.72	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.88	0.72
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.89	0.72
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.71	0.72
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.24	0.72
2:O:217:LYS:O	2:O:221:GLU:HG2	1.90	0.72
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.14	0.71
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.90	0.71
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.91	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.03	0.71
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.55	0.71
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.71
2:B:31:ASN:H	2:B:31:ASN:HD22	1.37	0.71
2:B:38:LEU:HD12	2:B:39:GLU:N	2.06	0.71
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.25	0.71
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.71
1:A:103:SER:HB3	1:A:202:GLY:O	1.90	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.71
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.26	0.71
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.71
2:B:76:THR:CG2	2:B:82:SER:H	2.00	0.70
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.73	0.70
9:I:70:LEU:HD23	9:I:71:ASN:H	1.56	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.91	0.70
5:E:52:LYS:C	5:E:52:LYS:HD3	2.15	0.70
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.55	0.70
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.70
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.74	0.70
1:N:178:THR:HB	1:N:181:ASP:OD1	1.89	0.70
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.70
2:B:31:ASN:HD22	2:B:31:ASN:N	1.90	0.70
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.17	0.70
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.70
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.57	0.70
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.73	0.69
10:J:7:ARG:HB3	10:J:7:ARG:NH1	2.07	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.57	0.69
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.69
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.75	0.69
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.74	0.69
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
8:H:10:GLU:O	8:H:11:GLU:HG3	1.92	0.69
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.69
2:O:361:LYS:O	2:O:365:LYS:HG3	1.93	0.69
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.07	0.69
3:C:49:GLY:C	12:C:501:HEM:HAC	2.17	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.75	0.68
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
2:O:225:ASN:O	2:O:227:ARG:HG3	1.93	0.68
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:52:LYS:HD3	5:R:52:LYS:C	2.18	0.68
4:Q:164:ILE:O	4:Q:179:MET:HE2	1.93	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.24	0.68
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.73	0.68
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.59	0.68
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.23	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.94	0.68
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.29	0.68
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.23	0.68
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.75	0.68
1:A:106:MET:HE2	1:A:107:PRO:HA	1.76	0.68
4:D:231:LYS:O	6:F:71:LYS:HE3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.28	0.68
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.75	0.67
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.09	0.67
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.76	0.67
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.29	0.67
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.94	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.29	0.67
2:B:252:LEU:HD13	9:I:55:MET:HE3	1.77	0.67
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.67
3:P:49:GLY:C	12:P:501:HEM:HAC	2.19	0.67
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.67
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.95	0.67
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.76	0.66
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.66
1:A:350:THR:HG22	1:A:352:SER:H	1.60	0.66
3:P:101:ARG:C	3:P:101:ARG:HD2	2.20	0.66
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.25	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.76	0.66
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.77	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.76	0.66
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.77	0.66
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.77	0.66
5:E:106:ILE:C	5:E:110:ALA:HB3	2.20	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.10	0.66
2:O:252:LEU:HD13	9:V:55:MET:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.66
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.78	0.65
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.78	0.65
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.76	0.65
1:N:112:LEU:O	1:N:116:VAL:HG23	1.96	0.65
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.05	0.65
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.77	0.65
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.61	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
5:E:130:PRO:HG2	5:E:131:GLU:H	1.61	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.76	0.65
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.30	0.65
4:D:235:MET:HB3	7:G:15:THR:HG22	1.78	0.65
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.77	0.65
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.78	0.65
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.65
2:O:150:VAL:O	2:O:153:GLN:HG3	1.97	0.65
2:O:422:LYS:O	2:O:436:LEU:HD21	1.95	0.65
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.31	0.64
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.63	0.64
2:B:341:MET:HE2	2:B:341:MET:HA	1.79	0.64
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.78	0.64
2:B:270:ASN:H	2:B:270:ASN:ND2	1.94	0.64
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.79	0.64
6:S:53:ASP:OD1	6:S:54:LEU:N	2.30	0.64
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.12	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64
8:H:27:THR:O	8:H:31:VAL:HG23	1.97	0.64
1:N:269:VAL:HG22	1:N:406:MET:HE3	1.80	0.64
2:O:353:THR:HG22	2:O:355:GLU:N	2.00	0.64
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.64
4:D:164:ILE:O	4:D:179:MET:HE2	1.97	0.64
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.12	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.33	0.64
2:B:422:LYS:O	2:B:436:LEU:HD21	1.98	0.64
6:F:53:ASP:OD1	6:F:54:LEU:N	2.30	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.78	0.64
1:A:190:PHE:C	1:A:195:MET:HE2	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.13	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
1:N:282:ARG:NH2	9:V:37:UNK:N	2.45	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.62	0.64
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.64
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.28	0.63
3:C:247:SER:OG	3:C:250:LEU:HB2	1.99	0.63
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.79	0.63
8:H:28:GLU:O	8:H:32:LYS:HG3	1.97	0.63
1:N:143:ASN:HD22	9:V:48:PRO:CD	2.11	0.63
2:O:192:HIS:O	2:O:196:GLN:HG3	1.98	0.63
8:U:43:ARG:O	8:U:47:ARG:HG3	1.97	0.63
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.81	0.63
2:O:341:MET:HE2	2:O:341:MET:HA	1.79	0.63
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.63	0.63
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.80	0.63
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.63
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.80	0.63
7:T:79:ASN:O	7:T:80:ASP:HB2	1.97	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.80	0.63
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.80	0.63
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.63
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.81	0.63
2:B:341:MET:HA	2:B:341:MET:CE	2.29	0.62
1:N:15:ASN:O	1:N:26:ALA:HA	1.98	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.34	0.62
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.81	0.62
2:B:248:ASN:C	2:B:248:ASN:ND2	2.58	0.62
10:J:7:ARG:CB	10:J:7:ARG:HH11	2.11	0.62
1:N:269:VAL:CG2	1:N:406:MET:HE3	2.28	0.62
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.33	0.62
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.81	0.62
2:B:150:VAL:O	2:B:153:GLN:HG3	1.99	0.62
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.64	0.62
2:O:207:VAL:HG12	2:O:208:GLY:H	1.64	0.62
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.62
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.14	0.62
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.62
2:B:361:LYS:O	2:B:365:LYS:HG3	2.00	0.62
2:O:248:ASN:C	2:O:248:ASN:ND2	2.55	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.29	0.62
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.35	0.62
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.32	0.62
5:E:55:VAL:O	5:E:59:ILE:HG12	2.00	0.62
2:B:207:VAL:HG12	2:B:208:GLY:H	1.64	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.81	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.80	0.62
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.99	0.62
2:O:38:LEU:HD12	2:O:39:GLU:N	2.15	0.62
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.34	0.61
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.64	0.61
5:E:147:ILE:O	5:E:156:TYR:HA	1.99	0.61
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.24	0.61
2:B:62:ASN:O	2:B:65:THR:HG22	2.00	0.61
1:N:106:MET:O	1:N:110:VAL:HG23	2.00	0.61
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.30	0.61
2:B:201:SER:OG	2:B:228:SER:HA	1.99	0.61
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.82	0.61
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.81	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.00	0.61
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.83	0.61
3:C:37:LEU:O	3:C:41:CYS:HB2	2.01	0.61
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.00	0.61
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.28	0.61
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.60
8:U:28:GLU:O	8:U:32:LYS:HG3	2.01	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.01	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.36	0.60
1:A:402:VAL:HG22	1:A:406:MET:CE	2.32	0.60
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.17	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.02	0.60
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.83	0.60
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.00	0.60
1:N:106:MET:HE2	1:N:107:PRO:HA	1.83	0.60
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.84	0.60
1:N:170:THR:HG22	1:N:171:THR:N	2.16	0.60
9:I:31:UNK:C	9:I:73:PRO:HG2	2.31	0.60
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.84	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.17	0.60
2:B:192:HIS:O	2:B:196:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.31	0.60
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.17	0.60
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.01	0.60
2:O:341:MET:HA	2:O:341:MET:CE	2.31	0.60
1:A:402:VAL:HA	1:A:406:MET:HE2	1.83	0.60
2:B:202:ALA:HB3	2:B:229:GLY:O	2.02	0.60
10:W:7:ARG:CB	10:W:7:ARG:HH11	2.15	0.60
5:E:131:GLU:CD	5:E:131:GLU:H	2.10	0.59
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.32	0.59
2:O:402:ILE:C	2:O:402:ILE:HD13	2.27	0.59
2:O:156:GLN:HE22	9:V:77:ARG:C	2.09	0.59
2:O:221:GLU:C	2:O:223:PHE:H	2.10	0.59
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.59
1:A:15:ASN:O	1:A:26:ALA:HA	2.02	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.66	0.59
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.03	0.59
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.59
3:P:37:LEU:O	3:P:41:CYS:HB2	2.02	0.59
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.37	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.02	0.59
1:A:191:LYS:N	1:A:195:MET:HE2	2.17	0.59
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.59
2:B:264:VAL:HG23	2:B:316:TYR:C	2.28	0.59
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.59
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.03	0.59
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.36	0.59
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD2	2.02	0.58
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.83	0.58
1:N:190:PHE:C	1:N:195:MET:HE2	2.27	0.58
3:P:199:THR:HA	18:P:2010:BOG:O1	2.03	0.58
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.31	0.58
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.84	0.58
8:H:40:CYS:O	8:H:44:VAL:HG23	2.03	0.58
5:E:106:ILE:O	5:E:110:ALA:HB3	2.03	0.58
1:N:402:VAL:HA	1:N:406:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.84	0.58
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.38	0.58
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.17	0.58
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.69	0.58
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.32	0.58
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.70	0.58
9:I:70:LEU:HD23	9:I:71:ASN:N	2.19	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.84	0.58
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.18	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.66	0.58
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.85	0.58
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.19	0.58
2:O:372:VAL:HG12	2:O:372:VAL:O	2.02	0.58
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.86	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.19	0.58
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.85	0.58
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.69	0.58
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.34	0.58
5:E:163:SER:HA	5:E:174:GLY:HA3	1.86	0.58
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.58
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.18	0.57
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.86	0.57
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.57
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.44	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.67	0.57
2:B:372:VAL:HG12	2:B:372:VAL:O	2.04	0.57
1:N:173:ASN:O	1:N:177:LEU:HG	2.04	0.57
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.34	0.57
1:N:371:GLY:O	1:N:375:VAL:HG23	2.05	0.57
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.20	0.57
1:A:131:ARG:NH2	1:A:177:LEU:O	2.37	0.57
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.40	0.57
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.57
9:V:65:VAL:HG12	9:V:66:ALA:N	2.19	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.20	0.57
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.03	0.57
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.57
9:V:70:LEU:HD23	9:V:71:ASN:N	2.20	0.57
2:O:334:GLY:O	2:O:338:ARG:HG2	2.05	0.57
1:N:317:THR:HG23	1:N:318:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.87	0.57
2:O:318:ASP:O	2:O:319:SER:HB2	2.05	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57
5:R:163:SER:H	5:R:175:PRO:HD2	1.70	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.04	0.56
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.85	0.56
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.87	0.56
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.56
5:R:188:VAL:HG23	5:R:192:LEU:HB2	1.86	0.56
2:B:24:LEU:HD12	2:B:37:SER:O	2.05	0.56
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.40	0.56
2:O:407:SER:O	2:O:411:VAL:HG23	2.05	0.56
1:A:106:MET:HE2	1:A:106:MET:C	2.31	0.56
1:A:106:MET:O	1:A:110:VAL:HG23	2.04	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.67	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.56
3:P:9:HIS:CD2	3:P:12:LEU:H	2.15	0.56
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.87	0.56
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.70	0.56
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.71	0.56
2:B:225:ASN:O	2:B:227:ARG:N	2.38	0.56
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.69	0.56
5:E:187:PHE:C	5:E:189:GLY:H	2.13	0.56
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.88	0.56
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.20	0.56
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.87	0.56
6:F:84:GLU:H	6:F:84:GLU:CD	2.14	0.56
5:R:161:HIS:HB2	5:R:175:PRO:HG3	1.88	0.56
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.69	0.56
1:A:106:MET:HE2	1:A:107:PRO:CA	2.35	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.87	0.56
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.86	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.87	0.56
3:C:101:ARG:HD2	3:C:101:ARG:C	2.30	0.56
1:N:131:ARG:NH2	1:N:177:LEU:O	2.37	0.56
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.56
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.56
1:N:103:SER:HB3	1:N:202:GLY:O	2.06	0.56
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.87	0.55
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.88	0.55
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.89	0.55
3:P:40:VAL:HA	3:P:43:MET:HE3	1.88	0.55
5:R:73:LYS:HB3	5:R:196:GLY:O	2.05	0.55
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.55
1:A:7:THR:HG21	2:B:113:ARG:CD	2.32	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.07	0.55
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.89	0.55
10:W:49:GLY:N	10:W:54:HIS:ND1	2.54	0.55
5:E:116:LYS:HD2	5:E:116:LYS:N	2.22	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.36	0.55
1:N:130:GLU:O	1:N:134:ILE:HG13	2.07	0.55
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.25	0.55
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.41	0.55
2:O:207:VAL:HG12	2:O:208:GLY:N	2.22	0.55
1:A:365:MET:HE3	1:A:392:LEU:HD22	1.88	0.55
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.55
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.32	0.55
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.71	0.55
5:R:55:VAL:O	5:R:59:ILE:HG12	2.06	0.55
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.50	0.55
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.40	0.55
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.89	0.55
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.87	0.55
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.72	0.55
2:O:221:GLU:O	2:O:223:PHE:N	2.40	0.55
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.37	0.55
9:I:65:VAL:HG12	9:I:66:ALA:N	2.22	0.54
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.89	0.54
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.54
2:B:397:VAL:O	2:B:401:LYS:HG2	2.07	0.54
5:E:84:GLY:CA	5:E:102:THR:HG23	2.37	0.54
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.08	0.54
10:J:7:ARG:HB3	10:J:7:ARG:HH11	1.72	0.54
3:P:156:TYR:C	3:P:158:GLY:H	2.13	0.54
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.54
4:D:169:LEU:C	4:D:169:LEU:HD23	2.32	0.54
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.71	0.54
1:A:23:LEU:HD23	1:A:24:ARG:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
1:N:187:ASP:O	1:N:191:LYS:HE3	2.07	0.54
2:O:24:LEU:HD12	2:O:37:SER:O	2.08	0.54
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.54
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.43	0.54
2:B:96:LEU:H	9:I:70:LEU:HD22	1.72	0.54
2:O:59:THR:HG22	2:O:61:ALA:H	1.73	0.54
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.41	0.54
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.06	0.54
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.89	0.54
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.36	0.54
3:C:150:LEU:HB3	3:C:292:VAL:HG22	1.90	0.54
8:H:18:THR:O	8:H:22:GLU:HG3	2.08	0.54
1:N:106:MET:HE2	1:N:106:MET:C	2.32	0.54
2:O:140:LEU:O	2:O:143:GLN:HB3	2.07	0.54
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.43	0.54
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.08	0.54
1:N:295:ALA:O	1:N:299:VAL:HG23	2.08	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.06	0.54
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.90	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.54
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.38	0.54
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.72	0.54
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.08	0.54
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.33	0.54
2:O:31:ASN:H	2:O:31:ASN:ND2	2.04	0.54
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.08	0.54
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.07	0.54
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.43	0.54
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.44	0.53
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.08	0.53
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.23	0.53
1:N:49:ASN:ND2	1:N:51:LYS:H	2.04	0.53
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.88	0.53
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.89	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.53
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.38	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.09	0.53
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.43	0.53
3:P:121:LEU:O	3:P:125:MET:HG3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.89	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.89	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.89	0.53
5:R:77:LYS:HA	5:R:191:ASP:O	2.09	0.53
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.90	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
3:C:334:LEU:HD21	11:C:2007:PEE:H65	1.89	0.53
6:F:11:ARG:O	6:F:15:ARG:HG3	2.08	0.53
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.53
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.90	0.53
6:S:84:GLU:CD	6:S:84:GLU:H	2.16	0.53
4:D:47:ALA:HA	4:D:90:TYR:HA	1.90	0.53
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.91	0.53
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.90	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.42	0.53
5:E:83:GLU:C	5:E:85:LYS:H	2.16	0.53
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.53
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.91	0.53
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.53
4:D:102:ARG:HA	4:D:108:ALA:O	2.08	0.53
9:I:29:UNK:O	9:I:30:UNK:HB2	2.08	0.53
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.53
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.73	0.53
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.43	0.53
1:A:269:VAL:HG22	1:A:406:MET:HE3	1.92	0.52
5:R:162:GLY:O	5:R:163:SER:C	2.51	0.52
2:B:21:ALA:O	2:B:22:GLU:HB3	2.08	0.52
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.90	0.52
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.24	0.52
2:B:140:LEU:O	2:B:143:GLN:HB3	2.08	0.52
2:B:153:GLN:HE22	9:I:34:UNK:CG	2.22	0.52
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.09	0.52
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.27	0.52
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.92	0.52
6:F:13:MET:HA	6:F:13:MET:HE2	1.90	0.52
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.24	0.52
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.09	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
1:A:268:VAL:O	1:A:272:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.09	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.09	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.56	0.52
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.92	0.52
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.91	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
4:Q:240:PRO:O	4:Q:241:LYS:C	2.53	0.52
5:R:188:VAL:HG23	5:R:192:LEU:CB	2.40	0.52
6:S:40:ASP:O	6:S:44:LYS:HG3	2.10	0.52
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.45	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.92	0.52
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.10	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.67	0.52
5:R:178:TYR:N	5:R:178:TYR:CD1	2.78	0.52
8:U:18:THR:O	8:U:22:GLU:HG3	2.10	0.52
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.37	0.52
5:E:178:TYR:HD1	5:E:178:TYR:H	1.58	0.52
1:A:217:SER:O	1:A:218:GLY:C	2.53	0.52
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.75	0.52
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.90	0.51
2:B:27:THR:CG2	2:B:28:LYS:H	2.17	0.51
2:B:334:GLY:O	2:B:338:ARG:HG2	2.10	0.51
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.51
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.91	0.51
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.40	0.51
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.51
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.51
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.55	0.51
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.91	0.51
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.39	0.51
2:B:57:TYR:N	2:B:57:TYR:CD1	2.78	0.51
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.44	0.51
1:N:364:ALA:O	1:N:368:GLN:HG3	2.10	0.51
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.73	0.51
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.93	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
2:O:259:THR:CG2	2:O:260:GLU:N	2.74	0.51
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.51
3:C:216:SER:CB	6:F:59:MET:HE2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.74	0.51
8:U:22:GLU:O	8:U:26:GLN:HG2	2.10	0.51
9:V:70:LEU:HD23	9:V:71:ASN:H	1.74	0.51
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.91	0.51
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.93	0.51
2:B:76:THR:HG23	2:B:82:SER:HB2	1.92	0.51
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.50	0.51
5:E:187:PHE:C	5:E:189:GLY:N	2.68	0.51
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.26	0.51
2:O:156:GLN:NE2	9:V:77:ARG:C	2.68	0.51
3:P:138:GLN:HA	3:P:138:GLN:OE1	2.11	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.11	0.51
10:W:4:ALA:O	10:W:8:GLN:HG3	2.10	0.51
1:A:187:ASP:O	1:A:191:LYS:HE3	2.10	0.51
4:D:57:THR:HB	4:D:60:GLU:HG3	1.92	0.51
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
1:N:106:MET:HE2	1:N:107:PRO:CA	2.41	0.51
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.51
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.91	0.51
7:T:36:ASN:O	7:T:40:ARG:HG3	2.11	0.51
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.51
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.76	0.51
4:Q:2:GLU:O	4:Q:3:LEU:O	2.29	0.51
2:B:225:ASN:O	2:B:226:ILE:C	2.53	0.51
2:B:292:THR:HG22	2:B:292:THR:O	2.11	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.10	0.51
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.92	0.51
17:D:2003:CDL:H721	17:D:2003:CDL:HA61	1.93	0.51
5:E:155:GLY:HA3	5:E:166:ASP:O	2.11	0.51
9:I:64:LEU:HD12	9:I:77:ARG:O	2.11	0.51
2:O:164:HIS:O	2:O:173:ALA:HA	2.11	0.51
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.11	0.51
2:O:31:ASN:HB2	2:O:201:SER:OG	2.11	0.50
2:O:57:TYR:CD1	2:O:57:TYR:N	2.79	0.50
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.46	0.50
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.40	0.50
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.25	0.50
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.41	0.50
1:N:137:GLU:O	1:N:141:MET:HG3	2.10	0.50
1:N:191:LYS:N	1:N:195:MET:HE2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:122:TYR:O	2:O:126:VAL:HG23	2.10	0.50
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.75	0.50
3:P:350:ILE:O	3:P:354:MET:HG2	2.11	0.50
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.50
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.40	0.50
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.12	0.50
10:W:7:ARG:HB3	10:W:7:ARG:HH11	1.73	0.50
6:F:13:MET:HE2	6:F:16:ILE:HD12	1.92	0.50
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.50
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.36	0.50
3:P:313:GLN:HE21	6:S:36:THR:CB	2.24	0.50
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.50
2:B:28:LYS:O	2:B:29:LEU:O	2.29	0.50
2:B:156:GLN:HE22	9:I:77:ARG:C	2.20	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:332:HIS:O	2:B:336:VAL:HG23	2.12	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.47	0.50
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.93	0.50
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.93	0.50
2:B:104:LYS:HD2	2:B:104:LYS:C	2.37	0.50
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.41	0.50
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.94	0.50
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
2:O:52:LYS:O	2:O:203:ARG:NH2	2.35	0.50
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.93	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.93	0.50
2:B:338:ARG:NH1	2:B:338:ARG:CG	2.69	0.50
5:E:189:GLY:O	5:E:192:LEU:N	2.45	0.50
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.42	0.50
3:P:34:PHE:HB2	20:P:381:HOH:O	2.10	0.50
2:B:59:THR:HG22	2:B:61:ALA:H	1.75	0.50
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.42	0.50
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.50
3:C:313:GLN:HE21	6:F:36:THR:CB	2.25	0.50
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.32	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.23	0.50
1:N:281:ASP:O	1:N:283:THR:N	2.45	0.50
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.27	0.50
5:R:131:GLU:OE1	5:R:131:GLU:N	2.45	0.50
2:B:52:LYS:O	2:B:203:ARG:NH2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.35	0.50
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.50
1:N:280:TYR:CG	1:N:281:ASP:N	2.79	0.50
3:P:216:SER:CB	6:S:59:MET:HE2	2.40	0.50
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.72	0.50
3:C:286:PRO:O	3:C:287:ASN:HB2	2.12	0.49
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.94	0.49
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.94	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
2:O:286:LYS:C	2:O:288:GLY:H	2.20	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.12	0.49
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.94	0.49
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.94	0.49
5:E:165:TYR:HA	5:E:170:ARG:O	2.12	0.49
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.49
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.93	0.49
1:A:137:GLU:O	1:A:141:MET:HG3	2.12	0.49
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.49
1:N:382:HIS:HB3	1:N:388:ARG:O	2.12	0.49
5:R:97:PHE:O	5:R:134:ILE:HA	2.13	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.51	0.49
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.48	0.49
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.40	0.49
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.48	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.11	0.49
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.12	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.93	0.49
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.27	0.49
1:A:49:ASN:ND2	1:A:51:LYS:H	2.10	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.12	0.49
1:A:371:GLY:O	1:A:375:VAL:HG23	2.12	0.49
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.48	0.49
4:D:169:LEU:HD23	4:D:169:LEU:O	2.11	0.49
3:P:334:LEU:HD21	11:P:3007:PEE:H65	1.93	0.49
4:Q:79:GLU:OE2	4:Q:79:GLU:HA	2.13	0.49
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.95	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.71	0.49
3:P:263:LEU:O	3:P:264:VAL:CG2	2.61	0.49
3:P:286:PRO:O	3:P:287:ASN:HB2	2.13	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.95	0.49
5:E:97:PHE:O	5:E:134:ILE:HA	2.12	0.49
5:E:188:VAL:HG12	5:E:188:VAL:O	2.12	0.49
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.49
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.93	0.49
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.49
5:R:177:PRO:HG2	5:R:178:TYR:H	1.77	0.49
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.95	0.49
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.95	0.49
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.49
5:R:118:ARG:NH1	5:R:174:GLY:O	2.45	0.49
5:R:179:ASN:O	5:R:180:LEU:C	2.56	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.11	0.49
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.48	0.49
3:C:50:LEU:O	3:C:54:MET:HG3	2.12	0.49
2:O:54:GLY:C	2:O:56:ARG:H	2.20	0.49
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.13	0.49
2:B:27:THR:CG2	2:B:28:LYS:N	2.74	0.49
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.78	0.49
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.48	0.49
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.49
2:O:292:THR:HG22	2:O:292:THR:O	2.13	0.49
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.49
2:B:164:HIS:O	2:B:173:ALA:HA	2.13	0.48
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.48
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.48
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.13	0.48
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.94	0.48
2:O:59:THR:HG22	2:O:60:THR:N	2.27	0.48
3:P:125:MET:HE2	3:P:275:PHE:CE2	2.48	0.48
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.31	0.48
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.43	0.48
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.48
4:Q:1:GLY:O	4:Q:2:GLU:HB2	2.13	0.48
4:D:171:TYR:OH	4:D:182:ILE:HA	2.13	0.48
5:E:73:LYS:HB3	5:E:196:GLY:O	2.12	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.94	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:402:ILE:HG23	2:O:403:ASP:N	2.28	0.48
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.48	0.48
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.13	0.48
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.96	0.48
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.28	0.48
4:D:57:THR:CG2	4:D:58:GLU:N	2.75	0.48
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.93	0.48
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.13	0.48
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.94	0.48
9:I:34:UNK:CG	9:I:35:UNK:N	2.76	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.32	0.48
3:P:263:LEU:O	3:P:264:VAL:HG23	2.13	0.48
5:R:78:LEU:HD11	5:R:187:PHE:HD1	1.77	0.48
5:R:155:GLY:HA3	5:R:166:ASP:O	2.13	0.48
5:R:186:GLN:O	5:R:193:VAL:HG23	2.14	0.48
1:A:27:SER:HA	1:A:199:ALA:O	2.13	0.48
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.48	0.48
5:E:178:TYR:N	5:E:178:TYR:CD1	2.82	0.48
3:P:263:LEU:C	3:P:264:VAL:HG23	2.39	0.48
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.96	0.48
5:R:170:ARG:HA	5:R:179:ASN:CB	2.39	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.94	0.48
2:O:31:ASN:N	2:O:31:ASN:ND2	2.58	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.47	0.48
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.79	0.48
2:B:264:VAL:HG23	2:B:316:TYR:O	2.13	0.48
5:E:189:GLY:O	5:E:192:LEU:O	2.32	0.48
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.95	0.48
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.43	0.48
3:P:279:TYR:O	3:P:282:LEU:HB3	2.14	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.48
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.76	0.48
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.48
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.79	0.48
1:N:365:MET:HE3	1:N:392:LEU:HD22	1.96	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.48	0.48
1:A:223:TYR:H	1:A:223:TYR:HD2	1.60	0.48
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.48
2:B:54:GLY:C	2:B:56:ARG:H	2.21	0.48
2:B:353:THR:HG22	2:B:354:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.48
3:P:30:ALA:HB1	17:Q:3003:CDL:H111	1.95	0.48
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.96	0.48
7:T:65:GLU:O	7:T:69:LEU:HG	2.13	0.48
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.94	0.48
5:E:77:LYS:HA	5:E:192:LEU:HD23	1.96	0.48
1:N:45:SER:HA	1:N:48:GLU:HG3	1.95	0.48
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.95	0.48
1:A:358:LYS:HE3	1:A:399:ILE:O	2.14	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47
5:E:162:GLY:O	5:E:163:SER:C	2.57	0.47
10:J:40:ASP:O	10:J:44:GLU:HG3	2.14	0.47
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.44	0.47
8:U:65:ARG:O	8:U:68:CYS:HB3	2.14	0.47
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.47	0.47
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.95	0.47
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.74	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.37	0.47
1:N:358:LYS:HE3	1:N:399:ILE:O	2.14	0.47
5:R:178:TYR:N	5:R:178:TYR:HD1	2.12	0.47
6:S:95:LYS:O	6:S:99:ARG:HG3	2.14	0.47
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.50	0.47
2:B:28:LYS:O	2:B:28:LYS:HG2	2.14	0.47
3:C:121:LEU:O	3:C:125:MET:HG3	2.14	0.47
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.47
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.49	0.47
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.31	0.47
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.28	0.47
2:O:227:ARG:HB3	2:O:228:SER:H	1.52	0.47
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.47
3:P:92:PHE:O	3:P:95:ILE:HG22	2.14	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.79	0.47
2:B:215:ASP:O	2:B:219:VAL:HG23	2.15	0.47
5:E:130:PRO:C	5:E:132:TRP:H	2.21	0.47
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.49	0.47
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.96	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.79	0.47
4:Q:222:MET:HE3	5:R:40:THR:OG1	2.14	0.47
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.33	0.47
3:C:92:PHE:O	3:C:95:ILE:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.97	0.47
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.49	0.47
1:N:320:PHE:CE2	1:N:415:ILE:HD11	2.49	0.47
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.14	0.47
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.75	0.47
2:B:259:THR:CG2	2:B:260:GLU:N	2.77	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.50	0.47
5:E:127:VAL:O	5:E:128:LYS:HB2	2.15	0.47
2:O:76:THR:HG23	2:O:82:SER:HB2	1.97	0.47
2:O:303:THR:HA	2:O:335:GLU:OE1	2.15	0.47
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.50	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.50	0.47
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.96	0.47
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.96	0.47
5:R:185:TYR:O	5:R:186:GLN:HB3	2.14	0.47
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.15	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.30	0.47
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.47
2:O:385:GLU:O	2:O:389:SER:HB3	2.14	0.47
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.47
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.95	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.45	0.47
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.15	0.47
4:D:208:MET:O	4:D:212:SER:HB2	2.15	0.47
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.50	0.47
8:U:34:ARG:O	8:U:38:GLU:HG3	2.15	0.47
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.80	0.47
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.50	0.47
4:D:235:MET:CB	7:G:15:THR:HG22	2.45	0.47
1:N:205:HIS:O	1:N:208:LEU:HB3	2.15	0.47
3:P:50:LEU:O	3:P:54:MET:HG3	2.15	0.47
5:R:84:GLY:O	5:R:85:LYS:HD3	2.14	0.47
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.42	0.47
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.97	0.46
7:G:36:ASN:O	7:G:40:ARG:HG3	2.15	0.46
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.46
3:P:156:TYR:CD2	3:P:156:TYR:N	2.80	0.46
3:P:238:THR:HB	3:P:239:PRO:CD	2.40	0.46
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.46	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.29	0.46
5:E:75:GLU:HG3	5:E:75:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.46
2:O:332:HIS:O	2:O:336:VAL:HG23	2.15	0.46
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.97	0.46
1:A:269:VAL:CG2	1:A:406:MET:HE3	2.45	0.46
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.15	0.46
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.45	0.46
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.79	0.46
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.15	0.46
2:B:402:ILE:O	2:B:405:VAL:HG23	2.16	0.46
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.49	0.46
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.44	0.46
5:R:83:GLU:CD	5:R:102:THR:HA	2.40	0.46
10:W:32:GLU:HG2	10:W:36:ASP:OD2	2.15	0.46
2:B:24:LEU:HG	2:B:24:LEU:O	2.16	0.46
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.46
2:B:355:GLU:CD	2:B:359:LYS:HE3	2.41	0.46
9:I:71:ASN:H	9:I:71:ASN:HD22	1.64	0.46
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.46
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.81	0.46
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.41	0.46
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.46	0.46
2:B:411:VAL:O	2:B:415:LYS:HG3	2.15	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
1:N:158:PHE:O	1:N:164:ALA:HB2	2.15	0.46
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.46
1:N:282:ARG:NH2	9:V:36:UNK:HA	2.24	0.46
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.35	0.46
4:Q:3:LEU:N	4:Q:3:LEU:HD12	2.31	0.46
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.16	0.46
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.16	0.46
2:B:385:GLU:O	2:B:387:LEU:N	2.49	0.46
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.97	0.46
5:E:91:TRP:HZ2	5:E:196:GLY:HA2	1.80	0.46
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
2:B:274:VAL:O	2:B:278:VAL:HG23	2.15	0.46
2:B:385:GLU:C	2:B:387:LEU:H	2.24	0.46
3:C:279:TYR:O	3:C:282:LEU:HB3	2.16	0.46
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.14	0.46
1:N:27:SER:HA	1:N:199:ALA:O	2.16	0.46
2:O:110:GLU:O	2:O:111:CYS:HB3	2.15	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:22:GLY:O	1:N:193:PRO:HA	2.15	0.46
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.46
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.98	0.46
5:R:106:ILE:HG21	5:R:130:PRO:HB3	1.97	0.46
1:A:26:ALA:O	1:A:198:ALA:HA	2.16	0.46
1:A:239:SER:HB2	7:G:17:SER:O	2.16	0.46
3:C:138:GLN:HB2	3:C:255:GLU:O	2.16	0.46
5:E:102:THR:C	5:E:103:GLN:HG3	2.41	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
5:E:179:ASN:O	5:E:180:LEU:C	2.57	0.46
5:E:191:ASP:OD2	5:E:191:ASP:N	2.48	0.46
3:P:377:MET:HE2	6:S:20:TYR:CG	2.51	0.46
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.46
5:R:76:ILE:O	5:R:193:VAL:HG12	2.16	0.46
5:R:137:GLY:O	5:R:145:VAL:HG13	2.15	0.46
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.45
1:N:383:LEU:O	1:N:387:GLY:HA2	2.16	0.45
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.98	0.45
2:O:353:THR:HG22	2:O:354:GLU:N	2.31	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.45
5:R:75:GLU:O	5:R:75:GLU:HG3	2.15	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.15	0.45
6:S:16:ILE:O	6:S:19:TRP:HB3	2.16	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
1:A:49:ASN:HD21	1:A:51:LYS:CE	2.28	0.45
2:B:22:GLU:O	2:B:23:ASP:CG	2.59	0.45
2:O:225:ASN:C	2:O:227:ARG:HG3	2.41	0.45
5:R:96:LEU:HD12	5:R:135:LEU:O	2.16	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.45
6:S:10:GLY:C	6:S:12:LEU:H	2.24	0.45
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.81	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.45
3:C:272:GLU:O	3:C:273:TRP:C	2.59	0.45
4:D:102:ARG:HG2	4:D:102:ARG:NH1	2.31	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.16	0.45
1:N:223:TYR:H	1:N:223:TYR:HD2	1.64	0.45
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.79	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45
5:R:188:VAL:O	5:R:192:LEU:HB2	2.16	0.45
10:W:59:TYR:N	10:W:59:TYR:CD1	2.84	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
1:N:240:GLU:HA	1:N:422:LEU:O	2.17	0.45
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.80	0.45
5:R:77:LYS:HA	5:R:192:LEU:HD23	1.97	0.45
5:R:184:THR:O	5:R:185:TYR:HB3	2.16	0.45
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.49	0.45
1:A:178:THR:HG22	1:A:179:ARG:N	2.31	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.16	0.45
7:G:81:GLN:OXT	7:G:81:GLN:HG3	2.17	0.45
1:N:48:GLU:CD	1:N:54:GLY:H	2.24	0.45
2:O:169:LYS:O	2:O:170:THR:HG23	2.15	0.45
2:O:221:GLU:C	2:O:223:PHE:N	2.74	0.45
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.82	0.45
3:P:18:SER:CB	3:P:202:HIS:HE1	2.30	0.45
1:A:382:HIS:HB3	1:A:388:ARG:O	2.17	0.45
2:B:86:THR:O	2:B:90:GLU:HG3	2.17	0.45
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.52	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
2:O:403:ASP:C	2:O:405:VAL:H	2.24	0.45
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.81	0.45
2:B:303:THR:HA	2:B:335:GLU:OE1	2.17	0.45
5:E:84:GLY:N	5:E:100:HIS:O	2.44	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.99	0.45
7:G:28:ASN:HB3	7:G:31:SER:OG	2.17	0.45
1:N:26:ALA:O	1:N:198:ALA:HA	2.17	0.45
1:N:49:ASN:HD21	1:N:51:LYS:CE	2.30	0.45
1:N:143:ASN:ND2	9:V:48:PRO:HD3	2.25	0.45
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.46	0.45
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.99	0.45
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.32	0.45
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.45
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.97	0.45
6:F:40:ASP:O	6:F:44:LYS:HG3	2.17	0.45
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.99	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.99	0.45
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.45
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.99	0.45
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.98	0.45
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.17	0.45
2:B:38:LEU:HD12	2:B:38:LEU:C	2.41	0.45
3:C:377:MET:HE2	6:F:20:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:GLY:O	5:E:145:VAL:HG13	2.16	0.45
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.32	0.45
3:C:263:LEU:C	3:C:264:VAL:HG23	2.41	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
3:P:376:LYS:O	6:S:17:ARG:NH1	2.47	0.45
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.46	0.44
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.99	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.44
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.83	0.44
10:J:32:GLU:HG2	10:J:36:ASP:OD2	2.17	0.44
5:R:161:HIS:CB	5:R:175:PRO:HG3	2.47	0.44
5:R:169:GLY:O	5:R:179:ASN:HB3	2.17	0.44
1:A:205:HIS:O	1:A:208:LEU:HB3	2.18	0.44
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.44
5:E:127:VAL:CG1	5:E:128:LYS:H	2.13	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.85	0.44
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.99	0.44
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.82	0.44
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.82	0.44
2:O:54:GLY:C	2:O:56:ARG:N	2.73	0.44
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.44
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.44
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.44
2:O:26:ILE:O	2:O:26:ILE:HG12	2.16	0.44
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.44
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.43	0.44
5:R:171:ILE:HG12	5:R:176:ALA:O	2.18	0.44
2:B:295:LEU:O	2:B:299:VAL:HG23	2.18	0.44
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.81	0.44
1:N:439:SER:C	1:N:441:MET:H	2.26	0.44
2:O:225:ASN:O	2:O:226:ILE:C	2.60	0.44
17:Q:3003:CDL:HA61	17:Q:3003:CDL:H721	1.99	0.44
2:B:170:THR:O	2:B:172:LEU:N	2.50	0.44
3:C:286:PRO:O	3:C:287:ASN:CB	2.65	0.44
5:E:52:LYS:C	5:E:52:LYS:CD	2.87	0.44
1:N:438:ARG:HG3	1:N:438:ARG:HH11	1.83	0.44
3:P:275:PHE:HB3	13:P:3001:AZO:C11	2.48	0.44
2:B:399:ALA:C	2:B:402:ILE:HG22	2.43	0.44
8:H:10:GLU:C	8:H:11:GLU:HG3	2.43	0.44
1:N:402:VAL:HA	1:N:406:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
2:O:411:VAL:O	2:O:415:LYS:HG3	2.18	0.44
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.82	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.53	0.44
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.16	0.44
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.53	0.44
9:V:33:UNK:HA	9:V:73:PRO:HB3	2.00	0.44
1:A:402:VAL:HA	1:A:406:MET:CE	2.46	0.44
2:B:333:ALA:O	2:B:337:ILE:HG13	2.18	0.44
2:O:104:LYS:HD2	2:O:104:LYS:C	2.43	0.44
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.43
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.33	0.43
3:C:106:GLY:HA2	3:C:108:TYR:CZ	2.53	0.43
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.53	0.43
5:E:96:LEU:HD12	5:E:135:LEU:O	2.18	0.43
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.83	0.43
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.53	0.43
5:E:133:VAL:O	5:E:133:VAL:HG13	2.18	0.43
8:H:34:ARG:O	8:H:38:GLU:HG3	2.18	0.43
10:J:52:TRP:O	10:J:53:LYS:C	2.61	0.43
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.53	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.46	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
3:P:101:ARG:C	3:P:101:ARG:CD	2.88	0.43
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	2.00	0.43
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.18	0.43
1:A:217:SER:O	1:A:219:VAL:HG23	2.18	0.43
3:C:49:GLY:O	12:C:501:HEM:HAC	2.17	0.43
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.48	0.43
1:N:239:SER:HB2	7:T:17:SER:O	2.18	0.43
2:O:341:MET:HE2	2:O:341:MET:CA	2.48	0.43
5:R:103:GLN:O	5:R:107:ASN:ND2	2.51	0.43
6:S:82:LYS:O	6:S:83:TYR:C	2.60	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.18	0.43
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.53	0.43
3:C:153:ALA:CB	3:C:288:LYS:HG2	2.49	0.43
2:O:371:SER:C	2:O:372:VAL:HG23	2.43	0.43
3:P:286:PRO:O	3:P:287:ASN:CB	2.66	0.43
2:B:68:LEU:HD23	2:B:186:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ALA:O	2:B:224:LEU:HB2	2.18	0.43
2:B:286:LYS:C	2:B:288:GLY:N	2.77	0.43
2:B:403:ASP:C	2:B:405:VAL:H	2.26	0.43
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.00	0.43
1:N:134:ILE:HG22	1:N:174:ILE:HD13	2.00	0.43
3:P:101:ARG:HD2	3:P:101:ARG:O	2.18	0.43
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.43
2:B:33:LEU:HD12	2:B:204:MET:O	2.19	0.43
2:B:46:ARG:HD2	2:B:110:GLU:HG2	2.00	0.43
1:N:362:ARG:O	1:N:365:MET:HG2	2.18	0.43
2:O:33:LEU:HD12	2:O:204:MET:O	2.17	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
1:A:48:GLU:CD	1:A:54:GLY:H	2.26	0.43
2:B:167:ALA:C	2:B:168:TYR:CD1	2.96	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.00	0.43
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.34	0.43
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.83	0.43
1:A:274:ASN:ND2	1:A:309:THR:HB	2.34	0.43
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.43
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.48	0.43
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.43
2:O:222:GLN:O	2:O:222:GLN:HG2	2.19	0.43
5:R:79:SER:OG	5:R:191:ASP:HB2	2.18	0.43
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.00	0.43
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.41	0.43
3:C:125:MET:HE2	3:C:275:PHE:CE2	2.54	0.43
9:I:39:UNK:HA	9:V:40:UNK:O	2.19	0.43
1:N:178:THR:HG22	1:N:179:ARG:N	2.33	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.34	0.43
1:A:21:ASN:OD1	1:A:21:ASN:N	2.49	0.43
2:B:297:GLN:O	2:B:301:LYS:HG3	2.18	0.43
4:D:227:TRP:O	4:D:228:SER:C	2.59	0.43
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.34	0.43
2:O:141:GLN:N	2:O:142:PRO:HD2	2.34	0.43
2:O:286:LYS:C	2:O:288:GLY:N	2.74	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.43
1:A:418:LYS:O	1:A:420:PRO:HD3	2.19	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.84	0.43
2:B:286:LYS:C	2:B:288:GLY:H	2.26	0.43
4:D:161:ALA:O	4:D:162:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.48	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.18	0.43
4:Q:235:MET:CB	7:T:15:THR:HG22	2.45	0.43
5:R:133:VAL:O	5:R:133:VAL:HG13	2.19	0.43
8:U:21:ARG:HD2	8:U:65:ARG:NH1	2.33	0.43
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.01	0.42
2:B:209:ILE:HG22	2:B:210:GLY:N	2.34	0.42
2:B:395:PRO:O	2:B:398:VAL:CG1	2.67	0.42
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.84	0.42
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.42
2:O:399:ALA:C	2:O:402:ILE:HG22	2.43	0.42
2:O:402:ILE:HG23	2:O:403:ASP:H	1.84	0.42
5:R:184:THR:HG22	5:R:185:TYR:N	2.34	0.42
2:B:399:ALA:O	2:B:402:ILE:CG2	2.63	0.42
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.42
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.62	0.42
2:O:18:CYS:CB	2:O:19:PRO:CD	2.97	0.42
2:O:141:GLN:C	2:O:143:GLN:N	2.77	0.42
3:P:345:GLU:C	3:P:349:ILE:HG13	2.44	0.42
1:A:119:ASN:O	1:A:120:CYS:C	2.61	0.42
4:D:105:ASN:O	4:D:106:ASN:HB2	2.18	0.42
5:E:77:LYS:HG3	5:E:191:ASP:O	2.18	0.42
5:E:151:GLY:O	5:E:154:GLY:N	2.52	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.53	0.42
5:E:171:ILE:O	5:E:171:ILE:HG23	2.18	0.42
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.42
8:U:65:ARG:O	8:U:69:VAL:HG23	2.20	0.42
2:B:385:GLU:C	2:B:387:LEU:N	2.78	0.42
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.84	0.42
17:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.52	0.42
1:N:271:HIS:CE1	1:N:311:ASN:HD22	2.37	0.42
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.84	0.42
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.54	0.42
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.19	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42
6:S:98:ILE:O	6:S:102:LEU:HG	2.20	0.42
1:A:143:ASN:HB2	9:I:48:PRO:HD2	2.01	0.42
2:B:353:THR:CG2	2:B:354:GLU:N	2.82	0.42
1:N:351:GLU:O	1:N:355:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:129:PHE:CE1	13:P:3001:AZO:H223	2.55	0.42
4:Q:169:LEU:HD23	4:Q:169:LEU:O	2.20	0.42
5:R:74:ILE:HG22	5:R:91:TRP:CD1	2.54	0.42
1:A:23:LEU:HD23	1:A:23:LEU:C	2.44	0.42
1:A:140:GLU:OE2	9:I:50:LEU:N	2.39	0.42
4:D:186:VAL:O	4:D:190:LEU:HG	2.19	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
8:H:50:THR:HG23	8:H:50:THR:O	2.19	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.82	0.42
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.01	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.72	0.42
2:O:385:GLU:C	2:O:387:LEU:H	2.28	0.42
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	2.01	0.42
4:Q:227:TRP:O	4:Q:228:SER:C	2.61	0.42
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.50	0.42
4:D:211:ILE:HD13	4:D:211:ILE:HA	1.89	0.42
1:N:270:LEU:HD23	1:N:270:LEU:HA	1.88	0.42
3:P:240:PHE:C	3:P:240:PHE:CD2	2.97	0.42
1:A:206:LYS:HA	1:A:209:VAL:HG12	2.01	0.42
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.27	0.42
2:B:26:ILE:O	2:B:26:ILE:HG12	2.20	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.00	0.42
5:E:161:HIS:HB2	19:E:501:FES:S1	2.60	0.42
2:O:399:ALA:HA	2:O:402:ILE:HG22	2.01	0.42
3:P:70:THR:O	3:P:77:GLY:HA3	2.20	0.42
4:Q:167:GLU:C	4:Q:169:LEU:H	2.27	0.42
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.37	0.42
10:W:38:GLY:O	10:W:41:ALA:HB3	2.19	0.42
1:A:240:GLU:HA	1:A:422:LEU:O	2.20	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.55	0.42
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.42
1:N:119:ASN:O	1:N:120:CYS:C	2.62	0.42
2:O:54:GLY:O	2:O:56:ARG:N	2.53	0.42
3:P:288:LYS:O	3:P:292:VAL:HG23	2.19	0.42
4:Q:41:HIS:CE1	4:Q:110:PRO:HB2	2.54	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
2:B:50:PHE:N	2:B:50:PHE:CD1	2.88	0.42
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.02	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
1:N:51:LYS:HE3	1:N:51:LYS:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.35	0.42
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.35	0.42
4:Q:167:GLU:C	4:Q:169:LEU:N	2.76	0.42
2:B:169:LYS:O	2:B:170:THR:HG23	2.19	0.41
2:B:246:GLU:HB3	2:B:427:SER:HB3	2.01	0.41
3:C:151:PHE:C	3:C:153:ALA:H	2.28	0.41
5:E:114:VAL:O	5:E:115:SER:C	2.62	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
1:N:418:LYS:O	1:N:420:PRO:HD3	2.20	0.41
2:O:67:HIS:O	2:O:70:ARG:HB3	2.19	0.41
6:S:89:TYR:CD1	6:S:89:TYR:C	2.98	0.41
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.85	0.41
1:A:89:TYR:CD1	1:A:89:TYR:C	2.97	0.41
1:A:106:MET:HE2	1:A:107:PRO:N	2.35	0.41
1:A:271:HIS:CE1	1:A:311:ASN:HD22	2.38	0.41
1:A:281:ASP:O	1:A:283:THR:N	2.53	0.41
1:A:373:THR:HB	1:A:374:PRO:CD	2.50	0.41
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.50	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.53	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HB2	2.01	0.41
5:E:117:LEU:HD23	5:E:119:ASP:O	2.20	0.41
3:P:151:PHE:C	3:P:153:ALA:H	2.28	0.41
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.50	0.41
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.51	0.41
2:B:59:THR:CG2	2:B:60:THR:N	2.83	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.71	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.46	0.41
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.02	0.41
6:S:13:MET:HA	6:S:16:ILE:HD12	2.02	0.41
9:V:69:SER:HB2	9:V:72:ALA:H	1.84	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.54	0.41
2:B:361:LYS:HD3	2:B:403:ASP:HA	2.02	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.03	0.41
5:E:189:GLY:O	5:E:190:ASP:C	2.64	0.41
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.20	0.41
1:N:117:VAL:HG23	1:N:118:GLN:HG3	2.03	0.41
9:V:35:UNK:CG	9:V:36:UNK:N	2.75	0.41
1:A:295:ALA:O	1:A:299:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.41
4:D:68:VAL:HG11	4:D:92:PRO:HG3	2.03	0.41
5:E:185:TYR:O	5:E:186:GLN:HB3	2.21	0.41
1:N:90:THR:O	1:N:167:VAL:HG11	2.21	0.41
1:N:163:LEU:HD23	1:N:163:LEU:HA	1.93	0.41
2:O:37:SER:CB	2:O:213:HIS:ND1	2.68	0.41
5:R:185:TYR:N	5:R:185:TYR:CD2	2.88	0.41
2:B:29:LEU:HD12	2:B:33:LEU:HD23	2.02	0.41
3:C:242:THR:O	3:C:246:PHE:HB2	2.20	0.41
8:H:21:ARG:HD2	8:H:65:ARG:NH1	2.36	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.20	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.21	0.41
3:P:49:GLY:O	12:P:501:HEM:HAC	2.20	0.41
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.55	0.41
5:R:161:HIS:HB2	19:R:501:FES:S1	2.61	0.41
7:T:34:LEU:O	7:T:35:PRO:C	2.63	0.41
9:V:32:UNK:N	9:V:73:PRO:HG2	2.36	0.41
1:A:106:MET:N	1:A:107:PRO:HD2	2.35	0.41
1:A:279:ARG:HH22	9:I:30:UNK:C	2.33	0.41
7:G:2:ILE:HG22	7:G:6:ASN:HD21	1.86	0.41
1:N:47:TYR:CZ	1:N:231:LEU:HD11	2.55	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
2:O:227:ARG:O	2:O:228:SER:O	2.39	0.41
3:P:41:CYS:SG	3:P:90:PHE:HD2	2.44	0.41
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.21	0.41
5:R:75:GLU:HB3	5:R:194:VAL:HG22	2.01	0.41
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.51	0.41
3:C:139:MET:HE3	3:C:253:ASP:OD2	2.19	0.41
3:C:240:PHE:CD2	3:C:240:PHE:C	2.98	0.41
4:D:220:TYR:O	4:D:224:ARG:HG2	2.20	0.41
5:E:119:ASP:O	5:E:121:GLN:N	2.53	0.41
5:E:125:ASP:C	5:E:126:ARG:HG3	2.46	0.41
6:F:89:TYR:CD1	6:F:89:TYR:C	2.98	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:205:HIS:O	1:N:209:VAL:HG12	2.20	0.41
1:N:342:TRP:O	1:N:345:LEU:HB2	2.20	0.41
2:O:98:VAL:HA	2:O:106:THR:O	2.21	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.63	0.41
3:P:141:PHE:HE1	3:P:171:VAL:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:165:TYR:CZ	4:Q:168:ILE:HG13	2.56	0.41
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.50	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.65	0.41
1:A:351:GLU:O	1:A:355:LYS:HB2	2.20	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.51	0.41
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.36	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
8:H:39:LEU:O	8:H:42:ALA:HB3	2.20	0.41
1:N:106:MET:HE2	1:N:107:PRO:N	2.35	0.41
1:N:268:VAL:O	1:N:272:VAL:HG23	2.21	0.41
2:O:306:PRO:HA	9:V:52:ARG:CG	2.50	0.41
2:O:417:PHE:CD2	2:O:417:PHE:C	2.98	0.41
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.20	0.41
5:R:185:TYR:N	5:R:185:TYR:HD2	2.19	0.41
6:S:17:ARG:HG2	6:S:17:ARG:NH1	2.35	0.41
6:S:104:ARG:O	6:S:105:GLU:C	2.64	0.41
1:A:403:ASP:O	1:A:404:ALA:C	2.63	0.41
1:A:422:LEU:HD22	1:A:437:ILE:HD13	2.03	0.41
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.03	0.41
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.35	0.41
5:E:75:GLU:HA	5:E:193:VAL:O	2.21	0.41
1:N:4:TYR:HE2	1:N:396:ASP:OD2	2.04	0.41
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.50	0.41
2:O:43:PRO:O	2:O:113:ARG:HG3	2.21	0.41
2:O:412:ASN:O	2:O:413:ALA:C	2.64	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.52	0.41
6:S:71:LYS:O	6:S:72:HIS:HB2	2.21	0.41
1:A:106:MET:CE	1:A:110:VAL:HG21	2.50	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.82	0.40
3:C:19:LEU:C	3:C:20:ILE:HG13	2.45	0.40
4:D:116:ILE:HG12	16:D:501:HEC:HMA3	2.03	0.40
2:O:209:ILE:HG22	2:O:210:GLY:N	2.36	0.40
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.03	0.40
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.51	0.40
2:B:141:GLN:N	2:B:142:PRO:HD2	2.35	0.40
4:D:158:ILE:HG12	4:D:160:MET:H	1.86	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.85	0.40
2:O:150:VAL:CG2	2:O:151:ALA:N	2.84	0.40
3:P:287:ASN:O	3:P:288:LYS:C	2.63	0.40
1:A:270:LEU:O	1:A:273:ALA:HB3	2.20	0.40
2:B:437:ASP:OD1	2:B:437:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:TRP:HE1	17:G:2004:CDL:H1	1.87	0.40
3:C:377:MET:HE1	6:F:19:TRP:HZ3	1.85	0.40
5:E:172:ARG:HB2	5:E:173:LYS:H	1.74	0.40
2:O:297:GLN:O	2:O:301:LYS:HG3	2.21	0.40
3:P:81:ARG:HD3	3:P:81:ARG:C	2.47	0.40
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.40
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.56	0.40
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.54	0.40
1:A:51:LYS:HE3	1:A:51:LYS:HB2	1.89	0.40
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.86	0.40
1:A:383:LEU:O	1:A:387:GLY:HA2	2.22	0.40
3:C:30:ALA:HB1	17:D:2003:CDL:H111	2.02	0.40
4:D:197:GLU:O	4:D:198:HIS:C	2.63	0.40
5:E:101:ARG:NH2	5:E:130:PRO:O	2.55	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.04	0.40
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.56	0.40
2:O:246:GLU:HB3	2:O:427:SER:HB3	2.02	0.40
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.69	0.40
16:Q:501:HEC:CMB	16:Q:501:HEC:HBB3	2.51	0.40
5:R:141:HIS:HB3	19:R:501:FES:S2	2.62	0.40
2:B:206:LEU:HG	2:B:206:LEU:O	2.22	0.40
7:G:29:ILE:HA	7:G:33:ALA:HB3	2.04	0.40
1:N:233:ARG:NH2	1:N:316:ASP:O	2.53	0.40
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/446 (99%)	411 (93%)	25 (6%)	6 (1%)	9 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	440/446 (99%)	408 (93%)	25 (6%)	7 (2%)	7	16
2	B	418/441 (95%)	353 (84%)	50 (12%)	15 (4%)	2	5
2	O	420/441 (95%)	364 (87%)	42 (10%)	14 (3%)	3	6
3	C	378/380 (100%)	360 (95%)	14 (4%)	4 (1%)	11	23
3	P	377/380 (99%)	353 (94%)	19 (5%)	5 (1%)	9	20
4	D	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
4	Q	239/241 (99%)	221 (92%)	16 (7%)	2 (1%)	16	31
5	E	194/196 (99%)	148 (76%)	34 (18%)	12 (6%)	1	1
5	R	194/196 (99%)	162 (84%)	23 (12%)	9 (5%)	2	3
6	F	99/110 (90%)	96 (97%)	2 (2%)	1 (1%)	12	24
6	S	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	12	24
7	G	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	9	20
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	4	9
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100	100
8	U	65/77 (84%)	61 (94%)	2 (3%)	2 (3%)	3	7
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100	100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100	100
10	J	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	15
All	All	4002/4160 (96%)	3619 (90%)	301 (8%)	82 (2%)	6	12

