



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:15 AM EDT

PDB ID : 3TGU / pdb_00003tgu
Title : Cytochrome bc1 complex from chicken with pfvs-designed moa inhibitor bound
Authors : Huang, L.-S.; Yang, G.-F.; Berry, E.A.
Deposited on : 2011-08-17
Resolution : 2.70 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

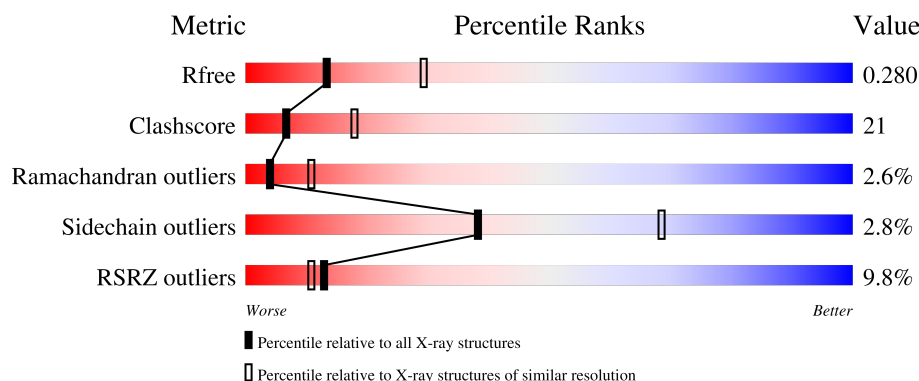
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



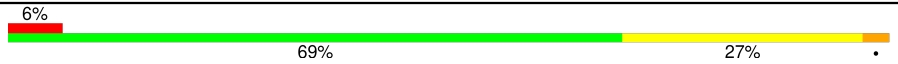
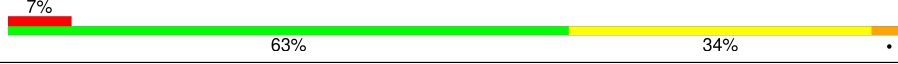
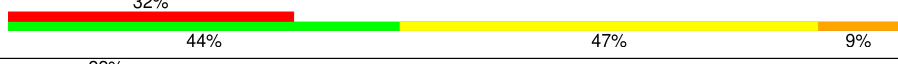
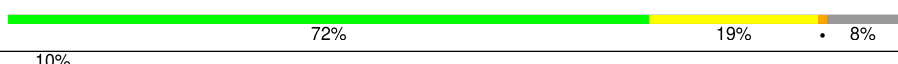
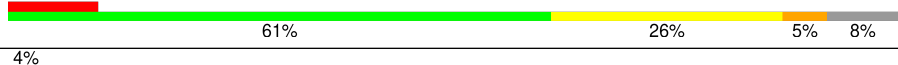
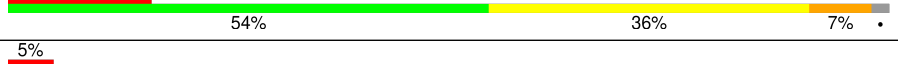
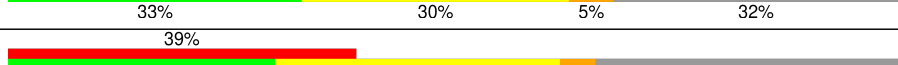
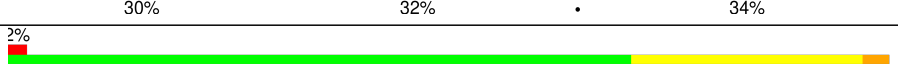
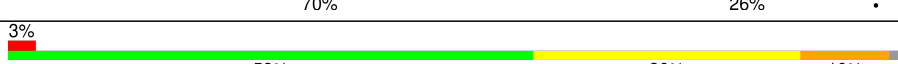
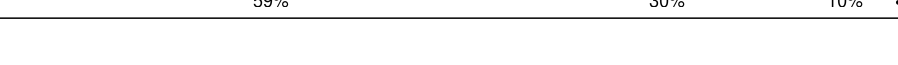
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	4% 62% 34% ..
1	N	446	7% 61% 35% ..
2	B	441	7% 51% 41% 5%
2	O	441	7% 50% 39% 6% .
3	C	380	3% 72% 25% .

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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	76	
9	V	76	
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
16	PEE	N	502	-	X	-	-
18	HEC	D	501	X	-	-	-
18	HEC	Q	501	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32733 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	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	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	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	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
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	initiating methionine	UNP P18946
P	1	FME	-	initiating methionine	UNP P18946

- 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			

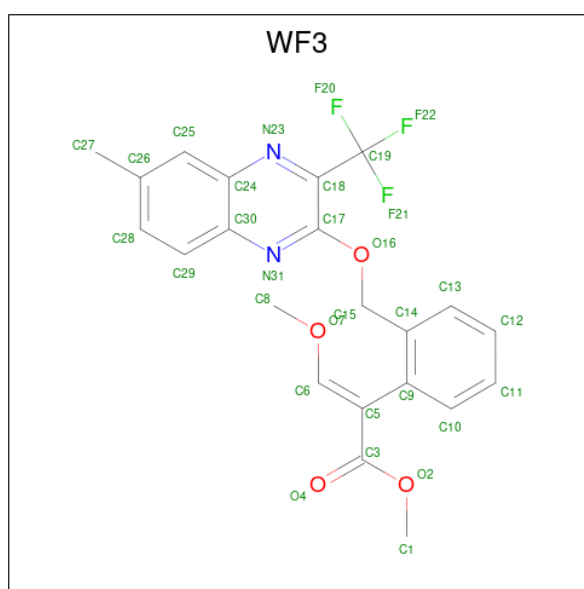
- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

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.

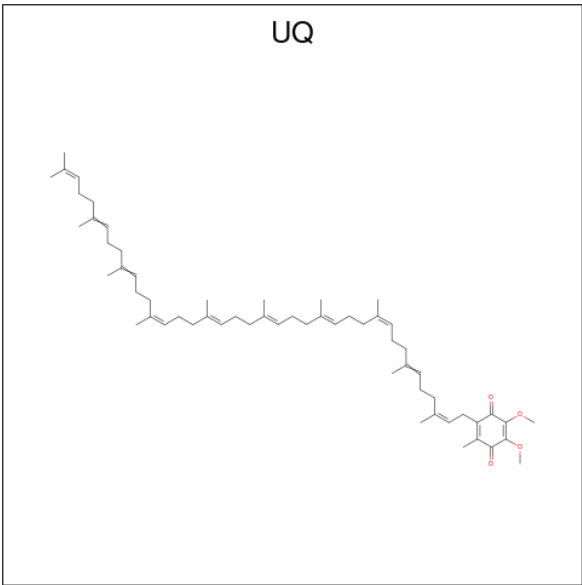
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 13 is methyl (2E)-3-methoxy-2-[2-({[6-methyl-3-(trifluoromethyl)quinoxalin-2-yl]oxy}methyl)phenyl]prop-2-enoate (CCD ID: WF3) (formula: C₂₂H₁₉F₃N₂O₄).



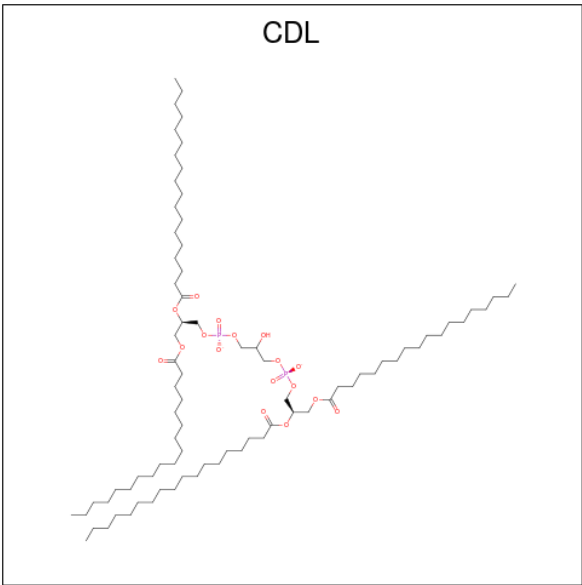
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	
			31	22	3	2	4	
13	P	1	Total	C	F	N	O	
			31	22	3	2	4	

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



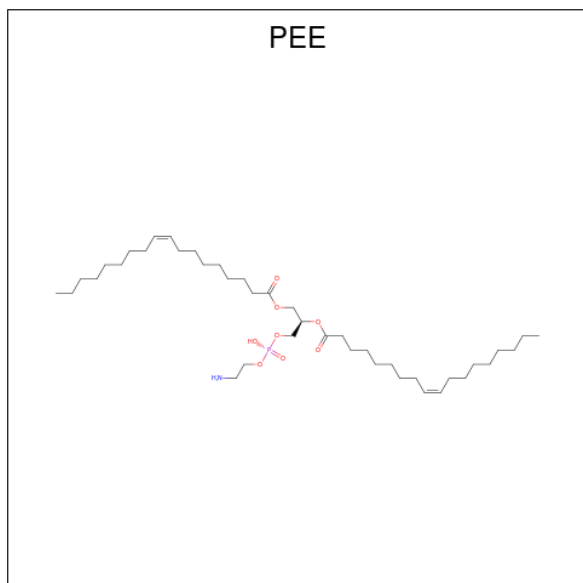
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			42	23	17	2		
15	G	1	Total	C	O	P	0	0
			40	21	17	2		

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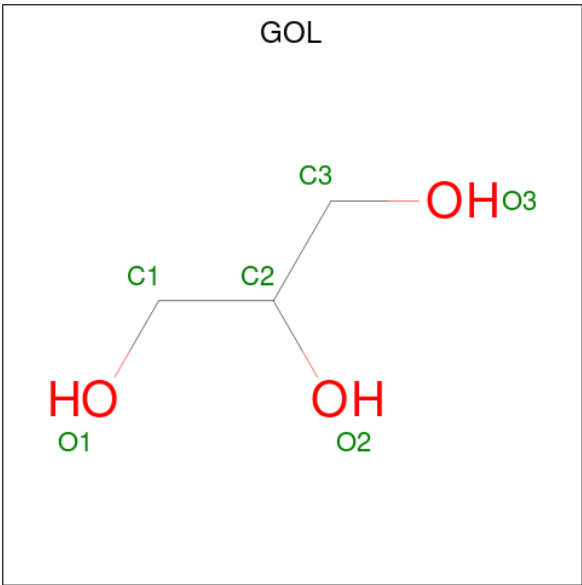
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



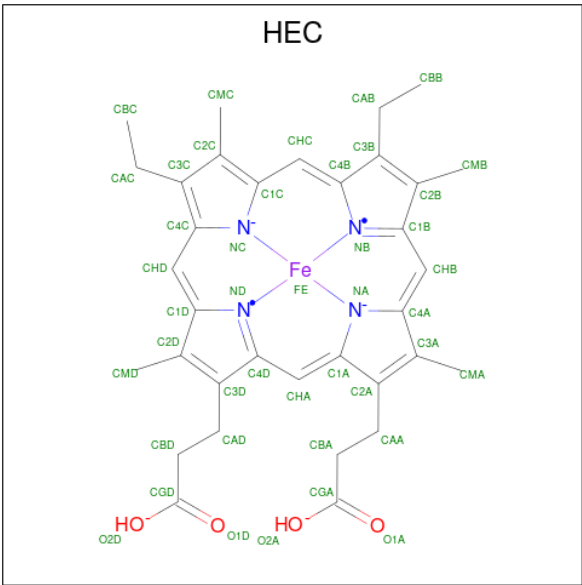
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	C	1	Total	C	O	P		0	0
			21	12	8	1			
16	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
16	N	1	Total	O	P			0	0
			5	4	1				
16	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	R	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 17 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



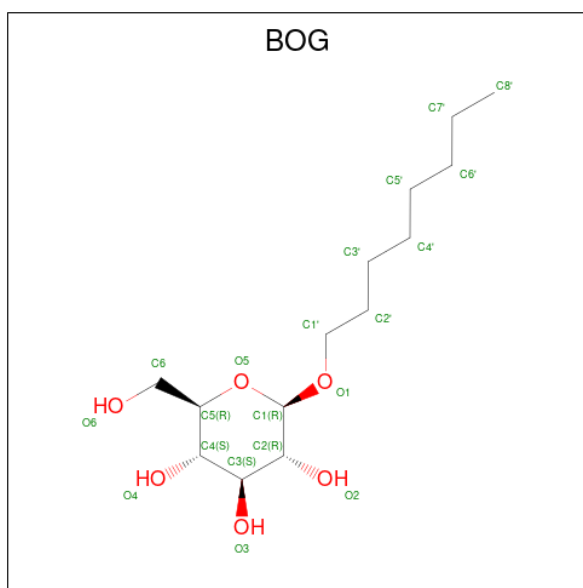
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			6	3	3		
17	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



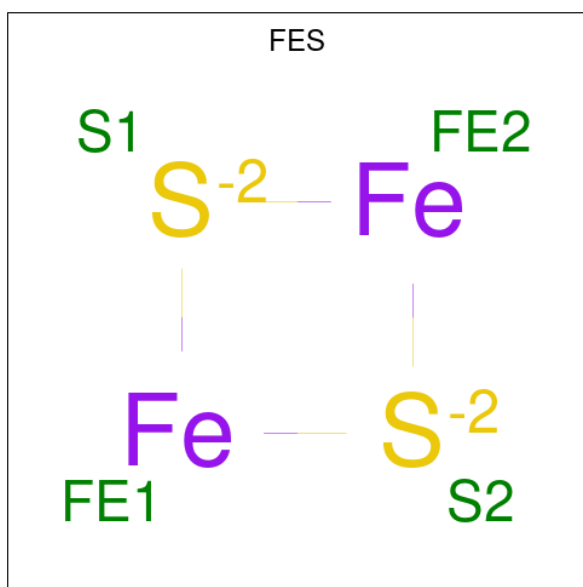
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
18	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 19 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

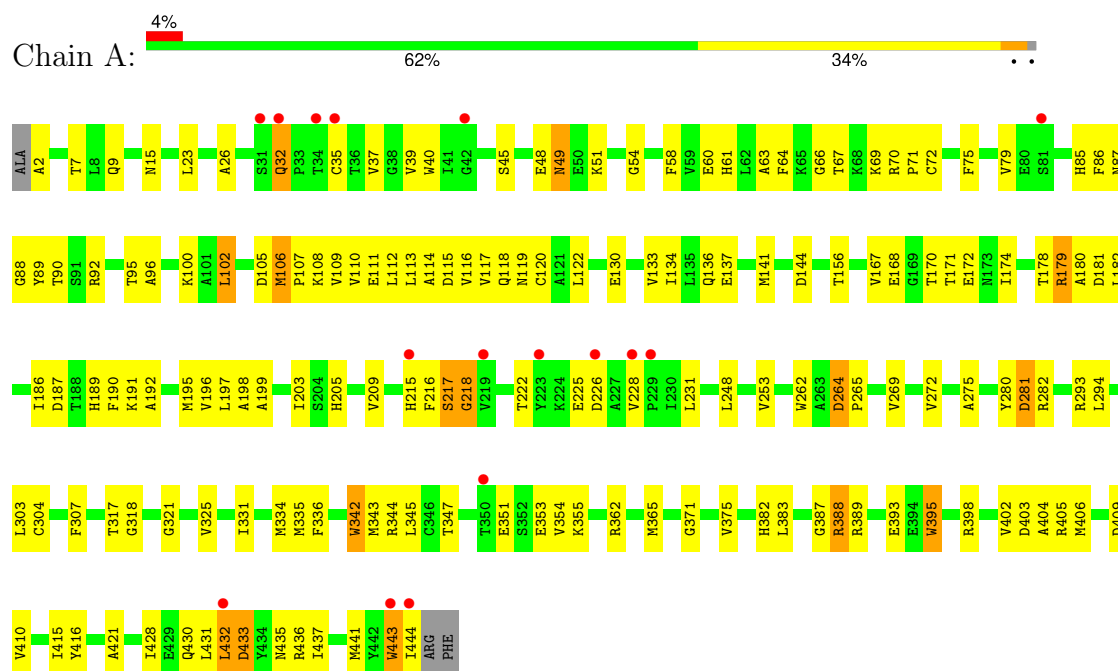
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	C	9	Total	O	0	0
			9	9		
21	E	1	Total	O	0	0
			1	1		
21	P	10	Total	O	0	0
			10	10		
21	R	1	Total	O	0	0
			1	1		

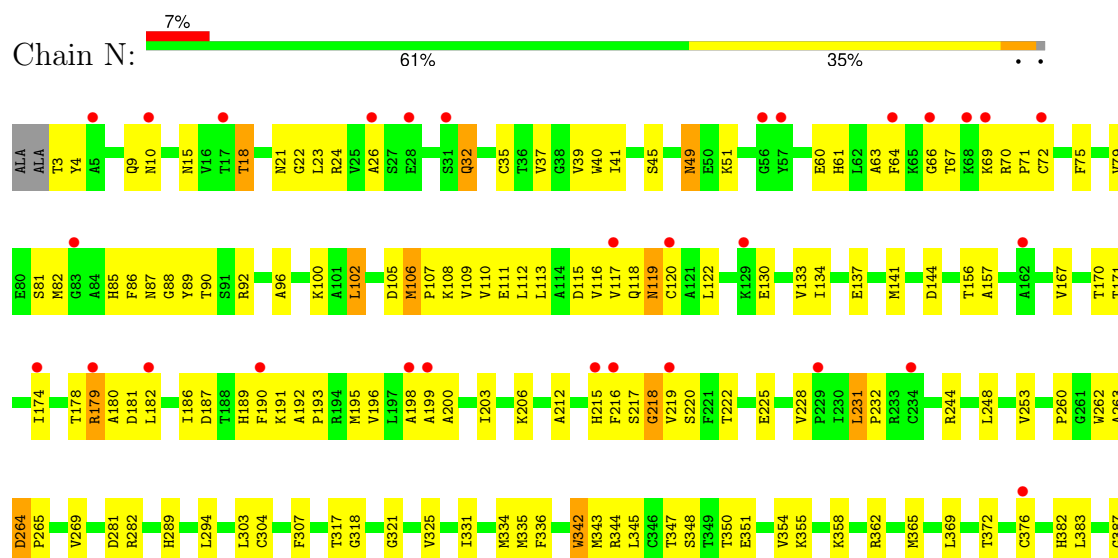
3 Residue-property plots [i](#)

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

- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

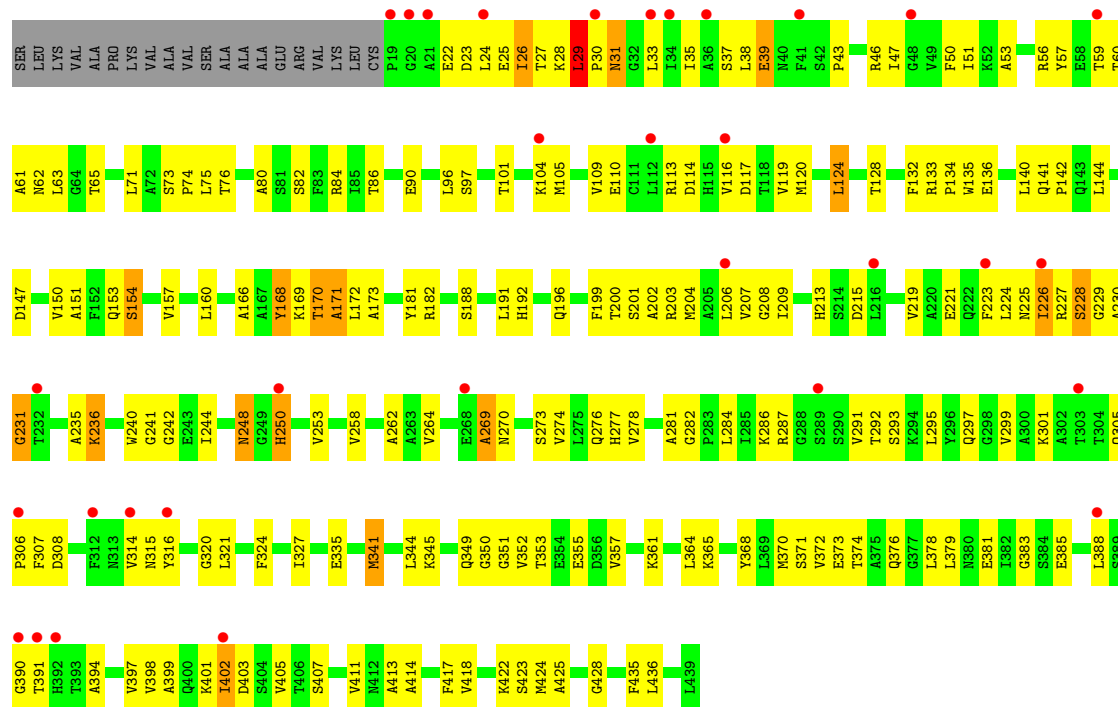


- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

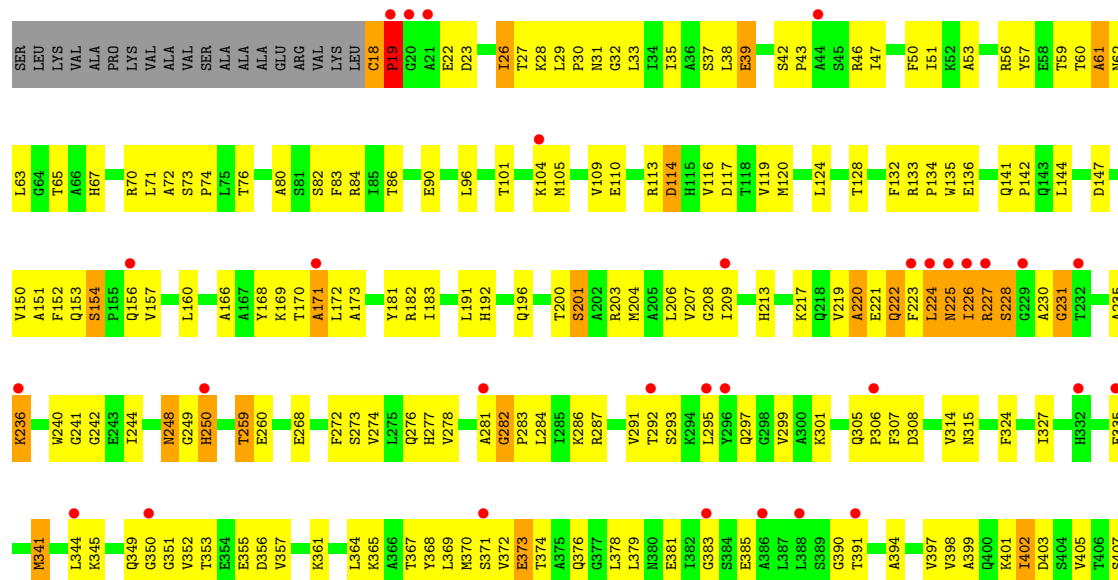


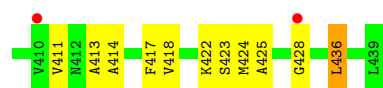


- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

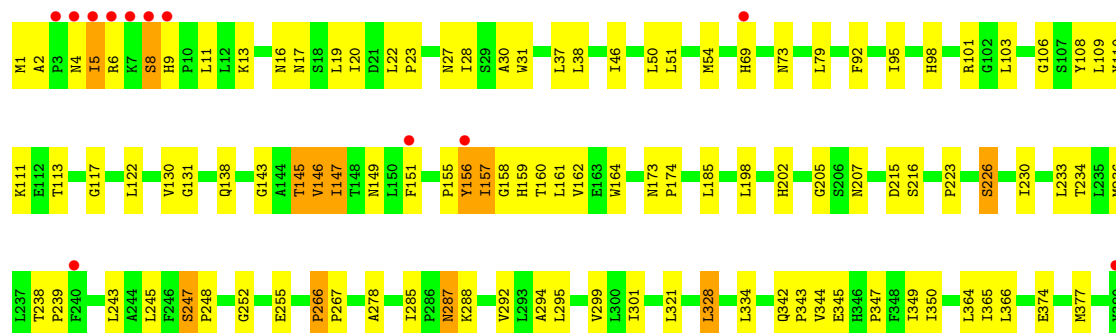


- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

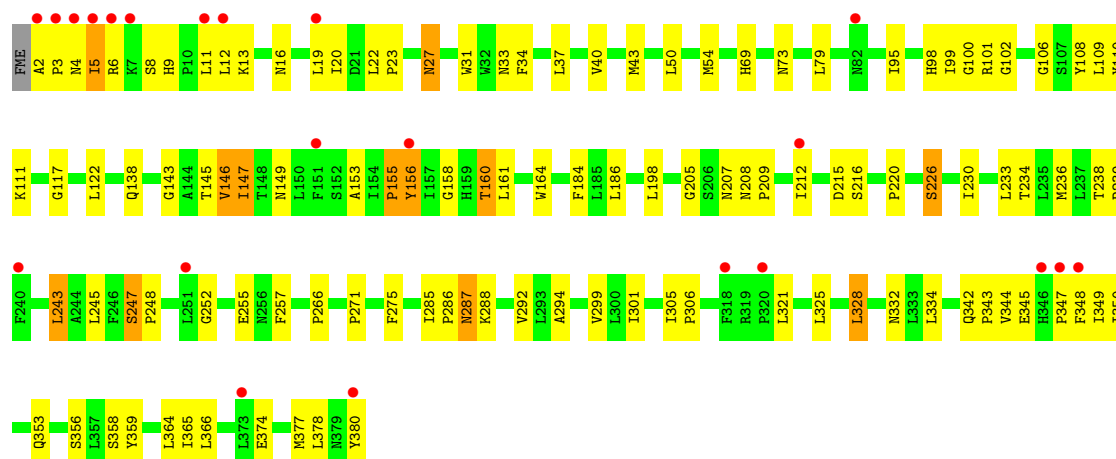




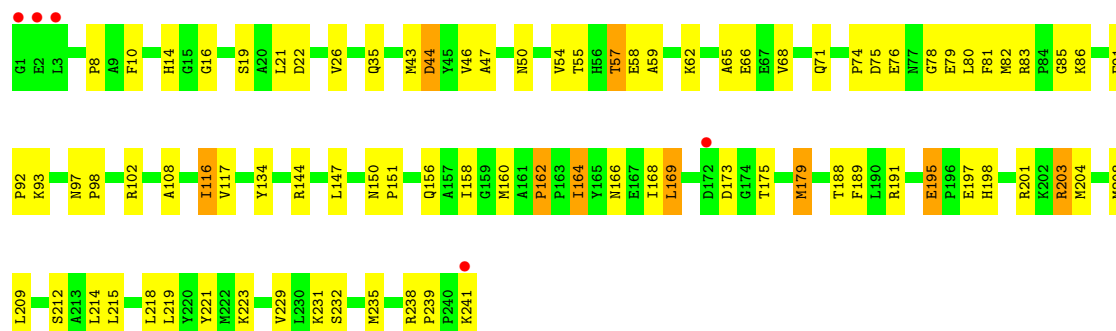
• Molecule 3: Cytochrome b



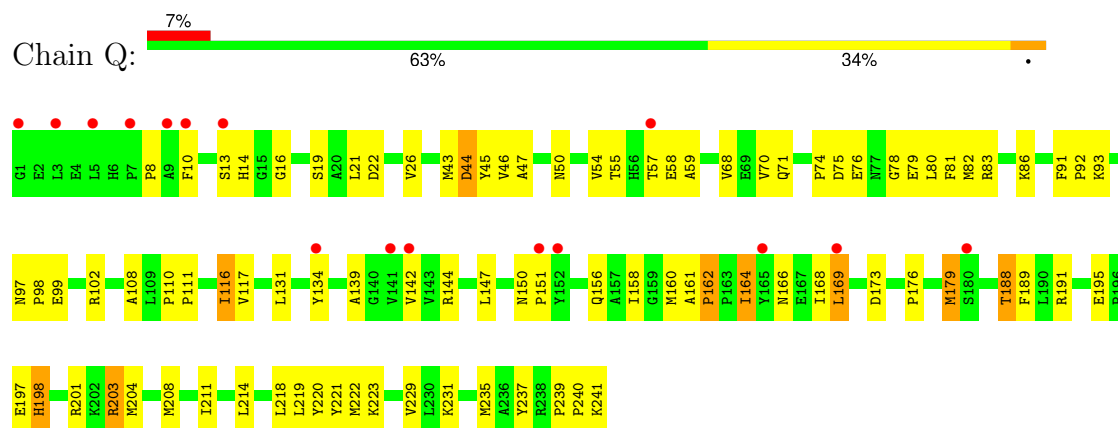
• Molecule 3: Cytochrome b



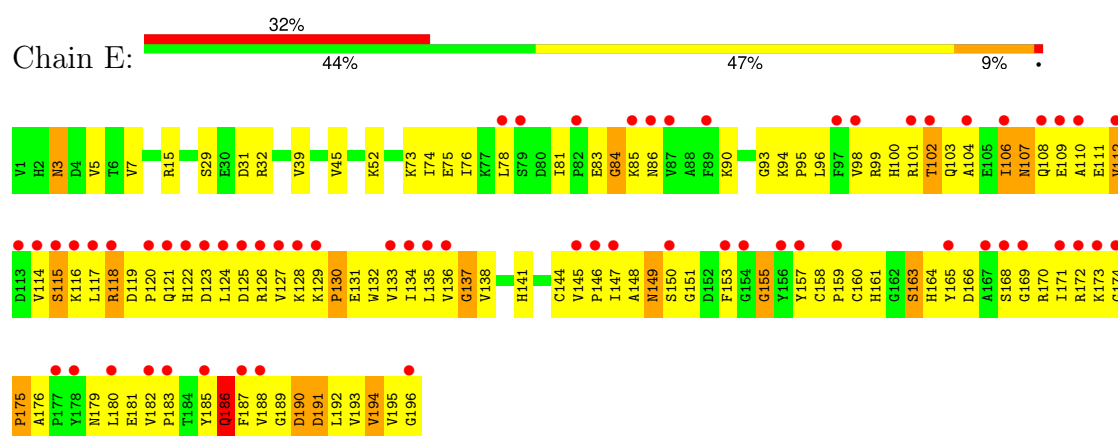
• Molecule 4: Mitochondrial cytochrome c1, heme protein



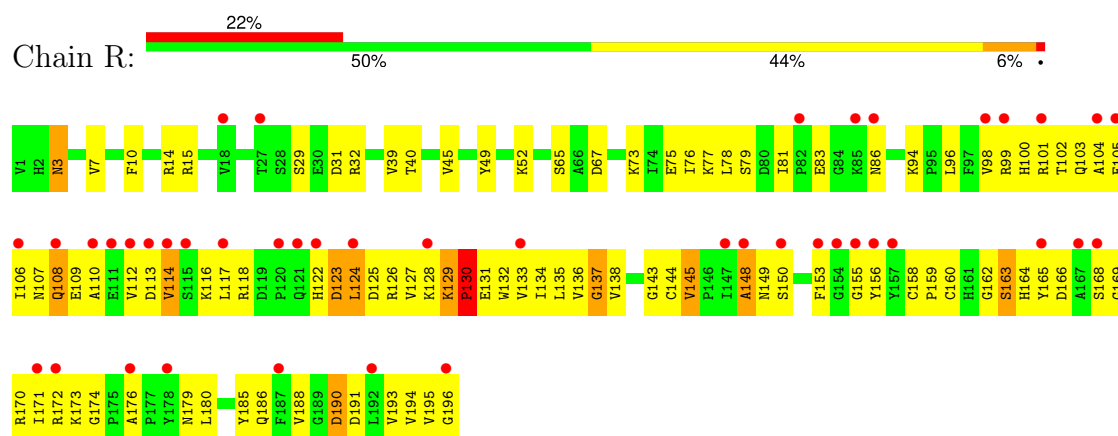
• Molecule 4: Mitochondrial cytochrome c1, heme protein



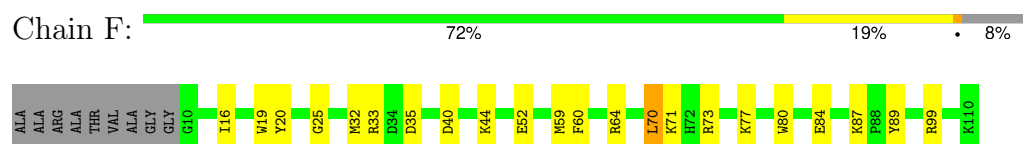
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



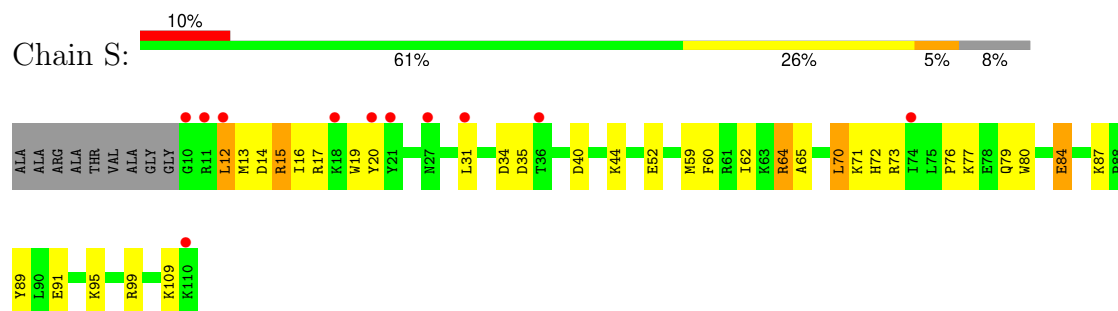
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



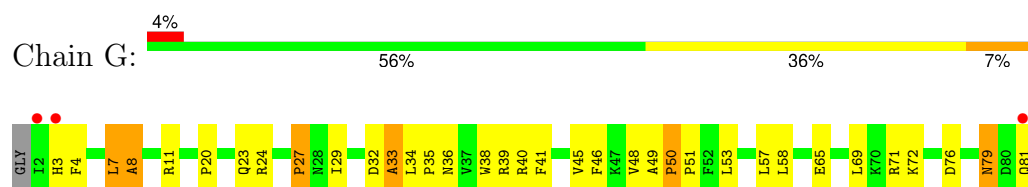
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



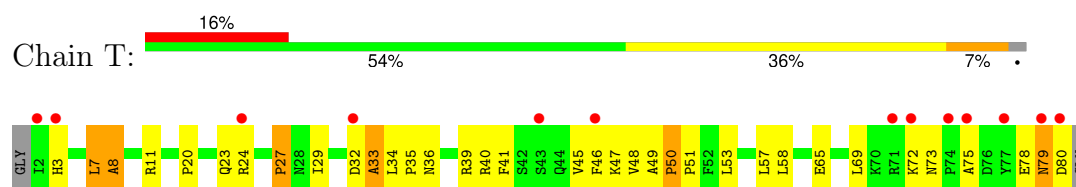
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



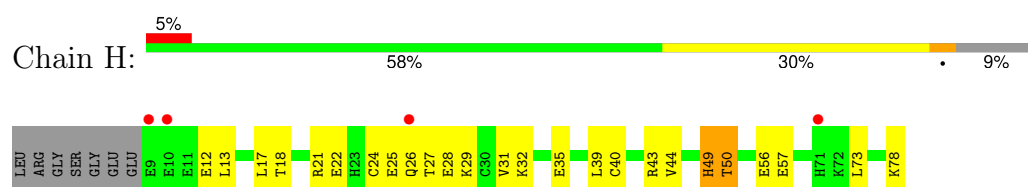
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



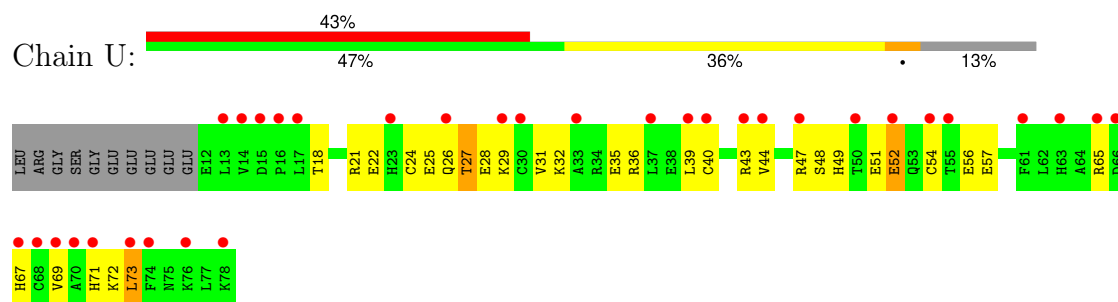
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



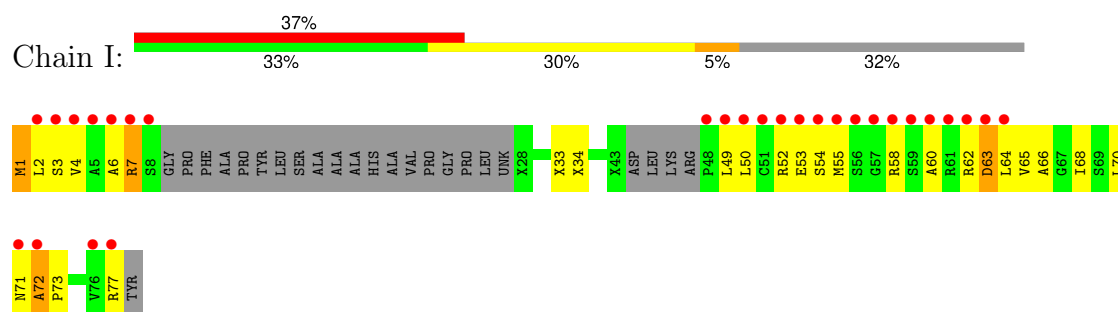
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



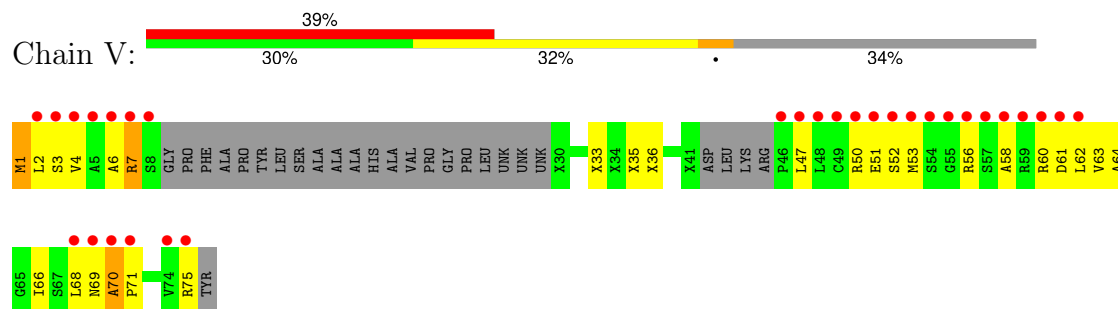
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



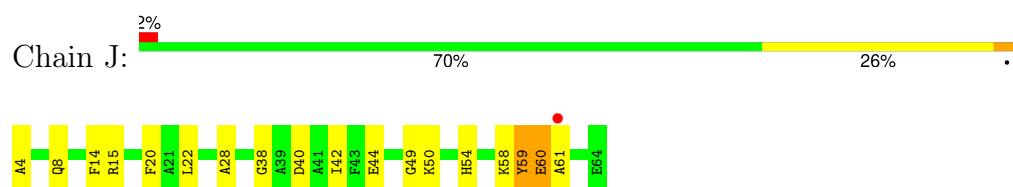
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



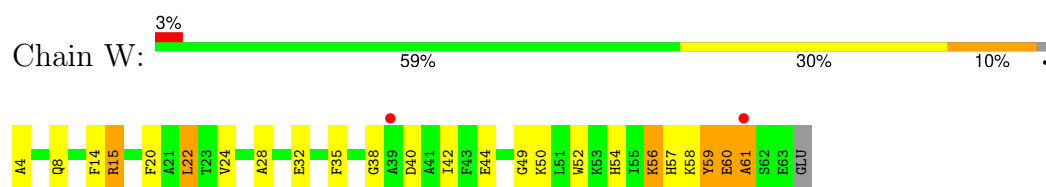
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- 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	172.68Å 183.31Å 241.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.70 24.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.98-2.70) 91.0 (24.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.289 0.246 , 0.280	Depositor DCC
R_{free} test set	3737 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32733	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: FME, AME, HEM, UNL, WF3, UQ, BOG, CDL, PEE, GOL, FES, HEC

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	0.47	0/3513	1.00	20/4760 (0.4%)
1	N	0.46	0/3508	1.01	26/4753 (0.5%)
2	B	0.43	0/3196	0.96	8/4334 (0.2%)
2	O	0.47	0/3202	0.99	11/4343 (0.3%)
3	C	0.56	0/3114	1.01	18/4263 (0.4%)
3	P	0.50	0/3114	1.00	17/4263 (0.4%)
4	D	0.53	0/1956	1.02	8/2658 (0.3%)
4	Q	0.45	0/1956	0.97	7/2658 (0.3%)
5	E	0.43	0/1547	0.89	4/2103 (0.2%)
5	R	0.42	0/1543	0.96	10/2098 (0.5%)
6	F	0.53	0/911	0.89	1/1219 (0.1%)
6	S	0.42	0/911	0.94	2/1219 (0.2%)
7	G	0.47	0/694	1.01	2/941 (0.2%)
7	T	0.43	0/684	1.00	4/929 (0.4%)
8	H	0.47	0/582	0.91	0/779
8	U	0.37	0/561	0.88	2/751 (0.3%)
9	I	0.51	0/251	1.07	3/336 (0.9%)
9	V	0.49	0/251	0.95	0/336
10	J	0.48	0/508	0.86	0/682
10	W	0.46	0/490	0.84	1/660 (0.2%)
All	All	0.47	0/32492	0.98	144/44085 (0.3%)

There are no bond length outliers.