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	24	LEU
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO

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Mol	Chain	Res	Type
5	E	163	SER
1	N	282	ARG
2	O	171	ALA
2	O	222	GLN
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	49	HIS
8	U	52	GLU
1	A	218	GLY
1	A	262	TRP
1	A	282	ARG
2	B	26	ILE
2	B	231	GLY
2	B	386	ALA
2	B	389	SER
5	E	80	ASP
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	26	ILE
2	O	231	GLY
2	O	372	VAL
2	O	389	SER
3	P	157	ILE
10	W	61	ALA
1	A	72	CYS
1	A	433	ASP
2	B	221	GLU
2	B	372	VAL
3	C	264	VAL
1	N	72	CYS
1	N	433	ASP
2	O	19	PRO
2	O	24	LEU
5	R	185	TYR
5	R	191	ASP
6	S	11	ARG
2	B	222	GLN
2	B	224	LEU

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Mol	Chain	Res	Type
3	C	3	PRO
5	E	115	SER
1	N	63	ALA
2	O	319	SER
2	O	386	ALA
3	P	156	TYR
3	P	264	VAL
2	B	55	SER
1	N	443	TRP
2	O	55	SER
2	O	221	GLU
3	P	3	PRO
4	Q	177	ALA
5	R	127	VAL
7	T	33	ALA
5	E	137	GLY
6	F	77	LYS
5	R	113	ASP
5	R	120	PRO
5	R	177	PRO
7	T	50	PRO
3	C	158	GLY
5	E	120	PRO
5	R	137	GLY
7	G	50	PRO
2	O	208	GLY
1	A	71	PRO
5	E	154	GLY
5	R	154	GLY

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	365/368 (99%)	356 (98%)	9 (2%)	42 66
1	N	365/368 (99%)	354 (97%)	11 (3%)	36 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	331/347 (95%)	316 (96%)	15 (4%)	24	48
2	O	333/347 (96%)	320 (96%)	13 (4%)	28	53
3	C	328/329 (100%)	324 (99%)	4 (1%)	63	80
3	P	328/329 (100%)	326 (99%)	2 (1%)	78	89
4	D	200/200 (100%)	196 (98%)	4 (2%)	48	72
4	Q	200/200 (100%)	196 (98%)	4 (2%)	48	72
5	E	166/166 (100%)	164 (99%)	2 (1%)	63	80
5	R	165/166 (99%)	163 (99%)	2 (1%)	63	80
6	F	93/96 (97%)	89 (96%)	4 (4%)	26	50
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	42
7	G	71/71 (100%)	70 (99%)	1 (1%)	59	78
7	T	70/71 (99%)	70 (100%)	0	100	100
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	55	76
9	I	23/26 (88%)	21 (91%)	2 (9%)	9	21
9	V	23/26 (88%)	21 (91%)	2 (9%)	9	21
10	J	49/49 (100%)	48 (98%)	1 (2%)	48	72
10	W	47/49 (96%)	47 (100%)	0	100	100
All	All	3378/3446 (98%)	3296 (98%)	82 (2%)	43	67

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	106	MET
1	A	108	LYS
1	A	281	ASP
1	A	352	SER
1	A	395	TRP
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	26	ILE
2	B	31	ASN
2	B	38	LEU

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Mol	Chain	Res	Type
2	B	57	TYR
2	B	124	LEU
2	B	150	VAL
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	291	VAL
2	B	338	ARG
2	B	341	MET
2	B	402	ILE
3	C	22	LEU
3	C	41	CYS
3	C	223	PRO
3	C	328	LEU
4	D	43	MET
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG
5	E	178	TYR
5	E	185	TYR
6	F	52	GLU
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
7	G	35	PRO
9	I	68	ILE
9	I	71	ASN
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	50	GLU
1	N	106	MET
1	N	108	LYS
1	N	281	ASP
1	N	352	SER
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO

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Mol	Chain	Res	Type
2	O	26	ILE
2	O	31	ASN
2	O	124	LEU
2	O	150	VAL
2	O	248	ASN
2	O	250	HIS
2	O	260	GLU
2	O	291	VAL
2	O	341	MET
2	O	367	THR
2	O	402	ILE
3	P	22	LEU
3	P	328	LEU
4	Q	43	MET
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	52	GLU
6	S	64	ARG
6	S	70	LEU
6	S	73	ARG
8	U	49	HIS
9	V	68	ILE
9	V	75	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	49	ASN
1	A	61	HIS
1	A	85	HIS
1	A	94	GLN
1	A	118	GLN
1	A	173	ASN
1	A	176	HIS
1	A	214	GLN
1	A	274	ASN
1	A	289	HIS

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Mol	Chain	Res	Type
1	A	311	ASN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	162	ASN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	315	ASN
2	B	329	GLN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN
3	C	55	HIS
3	C	69	HIS
3	C	73	ASN
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	31	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
4	D	225	HIS
5	E	3	ASN
5	E	57	GLN
5	E	103	GLN
5	E	121	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
5	E	179	ASN
6	F	22	ASN
7	G	6	ASN
7	G	23	GLN
7	G	28	ASN

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Mol	Chain	Res	Type
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	176	HIS
1	N	274	ASN
1	N	289	HIS
1	N	311	ASN
2	O	31	ASN
2	O	115	HIS
2	O	153	GLN
2	O	156	GLN
2	O	162	ASN
2	O	196	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	329	GLN
2	O	342	ASN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	73	ASN
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	31	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS

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Mol	Chain	Res	Type
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	121	GLN
5	R	164	HIS
5	R	186	GLN
6	S	22	ASN
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN

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](#)

29 ligands are modelled in this entry.

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	$\# Z > 2$
17	CDL	T	3004	-	39,39,99	1.22	2 (5%)	45,51,111	1.12	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CDL	G	2004	-	39,39,99	1.22	1 (2%)	45,51,111	1.11	3 (6%)
13	AZO	P	3001	-	32,32,32	3.30	17 (53%)	42,42,42	3.03	13 (30%)
15	GOL	P	3011	-	5,5,5	1.43	0	5,5,5	0.66	0
16	HEC	D	501	4	50,50,50	1.49	10 (20%)	68,82,82	1.90	21 (30%)
16	HEC	Q	501	4	50,50,50	1.23	6 (12%)	68,82,82	1.56	9 (13%)
11	PEE	C	2007	-	48,48,50	1.42	7 (14%)	51,53,55	0.83	2 (3%)
12	HEM	C	502	3	50,50,50	1.54	7 (14%)	67,82,82	1.50	12 (17%)
12	HEM	P	502	3	50,50,50	1.50	6 (12%)	67,82,82	1.32	8 (11%)
17	CDL	Q	3003	-	41,41,99	1.20	1 (2%)	47,53,111	1.06	3 (6%)
11	PEE	P	3007	-	48,48,50	1.36	6 (12%)	51,53,55	0.78	2 (3%)
19	FES	E	501	5	0,4,4	-	-	-	-	-
11	PEE	A	2008	-	20,20,50	1.83	6 (30%)	23,25,55	0.70	0
18	BOG	P	2010	-	12,12,20	1.31	2 (16%)	17,17,25	0.60	0
13	AZO	C	2001	-	32,32,32	3.12	16 (50%)	42,42,42	3.00	13 (30%)
11	PEE	N	3008	-	4,4,50	3.73	4 (100%)	6,6,55	0.65	0
19	FES	R	501	5	0,4,4	-	-	-	-	-
11	PEE	P	3005	-	49,49,50	1.52	10 (20%)	52,54,55	0.85	3 (5%)
18	BOG	Q	3009	-	20,20,20	0.98	1 (5%)	25,25,25	0.83	1 (4%)
15	GOL	C	2011	-	5,5,5	1.42	0	5,5,5	0.64	0
17	CDL	D	2003	-	41,41,99	1.19	1 (2%)	47,53,111	1.05	2 (4%)
18	BOG	Q	3091	-	13,13,20	1.35	2 (15%)	18,18,25	1.15	2 (11%)
14	UQ	P	3002	-	19,19,63	2.65	10 (52%)	24,26,79	1.33	3 (12%)
11	PEE	A	2005	-	49,49,50	1.54	10 (20%)	52,54,55	0.86	3 (5%)
14	UQ	C	2002	-	19,19,63	2.68	10 (52%)	24,26,79	1.37	3 (12%)
12	HEM	C	501	3	50,50,50	1.51	8 (16%)	67,82,82	1.34	8 (11%)
18	BOG	D	2091	-	13,13,20	1.29	2 (15%)	18,18,25	1.13	2 (11%)
18	BOG	D	2009	-	20,20,20	1.03	1 (5%)	25,25,25	0.87	2 (8%)
12	HEM	P	501	3	50,50,50	1.37	4 (8%)	67,82,82	1.33	9 (13%)

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
17	CDL	T	3004	-	-	21/49/49/110	-
17	CDL	G	2004	-	-	21/49/49/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEC	D	501	4	1/1/3/7	9/14/54/54	-
16	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
13	AZO	P	3001	-	-	1/23/23/23	0/3/3/3
15	GOL	P	3011	-	-	2/4/4/4	-
11	PEE	C	2007	-	-	20/52/52/54	-
12	HEM	C	502	3	-	5/14/54/54	-
12	HEM	P	502	3	-	5/14/54/54	-
17	CDL	Q	3003	-	-	23/51/51/110	-
11	PEE	P	3007	-	-	23/52/52/54	-
19	FES	E	501	5	-	-	0/1/1/1
11	PEE	A	2008	-	-	11/24/24/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	AZO	C	2001	-	-	1/23/23/23	0/3/3/3
19	FES	R	501	5	-	-	0/1/1/1
11	PEE	P	3005	-	-	26/53/53/54	-
18	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
15	GOL	C	2011	-	-	4/4/4/4	-
17	CDL	D	2003	-	-	23/51/51/110	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
11	PEE	A	2005	-	-	25/53/53/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
12	HEM	C	501	3	-	8/14/54/54	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
18	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
12	HEM	P	501	3	-	6/14/54/54	-

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	AZO	C21-C18	8.42	1.51	1.34
13	C	2001	AZO	C21-C18	8.04	1.50	1.34
13	P	3001	AZO	C18-C19	-6.54	1.32	1.48
13	P	3001	AZO	C2-C7	6.30	1.53	1.40
13	C	2001	AZO	C18-C19	-6.24	1.33	1.48
13	P	3001	AZO	C17-C12	6.08	1.51	1.40
13	C	2001	AZO	O4-C19	6.05	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	2001	AZO	C2-C7	5.91	1.52	1.40
13	P	3001	AZO	O4-C19	5.66	1.45	1.33
13	C	2001	AZO	C17-C12	5.38	1.50	1.40
12	C	502	HEM	CBB-CAB	5.21	1.55	1.30
14	C	2002	UQ	C6-C5	5.04	1.44	1.35
14	P	3002	UQ	C7-C6	5.02	1.60	1.51
11	N	3008	PEE	P-O1P	5.00	1.62	1.50
14	C	2002	UQ	C7-C6	4.93	1.60	1.51
13	P	3001	AZO	C10-N3	4.84	1.39	1.32
14	P	3002	UQ	C6-C5	4.83	1.43	1.35
12	P	501	HEM	CBB-CAB	4.51	1.52	1.30
12	P	502	HEM	CBB-CAB	4.47	1.51	1.30
12	P	501	HEM	CBC-CAC	4.45	1.51	1.30
12	C	501	HEM	CBC-CAC	4.27	1.50	1.30
12	C	501	HEM	CBB-CAB	4.20	1.50	1.30
11	C	2007	PEE	C39-C38	4.19	1.55	1.31
11	P	3007	PEE	C39-C38	4.19	1.55	1.31
11	A	2005	PEE	C39-C38	4.10	1.55	1.31
13	P	3001	AZO	C8-N2	4.04	1.38	1.32
11	P	3005	PEE	C39-C38	4.03	1.54	1.31
12	P	502	HEM	CBC-CAC	3.91	1.49	1.30
14	P	3002	UQ	C6-C1	3.90	1.57	1.46
14	C	2002	UQ	C6-C1	3.81	1.57	1.46
13	C	2001	AZO	C10-N3	3.65	1.38	1.32
11	N	3008	PEE	P-O4P	3.61	1.65	1.54
11	A	2005	PEE	O3-C30	3.53	1.43	1.33
11	P	3005	PEE	O2-C10	3.52	1.44	1.34
13	C	2001	AZO	C8-N2	3.44	1.37	1.32
14	P	3002	UQ	O3-C3	3.43	1.45	1.36
13	C	2001	AZO	C4-C3	3.39	1.44	1.38
16	D	501	HEC	C4B-NB	-3.38	1.34	1.40
11	N	3008	PEE	P-O3P	3.38	1.64	1.54
12	C	502	HEM	CBC-CAC	3.36	1.46	1.30
11	P	3007	PEE	C21-C22	-3.35	1.35	1.51
11	P	3005	PEE	O3-C30	3.34	1.43	1.33
11	P	3005	PEE	P-O1P	3.29	1.62	1.50
11	A	2005	PEE	O2-C10	3.28	1.43	1.34
11	P	3005	PEE	C21-C22	-3.27	1.35	1.51
11	A	2005	PEE	P-O1P	3.27	1.62	1.50
11	A	2008	PEE	O3-C30	3.27	1.42	1.33
16	D	501	HEC	C4D-C3D	3.26	1.50	1.45
11	A	2005	PEE	C21-C22	-3.21	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2008	PEE	P-O1P	3.21	1.61	1.50
14	C	2002	UQ	O3-C3	3.20	1.44	1.36
11	A	2008	PEE	O2-C10	3.17	1.43	1.34
11	C	2007	PEE	O3-C30	3.16	1.42	1.33
12	C	501	HEM	CAB-C3B	-3.16	1.39	1.47
12	P	502	HEM	CAB-C3B	-3.12	1.39	1.47
11	C	2007	PEE	P-O1P	3.10	1.61	1.50
11	C	2007	PEE	C21-C22	-3.10	1.36	1.51
16	D	501	HEC	C4C-NC	-3.09	1.33	1.39
11	P	3007	PEE	O3-C30	3.08	1.42	1.33
14	C	2002	UQ	C2-C1	3.05	1.57	1.48
11	P	3007	PEE	P-O1P	2.92	1.60	1.50
12	C	502	HEM	CAB-C3B	-2.90	1.39	1.47
13	P	3001	AZO	O5-C21	2.89	1.40	1.34
11	C	2007	PEE	O2-C10	2.88	1.42	1.34
12	C	502	HEM	C3B-C4B	2.88	1.50	1.44
12	C	502	HEM	CAC-C3C	-2.87	1.39	1.47
13	P	3001	AZO	C5-C4	2.83	1.44	1.38
13	C	2001	AZO	C15-C16	2.82	1.43	1.38
13	C	2001	AZO	C13-C12	2.82	1.45	1.39
12	C	501	HEM	CAC-C3C	-2.79	1.39	1.47
13	C	2001	AZO	C5-C4	2.79	1.44	1.38
14	C	2002	UQ	CM5-C5	2.78	1.56	1.50
13	P	3001	AZO	C4-C3	2.77	1.43	1.38
14	C	2002	UQ	O2-C2	2.76	1.43	1.36
12	P	502	HEM	CAC-C3C	-2.76	1.40	1.47
14	C	2002	UQ	C5-C4	2.74	1.56	1.47
13	C	2001	AZO	C6-C7	2.74	1.45	1.39
14	P	3002	UQ	C2-C1	2.74	1.56	1.48
16	D	501	HEC	CHD-C1D	-2.72	1.33	1.38
14	P	3002	UQ	C5-C4	2.72	1.56	1.47
14	P	3002	UQ	O2-C2	2.72	1.43	1.36
13	P	3001	AZO	C15-C16	2.70	1.43	1.38
14	P	3002	UQ	CM5-C5	2.67	1.56	1.50
14	P	3002	UQ	C7-C8	2.67	1.54	1.50
11	P	3007	PEE	O2-C10	2.67	1.41	1.34
16	D	501	HEC	C1D-ND	-2.65	1.35	1.40
14	P	3002	UQ	C3-C4	2.63	1.56	1.48
14	C	2002	UQ	C7-C8	2.60	1.54	1.50
11	A	2005	PEE	C31-C30	2.59	1.58	1.50
12	P	501	HEM	CAB-C3B	-2.58	1.40	1.47
14	C	2002	UQ	C3-C4	2.57	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	AZO	C6-C7	2.56	1.44	1.39
12	C	502	HEM	CMD-C2D	2.54	1.56	1.50
16	Q	501	HEC	CHD-C1D	-2.50	1.33	1.38
11	N	3008	PEE	P-O2P	2.50	1.61	1.54
18	Q	3091	BOG	O5-C1	2.46	1.48	1.41
16	Q	501	HEC	C4C-NC	-2.41	1.35	1.39
16	D	501	HEC	CHD-C4C	-2.41	1.34	1.39
16	D	501	HEC	C3B-C2B	-2.40	1.31	1.36
12	P	501	HEM	CAC-C3C	-2.40	1.41	1.47
16	Q	501	HEC	C1D-ND	-2.39	1.36	1.40
16	Q	501	HEC	C3B-C2B	-2.39	1.31	1.36
18	D	2009	BOG	O5-C1	2.38	1.48	1.41
12	C	502	HEM	C1C-NC	-2.38	1.35	1.39
12	C	501	HEM	C2A-C3A	-2.38	1.32	1.38
11	P	3005	PEE	C3-C2	2.36	1.58	1.50
18	Q	3009	BOG	O5-C1	2.34	1.47	1.41
11	A	2008	PEE	C3-C2	2.33	1.58	1.50
18	D	2091	BOG	O5-C1	2.33	1.47	1.41
16	D	501	HEC	FE-NC	-2.33	1.87	1.95
17	Q	3003	CDL	O1-C1	2.33	1.50	1.43
11	A	2005	PEE	C3-C2	2.33	1.58	1.50
11	P	3005	PEE	C31-C30	2.32	1.57	1.50
11	A	2005	PEE	C11-C10	2.31	1.57	1.50
13	C	2001	AZO	C5-C6	2.30	1.42	1.38
11	A	2008	PEE	C1-C2	2.29	1.58	1.50
18	P	2010	BOG	C4-C5	2.27	1.57	1.53
18	Q	3091	BOG	C4-C5	2.27	1.57	1.53
11	P	3005	PEE	C11-C10	2.27	1.57	1.50
17	T	3004	CDL	O1-C1	2.27	1.50	1.43
11	A	2005	PEE	C1-C2	2.26	1.57	1.50
18	D	2091	BOG	C4-C5	2.23	1.57	1.53
13	P	3001	AZO	C13-C12	2.23	1.44	1.39
13	P	3001	AZO	C17-C18	2.21	1.51	1.49
13	P	3001	AZO	C15-C14	2.20	1.43	1.38
13	C	2001	AZO	C17-C18	2.20	1.51	1.49
17	G	2004	CDL	O1-C1	2.20	1.49	1.43
16	Q	501	HEC	C4B-NB	-2.19	1.36	1.40
16	D	501	HEC	C1A-C2A	2.19	1.49	1.45
11	A	2008	PEE	C11-C10	2.18	1.57	1.50
11	C	2007	PEE	O2-C2	2.18	1.51	1.46
17	T	3004	CDL	OB2-CB2	-2.17	1.36	1.44
13	C	2001	AZO	C15-C14	2.17	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	AZO	O2-C10	2.16	1.39	1.36
12	C	501	HEM	C3C-C4C	-2.15	1.42	1.46
16	D	501	HEC	C1C-NC	-2.14	1.35	1.39
12	C	501	HEM	CMB-C2B	2.14	1.55	1.50
17	D	2003	CDL	O1-C1	2.14	1.49	1.43
11	P	3005	PEE	C1-C2	2.13	1.57	1.50
13	P	3001	AZO	C9-C10	2.12	1.42	1.38
12	P	502	HEM	C3B-C4B	2.10	1.49	1.44
18	P	2010	BOG	C1-C2	2.09	1.57	1.52
12	C	501	HEM	CMA-C3A	2.07	1.55	1.50
12	P	502	HEM	C1A-C2A	2.06	1.48	1.44
11	A	2005	PEE	P-O4P	2.05	1.67	1.59
11	C	2007	PEE	C3-C2	2.05	1.57	1.50
11	P	3007	PEE	C31-C30	2.05	1.56	1.50
11	P	3005	PEE	O2-C2	2.05	1.51	1.46
13	C	2001	AZO	C16-C17	2.03	1.43	1.39
16	Q	501	HEC	C3C-C2C	-2.03	1.33	1.38

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	2001	AZO	C11-N3-C10	10.06	122.16	114.50
13	P	3001	AZO	C11-N3-C10	9.85	122.00	114.50
13	P	3001	AZO	C11-N2-C8	9.68	121.88	114.50
13	C	2001	AZO	C11-N2-C8	9.57	121.79	114.50
13	C	2001	AZO	N2-C11-N3	-6.66	118.50	128.58
13	P	3001	AZO	N2-C11-N3	-6.37	118.93	128.58
13	C	2001	AZO	O4-C19-C18	5.55	119.61	112.05
13	P	3001	AZO	O4-C19-C18	5.49	119.53	112.05
16	Q	501	HEC	CAA-C2A-C1A	4.72	134.44	124.85
13	C	2001	AZO	C22-O5-C21	-4.50	108.29	115.65
13	P	3001	AZO	C22-O5-C21	-4.50	108.29	115.65
14	C	2002	UQ	C8-C7-C6	4.41	122.94	112.08
16	D	501	HEC	CAA-C2A-C1A	4.37	133.75	124.85
14	P	3002	UQ	C8-C7-C6	4.33	122.76	112.08
13	C	2001	AZO	O5-C21-C18	-4.25	113.58	121.30
16	D	501	HEC	CAA-C2A-C3A	-4.21	119.98	127.87
13	P	3001	AZO	O5-C21-C18	-4.18	113.70	121.30
16	Q	501	HEC	CAA-C2A-C3A	-4.07	120.23	127.87
16	Q	501	HEC	CAC-C3C-C4C	-4.02	119.38	124.91
16	D	501	HEC	CAC-C3C-C2C	4.01	133.23	126.89
16	D	501	HEC	CAB-C3B-C4B	-3.77	119.89	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	C3B-C2B-C1B	-3.75	103.59	106.41
16	Q	501	HEC	CAC-C3C-C2C	3.68	132.72	126.89
18	Q	3091	BOG	C1'-O1-C1	3.65	118.80	113.26
13	P	3001	AZO	C9-C10-N3	-3.62	119.36	124.47
12	C	501	HEM	C3B-C4B-NB	3.58	112.04	109.47
16	D	501	HEC	C2D-C1D-ND	3.54	113.91	109.84
16	D	501	HEC	CAD-C3D-C4D	3.51	130.81	124.70
16	D	501	HEC	CAC-C3C-C4C	-3.49	120.11	124.91
12	C	502	HEM	CAD-C3D-C4D	3.46	130.73	124.70
18	D	2091	BOG	C1'-O1-C1	3.45	118.50	113.26
14	C	2002	UQ	C7-C6-C1	-3.42	114.54	118.52
13	C	2001	AZO	C12-O2-C10	3.32	125.16	118.43
13	C	2001	AZO	C9-C10-N3	-3.31	119.79	124.47
17	T	3004	CDL	CB4-OB6-CB5	-3.29	109.91	117.80
13	C	2001	AZO	C7-O1-C8	3.27	125.06	118.43
13	P	3001	AZO	C7-O1-C8	3.24	124.99	118.43
16	D	501	HEC	CMD-C2D-C1D	3.21	130.05	125.03
16	D	501	HEC	C2B-C1B-NB	3.18	113.58	109.90
12	P	501	HEM	CAD-C3D-C2D	-3.15	121.97	127.87
12	C	502	HEM	C3B-C4B-NB	3.14	111.73	109.47
16	Q	501	HEC	CMB-C2B-C1B	3.13	129.93	125.03
12	C	502	HEM	CAA-C2A-C1A	3.12	131.03	124.94
12	P	501	HEM	C3B-C4B-NB	3.12	111.71	109.47
13	P	3001	AZO	C12-O2-C10	3.11	124.74	118.43
12	C	501	HEM	C2B-C1B-NB	3.11	113.42	109.84
17	G	2004	CDL	CA4-OA6-CA5	-3.09	110.39	117.80
14	P	3002	UQ	C7-C6-C1	-3.07	114.95	118.52
12	P	502	HEM	C4C-C3C-C2C	-3.06	104.16	106.81
12	P	502	HEM	CAD-C3D-C4D	3.06	130.03	124.70
13	P	3001	AZO	C9-C8-N2	-3.05	120.15	124.47
17	G	2004	CDL	CB4-OB6-CB5	-3.05	110.50	117.80
12	C	502	HEM	C2B-C1B-NB	3.00	113.29	109.84
12	C	502	HEM	C4C-C3C-C2C	-2.98	104.23	106.81
12	C	502	HEM	C3B-C2B-C1B	-2.97	104.18	106.41
16	D	501	HEC	CAB-C3B-C2B	2.96	132.99	127.56
12	C	502	HEM	C2A-C1A-NA	2.92	113.39	110.15
18	Q	3009	BOG	C1'-O1-C1	2.86	118.56	113.68
12	C	502	HEM	C2D-C1D-ND	2.86	113.21	109.90
13	P	3001	AZO	C10-C9-C8	2.85	117.67	115.20
11	A	2005	PEE	C22-C21-C20	2.85	127.56	113.86
12	P	502	HEM	C3B-C4B-NB	2.84	111.51	109.47
12	P	501	HEM	CAD-C3D-C4D	2.84	129.64	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	3005	PEE	C22-C21-C20	2.83	127.47	113.86
12	P	501	HEM	C3B-C2B-C1B	-2.83	104.29	106.41
18	D	2009	BOG	C1'-O1-C1	2.82	118.50	113.68
13	P	3001	AZO	C20-O4-C19	2.78	121.01	115.85
12	P	502	HEM	CAA-C2A-C1A	2.76	130.34	124.94
11	C	2007	PEE	C22-C21-C20	2.74	127.05	113.86
12	P	501	HEM	C2B-C1B-NB	2.74	112.99	109.84
13	C	2001	AZO	C9-C8-N2	-2.69	120.67	124.47
16	Q	501	HEC	CAD-C3D-C4D	2.67	129.35	124.70
17	T	3004	CDL	CA4-OA6-CA5	-2.67	111.41	117.80
11	P	3007	PEE	C22-C21-C20	2.66	126.66	113.86
18	D	2091	BOG	O1-C1-C2	2.62	111.16	108.14
16	Q	501	HEC	C2D-C1D-ND	2.61	112.84	109.84
11	C	2007	PEE	C21-C22-C23	2.58	127.39	114.37
12	C	501	HEM	CAD-C3D-C2D	-2.55	123.09	127.87
18	Q	3091	BOG	O1-C1-C2	2.55	111.08	108.14
12	P	502	HEM	C3B-C2B-C1B	-2.55	104.50	106.41
16	D	501	HEC	CMA-C3A-C4A	2.53	129.19	124.73
17	D	2003	CDL	CB4-OB6-CB5	-2.53	111.74	117.80
12	P	502	HEM	C2B-C1B-NB	2.52	112.73	109.84
16	Q	501	HEC	CMD-C2D-C1D	2.48	128.91	125.03
11	A	2005	PEE	C21-C22-C23	2.46	126.80	114.37
12	C	502	HEM	CAD-C3D-C2D	-2.45	123.28	127.87
12	C	501	HEM	CAD-C3D-C4D	2.44	128.96	124.70
11	P	3007	PEE	C21-C22-C23	2.44	126.68	114.37
16	D	501	HEC	C4B-NB-C1B	-2.41	102.35	105.21
11	P	3005	PEE	C21-C22-C23	2.40	126.51	114.37
17	Q	3003	CDL	CB4-OB6-CB5	-2.40	112.05	117.80
12	C	502	HEM	C4D-ND-C1D	-2.36	102.41	105.21
13	C	2001	AZO	C20-O4-C19	2.36	120.23	115.85
11	P	3005	PEE	O3-C3-C2	2.34	115.14	108.40
16	D	501	HEC	CMB-C2B-C1B	2.34	128.68	125.03
16	D	501	HEC	C3D-C4D-ND	2.32	112.59	110.35
12	P	502	HEM	CHC-C4B-NB	-2.31	121.93	124.42
12	P	501	HEM	C3C-C2C-C1C	-2.30	104.87	107.05
12	P	501	HEM	CMC-C2C-C1C	2.29	128.77	124.73
12	C	501	HEM	C2D-C1D-ND	2.29	112.55	109.90
17	T	3004	CDL	CA6-CA4-CA3	-2.28	106.47	111.78
17	D	2003	CDL	CA6-CA4-CA3	-2.27	106.48	111.78
11	A	2005	PEE	O3-C3-C2	2.26	114.91	108.40
16	D	501	HEC	C1C-C2C-C3C	-2.26	104.23	106.82
14	P	3002	UQ	C10-C9-C8	-2.23	117.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	3003	CDL	CA6-CA4-CA3	-2.23	106.58	111.78
18	D	2009	BOG	O1-C1-C2	2.21	111.63	108.27
16	D	501	HEC	C1D-ND-C4D	-2.21	102.59	105.21
16	Q	501	HEC	CAB-C3B-C4B	-2.19	121.94	124.79
13	C	2001	AZO	C10-C9-C8	2.17	117.08	115.20
16	D	501	HEC	C3C-C4C-NC	2.16	112.55	110.15
16	D	501	HEC	C2A-C1A-NA	2.16	112.40	110.32
14	C	2002	UQ	C10-C9-C8	-2.16	118.09	123.63
17	G	2004	CDL	CA6-CA4-CA3	-2.15	106.78	111.78
13	P	3001	AZO	O4-C19-O3	-2.14	119.41	123.50
12	P	501	HEM	C1D-C2D-C3D	-2.13	104.74	106.98
16	D	501	HEC	CHA-C1A-NA	-2.12	122.15	124.45
17	Q	3003	CDL	CA4-OA6-CA5	-2.12	112.73	117.80
12	C	501	HEM	CMD-C2D-C1D	2.11	128.32	125.03
12	P	502	HEM	CHD-C4C-C3C	-2.10	121.66	125.21
12	C	502	HEM	C3D-C4D-ND	2.10	112.48	110.17
12	C	502	HEM	CMC-C2C-C1C	2.07	128.37	124.73
16	D	501	HEC	CHC-C4B-NB	-2.05	121.83	124.37
12	C	501	HEM	C4A-NA-C1A	-2.04	102.49	105.82
12	P	501	HEM	C2D-C1D-ND	2.04	112.26	109.90
13	C	2001	AZO	O4-C19-O3	-2.03	119.63	123.50
16	D	501	HEC	C4A-NA-C1A	-2.01	102.55	105.82
17	T	3004	CDL	CB6-CB4-CB3	-2.00	107.11	111.78

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	D	501	HEC	NA
16	Q	501	HEC	NA