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	116	ILE	N-CA-C	7.59	117.71	110.42
5	E	106	ILE	N-CA-C	-7.58	104.08	112.80
1	A	248	LEU	CA-C-N	7.53	126.80	118.97
1	A	248	LEU	C-N-CA	7.53	126.80	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLN	N-CA-C	7.31	118.01	109.60
1	A	432	LEU	N-CA-C	7.21	119.70	108.96
1	A	189	HIS	N-CA-C	7.18	122.10	113.12
1	A	264	ASP	CA-C-N	7.12	126.82	119.56
1	A	264	ASP	C-N-CA	7.12	126.82	119.56
2	B	282	GLY	CA-C-N	7.03	128.63	119.84
2	B	282	GLY	C-N-CA	7.03	128.63	119.84
8	U	72	LYS	N-CA-C	7.03	119.98	111.40
1	N	432	LEU	N-CA-C	7.03	118.86	108.60
4	Q	116	ILE	N-CA-C	7.02	117.16	110.42
1	N	264	ASP	CA-C-N	6.99	126.69	119.56
1	N	264	ASP	C-N-CA	6.99	126.69	119.56
2	O	227	ARG	N-CA-C	6.99	117.88	108.23
3	C	226	SER	N-CA-C	-6.96	103.77	111.36
5	R	145	VAL	CA-C-N	6.93	126.92	119.78
5	R	145	VAL	C-N-CA	6.93	126.92	119.78
1	A	415	ILE	N-CA-C	6.92	118.25	111.67
5	R	15	ARG	N-CA-C	-6.90	101.43	110.53
2	O	282	GLY	CA-C-N	6.87	128.43	119.84
2	O	282	GLY	C-N-CA	6.87	128.43	119.84
3	P	328	LEU	N-CA-C	-6.74	104.01	111.36
3	C	328	LEU	N-CA-C	-6.67	103.93	111.14
4	Q	44	ASP	N-CA-C	6.64	119.35	111.71
3	P	205	GLY	N-CA-C	-6.64	104.30	112.33
6	S	15	ARG	N-CA-C	-6.64	104.20	112.90
1	N	189	HIS	N-CA-C	6.58	121.35	113.12
3	C	205	GLY	N-CA-C	-6.54	104.42	112.33
1	N	32	GLN	N-CA-C	6.52	117.10	109.60
1	A	347	THR	N-CA-C	6.50	122.69	114.31
1	N	347	THR	N-CA-C	6.47	122.65	114.31
1	A	179	ARG	N-CA-C	-6.45	103.52	111.33
5	R	190	ASP	N-CA-C	-6.44	105.25	113.23
5	E	15	ARG	N-CA-C	-6.41	102.07	110.53
2	O	18	CYS	CA-C-N	6.40	127.84	119.84
2	O	18	CYS	C-N-CA	6.40	127.84	119.84
3	C	207	ASN	N-CA-C	-6.38	100.46	110.36
4	Q	164	ILE	N-CA-C	6.38	117.97	108.46
3	P	143	GLY	N-CA-C	-6.37	104.78	112.49
3	P	207	ASN	N-CA-C	-6.33	101.41	110.59
1	N	415	ILE	N-CA-C	6.31	116.99	111.56
3	P	252	GLY	N-CA-C	6.30	120.27	112.14
3	P	164	TRP	N-CA-C	-6.20	103.83	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	266	PRO	CA-C-N	6.20	125.41	118.97
3	C	266	PRO	C-N-CA	6.20	125.41	118.97
5	R	174	GLY	CA-C-N	6.16	125.86	119.64
5	R	174	GLY	C-N-CA	6.16	125.86	119.64
3	C	111	LYS	N-CA-C	6.10	121.44	111.37
1	N	248	LEU	CA-C-N	6.10	125.58	119.24
1	N	248	LEU	C-N-CA	6.10	125.58	119.24
4	D	44	ASP	N-CA-C	6.09	119.81	112.38
2	O	61	ALA	N-CA-C	6.09	118.00	111.36
2	O	225	ASN	N-CA-C	6.08	118.52	108.48
1	N	179	ARG	N-CA-C	-6.04	104.02	111.33
2	O	224	LEU	N-CA-C	6.04	118.99	110.23
1	N	32	GLN	CA-C-N	6.02	125.72	119.64
1	N	32	GLN	C-N-CA	6.02	125.72	119.64
3	C	143	GLY	N-CA-C	-5.97	105.57	112.50
2	O	373	GLU	N-CA-C	-5.96	105.10	112.90
1	A	264	ASP	N-CA-C	5.93	118.02	109.48
4	D	164	ILE	N-CA-C	5.90	117.25	108.46
4	D	195	GLU	CA-C-N	5.90	126.31	119.47
4	D	195	GLU	C-N-CA	5.90	126.31	119.47
5	R	129	LYS	CA-C-N	5.83	127.13	119.84
5	R	129	LYS	C-N-CA	5.83	127.13	119.84
3	P	226	SER	N-CA-C	-5.83	104.84	111.14
6	S	109	LYS	N-CA-C	-5.81	104.38	112.45
1	N	428	ILE	N-CA-C	5.80	121.40	109.34
3	C	247	SER	CA-C-N	5.80	127.09	119.84
3	C	247	SER	C-N-CA	5.80	127.09	119.84
2	B	61	ALA	N-CA-C	5.78	118.53	111.82
1	A	66	GLY	N-CA-C	5.77	119.95	112.68
1	N	264	ASP	N-CA-C	5.77	117.79	109.48
1	N	263	ALA	N-CA-C	5.76	118.02	111.11
3	P	111	LYS	N-CA-C	5.75	120.86	111.37
3	C	110	TYR	N-CA-C	-5.75	101.00	109.62
3	C	147	ILE	N-CA-C	5.73	115.92	110.53
9	I	72	ALA	N-CA-C	5.72	114.72	108.14
9	I	72	ALA	CA-C-N	5.71	126.98	119.84
9	I	72	ALA	C-N-CA	5.71	126.98	119.84
3	C	252	GLY	N-CA-C	5.71	120.37	112.37
8	U	73	LEU	N-CA-C	5.70	120.77	111.37
1	N	66	GLY	N-CA-C	5.68	119.84	112.68
1	N	416	TYR	N-CA-C	5.66	118.79	110.30
1	N	415	ILE	CB-CA-C	-5.65	106.07	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	148	ALA	N-CA-C	5.64	122.82	110.80
1	A	231	LEU	N-CA-C	5.62	117.83	110.08
3	C	8	SER	N-CA-C	5.58	118.20	111.40
4	D	173	ASP	N-CA-C	-5.54	105.87	113.30
1	A	416	TYR	N-CA-C	5.50	118.56	110.30
3	C	185	LEU	N-CA-C	5.48	118.31	111.24
4	D	80	LEU	N-CA-C	-5.48	103.46	110.53
7	G	8	ALA	N-CA-C	5.47	117.50	109.24
1	N	244	ARG	N-CA-C	5.47	118.16	109.24
1	A	428	ILE	N-CA-C	5.46	120.70	109.34
4	D	35	GLN	N-CA-C	5.46	119.94	113.28
7	G	76	ASP	N-CA-C	-5.45	106.49	114.39
3	P	27	ASN	N-CA-C	5.42	119.45	112.41
3	C	113	THR	N-CA-C	-5.41	105.38	111.28
3	P	257	PHE	N-CA-C	-5.40	106.27	112.92
3	C	27	ASN	N-CA-C	5.39	119.47	111.87
2	B	413	ALA	N-CA-C	-5.36	105.44	111.28
3	P	110	TYR	N-CA-C	-5.35	101.60	109.62
4	Q	80	LEU	N-CA-C	-5.30	103.70	110.53
1	N	303	LEU	N-CA-C	5.29	117.95	111.82
3	C	164	TRP	N-CA-C	-5.28	104.96	111.40
1	N	348	SER	N-CA-C	5.26	120.48	112.54
3	P	147	ILE	N-CA-C	5.24	115.46	110.53
1	A	58	PHE	N-CA-C	-5.23	105.58	111.28
7	T	47	LYS	N-CA-C	-5.22	106.59	113.12
2	O	369	LEU	N-CA-C	5.22	116.66	111.07
6	F	25	GLY	N-CA-C	5.21	122.54	115.30
7	T	8	ALA	N-CA-C	5.21	117.11	109.24
1	A	303	LEU	N-CA-C	5.21	117.86	111.82
1	A	415	ILE	CB-CA-C	-5.20	105.66	111.80
2	O	413	ALA	N-CA-C	-5.20	105.61	111.28
5	R	143	GLY	N-CA-C	5.19	125.47	113.18
7	T	78	GLU	N-CA-C	-5.18	106.65	113.12
3	P	247	SER	CA-C-N	5.17	126.30	119.84
3	P	247	SER	C-N-CA	5.17	126.30	119.84
3	P	266	PRO	CA-C-N	5.16	124.34	118.97
3	P	266	PRO	C-N-CA	5.16	124.34	118.97
1	N	437	ILE	CB-CA-C	-5.15	105.19	112.14
1	N	119	ASN	N-CA-C	5.14	118.86	112.59
1	A	421	ALA	N-CA-C	-5.14	101.32	109.59
1	A	437	ILE	CB-CA-C	-5.14	105.21	112.14
10	W	56	LYS	N-CA-C	5.11	116.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	TYR	N-CA-C	5.10	116.43	109.18
2	B	188	SER	N-CA-C	-5.10	105.91	111.82
4	Q	188	THR	N-CA-C	-5.10	105.62	111.07
3	P	378	LEU	N-CA-C	-5.09	106.48	113.30
1	N	231	LEU	N-CA-C	5.08	117.09	110.08
1	N	260	PRO	N-CA-C	5.06	120.18	113.40
2	B	29	LEU	CA-C-N	5.04	126.14	119.84
2	B	29	LEU	C-N-CA	5.04	126.14	119.84
5	E	194	VAL	N-CA-C	5.04	114.00	106.85
1	N	434	TYR	N-CA-C	-5.04	105.68	111.07
4	Q	45	TYR	N-CA-C	5.03	119.39	113.16
7	T	23	GLN	N-CA-C	5.02	117.18	109.95
4	Q	173	ASP	N-CA-C	-5.02	106.85	113.17
5	E	181	GLU	N-CA-C	5.01	117.36	110.35