All (265) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2005	PEE	C11-C10-O2-C2
11	A	2005	PEE	C4-O4P-P-O3P
11	A	2005	PEE	C4-O4P-P-O2P
11	A	2005	PEE	C4-O4P-P-O1P
11	A	2005	PEE	O4P-C4-C5-N
11	C	2007	PEE	C4-O4P-P-O3P
11	C	2007	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C11-C10-O2-C2
11	P	3005	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
11	P	3005	PEE	C4-O4P-P-O2P
11	P	3005	PEE	C4-O4P-P-O1P
11	P	3005	PEE	O4P-C4-C5-N
11	P	3007	PEE	C4-O4P-P-O3P
11	P	3007	PEE	C4-O4P-P-O2P
14	C	2002	UQ	C1-C6-C7-C8
14	C	2002	UQ	C5-C6-C7-C8
14	C	2002	UQ	C12-C11-C9-C8
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
14	P	3002	UQ	C12-C11-C9-C8
15	C	2011	GOL	C1-C2-C3-O3
15	P	3011	GOL	C1-C2-C3-O3
17	D	2003	CDL	CA3-OA5-PA1-OA4
17	D	2003	CDL	CB2-OB2-PB2-OB4
17	D	2003	CDL	CB2-OB2-PB2-OB5
17	D	2003	CDL	CB3-OB5-PB2-OB2
17	D	2003	CDL	CB3-OB5-PB2-OB4
17	G	2004	CDL	O1-C1-CA2-OA2
17	G	2004	CDL	CA3-OA5-PA1-OA2
17	G	2004	CDL	CA3-OA5-PA1-OA3
17	G	2004	CDL	CA3-OA5-PA1-OA4
17	G	2004	CDL	CB3-OB5-PB2-OB3
17	G	2004	CDL	OB7-CB5-OB6-CB4
17	G	2004	CDL	C51-CB5-OB6-CB4
17	Q	3003	CDL	CA3-OA5-PA1-OA4
17	Q	3003	CDL	CB2-OB2-PB2-OB4
17	Q	3003	CDL	CB2-OB2-PB2-OB5
17	Q	3003	CDL	CB3-OB5-PB2-OB2
17	Q	3003	CDL	CB3-OB5-PB2-OB4
17	T	3004	CDL	O1-C1-CA2-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA3
17	T	3004	CDL	CA3-OA5-PA1-OA4
17	T	3004	CDL	CB3-OB5-PB2-OB3
17	T	3004	CDL	C51-CB5-OB6-CB4
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
11	A	2005	PEE	O5-C30-O3-C3
11	P	3005	PEE	O5-C30-O3-C3
11	P	3005	PEE	C31-C30-O3-C3
17	G	2004	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
17	T	3004	CDL	OB9-CB7-OB8-CB6
17	G	2004	CDL	C31-CA7-OA8-CA6
17	T	3004	CDL	C31-CA7-OA8-CA6
11	A	2008	PEE	O5-C30-O3-C3
17	T	3004	CDL	OB7-CB5-OB6-CB4
11	A	2005	PEE	C31-C30-O3-C3
17	G	2004	CDL	OA9-CA7-OA8-CA6
17	T	3004	CDL	OA9-CA7-OA8-CA6
16	Q	501	HEC	C3A-C2A-CAA-CBA
17	G	2004	CDL	C71-CB7-OB8-CB6
17	T	3004	CDL	C71-CB7-OB8-CB6
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
11	A	2005	PEE	O4-C10-O2-C2
11	P	3005	PEE	O4-C10-O2-C2
17	D	2003	CDL	C31-CA7-OA8-CA6
17	Q	3003	CDL	C31-CA7-OA8-CA6
17	D	2003	CDL	O1-C1-CA2-OA2
17	Q	3003	CDL	O1-C1-CA2-OA2
11	A	2008	PEE	C31-C30-O3-C3
18	Q	3091	BOG	O5-C5-C6-O6
18	D	2009	BOG	O5-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
16	Q	501	HEC	C2B-C3B-CAB-CBB
18	D	2091	BOG	C2-C1-O1-C1'
18	D	2009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	C2-C1-O1-C1'
16	D	501	HEC	C3A-C2A-CAA-CBA
18	D	2091	BOG	O5-C1-O1-C1'
17	D	2003	CDL	C71-CB7-OB8-CB6
17	Q	3003	CDL	C71-CB7-OB8-CB6
18	Q	3091	BOG	C4-C5-C6-O6
17	D	2003	CDL	OA9-CA7-OA8-CA6
17	D	2003	CDL	CB7-C71-C72-C73
17	Q	3003	CDL	OA9-CA7-OA8-CA6
17	Q	3003	CDL	CB7-C71-C72-C73
17	D	2003	CDL	OB9-CB7-OB8-CB6
17	Q	3003	CDL	OB9-CB7-OB8-CB6
16	Q	501	HEC	C1A-C2A-CAA-CBA
11	C	2007	PEE	C10-C11-C12-C13
17	G	2004	CDL	CB2-C1-CA2-OA2
17	T	3004	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C10-C11-C12-C13
17	G	2004	CDL	C11-CA5-OA6-CA4
17	T	3004	CDL	C11-CA5-OA6-CA4
17	T	3004	CDL	OA7-CA5-OA6-CA4
15	C	2011	GOL	O1-C1-C2-C3
18	D	2009	BOG	O1-C1'-C2'-C3'
18	Q	3009	BOG	O1-C1'-C2'-C3'
17	G	2004	CDL	OA7-CA5-OA6-CA4
11	P	3005	PEE	C34-C35-C36-C37
11	A	2005	PEE	C34-C35-C36-C37
11	C	2007	PEE	C33-C34-C35-C36
11	P	3007	PEE	C33-C34-C35-C36
15	C	2011	GOL	O2-C2-C3-O3
15	P	3011	GOL	O2-C2-C3-O3
17	G	2004	CDL	CB5-C51-C52-C53
11	A	2005	PEE	C20-C21-C22-C23
18	Q	3009	BOG	C1'-C2'-C3'-C4'
18	D	2009	BOG	C1'-C2'-C3'-C4'
11	C	2007	PEE	C40-C41-C42-C43
11	P	3005	PEE	C20-C21-C22-C23
11	A	2008	PEE	C11-C10-O2-C2
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C40-C41-C42-C43
17	D	2003	CDL	C51-CB5-OB6-CB4
17	Q	3003	CDL	C51-CB5-OB6-CB4
16	Q	501	HEC	C4B-C3B-CAB-CBB
11	P	3005	PEE	C39-C40-C41-C42
12	C	501	HEM	C2C-C3C-CAC-CBC
12	P	501	HEM	C2C-C3C-CAC-CBC
17	G	2004	CDL	OB5-CB3-CB4-OB6
17	T	3004	CDL	OB5-CB3-CB4-OB6
11	P	3005	PEE	C30-C31-C32-C33
11	C	2007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C39-C40-C41-C42
11	P	3007	PEE	C15-C16-C17-C18
16	D	501	HEC	C2B-C3B-CAB-CBB
17	Q	3003	CDL	OB7-CB5-OB6-CB4
16	D	501	HEC	C4B-C3B-CAB-CBB
11	A	2005	PEE	C11-C12-C13-C14
15	C	2011	GOL	O1-C1-C2-O2
11	C	2007	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	C39-C40-C41-C42
11	A	2008	PEE	O4-C10-O2-C2
17	D	2003	CDL	OB7-CB5-OB6-CB4
11	A	2005	PEE	C30-C31-C32-C33
11	A	2005	PEE	C41-C42-C43-C44
16	D	501	HEC	C1A-C2A-CAA-CBA
11	P	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C35-C36-C37-C38
11	A	2005	PEE	C39-C40-C41-C42
11	P	3005	PEE	O3P-C1-C2-O2
11	P	3005	PEE	C41-C42-C43-C44
11	A	2008	PEE	O2-C2-C3-O3
17	D	2003	CDL	OA6-CA4-CA6-OA8
17	Q	3003	CDL	OA6-CA4-CA6-OA8
17	Q	3003	CDL	C71-C72-C73-C74
11	P	3007	PEE	C11-C12-C13-C14
17	D	2003	CDL	C71-C72-C73-C74
11	P	3007	PEE	C43-C44-C45-C46
11	C	2007	PEE	C43-C44-C45-C46
11	P	3005	PEE	O3P-C1-C2-C3
17	D	2003	CDL	OB5-CB3-CB4-CB6
17	G	2004	CDL	OB5-CB3-CB4-CB6
17	Q	3003	CDL	OB5-CB3-CB4-CB6
17	T	3004	CDL	OB5-CB3-CB4-CB6
11	C	2007	PEE	C11-C12-C13-C14
11	A	2005	PEE	C43-C44-C45-C46
17	T	3004	CDL	CB5-C51-C52-C53
11	P	3005	PEE	C23-C24-C25-C26
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10
11	A	2005	PEE	C23-C24-C25-C26
17	D	2003	CDL	CA3-CA4-CA6-OA8
17	Q	3003	CDL	CA3-CA4-CA6-OA8
11	A	2005	PEE	O3P-C1-C2-O2
11	A	2008	PEE	O3P-C1-C2-O2
11	P	3007	PEE	C42-C43-C44-C45
11	P	3005	PEE	C43-C44-C45-C46
11	A	2005	PEE	O3P-C1-C2-C3
11	A	2008	PEE	O3P-C1-C2-C3
12	C	501	HEM	C2B-C3B-CAB-CBB
11	A	2005	PEE	C35-C36-C37-C38
11	C	2007	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
12	P	502	HEM	C4D-C3D-CAD-CBD
17	D	2003	CDL	OB5-CB3-CB4-OB6
17	Q	3003	CDL	OB5-CB3-CB4-OB6
11	A	2005	PEE	C10-C11-C12-C13
16	D	501	HEC	C4C-C3C-CAC-CBC
11	P	3005	PEE	C10-C11-C12-C13
12	C	502	HEM	C4D-C3D-CAD-CBD
11	C	2007	PEE	C34-C35-C36-C37
11	P	3005	PEE	C22-C23-C24-C25
17	D	2003	CDL	CA2-OA2-PA1-OA5
17	D	2003	CDL	CA3-OA5-PA1-OA2
17	D	2003	CDL	CA3-OA5-PA1-OA3
17	G	2004	CDL	CB3-OB5-PB2-OB2
17	G	2004	CDL	CB3-OB5-PB2-OB4
17	Q	3003	CDL	CA2-OA2-PA1-OA5
17	Q	3003	CDL	CA3-OA5-PA1-OA2
17	Q	3003	CDL	CA3-OA5-PA1-OA3
17	T	3004	CDL	CB3-OB5-PB2-OB2
17	T	3004	CDL	CB3-OB5-PB2-OB4
11	P	3005	PEE	C35-C36-C37-C38
11	A	2005	PEE	C1-C2-O2-C10
11	P	3005	PEE	C1-C2-O2-C10
11	A	2005	PEE	C22-C23-C24-C25
11	A	2005	PEE	C14-C15-C16-C17
11	P	3007	PEE	C31-C32-C33-C34
11	P	3005	PEE	C31-C32-C33-C34
11	P	3007	PEE	C30-C31-C32-C33
11	P	3005	PEE	C14-C15-C16-C17
11	A	2008	PEE	C10-C11-C12-C13
16	Q	501	HEC	C4C-C3C-CAC-CBC
11	A	2005	PEE	C31-C32-C33-C34
11	P	3007	PEE	C34-C35-C36-C37
11	P	3007	PEE	C20-C21-C22-C23
12	P	502	HEM	CAD-CBD-CGD-O1D
11	P	3007	PEE	O5-C30-O3-C3
12	C	501	HEM	CAA-CBA-CGA-O1A
12	C	502	HEM	CAD-CBD-CGD-O1D
11	P	3007	PEE	C31-C30-O3-C3
12	P	502	HEM	CAA-CBA-CGA-O1A
11	C	2007	PEE	C30-C31-C32-C33
12	C	502	HEM	CAA-CBA-CGA-O1A
12	C	502	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	P	502	HEM	CAD-CBD-CGD-O2D
12	C	501	HEM	CAA-CBA-CGA-O2A
11	C	2007	PEE	C31-C32-C33-C34
12	P	501	HEM	CAA-CBA-CGA-O2A
12	P	501	HEM	CAA-CBA-CGA-O1A
11	A	2005	PEE	C12-C13-C14-C15
17	T	3004	CDL	C1-CB2-OB2-PB2
12	P	502	HEM	CAA-CBA-CGA-O2A
16	D	501	HEC	CAD-CBD-CGD-O2D
16	Q	501	HEC	CAA-CBA-CGA-O2A
11	P	3007	PEE	C12-C13-C14-C15
12	C	501	HEM	CAD-CBD-CGD-O2D
12	C	502	HEM	CAA-CBA-CGA-O2A
17	G	2004	CDL	CA2-C1-CB2-OB2
17	T	3004	CDL	CA2-C1-CB2-OB2
11	A	2008	PEE	O3-C30-C31-C32
11	C	2007	PEE	C38-C39-C40-C41
17	G	2004	CDL	C1-CB2-OB2-PB2
16	Q	501	HEC	CAA-CBA-CGA-O1A
13	C	2001	AZO	N1-C1-C2-C7
11	P	3007	PEE	C38-C39-C40-C41
11	C	2007	PEE	C20-C21-C22-C23
16	D	501	HEC	CAD-CBD-CGD-O1D
16	Q	501	HEC	CAD-CBD-CGD-O2D
12	C	501	HEM	CAD-CBD-CGD-O1D
12	C	501	HEM	C4B-C3B-CAB-CBB
12	C	501	HEM	C4C-C3C-CAC-CBC
12	P	501	HEM	C4C-C3C-CAC-CBC
11	A	2008	PEE	O5-C30-C31-C32
11	P	3005	PEE	C12-C13-C14-C15
16	Q	501	HEC	CAD-CBD-CGD-O1D
16	D	501	HEC	CAA-CBA-CGA-O2A
11	C	2007	PEE	O2-C10-C11-C12
12	P	501	HEM	CAD-CBD-CGD-O2D
11	P	3007	PEE	O2-C10-C11-C12
16	D	501	HEC	CAA-CBA-CGA-O1A
13	P	3001	AZO	C12-C17-C18-C21
17	Q	3003	CDL	C72-C71-CB7-OB8
11	A	2008	PEE	C1-C2-C3-O3
17	D	2003	CDL	C72-C71-CB7-OB8
12	P	501	HEM	CAD-CBD-CGD-O1D
17	D	2003	CDL	C72-C71-CB7-OB9

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Mol	Chain	Res	Type	Atoms
17	Q	3003	CDL	C72-C71-CB7-OB9
11	C	2007	PEE	O4-C10-C11-C12
11	P	3007	PEE	O4-C10-C11-C12
11	P	3005	PEE	C19-C20-C21-C22

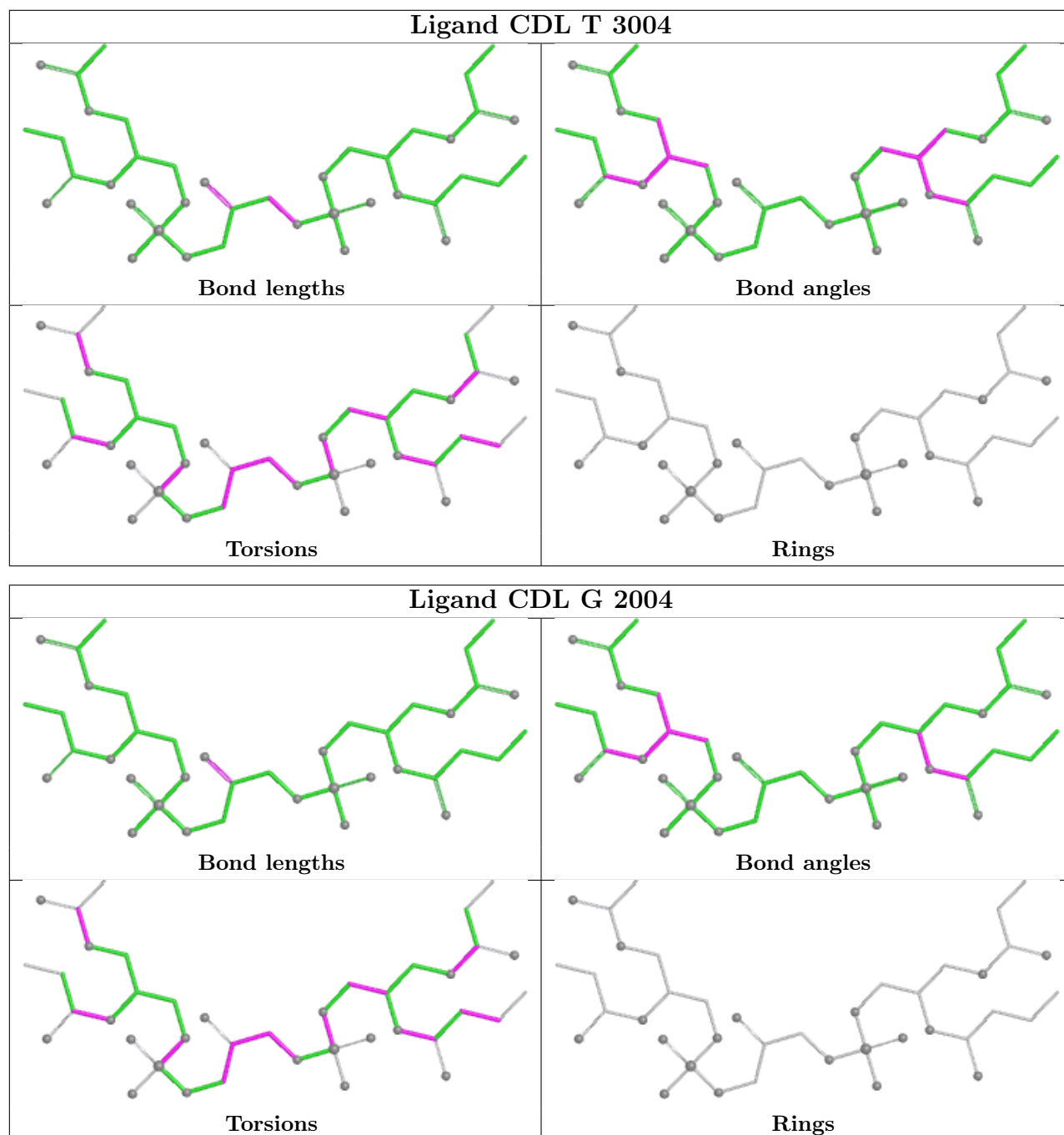
There are no ring outliers.

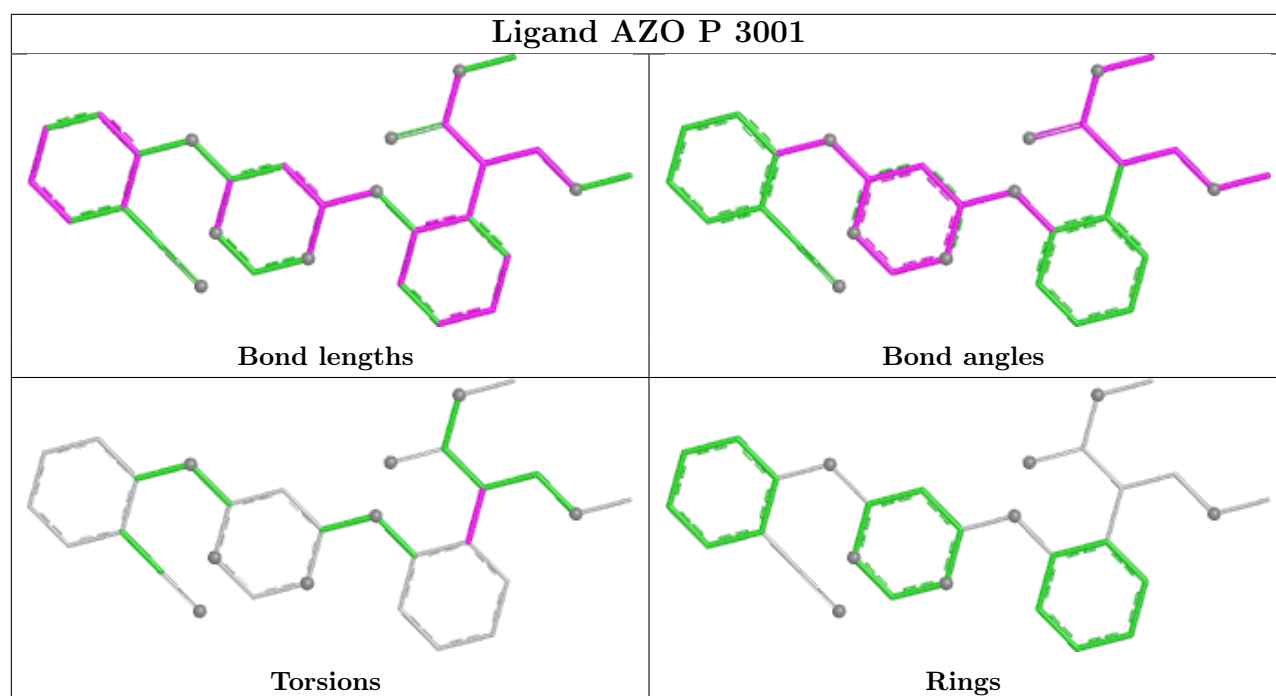
21 monomers are involved in 46 short contacts:

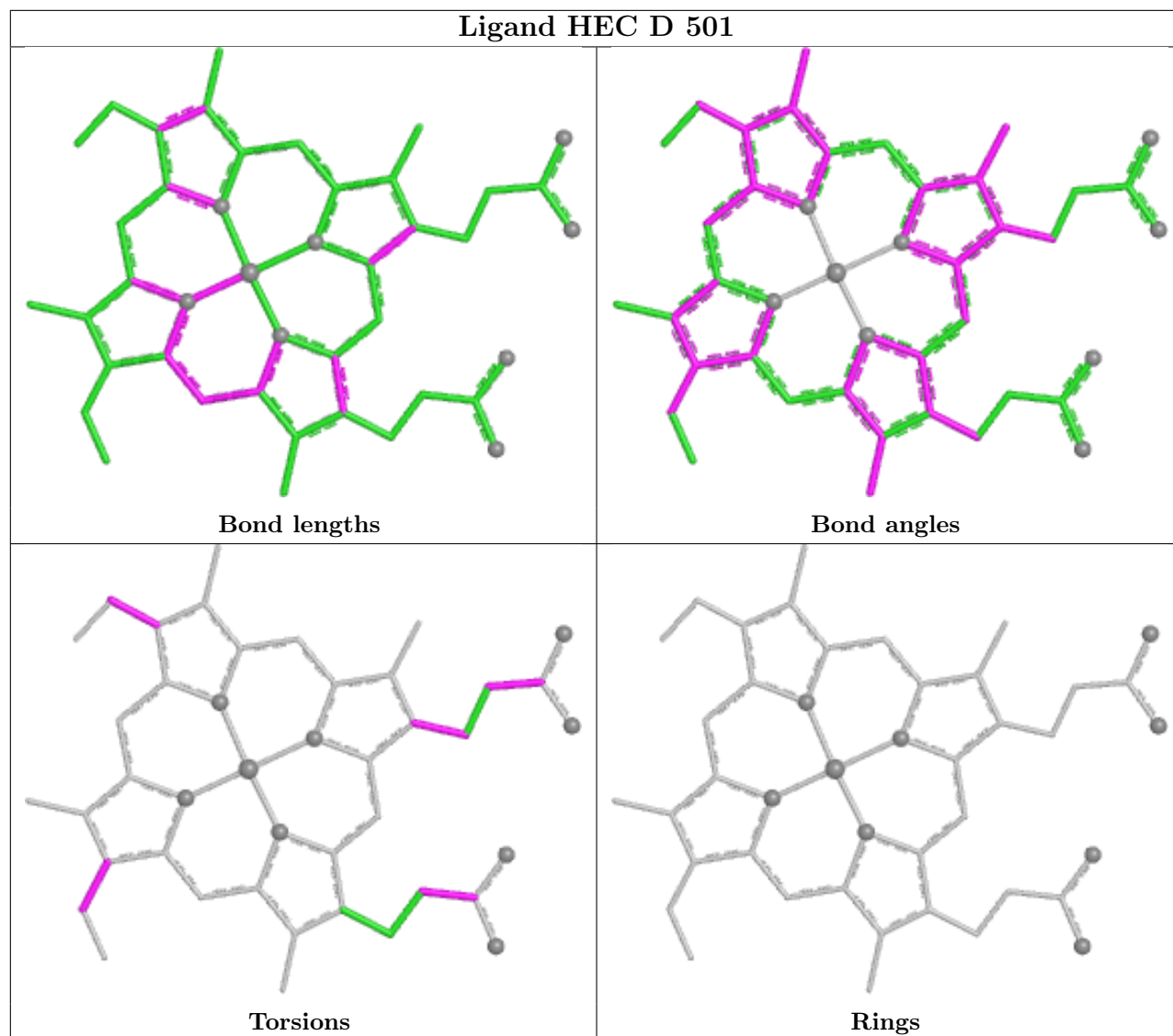
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	3004	CDL	3	0
17	G	2004	CDL	4	0
13	P	3001	AZO	2	0
16	D	501	HEC	1	0
16	Q	501	HEC	1	0
11	C	2007	PEE	5	0
12	C	502	HEM	2	0
12	P	502	HEM	2	0
17	Q	3003	CDL	3	0
11	P	3007	PEE	3	0
19	E	501	FES	2	0
18	P	2010	BOG	1	0
19	R	501	FES	2	0
15	C	2011	GOL	1	0
17	D	2003	CDL	4	0
18	Q	3091	BOG	1	0
14	P	3002	UQ	3	0
14	C	2002	UQ	2	0
12	C	501	HEM	3	0
18	D	2091	BOG	1	0
12	P	501	HEM	2	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

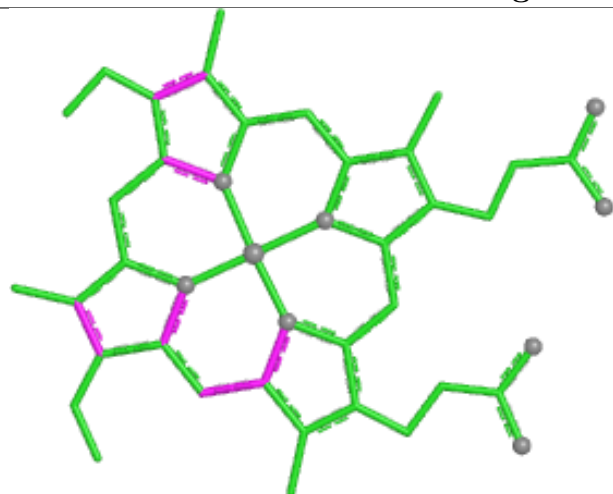
equivalents in the CSD to analyse the geometry.



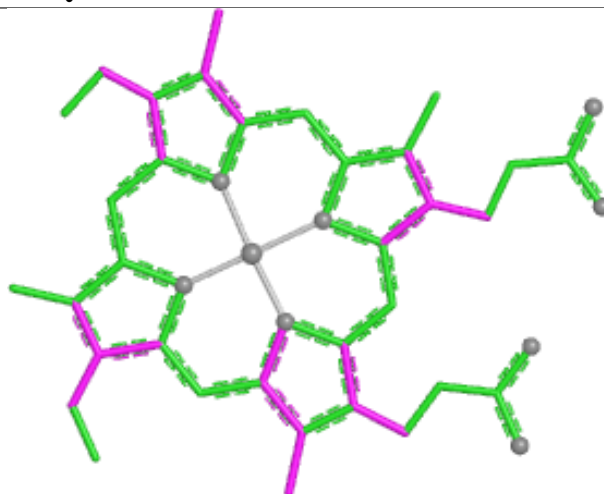




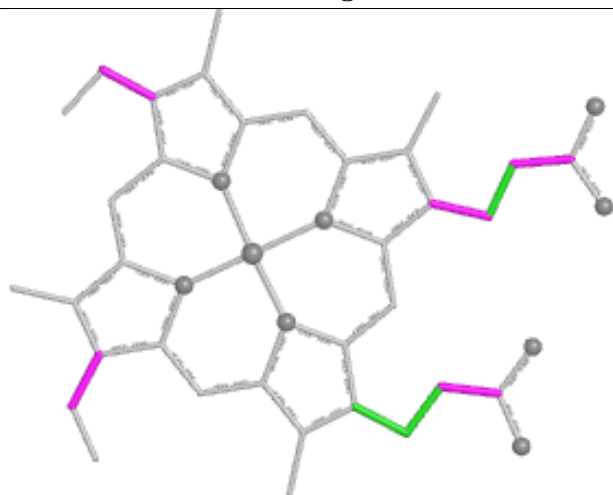
Ligand HEC Q 501



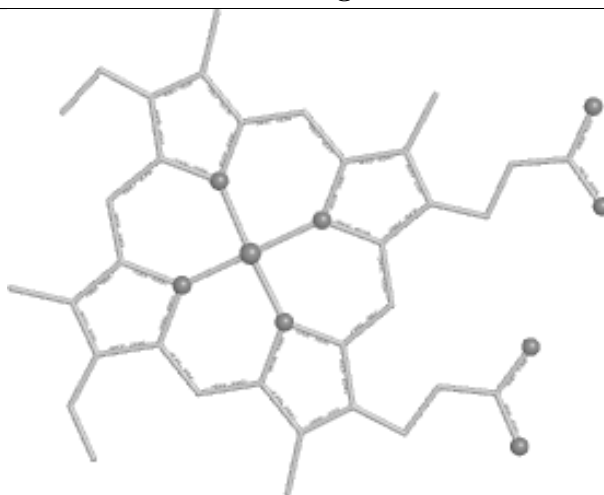
Bond lengths



Bond angles

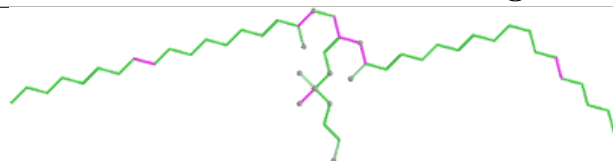


Torsions



Rings

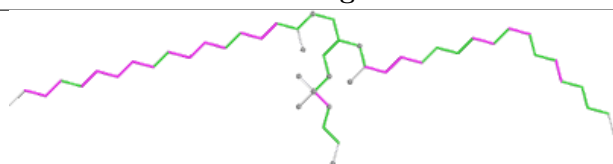
Ligand PEE C 2007



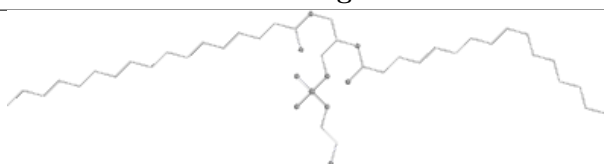
Bond lengths



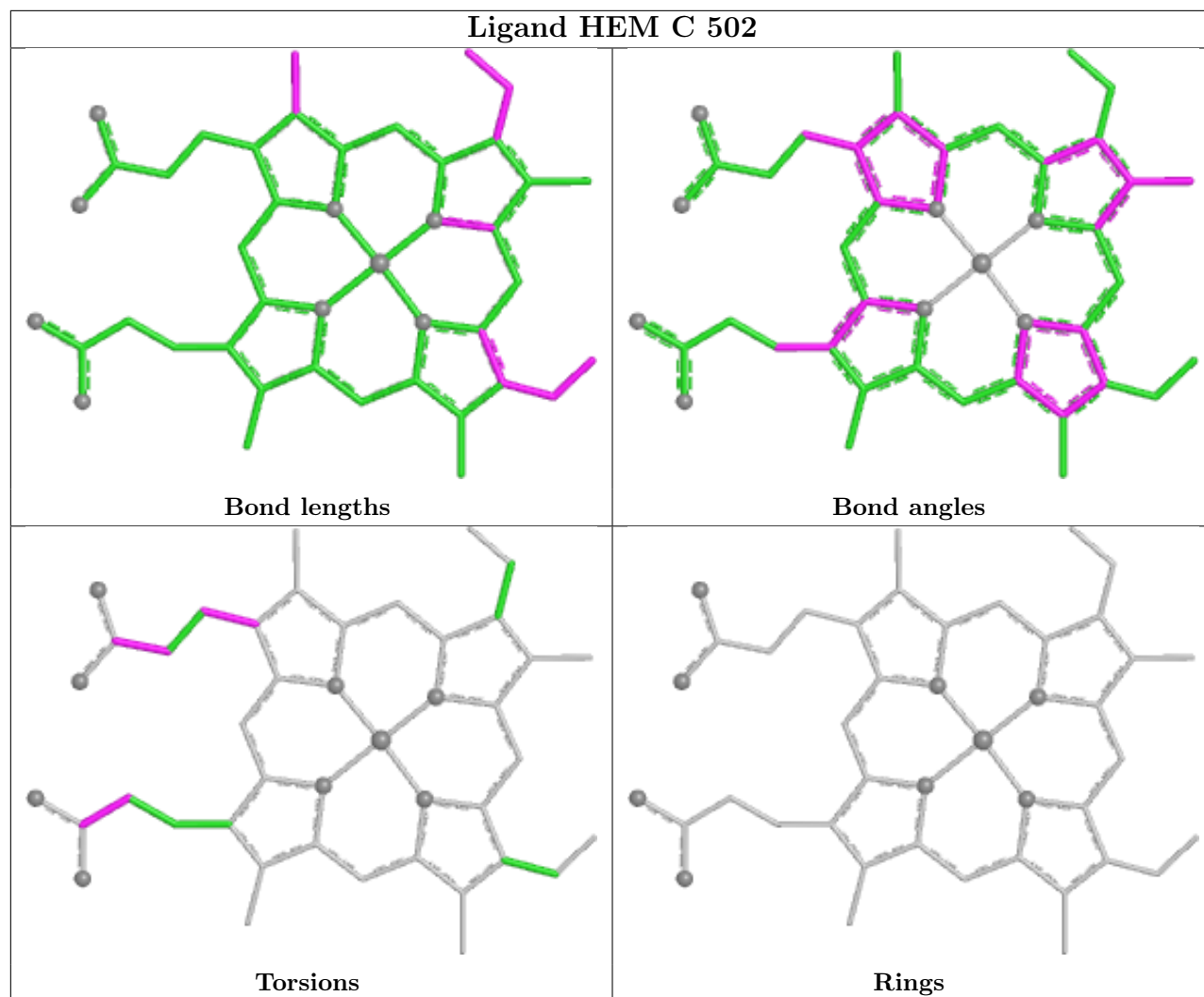
Bond angles

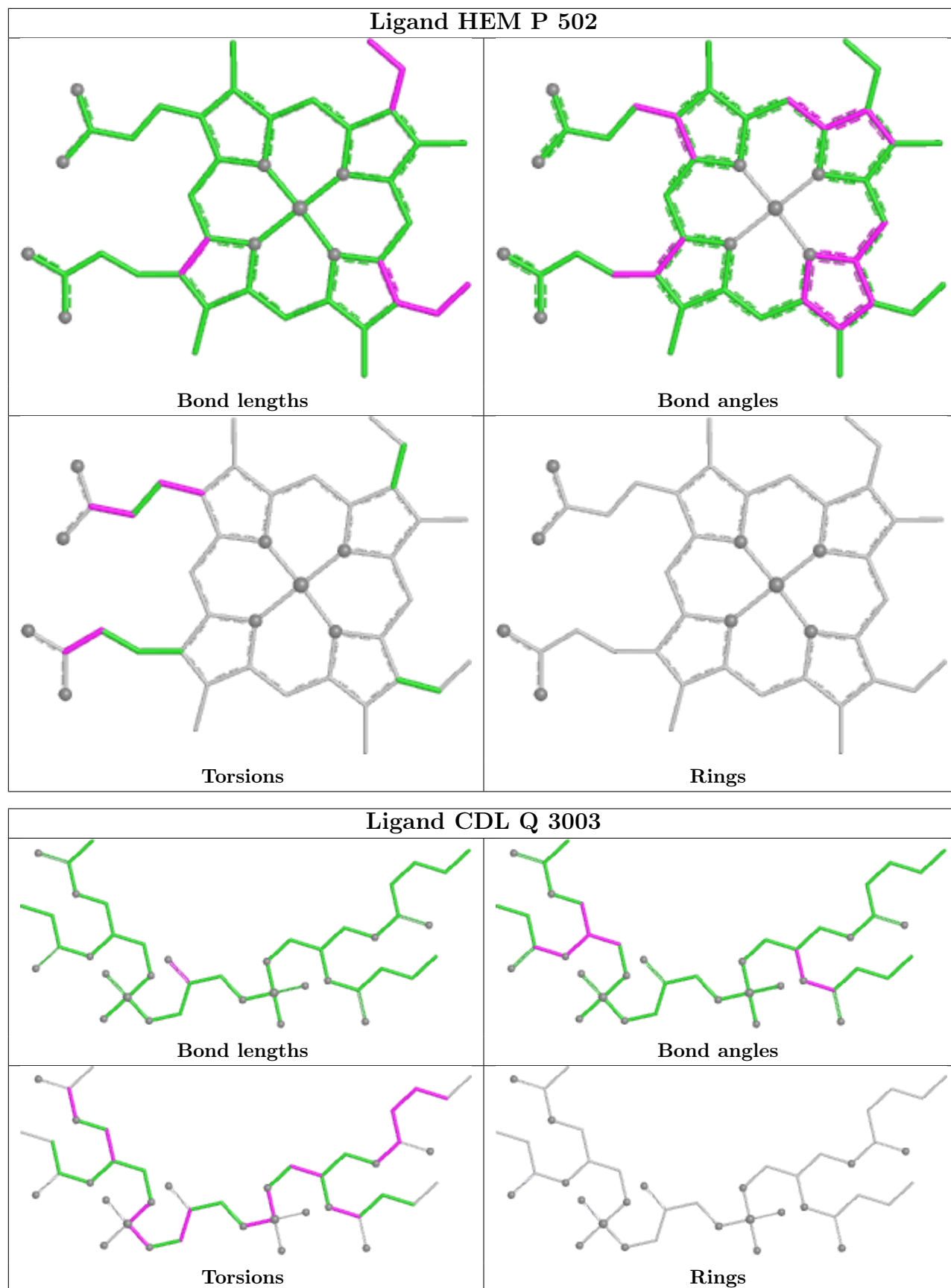


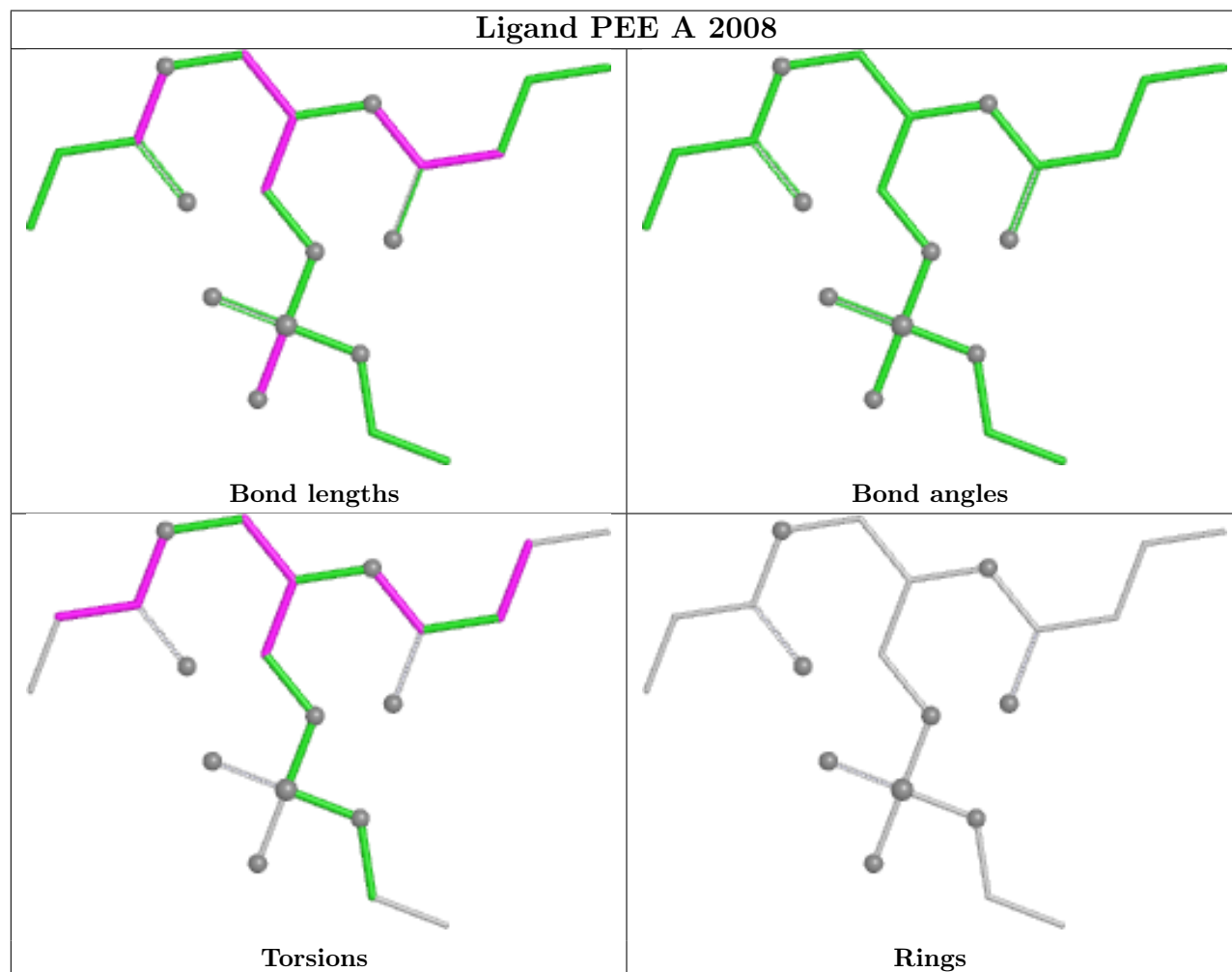
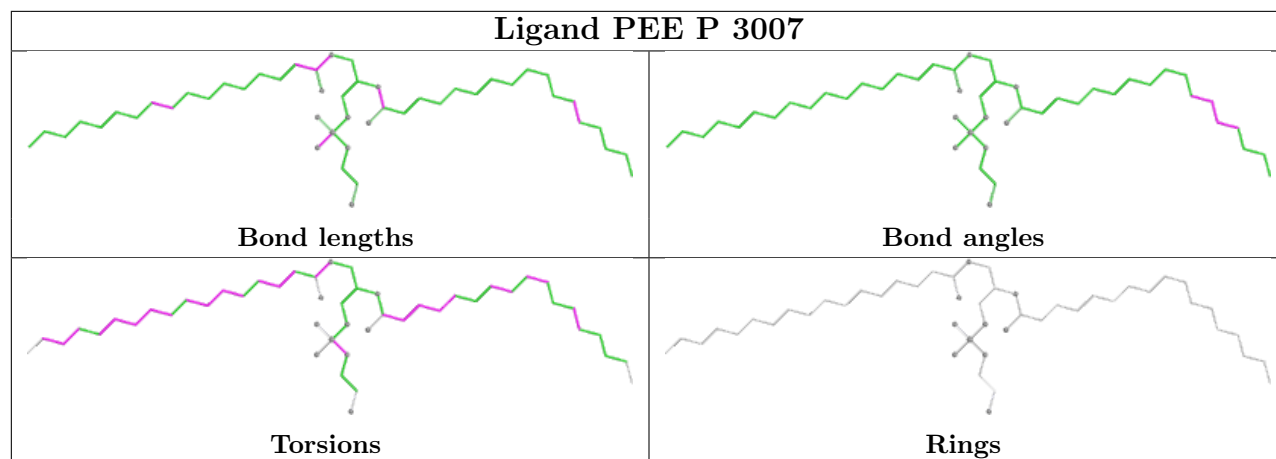
Torsions



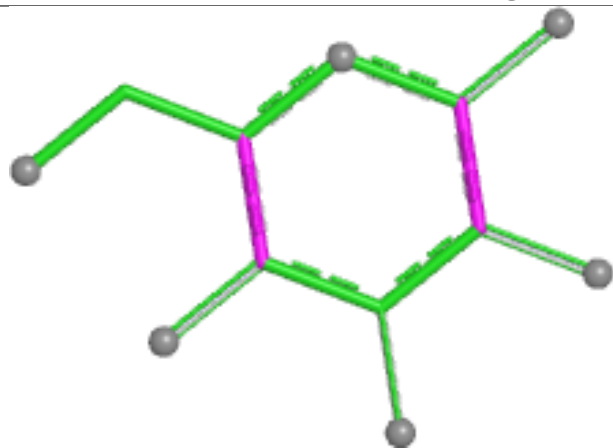
Rings



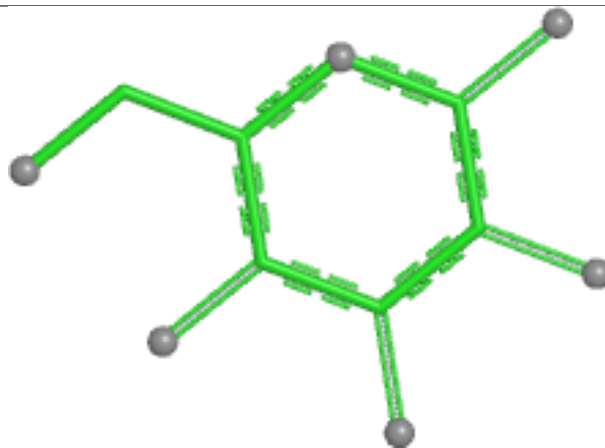




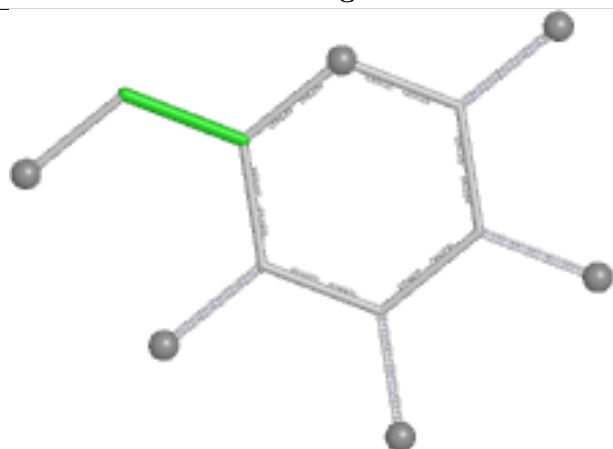
Ligand BOG P 2010



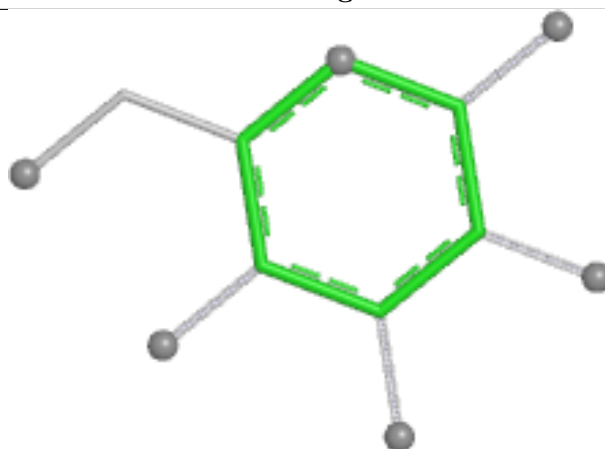
Bond lengths



Bond angles

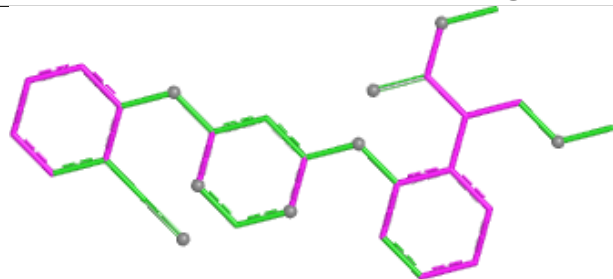


Torsions

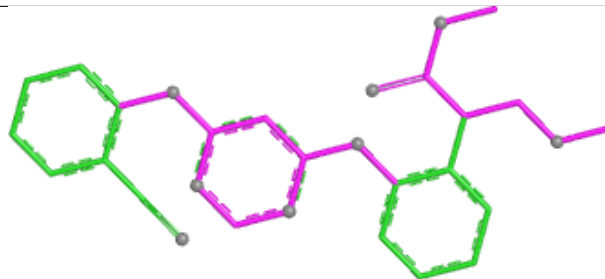


Rings

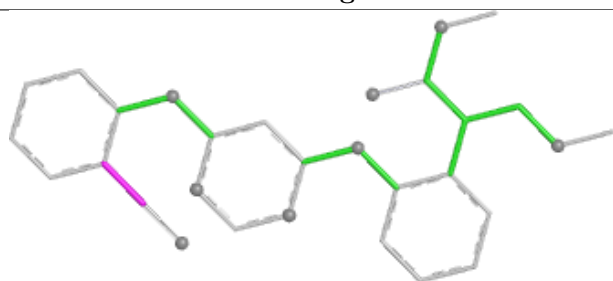
Ligand AZO C 2001



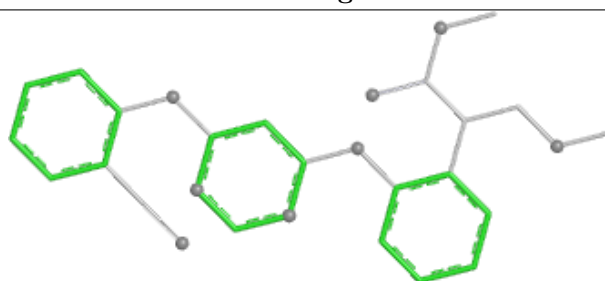
Bond lengths



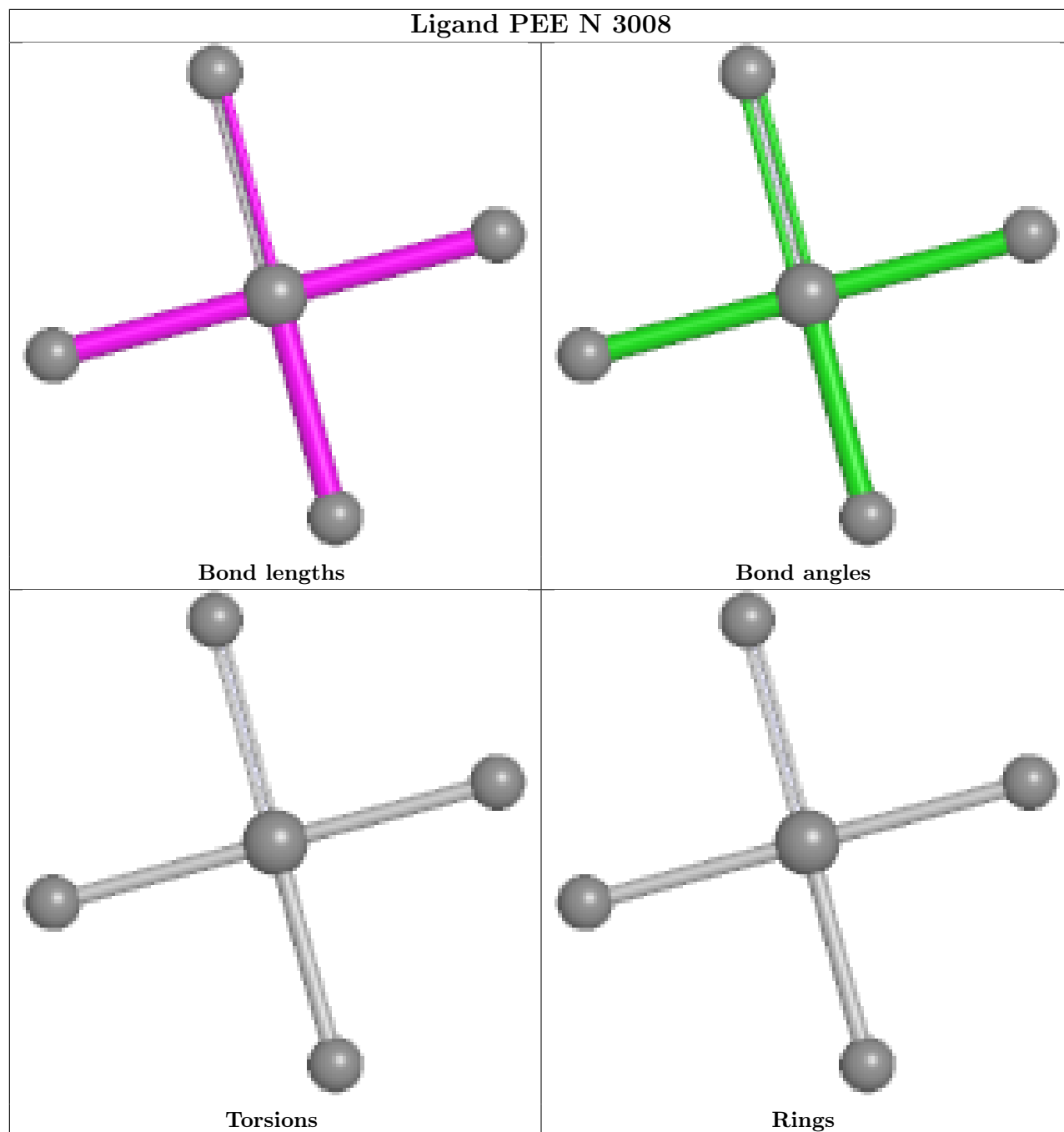
Bond angles

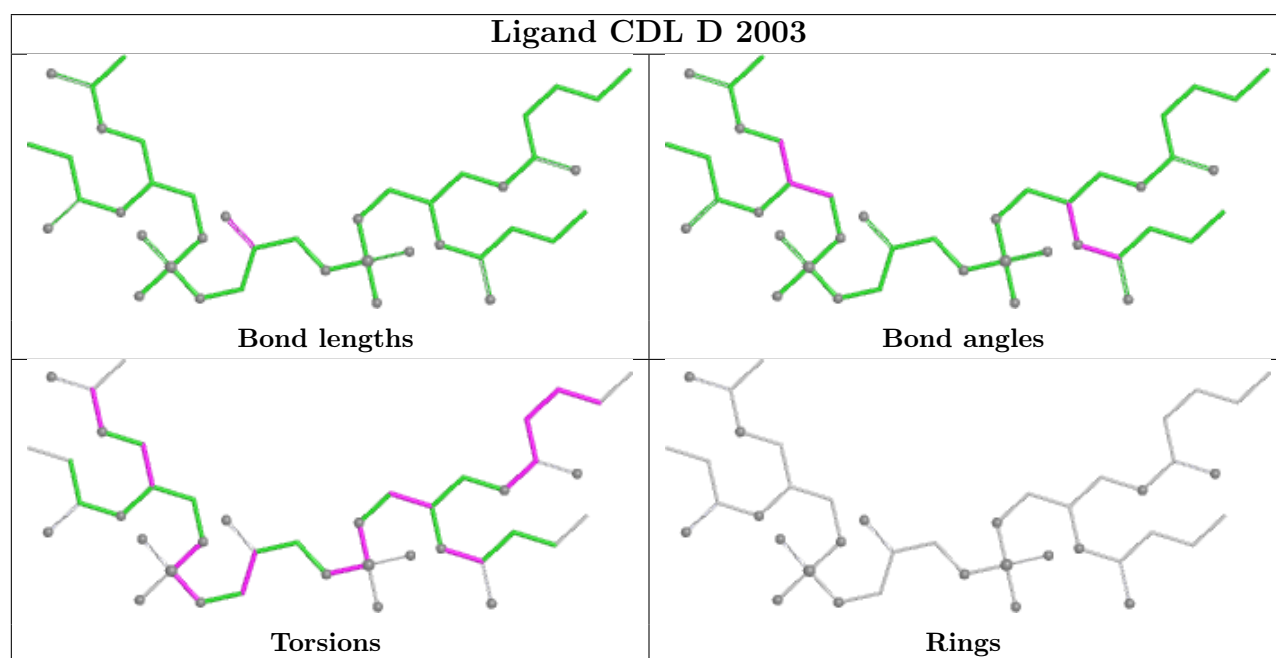
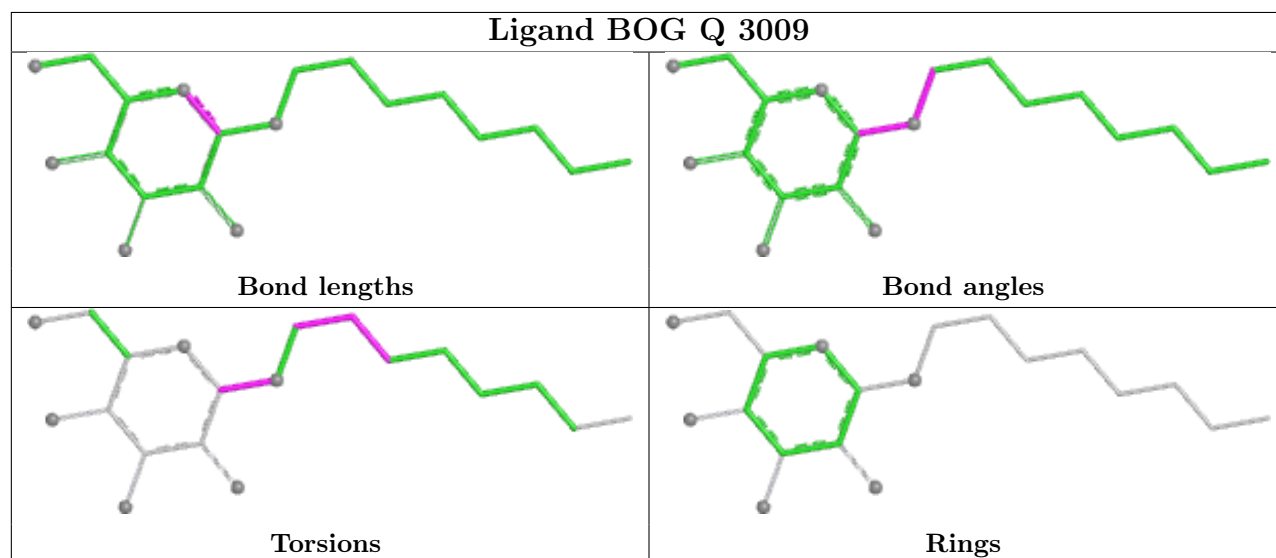
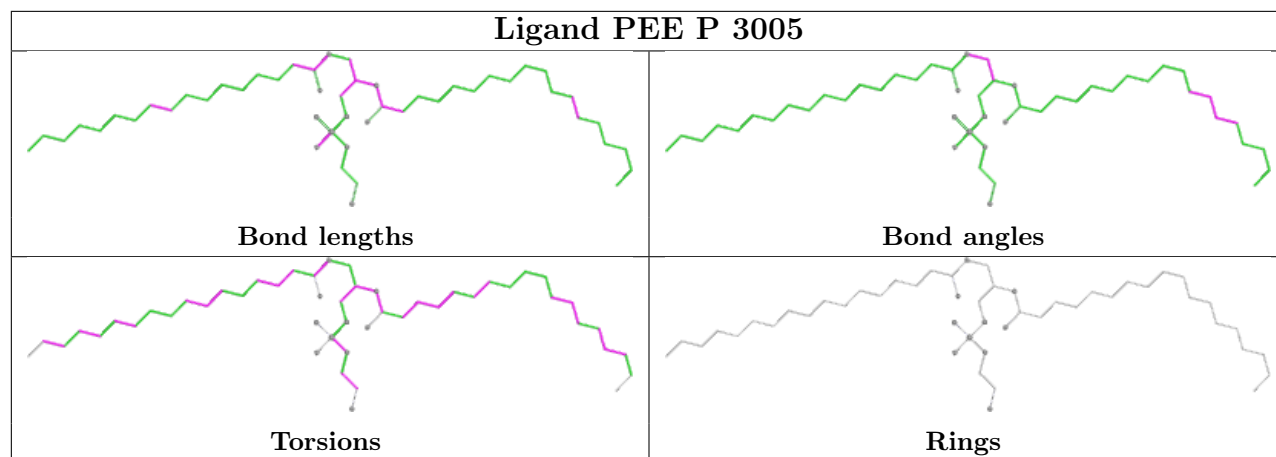