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	3442	0	3354	129	0
1	N	3437	0	3349	142	0
2	B	3141	0	3142	204	0
2	O	3147	0	3146	221	0
3	C	3021	0	3068	84	0
3	P	3012	0	3058	90	0
4	D	1898	0	1846	70	0
4	Q	1898	0	1846	75	0
5	E	1513	0	1478	113	0
5	R	1509	0	1474	102	0
6	F	891	0	893	21	0
6	S	891	0	893	34	0
7	G	672	0	653	31	0
7	T	662	0	645	33	0
8	H	574	0	548	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	553	0	535	31	0
9	I	319	0	281	45	0
9	V	311	0	283	50	0
10	J	497	0	490	14	0
10	W	479	0	478	22	0
11	A	1	0	0	0	0
11	N	1	0	0	0	0
12	C	86	0	60	4	0
12	P	86	0	60	5	0
13	C	31	0	19	1	0
13	P	31	0	19	1	0
14	C	19	0	17	3	0
14	P	19	0	17	1	0
15	C	42	0	28	1	0
15	G	40	0	24	1	0
15	P	40	0	24	3	0
15	Q	42	0	28	1	0
16	C	70	0	85	2	0
16	E	50	0	77	0	0
16	N	5	0	0	0	0
16	P	49	0	72	2	0
16	R	49	0	71	1	0
17	C	6	0	8	0	0
17	P	6	0	8	0	0
18	D	43	0	30	1	0
18	Q	43	0	30	1	0
19	D	33	0	39	0	0
19	P	12	0	11	0	0
19	Q	33	0	39	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	C	9	0	0	0	0
21	E	1	0	0	0	0
21	P	10	0	0	2	0
21	R	1	0	0	0	0
All	All	32733	0	32226	1395	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 (1395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:76:THR:HG22	2:O:82:SER:H	1.05	1.19
1:N:178:THR:HG22	1:N:180:ALA:H	1.10	1.14
1:A:178:THR:HG22	1:A:180:ALA:H	1.11	1.13
2:B:76:THR:HG22	2:B:82:SER:H	1.12	1.12
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.12	1.10
8:U:36:ARG:HH11	8:U:36:ARG:HB3	1.18	1.08
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.17	1.07
1:N:102:LEU:HD12	1:N:102:LEU:H	1.18	1.06
9:V:35:UNK:HG3	9:V:36:UNK:H	1.15	1.05
2:B:22:GLU:HG3	2:B:23:ASP:H	1.20	1.05
9:I:33:UNK:HG3	9:I:34:UNK:H	1.19	1.02
1:A:102:LEU:HD12	1:A:102:LEU:H	1.23	1.02
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.39	1.01
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.44	0.98
4:D:47:ALA:H	4:D:50:ASN:HD22	1.02	0.98
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.28	0.97
8:U:36:ARG:HB3	8:U:36:ARG:NH1	1.80	0.96
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.80	0.96
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.00	0.95
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.51	0.93
2:O:101:THR:HG21	9:V:4:VAL:HG11	1.48	0.93
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.34	0.93
5:E:116:LYS:H	5:E:116:LYS:HD2	1.33	0.93
2:B:353:THR:HG22	2:B:355:GLU:H	1.33	0.92
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.52	0.91
2:O:353:THR:HG22	2:O:355:GLU:H	1.33	0.90
2:O:157:VAL:HG23	9:V:62:LEU:HD21	1.53	0.90
1:N:206:LYS:H	1:N:206:LYS:HD2	1.37	0.89
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.71	0.88
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.54	0.88
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.09	0.87
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.55	0.87
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.53	0.87
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:N	1.89	0.86
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.91	0.86
5:R:117:LEU:HD21	5:R:172:ARG:NH1	1.91	0.86
2:O:385:GLU:HG2	9:V:2:LEU:HD13	1.58	0.85
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.41	0.84
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.75	0.84
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.83
3:P:40:VAL:HA	3:P:43:MET:HE3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.83
2:B:315:ASN:HD22	9:I:7:ARG:HD3	1.43	0.82
6:S:13:MET:HA	6:S:16:ILE:HD12	1.62	0.82
5:E:107:ASN:N	5:E:107:ASN:HD22	1.78	0.82
2:O:27:THR:HG22	2:O:28:LYS:H	1.42	0.82
4:D:57:THR:HG22	4:D:59:ALA:H	1.43	0.82
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.60	0.82
1:A:178:THR:HB	1:A:181:ASP:OD1	1.78	0.82
1:N:178:THR:HG22	1:N:180:ALA:N	1.92	0.82
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.63	0.81
2:O:96:LEU:HB3	9:V:68:LEU:HD22	1.62	0.81
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.62	0.81
2:O:221:GLU:HG3	2:O:222:GLN:H	1.45	0.81
8:H:27:THR:HG22	8:H:29:LYS:H	1.45	0.80
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.44	0.80
8:U:27:THR:HG22	8:U:29:LYS:H	1.44	0.80
2:B:76:THR:HG22	2:B:82:SER:N	1.94	0.80
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.64	0.80
1:A:69:LYS:HD2	1:A:70:ARG:NH2	1.95	0.80
2:O:38:LEU:HG	2:O:39:GLU:H	1.47	0.80
4:D:47:ALA:H	4:D:50:ASN:ND2	1.77	0.80
2:O:291:VAL:HA	2:O:297:GLN:NE2	1.96	0.79
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.65	0.79
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.65	0.79
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.62	0.79
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.46	0.79
10:W:60:GLU:O	10:W:60:GLU:HG2	1.80	0.78
2:O:381:GLU:OE1	9:V:3:SER:HB2	1.83	0.78
2:B:38:LEU:HG	2:B:39:GLU:H	1.49	0.78
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.48	0.78
2:B:27:THR:HG22	2:B:28:LYS:H	1.48	0.78
3:P:238:THR:HB	3:P:239:PRO:HD3	1.66	0.78
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.66	0.77
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.63	0.77
9:I:64:LEU:HD12	9:I:77:ARG:C	2.10	0.77
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.00	0.77
4:D:57:THR:HG22	4:D:59:ALA:N	2.00	0.77
1:N:69:LYS:HD2	1:N:70:ARG:NH2	1.98	0.77
2:O:248:ASN:HD22	2:O:248:ASN:C	1.89	0.77
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.49	0.76
2:B:291:VAL:HA	2:B:297:GLN:NE2	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.67	0.76
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.01	0.76
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.21	0.75
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.75
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.18	0.75
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.22	0.75
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.75
2:O:62:ASN:O	2:O:65:THR:HG22	1.86	0.75
9:V:3:SER:HB3	9:V:6:ALA:HB3	1.69	0.75
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.68	0.75
2:O:154:SER:O	2:O:157:VAL:HG12	1.87	0.75
1:A:2:ALA:HB3	2:B:113:ARG:HH21	1.52	0.74
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.74
9:I:49:LEU:HD22	9:I:54:SER:O	1.87	0.74
1:N:102:LEU:HD12	1:N:102:LEU:N	2.00	0.74
9:V:47:LEU:HD22	9:V:52:SER:O	1.86	0.74
1:N:178:THR:HB	1:N:181:ASP:OD1	1.85	0.74
2:O:368:TYR:HB2	9:V:1:AME:HE2	1.67	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.68	0.74
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.23	0.74
1:N:187:ASP:O	1:N:191:LYS:HE3	1.88	0.73
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.69	0.73
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.22	0.73
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.71	0.73
2:O:315:ASN:HD22	9:V:7:ARG:HD3	1.53	0.73
18:D:501:HEC:HMB3	18:D:501:HEC:HBB3	1.71	0.73
1:N:206:LYS:HD2	1:N:206:LYS:N	2.04	0.73
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.69	0.73
2:O:327:ILE:HD11	9:V:56:ARG:O	1.89	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.89	0.73
9:I:3:SER:HB3	9:I:6:ALA:HB3	1.71	0.73
2:B:22:GLU:HG3	2:B:23:ASP:N	2.01	0.72
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.72
9:V:63:VAL:HB	9:V:75:ARG:HD3	1.70	0.72
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.03	0.72
1:A:187:ASP:O	1:A:191:LYS:HE3	1.88	0.72
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.71	0.72
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.90	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
1:N:102:LEU:H	1:N:102:LEU:CD1	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:216:SER:HB3	6:S:59:MET:HE2	1.71	0.72
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.72	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.04	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.72
1:N:443:TRP:HA	1:N:443:TRP:HE3	1.54	0.72
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.71	0.72
2:B:62:ASN:O	2:B:65:THR:HG22	1.90	0.72
2:B:248:ASN:C	2:B:248:ASN:HD22	1.98	0.72
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.24	0.72
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.72	0.72
10:W:40:ASP:O	10:W:44:GLU:HG3	1.89	0.71
1:A:443:TRP:HA	1:A:443:TRP:HE3	1.55	0.71
9:I:70:LEU:HD23	9:I:71:ASN:HD22	1.55	0.71
9:V:62:LEU:HD12	9:V:75:ARG:C	2.15	0.71
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.72	0.71
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.70	0.71
1:A:182:LEU:O	1:A:186:ILE:HG13	1.89	0.71
4:D:231:LYS:O	6:F:71:LYS:HE3	1.90	0.71
2:O:221:GLU:HG3	2:O:222:GLN:N	2.05	0.71
2:O:295:LEU:O	2:O:299:VAL:HG23	1.91	0.71
2:O:314:VAL:HG13	9:V:61:ASP:HB3	1.73	0.71
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.71	0.71
2:B:38:LEU:CG	2:B:39:GLU:H	2.04	0.70
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.70
3:C:79:LEU:HD22	4:D:204:MET:HE1	1.72	0.70
2:O:38:LEU:CG	2:O:39:GLU:H	2.05	0.70
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.92	0.70
1:A:102:LEU:HD12	1:A:102:LEU:N	2.02	0.70
5:E:78:LEU:HD12	5:E:190:ASP:O	1.92	0.70
2:O:22:GLU:HG3	2:O:23:ASP:H	1.56	0.70
2:B:150:VAL:O	2:B:153:GLN:HG3	1.91	0.70
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.73	0.70
2:B:399:ALA:O	2:B:402:ILE:HG22	1.92	0.69
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.27	0.69
4:D:164:ILE:O	4:D:179:MET:HE2	1.92	0.69
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.57	0.69
9:V:35:UNK:HG3	9:V:36:UNK:N	1.95	0.69
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.72	0.69
15:P:506:CDL:OA4	7:T:40:ARG:HD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:150:VAL:O	2:O:153:GLN:HG3	1.92	0.69
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.69
2:B:368:TYR:HB2	9:I:1:AME:HE2	1.74	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.68
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.28	0.68
5:R:169:GLY:O	5:R:179:ASN:HB3	1.92	0.68
2:B:31:ASN:HD22	2:B:31:ASN:N	1.91	0.68
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.09	0.68
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.93	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.59	0.68
2:O:225:ASN:O	2:O:226:ILE:C	2.35	0.68
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.68
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.76	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.93	0.68
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.76	0.67
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.29	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.28	0.67
2:O:26:ILE:HD13	2:O:391:THR:HA	1.76	0.67
2:B:361:LYS:O	2:B:365:LYS:HG3	1.94	0.67
10:J:40:ASP:O	10:J:44:GLU:HG3	1.95	0.67
3:P:22:LEU:HD21	14:P:505:UQ:HM32	1.77	0.67
1:A:69:LYS:CD	1:A:70:ARG:HH21	1.99	0.67
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
2:B:264:VAL:HG23	2:B:316:TYR:C	2.19	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.94	0.67
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.77	0.67
2:B:101:THR:HG21	9:I:4:VAL:HG11	1.77	0.66
4:D:102:ARG:HA	4:D:108:ALA:O	1.94	0.66
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.20	0.66
7:G:40:ARG:HD2	15:G:101:CDL:OA4	1.95	0.66
10:J:15:ARG:HG2	10:J:15:ARG:HH11	1.59	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.77	0.66
1:A:102:LEU:H	1:A:102:LEU:CD1	2.01	0.66
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.31	0.66
2:B:307:PHE:H	9:I:52:ARG:HG2	1.58	0.66
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.66
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.10	0.66
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.02	0.66
5:E:84:GLY:N	5:E:102:THR:HG23	2.10	0.66
1:N:85:HIS:NE2	2:O:370:MET:HE1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:THR:HG22	1:N:171:THR:N	2.11	0.66
7:T:29:ILE:O	7:T:33:ALA:HB3	1.95	0.66
8:H:40:CYS:O	8:H:44:VAL:HG23	1.96	0.66
9:V:35:UNK:CG	9:V:36:UNK:H	2.00	0.66
2:B:169:LYS:O	2:B:170:THR:HG23	1.95	0.66
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.78	0.65
5:E:96:LEU:HD12	5:E:135:LEU:O	1.96	0.65
10:W:15:ARG:HG2	10:W:15:ARG:HH11	1.61	0.65
3:P:9:HIS:O	3:P:13:LYS:HB3	1.95	0.65
1:N:105:ASP:O	1:N:109:VAL:HG23	1.96	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
2:O:414:ALA:O	2:O:418:VAL:HG23	1.96	0.65
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.61	0.65
5:E:117:LEU:HD21	5:E:170:ARG:HD2	1.78	0.65
5:E:163:SER:HA	5:E:174:GLY:HA3	1.79	0.65
1:N:69:LYS:CD	1:N:70:ARG:HH21	2.03	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
1:N:32:GLN:OE1	2:O:373:GLU:HG2	1.97	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.62	0.65
2:B:26:ILE:HD13	2:B:391:THR:HA	1.79	0.65
3:C:216:SER:HB3	6:F:59:MET:HE2	1.79	0.65
5:R:73:LYS:HB3	5:R:196:GLY:O	1.97	0.65
5:R:96:LEU:HD12	5:R:135:LEU:O	1.97	0.65
5:R:128:LYS:O	5:R:130:PRO:HD3	1.97	0.64
5:E:190:ASP:C	5:E:192:LEU:H	2.04	0.64
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.64
5:E:186:GLN:HG3	5:E:188:VAL:HG23	1.78	0.64
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.64
3:C:9:HIS:O	3:C:13:LYS:HB3	1.96	0.64
5:E:106:ILE:C	5:E:107:ASN:HD22	2.06	0.64
5:R:101:ARG:HA	5:R:105:GLU:OE1	1.97	0.64
2:B:327:ILE:HD11	9:I:58:ARG:O	1.97	0.64
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.63	0.64
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.78	0.64
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.80	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.98	0.64
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.80	0.63
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.33	0.63
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.63	0.63
1:N:206:LYS:H	1:N:206:LYS:CD	2.10	0.63
6:S:13:MET:HE3	6:S:17:ARG:HH12	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:THR:HG23	8:H:78:LYS:HD2	1.79	0.63
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.80	0.63
3:P:155:PRO:O	3:P:156:TYR:HB2	1.97	0.63
9:V:47:LEU:HD13	9:V:53:MET:HG2	1.80	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.81	0.63
4:Q:102:ARG:HA	4:Q:108:ALA:O	1.99	0.63
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.99	0.63
3:C:117:GLY:O	12:C:502:HEM:HMC3	1.98	0.63
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.98	0.63
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.14	0.63
1:A:85:HIS:NE2	2:B:370:MET:HE1	2.14	0.62
1:N:112:LEU:O	1:N:116:VAL:HG23	1.99	0.62
2:O:47:ILE:HD13	2:O:120:MET:CE	2.29	0.62
2:B:341:MET:HE2	2:B:341:MET:HA	1.81	0.62
9:V:1:AME:C	9:V:3:SER:H	2.12	0.62
3:C:101:ARG:HD2	3:C:101:ARG:C	2.24	0.62
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
10:W:57:HIS:HA	10:W:60:GLU:OE2	1.99	0.62
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.38	0.62
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.81	0.62
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.80	0.62
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.64	0.62
2:O:306:PRO:HA	9:V:50:ARG:HG3	1.81	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.62
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.62
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.81	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.35	0.62
2:B:47:ILE:HD13	2:B:120:MET:CE	2.30	0.61
7:T:46:PHE:O	7:T:50:PRO:HG2	2.00	0.61
5:R:102:THR:O	5:R:106:ILE:HG13	2.01	0.61
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.82	0.61
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.83	0.61
1:A:170:THR:HG22	1:A:171:THR:N	2.15	0.61
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.83	0.61
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.29	0.61
8:U:21:ARG:O	8:U:25:GLU:HG3	2.01	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
3:P:117:GLY:O	12:P:502:HEM:HMC3	2.00	0.61
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.16	0.61
1:A:32:GLN:OE1	2:B:373:GLU:HG2	2.01	0.61
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:225:ASN:O	2:O:227:ARG:HB3	2.01	0.61
5:E:144:CYS:O	5:E:146:PRO:HD3	2.01	0.61
9:I:33:UNK:HG3	9:I:34:UNK:N	1.99	0.61
9:V:68:LEU:HD21	9:V:69:ASN:ND2	2.15	0.61
10:W:49:GLY:N	10:W:54:HIS:ND1	2.48	0.61
2:B:397:VAL:O	2:B:401:LYS:HG2	2.01	0.61
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.30	0.61
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.61
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.60
5:E:163:SER:H	5:E:175:PRO:HD2	1.66	0.60
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.83	0.60
2:O:248:ASN:ND2	2:O:250:HIS:H	1.99	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:B:76:THR:CG2	2:B:82:SER:H	2.01	0.60
5:E:73:LYS:HB3	5:E:196:GLY:O	2.01	0.60
5:R:112:VAL:HG11	5:R:170:ARG:NH1	2.16	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.01	0.60
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.84	0.60
6:F:99:ARG:HH11	6:F:99:ARG:HG3	1.66	0.60
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.83	0.60
2:O:169:LYS:O	2:O:170:THR:HG23	2.01	0.60
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.66	0.60
2:B:385:GLU:HG2	9:I:2:LEU:HD13	1.81	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.35	0.60
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.84	0.60
2:O:341:MET:HE2	2:O:341:MET:HA	1.84	0.60
1:A:67:THR:HG21	1:A:115:ASP:CG	2.26	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.87	0.60
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.02	0.60
1:A:402:VAL:HA	1:A:406:MET:HE2	1.83	0.60
2:B:43:PRO:O	2:B:113:ARG:HG3	2.00	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.82	0.60
1:N:402:VAL:HA	1:N:406:MET:HE2	1.84	0.60
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.67	0.60
1:N:106:MET:C	1:N:106:MET:HE2	2.26	0.60
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.67	0.60
7:T:79:ASN:N	7:T:79:ASN:HD22	1.99	0.60
8:U:40:CYS:O	8:U:44:VAL:HG23	2.02	0.59
9:V:6:ALA:O	9:V:7:ARG:HG3	2.01	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.83	0.59
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.83	0.59
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.37	0.59
6:F:32:MET:HE3	6:F:87:LYS:CE	2.32	0.59
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.02	0.59
8:H:27:THR:HG22	8:H:29:LYS:N	2.16	0.59
9:I:70:LEU:HD23	9:I:71:ASN:N	2.17	0.59
2:O:374:THR:HG22	2:O:376:GLN:H	1.68	0.59
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.02	0.59
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.59
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.83	0.59
2:B:407:SER:O	2:B:411:VAL:HG23	2.01	0.59
8:H:21:ARG:O	8:H:25:GLU:HG3	2.02	0.59
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.85	0.59
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.59
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.85	0.59
3:C:46:ILE:HA	12:C:501:HEM:HMC3	1.85	0.59
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.03	0.59
1:N:67:THR:HG21	1:N:115:ASP:CG	2.27	0.59
2:O:53:ALA:O	2:O:105:MET:HG3	2.03	0.59
2:O:101:THR:CG2	2:O:104:LYS:HE3	2.29	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.67	0.59
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.03	0.58
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.38	0.58
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.18	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.02	0.58
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.58
5:R:118:ARG:NH1	5:R:118:ARG:HB2	2.18	0.58
2:B:22:GLU:CG	2:B:23:ASP:H	1.99	0.58
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.68	0.58
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.84	0.58
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.39	0.58
3:C:288:LYS:O	3:C:292:VAL:HG23	2.03	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.32	0.58
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.17	0.58
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.35	0.58
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.19	0.58
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.58
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.85	0.58
2:B:315:ASN:ND2	9:I:7:ARG:HD3	2.17	0.58
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.26	0.58
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.85	0.58
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.85	0.58
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.58
1:A:106:MET:HE2	1:A:106:MET:C	2.28	0.58
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.86	0.58
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.39	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.33	0.58
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.58
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.84	0.58
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.39	0.57
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.34	0.57
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.69	0.57
9:I:6:ALA:O	9:I:7:ARG:HG3	2.03	0.57
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.85	0.57
9:V:69:ASN:O	9:V:70:ALA:HB2	2.03	0.57
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.85	0.57
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.04	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.57
2:B:374:THR:HG22	2:B:376:GLN:H	1.69	0.57
2:O:59:THR:HG22	2:O:60:THR:N	2.19	0.57
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.57
1:A:133:VAL:O	1:A:137:GLU:HG3	2.04	0.57
2:O:402:ILE:C	2:O:402:ILE:HD13	2.28	0.57
7:T:41:PHE:O	7:T:45:VAL:HG23	2.04	0.57
7:G:29:ILE:O	7:G:33:ALA:HB3	2.04	0.57
9:I:33:UNK:CG	9:I:34:UNK:H	2.03	0.57
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.57
1:N:402:VAL:HG22	1:N:406:MET:CE	2.35	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.40	0.57
3:P:5:ILE:O	3:P:5:ILE:HG22	2.05	0.57
5:R:155:GLY:HA3	5:R:166:ASP:C	2.30	0.57
2:B:381:GLU:OE1	9:I:3:SER:HB2	2.05	0.57
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.23	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.87	0.57
4:D:22:ASP:HA	10:J:50:LYS:HB3	1.87	0.57
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.04	0.57
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.85	0.57
1:A:362:ARG:O	1:A:365:MET:HG2	2.05	0.56
3:P:79:LEU:HD22	4:Q:204:MET:HE1	1.86	0.56
3:P:138:GLN:HB2	3:P:255:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.05	0.56
1:N:21:ASN:HB3	1:N:219:VAL:HG22	1.86	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.35	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.56
3:C:22:LEU:HD21	14:C:504:UQ:HM32	1.88	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.87	0.56
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.86	0.56
2:O:192:HIS:O	2:O:196:GLN:HG3	2.04	0.56
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.23	0.56
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.87	0.56
3:C:5:ILE:O	3:C:5:ILE:HG22	2.06	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.35	0.56
5:R:117:LEU:HD21	5:R:172:ARG:HH11	1.70	0.56
2:B:53:ALA:O	2:B:105:MET:HG3	2.06	0.56
6:F:32:MET:HE3	6:F:87:LYS:HE3	1.87	0.56
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.56
2:O:182:ARG:HG2	2:O:182:ARG:HH11	1.70	0.56
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.40	0.56
1:A:2:ALA:HB3	2:B:113:ARG:NH2	2.20	0.56
2:B:297:GLN:O	2:B:301:LYS:HG3	2.05	0.56
7:G:65:GLU:O	7:G:69:LEU:HG	2.06	0.56
1:N:90:THR:O	1:N:167:VAL:HG11	2.05	0.56
10:W:38:GLY:O	10:W:42:ILE:HG13	2.05	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.88	0.56
4:D:203:ARG:HB2	4:D:203:ARG:HH11	1.70	0.56
2:O:273:SER:O	2:O:276:GLN:HB3	2.06	0.56
3:P:153:ALA:O	3:P:155:PRO:HD3	2.06	0.56
7:T:80:ASP:C	8:U:47:ARG:HD3	2.30	0.55
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.70	0.55
2:B:31:ASN:N	2:B:31:ASN:ND2	2.52	0.55
2:B:101:THR:CG2	2:B:104:LYS:HE3	2.33	0.55
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.71	0.55
6:S:13:MET:O	6:S:16:ILE:HB	2.05	0.55
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.21	0.55
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.41	0.55
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.21	0.55
2:O:297:GLN:O	2:O:301:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:PHE:O	7:G:50:PRO:HG2	2.06	0.55
9:I:1:AME:HE1	9:I:6:ALA:O	2.06	0.55
3:P:230:ILE:HG23	16:R:502:PEE:H25	1.89	0.55
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.05	0.55
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.88	0.55
7:G:41:PHE:O	7:G:45:VAL:HG23	2.07	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.42	0.55
2:B:414:ALA:O	2:B:418:VAL:HG23	2.07	0.55
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.42	0.55
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.41	0.55
3:P:365:ILE:HG22	3:P:366:LEU:N	2.22	0.55
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.22	0.55
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.88	0.55
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.89	0.55
6:F:40:ASP:O	6:F:44:LYS:HG2	2.07	0.55
1:A:112:LEU:O	1:A:116:VAL:HG23	2.07	0.55
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.55
2:O:292:THR:HG22	2:O:292:THR:O	2.07	0.55
1:A:387:GLY:O	1:A:388:ARG:HB3	2.07	0.54
2:B:38:LEU:HG	2:B:39:GLU:N	2.21	0.54
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.42	0.54
8:U:43:ARG:HD2	8:U:47:ARG:HH22	1.72	0.54
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.88	0.54
5:E:189:GLY:O	5:E:192:LEU:N	2.39	0.54
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.89	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.69	0.54
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.07	0.54
9:V:47:LEU:HD11	9:V:56:ARG:HH11	1.72	0.54
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.42	0.54
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.43	0.54
5:R:3:ASN:ND2	5:R:3:ASN:H	2.06	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.89	0.54
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.23	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.08	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.38	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.08	0.54
5:R:3:ASN:H	5:R:3:ASN:HD22	1.55	0.54
4:Q:203:ARG:HH11	4:Q:203:ARG:HB2	1.73	0.54
2:B:166:ALA:O	2:B:242:GLY:N	2.35	0.54
3:C:145:THR:O	3:C:149:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:ASN:O	4:D:156:GLN:HA	2.06	0.54
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.38	0.54
8:U:32:LYS:O	8:U:36:ARG:HG3	2.06	0.54
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.23	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.90	0.54
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.90	0.54
5:R:126:ARG:NH2	5:R:169:GLY:O	2.41	0.54
6:S:40:ASP:O	6:S:44:LYS:HG2	2.06	0.54
5:E:169:GLY:O	5:E:179:ASN:HB3	2.07	0.54
5:E:194:VAL:HG12	5:E:194:VAL:O	2.07	0.54
2:O:160:LEU:HD12	9:V:62:LEU:HD13	1.90	0.54
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.89	0.54
2:O:227:ARG:HG3	2:O:228:SER:N	2.22	0.54
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.89	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.54
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.71	0.54
2:O:307:PHE:H	9:V:50:ARG:HG2	1.72	0.54
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.43	0.54
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.07	0.54
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.89	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
2:B:292:THR:HG22	2:B:292:THR:O	2.07	0.53
3:C:28:ILE:CD1	14:C:504:UQ:HM21	2.38	0.53
5:R:10:PHE:O	5:R:14:ARG:HG3	2.08	0.53
5:R:83:GLU:HB3	5:R:102:THR:CG2	2.27	0.53
5:E:3:ASN:HD22	5:E:3:ASN:H	1.56	0.53
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.26	0.53
4:Q:83:ARG:HH12	4:Q:86:LYS:HG3	1.73	0.53
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.08	0.53
3:C:245:LEU:O	4:D:201:ARG:HD2	2.08	0.53
5:E:109:GLU:OE2	5:E:166:ASP:HB2	2.08	0.53
2:O:27:THR:CG2	2:O:28:LYS:H	2.16	0.53
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.38	0.53
5:E:191:ASP:OD2	5:E:191:ASP:N	2.42	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.91	0.53
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.48	0.53
7:G:79:ASN:N	7:G:79:ASN:ND2	2.56	0.53
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.90	0.53
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:HD11	2:B:223:PHE:CD2	2.43	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.89	0.53
2:O:417:PHE:O	2:O:422:LYS:HE3	2.09	0.53
3:P:243:LEU:O	3:P:243:LEU:HD12	2.08	0.53
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.69	0.53
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.90	0.53
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.38	0.53
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53
2:O:402:ILE:HD13	2:O:402:ILE:O	2.09	0.53
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.91	0.53
5:R:148:ALA:O	5:R:155:GLY:O	2.26	0.53
7:T:79:ASN:N	7:T:79:ASN:ND2	2.54	0.53
2:B:35:ILE:O	2:B:213:HIS:HE1	1.92	0.53
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.90	0.53
2:B:199:PHE:O	2:B:226:ILE:HG21	2.08	0.53
5:R:166:ASP:OD1	5:R:168:SER:HB3	2.09	0.53
3:C:122:LEU:HD21	3:C:299:VAL:HG11	1.90	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.90	0.53
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.53
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.91	0.53
1:A:398:ARG:HG2	1:A:398:ARG:HH11	1.74	0.52
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.90	0.52
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.73	0.52
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.24	0.52
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.91	0.52
5:E:96:LEU:HD21	5:E:195:VAL:HG21	1.91	0.52
5:E:155:GLY:HA3	5:E:166:ASP:C	2.34	0.52
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.08	0.52
2:O:219:VAL:O	2:O:223:PHE:HB2	2.09	0.52
3:C:377:MET:HE2	6:F:20:TYR:CG	2.44	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.73	0.52
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.90	0.52
1:A:178:THR:CG2	1:A:179:ARG:N	2.73	0.52
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.91	0.52
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.43	0.52
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.91	0.52
7:G:79:ASN:N	7:G:79:ASN:HD22	2.07	0.52
2:O:341:MET:HA	2:O:341:MET:CE	2.38	0.52
2:O:403:ASP:C	2:O:405:VAL:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.92	0.52
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.45	0.52
2:B:207:VAL:HG12	2:B:208:GLY:N	2.25	0.52
2:B:225:ASN:O	2:B:226:ILE:C	2.52	0.52
9:I:49:LEU:HB3	9:I:55:MET:HG3	1.92	0.52
2:O:76:THR:CG2	2:O:82:SER:H	1.98	0.52
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.25	0.52
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.39	0.52
2:O:147:ASP:OD1	9:V:66:ILE:HD11	2.09	0.52
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.91	0.52
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.10	0.52
1:A:49:ASN:ND2	1:A:51:LYS:H	2.06	0.52
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.52
2:O:156:GLN:NE2	9:V:75:ARG:C	2.68	0.52
2:B:341:MET:HA	2:B:341:MET:CE	2.39	0.52
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.75	0.52
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.24	0.52
6:S:95:LYS:O	6:S:99:ARG:HG3	2.10	0.52
2:B:38:LEU:CG	2:B:39:GLU:N	2.72	0.52
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.23	0.52
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.52
2:B:403:ASP:C	2:B:405:VAL:H	2.18	0.52
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.40	0.52
1:N:49:ASN:HD21	1:N:51:LYS:H	1.58	0.52
2:O:314:VAL:CG1	9:V:61:ASP:HB3	2.38	0.52
6:S:70:LEU:HD12	6:S:70:LEU:C	2.35	0.52
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.45	0.51
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.51
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.40	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.72	0.51
1:N:294:LEU:HD11	1:N:334:MET:CE	2.40	0.51
2:O:29:LEU:CD1	2:O:221:GLU:HB3	2.39	0.51
1:A:191:LYS:O	1:A:195:MET:HG3	2.10	0.51
3:C:202:HIS:NE2	14:C:504:UQ:O4	2.43	0.51
5:E:95:PRO:HG2	5:E:145:VAL:CG1	2.40	0.51
2:O:38:LEU:CG	2:O:39:GLU:N	2.73	0.51
2:O:235:ALA:O	2:O:236:LYS:C	2.53	0.51
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.51
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.27	0.51
1:A:105:ASP:O	1:A:109:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
10:J:60:GLU:OE2	10:J:60:GLU:HA	2.09	0.51
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.51
5:E:107:ASN:N	5:E:107:ASN:ND2	2.51	0.51
8:U:27:THR:HG22	8:U:29:LYS:N	2.20	0.51
2:B:235:ALA:O	2:B:236:LYS:C	2.53	0.51
3:C:365:ILE:HG22	3:C:366:LEU:N	2.26	0.51
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.46	0.51
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.45	0.51
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.76	0.51
3:P:95:ILE:O	3:P:99:ILE:HG13	2.10	0.51
5:R:52:LYS:HD3	5:R:52:LYS:C	2.35	0.51
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.40	0.51
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.93	0.51
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.51
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.51
1:N:137:GLU:O	1:N:141:MET:HG3	2.11	0.51
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.74	0.51
7:T:3:HIS:O	7:T:7:LEU:HG	2.11	0.51
2:O:273:SER:OG	9:V:7:ARG:NH1	2.44	0.51
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.11	0.51
2:B:230:ALA:O	2:B:231:GLY:C	2.54	0.51
7:G:53:LEU:O	7:G:57:LEU:HG	2.11	0.51
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.46	0.51
1:A:269:VAL:HG22	1:A:406:MET:HE3	1.93	0.51
1:A:343:MET:HB3	1:A:444:ILE:HA	1.92	0.51
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.51
2:B:273:SER:OG	9:I:7:ARG:NH1	2.44	0.51
8:H:12:GLU:HG2	8:H:13:LEU:N	2.25	0.51
2:B:287:ARG:HD3	9:I:53:GLU:HG2	1.92	0.50
1:N:75:PHE:O	1:N:79:VAL:HG23	2.11	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.74	0.50
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.92	0.50
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.92	0.50
1:A:307:PHE:CD1	1:A:307:PHE:C	2.89	0.50
2:B:50:PHE:N	2:B:50:PHE:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.76	0.50
5:E:3:ASN:H	5:E:3:ASN:ND2	2.09	0.50
5:E:147:ILE:HG22	5:E:149:ASN:H	1.76	0.50
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.93	0.50
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.27	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.50
2:O:38:LEU:HG	2:O:39:GLU:N	2.21	0.50
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.50
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.94	0.50
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.41	0.50
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.77	0.50
9:I:49:LEU:HD11	9:I:58:ARG:HH11	1.74	0.50
3:P:50:LEU:O	3:P:54:MET:HG3	2.11	0.50
4:Q:71:GLN:HG3	4:Q:82:MET:HE1	1.93	0.50
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.52	0.50
1:A:405:ARG:HD3	1:A:409:ASP:OD2	2.11	0.50
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.93	0.50
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.50
1:N:343:MET:HB3	1:N:444:ILE:HA	1.93	0.50
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.50
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.41	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.94	0.50
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.42	0.50
9:V:1:AME:HE1	9:V:6:ALA:O	2.11	0.50
3:C:156:TYR:C	3:C:158:GLY:H	2.19	0.50
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.12	0.50
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.93	0.50
1:N:405:ARG:HG2	1:N:405:ARG:HH11	1.77	0.50
9:V:1:AME:C	9:V:3:SER:N	2.73	0.50
10:W:14:PHE:N	10:W:14:PHE:CD2	2.79	0.50
3:C:147:ILE:HG13	13:C:503:WF3:H15	1.94	0.50
4:D:239:PRO:C	4:D:241:LYS:H	2.18	0.50
9:I:49:LEU:HB3	9:I:55:MET:CG	2.42	0.50
10:W:22:LEU:O	10:W:22:LEU:HD23	2.12	0.50
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.47	0.49
9:I:65:VAL:HG12	9:I:66:ALA:N	2.26	0.49
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.38	0.49
6:S:91:GLU:O	6:S:95:LYS:HG3	2.11	0.49
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.12	0.49
2:B:150:VAL:HG23	2:B:151:ALA:N	2.26	0.49
7:G:81:GLN:OXT	7:G:81:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:ASN:HD21	9:V:7:ARG:HH11	1.60	0.49
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.12	0.49
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.60	0.49
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.31	0.49
6:F:70:LEU:C	6:F:70:LEU:HD12	2.36	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.44	0.49
2:O:166:ALA:HB1	2:O:242:GLY:C	2.37	0.49
2:O:287:ARG:HD3	9:V:51:GLU:HG2	1.93	0.49
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.94	0.49
5:R:118:ARG:CB	5:R:118:ARG:HH11	2.26	0.49
5:R:130:PRO:C	5:R:132:TRP:H	2.20	0.49
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
7:T:48:VAL:O	7:T:51:PRO:HD2	2.11	0.49
1:A:95:THR:HG22	1:A:96:ALA:N	2.27	0.49
2:B:27:THR:CG2	2:B:28:LYS:H	2.21	0.49
4:D:169:LEU:C	4:D:169:LEU:HD23	2.38	0.49
2:O:71:LEU:HD23	9:V:66:ILE:HG13	1.94	0.49
2:O:73:SER:N	2:O:74:PRO:HD2	2.28	0.49
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.94	0.49
3:P:287:ASN:O	3:P:288:LYS:C	2.56	0.49
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.38	0.49
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
3:P:288:LYS:O	3:P:292:VAL:HG23	2.12	0.49
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.76	0.49
2:B:262:ALA:CB	2:B:269:ALA:HA	2.43	0.49
3:C:173:ASN:N	3:C:174:PRO:HD2	2.27	0.49
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.26	0.49
5:E:107:ASN:O	5:E:111:GLU:HG3	2.13	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.13	0.49
2:O:268:GLU:HG2	2:O:272:PHE:CE1	2.47	0.49
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.42	0.49
10:W:20:PHE:CD1	10:W:20:PHE:C	2.90	0.49
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.47	0.49
4:Q:222:MET:HE3	5:R:40:THR:OG1	2.13	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.49
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.42	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
2:B:315:ASN:HD21	9:I:7:ARG:HH11	1.61	0.49
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.47	0.49
2:B:398:VAL:HG13	2:B:399:ALA:N	2.28	0.49
4:D:166:ASN:H	4:D:166:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.94	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.49
2:B:248:ASN:ND2	2:B:250:HIS:H	2.11	0.49
2:O:306:PRO:HA	9:V:50:ARG:CG	2.43	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.49
3:P:334:LEU:HD21	16:P:507:PEE:H65	1.95	0.49
5:R:114:VAL:HG12	5:R:114:VAL:O	2.13	0.49
1:A:106:MET:HE2	1:A:107:PRO:HA	1.94	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.42	0.48
6:F:32:MET:CE	6:F:87:LYS:HG2	2.42	0.48
1:N:35:CYS:HB2	1:N:200:ALA:O	2.13	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.48	0.48
1:N:269:VAL:HG22	1:N:406:MET:HE3	1.95	0.48
2:O:156:GLN:HE22	9:V:75:ARG:C	2.21	0.48
2:O:370:MET:C	2:O:372:VAL:H	2.21	0.48
3:P:33:ASN:HB3	21:P:608:HOH:O	2.13	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.95	0.48
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.95	0.48
4:Q:131:LEU:HD11	18:Q:501:HEC:HMB2	1.95	0.48
5:R:186:GLN:HE21	5:R:188:VAL:CG1	2.25	0.48
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.48
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.78	0.48
5:E:137:GLY:O	5:E:145:VAL:HG13	2.13	0.48
4:Q:81:PHE:C	4:Q:82:MET:HE2	2.38	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.48
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.94	0.48
2:B:206:LEU:HG	2:B:206:LEU:O	2.12	0.48
5:R:118:ARG:NH1	5:R:118:ARG:CB	2.77	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.46	0.48
8:U:28:GLU:O	8:U:32:LYS:HG3	2.14	0.48
2:B:27:THR:CG2	2:B:28:LYS:N	2.76	0.48
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.48
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.95	0.48
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.14	0.48
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.48	0.48
3:P:101:ARG:C	3:P:101:ARG:CD	2.85	0.48
5:R:29:SER:HA	5:R:32:ARG:NH2	2.28	0.48
9:V:33:UNK:C	9:V:71:PRO:HG2	2.43	0.48
2:B:402:ILE:HD13	2:B:402:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
5:E:130:PRO:HG2	5:E:131:GLU:H	1.79	0.48
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.95	0.48
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.49	0.48
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.96	0.48
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.94	0.48
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.12	0.48
5:R:107:ASN:O	5:R:110:ALA:N	2.43	0.48
9:V:47:LEU:HB3	9:V:53:MET:CG	2.44	0.48
2:B:38:LEU:O	2:B:39:GLU:HB2	2.14	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.96	0.48
2:B:370:MET:O	2:B:373:GLU:HG3	2.14	0.48
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.79	0.48
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.48
2:B:274:VAL:O	2:B:278:VAL:HG23	2.14	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.48
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.43	0.48
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.79	0.48
5:R:133:VAL:O	5:R:133:VAL:HG13	2.12	0.48
8:U:73:LEU:HD12	8:U:73:LEU:O	2.13	0.48
1:A:170:THR:HG22	1:A:172:GLU:H	1.79	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.48
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.48
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.14	0.48
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.95	0.48
5:E:119:ASP:O	5:E:121:GLN:N	2.46	0.48
1:N:342:TRP:O	1:N:345:LEU:HB2	2.12	0.48
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.48
2:O:341:MET:CE	2:O:417:PHE:HE2	2.14	0.48
3:P:377:MET:HE2	6:S:20:TYR:CG	2.49	0.48
5:R:194:VAL:O	5:R:194:VAL:HG12	2.14	0.48
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.13	0.48
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.78	0.48
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.95	0.48
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.08	0.48
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.29	0.47
9:I:1:AME:C	9:I:3:SER:H	2.27	0.47
2:O:38:LEU:O	2:O:39:GLU:HB2	2.14	0.47
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.85	0.47
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.95	0.47
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.76	0.47
8:H:35:GLU:O	8:H:39:LEU:HG	2.14	0.47
2:O:230:ALA:O	2:O:231:GLY:C	2.56	0.47
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.96	0.47
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.96	0.47
2:B:307:PHE:N	9:I:52:ARG:HG2	2.27	0.47
2:B:368:TYR:HB2	9:I:1:AME:CE	2.42	0.47
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.14	0.47
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.38	0.47
3:P:332:ASN:ND2	3:P:358:SER:OG	2.47	0.47
5:R:166:ASP:OD2	5:R:172:ARG:HD3	2.13	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.47
3:C:103:LEU:HD12	3:C:103:LEU:O	2.13	0.47
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.97	0.47
4:D:71:GLN:HG3	4:D:82:MET:HE1	1.95	0.47
1:N:387:GLY:O	1:N:388:ARG:HB3	2.13	0.47
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.47
2:O:72:ALA:C	2:O:74:PRO:HD2	2.39	0.47
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.49	0.47
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.96	0.47
2:B:207:VAL:HG12	2:B:208:GLY:H	1.79	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.13	0.47
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.47
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.32	0.47
5:E:125:ASP:C	5:E:126:ARG:HG3	2.39	0.47
5:E:161:HIS:HB2	5:E:175:PRO:HG3	1.96	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
1:N:119:ASN:O	1:N:120:CYS:C	2.57	0.47
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.47
5:R:129:LYS:HG2	5:R:131:GLU:OE1	2.14	0.47
6:S:16:ILE:O	6:S:19:TRP:HB3	2.15	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.14	0.47
3:C:138:GLN:HB2	3:C:255:GLU:O	2.15	0.47
5:E:153:PHE:C	5:E:155:GLY:H	2.23	0.47
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.14	0.47
8:H:26:GLN:HA	8:H:26:GLN:OE1	2.14	0.47
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.47
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.97	0.47
1:N:317:THR:HG23	1:N:318:GLY:N	2.30	0.47
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.47
2:O:166:ALA:O	2:O:242:GLY:N	2.45	0.47
2:O:207:VAL:HG12	2:O:208:GLY:N	2.30	0.47
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.47
3:P:34:PHE:HB2	21:P:601:HOH:O	2.14	0.47
5:R:65:SER:OG	5:R:67:ASP:OD1	2.33	0.47
5:R:153:PHE:C	5:R:155:GLY:H	2.22	0.47
5:E:116:LYS:HD2	5:E:116:LYS:N	2.13	0.47
5:E:127:VAL:HG12	5:E:128:LYS:N	2.30	0.47
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.47
1:A:75:PHE:O	1:A:79:VAL:HG23	2.15	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
3:C:243:LEU:HD12	3:C:243:LEU:O	2.14	0.47
2:O:150:VAL:HG23	2:O:151:ALA:N	2.29	0.47
5:R:100:HIS:HA	5:R:131:GLU:O	2.14	0.47
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.47
5:E:133:VAL:O	5:E:133:VAL:HG13	2.15	0.47
2:O:398:VAL:HG13	2:O:399:ALA:N	2.30	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.47
5:R:156:TYR:N	5:R:165:TYR:O	2.37	0.47
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.50	0.47
3:C:156:TYR:C	3:C:158:GLY:N	2.73	0.46
3:C:158:GLY:C	3:C:160:THR:N	2.73	0.46
5:E:151:GLY:HA2	5:E:157:TYR:HB2	1.96	0.46
1:N:23:LEU:HA	1:N:192:ALA:O	2.16	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
2:O:28:LYS:CE	2:O:32:GLY:HA2	2.45	0.46
9:V:47:LEU:HB3	9:V:53:MET:HG3	1.95	0.46
2:B:46:ARG:HH22	2:B:376:GLN:HG3	1.80	0.46
5:E:190:ASP:C	5:E:192:LEU:N	2.71	0.46
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.50	0.46
2:O:73:SER:N	2:O:74:PRO:CD	2.78	0.46
3:P:146:VAL:HG12	3:P:147:ILE:N	2.31	0.46
3:P:147:ILE:HG13	13:P:504:WF3:H15	1.97	0.46
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.15	0.46
6:S:13:MET:CE	6:S:17:ARG:HH12	2.27	0.46
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.48	0.46
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.79	0.46
4:D:16:GLY:N	4:D:19:SER:OG	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ILE:HG12	4:D:160:MET:H	1.80	0.46
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.46
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.44	0.46
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.46
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.74	0.46
5:R:83:GLU:OE1	5:R:103:GLN:NE2	2.49	0.46
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.79	0.46
1:A:342:TRP:O	1:A:345:LEU:HB2	2.16	0.46
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.45	0.46
3:C:146:VAL:HG12	3:C:147:ILE:N	2.30	0.46
5:E:29:SER:HA	5:E:32:ARG:NH2	2.30	0.46
5:E:102:THR:HB	5:E:103:GLN:OE1	2.15	0.46
5:E:104:ALA:O	5:E:108:GLN:HB3	2.15	0.46
5:E:134:ILE:O	5:E:182:VAL:HG13	2.15	0.46
2:O:67:HIS:O	2:O:70:ARG:HB3	2.15	0.46
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.83	0.46
4:Q:13:SER:O	10:W:50:LYS:NZ	2.46	0.46
9:V:2:LEU:HD12	9:V:2:LEU:H	1.78	0.46
2:B:166:ALA:HB1	2:B:242:GLY:C	2.40	0.46
2:B:341:MET:CE	2:B:417:PHE:HE2	2.15	0.46
4:D:57:THR:CG2	4:D:59:ALA:H	2.23	0.46
4:D:81:PHE:C	4:D:82:MET:HE2	2.40	0.46
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.46
1:A:15:ASN:O	1:A:26:ALA:HA	2.16	0.46
1:A:294:LEU:HD11	1:A:334:MET:CE	2.46	0.46
2:B:86:THR:O	2:B:90:GLU:HG3	2.15	0.46
2:B:141:GLN:N	2:B:142:PRO:HD2	2.31	0.46
5:E:186:GLN:O	5:E:193:VAL:HA	2.16	0.46
9:I:49:LEU:CD1	9:I:55:MET:HG2	2.44	0.46
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.46
4:Q:22:ASP:HA	10:W:50:LYS:HB3	1.98	0.46
3:C:157:ILE:O	3:C:157:ILE:HG12	2.15	0.46
1:N:87:ASN:CG	1:N:88:GLY:N	2.73	0.46
7:T:53:LEU:O	7:T:57:LEU:HG	2.15	0.46
1:A:405:ARG:HG2	1:A:405:ARG:NH1	2.30	0.46
2:B:370:MET:C	2:B:372:VAL:H	2.23	0.46
3:C:334:LEU:HD21	16:C:506:PEE:H65	1.97	0.46
1:N:253:VAL:HG11	1:N:335:MET:HE2	1.98	0.46
2:O:35:ILE:O	2:O:213:HIS:HE1	1.98	0.46
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.46
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.96	0.46
6:F:16:ILE:O	6:F:19:TRP:HB3	2.16	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.98	0.46
2:B:76:THR:HG23	2:B:82:SER:HB2	1.98	0.46
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.46	0.46
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.49	0.46
4:D:208:MET:O	4:D:212:SER:HB2	2.16	0.45
1:N:398:ARG:NH1	1:N:398:ARG:HG2	2.30	0.45
2:O:201:SER:H	2:O:227:ARG:HA	1.81	0.45
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.98	0.45
2:O:350:GLY:C	2:O:352:VAL:H	2.24	0.45
9:V:63:VAL:HG12	9:V:64:ALA:N	2.31	0.45
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.71	0.45
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.98	0.45
4:Q:240:PRO:O	4:Q:241:LYS:C	2.58	0.45
5:R:109:GLU:HA	5:R:109:GLU:OE2	2.17	0.45
6:S:76:PRO:HD2	6:S:79:GLN:OE1	2.16	0.45
8:U:51:GLU:O	8:U:52:GLU:C	2.58	0.45
1:A:354:VAL:HG23	1:A:355:LYS:N	2.32	0.45
2:B:262:ALA:O	2:B:320:GLY:HA3	2.16	0.45
5:E:128:LYS:O	5:E:129:LYS:C	2.58	0.45
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.76	0.45
5:R:79:SER:C	5:R:81:ILE:H	2.22	0.45
8:U:27:THR:O	8:U:31:VAL:HG23	2.17	0.45
1:A:272:VAL:O	1:A:275:ALA:HB3	2.17	0.45
2:B:345:LYS:O	2:B:349:GLN:HG3	2.16	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.49	0.45
4:D:65:ALA:O	4:D:85:GLY:HA3	2.16	0.45
5:E:185:TYR:O	5:E:186:GLN:HB3	2.16	0.45
10:J:4:ALA:O	10:J:8:GLN:HG3	2.17	0.45
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.45
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.45
1:A:119:ASN:O	1:A:120:CYS:C	2.58	0.45
1:A:217:SER:O	1:A:218:GLY:C	2.60	0.45
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.65	0.45
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.74	0.45
3:C:122:LEU:HD21	3:C:299:VAL:CG1	2.47	0.45
5:E:131:GLU:H	5:E:131:GLU:CD	2.23	0.45
10:J:14:PHE:CD2	10:J:14:PHE:N	2.82	0.45
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.98	0.45
3:C:377:MET:HE1	6:F:19:TRP:HZ3	1.82	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.98	0.45
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.99	0.45
5:R:136:VAL:O	5:R:138:VAL:N	2.46	0.45
7:T:57:LEU:O	7:T:58:LEU:C	2.59	0.45
5:E:130:PRO:C	5:E:132:TRP:H	2.24	0.45
3:P:4:ASN:C	3:P:6:ARG:H	2.25	0.45
1:A:130:GLU:O	1:A:134:ILE:HG13	2.17	0.45
1:A:136:GLN:NE2	9:I:50:LEU:HB3	2.32	0.45
2:B:368:TYR:O	2:B:372:VAL:HG23	2.17	0.45
3:C:31:TRP:CZ3	16:C:506:PEE:H20	2.52	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.47	0.45
1:N:395:TRP:CE3	1:N:398:ARG:HD2	2.52	0.45
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.47	0.45
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.45
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.80	0.45
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.31	0.45
4:Q:214:LEU:O	4:Q:218:LEU:HG	2.17	0.45
4:Q:239:PRO:C	4:Q:241:LYS:H	2.25	0.45
1:A:122:LEU:HD11	1:A:186:ILE:HD12	1.99	0.45
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.32	0.45
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.50	0.45
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.45
1:A:90:THR:O	1:A:167:VAL:HG11	2.17	0.45
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.52	0.45
3:C:155:PRO:O	3:C:157:ILE:HG22	2.16	0.45
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.99	0.45
7:G:71:ARG:NH1	8:H:56:GLU:HG3	2.32	0.45
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.45
3:P:122:LEU:HD21	3:P:299:VAL:HG11	1.98	0.45
4:Q:16:GLY:N	4:Q:19:SER:OG	2.50	0.45
5:R:122:HIS:C	5:R:124:LEU:N	2.73	0.45
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.52	0.45
3:C:122:LEU:CD2	3:C:299:VAL:HG11	2.46	0.44
5:E:100:HIS:HA	5:E:131:GLU:O	2.17	0.44
1:N:10:ASN:OD1	2:O:18:CYS:HB3	2.16	0.44
1:N:144:ASP:OD1	1:N:144:ASP:C	2.59	0.44
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.99	0.44
3:P:31:TRP:CZ3	16:P:507:PEE:H20	2.51	0.44
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:OD1	1:A:144:ASP:C	2.60	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
1:N:405:ARG:HD3	1:N:409:ASP:OD2	2.18	0.44
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.52	0.44
3:P:19:LEU:C	3:P:20:ILE:HG13	2.41	0.44
9:V:47:LEU:CD1	9:V:53:MET:HG2	2.46	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
1:A:269:VAL:HG21	1:A:410:VAL:HG21	2.00	0.44
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.17	0.44
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.98	0.44
5:E:171:ILE:HG12	5:E:176:ALA:O	2.18	0.44
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.99	0.44
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.44
4:Q:197:GLU:O	4:Q:198:HIS:C	2.60	0.44
9:V:69:ASN:O	9:V:70:ALA:CB	2.65	0.44
2:B:399:ALA:C	2:B:402:ILE:HG22	2.41	0.44
3:C:215:ASP:HB3	7:G:8:ALA:HB2	2.00	0.44
5:E:74:ILE:CG2	5:E:195:VAL:HB	2.47	0.44
1:N:15:ASN:O	1:N:26:ALA:HA	2.18	0.44
2:O:50:PHE:CD1	2:O:50:PHE:N	2.85	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
2:O:248:ASN:HD22	2:O:250:HIS:H	1.63	0.44
5:R:122:HIS:O	5:R:124:LEU:N	2.51	0.44
2:B:350:GLY:C	2:B:352:VAL:H	2.25	0.44
2:O:26:ILE:HG23	2:O:26:ILE:O	2.18	0.44
2:O:150:VAL:CG2	2:O:151:ALA:N	2.81	0.44
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.44
4:Q:208:MET:SD	4:Q:208:MET:C	3.01	0.44
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.82	0.44
8:U:24:CYS:C	8:U:26:GLN:H	2.24	0.44
8:U:35:GLU:O	8:U:39:LEU:HG	2.17	0.44
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.44
5:E:191:ASP:O	5:E:192:LEU:HD23	2.18	0.44
7:G:57:LEU:O	7:G:58:LEU:C	2.60	0.44
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.47	0.44
2:O:182:ARG:HG2	2:O:182:ARG:NH1	2.32	0.44
2:O:402:ILE:O	2:O:405:VAL:HG23	2.18	0.44
4:Q:71:GLN:CG	4:Q:82:MET:HE1	2.47	0.44
8:U:18:THR:O	8:U:22:GLU:HG3	2.17	0.44
2:B:150:VAL:CG2	2:B:151:ALA:N	2.80	0.44
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.98	0.44
10:J:20:PHE:CD1	10:J:20:PHE:C	2.95	0.44
2:O:42:SER:O	2:O:113:ARG:HD2	2.17	0.44
3:P:50:LEU:HD23	12:P:501:HEM:HBC1	1.99	0.44
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.99	0.44
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.57	0.44
5:R:166:ASP:C	5:R:168:SER:H	2.26	0.44
1:A:253:VAL:HG11	1:A:335:MET:HE2	2.00	0.44
3:C:158:GLY:C	3:C:160:THR:H	2.25	0.44
5:E:166:ASP:OD2	5:E:172:ARG:HD3	2.17	0.44
1:N:106:MET:CG	1:N:203:ILE:HD13	2.40	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
2:B:424:MET:HG2	2:B:425:ALA:N	2.33	0.44
1:N:22:GLY:O	1:N:193:PRO:HA	2.18	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.44
2:B:182:ARG:HH11	2:B:182:ARG:HG2	1.83	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43
4:D:71:GLN:CG	4:D:82:MET:HE1	2.48	0.43
2:O:206:LEU:O	2:O:206:LEU:HG	2.17	0.43
5:R:118:ARG:NH1	5:R:171:ILE:HG13	2.33	0.43
2:B:422:LYS:O	2:B:436:LEU:HD21	2.18	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.89	0.43
1:N:87:ASN:CG	1:N:88:GLY:H	2.26	0.43
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.43
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.99	0.43
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.48	0.43
5:E:185:TYR:HB3	5:E:195:VAL:HA	1.99	0.43
8:H:28:GLU:O	8:H:32:LYS:HG3	2.18	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.33	0.43
2:O:181:TYR:CD1	2:O:181:TYR:C	2.96	0.43
4:Q:166:ASN:ND2	4:Q:166:ASN:H	2.14	0.43
1:A:168:GLU:H	1:A:168:GLU:CD	2.26	0.43
1:A:436:ARG:HA	1:A:436:ARG:HD2	1.89	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
2:B:258:VAL:HG21	2:B:321:LEU:HD22	2.00	0.43
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.83	0.43
2:O:315:ASN:ND2	9:V:7:ARG:HD3	2.27	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.99	0.43
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.54	0.43
1:A:23:LEU:HA	1:A:192:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.18	0.43
3:C:101:ARG:C	3:C:101:ARG:CD	2.92	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.60	0.43
2:O:315:ASN:HD21	9:V:7:ARG:NH1	2.16	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.48	0.43
1:A:105:ASP:O	1:A:106:MET:C	2.61	0.43
1:A:331:ILE:HG21	1:A:431:LEU:HB2	2.01	0.43
8:H:49:HIS:O	8:H:50:THR:HB	2.18	0.43
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.84	0.43
1:N:430:GLN:O	1:N:430:GLN:HG2	2.19	0.43
3:P:247:SER:N	3:P:248:PRO:HD3	2.33	0.43
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.43
8:U:24:CYS:C	8:U:26:GLN:N	2.77	0.43
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.54	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.19	0.43
2:B:26:ILE:O	2:B:26:ILE:HG12	2.18	0.43
2:B:59:THR:HG22	2:B:60:THR:HG22	2.01	0.43
3:C:9:HIS:CD2	3:C:11:LEU:H	2.36	0.43
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.84	0.43
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.43
1:N:304:CYS:HB2	1:N:325:VAL:O	2.19	0.43
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.01	0.43
2:O:424:MET:HG2	2:O:425:ALA:N	2.33	0.43
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.54	0.43
8:U:65:ARG:O	8:U:69:VAL:HG23	2.19	0.43
10:W:52:TRP:O	10:W:56:LYS:HB2	2.18	0.43
1:A:317:THR:HG23	1:A:318:GLY:N	2.34	0.43
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.01	0.43
1:A:395:TRP:CE3	1:A:398:ARG:HD2	2.54	0.43
2:B:38:LEU:CD1	2:B:39:GLU:H	2.32	0.43
5:E:83:GLU:O	5:E:85:LYS:N	2.43	0.43
1:N:106:MET:HE2	1:N:106:MET:O	2.19	0.43
3:P:365:ILE:HG22	3:P:366:LEU:HD23	2.01	0.43
5:R:158:CYS:C	5:R:160:CYS:H	2.27	0.43
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.19	0.43
5:R:186:GLN:O	5:R:193:VAL:HG23	2.19	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
3:C:50:LEU:O	3:C:54:MET:HG3	2.19	0.43
4:D:208:MET:SD	4:D:208:MET:C	3.02	0.43
2:O:47:ILE:HD11	2:O:116:VAL:HG13	2.01	0.43
2:O:59:THR:HG22	2:O:60:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:344:VAL:O	3:P:345:GLU:HG3	2.18	0.43
5:R:104:ALA:HA	5:R:107:ASN:HD22	1.83	0.43
1:A:63:ALA:O	1:A:116:VAL:HG13	2.19	0.43
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.49	0.43
3:C:198:LEU:HD21	12:C:502:HEM:HMA3	2.00	0.43
3:P:9:HIS:ND1	3:P:12:LEU:HD12	2.34	0.43
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.43
10:W:15:ARG:HH11	10:W:15:ARG:CG	2.31	0.43
2:B:31:ASN:ND2	2:B:31:ASN:H	2.16	0.42
2:B:372:VAL:HG12	2:B:372:VAL:O	2.19	0.42
3:C:347:PRO:O	3:C:350:ILE:HG22	2.18	0.42
5:E:101:ARG:HB2	5:E:131:GLU:HA	2.00	0.42
6:F:59:MET:HE3	6:F:59:MET:HA	2.01	0.42
8:H:27:THR:O	8:H:31:VAL:HG23	2.19	0.42
2:O:33:LEU:HD22	2:O:224:LEU:HD12	2.01	0.42
2:O:152:PHE:HA	2:O:157:VAL:HG11	2.01	0.42
2:O:268:GLU:HG2	2:O:268:GLU:O	2.18	0.42
4:Q:223:LYS:HD3	4:Q:223:LYS:C	2.44	0.42
5:R:122:HIS:O	5:R:123:ASP:C	2.62	0.42
9:V:47:LEU:HD11	9:V:56:ARG:NH1	2.34	0.42
3:C:344:VAL:C	3:C:345:GLU:HG3	2.44	0.42
5:E:187:PHE:O	5:E:188:VAL:C	2.62	0.42
1:N:191:LYS:O	1:N:195:MET:HG3	2.19	0.42
2:O:28:LYS:HE3	2:O:32:GLY:HA2	2.01	0.42
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.47	0.42
2:O:374:THR:HG22	2:O:376:GLN:N	2.33	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.42
8:U:48:SER:O	8:U:49:HIS:HB2	2.18	0.42
2:B:253:VAL:O	2:B:327:ILE:HA	2.20	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.00	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
5:E:117:LEU:O	5:E:118:ARG:C	2.62	0.42
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
1:N:358:LYS:HE3	1:N:399:ILE:O	2.19	0.42
3:P:215:ASP:HB3	7:T:8:ALA:HB2	2.01	0.42
5:R:170:ARG:HG2	5:R:179:ASN:CG	2.44	0.42
2:B:28:LYS:O	2:B:28:LYS:HG2	2.18	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.44	0.42
2:O:368:TYR:O	2:O:372:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:ALA:CB	3:P:8:SER:HB3	2.41	0.42
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	2.02	0.42
6:S:17:ARG:HH11	6:S:17:ARG:HG2	1.82	0.42
1:A:443:TRP:CE3	1:A:443:TRP:CA	3.00	0.42
5:E:114:VAL:HG11	5:E:117:LEU:HD12	2.01	0.42
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.37	0.42
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.34	0.42
2:O:86:THR:O	2:O:90:GLU:HG3	2.20	0.42
3:P:9:HIS:CD2	3:P:11:LEU:H	2.37	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
9:V:75:ARG:N	9:V:75:ARG:HD2	2.34	0.42
10:W:20:PHE:O	10:W:24:VAL:HG23	2.20	0.42
3:C:151:PHE:HB2	3:C:162:VAL:HG22	2.00	0.42
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.20	0.42
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.60	0.42
2:O:367:THR:HA	2:O:370:MET:HE3	2.00	0.42
3:P:349:ILE:O	3:P:353:GLN:HG3	2.19	0.42
4:Q:235:MET:CE	6:S:64:ARG:HA	2.49	0.42
5:R:107:ASN:O	5:R:108:GLN:C	2.63	0.42
5:R:124:LEU:C	5:R:126:ARG:H	2.27	0.42
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.69	0.42
1:A:49:ASN:HD21	1:A:51:LYS:H	1.68	0.42
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.50	0.42
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.50	0.42
3:C:160:THR:O	3:C:161:LEU:C	2.63	0.42
4:D:62:LYS:O	4:D:66:GLU:HG3	2.19	0.42
4:D:223:LYS:HD3	4:D:223:LYS:C	2.45	0.42
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.84	0.42
3:P:23:PRO:HG2	7:T:3:HIS:HB2	2.00	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.54	0.42
6:S:12:LEU:C	6:S:14:ASP:N	2.76	0.42
1:A:37:VAL:HG12	1:A:199:ALA:HB1	2.01	0.42
1:A:48:GLU:CD	1:A:54:GLY:H	2.28	0.42
3:C:130:VAL:HG23	3:C:131:GLY:N	2.34	0.42
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.20	0.42
4:D:76:GLU:OE1	4:D:76:GLU:N	2.43	0.42
4:D:232:SER:CB	7:G:23:GLN:HE22	2.32	0.42
5:E:158:CYS:C	5:E:160:CYS:H	2.28	0.42
5:E:166:ASP:C	5:E:168:SER:H	2.28	0.42
1:N:106:MET:HE2	1:N:107:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:269:VAL:HG21	1:N:410:VAL:HG21	2.02	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.42
3:P:31:TRP:CH2	15:P:506:CDL:H512	2.55	0.42
8:U:51:GLU:O	8:U:52:GLU:O	2.38	0.42
2:B:73:SER:N	2:B:74:PRO:HD2	2.34	0.42
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.93	0.42
3:C:4:ASN:C	3:C:6:ARG:H	2.27	0.42
2:O:315:ASN:ND2	9:V:7:ARG:HH11	2.18	0.42
2:O:372:VAL:HG12	2:O:372:VAL:O	2.20	0.42
2:O:374:THR:HG22	2:O:376:GLN:HB3	2.01	0.42
3:P:100:GLY:O	3:P:101:ARG:C	2.63	0.42
3:P:160:THR:O	3:P:161:LEU:C	2.61	0.42
3:P:184:PHE:HD2	3:P:184:PHE:O	2.03	0.42
4:Q:239:PRO:C	4:Q:241:LYS:N	2.77	0.42
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.55	0.42
9:V:4:VAL:HG12	9:V:61:ASP:OD2	2.19	0.42
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.42
1:A:294:LEU:HD11	1:A:334:MET:HE3	2.02	0.42
2:B:215:ASP:O	2:B:219:VAL:HG23	2.20	0.42
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.42
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.50	0.42
5:E:116:LYS:H	5:E:116:LYS:CD	2.14	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
1:N:382:HIS:HB3	1:N:388:ARG:O	2.20	0.42
3:P:377:MET:HE2	6:S:20:TYR:CB	2.50	0.42
2:B:128:THR:HG21	2:B:224:LEU:HD22	2.01	0.41
4:D:57:THR:HG22	4:D:58:GLU:N	2.34	0.41
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.35	0.41
10:J:15:ARG:HG2	10:J:15:ARG:NH1	2.30	0.41
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.20	0.41
1:N:405:ARG:HG2	1:N:405:ARG:NH1	2.35	0.41
2:O:151:ALA:O	2:O:157:VAL:HG11	2.20	0.41
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.20	0.41
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.63	0.41
3:P:286:PRO:O	3:P:287:ASN:HB2	2.20	0.41
2:B:62:ASN:O	2:B:65:THR:CG2	2.63	0.41
2:B:140:LEU:C	2:B:142:PRO:HD2	2.45	0.41
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
5:E:126:ARG:O	5:E:127:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:146:PRO:HG2	5:E:180:LEU:HD21	2.01	0.41
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.50	0.41
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
5:R:148:ALA:O	5:R:150:SER:N	2.53	0.41
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41
2:B:57:TYR:N	2:B:57:TYR:CD1	2.87	0.41
3:C:13:LYS:HG3	3:C:17:ASN:ND2	2.36	0.41
1:N:35:CYS:HA	1:N:372:THR:HG21	2.02	0.41
2:O:207:VAL:HG12	2:O:208:GLY:H	1.86	0.41
12:P:501:HEM:HMC1	12:P:501:HEM:HBC2	2.02	0.41
4:Q:142:VAL:HG23	4:Q:142:VAL:O	2.19	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.62	0.41
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.54	0.41
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.29	0.41
1:A:430:GLN:O	1:A:430:GLN:HG2	2.19	0.41
2:B:327:ILE:CG2	9:I:55:MET:HE3	2.50	0.41
3:C:30:ALA:HB1	15:C:505:CDL:H111	2.02	0.41
1:N:45:SER:OG	1:N:92:ARG:HG2	2.20	0.41
2:O:59:THR:HG22	2:O:60:THR:H	1.83	0.41
2:O:96:LEU:HB3	9:V:68:LEU:CD2	2.41	0.41
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.55	0.41
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.35	0.41
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.55	0.41
1:A:403:ASP:O	1:A:404:ALA:C	2.63	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.83	0.41
4:D:16:GLY:CA	4:D:19:SER:OG	2.68	0.41
5:E:106:ILE:O	5:E:106:ILE:HG22	2.21	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.56	0.41
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.55	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
2:O:59:THR:C	2:O:61:ALA:N	2.77	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.25	0.41
3:P:2:ALA:HA	3:P:3:PRO:HD2	1.86	0.41
15:P:506:CDL:HA32	7:T:40:ARG:HB3	2.03	0.41
5:R:83:GLU:HA	5:R:100:HIS:O	2.20	0.41
5:R:137:GLY:O	5:R:145:VAL:HG13	2.21	0.41
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.49	0.41
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.92	0.41
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.36	0.41
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ILE:HD12	3:C:294:ALA:HB2	2.03	0.41
4:D:68:VAL:HG11	4:D:92:PRO:CG	2.50	0.41
4:D:235:MET:HE3	6:F:60:PHE:CE1	2.55	0.41
1:N:23:LEU:C	1:N:23:LEU:HD23	2.46	0.41
1:N:156:THR:CG2	1:N:157:ALA:N	2.83	0.41
1:N:350:THR:HG22	1:N:351:GLU:N	2.35	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:22:GLU:HG3	2:O:23:ASP:N	2.30	0.41
4:Q:220:TYR:CE2	15:Q:502:CDL:H722	2.55	0.41
5:R:77:LYS:HG3	5:R:191:ASP:OD2	2.20	0.41
1:A:106:MET:HG3	1:A:203:ILE:HG21	2.02	0.41
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.02	0.41
2:O:144:LEU:HB2	2:O:183:ILE:HD12	2.03	0.41
2:O:248:ASN:HD22	2:O:249:GLY:N	2.18	0.41
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.41
5:R:162:GLY:O	5:R:163:SER:C	2.64	0.41
5:R:193:VAL:O	5:R:193:VAL:HG13	2.21	0.41
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	0.41
8:U:67:HIS:CE1	8:U:71:HIS:HE1	2.38	0.41
10:W:4:ALA:O	10:W:8:GLN:HG3	2.21	0.41
1:A:87:ASN:CG	1:A:88:GLY:H	2.29	0.41
1:A:388:ARG:HH21	1:A:388:ARG:HG3	1.86	0.41
2:B:59:THR:O	2:B:60:THR:C	2.63	0.41
2:B:75:LEU:HD22	2:B:136:GLU:HB3	2.02	0.41
2:B:374:THR:HG22	2:B:376:GLN:N	2.35	0.41
4:D:117:VAL:HG21	4:D:191:ARG:HA	2.03	0.41
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.41
8:H:17:LEU:HD13	8:H:73:LEU:HD22	2.01	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.21	0.41
1:N:212:ALA:O	1:N:216:PHE:HB2	2.21	0.41
1:N:331:ILE:HG21	1:N:431:LEU:HB2	2.03	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.55	0.41
3:P:186:LEU:HD23	3:P:186:LEU:HA	1.89	0.41
5:R:112:VAL:HG11	5:R:170:ARG:HH12	1.83	0.41
1:A:156:THR:HA	5:E:7:VAL:HG21	2.02	0.41
1:A:343:MET:HE3	1:A:441:MET:HA	2.02	0.41
2:B:26:ILE:CD1	2:B:391:THR:HA	2.48	0.41
2:B:181:TYR:CD1	2:B:181:TYR:C	2.98	0.41
3:C:285:ILE:O	3:C:285:ILE:HG22	2.19	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:216:SER:CB	6:S:59:MET:HE2	2.47	0.41
6:S:84:GLU:H	6:S:84:GLU:CD	2.29	0.41
1:A:109:VAL:HA	1:A:112:LEU:HD12	2.03	0.40
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.55	0.40
3:C:287:ASN:O	3:C:288:LYS:C	2.63	0.40
4:D:116:ILE:HG23	4:D:117:VAL:N	2.36	0.40
8:H:24:CYS:C	8:H:26:GLN:H	2.29	0.40
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.40
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.40
2:O:230:ALA:O	2:O:231:GLY:O	2.39	0.40
2:O:353:THR:HB	2:O:356:ASP:CG	2.46	0.40
3:P:109:LEU:HD23	3:P:109:LEU:HA	1.81	0.40
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.52	0.40
6:S:87:LYS:HA	6:S:87:LYS:HD3	1.93	0.40
1:A:87:ASN:CG	1:A:88:GLY:N	2.78	0.40
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.57	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
1:A:45:SER:OG	1:A:92:ARG:HA	2.22	0.40
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.40
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.40
6:F:32:MET:O	6:F:33:ARG:C	2.62	0.40
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.36	0.40
3:P:344:VAL:C	3:P:345:GLU:HG3	2.45	0.40
1:A:371:GLY:O	1:A:375:VAL:HG23	2.21	0.40
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.21	0.40
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.33	0.40
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.39	0.40
10:J:15:ARG:HH11	10:J:15:ARG:CG	2.30	0.40
1:N:156:THR:HG23	1:N:157:ALA:N	2.37	0.40
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.03	0.40
3:P:356:SER:O	3:P:359:TYR:HB3	2.21	0.40
5:R:78:LEU:N	5:R:191:ASP:O	2.48	0.40
6:S:71:LYS:O	6:S:72:HIS:HB2	2.22	0.40
2:B:291:VAL:C	2:B:293:SER:N	2.79	0.40
4:D:214:LEU:O	4:D:218:LEU:HG	2.21	0.40
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.57	0.40
7:G:38:TRP:O	7:G:39:ARG:C	2.65	0.40
9:I:65:VAL:HG12	9:I:66:ALA:H	1.85	0.40
1:N:82:MET:CE	1:N:105:ASP:HB3	2.51	0.40
2:O:291:VAL:C	2:O:293:SER:N	2.79	0.40
7:T:24:ARG:O	7:T:27:PRO:HD3	2.21	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	441/446 (99%)	408 (92%)	25 (6%)	8 (2%)	6	18
1	N	440/446 (99%)	409 (93%)	24 (6%)	7 (2%)	7	20
2	B	419/441 (95%)	351 (84%)	52 (12%)	16 (4%)	2	5
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	2	6
3	C	378/380 (100%)	350 (93%)	24 (6%)	4 (1%)	11	29
3	P	377/380 (99%)	348 (92%)	23 (6%)	6 (2%)	7	20
4	D	239/241 (99%)	222 (93%)	16 (7%)	1 (0%)	30	54
4	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	25
5	E	194/196 (99%)	147 (76%)	31 (16%)	16 (8%)	0	1
5	R	194/196 (99%)	151 (78%)	32 (16%)	11 (6%)	1	2
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	4	11
7	T	77/81 (95%)	66 (86%)	9 (12%)	2 (3%)	4	11
8	H	68/77 (88%)	63 (93%)	4 (6%)	1 (2%)	8	22
8	U	65/77 (84%)	55 (85%)	8 (12%)	2 (3%)	3	8
9	I	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0
9	V	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0
10	J	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
10	W	58/61 (95%)	52 (90%)	4 (7%)	2 (3%)	3	7
All	All	4012/4218 (95%)	3556 (89%)	352 (9%)	104 (3%)	4	11

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
1	A	433	ASP
2	B	26	ILE
2	B	39	GLU
2	B	226	ILE
3	C	287	ASN
5	E	102	THR
5	E	149	ASN
5	E	150	SER
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	39	GLU
2	O	228	SER
3	P	287	ASN
5	R	124	LEU
5	R	125	ASP
8	U	52	GLU
10	W	61	ALA
1	A	262	TRP
2	B	171	ALA
2	B	201	SER
2	B	227	ARG
2	B	228	SER
2	B	231	GLY
2	B	236	LYS
2	B	371	SER
5	E	118	ARG
5	E	163	SER
5	E	190	ASP
9	I	7	ARG
9	I	60	ALA
9	I	63	ASP
1	N	218	GLY
1	N	262	TRP
1	N	282	ARG
2	O	171	ALA
2	O	201	SER
2	O	220	ALA
2	O	231	GLY
2	O	371	SER
5	R	127	VAL
5	R	163	SER

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Mol	Chain	Res	Type
9	V	58	ALA
9	V	70	ALA
1	A	217	SER
1	A	282	ARG
2	B	29	LEU
3	C	159	HIS
5	E	84	GLY
5	E	115	SER
5	E	120	PRO
5	E	137	GLY
2	O	236	LYS
3	P	155	PRO
3	P	160	THR
5	R	149	ASN
7	T	33	ALA
9	V	7	ARG
9	V	60	ARG
1	A	71	PRO
1	A	72	CYS
2	B	221	GLU
3	C	5	ILE
5	E	112	VAL
7	G	33	ALA
1	N	81	SER
2	O	222	GLN
3	P	5	ILE
3	P	156	TYR
5	R	123	ASP
5	R	137	GLY
1	A	388	ARG
2	B	269	ALA
2	B	270	ASN
2	B	390	GLY
3	C	156	TYR
5	E	186	GLN
7	G	7	LEU
8	H	50	THR
9	I	62	ARG
1	N	71	PRO
1	N	72	CYS
2	O	390	GLY
4	Q	162	PRO

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Mol	Chain	Res	Type
5	R	108	GLN
7	T	7	LEU
8	U	27	THR
10	W	15	ARG
4	D	162	PRO
5	E	130	PRO
2	O	226	ILE
2	O	436	LEU
3	P	158	GLY
4	Q	198	HIS
5	R	130	PRO
5	R	159	PRO
4	Q	176	PRO
5	R	114	VAL
5	E	159	PRO
2	O	351	GLY
2	B	351	GLY
5	E	155	GLY
5	E	175	PRO

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%)	355 (97%)	10 (3%)	39	69
1	N	365/368 (99%)	353 (97%)	12 (3%)	33	63
2	B	332/347 (96%)	319 (96%)	13 (4%)	28	57
2	O	333/347 (96%)	321 (96%)	12 (4%)	31	60
3	C	328/328 (100%)	323 (98%)	5 (2%)	57	81
3	P	328/328 (100%)	325 (99%)	3 (1%)	70	87
4	D	200/200 (100%)	195 (98%)	5 (2%)	42	71
4	Q	200/200 (100%)	197 (98%)	3 (2%)	57	81
5	E	166/166 (100%)	160 (96%)	6 (4%)	31	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	165/166 (99%)	161 (98%)	4 (2%)	43	72
6	F	93/96 (97%)	90 (97%)	3 (3%)	34	64
6	S	93/96 (97%)	88 (95%)	5 (5%)	20	45
7	G	71/71 (100%)	68 (96%)	3 (4%)	26	55
7	T	70/71 (99%)	67 (96%)	3 (4%)	26	54
8	H	65/71 (92%)	64 (98%)	1 (2%)	57	81
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	26/45 (58%)	26 (100%)	0	100	100
9	V	26/45 (58%)	26 (100%)	0	100	100
10	J	49/49 (100%)	46 (94%)	3 (6%)	17	40
10	W	47/49 (96%)	44 (94%)	3 (6%)	16	38
All	All	3385/3482 (97%)	3291 (97%)	94 (3%)	38	68

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	102	LEU
1	A	106	MET
1	A	108	LYS
1	A	226	ASP
1	A	281	ASP
1	A	342	TRP
1	A	395	TRP
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	97	SER
2	B	114	ASP
2	B	117	ASP
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	228	SER
2	B	248	ASN
2	B	250	HIS
2	B	335	GLU
2	B	341	MET

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Mol	Chain	Res	Type
2	B	402	ILE
3	C	145	THR
3	C	146	VAL
3	C	157	ILE
3	C	223	PRO
3	C	226	SER
4	D	57	THR
4	D	169	LEU
4	D	179	MET
4	D	203	ARG
4	D	215	LEU
5	E	3	ASN
5	E	31	ASP
5	E	107	ASN
5	E	123	ASP
5	E	186	GLN
5	E	191	ASP
6	F	64	ARG
6	F	70	LEU
6	F	84	GLU
7	G	27	PRO
7	G	50	PRO
7	G	79	ASN
8	H	49	HIS
10	J	22	LEU
10	J	59	TYR
10	J	60	GLU
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	102	LEU
1	N	106	MET
1	N	108	LYS
1	N	281	ASP
1	N	342	TRP
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	114	ASP

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Mol	Chain	Res	Type
2	O	117	ASP
2	O	124	LEU
2	O	154	SER
2	O	248	ASN
2	O	250	HIS
2	O	259	THR
2	O	335	GLU
2	O	341	MET
2	O	402	ILE
3	P	146	VAL
3	P	226	SER
3	P	243	LEU
4	Q	169	LEU
4	Q	179	MET
4	Q	203	ARG
5	R	3	ASN
5	R	31	ASP
5	R	130	PRO
5	R	190	ASP
6	S	12	LEU
6	S	15	ARG
6	S	64	ARG
6	S	70	LEU
6	S	84	GLU
7	T	27	PRO
7	T	50	PRO
7	T	79	ASN
10	W	22	LEU
10	W	59	TYR
10	W	60	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
1	A	368	GLN
1	A	385	ASN
1	A	435	ASN

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Mol	Chain	Res	Type
2	B	31	ASN
2	B	156	GLN
2	B	248	ASN
2	B	276	GLN
2	B	315	ASN
2	B	332	HIS
2	B	343	GLN
2	B	349	GLN
2	B	362	ASN
3	C	9	HIS
3	C	17	ASN
3	C	73	ASN
3	C	82	ASN
3	C	159	HIS
3	C	207	ASN
3	C	342	GLN
4	D	31	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
4	D	166	ASN
5	E	3	ASN
5	E	57	GLN
5	E	107	ASN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	49	ASN
1	N	118	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	368	GLN
1	N	435	ASN
2	O	31	ASN

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Mol	Chain	Res	Type
2	O	156	GLN
2	O	197	ASN
2	O	248	ASN
2	O	276	GLN
2	O	313	ASN
2	O	315	ASN
2	O	332	HIS
2	O	343	GLN
2	O	349	GLN
2	O	362	ASN
2	O	380	ASN
3	P	9	HIS
3	P	17	ASN
3	P	73	ASN
3	P	149	ASN
3	P	159	HIS
3	P	207	ASN
3	P	332	ASN
3	P	342	GLN
4	Q	31	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	121	GLN
5	R	122	HIS
5	R	149	ASN
5	R	164	HIS
5	R	186	GLN
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	23	HIS
8	U	71	HIS
8	U	75	ASN
9	V	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
9	AME	V	1	9	7,8,11	2.10	1 (14%)	5,8,13	1.56	1 (20%)
3	FME	C	1	3	7,8,10	2.12	1 (14%)	5,8,11	1.45	1 (20%)
9	AME	I	1	9	7,8,11	2.09	1 (14%)	5,8,13	1.48	1 (20%)

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
9	AME	V	1	9	-	0/5/8/12	-
3	FME	C	1	3	-	1/5/8/11	-
9	AME	I	1	9	-	0/5/8/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	AME	CT1-N	-5.41	1.33	1.46
9	I	1	AME	CT1-N	-5.40	1.33	1.46
3	C	1	FME	CN-N	-5.36	1.33	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	AME	CT1-N-CA	2.72	121.83	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CN-N-CA	2.71	121.79	113.70
9	I	1	AME	CT1-N-CA	2.66	121.66	113.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	AME	4	0
9	I	1	AME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 2 are unknown - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	HEC	Q	501	4	50,50,50	1.04	1 (2%)	68,82,82	1.56	10 (14%)
12	HEM	C	502	3	50,50,50	1.38	4 (8%)	67,82,82	1.43	9 (13%)
14	UQ	P	505	-	19,19,63	2.59	10 (52%)	24,26,79	1.05	2 (8%)
12	HEM	P	501	3	50,50,50	1.47	5 (10%)	67,82,82	1.21	6 (8%)
19	BOG	D	502	-	20,20,20	0.86	0	25,25,25	0.89	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CDL	P	506	-	39,39,99	1.23	2 (5%)	45,51,111	1.14	4 (8%)
16	PEE	N	502	-	4,4,50	3.62	4 (100%)	6,6,55	0.59	0
12	HEM	C	501	3	50,50,50	1.51	6 (12%)	67,82,82	1.33	7 (10%)
15	CDL	C	505	-	41,41,99	1.19	2 (4%)	47,53,111	1.08	4 (8%)
19	BOG	Q	503	-	20,20,20	0.94	2 (10%)	25,25,25	0.90	1 (4%)
16	PEE	P	507	-	48,48,50	1.36	5 (10%)	51,53,55	0.76	2 (3%)
18	HEC	D	501	4	50,50,50	1.21	6 (12%)	68,82,82	1.67	11 (16%)
19	BOG	P	503	-	12,12,20	1.40	3 (25%)	17,17,25	0.53	0
13	WF3	C	503	-	32,33,33	2.97	15 (46%)	43,47,47	2.48	15 (34%)
15	CDL	G	101	-	39,39,99	1.22	1 (2%)	45,51,111	1.14	4 (8%)
15	CDL	Q	502	-	41,41,99	1.20	1 (2%)	47,53,111	1.09	4 (8%)
13	WF3	P	504	-	32,33,33	3.11	15 (46%)	43,47,47	2.47	15 (34%)
16	PEE	C	507	-	20,20,50	1.79	6 (30%)	23,25,55	0.63	0
16	PEE	C	506	-	48,48,50	1.39	6 (12%)	51,53,55	0.79	2 (3%)
19	BOG	D	503	-	13,13,20	1.39	2 (15%)	18,18,25	1.20	2 (11%)
20	FES	E	501	5	0,4,4	-	-	-	-	-
16	PEE	E	502	-	49,49,50	1.55	10 (20%)	52,54,55	0.92	3 (5%)
17	GOL	P	508	-	5,5,5	1.46	1 (20%)	5,5,5	0.68	0
14	UQ	C	504	-	19,19,63	2.61	9 (47%)	24,26,79	1.07	2 (8%)
19	BOG	Q	504	-	13,13,20	1.30	2 (15%)	18,18,25	1.11	2 (11%)
17	GOL	C	508	-	5,5,5	1.43	0	5,5,5	0.68	0
12	HEM	P	502	3	50,50,50	1.41	4 (8%)	67,82,82	1.22	7 (10%)
20	FES	R	501	5	0,4,4	-	-	-	-	-
16	PEE	R	502	-	47,47,50	1.49	8 (17%)	49,51,55	0.73	1 (2%)

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
18	HEC	Q	501	4	1/1/3/7	9/14/54/54	-
12	HEM	C	502	3	-	6/14/54/54	-
14	UQ	P	505	-	-	3/11/35/87	0/1/1/1
12	HEM	P	501	3	-	5/14/54/54	-
19	BOG	D	502	-	-	4/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	P	506	-	-	19/49/49/110	-
12	HEM	C	501	3	-	4/14/54/54	-
15	CDL	C	505	-	-	16/51/51/110	-
19	BOG	Q	503	-	-	4/11/31/31	0/1/1/1
16	PEE	P	507	-	-	20/52/52/54	-
18	HEC	D	501	4	1/1/3/7	10/14/54/54	-
19	BOG	P	503	-	-	0/2/22/31	0/1/1/1
13	WF3	C	503	-	-	1/24/24/24	0/3/3/3
15	CDL	G	101	-	-	17/49/49/110	-
15	CDL	Q	502	-	-	16/51/51/110	-
13	WF3	P	504	-	-	6/24/24/24	0/3/3/3
16	PEE	C	507	-	-	7/24/24/54	-
16	PEE	C	506	-	-	19/52/52/54	-
19	BOG	D	503	-	-	0/4/24/31	0/1/1/1
20	FES	E	501	5	-	-	0/1/1/1
16	PEE	E	502	-	-	27/53/53/54	-
17	GOL	P	508	-	-	3/4/4/4	-
14	UQ	C	504	-	-	3/11/35/87	0/1/1/1
19	BOG	Q	504	-	-	4/4/24/31	0/1/1/1
17	GOL	C	508	-	-	4/4/4/4	-
12	HEM	P	502	3	-	5/14/54/54	-
20	FES	R	501	5	-	-	0/1/1/1
16	PEE	R	502	-	-	25/49/49/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	504	WF3	C6-C5	9.85	1.54	1.34
13	C	503	WF3	C6-C5	9.44	1.53	1.34
13	P	504	WF3	C18-N23	6.30	1.38	1.30
13	P	504	WF3	C9-C5	-5.84	1.42	1.49
13	C	503	WF3	C18-N23	5.74	1.37	1.30
13	P	504	WF3	C9-C14	5.30	1.47	1.40
13	C	503	WF3	C9-C5	-5.25	1.42	1.49
13	C	503	WF3	C9-C14	4.97	1.47	1.40
14	C	504	UQ	C6-C5	4.96	1.44	1.35
14	P	505	UQ	C7-C6	4.96	1.60	1.51
14	C	504	UQ	C7-C6	4.94	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	502	PEE	P-O1P	4.94	1.62	1.50
12	P	501	HEM	CBC-CAC	4.93	1.54	1.30
12	C	501	HEM	CBC-CAC	4.93	1.54	1.30
12	P	502	HEM	CBC-CAC	4.91	1.54	1.30
14	P	505	UQ	C6-C5	4.83	1.43	1.35
12	C	502	HEM	CBC-CAC	4.69	1.52	1.30
12	P	501	HEM	CBB-CAB	4.62	1.52	1.30
12	C	501	HEM	CBB-CAB	4.45	1.51	1.30
12	C	502	HEM	CBB-CAB	4.42	1.51	1.30
16	R	502	PEE	C39-C38	4.20	1.55	1.31
13	P	504	WF3	C15-C14	-4.12	1.40	1.50
14	C	504	UQ	C6-C1	4.10	1.58	1.46
16	C	506	PEE	C39-C38	4.09	1.54	1.31
16	P	507	PEE	C39-C38	4.04	1.54	1.31
16	E	502	PEE	C39-C38	4.02	1.54	1.31
13	C	503	WF3	C15-C14	-3.98	1.40	1.50
12	P	502	HEM	CBB-CAB	3.90	1.49	1.30
18	D	501	HEC	FE-ND	-3.81	1.83	1.94
14	P	505	UQ	C6-C1	3.79	1.57	1.46
13	C	503	WF3	C25-C26	3.59	1.44	1.37
16	E	502	PEE	O2-C10	3.57	1.44	1.34
13	P	504	WF3	C17-N31	3.54	1.38	1.30
16	P	507	PEE	C21-C22	-3.49	1.34	1.51
16	N	502	PEE	P-O4P	3.44	1.64	1.54
16	C	506	PEE	O3-C30	3.35	1.43	1.33
16	E	502	PEE	P-O1P	3.33	1.62	1.50
13	C	503	WF3	C17-N31	3.33	1.37	1.30
16	R	502	PEE	O2-C10	3.32	1.43	1.34
16	C	506	PEE	C21-C22	-3.30	1.35	1.51
13	C	503	WF3	C10-C9	3.30	1.45	1.39
13	P	504	WF3	C13-C14	3.29	1.45	1.39
14	P	505	UQ	O3-C3	3.27	1.44	1.36
14	C	504	UQ	O3-C3	3.24	1.44	1.36
12	C	501	HEM	CAB-C3B	-3.22	1.38	1.47
16	E	502	PEE	O3-C30	3.21	1.42	1.33
16	E	502	PEE	C21-C22	-3.20	1.35	1.51
16	N	502	PEE	P-O3P	3.20	1.64	1.54
16	R	502	PEE	O3-C30	3.20	1.42	1.33
13	P	504	WF3	C29-C28	3.19	1.43	1.36
16	C	507	PEE	P-O1P	3.16	1.61	1.50
16	R	502	PEE	P-O1P	3.15	1.61	1.50
16	P	507	PEE	O3-C30	3.10	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	502	HEM	CAB-C3B	-3.10	1.39	1.47
13	C	503	WF3	C29-C28	3.10	1.43	1.36
12	C	502	HEM	CAB-C3B	-3.10	1.39	1.47
13	P	504	WF3	C25-C26	3.10	1.43	1.37
12	C	501	HEM	CAC-C3C	-3.07	1.39	1.47
12	P	501	HEM	CAC-C3C	-3.04	1.39	1.47
16	C	507	PEE	O2-C10	3.04	1.42	1.34
12	P	501	HEM	CAB-C3B	-3.03	1.39	1.47
14	C	504	UQ	C2-C1	2.97	1.57	1.48
16	C	506	PEE	P-O1P	2.95	1.61	1.50
13	P	504	WF3	C10-C9	2.89	1.44	1.39
16	P	507	PEE	P-O1P	2.89	1.60	1.50
14	P	505	UQ	CM5-C5	2.88	1.56	1.50
14	C	504	UQ	CM5-C5	2.87	1.56	1.50
16	P	507	PEE	O2-C10	2.85	1.42	1.34
16	C	507	PEE	O3-C30	2.83	1.41	1.33
14	P	505	UQ	C2-C1	2.82	1.57	1.48
16	C	506	PEE	O2-C10	2.73	1.42	1.34
13	C	503	WF3	C13-C14	2.72	1.44	1.39
13	P	504	WF3	C11-C10	2.71	1.43	1.38
14	P	505	UQ	O2-C2	2.70	1.43	1.36
14	C	504	UQ	C5-C4	2.67	1.56	1.47
14	P	505	UQ	C5-C4	2.66	1.56	1.47
14	C	504	UQ	C3-C4	2.65	1.56	1.48
13	P	504	WF3	C19-C18	2.65	1.55	1.51
13	C	503	WF3	C28-C26	2.64	1.45	1.38
19	D	503	BOG	C4-C5	2.64	1.58	1.53
15	C	505	CDL	O1-C1	2.63	1.51	1.43
18	D	501	HEC	C4D-C3D	2.60	1.49	1.45
18	D	501	HEC	CHD-C4C	-2.59	1.33	1.39
12	P	502	HEM	CAC-C3C	-2.57	1.40	1.47
16	R	502	PEE	C11-C10	2.55	1.58	1.50
14	C	504	UQ	O2-C2	2.52	1.42	1.36
15	Q	502	CDL	O1-C1	2.52	1.50	1.43
14	P	505	UQ	C3-C4	2.50	1.56	1.48
13	C	503	WF3	C19-C18	2.49	1.55	1.51
16	E	502	PEE	C11-C10	2.48	1.57	1.50
13	P	504	WF3	C28-C26	2.46	1.44	1.38
13	C	503	WF3	C11-C10	2.45	1.43	1.38
13	P	504	WF3	C12-C11	2.44	1.43	1.38
16	E	502	PEE	C3-C2	2.43	1.58	1.50
16	N	502	PEE	P-O2P	2.42	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	E	502	PEE	C1-C2	2.42	1.58	1.50
16	C	507	PEE	C1-C2	2.41	1.58	1.50
14	P	505	UQ	C7-C8	2.41	1.54	1.50
18	Q	501	HEC	C1D-ND	-2.36	1.36	1.40
15	P	506	CDL	O1-C1	2.36	1.50	1.43
19	P	503	BOG	C4-C5	2.35	1.58	1.53
19	Q	504	BOG	C4-C5	2.33	1.58	1.53
19	Q	504	BOG	O5-C1	2.33	1.47	1.41
12	C	501	HEM	C2A-C3A	-2.30	1.32	1.38
19	D	503	BOG	O5-C1	2.26	1.47	1.41
16	E	502	PEE	O2-C2	2.23	1.51	1.46
16	C	507	PEE	C11-C10	2.22	1.57	1.50
16	E	502	PEE	C31-C30	2.20	1.57	1.50
16	R	502	PEE	C31-C30	2.20	1.57	1.50
19	P	503	BOG	O5-C1	2.20	1.48	1.42
13	C	503	WF3	C12-C11	2.19	1.43	1.38
15	C	505	CDL	OA6-CA5	2.19	1.40	1.34
13	P	504	WF3	C12-C13	2.18	1.42	1.38
19	Q	503	BOG	C4-C5	2.18	1.57	1.53
16	C	507	PEE	P-O4P	2.18	1.67	1.59
16	R	502	PEE	C3-C2	2.17	1.57	1.50
12	P	501	HEM	C1A-NA	-2.17	1.35	1.39
19	P	503	BOG	C1-C2	2.16	1.57	1.52
18	D	501	HEC	CHD-C1D	-2.16	1.34	1.38
16	R	502	PEE	C1-C2	2.15	1.57	1.50
18	D	501	HEC	C1C-C2C	2.15	1.48	1.43
12	C	502	HEM	C3B-C4B	2.11	1.49	1.44
15	G	101	CDL	O1-C1	2.10	1.49	1.43
17	P	508	GOL	O2-C2	2.10	1.49	1.43
12	C	501	HEM	CMC-C2C	2.07	1.55	1.50
15	P	506	CDL	CB3-CB4	2.07	1.57	1.50
19	Q	503	BOG	O5-C1	2.06	1.47	1.41
16	C	506	PEE	C3-C2	2.04	1.57	1.50
18	D	501	HEC	CMA-C3A	2.04	1.54	1.50
13	C	503	WF3	C12-C13	2.01	1.42	1.38

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	504	WF3	O2-C3-C5	9.95	125.61	112.05
13	C	503	WF3	O2-C3-C5	9.67	125.22	112.05
18	D	501	HEC	CAC-C3C-C2C	4.92	134.68	126.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	501	HEC	CAC-C3C-C2C	4.81	134.50	126.89
18	Q	501	HEC	CAC-C3C-C4C	-4.55	118.65	124.91
13	C	503	WF3	C26-C25-C24	-4.40	118.09	121.19
18	Q	501	HEC	CAA-C2A-C1A	4.33	133.67	124.85
13	P	504	WF3	C8-O7-C6	-4.33	108.57	115.65
12	C	501	HEM	C3B-C4B-NB	4.22	112.50	109.47
12	C	502	HEM	CAD-C3D-C4D	4.18	131.99	124.70
18	D	501	HEC	CAC-C3C-C4C	-4.17	119.18	124.91
18	D	501	HEC	CAA-C2A-C3A	-4.15	120.09	127.87
13	P	504	WF3	C26-C25-C24	-4.08	118.32	121.19
12	P	501	HEM	C3B-C4B-NB	4.03	112.36	109.47
18	Q	501	HEC	CAA-C2A-C3A	-4.01	120.36	127.87
13	C	503	WF3	C8-O7-C6	-3.94	109.20	115.65
12	C	502	HEM	C4C-C3C-C2C	-3.93	103.41	106.81
13	C	503	WF3	C19-C18-N23	3.85	119.97	113.54
13	C	503	WF3	C1-O2-C3	3.84	122.97	115.85
19	D	503	BOG	C1'-O1-C1	3.73	118.93	113.26
18	D	501	HEC	CAA-C2A-C1A	3.73	132.43	124.85
13	C	503	WF3	O2-C3-O4	-3.71	116.42	123.50
13	P	504	WF3	C1-O2-C3	3.69	122.70	115.85
13	P	504	WF3	C18-N23-C24	3.69	122.81	115.17
13	C	503	WF3	C18-N23-C24	3.66	122.75	115.17
13	P	504	WF3	C19-C18-N23	3.65	119.63	113.54
12	P	502	HEM	CAD-C3D-C4D	3.64	131.04	124.70
13	P	504	WF3	O2-C3-O4	-3.57	116.69	123.50
19	Q	504	BOG	C1'-O1-C1	3.47	118.53	113.26
12	C	501	HEM	CAD-C3D-C4D	3.45	130.72	124.70
14	C	504	UQ	C8-C7-C6	3.45	120.58	112.08
15	P	506	CDL	CB4-OB6-CB5	-3.36	109.75	117.80
19	Q	503	BOG	C1'-O1-C1	3.33	119.36	113.68
14	P	505	UQ	C8-C7-C6	3.26	120.10	112.08
13	P	504	WF3	O4-C3-C5	-3.24	117.70	124.50
18	D	501	HEC	CAD-C3D-C4D	3.22	130.31	124.70
15	G	101	CDL	CB4-OB6-CB5	-3.21	110.12	117.80
13	C	503	WF3	C17-N31-C30	3.16	123.01	116.38
12	C	502	HEM	CAD-C3D-C2D	-3.10	122.06	127.87
19	D	502	BOG	C1'-O1-C1	3.07	118.92	113.68
13	P	504	WF3	C17-N31-C30	3.04	122.76	116.38
13	C	503	WF3	O4-C3-C5	-2.93	118.35	124.50
12	C	502	HEM	C3B-C4B-NB	2.90	111.55	109.47
12	C	502	HEM	C2B-C1B-NB	2.83	113.10	109.84
18	D	501	HEC	C2D-C1D-ND	2.83	113.10	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	502	HEM	C3B-C4B-NB	2.82	111.50	109.47
16	E	502	PEE	C22-C21-C20	2.80	127.31	113.86
12	C	501	HEM	C2B-C1B-NB	2.78	113.03	109.84
12	C	502	HEM	C2D-C1D-ND	2.78	113.11	109.90
13	C	503	WF3	C28-C26-C25	2.77	121.67	118.40
19	D	503	BOG	O1-C1-C2	2.73	111.29	108.14
12	P	501	HEM	CAD-C3D-C4D	2.70	129.41	124.70
12	P	502	HEM	CBA-CAA-C2A	2.70	119.99	112.53
12	P	502	HEM	CAD-C3D-C2D	-2.67	122.86	127.87
15	P	506	CDL	CA6-CA4-CA3	-2.65	105.61	111.78
13	C	503	WF3	C24-C30-N31	-2.64	117.95	121.18
18	D	501	HEC	CAD-C3D-C2D	-2.64	122.93	127.87
12	P	502	HEM	C4C-C3C-C2C	-2.62	104.54	106.81
13	P	504	WF3	C10-C9-C5	-2.61	115.53	119.60
18	Q	501	HEC	CMB-C2B-C1B	2.56	129.03	125.03
15	G	101	CDL	CA6-CA4-CA3	-2.56	105.82	111.78
12	P	501	HEM	C2B-C1B-NB	2.55	112.78	109.84
12	P	502	HEM	C2D-C1D-ND	2.55	112.85	109.90
18	Q	501	HEC	CBA-CAA-C2A	2.52	119.50	112.53
16	P	507	PEE	C22-C21-C20	2.52	125.97	113.86
18	Q	501	HEC	C2D-C1D-ND	2.52	112.73	109.84
13	C	503	WF3	C10-C9-C5	-2.51	115.68	119.60
16	C	506	PEE	C22-C21-C20	2.51	125.93	113.86
12	C	501	HEM	C3B-C2B-C1B	-2.51	104.53	106.41
12	C	501	HEM	CBD-CAD-C3D	2.50	119.45	112.53
16	E	502	PEE	C21-C22-C23	2.49	126.94	114.37
16	C	506	PEE	C21-C22-C23	2.48	126.90	114.37
19	Q	504	BOG	O1-C1-C2	2.46	110.98	108.14
12	C	501	HEM	C3D-C4D-ND	2.43	112.84	110.17
13	P	504	WF3	C28-C26-C25	2.43	121.27	118.40
16	P	507	PEE	C21-C22-C23	2.39	126.46	114.37
15	G	101	CDL	CA4-OA6-CA5	-2.38	112.11	117.80
15	C	505	CDL	CA6-CA4-CA3	-2.35	106.31	111.78
18	D	501	HEC	CHD-C1D-C2D	-2.32	120.35	126.95
12	P	501	HEM	C2D-C1D-ND	2.29	112.55	109.90
12	P	501	HEM	CBD-CAD-C3D	2.29	118.86	112.53
13	P	504	WF3	C24-C30-N31	-2.28	118.39	121.18
12	C	502	HEM	CBA-CAA-C2A	2.27	118.81	112.53
15	Q	502	CDL	CA6-CA4-CA3	-2.26	106.53	111.78
16	E	502	PEE	O3-C3-C2	2.26	114.90	108.40
15	C	505	CDL	CB4-OB6-CB5	-2.23	112.47	117.80
18	D	501	HEC	CMC-C2C-C1C	2.22	128.80	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	502	CDL	CA4-OA6-CA5	-2.22	112.48	117.80
15	Q	502	CDL	CA6-OA8-CA7	-2.21	111.63	117.08
15	C	505	CDL	CA6-OA8-CA7	-2.21	111.64	117.08
16	R	502	PEE	O3-C3-C2	2.20	114.74	108.40
15	P	506	CDL	OB6-CB4-CB3	2.19	116.19	108.34
14	P	505	UQ	C7-C6-C1	-2.18	115.98	118.52
15	P	506	CDL	CA4-OA6-CA5	-2.17	112.60	117.80
18	Q	501	HEC	CMC-C2C-C1C	2.16	128.71	125.42
12	P	501	HEM	CMA-C3A-C4A	2.16	128.70	125.42
15	Q	502	CDL	CB4-OB6-CB5	-2.15	112.66	117.80
13	P	504	WF3	C28-C29-C30	-2.15	118.23	120.80
13	C	503	WF3	C28-C29-C30	-2.14	118.24	120.80
12	C	501	HEM	CAD-C3D-C2D	-2.13	123.88	127.87
12	C	502	HEM	C4D-ND-C1D	-2.11	102.71	105.21
18	D	501	HEC	C4B-NB-C1B	-2.10	102.72	105.21
13	C	503	WF3	O16-C15-C14	2.10	115.45	109.26
18	Q	501	HEC	CAD-C3D-C4D	2.09	128.34	124.70
14	C	504	UQ	C7-C6-C1	-2.08	116.10	118.52
15	G	101	CDL	OB6-CB4-CB3	2.08	115.79	108.34
12	P	502	HEM	C2B-C1B-NB	2.07	112.22	109.84
13	P	504	WF3	C14-C9-C5	2.06	125.06	122.31
13	P	504	WF3	O16-C15-C14	2.05	115.30	109.26
18	Q	501	HEC	CAB-C3B-C2B	2.05	131.32	127.56
15	C	505	CDL	CA4-OA6-CA5	-2.04	112.92	117.80
13	C	503	WF3	C14-C9-C5	2.02	125.02	122.31
18	D	501	HEC	C3C-C4C-NC	2.02	112.39	110.15
12	C	502	HEM	C3B-C2B-C1B	-2.02	104.90	106.41