Torsions

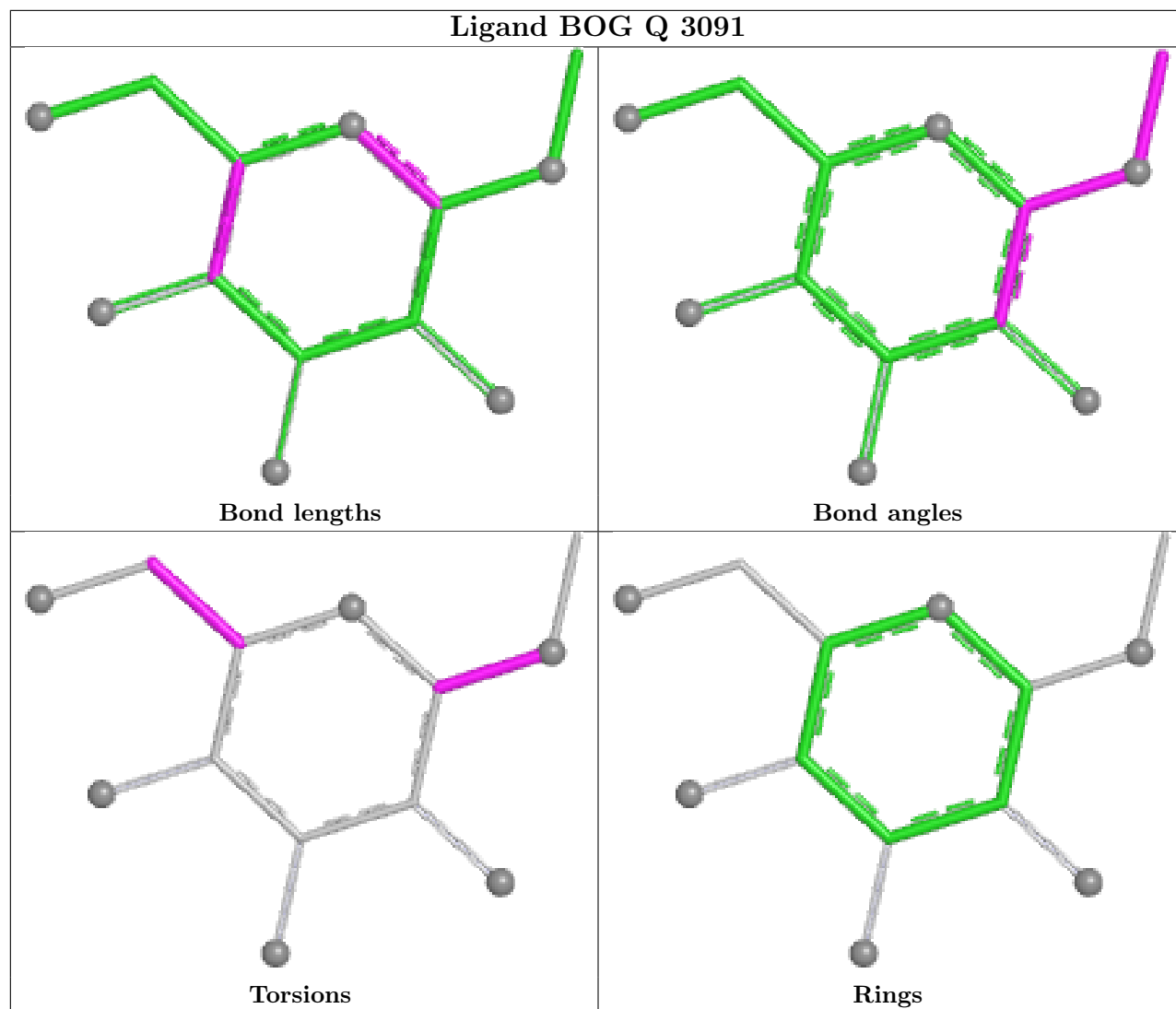


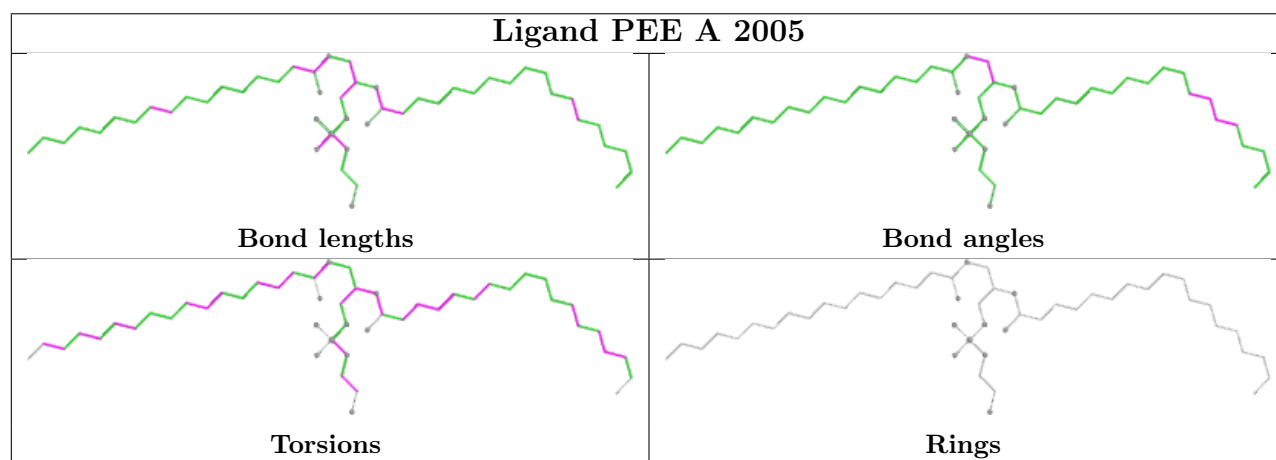
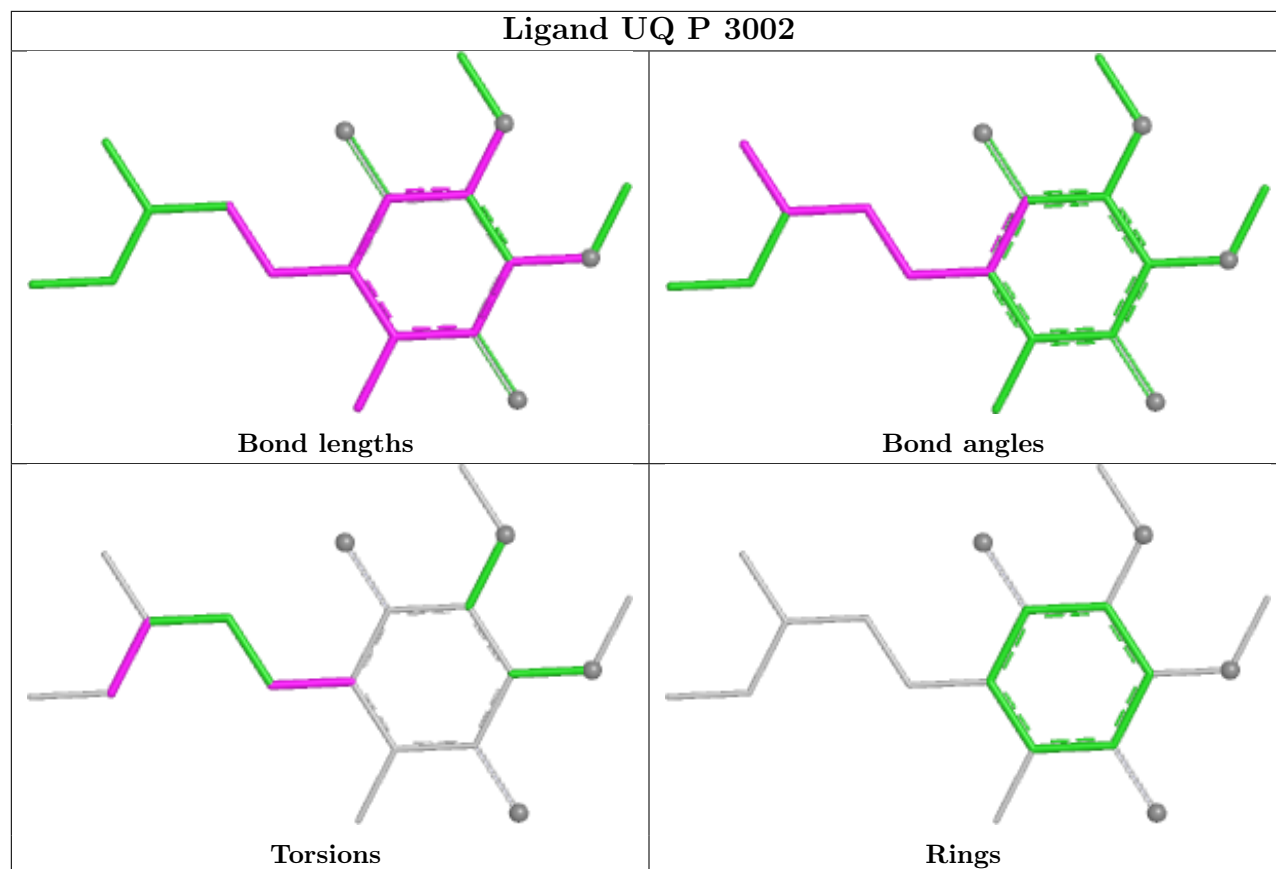
Rings