All (2) chirality outliers are listed below:

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

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	504	WF3	O2-C3-C5-C6
13	P	504	WF3	O4-C3-C5-C6
15	C	505	CDL	O1-C1-CB2-OB2
15	C	505	CDL	CB2-OB2-PB2-OB3
15	C	505	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	C	505	CDL	CB2-OB2-PB2-OB5
15	G	101	CDL	O1-C1-CA2-OA2
15	G	101	CDL	CA3-OA5-PA1-OA2
15	G	101	CDL	CA3-OA5-PA1-OA3
15	G	101	CDL	CA3-OA5-PA1-OA4
15	G	101	CDL	CB3-OB5-PB2-OB2
15	G	101	CDL	CB3-OB5-PB2-OB3
15	G	101	CDL	CB3-OB5-PB2-OB4
15	G	101	CDL	C51-CB5-OB6-CB4
15	P	506	CDL	O1-C1-CA2-OA2
15	P	506	CDL	CA3-OA5-PA1-OA2
15	P	506	CDL	CA3-OA5-PA1-OA3
15	P	506	CDL	CA3-OA5-PA1-OA4
15	P	506	CDL	CB3-OB5-PB2-OB2
15	P	506	CDL	CB3-OB5-PB2-OB3
15	P	506	CDL	C51-CB5-OB6-CB4
15	Q	502	CDL	O1-C1-CB2-OB2
15	Q	502	CDL	CB2-OB2-PB2-OB3
15	Q	502	CDL	CB2-OB2-PB2-OB4
15	Q	502	CDL	CB2-OB2-PB2-OB5
16	C	506	PEE	O4P-C4-C5-N
16	C	507	PEE	C1-O3P-P-O1P
16	E	502	PEE	C11-C10-O2-C2
16	E	502	PEE	O4-C10-O2-C2
16	E	502	PEE	C4-O4P-P-O3P
16	E	502	PEE	C4-O4P-P-O2P
16	E	502	PEE	C4-O4P-P-O1P
16	P	507	PEE	O4P-C4-C5-N
16	R	502	PEE	C17-C18-C19-C20
16	R	502	PEE	C11-C10-O2-C2
16	R	502	PEE	C1-O3P-P-O2P
16	R	502	PEE	C1-O3P-P-O4P
16	R	502	PEE	O4P-C4-C5-N
17	C	508	GOL	O1-C1-C2-C3
17	C	508	GOL	C1-C2-C3-O3
17	P	508	GOL	C1-C2-C3-O3
18	D	501	HEC	C3A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
15	G	101	CDL	OB9-CB7-OB8-CB6
15	P	506	CDL	OB9-CB7-OB8-CB6
16	R	502	PEE	O5-C30-O3-C3
15	C	505	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
15	Q	502	CDL	C31-CA7-OA8-CA6
16	E	502	PEE	O5-C30-O3-C3
16	R	502	PEE	C31-C30-O3-C3
19	Q	504	BOG	O5-C5-C6-O6
19	Q	504	BOG	O5-C1-O1-C1'
15	G	101	CDL	C71-CB7-OB8-CB6
15	P	506	CDL	C71-CB7-OB8-CB6
16	E	502	PEE	C31-C30-O3-C3
15	C	505	CDL	OA9-CA7-OA8-CA6
18	Q	501	HEC	C1A-C2A-CAA-CBA
15	G	101	CDL	OB7-CB5-OB6-CB4
15	P	506	CDL	OB7-CB5-OB6-CB4
16	R	502	PEE	O4-C10-O2-C2
15	Q	502	CDL	OA9-CA7-OA8-CA6
15	G	101	CDL	C31-CA7-OA8-CA6
15	P	506	CDL	C31-CA7-OA8-CA6
18	Q	501	HEC	C2B-C3B-CAB-CBB
19	Q	504	BOG	C2-C1-O1-C1'
18	D	501	HEC	C4B-C3B-CAB-CBB
15	C	505	CDL	C71-CB7-OB8-CB6
15	Q	502	CDL	C71-CB7-OB8-CB6
19	Q	504	BOG	C4-C5-C6-O6
15	C	505	CDL	OB9-CB7-OB8-CB6
15	Q	502	CDL	OB9-CB7-OB8-CB6
16	C	506	PEE	C17-C18-C19-C20
18	Q	501	HEC	C4B-C3B-CAB-CBB
15	G	101	CDL	OA9-CA7-OA8-CA6
15	P	506	CDL	OA9-CA7-OA8-CA6
19	D	502	BOG	O1-C1'-C2'-C3'
19	Q	503	BOG	O1-C1'-C2'-C3'
16	E	502	PEE	C30-C31-C32-C33
16	R	502	PEE	C30-C31-C32-C33
16	P	507	PEE	C17-C18-C19-C20
16	C	506	PEE	C10-C11-C12-C13
18	D	501	HEC	C1A-C2A-CAA-CBA
16	E	502	PEE	C10-C11-C12-C13
15	C	505	CDL	CA2-C1-CB2-OB2
15	G	101	CDL	CB2-C1-CA2-OA2
15	P	506	CDL	CB2-C1-CA2-OA2
15	Q	502	CDL	CA2-C1-CB2-OB2
18	D	501	HEC	C2B-C3B-CAB-CBB
19	D	502	BOG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
19	Q	503	BOG	C2-C1-O1-C1'
16	C	506	PEE	C37-C38-C39-C40
16	P	507	PEE	C37-C38-C39-C40
16	E	502	PEE	C34-C35-C36-C37
17	C	508	GOL	O1-C1-C2-O2
17	C	508	GOL	O2-C2-C3-O3
16	P	507	PEE	C10-C11-C12-C13
16	R	502	PEE	C11-C12-C13-C14
19	D	502	BOG	C1'-C2'-C3'-C4'
19	Q	503	BOG	C1'-C2'-C3'-C4'
16	C	507	PEE	C31-C30-O3-C3
16	E	502	PEE	C20-C21-C22-C23
16	E	502	PEE	C22-C23-C24-C25
19	D	502	BOG	O5-C1-O1-C1'
19	Q	503	BOG	O5-C1-O1-C1'
16	C	507	PEE	O5-C30-O3-C3
16	E	502	PEE	C32-C33-C34-C35
16	R	502	PEE	C39-C40-C41-C42
16	R	502	PEE	C34-C35-C36-C37
16	R	502	PEE	C41-C42-C43-C44
16	C	506	PEE	C35-C36-C37-C38
16	P	507	PEE	C35-C36-C37-C38
16	C	506	PEE	C21-C22-C23-C24
17	P	508	GOL	O2-C2-C3-O3
16	P	507	PEE	C21-C22-C23-C24
16	E	502	PEE	C35-C36-C37-C38
16	E	502	PEE	O3P-C1-C2-C3
16	P	507	PEE	C20-C21-C22-C23
16	C	506	PEE	C15-C16-C17-C18
16	P	507	PEE	C15-C16-C17-C18
16	R	502	PEE	C42-C43-C44-C45
16	R	502	PEE	C35-C36-C37-C38
16	C	506	PEE	C11-C12-C13-C14
12	C	502	HEM	C4D-C3D-CAD-CBD
15	C	505	CDL	OA5-CA3-CA4-OA6
16	P	507	PEE	C11-C12-C13-C14
16	C	506	PEE	C20-C21-C22-C23
15	Q	502	CDL	C71-C72-C73-C74
15	G	101	CDL	OA6-CA4-CA6-OA8
15	P	506	CDL	OA6-CA4-CA6-OA8
16	E	502	PEE	C14-C15-C16-C17
16	P	507	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
13	P	504	WF3	C5-C3-O2-C1
16	E	502	PEE	C19-C20-C21-C22
15	C	505	CDL	C71-C72-C73-C74
13	P	504	WF3	O2-C3-C5-C9
16	R	502	PEE	C24-C25-C26-C27
16	R	502	PEE	C14-C15-C16-C17
16	R	502	PEE	C43-C44-C45-C46
16	C	506	PEE	C33-C34-C35-C36
14	P	505	UQ	C12-C11-C9-C10
15	Q	502	CDL	OA5-CA3-CA4-OA6
16	C	506	PEE	C12-C13-C14-C15
16	R	502	PEE	C22-C23-C24-C25
16	E	502	PEE	C41-C42-C43-C44
16	E	502	PEE	C15-C16-C17-C18
17	P	508	GOL	O1-C1-C2-O2
18	D	501	HEC	C4D-C3D-CAD-CBD
18	D	501	HEC	C2D-C3D-CAD-CBD
14	C	504	UQ	C5-C6-C7-C8
14	P	505	UQ	C5-C6-C7-C8
16	P	507	PEE	C12-C13-C14-C15
16	E	502	PEE	C1-C2-O2-C10
12	P	502	HEM	C4D-C3D-CAD-CBD
14	C	504	UQ	C1-C6-C7-C8
14	P	505	UQ	C1-C6-C7-C8
15	Q	502	CDL	OA5-CA3-CA4-CA6
16	P	507	PEE	C43-C44-C45-C46
16	E	502	PEE	O3P-C1-C2-O2
13	P	504	WF3	O4-C3-O2-C1
16	R	502	PEE	C12-C13-C14-C15
16	E	502	PEE	C13-C14-C15-C16
16	C	506	PEE	C43-C44-C45-C46
15	P	506	CDL	CB3-OB5-PB2-OB4
16	C	507	PEE	C1-O3P-P-O4P
16	R	502	PEE	C1-O3P-P-O1P
15	C	505	CDL	OA5-CA3-CA4-CA6
13	P	504	WF3	O4-C3-C5-C9
16	P	507	PEE	C42-C43-C44-C45
16	C	507	PEE	C10-C11-C12-C13
16	E	502	PEE	C38-C39-C40-C41
15	G	101	CDL	CA3-CA4-CA6-OA8
15	P	506	CDL	CA3-CA4-CA6-OA8
16	C	507	PEE	O3-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
14	C	504	UQ	C12-C11-C9-C10
12	P	502	HEM	CAA-CBA-CGA-O1A
12	C	502	HEM	CAA-CBA-CGA-O1A
16	C	506	PEE	C42-C43-C44-C45
15	G	101	CDL	C1-CB2-OB2-PB2
12	P	502	HEM	CAA-CBA-CGA-O2A
16	E	502	PEE	C23-C24-C25-C26
12	C	502	HEM	CAA-CBA-CGA-O2A
16	P	507	PEE	C14-C15-C16-C17
16	E	502	PEE	C18-C19-C20-C21
18	D	501	HEC	CAD-CBD-CGD-O2D
15	C	505	CDL	C1-CA2-OA2-PA1
15	Q	502	CDL	C1-CA2-OA2-PA1
12	C	501	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAD-CBD-CGD-O2D
18	D	501	HEC	CAA-CBA-CGA-O2A
12	P	501	HEM	CAA-CBA-CGA-O2A
16	C	506	PEE	C14-C15-C16-C17
15	P	506	CDL	OA7-CA5-OA6-CA4
15	P	506	CDL	C1-CB2-OB2-PB2
18	Q	501	HEC	CAA-CBA-CGA-O2A
16	C	507	PEE	O5-C30-C31-C32
18	D	501	HEC	CAD-CBD-CGD-O1D
18	Q	501	HEC	CAD-CBD-CGD-O2D
12	P	502	HEM	CAD-CBD-CGD-O1D
12	P	502	HEM	CAD-CBD-CGD-O2D
16	P	507	PEE	C38-C39-C40-C41
12	P	501	HEM	CAA-CBA-CGA-O1A
18	D	501	HEC	CAA-CBA-CGA-O1A
16	E	502	PEE	C43-C44-C45-C46
12	C	501	HEM	CAD-CBD-CGD-O1D
16	C	506	PEE	C38-C39-C40-C41
12	P	501	HEM	CAD-CBD-CGD-O1D
18	Q	501	HEC	CAD-CBD-CGD-O1D
12	C	501	HEM	CAA-CBA-CGA-O1A
12	C	501	HEM	CAA-CBA-CGA-O2A
12	C	502	HEM	CAD-CBD-CGD-O1D
16	R	502	PEE	C36-C37-C38-C39
16	C	506	PEE	O3-C30-C31-C32
12	C	502	HEM	CAD-CBD-CGD-O2D
18	Q	501	HEC	CAA-CBA-CGA-O1A
16	P	507	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	R	502	PEE	C23-C24-C25-C26
16	P	507	PEE	O3-C30-C31-C32
16	C	506	PEE	O2-C10-C11-C12
15	P	506	CDL	C11-CA5-OA6-CA4
16	P	507	PEE	O2-C10-C11-C12
15	C	505	CDL	C72-C71-CB7-OB8
16	R	502	PEE	C10-C11-C12-C13
15	Q	502	CDL	C72-C71-CB7-OB8
15	Q	502	CDL	C52-C51-CB5-OB6
15	C	505	CDL	C52-C51-CB5-OB6
16	P	507	PEE	O5-C30-C31-C32
16	R	502	PEE	O3P-C1-C2-O2
15	C	505	CDL	C72-C71-CB7-OB9
16	C	506	PEE	O4-C10-C11-C12
16	C	506	PEE	O5-C30-C31-C32
15	Q	502	CDL	C72-C71-CB7-OB9
13	C	503	WF3	O4-C3-C5-C6
18	Q	501	HEC	C2D-C3D-CAD-CBD
16	E	502	PEE	C16-C17-C18-C19
12	C	502	HEM	C2B-C3B-CAB-CBB
12	P	501	HEM	C2B-C3B-CAB-CBB
16	P	507	PEE	O4-C10-C11-C12

There are no ring outliers.

17 monomers are involved in 28 short contacts:

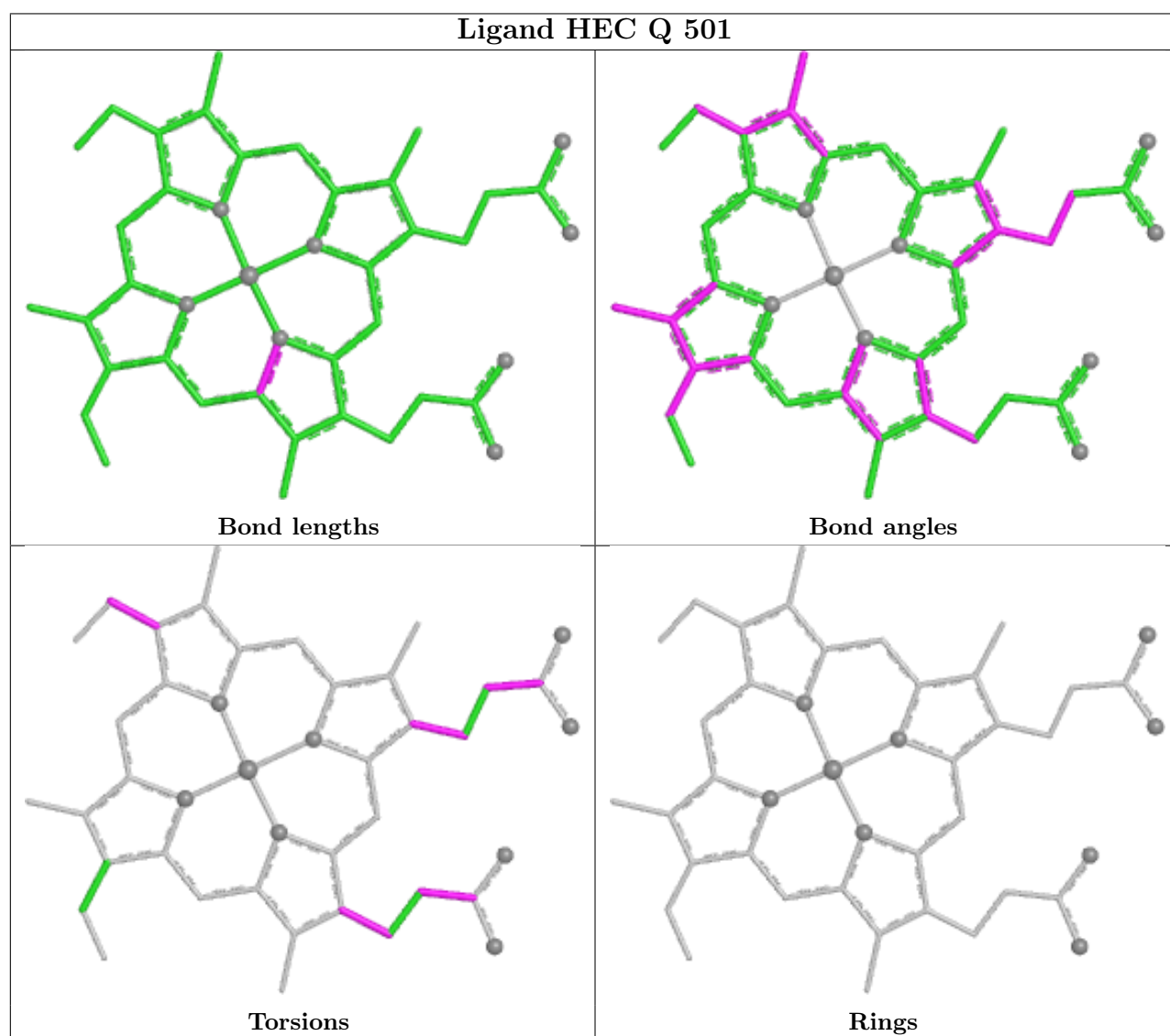
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	Q	501	HEC	1	0
12	C	502	HEM	3	0
14	P	505	UQ	1	0
12	P	501	HEM	2	0
15	P	506	CDL	3	0
12	C	501	HEM	1	0
15	C	505	CDL	1	0
16	P	507	PEE	2	0
18	D	501	HEC	1	0
13	C	503	WF3	1	0
15	G	101	CDL	1	0
15	Q	502	CDL	1	0
13	P	504	WF3	1	0
16	C	506	PEE	2	0
14	C	504	UQ	3	0

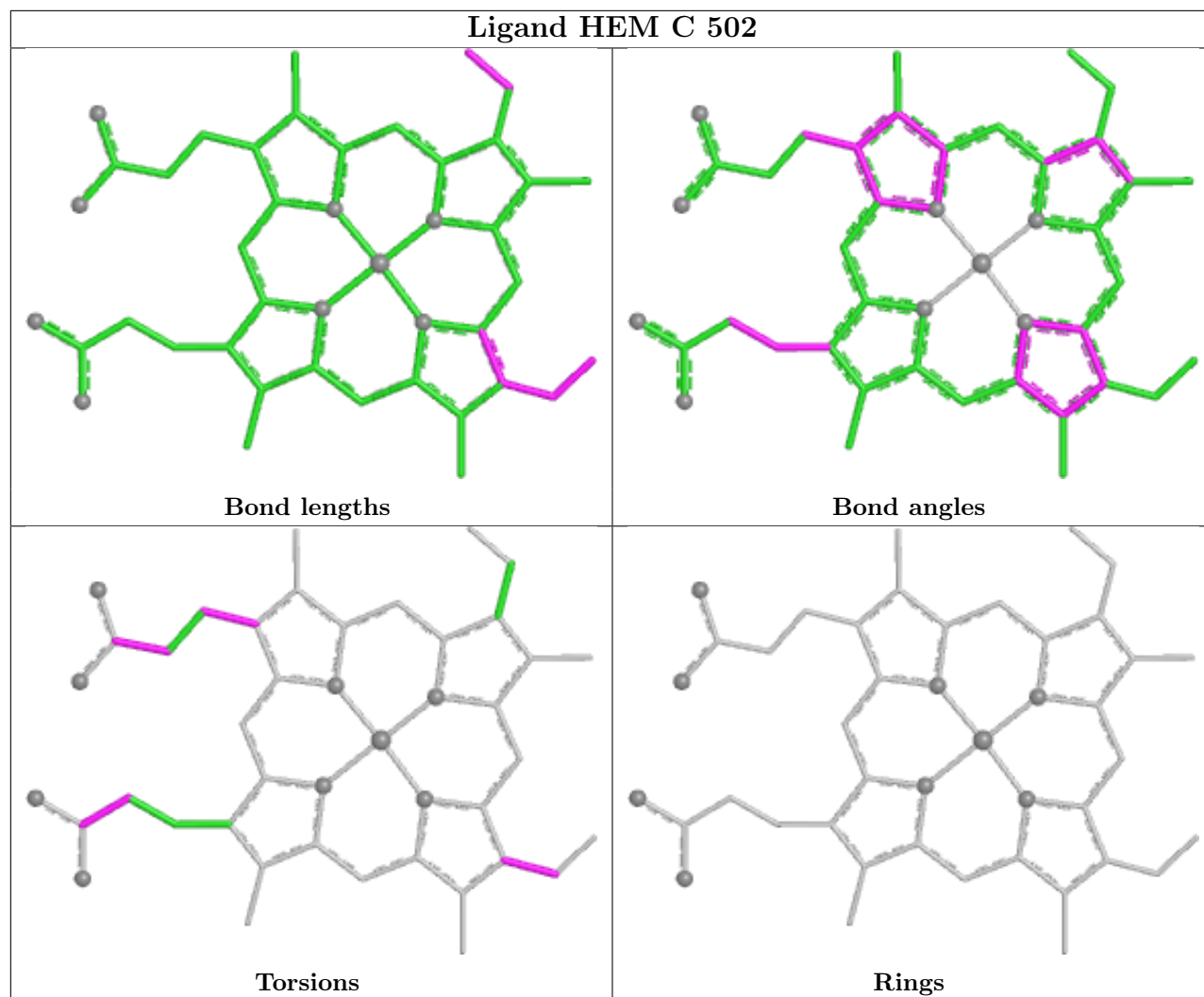
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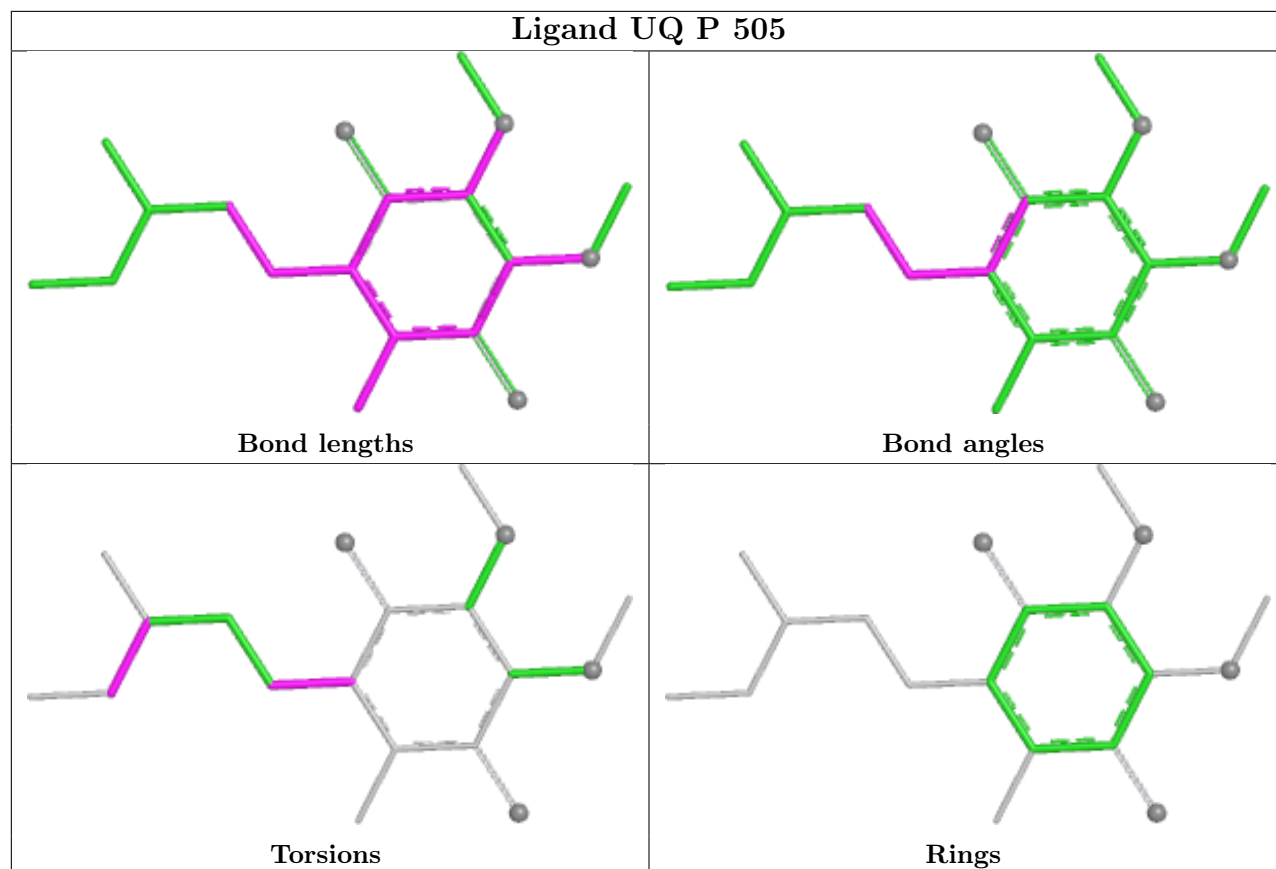
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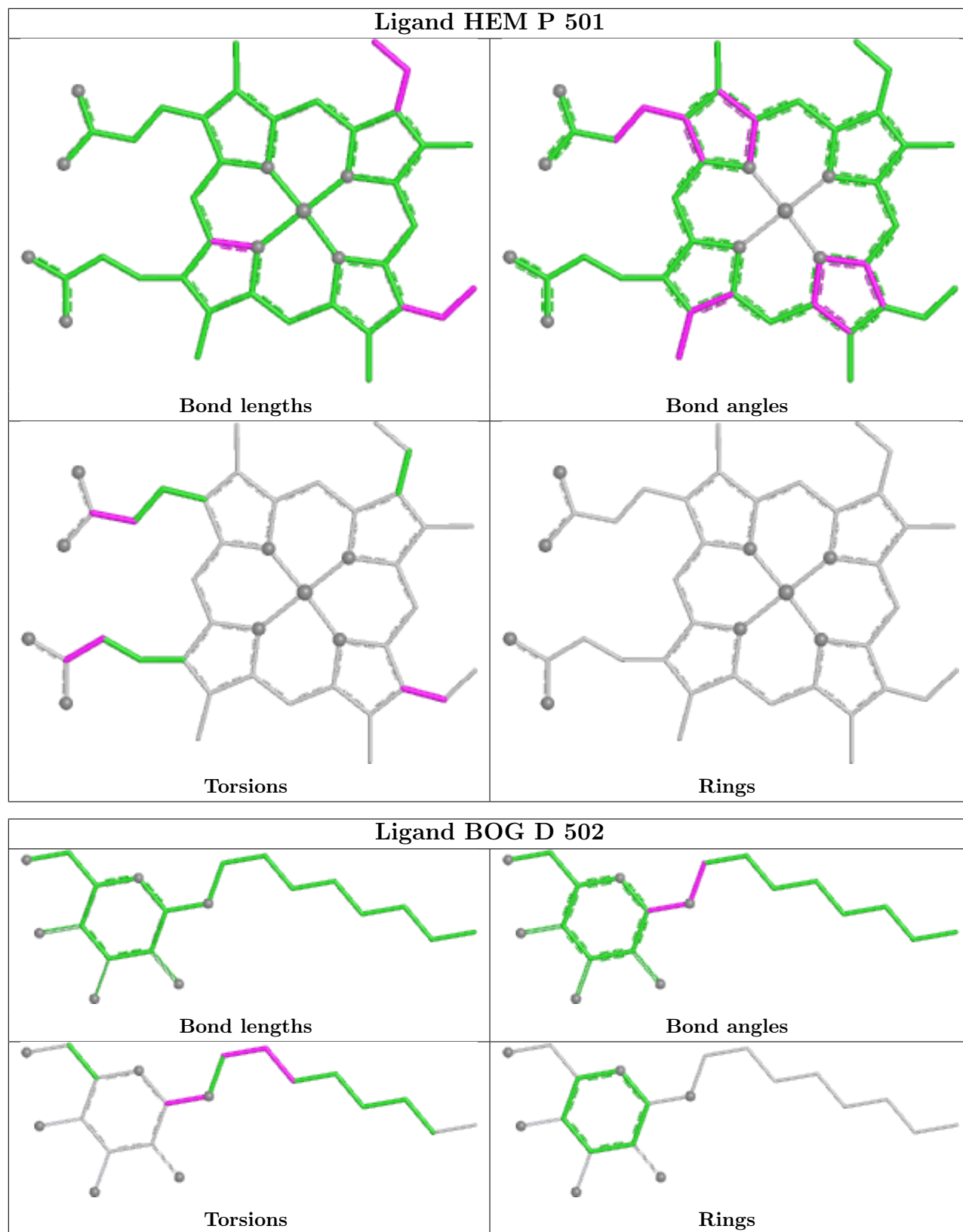
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	502	HEM	3	0
16	R	502	PEE	1	0

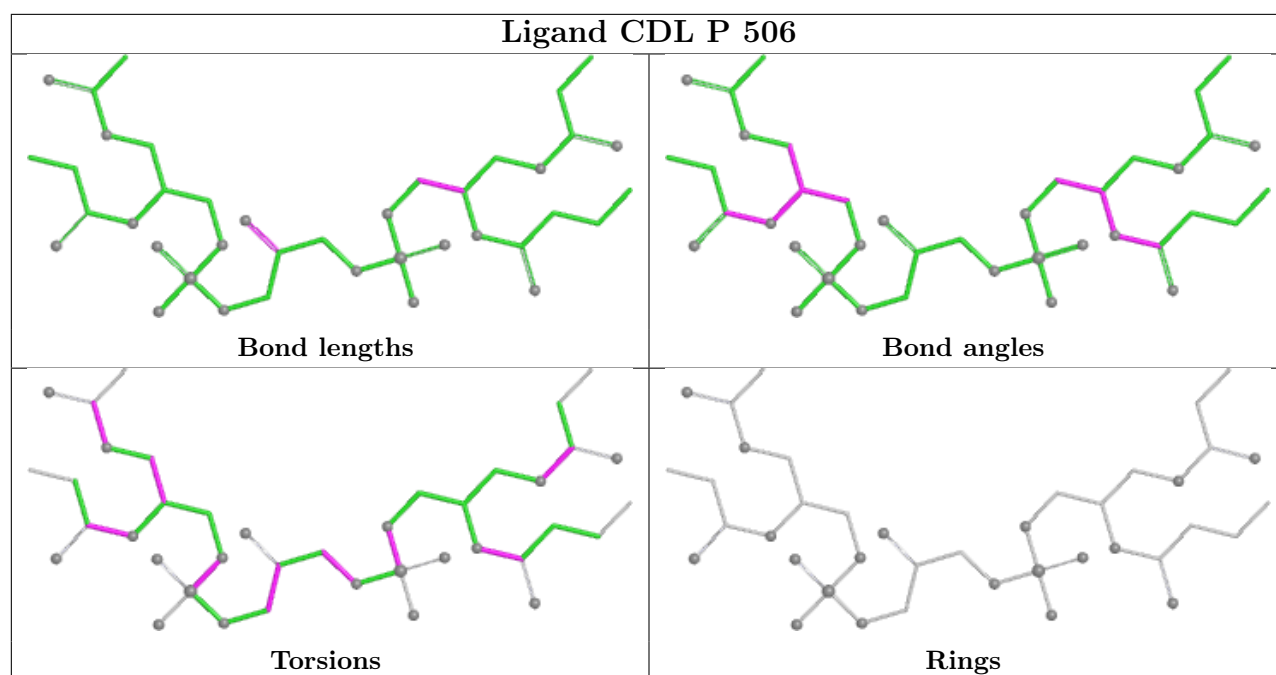
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

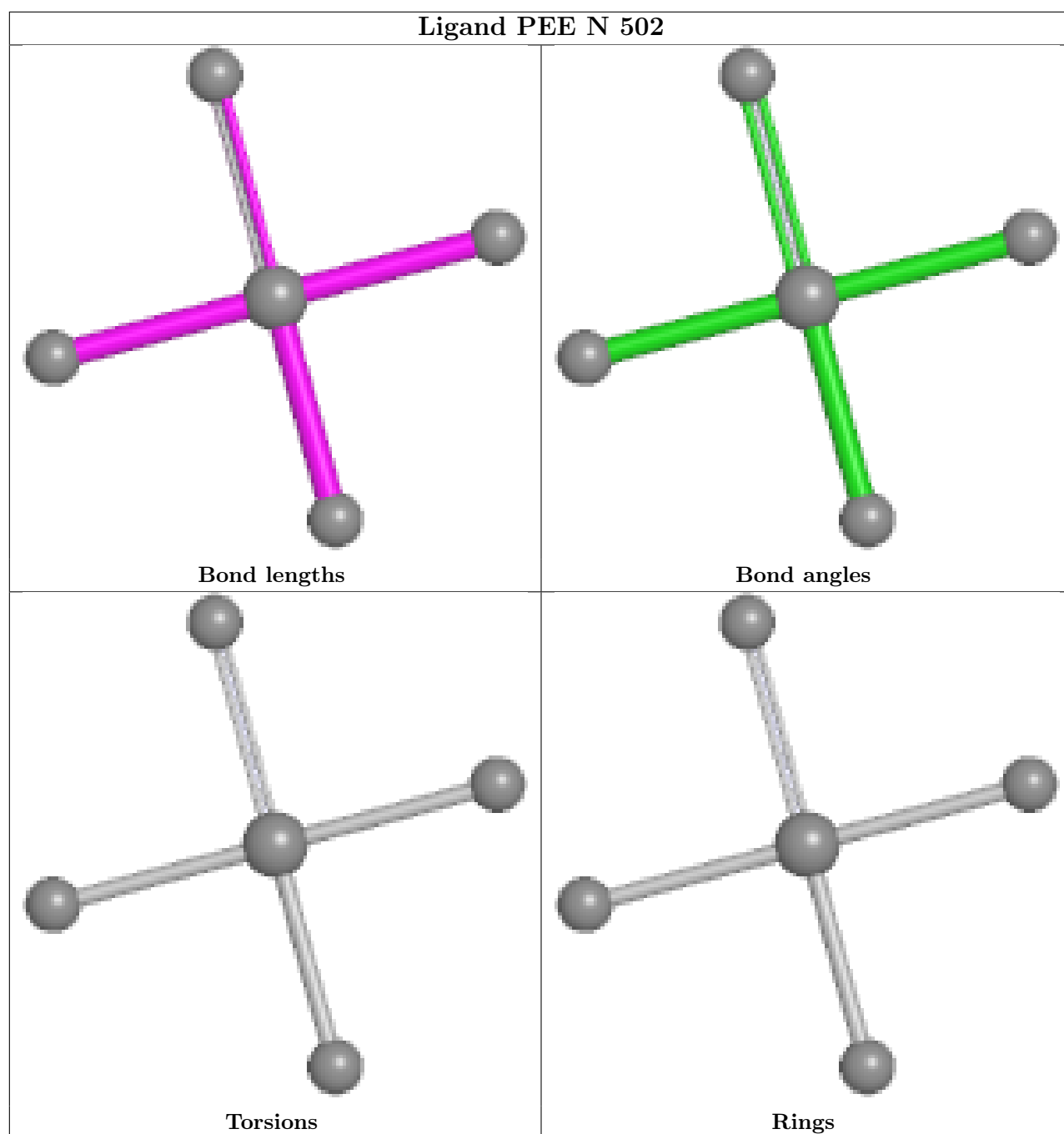


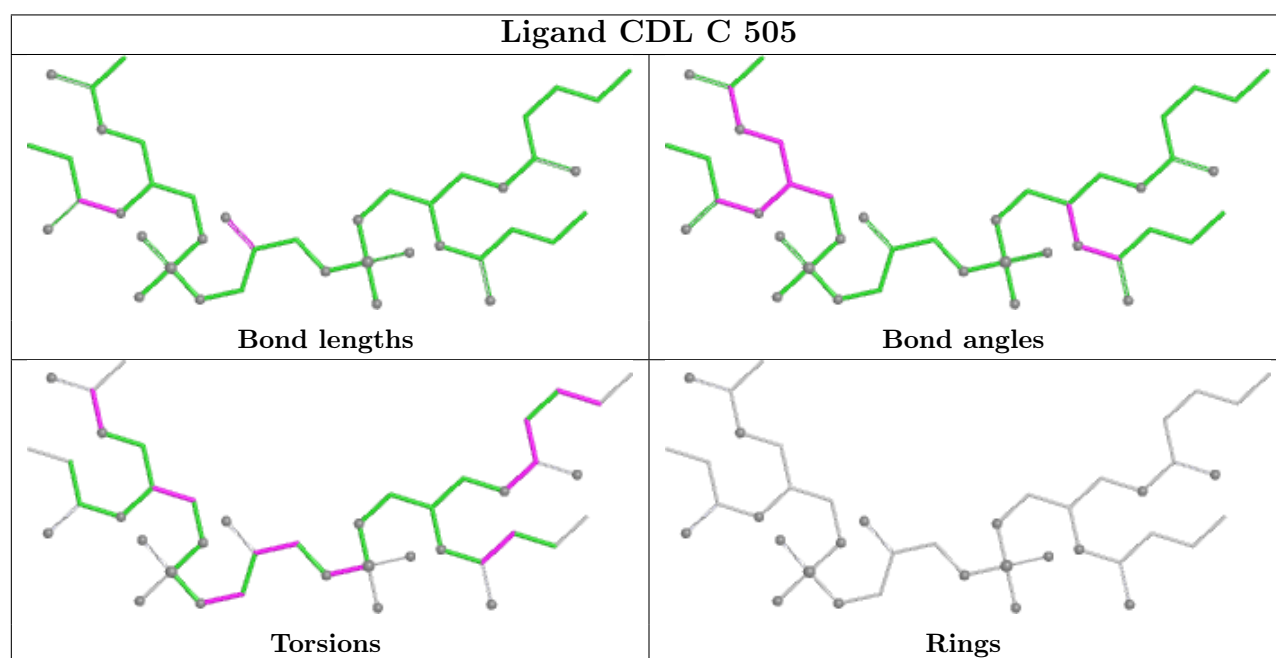
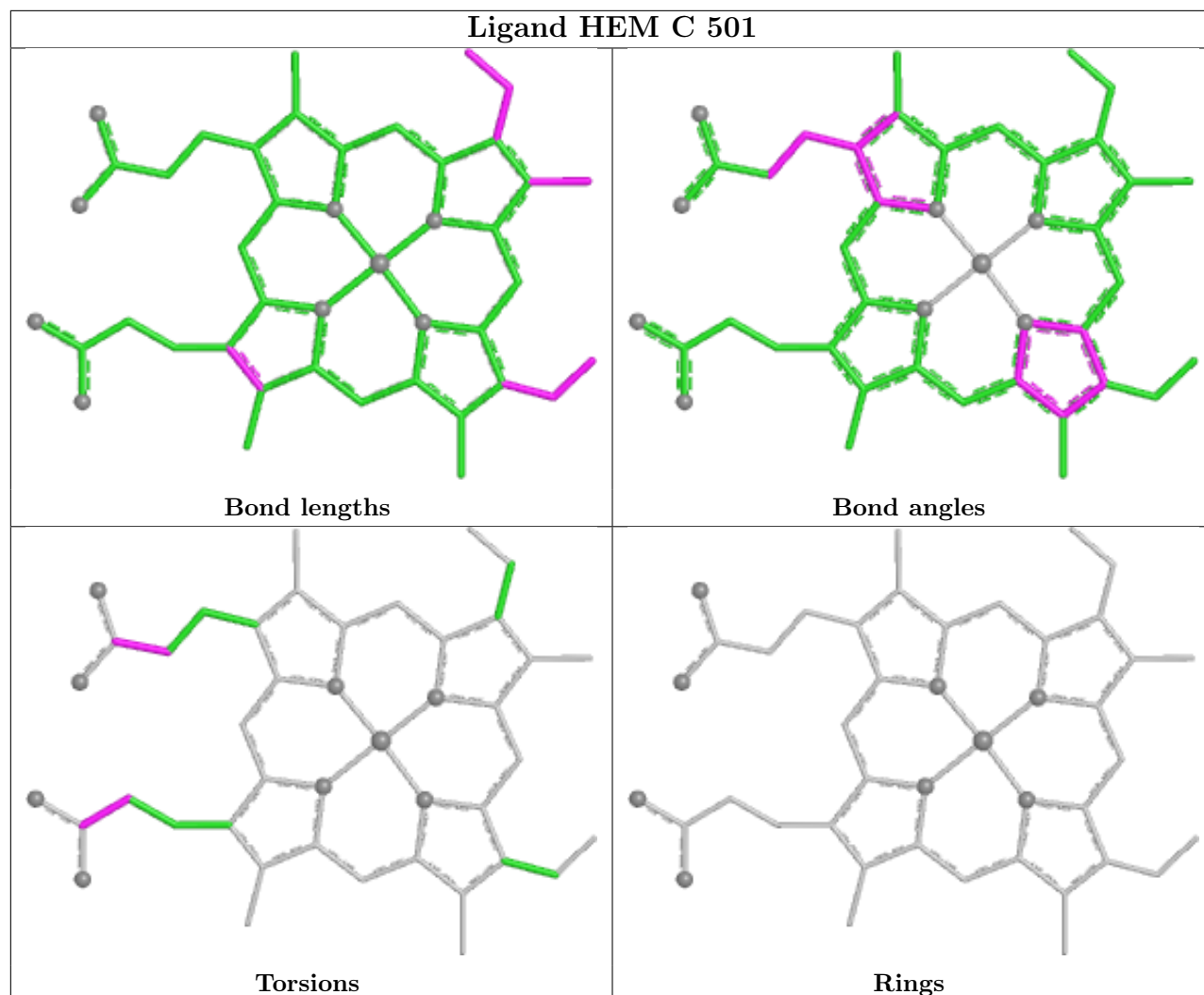


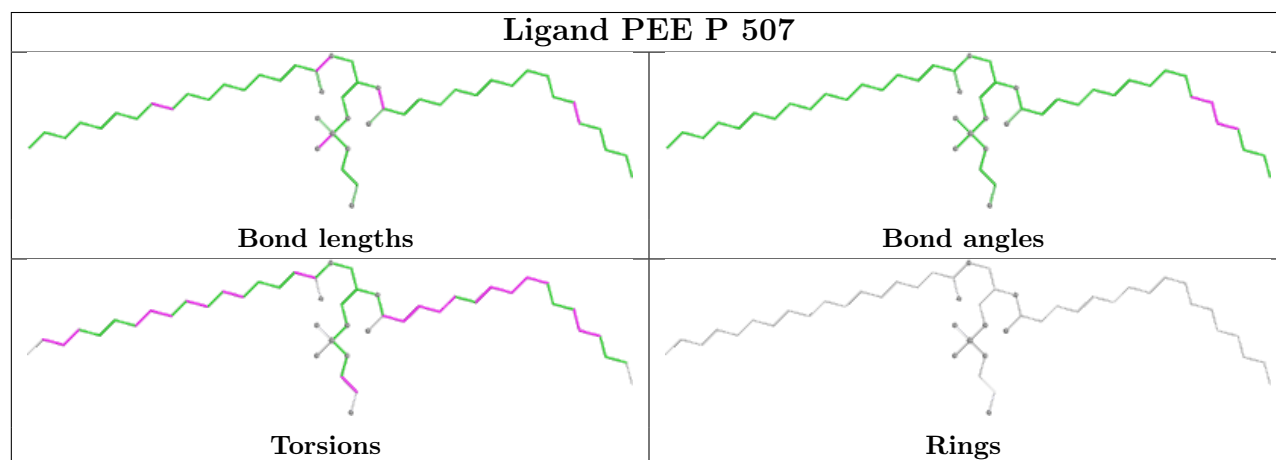
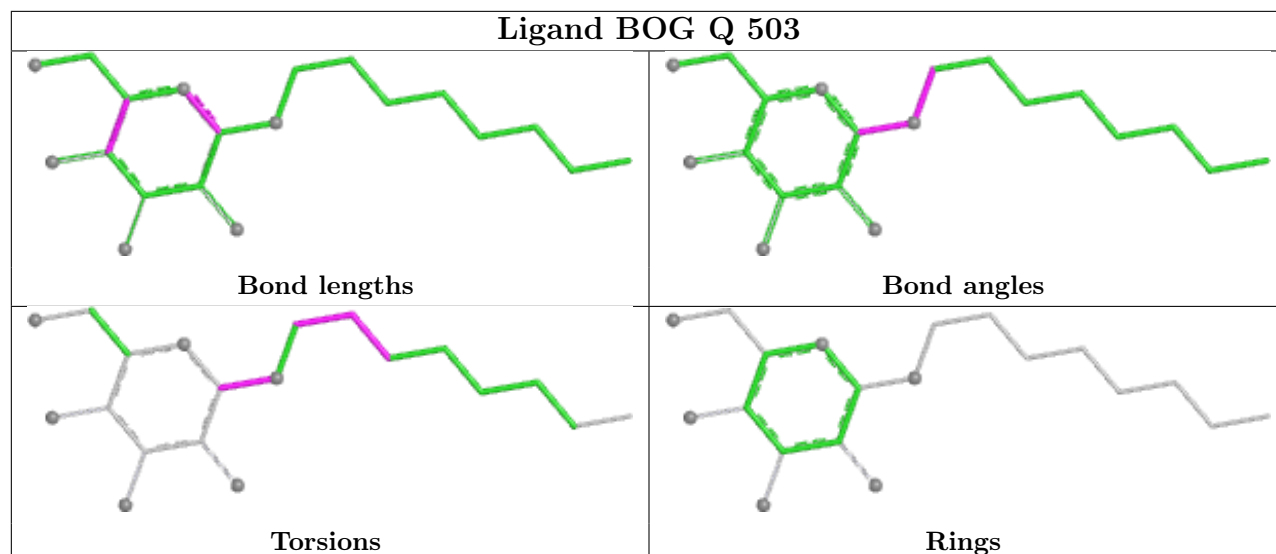




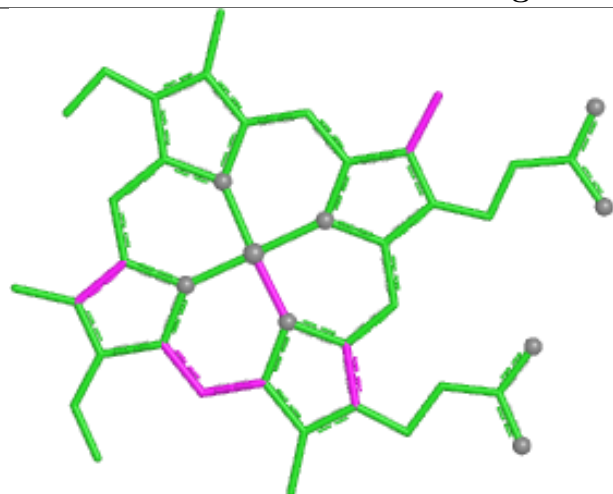




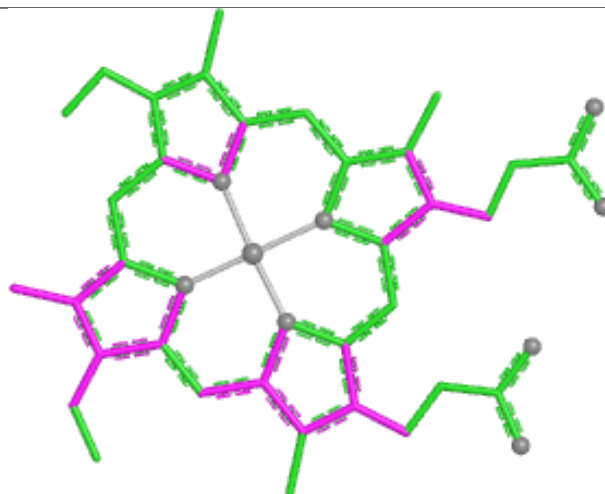




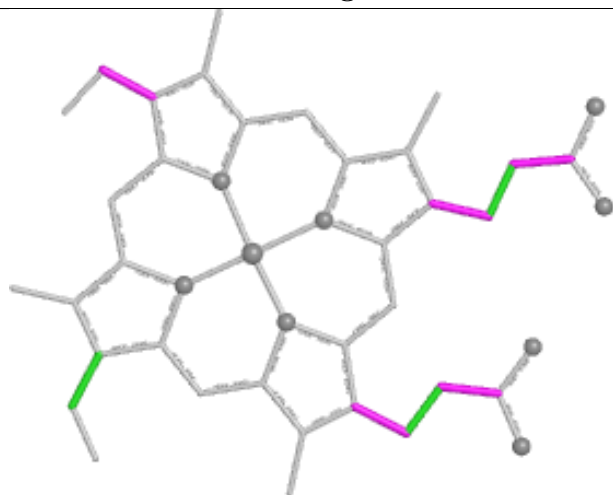
Ligand HEC D 501



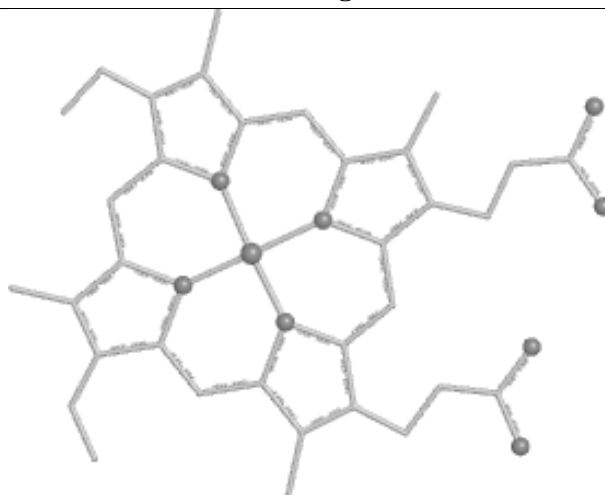
Bond lengths



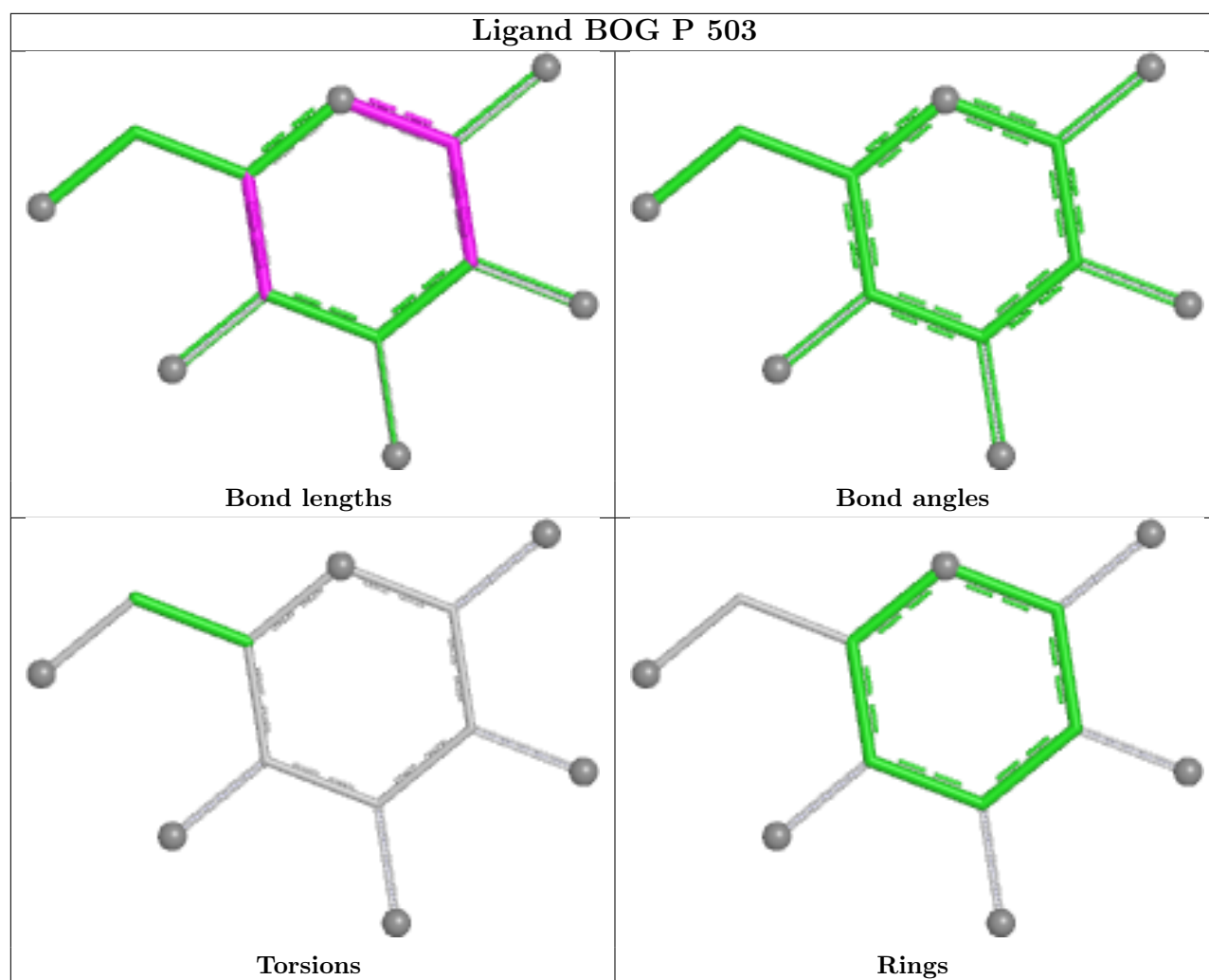
Bond angles



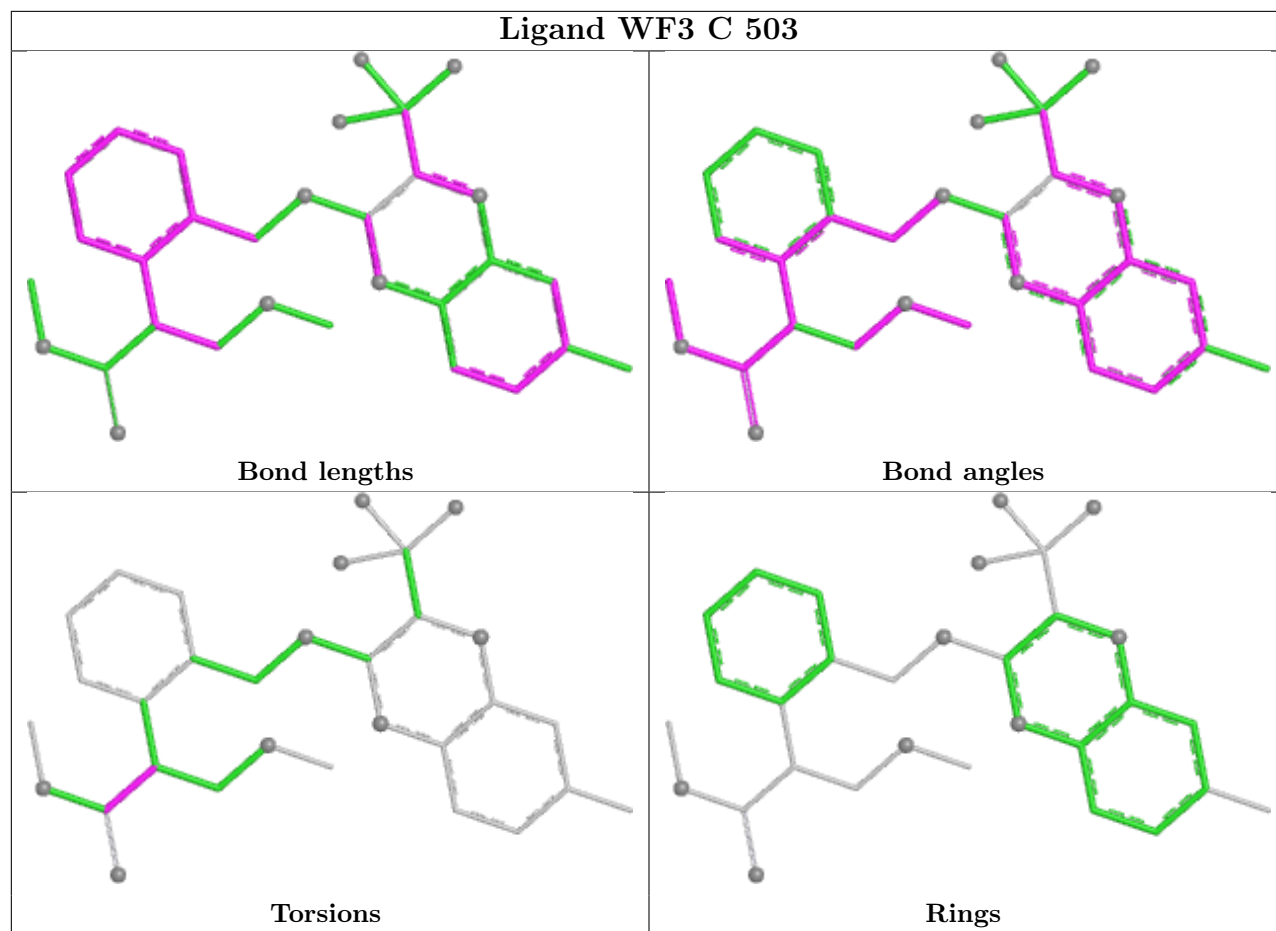
Torsions



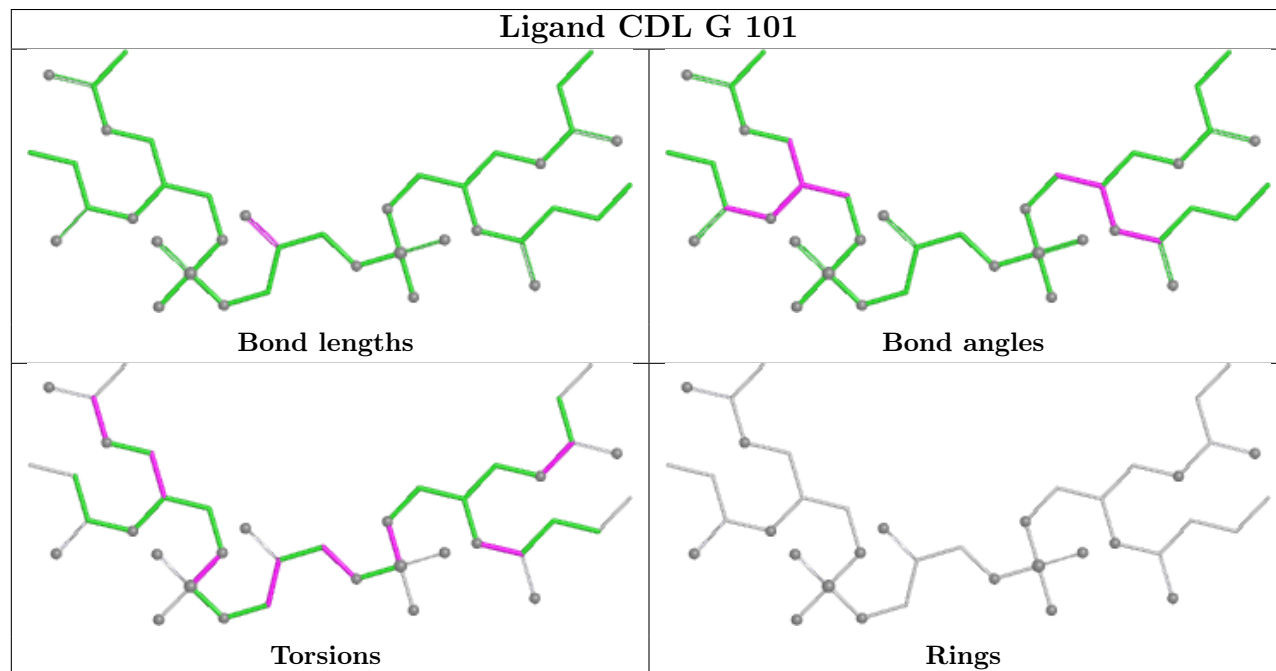
Rings

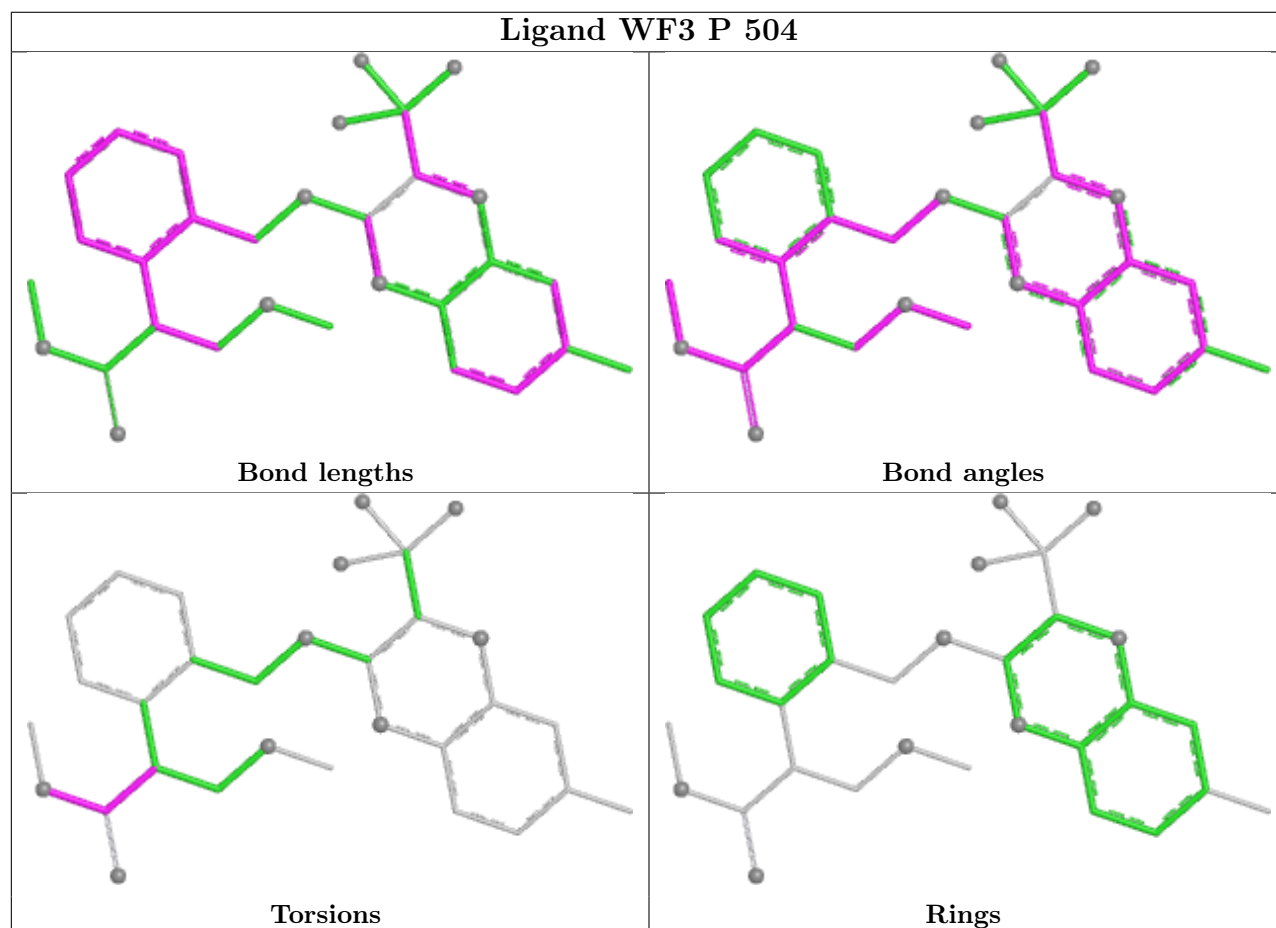
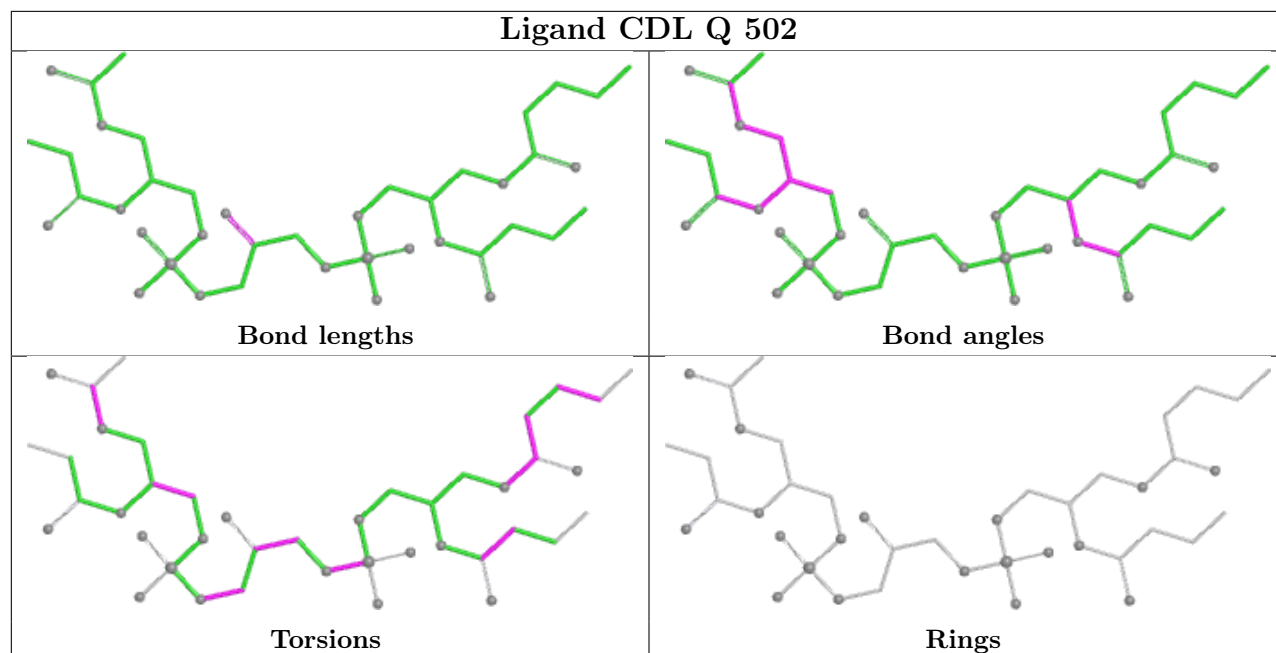


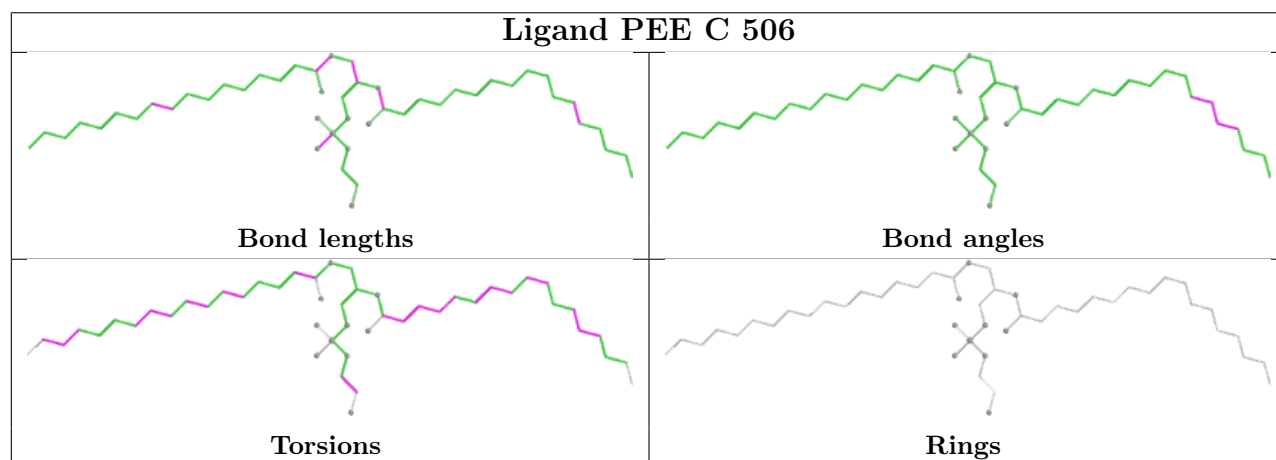
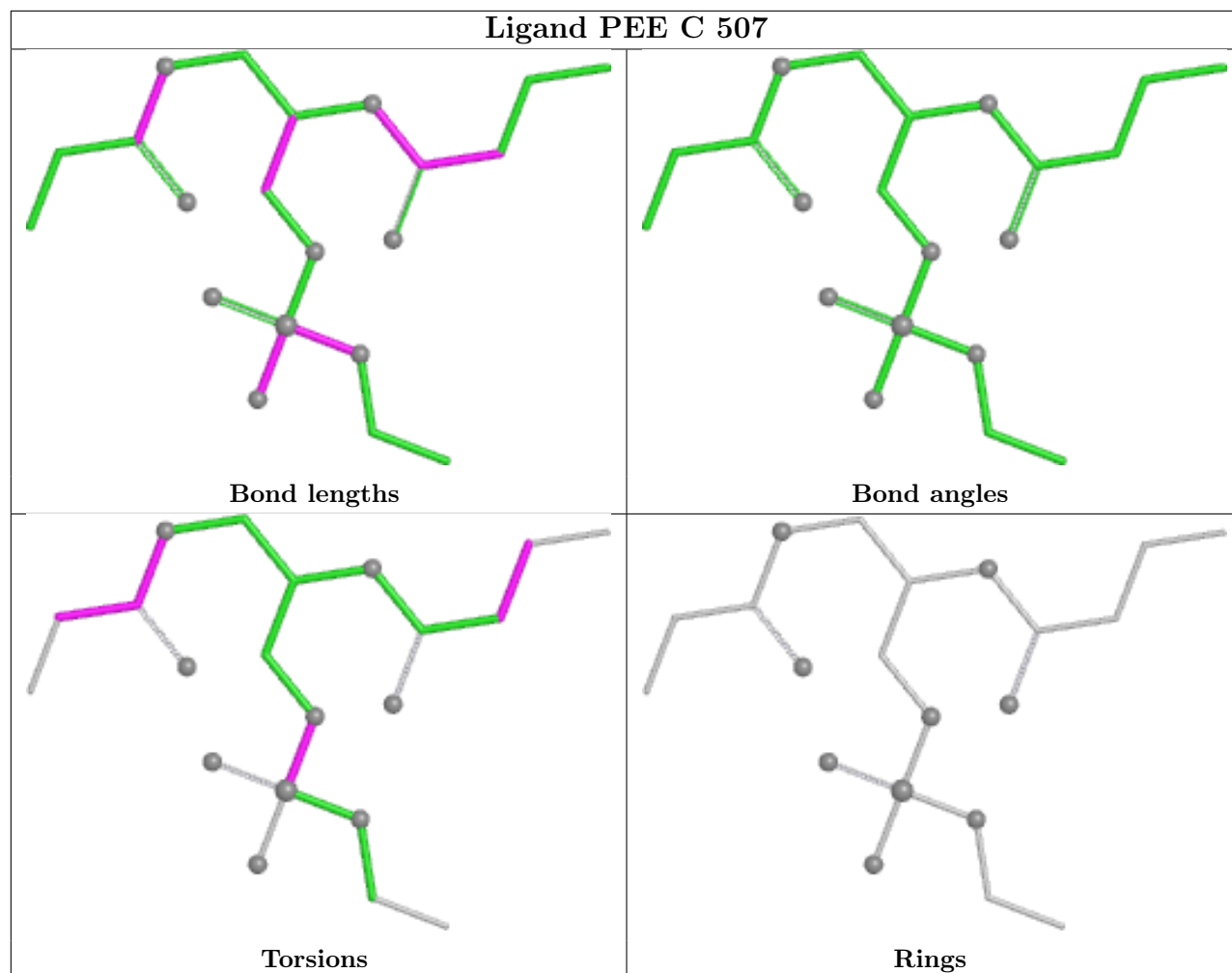
Ligand WF3 C 503

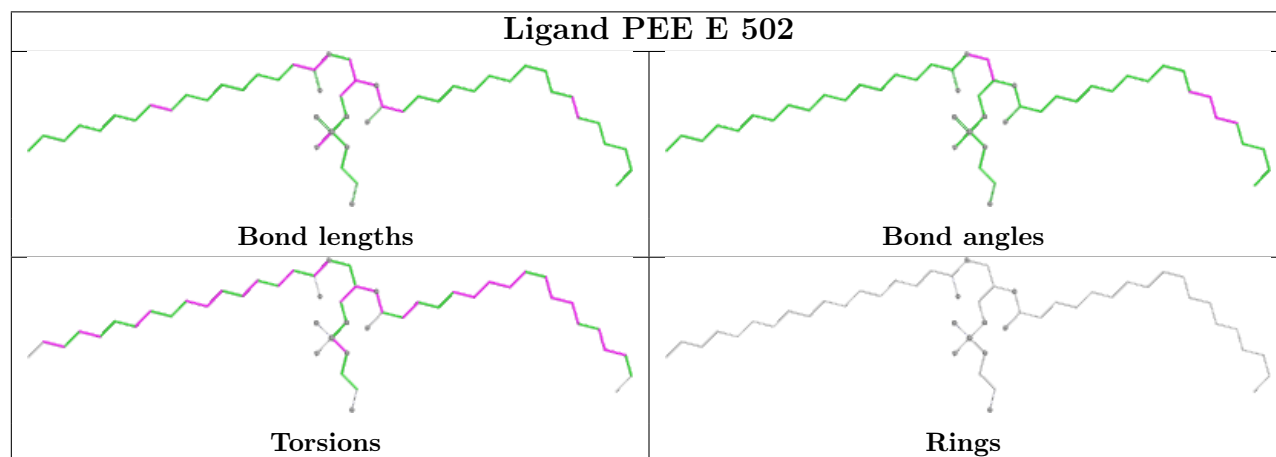
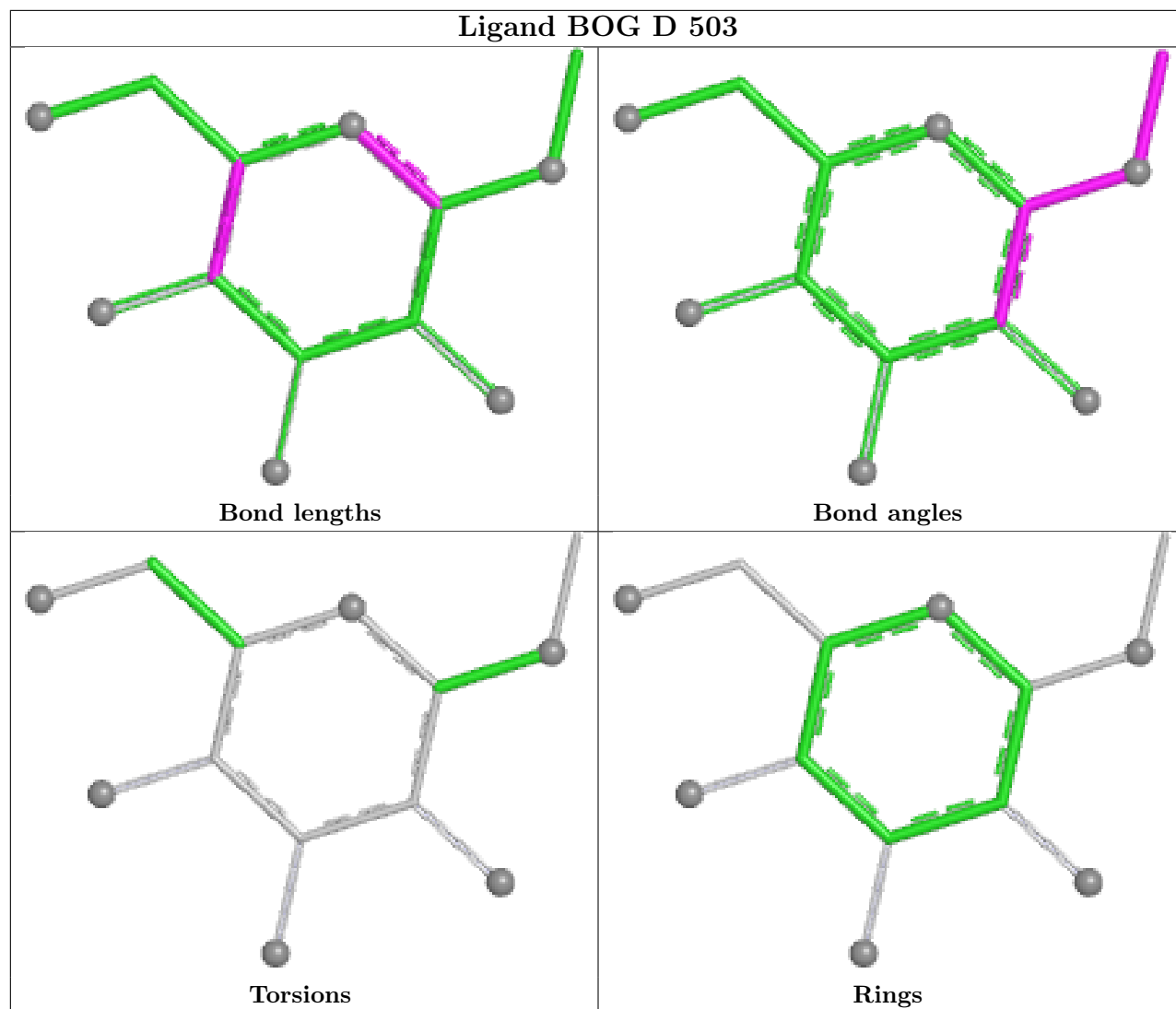