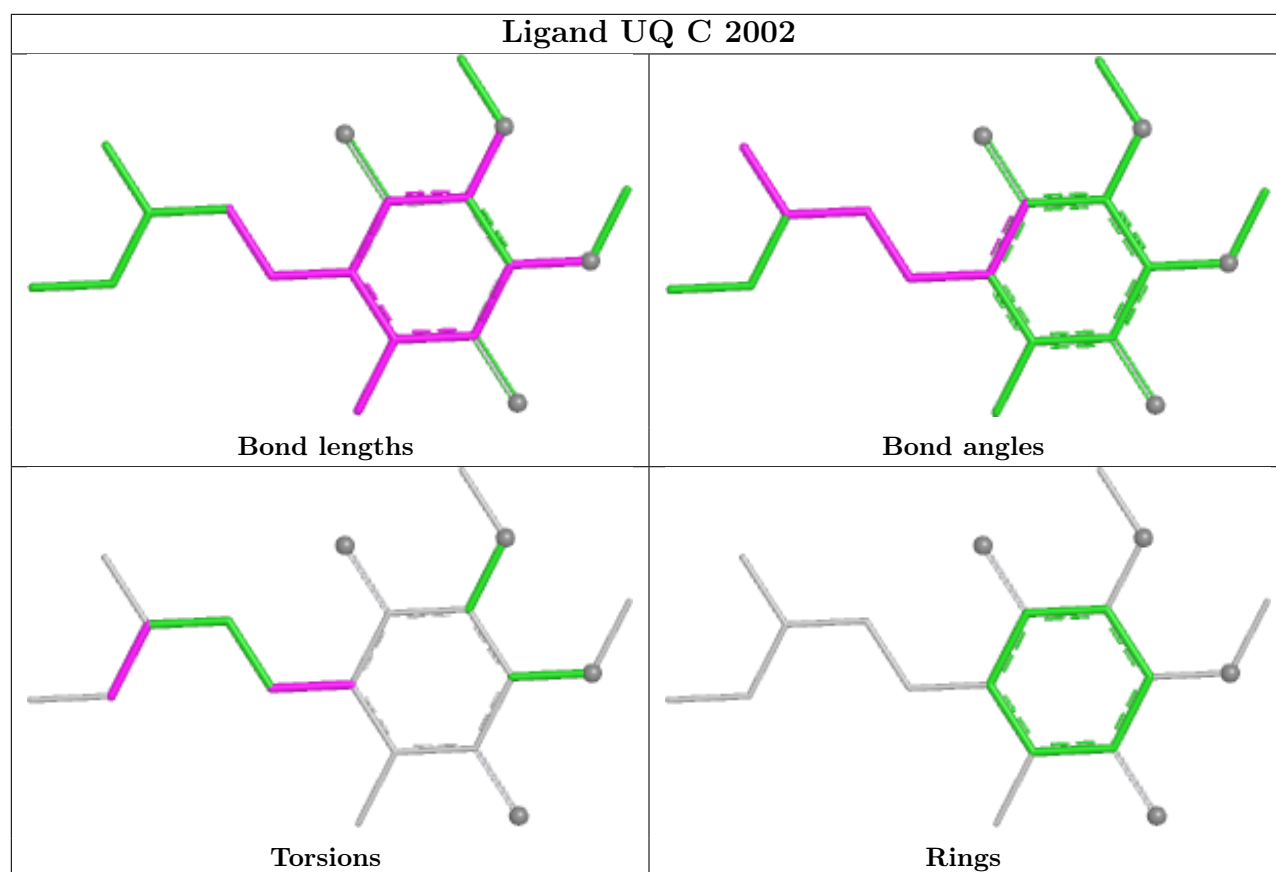


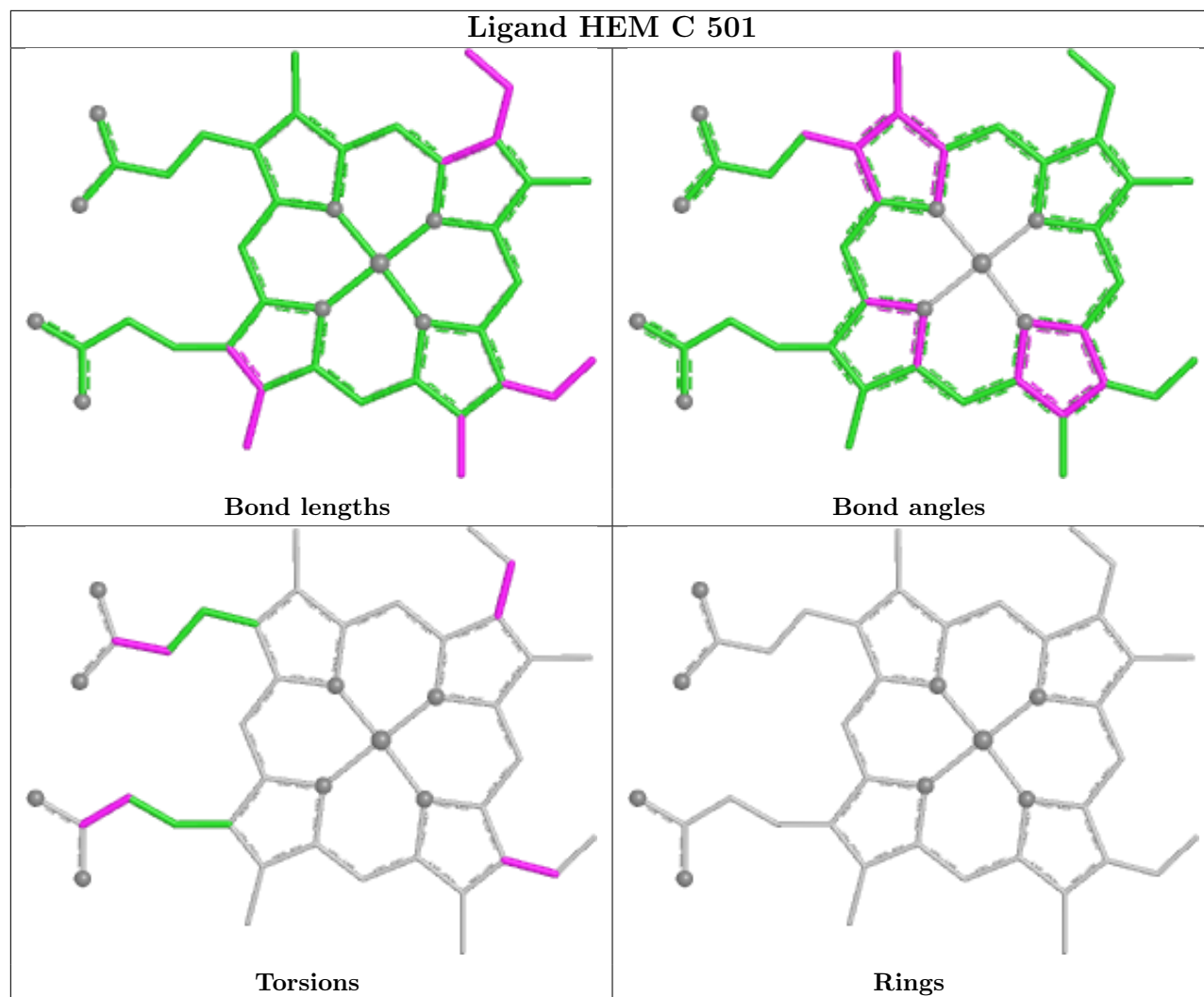


Ligand BOG Q 3091

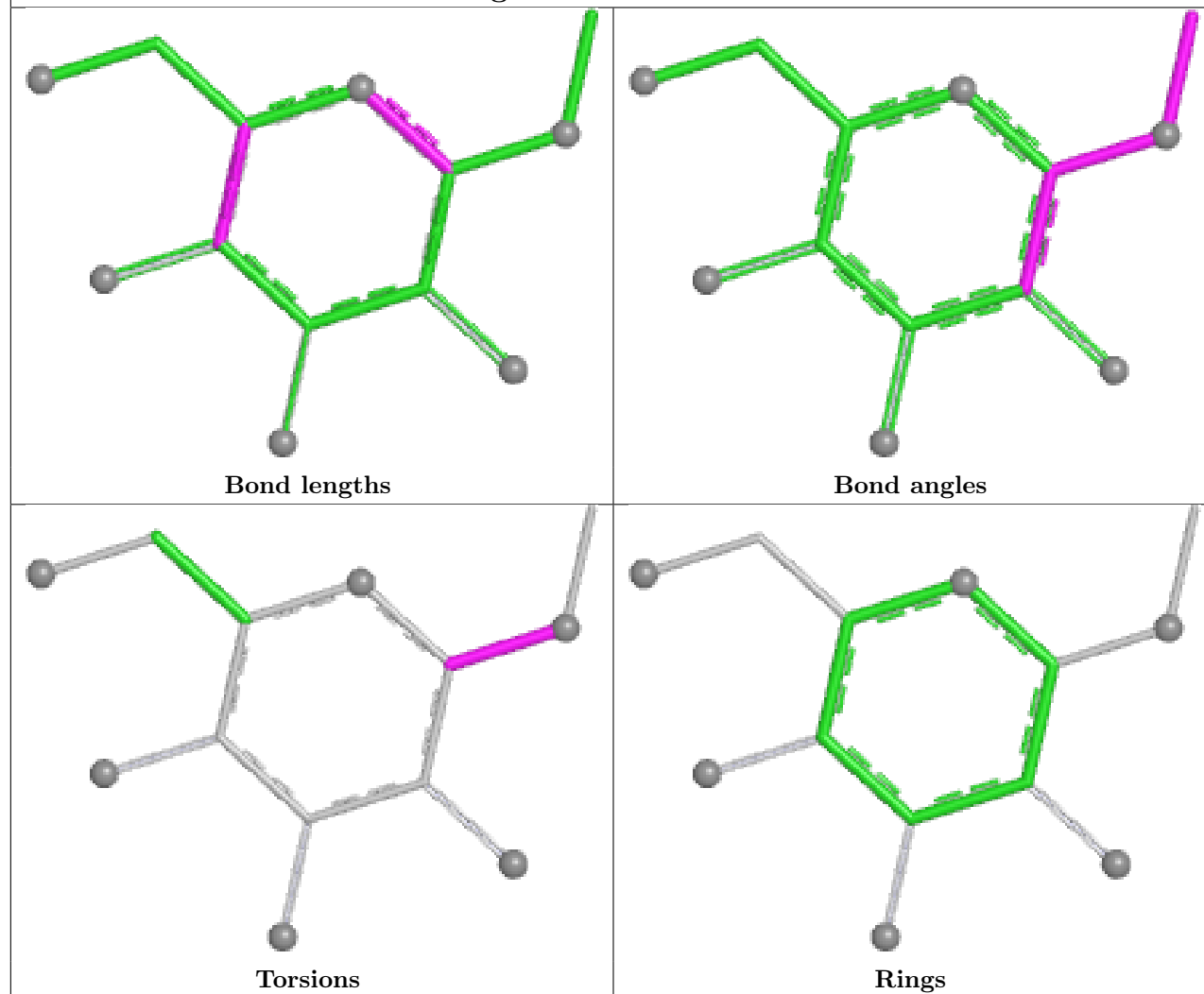




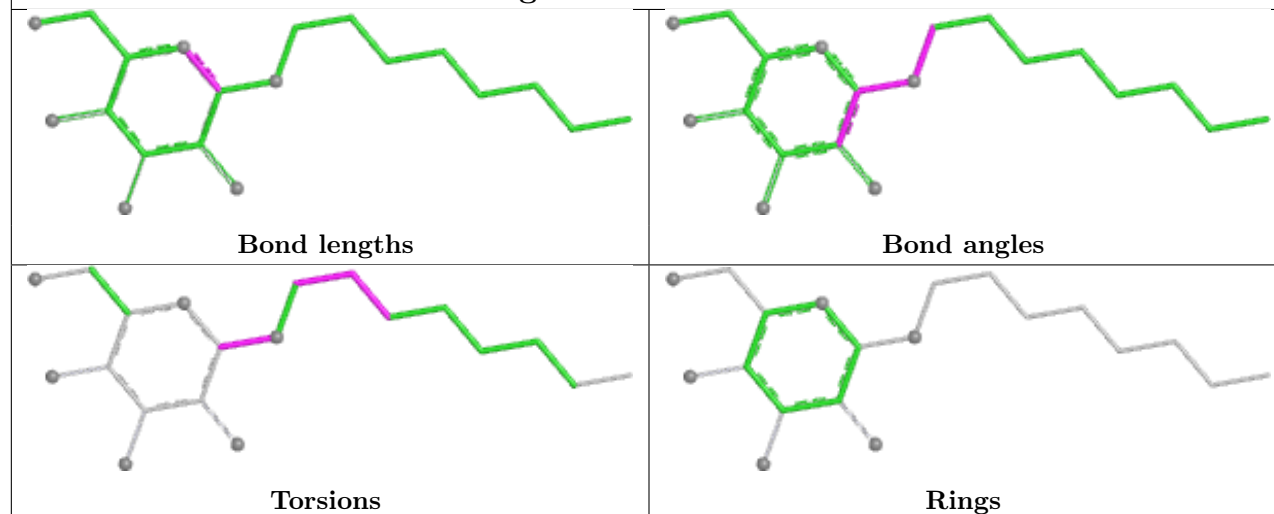


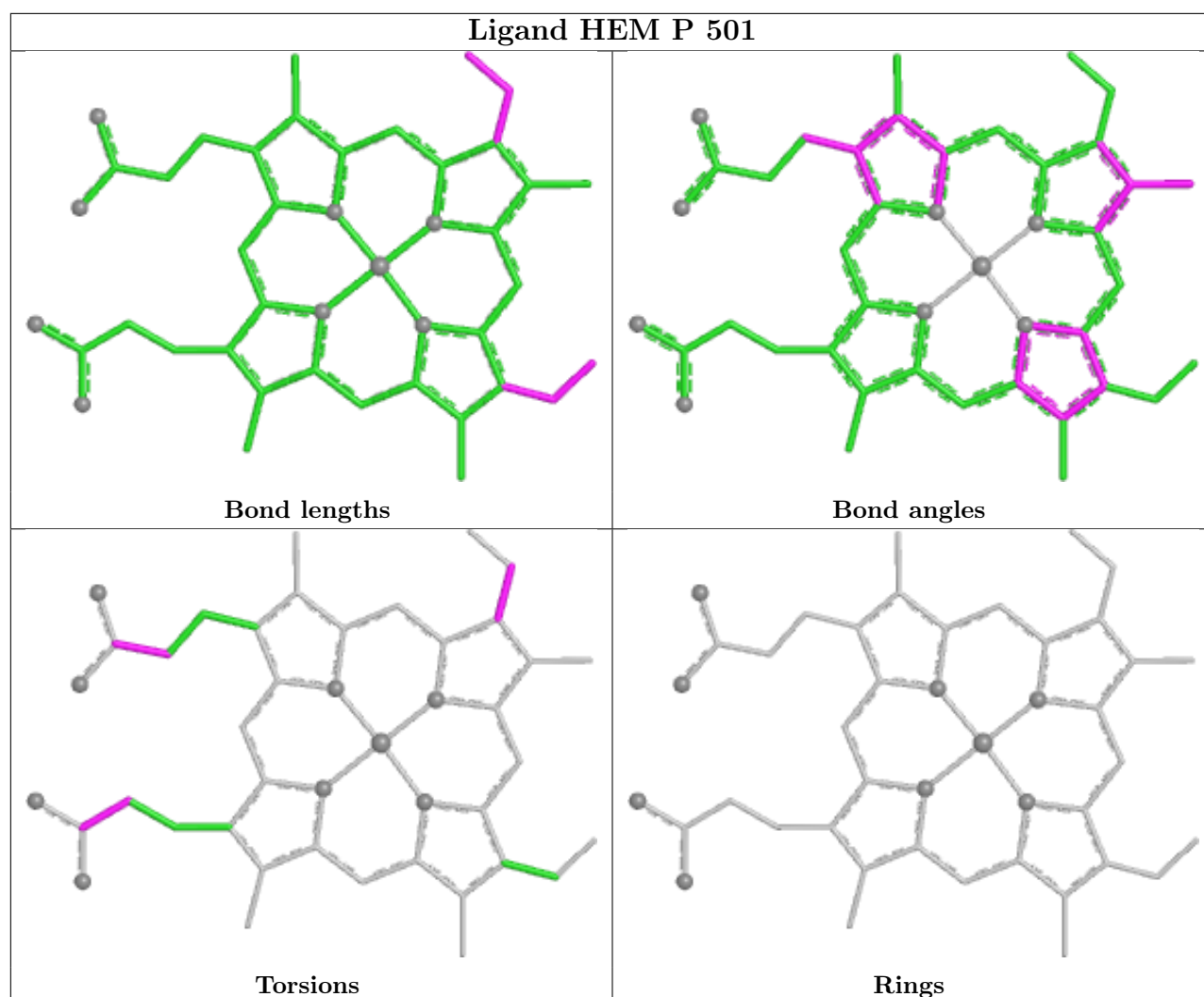


Ligand BOG D 2091



Ligand BOG D 2099





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	444/446 (99%)	0.22	12 (2%) 56 47	41, 68, 96, 110	0
1	N	442/446 (99%)	0.55	19 (4%) 40 31	48, 80, 103, 110	0
2	B	420/441 (95%)	0.66	16 (3%) 44 35	57, 87, 120, 142	0
2	O	422/441 (95%)	0.63	24 (5%) 29 22	49, 85, 113, 129	0
3	C	380/380 (100%)	-0.23	12 (3%) 50 40	30, 48, 88, 132	0
3	P	379/380 (99%)	0.12	7 (1%) 67 60	33, 63, 94, 132	0
4	D	241/241 (100%)	-0.27	1 (0%) 88 87	36, 51, 88, 109	0
4	Q	241/241 (100%)	0.33	3 (1%) 76 71	56, 76, 106, 127	0
5	E	196/196 (100%)	1.39	75 (38%) 1 0	41, 131, 160, 168	0
5	R	196/196 (100%)	0.89	24 (12%) 8 6	51, 95, 141, 153	0
6	F	101/110 (91%)	-0.31	0 100 100	38, 52, 70, 104	0
6	S	101/110 (91%)	0.37	3 (2%) 52 43	60, 74, 107, 131	0
7	G	80/81 (98%)	0.22	4 (5%) 34 27	42, 61, 106, 117	0
7	T	79/81 (97%)	0.68	5 (6%) 26 20	56, 85, 150, 159	0
8	H	70/77 (90%)	0.35	1 (1%) 73 67	45, 68, 91, 128	0
8	U	67/77 (87%)	1.22	9 (13%) 7 4	90, 117, 137, 141	0
9	I	31/47 (65%)	2.35	16 (51%) 0 0	80, 115, 142, 143	0
9	V	31/47 (65%)	2.65	18 (58%) 0 0	78, 115, 140, 145	0
10	J	61/61 (100%)	0.00	0 100 100	52, 65, 103, 147	0
10	W	60/61 (98%)	0.18	2 (3%) 49 39	63, 79, 109, 119	0
All	All	4042/4160 (97%)	0.41	251 (6%) 26 20	30, 73, 129, 168	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	7.9
9	V	56	SER	7.6
5	E	106	ILE	6.2
5	E	147	ILE	6.0
9	V	59	SER	5.9
2	B	226	ILE	5.9
5	E	120	PRO	5.7
2	O	226	ILE	5.4
9	I	47	ARG	5.3
5	R	196	GLY	5.2
9	I	61	ARG	5.1
5	E	98	VAL	4.9
8	H	9	GLU	4.8
9	I	63	ASP	4.8
9	V	58	ARG	4.7
1	N	444	ILE	4.7
9	I	49	LEU	4.6
5	R	167	ALA	4.6
3	C	4	ASN	4.6
7	G	2	ILE	4.6
5	E	183	PRO	4.5
5	E	143	GLY	4.4
5	E	104	ALA	4.3
2	B	20	GLY	4.3
7	T	2	ILE	4.3
5	E	167	ALA	4.2
5	E	124	LEU	4.2
9	V	50	LEU	4.2
5	E	109	GLU	4.2
5	E	97	PHE	4.0
1	A	444	ILE	3.9
9	V	60	ALA	3.9
9	V	49	LEU	3.9
8	U	24	CYS	3.9
5	E	117	LEU	3.9
5	R	124	LEU	3.8
3	P	380	TYR	3.8
5	E	180	LEU	3.8
9	V	57	GLY	3.8
5	E	177	PRO	3.8
1	A	28	GLU	3.8
7	G	32	ASP	3.7
5	E	82	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
5	E	168	SER	3.6
9	I	77	ARG	3.6
5	E	133	VAL	3.6
5	E	134	ILE	3.5
5	E	187	PHE	3.5
5	E	145	VAL	3.5
5	E	121	GLN	3.4
8	U	68	CYS	3.4
9	V	61	ARG	3.4
1	N	122	LEU	3.4
5	E	112	VAL	3.4
9	I	51	CYS	3.4
1	A	432	LEU	3.4
5	E	173	LYS	3.4
5	R	155	GLY	3.3
5	E	159	PRO	3.3
9	V	62	ARG	3.3
5	E	85	LYS	3.2
3	C	345	GLU	3.2
5	R	114	VAL	3.2
5	E	178	TYR	3.2
5	E	181	GLU	3.2
5	E	157	TYR	3.2
9	I	50	LEU	3.2
5	E	108	GLN	3.2
5	E	182	VAL	3.1
2	O	21	ALA	3.1
5	E	79	SER	3.1
5	R	154	GLY	3.1
5	E	184	THR	3.1
2	O	383	GLY	3.0
7	G	81	GLN	3.0
5	E	170	ARG	3.0
1	N	432	LEU	3.0
5	E	142	LEU	3.0
2	B	232	THR	3.0
1	N	26	ALA	3.0
9	V	64	LEU	3.0
5	E	114	VAL	3.0
5	E	118	ARG	3.0
1	A	392	LEU	3.0
5	E	87	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	135	LEU	2.9
5	E	169	GLY	2.9
4	Q	142	VAL	2.9
5	E	156	TYR	2.9
2	O	110	GLU	2.9
1	N	179	ARG	2.9
2	B	224	LEU	2.9
2	O	224	LEU	2.9
5	R	156	TYR	2.8
9	I	71	ASN	2.8
7	G	3	HIS	2.8
5	R	115	SER	2.8
8	U	76	LYS	2.8
2	O	156	GLN	2.8
3	C	380	TYR	2.8
5	E	136	VAL	2.8
9	V	77	ARG	2.8
9	V	53	GLU	2.8
1	N	223	TYR	2.8
9	I	64	LEU	2.8
5	R	178	TYR	2.7
5	E	102	THR	2.7
2	O	296	TYR	2.7
3	C	9	HIS	2.7
7	T	77	TYR	2.7
2	B	230	ALA	2.7
3	P	2	ALA	2.7
1	N	120	CYS	2.7
9	V	47	ARG	2.7
5	E	113	ASP	2.7
5	E	194	VAL	2.7
5	E	192	LEU	2.7
5	E	101	ARG	2.6
9	I	62	ARG	2.6
8	U	78	LYS	2.6
8	U	37	LEU	2.6
1	N	127	ILE	2.6
1	A	226	ASP	2.6
5	E	150	SER	2.6
2	O	371	SER	2.6
1	N	380	GLY	2.6
4	D	1	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	185	TYR	2.6
5	E	88	ALA	2.6
5	E	107	ASN	2.6
5	E	110	ALA	2.6
5	E	128	LYS	2.5
5	E	153	PHE	2.5
9	V	52	ARG	2.5
10	W	45	HIS	2.5
3	C	10	PRO	2.5
7	T	8	ALA	2.5
5	E	122	HIS	2.5
1	N	190	PHE	2.5
9	I	52	ARG	2.5
6	S	36	THR	2.5
4	Q	241	LYS	2.5
2	O	344	LEU	2.4
5	E	127	VAL	2.4
5	R	84	GLY	2.4
3	C	5	ILE	2.4
2	O	355	GLU	2.4
5	R	85	LYS	2.4
7	T	4	PHE	2.4
9	V	71	ASN	2.4
3	C	3	PRO	2.4
5	R	171	ILE	2.4
2	O	279	LEU	2.4
8	U	13	LEU	2.4
6	S	10	GLY	2.4
5	E	89	PHE	2.4
5	R	105	GLU	2.4
2	B	220	ALA	2.4
9	I	56	SER	2.4
5	E	175	PRO	2.4
5	E	154	GLY	2.3
1	A	433	ASP	2.3
9	I	53	GLU	2.3
2	B	216	LEU	2.3
3	P	5	ILE	2.3
4	Q	9	ALA	2.3
9	I	72	ALA	2.3
2	O	430	LEU	2.3
2	B	402	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
9	V	76	VAL	2.3
1	N	56	GLY	2.3
7	T	79	ASN	2.3
2	O	335	GLU	2.3
5	E	191	ASP	2.3
1	N	185	TYR	2.3
5	R	126	ARG	2.3
5	R	165	TYR	2.3
5	E	193	VAL	2.3
5	E	152	ASP	2.3
3	C	156	TYR	2.3
5	R	133	VAL	2.3
2	O	103	GLU	2.2
5	E	149	ASN	2.2
5	R	104	ALA	2.2
1	N	392	LEU	2.2
9	I	70	LEU	2.2
5	R	134	ILE	2.2
1	N	376	CYS	2.2
1	N	39	VAL	2.2
2	B	30	PRO	2.2
5	R	146	PRO	2.2
5	E	99	ARG	2.2
2	O	292	THR	2.2
5	R	175	PRO	2.2
2	B	368	TYR	2.2
2	O	289	SER	2.2
3	P	224	TYR	2.2
5	E	163	SER	2.2
6	S	13	MET	2.2
9	V	55	MET	2.2
1	A	86	PHE	2.2
5	R	5	VAL	2.2
1	A	443	TRP	2.2
3	C	8	SER	2.2
1	N	182	LEU	2.2
8	U	73	LEU	2.2
5	E	171	ILE	2.2
1	A	365	MET	2.2
2	O	238	THR	2.2
5	E	84	GLY	2.2
5	E	165	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	186	GLN	2.1
1	A	219	VAL	2.1
2	O	308	ASP	2.1
5	R	157	TYR	2.1
3	P	244	ALA	2.1
3	P	15	ILE	2.1
5	R	106	ILE	2.1
2	O	250	HIS	2.1
5	E	164	HIS	2.1
1	N	129	LYS	2.1
2	B	229	GLY	2.1
3	C	11	LEU	2.1
1	N	443	TRP	2.1
2	O	386	ALA	2.1
5	E	172	ARG	2.1
8	U	36	ARG	2.1
10	W	61	ALA	2.1
3	P	4	ASN	2.1
2	O	229	GLY	2.1
1	N	216	PHE	2.1
3	C	14	MET	2.1
5	E	116	LYS	2.1
1	A	107	PRO	2.1
5	R	82	PRO	2.1
2	O	387	LEU	2.1
2	B	94	GLY	2.1
9	I	58	ARG	2.1
2	B	35	ILE	2.1
2	B	386	ALA	2.1
1	A	31	SER	2.0
5	E	188	VAL	2.0
5	E	146	PRO	2.0
5	E	105	GLU	2.0
2	B	289	SER	2.0
2	O	193	HIS	2.0
5	E	103	GLN	2.0
2	B	388	LEU	2.0
8	U	20	ILE	2.0
2	O	232	THR	2.0
3	C	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

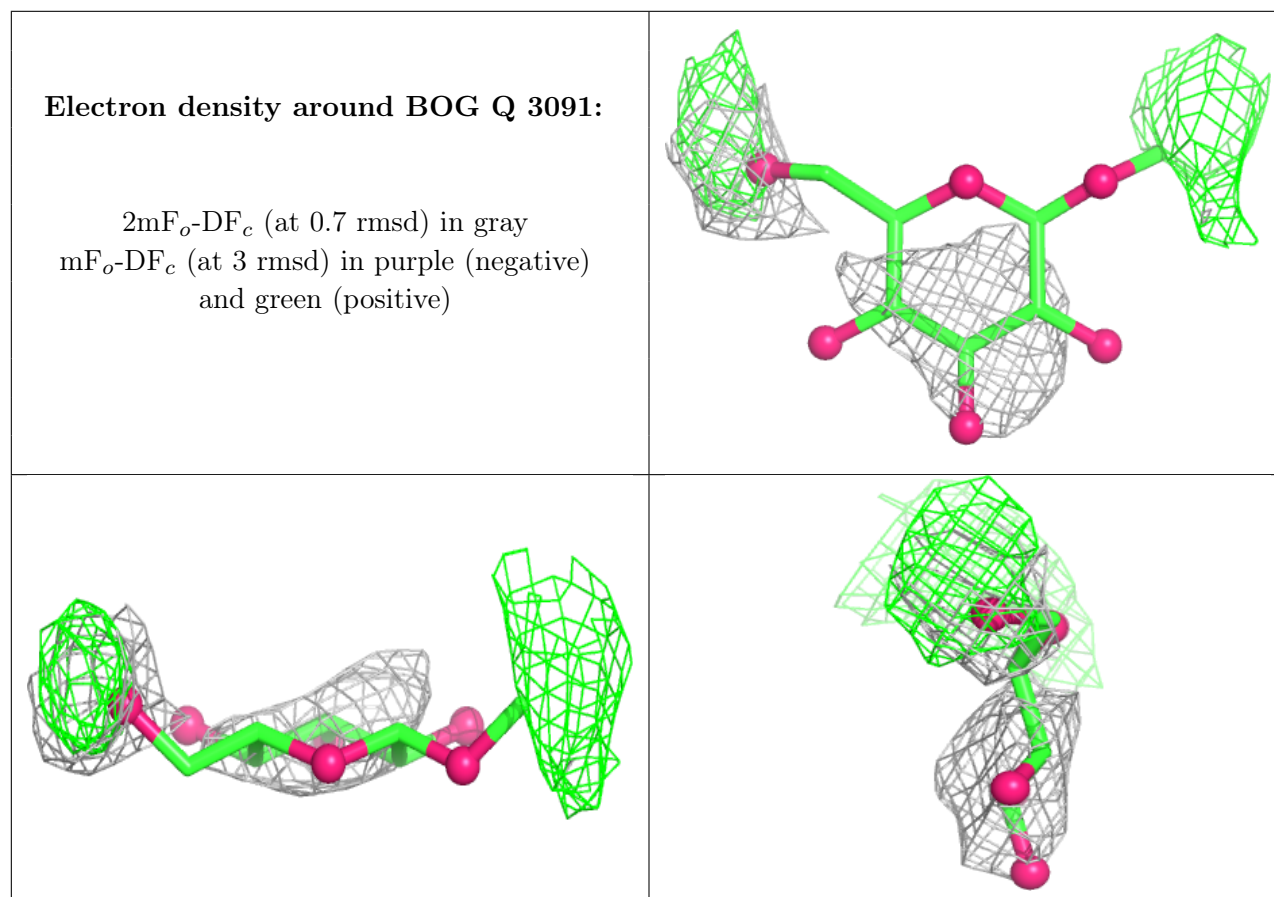
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	BOG	Q	3091	13/20	0.36	0.34	192,194,195,195	0
11	PEE	A	2008	21/51	0.46	0.30	132,136,139,140	0
18	BOG	P	2010	12/20	0.61	0.29	140,143,144,145	0
18	BOG	D	2091	13/20	0.70	0.35	207,208,208,208	0
11	PEE	N	3008	5/51	0.72	0.14	110,111,112,112	0
17	CDL	Q	3003	42/100	0.82	0.24	117,129,145,145	0
17	CDL	T	3004	40/100	0.83	0.18	97,104,113,114	0
14	UQ	P	3002	19/63	0.83	0.37	126,136,137,137	0
11	PEE	P	3005	50/51	0.84	0.28	92,105,114,115	0
17	CDL	D	2003	42/100	0.85	0.20	92,101,111,114	0
14	UQ	C	2002	19/63	0.86	0.27	91,92,94,95	0
11	PEE	A	2005	50/51	0.88	0.23	79,96,106,107	0
15	GOL	C	2011	6/6	0.88	0.27	80,84,85,86	0
17	CDL	G	2004	40/100	0.89	0.15	73,85,100,101	0
15	GOL	P	3011	6/6	0.90	0.22	84,86,87,88	0
18	BOG	Q	3009	20/20	0.90	0.17	74,89,91,93	0
11	PEE	P	3007	49/51	0.90	0.20	74,88,100,101	0
19	FES	E	501	4/4	0.90	0.10	153,153,154,154	0
18	BOG	D	2009	20/20	0.93	0.11	60,72,75,76	0
13	AZO	P	3001	30/30	0.93	0.13	52,60,66,67	0
11	PEE	C	2007	49/51	0.94	0.15	46,67,84,85	0
13	AZO	C	2001	30/30	0.95	0.09	36,39,41,41	0
16	HEC	Q	501	43/43	0.97	0.10	60,65,71,72	0
16	HEC	D	501	43/43	0.98	0.07	31,37,45,48	0
12	HEM	P	501	43/43	0.98	0.09	42,49,60,64	0
12	HEM	P	502	43/43	0.98	0.08	38,47,58,60	0
19	FES	R	501	4/4	0.98	0.04	88,89,90,91	0

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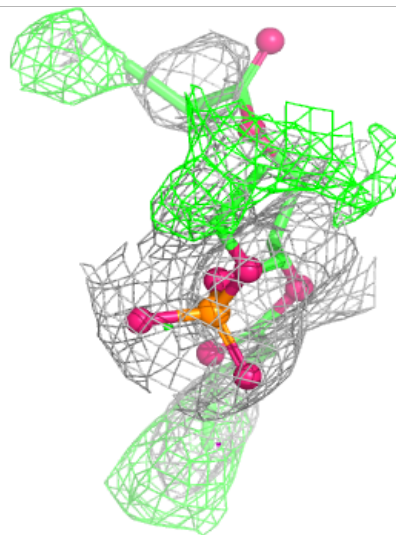
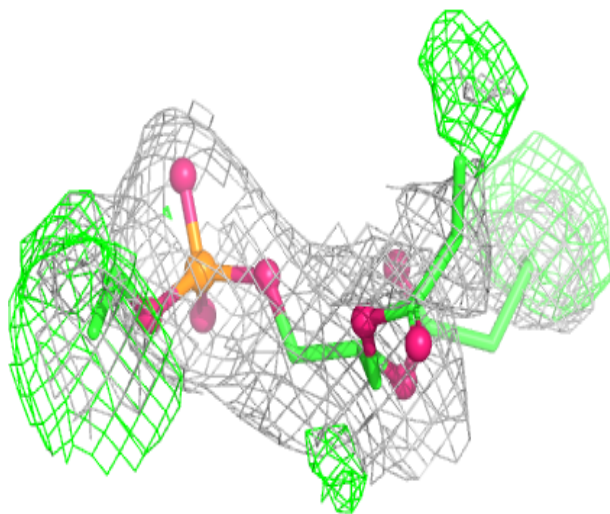
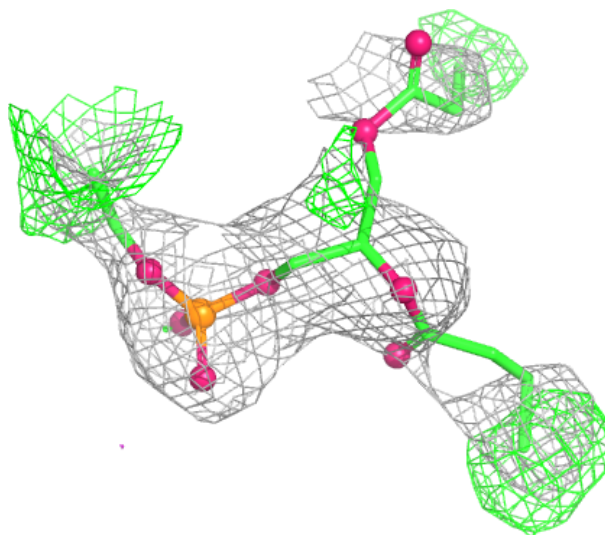
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	HEM	C	502	43/43	0.99	0.08	32,37,47,54	0
12	HEM	C	501	43/43	0.99	0.08	35,40,50,55	0

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.



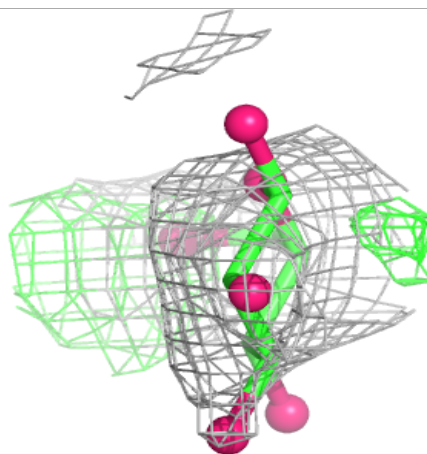
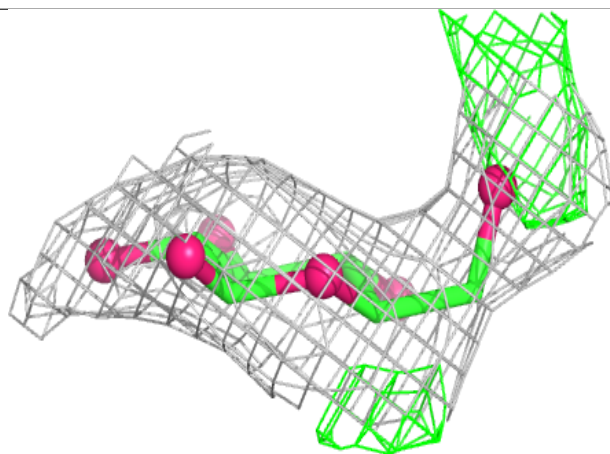
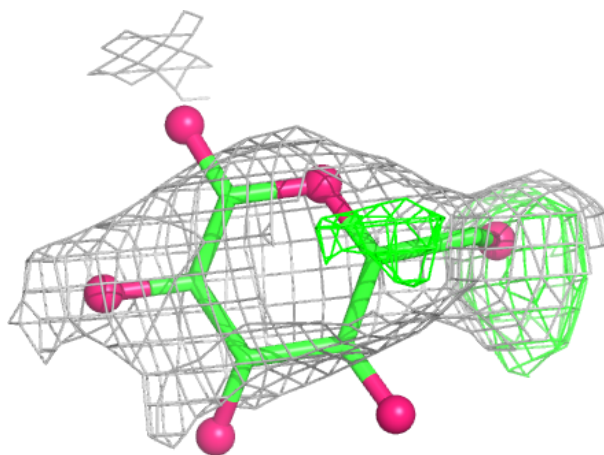
Electron density around PEE A 2008:

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



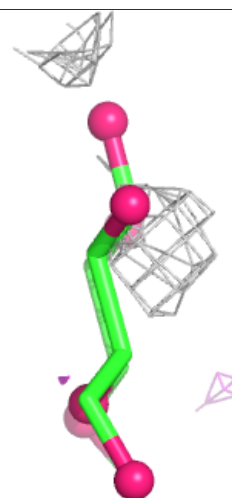
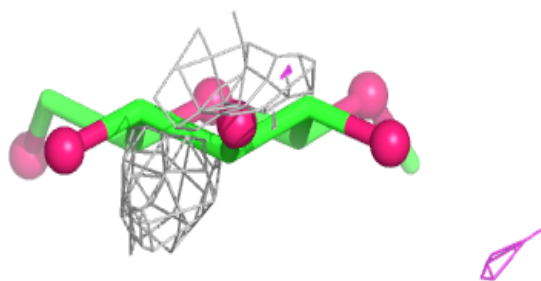
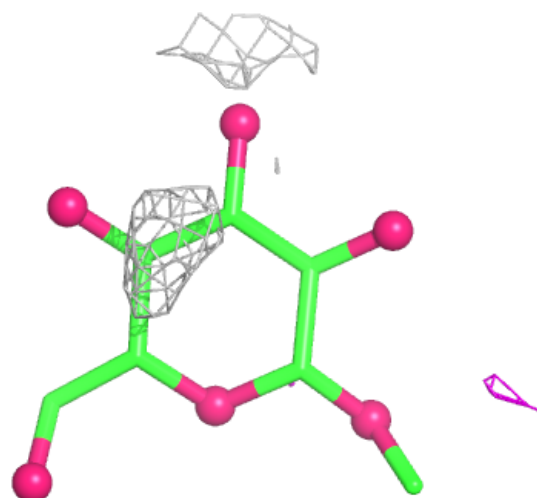
Electron density around BOG P 2010:

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



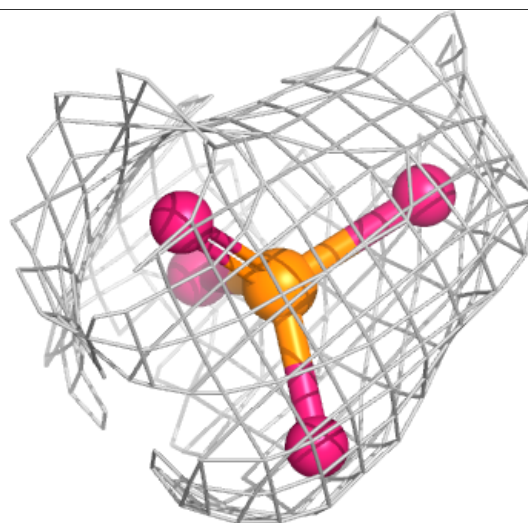
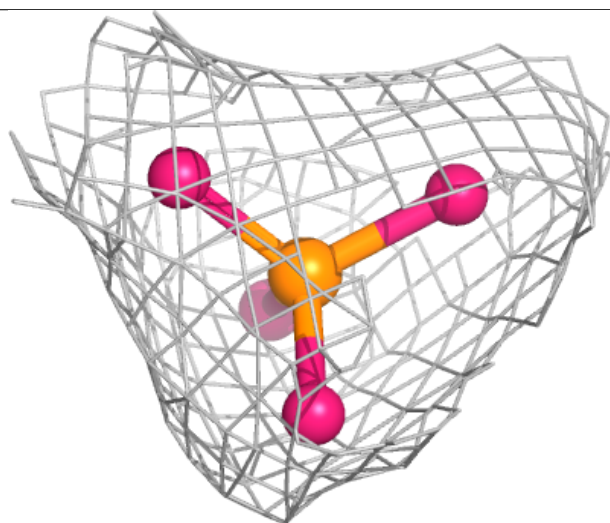
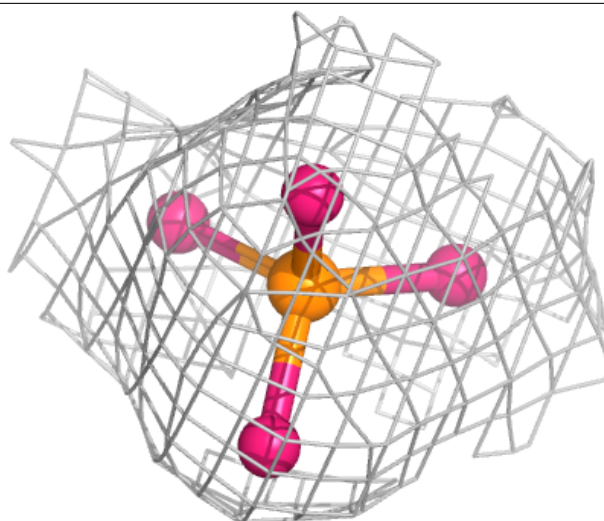
Electron density around BOG D 2091:

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



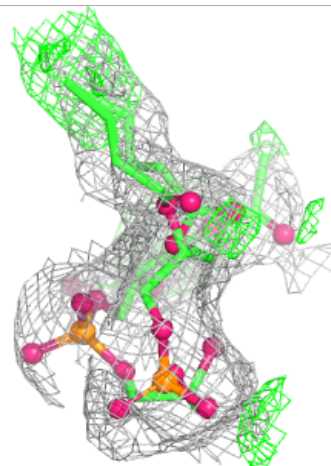
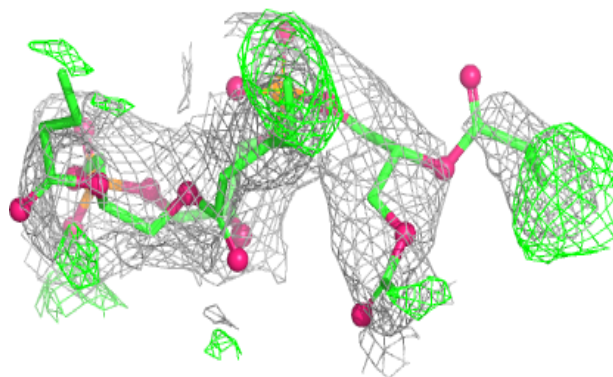
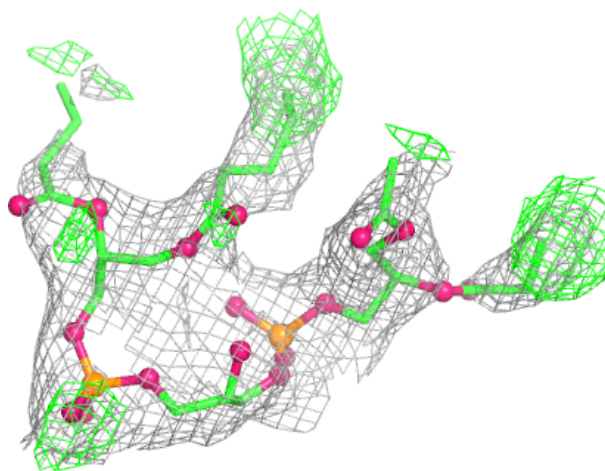
Electron density around PEE N 3008:

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



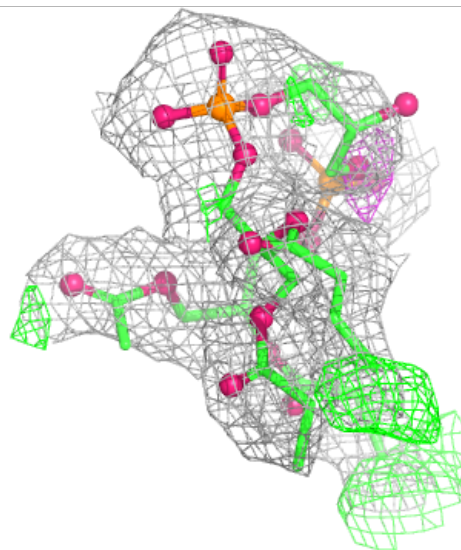
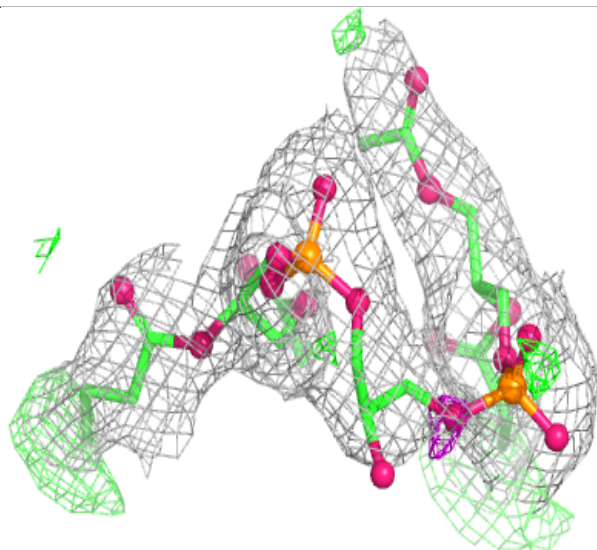
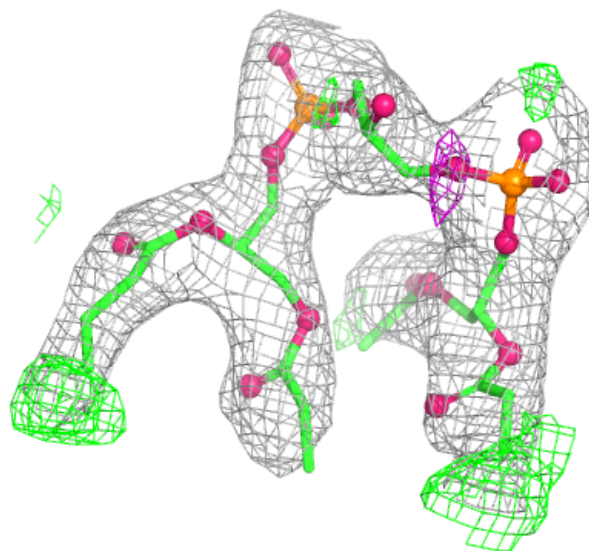
Electron density around CDL Q 3003:

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



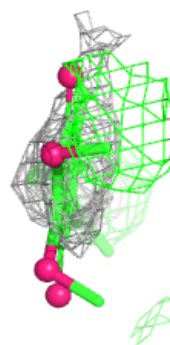
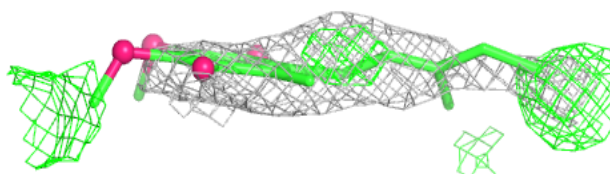
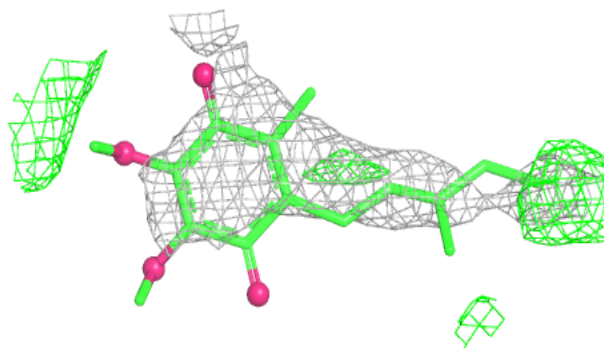
Electron density around CDL T 3004:

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

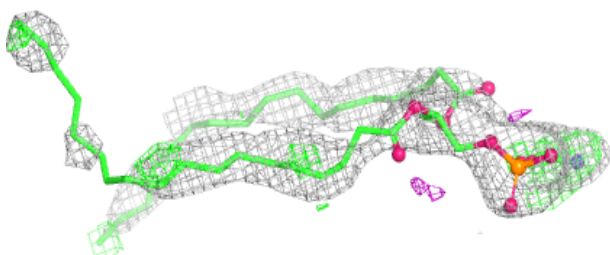
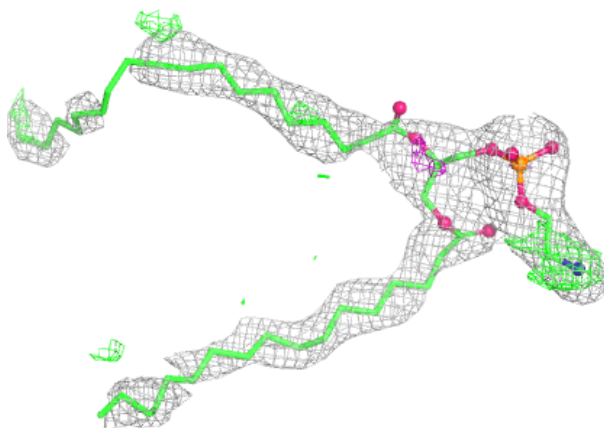


Electron density around UQ P 3002:

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

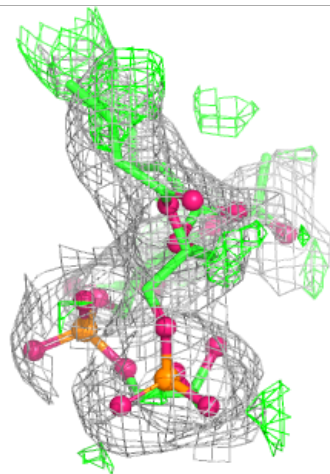
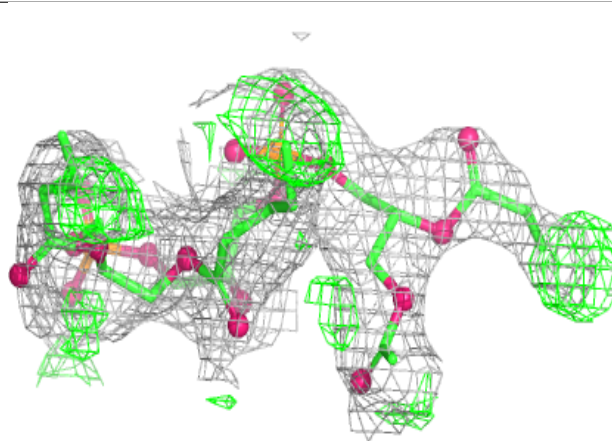
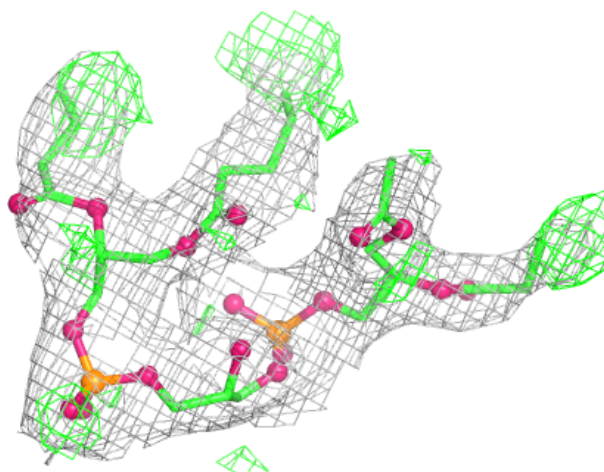
**Electron density around PEE P 3005:**

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



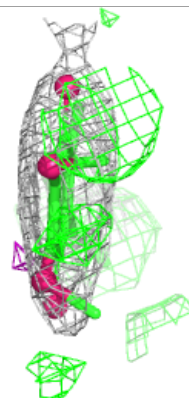
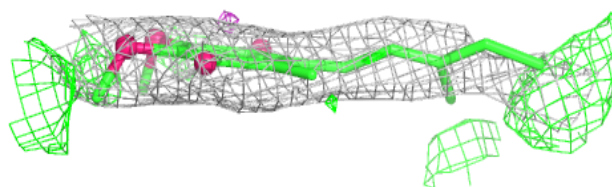
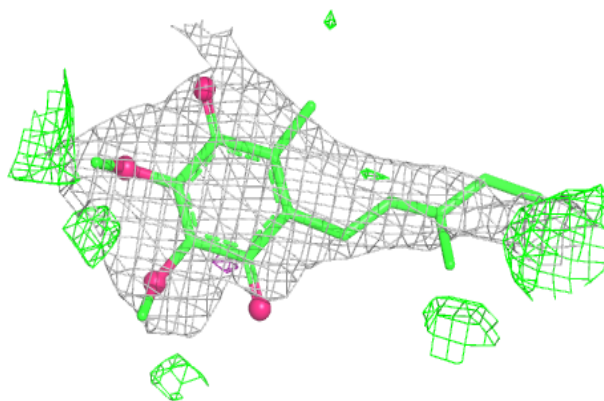
Electron density around CDL D 2003:

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

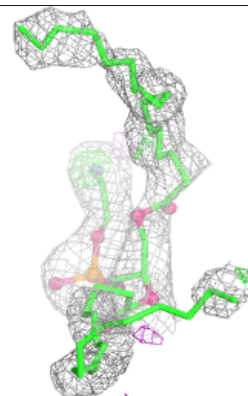
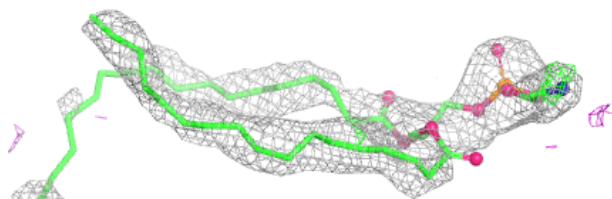
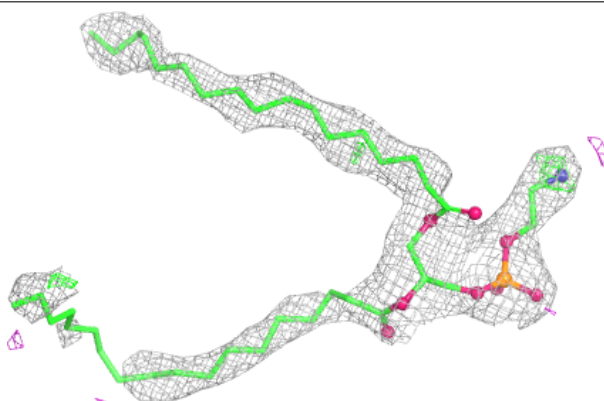


Electron density around UQ C 2002:

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

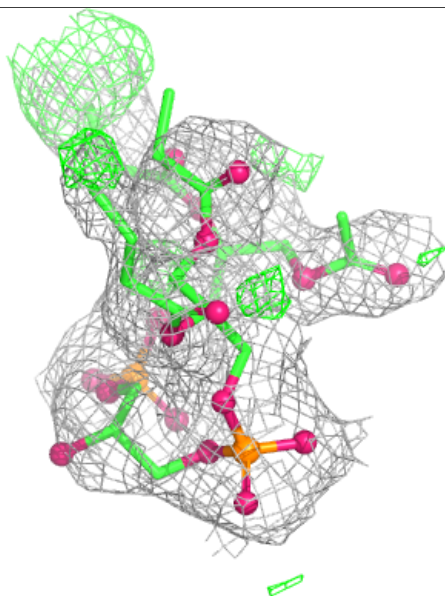
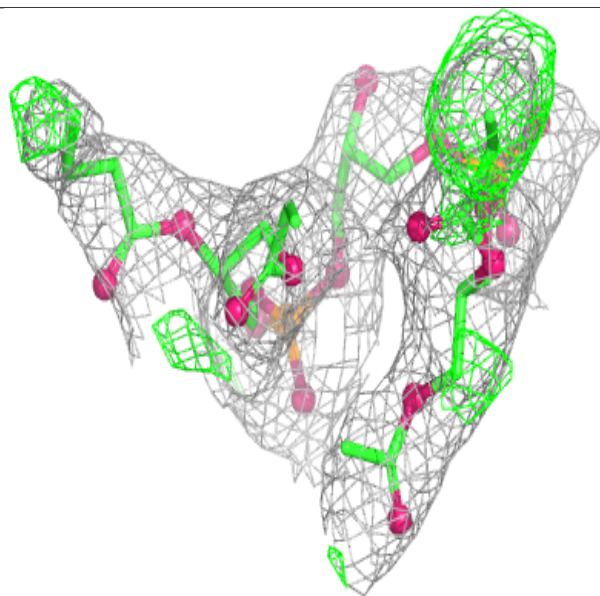
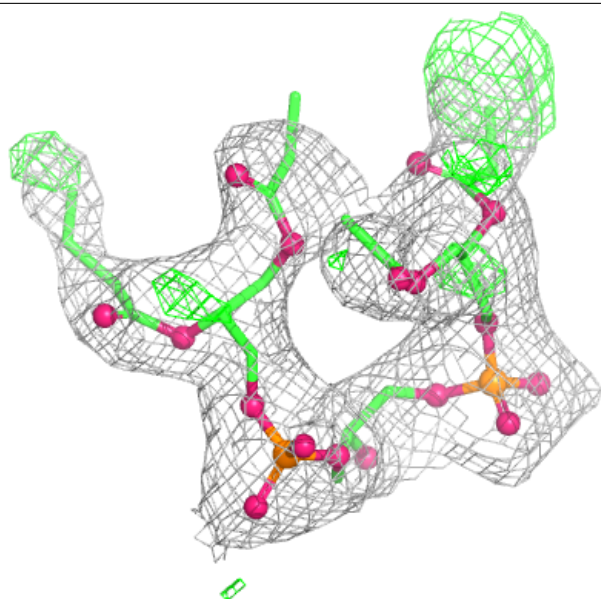
**Electron density around PEE A 2005:**

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



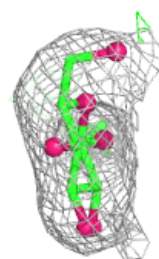
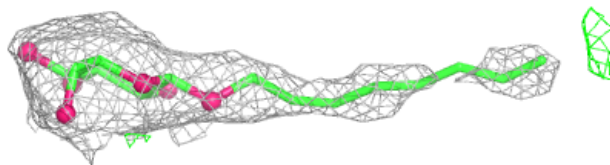
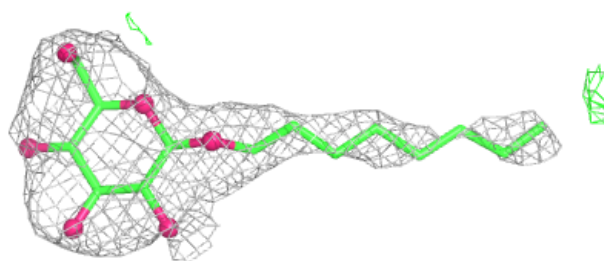
Electron density around CDL G 2004:

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and green (positive)

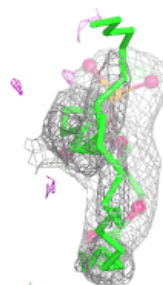
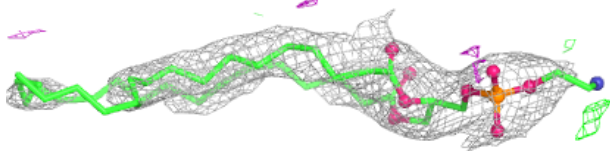
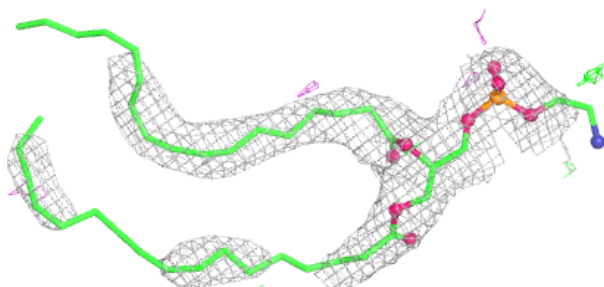


Electron density around BOG Q 3009:

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

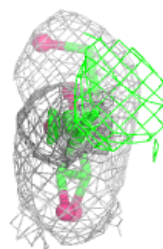
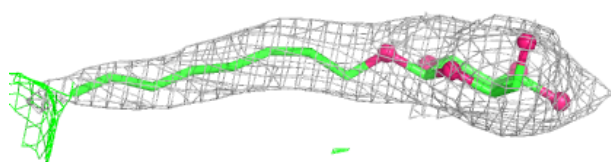
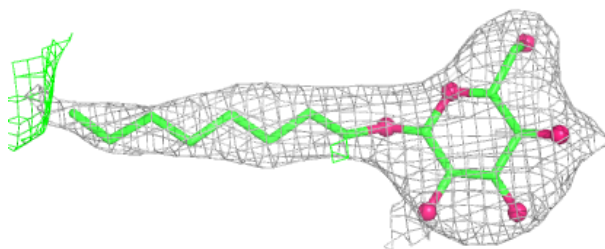
**Electron density around PEE P 3007:**

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

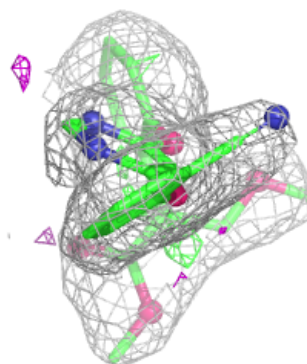
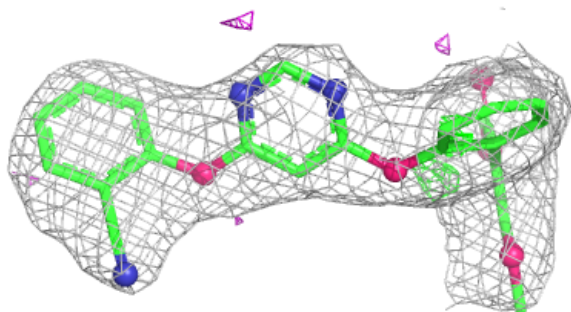
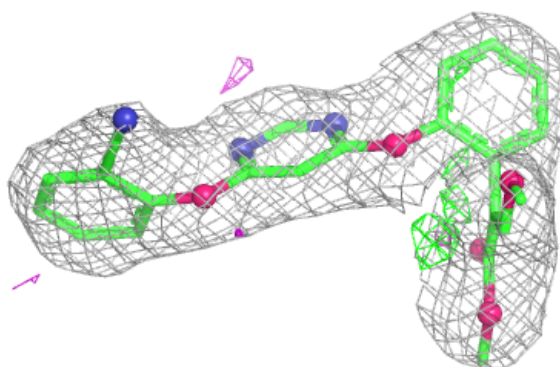


Electron density around BOG D 2009:

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

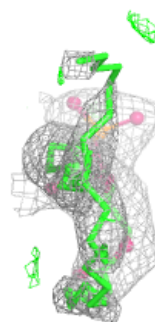
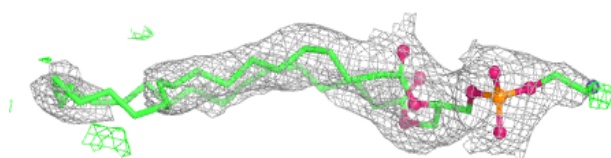
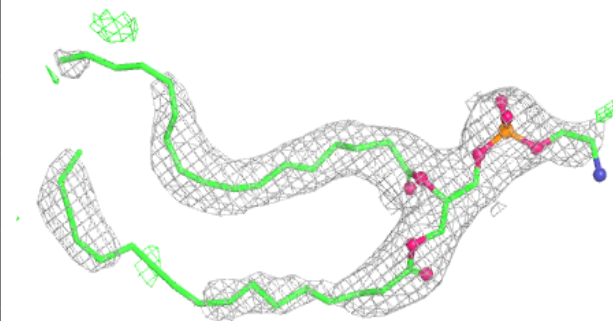
**Electron density around AZO P 3001:**

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

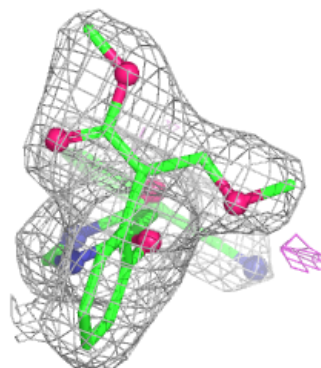
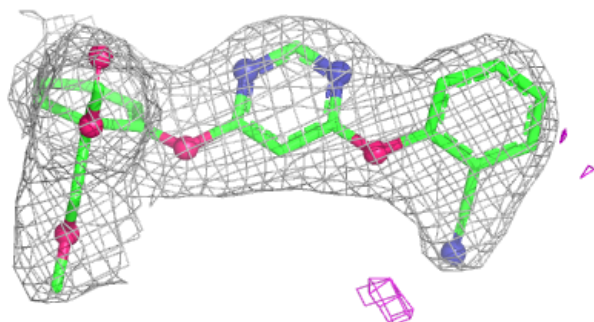
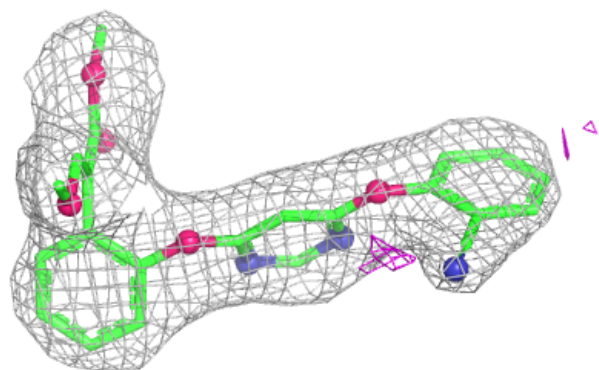


Electron density around PEE C 2007:

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and green (positive)

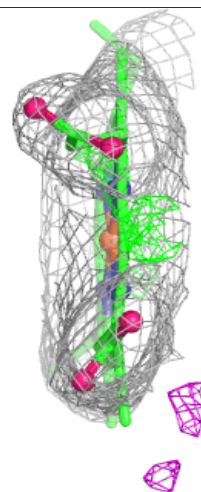
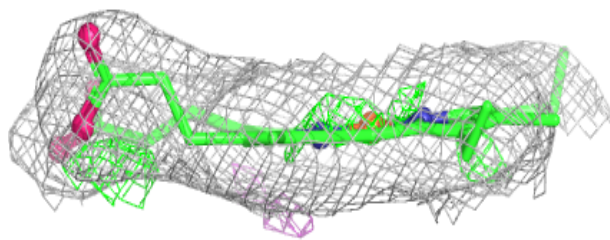
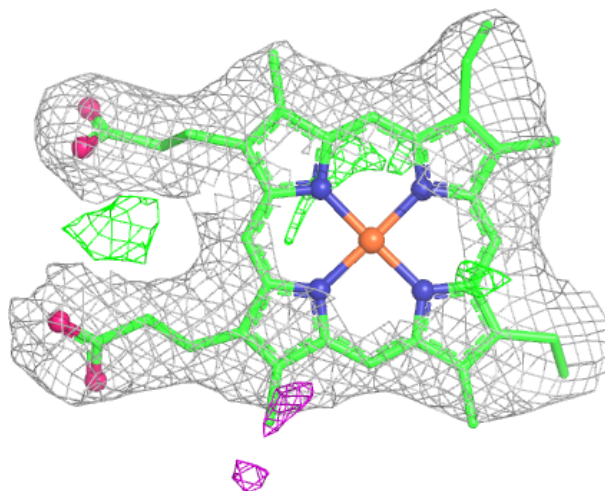
**Electron density around AZO C 2001:**

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



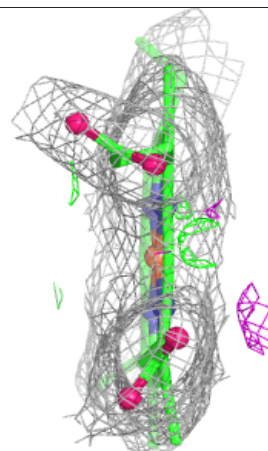
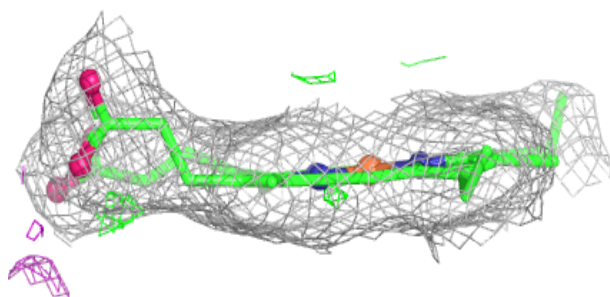
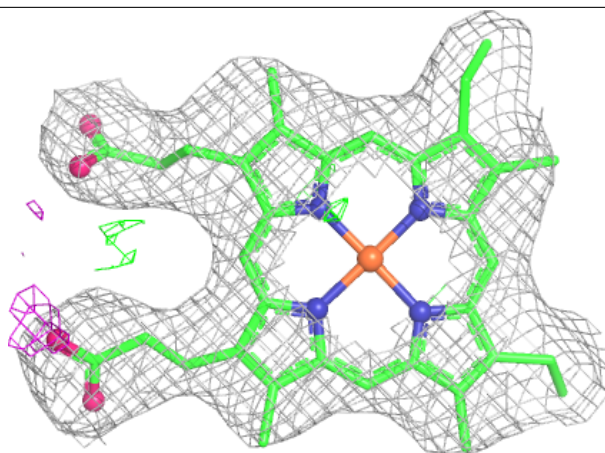
Electron density around HEC Q 501:

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



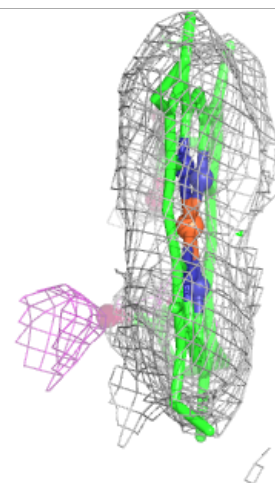
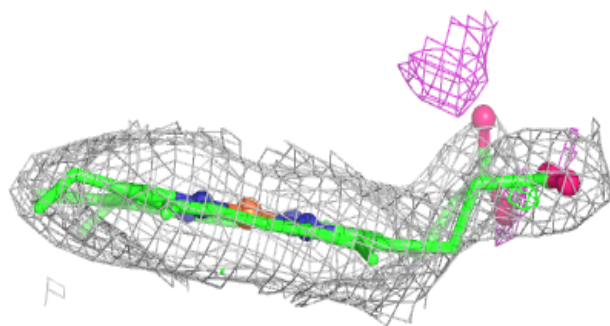
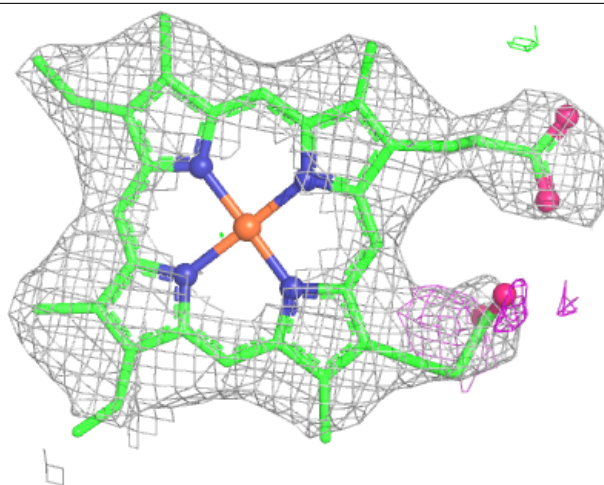
Electron density around HEC D 501:

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



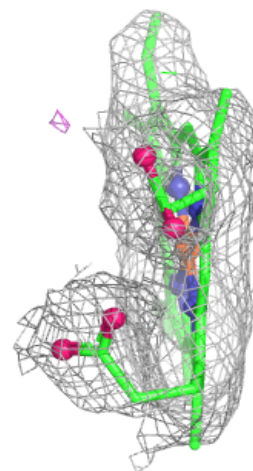
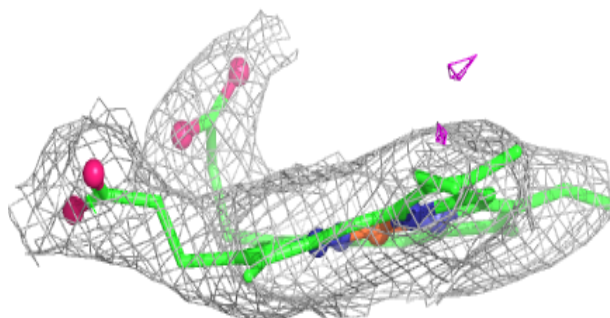
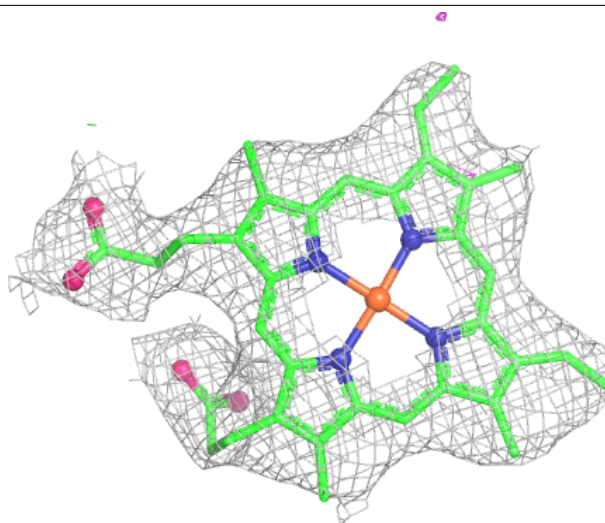
Electron density around HEM P 501:

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



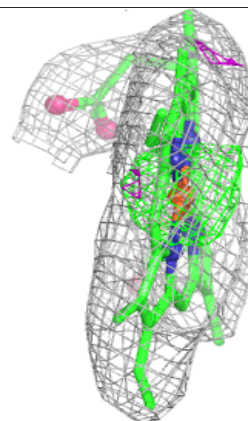
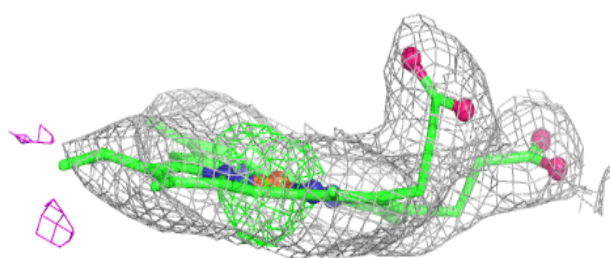
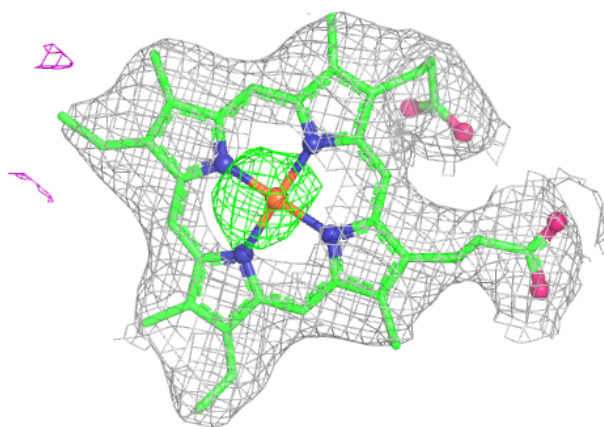
Electron density around HEM P 502:

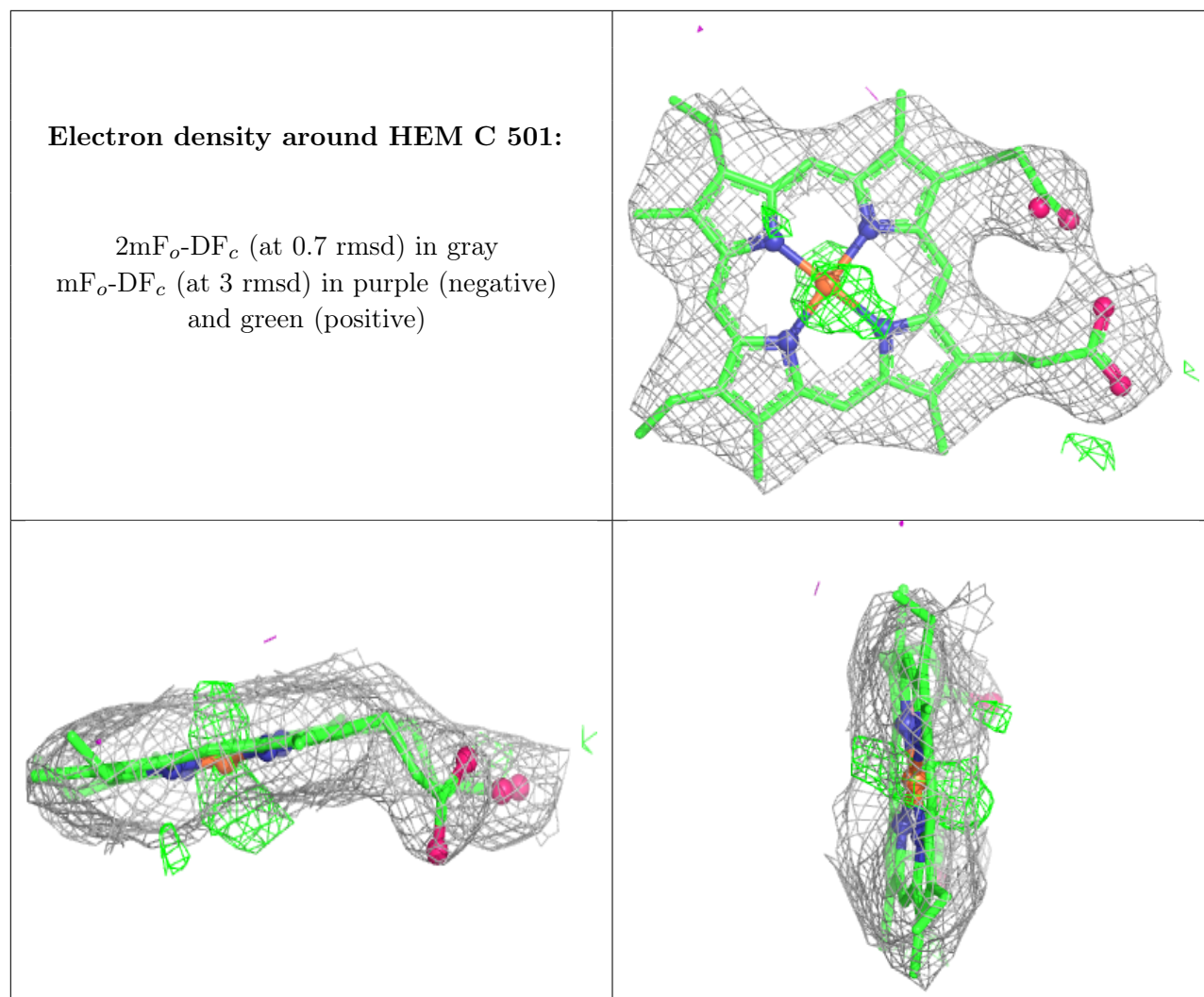
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

$2mF_o-DF_c$ (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.