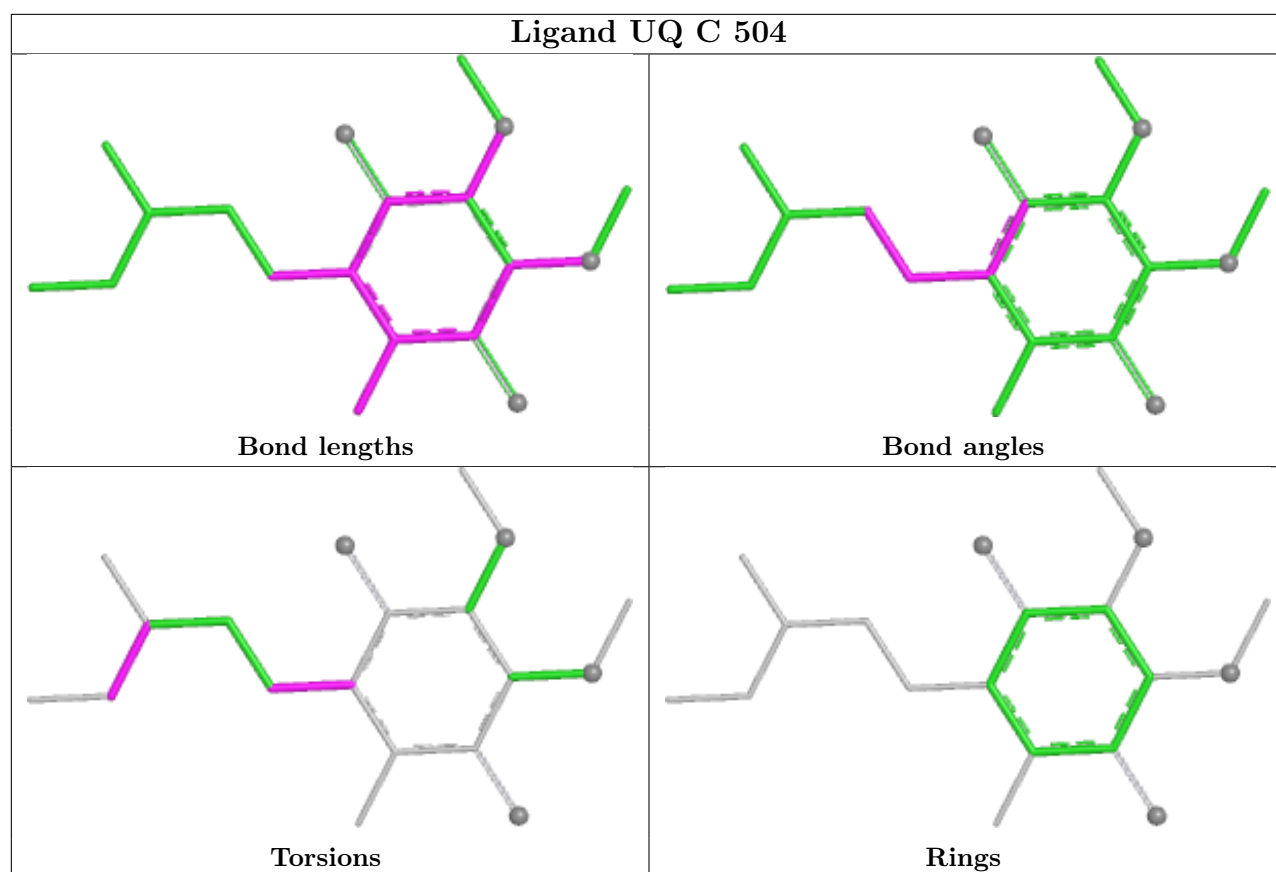
Ligand CDL G 101

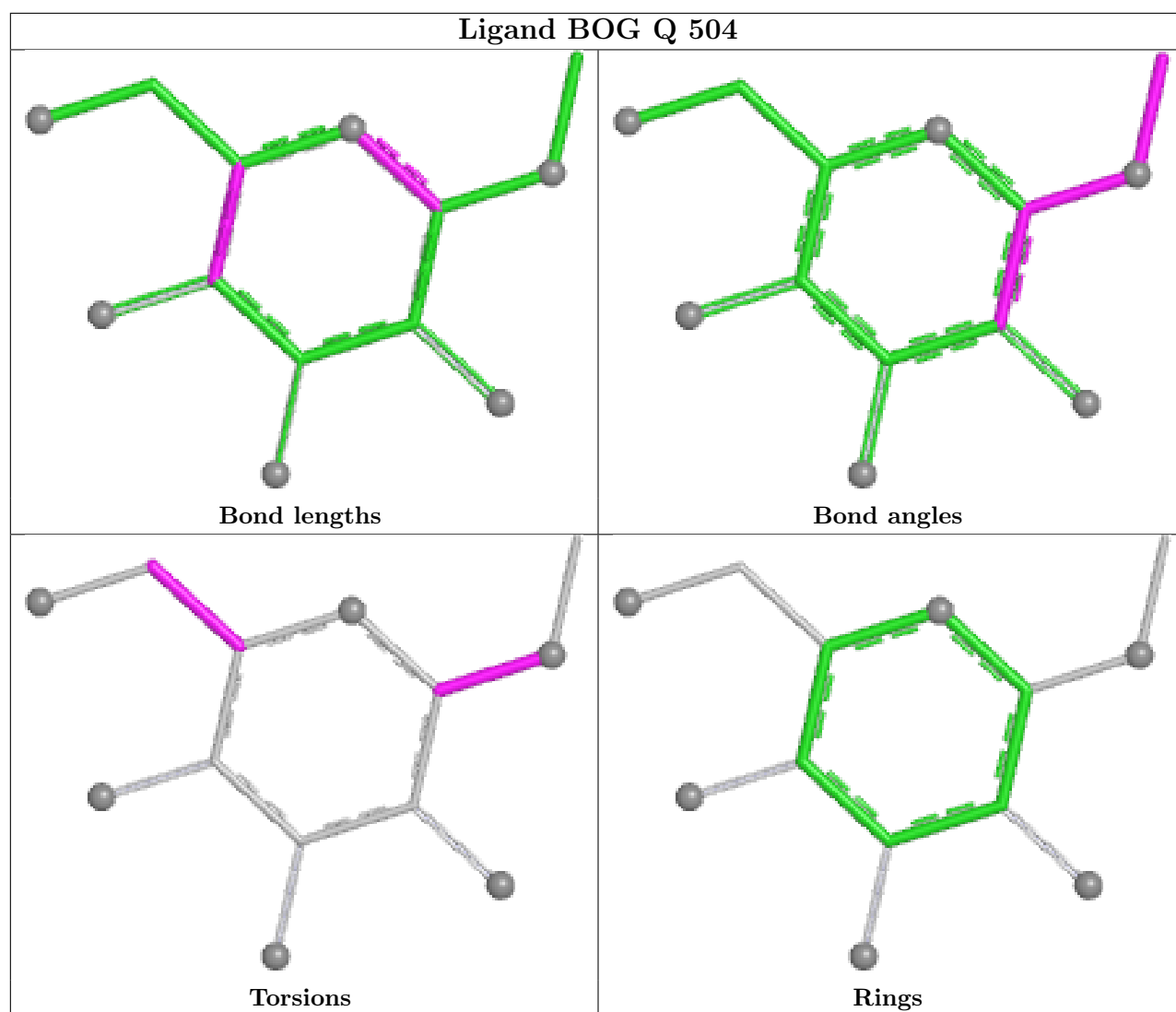


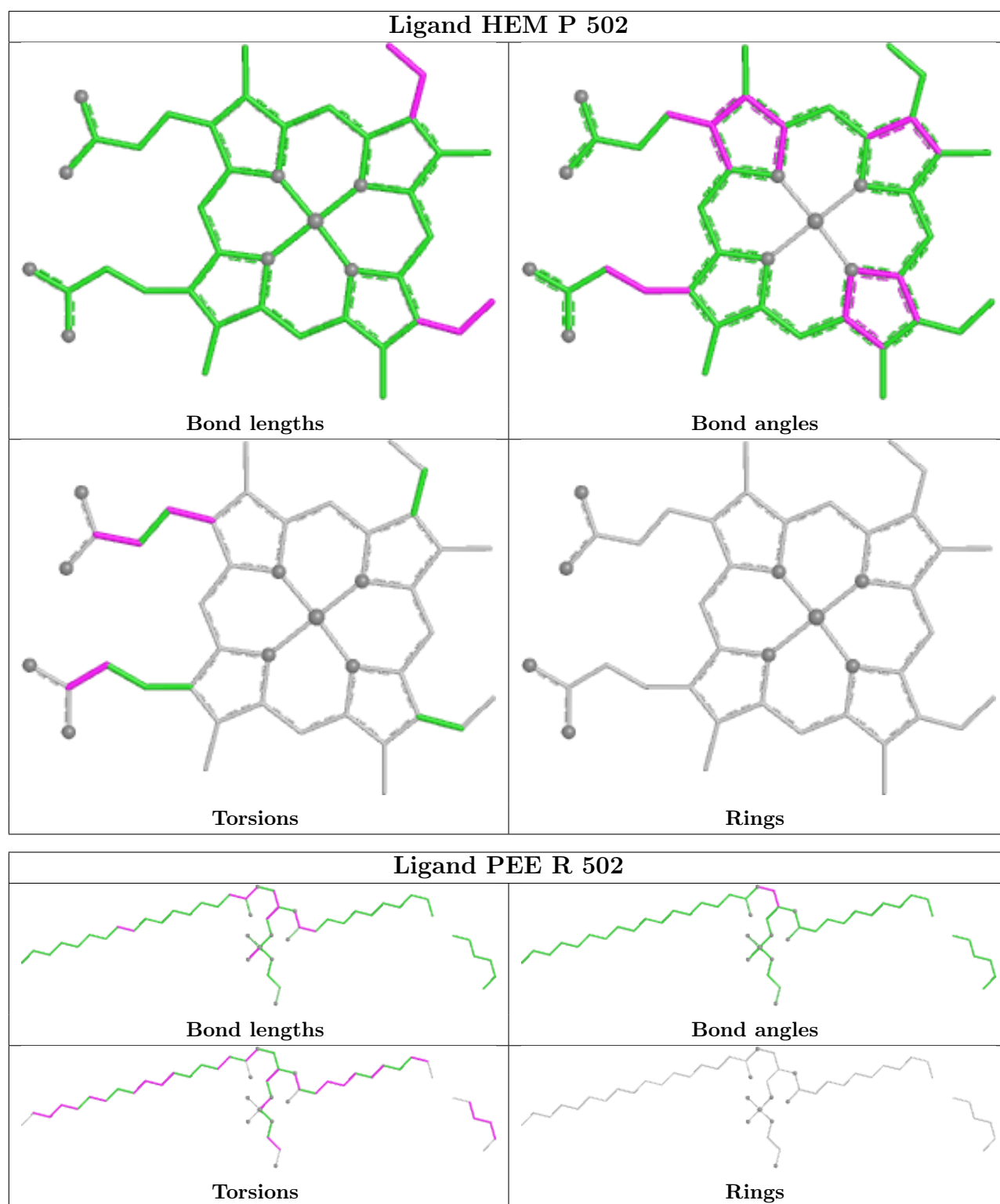












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	443/446 (99%)	0.33	16 (3%)	46	42	40, 70, 101, 123	0
1	N	442/446 (99%)	0.72	32 (7%)	21	18	44, 76, 104, 117	0
2	B	421/441 (95%)	0.85	32 (7%)	20	17	55, 88, 120, 147	0
2	O	422/441 (95%)	0.69	33 (7%)	19	16	49, 81, 114, 133	0
3	C	379/380 (99%)	-0.22	12 (3%)	50	46	29, 47, 92, 135	0
3	P	379/380 (99%)	0.36	22 (5%)	29	25	37, 68, 106, 127	0
4	D	241/241 (100%)	-0.23	5 (2%)	63	61	37, 49, 89, 118	0
4	Q	241/241 (100%)	0.88	16 (6%)	24	21	51, 82, 115, 128	0
5	E	196/196 (100%)	1.32	63 (32%)	1	1	41, 109, 159, 174	0
5	R	196/196 (100%)	1.18	43 (21%)	2	2	49, 96, 148, 168	0
6	F	101/110 (91%)	-0.35	0	100	100	31, 51, 71, 100	0
6	S	101/110 (91%)	0.75	11 (10%)	10	9	60, 79, 123, 146	0
7	G	80/81 (98%)	0.23	3 (3%)	44	40	37, 62, 116, 128	0
7	T	79/81 (97%)	1.26	13 (16%)	4	4	55, 91, 150, 165	0
8	H	70/77 (90%)	0.48	4 (5%)	29	26	45, 69, 101, 145	0
8	U	67/77 (87%)	2.05	33 (49%)	0	0	96, 129, 149, 155	0
9	I	37/76 (48%)	3.30	28 (75%)	0	0	80, 124, 163, 166	0
9	V	37/76 (48%)	3.30	30 (81%)	0	0	61, 126, 162, 163	0
10	J	61/61 (100%)	0.13	1 (1%)	70	68	46, 65, 107, 170	0
10	W	60/61 (98%)	0.72	2 (3%)	49	45	62, 81, 128, 138	0
All	All	4053/4218 (96%)	0.60	399 (9%)	13	11	29, 74, 131, 174	0

All (399) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	9	GLU	7.8
9	V	59	ARG	7.3
2	O	226	ILE	7.1
9	V	54	SER	7.0
9	I	2	LEU	6.3
9	I	61	ARG	6.2
9	V	61	ASP	6.1
9	I	51	CYS	5.9
2	B	226	ILE	5.8
5	E	106	ILE	5.8
5	E	147	ILE	5.6
9	I	50	LEU	5.6
9	V	48	LEU	5.6
7	T	2	ILE	5.6
5	E	167	ALA	5.6
9	I	57	GLY	5.5
9	V	46	PRO	5.5
5	R	124	LEU	5.4
9	V	8	SER	5.3
5	E	127	VAL	5.3
9	I	56	SER	5.3
7	T	74	PRO	5.2
9	V	55	GLY	5.2
7	G	2	ILE	5.1
9	V	47	LEU	5.1
9	I	4	VAL	5.0
5	E	113	ASP	4.9
9	I	63	ASP	4.9
5	E	120	PRO	4.8
9	V	57	SER	4.7
9	V	2	LEU	4.7
5	E	117	LEU	4.7
9	I	62	ARG	4.7
1	N	432	LEU	4.6
5	E	109	GLU	4.6
8	U	13	LEU	4.6
5	E	114	VAL	4.6
2	O	21	ALA	4.4
5	E	124	LEU	4.4
2	B	19	PRO	4.4
8	U	54	CYS	4.4
5	E	98	VAL	4.3
9	I	6	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	N	198	ALA	4.3
5	E	157	TYR	4.2
5	E	134	ILE	4.2
8	U	55	THR	4.2
9	V	4	VAL	4.2
9	I	8	SER	4.2
3	P	240	PHE	4.2
5	R	167	ALA	4.1
3	C	4	ASN	4.1
8	U	61	PHE	4.0
9	V	56	ARG	4.0
7	T	77	TYR	4.0
2	B	232	THR	3.9
9	I	55	MET	3.9
5	E	133	VAL	3.9
1	A	444	ILE	3.9
9	I	48	PRO	3.8
9	V	50	ARG	3.8
9	V	75	ARG	3.8
5	E	156	TYR	3.8
5	E	79	SER	3.8
1	N	66	GLY	3.8
4	D	241	LYS	3.8
5	R	157	TYR	3.8
8	U	37	LEU	3.8
2	O	383	GLY	3.8
5	E	104	ALA	3.7
10	W	61	ALA	3.7
6	S	10	GLY	3.7
9	I	53	GLU	3.7
5	E	85	LYS	3.7
5	E	110	ALA	3.7
9	I	60	ALA	3.7
2	B	250	HIS	3.7
2	B	388	LEU	3.7
5	R	192	LEU	3.7
3	P	4	ASN	3.7
9	I	77	ARG	3.7
5	R	154	GLY	3.7
3	C	240	PHE	3.7
5	E	97	PHE	3.6
5	E	180	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	Q	152	TYR	3.5
4	Q	5	LEU	3.5
2	O	281	ALA	3.5
5	R	117	LEU	3.5
5	E	135	LEU	3.5
9	I	49	LEU	3.5
9	I	58	ARG	3.5
5	R	171	ILE	3.5
9	I	5	ALA	3.5
5	R	120	PRO	3.5
5	E	121	GLN	3.5
2	B	216	LEU	3.4
7	G	81	GLN	3.4
5	E	183	PRO	3.4
2	O	386	ALA	3.4
9	V	5	ALA	3.4
5	E	177	PRO	3.4
2	B	206	LEU	3.4
5	E	168	SER	3.3
8	U	39	LEU	3.3
5	E	122	HIS	3.3
1	N	219	VAL	3.3
1	A	443	TRP	3.3
2	O	19	PRO	3.3
2	B	20	GLY	3.3
9	V	69	ASN	3.3
7	T	32	ASP	3.3
5	E	126	ARG	3.3
2	B	104	LYS	3.3
5	E	196	GLY	3.3
8	U	33	ALA	3.3
5	R	85	LYS	3.2
5	R	106	ILE	3.2
2	B	36	ALA	3.2
3	P	151	PHE	3.2
9	I	71	ASN	3.1
5	E	159	PRO	3.1
2	O	20	GLY	3.1
9	V	3	SER	3.1
5	R	112	VAL	3.1
3	P	380	TYR	3.1
1	A	350	THR	3.1

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Mol	Chain	Res	Type	RSRZ
4	Q	57	THR	3.1
5	E	145	VAL	3.1
5	R	114	VAL	3.1
3	C	3	PRO	3.1
9	V	49	CYS	3.1
9	V	7	ARG	3.1
7	T	79	ASN	3.1
1	N	444	ILE	3.1
3	P	2	ALA	3.1
5	R	99	ARG	3.1
5	R	153	PHE	3.1
9	V	53	MET	3.1
7	T	3	HIS	3.0
4	Q	1	GLY	3.0
5	R	156	TYR	3.0
6	S	21	TYR	3.0
3	C	5	ILE	3.0
5	E	169	GLY	3.0
9	V	60	ARG	3.0
1	A	219	VAL	3.0
9	I	7	ARG	3.0
8	U	78	LYS	3.0
9	I	52	ARG	3.0
5	E	116	LYS	2.9
8	U	76	LYS	2.9
1	N	120	CYS	2.9
2	B	21	ALA	2.9
2	B	289	SER	2.9
8	U	74	PHE	2.9
5	E	146	PRO	2.9
5	E	101	ARG	2.9
2	B	391	THR	2.9
9	V	74	VAL	2.9
8	U	29	LYS	2.9
1	N	56	GLY	2.9
4	Q	141	VAL	2.9
5	E	89	PHE	2.9
3	P	3	PRO	2.8
9	I	3	SER	2.8
9	V	70	ALA	2.8
5	E	118	ARG	2.8
3	P	5	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	115	SER	2.8
5	R	122	HIS	2.8
7	T	24	ARG	2.8
5	R	108	GLN	2.8
5	R	147	ILE	2.8
5	R	113	ASP	2.8
3	P	7	LYS	2.8
2	B	390	GLY	2.8
5	R	104	ALA	2.8
9	I	72	ALA	2.8
2	O	223	PHE	2.8
3	P	318	PHE	2.8
8	U	68	CYS	2.7
3	C	8	SER	2.7
5	E	86	ASN	2.7
5	R	111	GLU	2.7
10	J	61	ALA	2.7
8	U	65	ARG	2.7
5	R	165	TYR	2.7
8	U	26	GLN	2.7
8	U	30	CYS	2.7
1	N	182	LEU	2.7
3	P	11	LEU	2.7
1	A	215	HIS	2.7
3	P	6	ARG	2.7
4	Q	180	SER	2.7
9	V	58	ALA	2.7
5	E	128	LYS	2.7
2	O	224	LEU	2.7
5	E	172	ARG	2.7
5	E	112	VAL	2.7
5	E	173	LYS	2.7
5	E	187	PHE	2.7
8	U	69	VAL	2.7
3	P	12	LEU	2.6
5	E	78	LEU	2.6
4	Q	13	SER	2.6
3	P	320	PRO	2.6
6	S	36	THR	2.6
8	U	63	HIS	2.6
2	B	48	GLY	2.6
1	A	31	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	2.6
1	N	26	ALA	2.6
4	Q	10	PHE	2.6
4	Q	142	VAL	2.6
9	I	76	VAL	2.6
4	Q	151	PRO	2.6
9	V	62	LEU	2.6
5	E	153	PHE	2.6
5	R	110	ALA	2.6
1	N	174	ILE	2.6
8	U	73	LEU	2.6
3	C	156	TYR	2.6
3	C	380	TYR	2.6
5	R	178	TYR	2.6
6	S	20	TYR	2.6
2	B	223	PHE	2.6
3	C	151	PHE	2.6
2	O	391	THR	2.5
9	I	59	SER	2.5
1	A	223	TYR	2.5
5	E	108	GLN	2.5
4	D	3	LEU	2.5
9	I	64	LEU	2.5
1	N	28	GLU	2.5
2	B	41	PHE	2.5
3	C	6	ARG	2.5
4	Q	165	TYR	2.5
5	E	185	TYR	2.5
5	E	102	THR	2.5
2	O	209	ILE	2.5
9	I	54	SER	2.5
9	V	71	PRO	2.5
1	N	190	PHE	2.5
8	U	70	ALA	2.5
9	V	6	ALA	2.5
1	A	432	LEU	2.4
1	A	35	CYS	2.4
2	B	392	HIS	2.4
5	E	188	VAL	2.4
1	A	34	THR	2.4
2	B	112	LEU	2.4
5	R	150	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	104	LYS	2.4
2	O	410	VAL	2.4
7	T	75	ALA	2.4
8	U	47	ARG	2.4
6	S	12	LEU	2.4
5	R	168	SER	2.4
2	B	314	VAL	2.4
8	U	14	VAL	2.4
8	U	44	VAL	2.4
3	P	373	LEU	2.4
2	B	268	GLU	2.4
2	O	344	LEU	2.3
5	E	165	TYR	2.3
2	O	332	HIS	2.3
2	O	225	ASN	2.3
2	O	371	SER	2.3
5	E	129	LYS	2.3
7	T	80	ASP	2.3
8	U	66	ASP	2.3
1	A	229	PRO	2.3
2	O	388	LEU	2.3
2	O	250	HIS	2.3
5	R	27	THR	2.3
9	V	51	GLU	2.3
8	U	15	ASP	2.3
1	N	234	CYS	2.3
2	O	156	GLN	2.3
5	R	18	VAL	2.3
6	S	31	LEU	2.3
5	R	172	ARG	2.3
5	R	155	GLY	2.3
2	B	116	VAL	2.3
5	E	87	VAL	2.3
1	N	17	THR	2.3
3	P	156	TYR	2.3
5	E	82	PRO	2.3
4	D	1	GLY	2.3
5	R	196	GLY	2.3
4	Q	169	LEU	2.3
2	O	236	LYS	2.2
2	O	335	GLU	2.2
8	H	10	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	57	TYR	2.2
1	A	32	GLN	2.2
7	T	43	SER	2.2
2	O	350	GLY	2.2
2	B	33	LEU	2.2
1	N	68	LYS	2.2
8	U	67	HIS	2.2
4	Q	134	TYR	2.2
2	O	227	ARG	2.2
5	R	86	ASN	2.2
1	A	81	SER	2.2
4	D	172	ASP	2.2
5	R	115	SER	2.2
1	N	129	LYS	2.2
3	C	7	LYS	2.2
6	S	18	LYS	2.2
3	C	9	HIS	2.2
3	P	348	PHE	2.2
8	H	71	HIS	2.2
8	U	71	HIS	2.2
4	Q	9	ALA	2.2
1	N	72	CYS	2.2
8	U	50	THR	2.2
1	N	179	ARG	2.2
2	B	30	PRO	2.2
1	A	226	ASP	2.2
5	E	125	ASP	2.2
5	E	136	VAL	2.2
2	B	402	ILE	2.2
3	P	212	ILE	2.2
5	E	171	ILE	2.2
6	S	74	ILE	2.2
7	T	46	PHE	2.2
5	R	105	GLU	2.2
8	U	52	GLU	2.2
2	O	232	THR	2.2
3	P	347	PRO	2.2
5	R	121	GLN	2.2
6	S	110	LYS	2.2
7	T	72	LYS	2.2
9	V	52	SER	2.2
7	G	3	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	312	PHE	2.2
5	R	187	PHE	2.2
2	O	171	ALA	2.1
2	B	303	THR	2.1
8	U	43	ARG	2.1
2	B	306	PRO	2.1
8	H	26	GLN	2.1
3	C	69	HIS	2.1
5	R	133	VAL	2.1
5	R	176	ALA	2.1
6	S	11	ARG	2.1
2	O	292	THR	2.1
5	E	178	TYR	2.1
1	N	83	GLY	2.1
2	O	229	GLY	2.1
2	B	34	ILE	2.1
5	E	182	VAL	2.1
1	N	5	ALA	2.1
1	N	162	ALA	2.1
2	O	44	ALA	2.1
5	R	148	ALA	2.1
4	D	2	GLU	2.1
2	B	59	THR	2.1
1	N	69	LYS	2.1
2	O	306	PRO	2.1
2	B	24	LEU	2.1
4	Q	3	LEU	2.1
2	B	316	TYR	2.1
5	E	123	ASP	2.1
7	T	71	ARG	2.1
10	W	39	ALA	2.1
1	N	229	PRO	2.1
5	R	82	PRO	2.1
8	U	17	LEU	2.1
1	N	10	ASN	2.1
3	P	82	ASN	2.1
1	N	215	HIS	2.1
8	U	40	CYS	2.1
5	E	150	SER	2.0
5	R	128	LYS	2.0
8	U	16	PRO	2.0
2	O	295	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	P	19	LEU	2.0
3	P	251	LEU	2.0
8	U	23	HIS	2.0
1	A	42	GLY	2.0
1	N	117	VAL	2.0
1	N	376	CYS	2.0
1	N	64	PHE	2.0
1	N	216	PHE	2.0
5	R	101	ARG	2.0
1	N	199	ALA	2.0
1	N	31	SER	2.0
4	Q	7	PRO	2.0
9	V	68	LEU	2.0
3	P	346	HIS	2.0
2	O	428	GLY	2.0
5	E	154	GLY	2.0
5	E	174	GLY	2.0
6	S	27	ASN	2.0
5	R	98	VAL	2.0
2	O	296	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
3	FME	C	1	9/11	0.44	0.25	139,141,148,153	0
9	AME	V	1	9/12	0.77	0.25	136,148,153,154	0
9	AME	I	1	9/12	0.80	0.24	150,155,160,160	0

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,

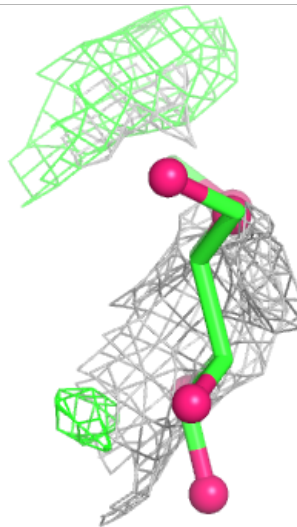
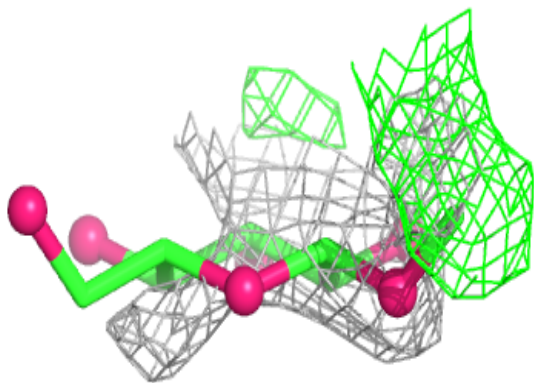
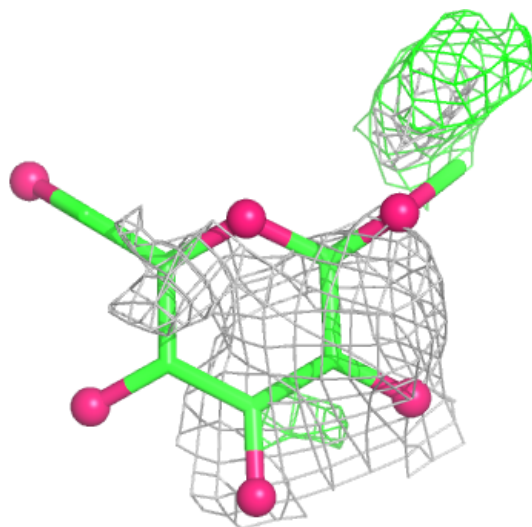
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	BOG	Q	504	13/20	0.37	0.27	179,186,190,192	0
19	BOG	D	503	13/20	0.56	0.30	140,156,162,164	0
16	PEE	C	507	21/51	0.57	0.25	64,135,154,156	0
16	PEE	N	502	5/51	0.63	0.15	132,134,139,140	0
15	CDL	Q	502	42/100	0.67	0.34	79,169,202,203	0
19	BOG	P	503	12/20	0.69	0.22	126,144,149,158	0
15	CDL	C	505	42/100	0.72	0.31	65,134,159,163	0
15	CDL	P	506	40/100	0.72	0.23	110,125,138,141	0
11	UNL	N	501	1/-	0.77	0.12	47,47,47,47	0
11	UNL	A	501	1/-	0.81	0.15	48,48,48,48	0
16	PEE	R	502	49/51	0.84	0.23	51,98,121,125	0
14	UQ	P	505	19/63	0.85	0.33	80,127,140,146	0
15	CDL	G	101	40/100	0.85	0.16	46,83,125,131	0
16	PEE	E	502	50/51	0.86	0.19	59,86,114,117	0
14	UQ	C	504	19/63	0.86	0.28	73,96,104,108	0
16	PEE	P	507	49/51	0.88	0.20	72,91,119,123	0
19	BOG	Q	503	20/20	0.89	0.17	72,100,105,113	0
16	PEE	C	506	49/51	0.92	0.14	33,60,91,103	0
19	BOG	D	502	20/20	0.92	0.10	44,64,72,76	0
17	GOL	C	508	6/6	0.93	0.16	64,72,75,76	0
17	GOL	P	508	6/6	0.94	0.15	67,76,82,84	0
13	WF3	P	504	31/31	0.94	0.10	51,64,73,78	0
20	FES	E	501	4/4	0.96	0.07	125,129,129,130	0
13	WF3	C	503	31/31	0.97	0.07	30,40,53,60	0
12	HEM	P	501	43/43	0.98	0.10	39,58,68,81	0
12	HEM	P	502	43/43	0.98	0.07	36,50,69,74	0
18	HEC	Q	501	43/43	0.98	0.08	48,60,77,85	0
20	FES	R	501	4/4	0.98	0.05	78,88,91,94	0
18	HEC	D	501	43/43	0.99	0.05	7,31,49,55	0
12	HEM	C	501	43/43	0.99	0.07	23,41,51,66	0
12	HEM	C	502	43/43	0.99	0.07	21,39,48,59	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.

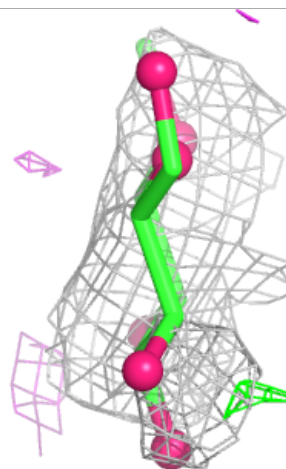
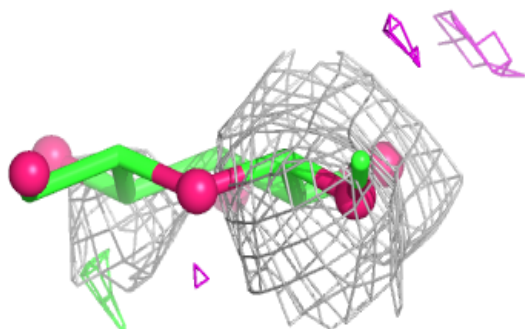
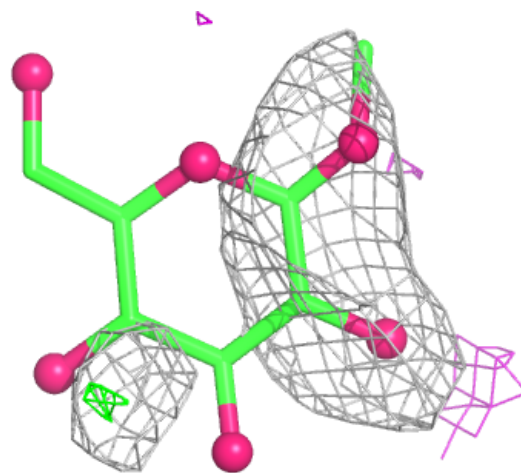
Electron density around BOG Q 504:

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



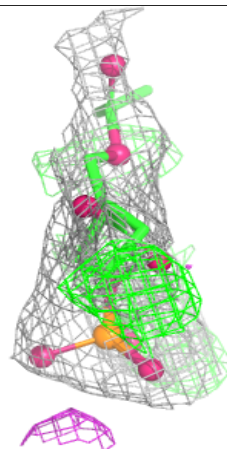
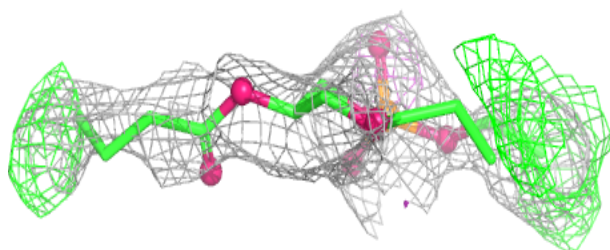
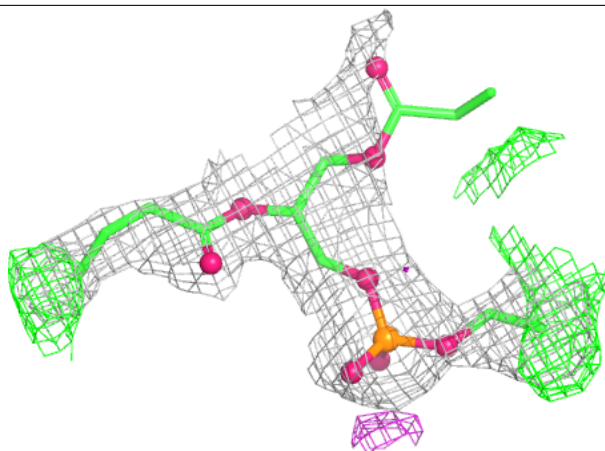
Electron density around BOG D 503:

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and green (positive)



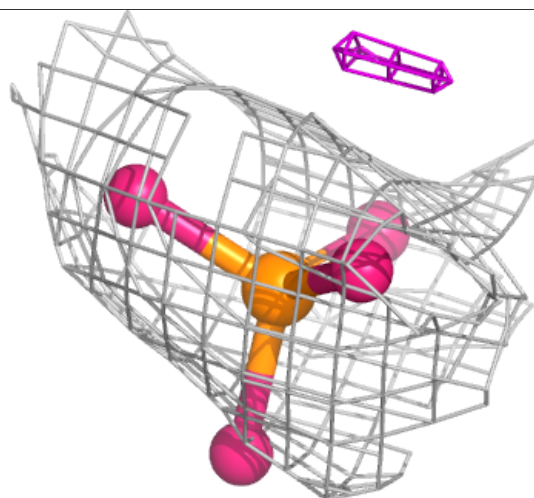
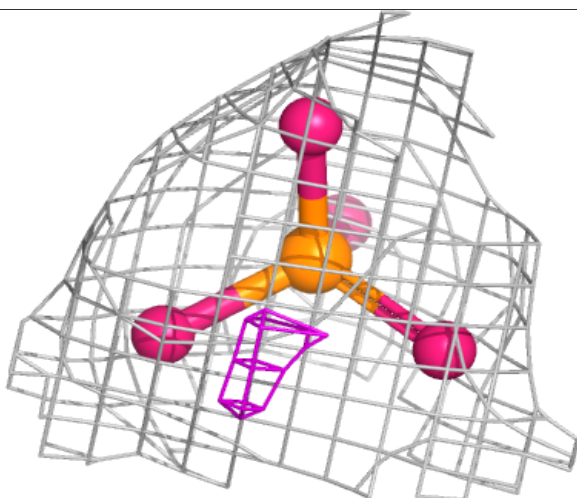
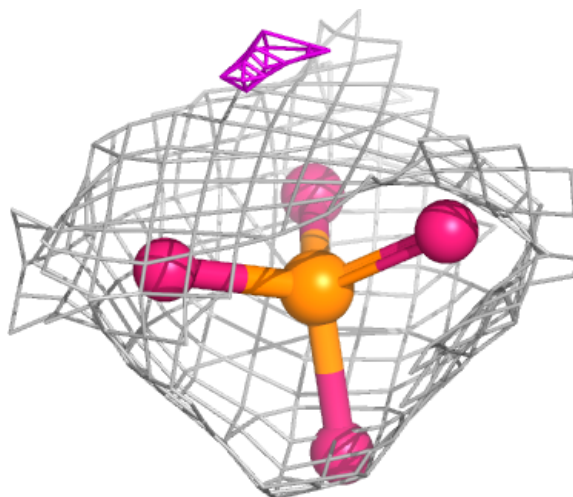
Electron density around PEE C 507:

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and green (positive)



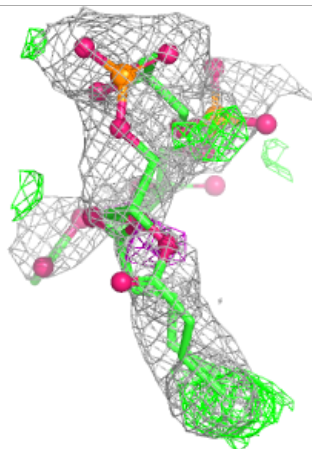
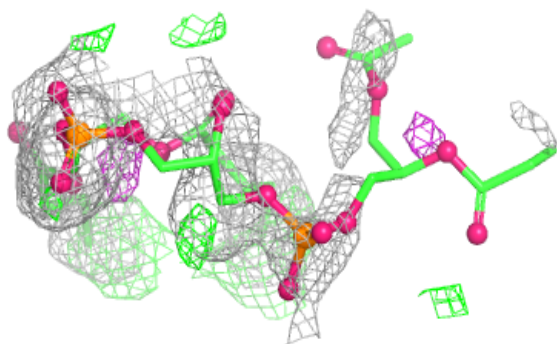
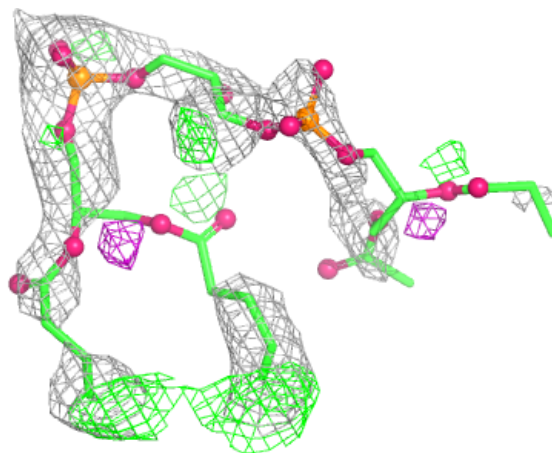
Electron density around PEE N 502:

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and green (positive)



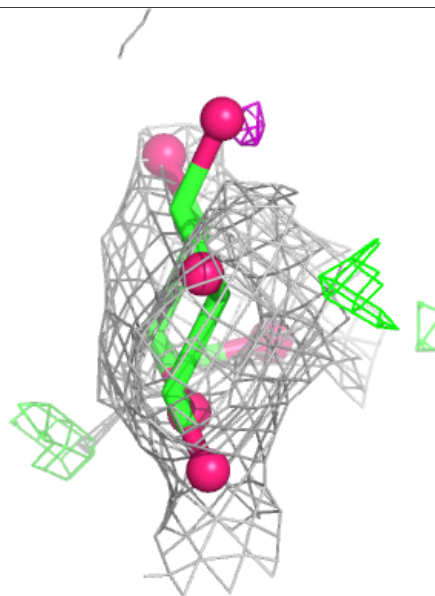
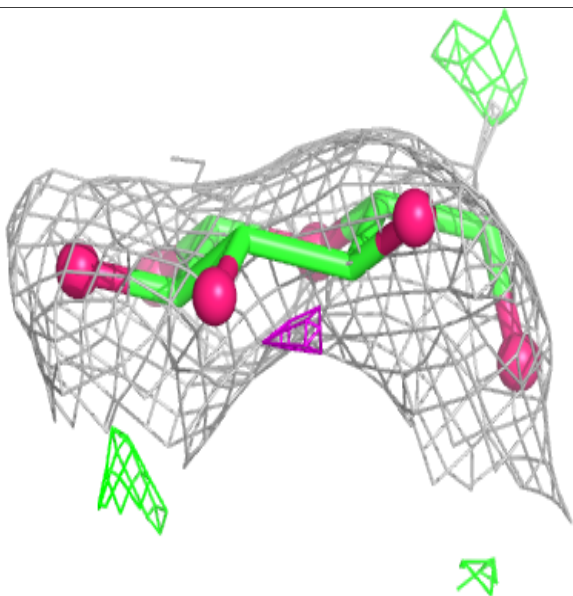
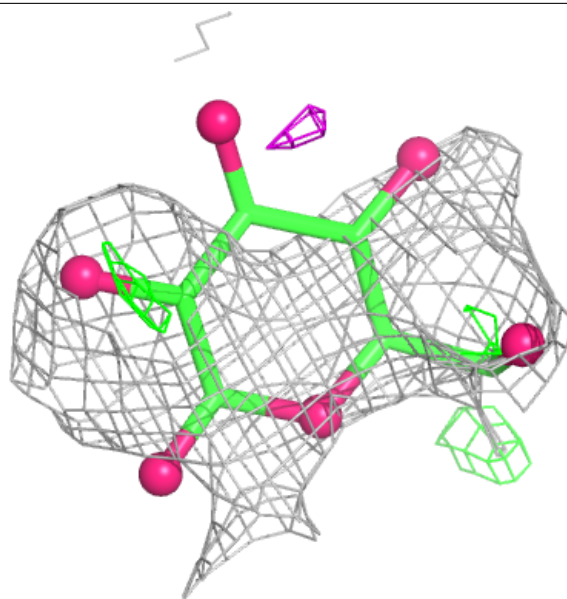
Electron density around CDL Q 502:

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and green (positive)



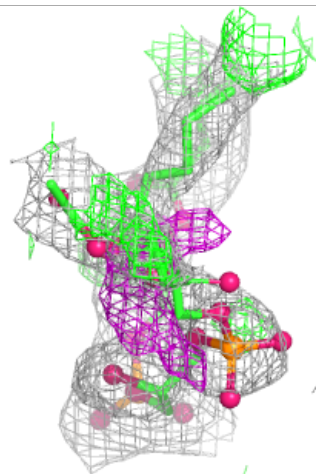
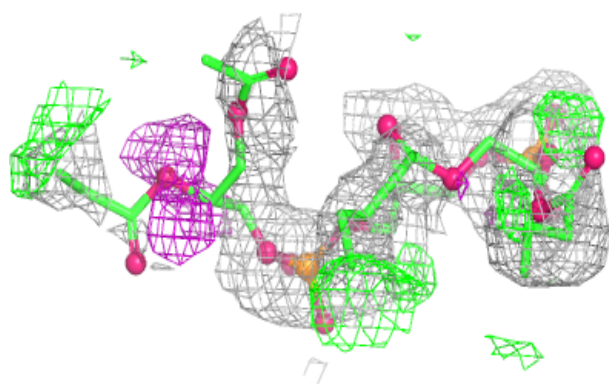
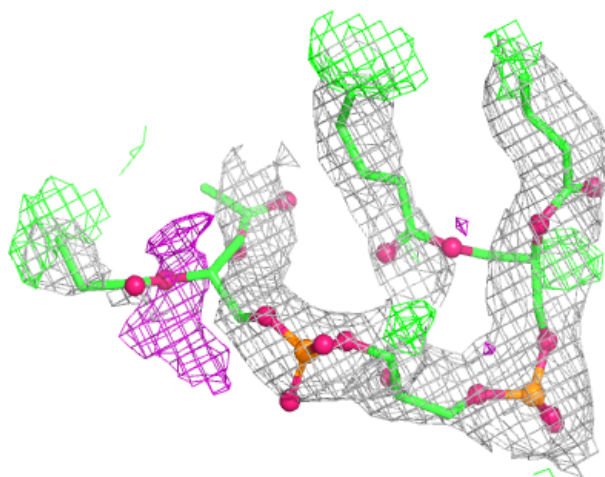
Electron density around BOG P 503:

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and green (positive)



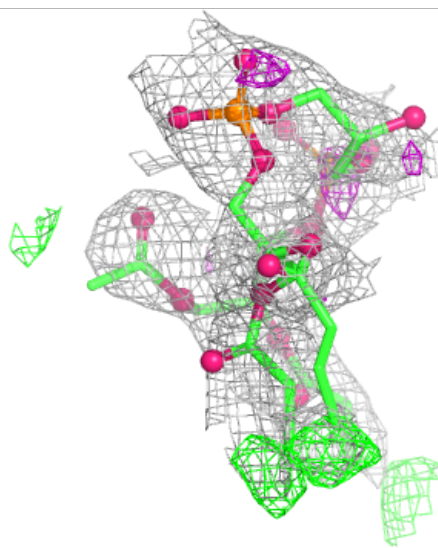
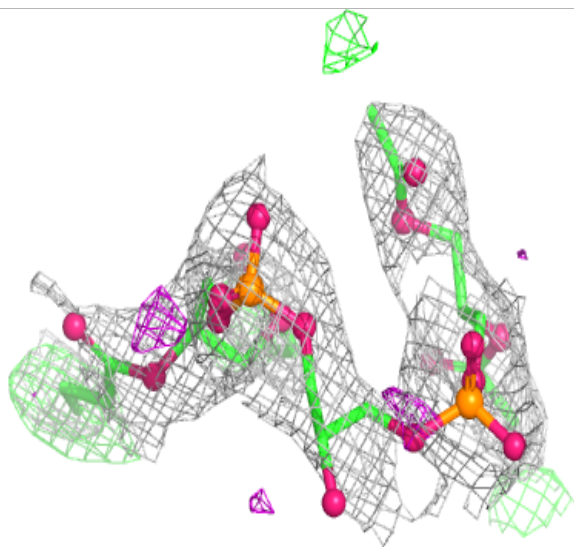
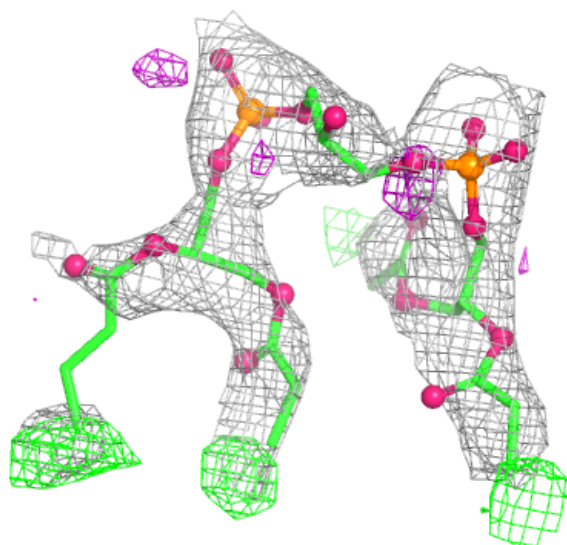
Electron density around CDL C 505:

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and green (positive)



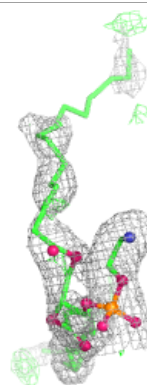
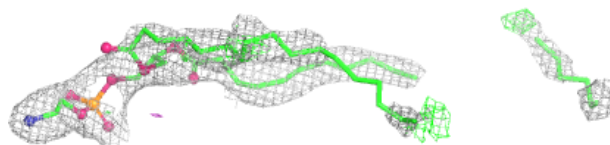
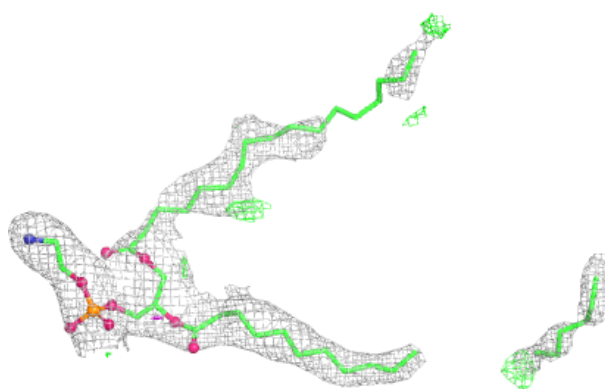
Electron density around CDL P 506:

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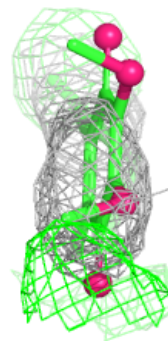
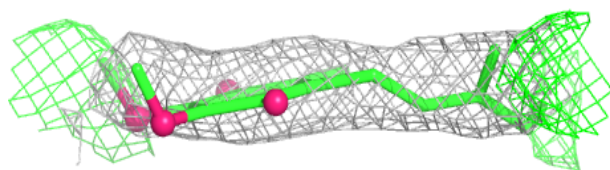
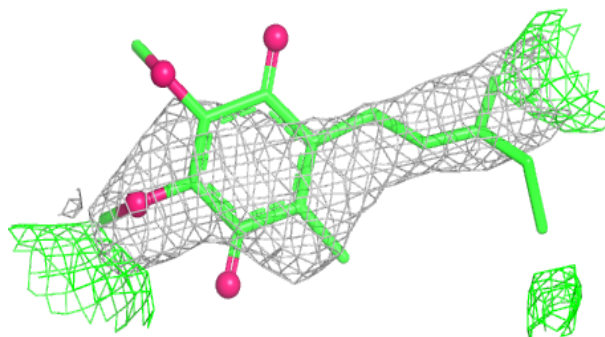


Electron density around PEE R 502:

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and green (positive)

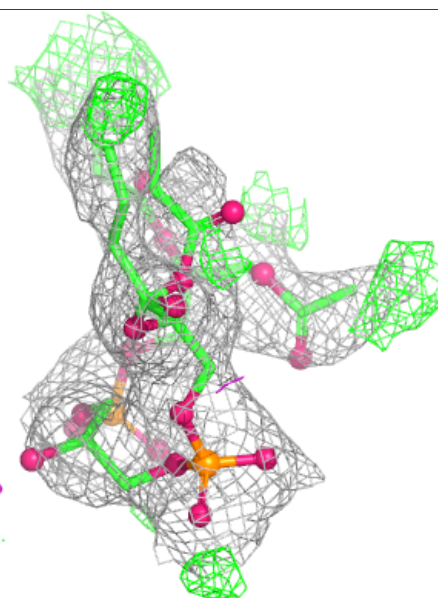
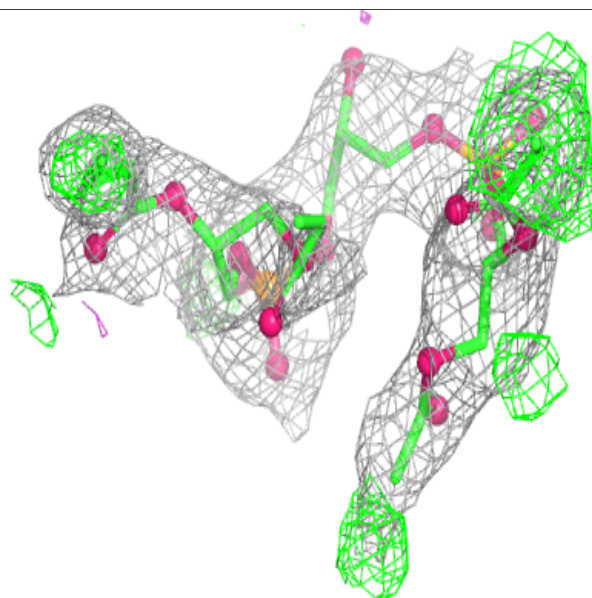
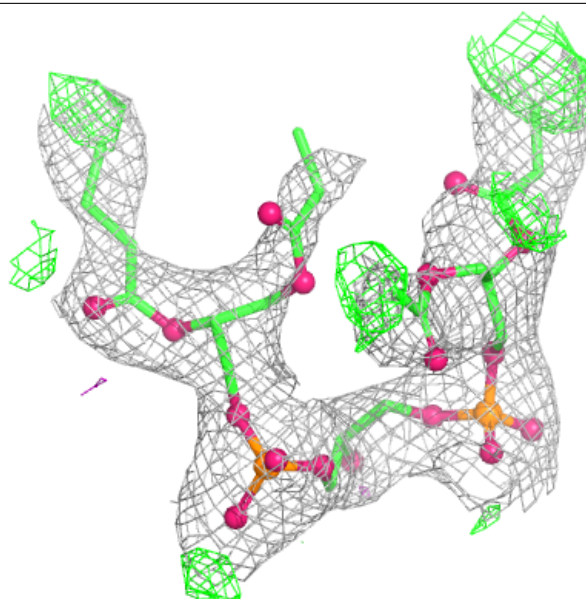
**Electron density around UQ P 505:**

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and green (positive)



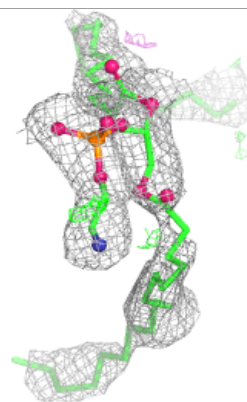
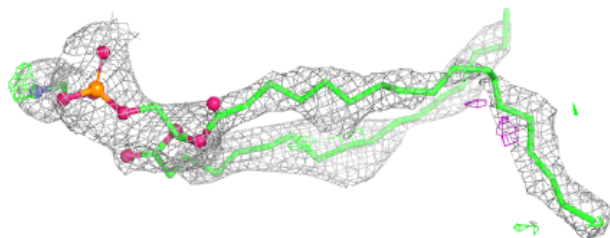
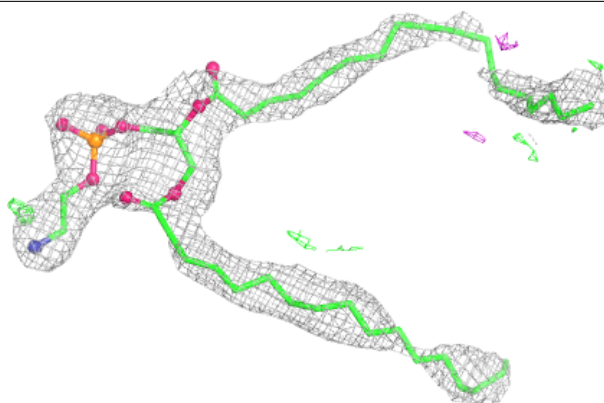
Electron density around CDL G 101:

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and green (positive)

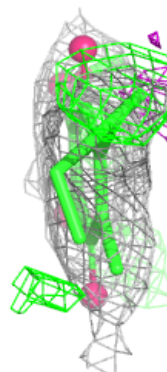
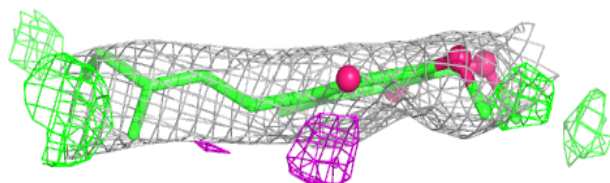
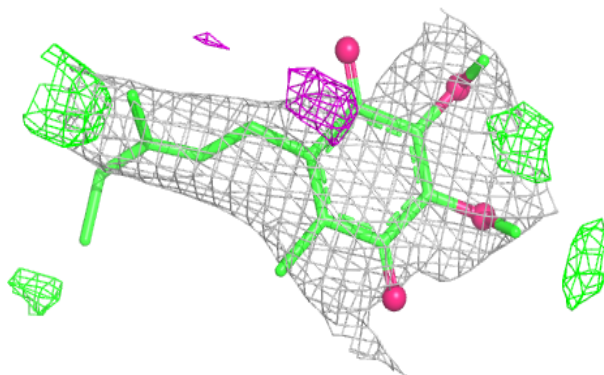


Electron density around PEE E 502:

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and green (positive)

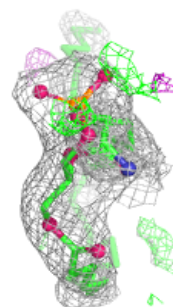
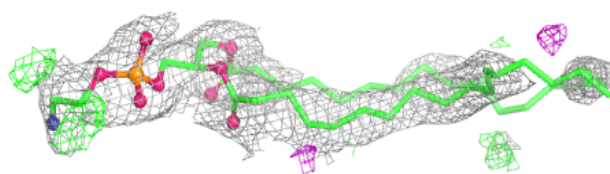
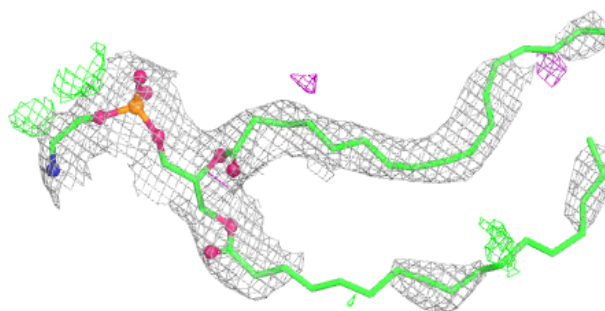
**Electron density around UQ C 504:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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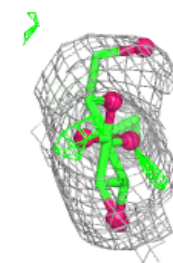
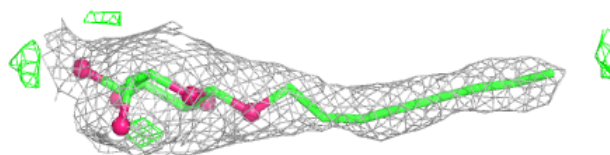
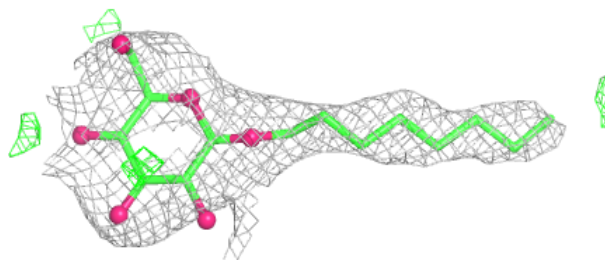


Electron density around PEE P 507:

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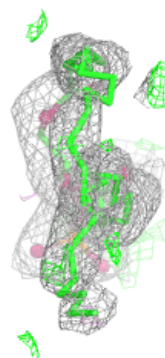
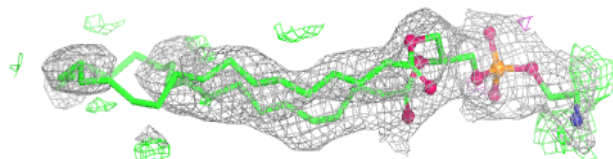
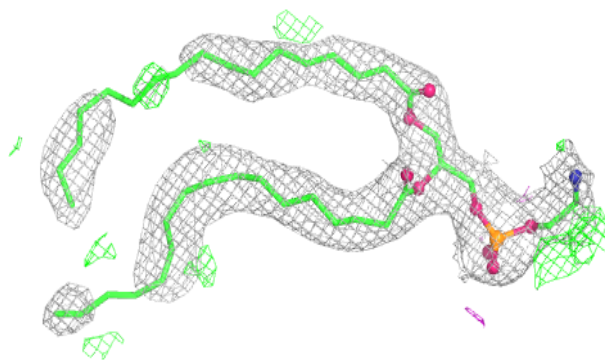
**Electron density around BOG Q 503:**

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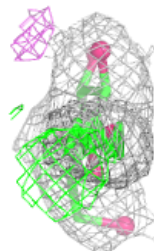
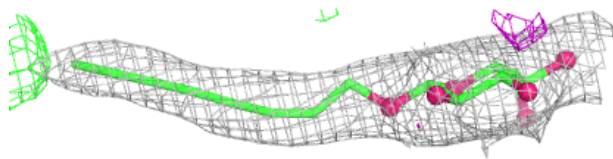
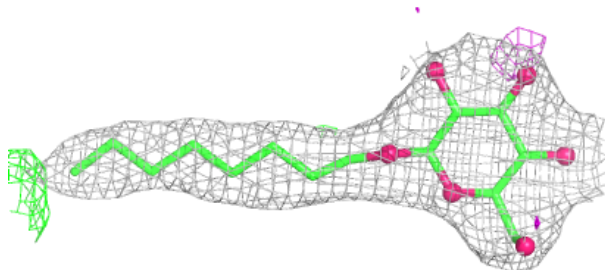


Electron density around PEE C 506:

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and green (positive)

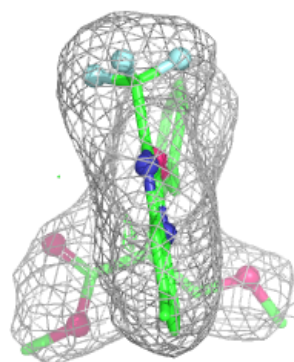
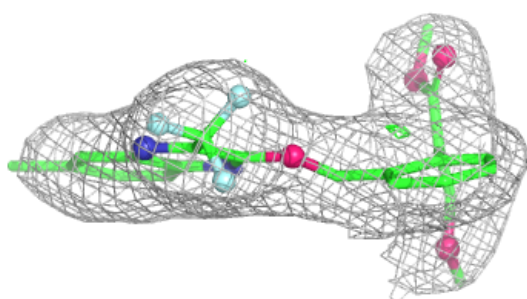
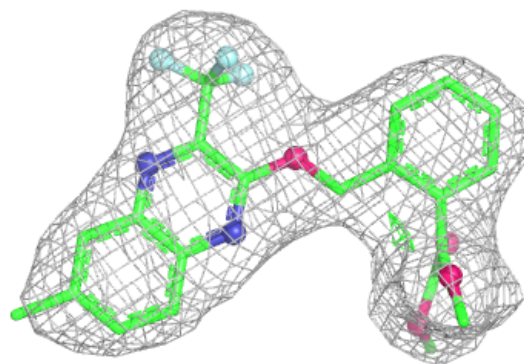
**Electron density around BOG D 502:**

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and green (positive)

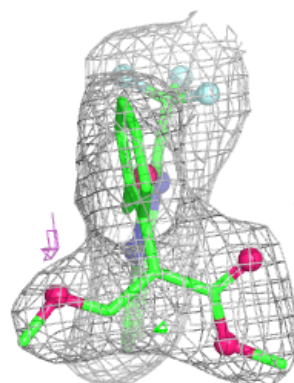
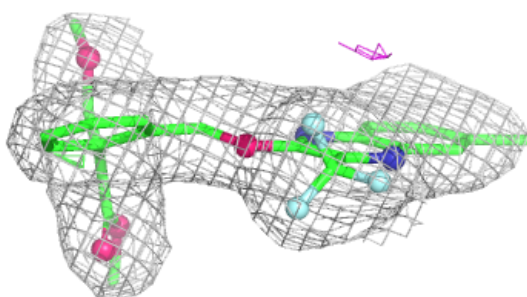
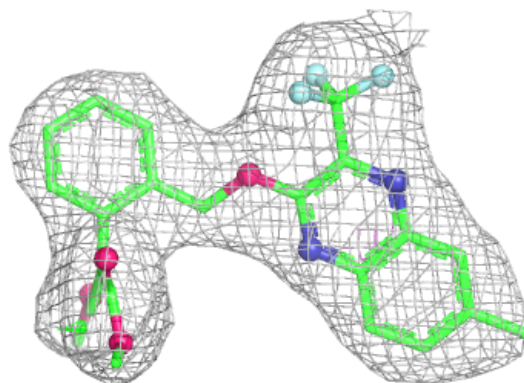


Electron density around WF3 P 504:

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

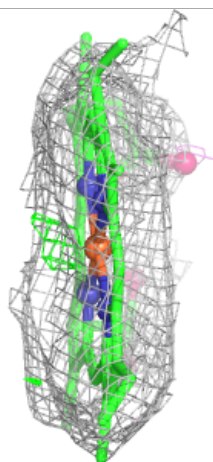
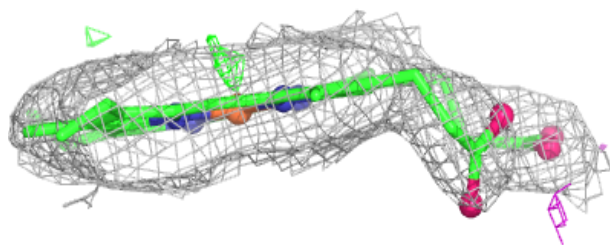
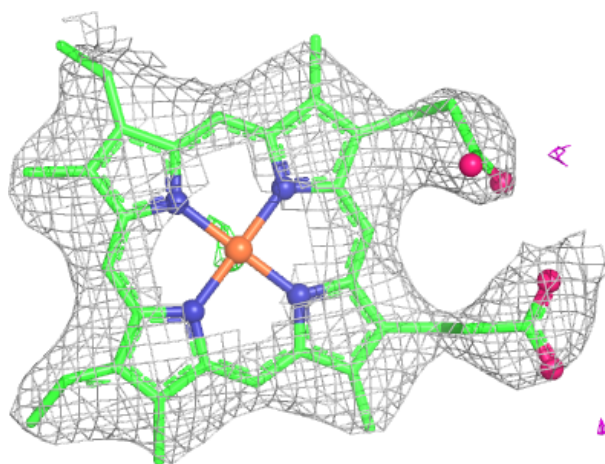
**Electron density around WF3 C 503:**

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



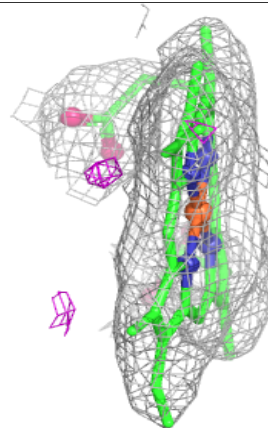
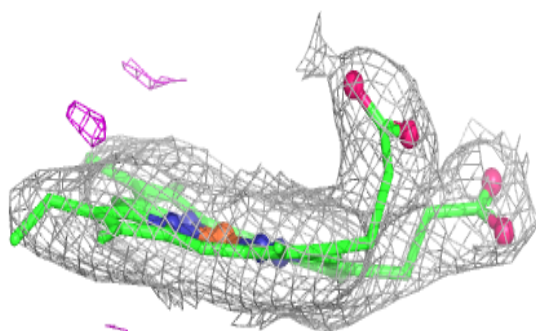
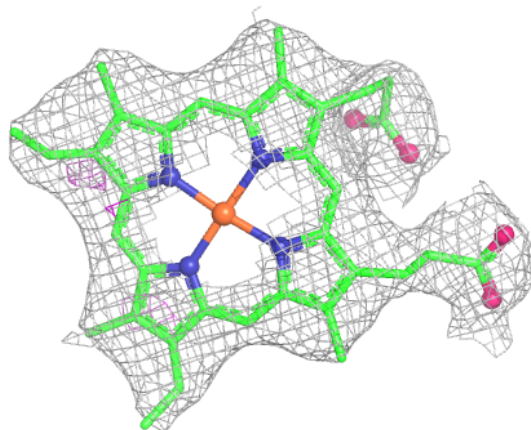
Electron density around HEM P 501:

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



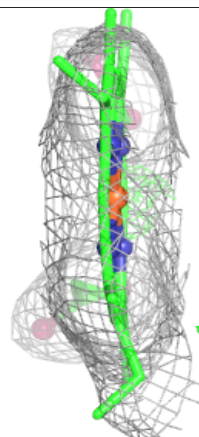
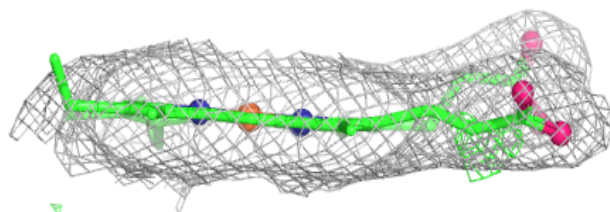
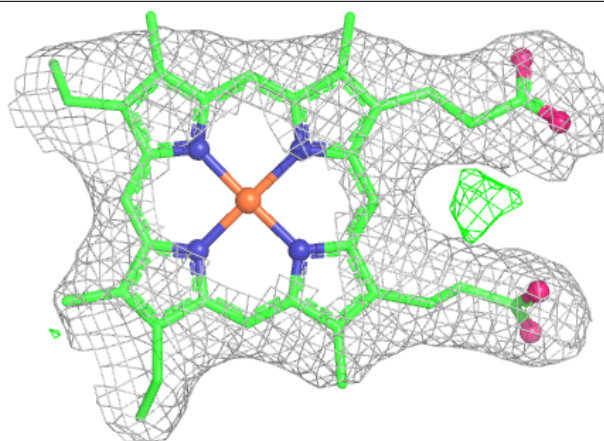
Electron density around HEM P 502:

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



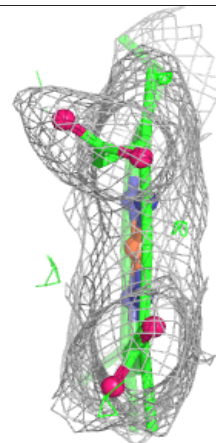
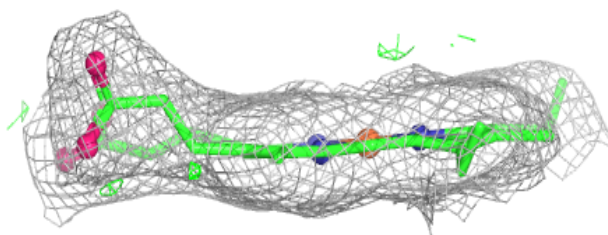
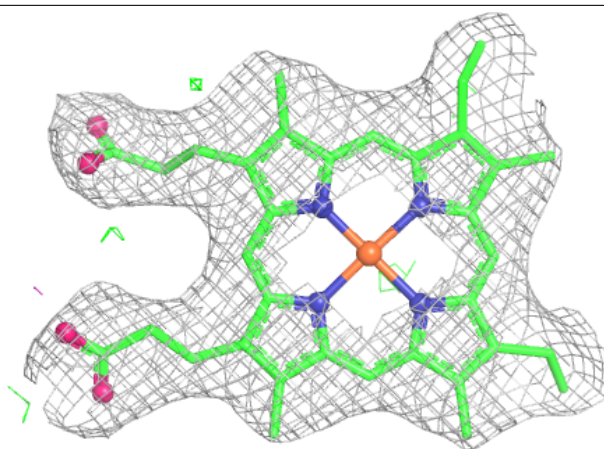
Electron density around HEC Q 501:

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



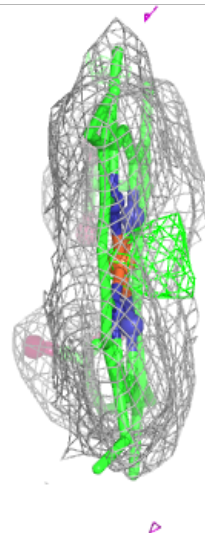
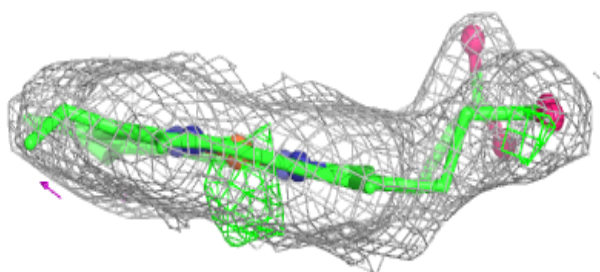
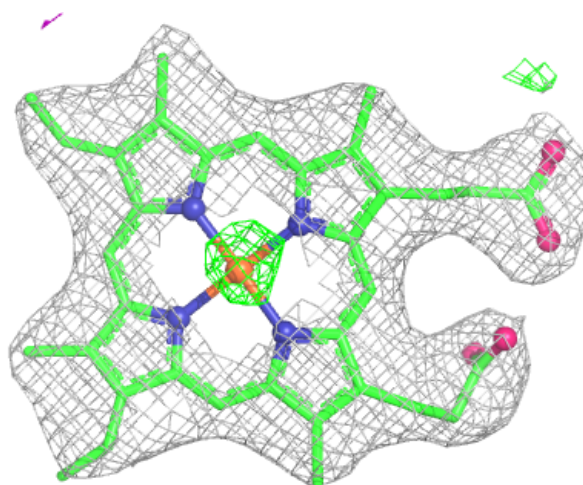
Electron density around HEC D 501:

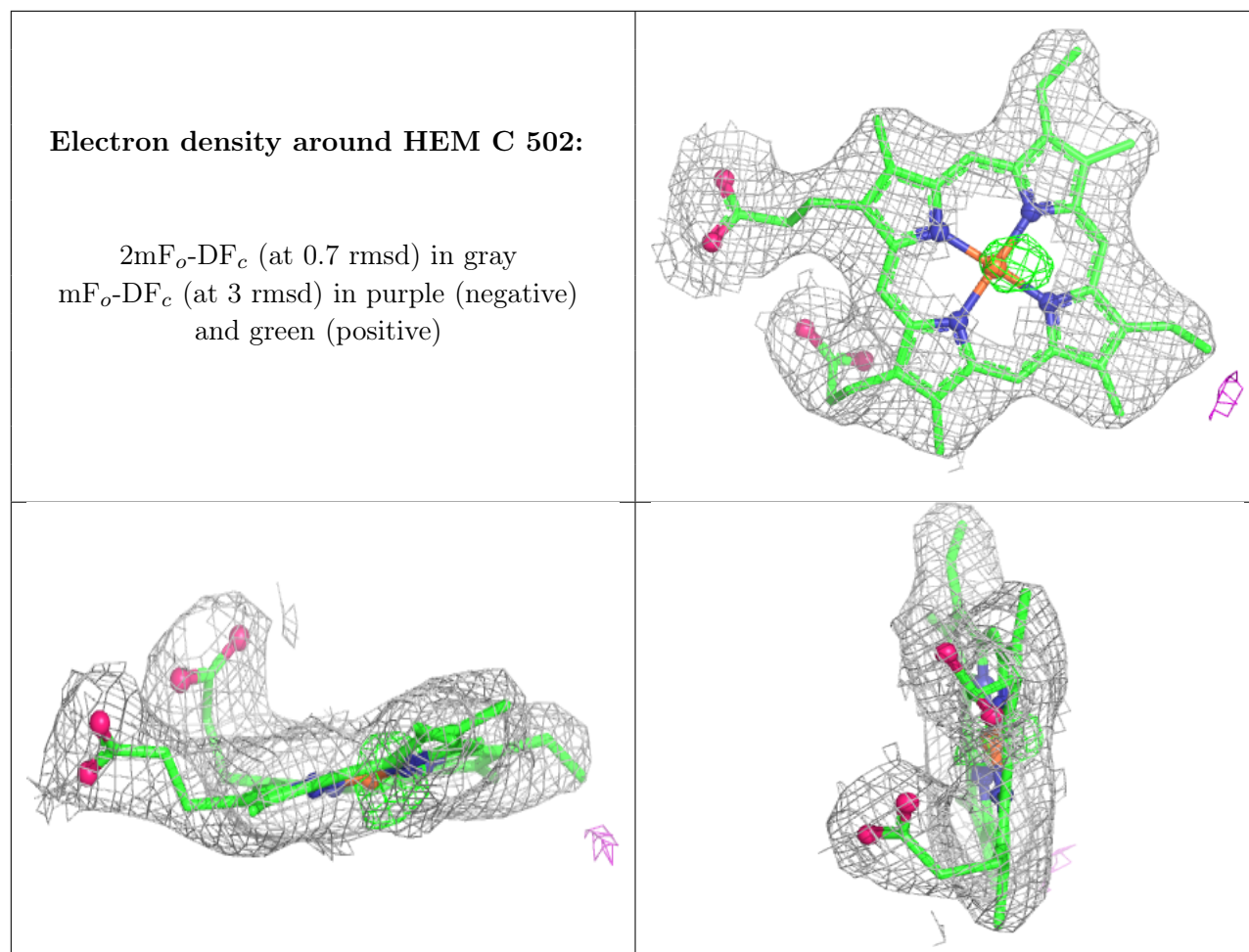
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.