



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:04 AM BST

PDB ID : 3L74
Title : Cytochrome BC1 complex from chicken with famoxadone bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-28
Resolution : 2.76 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

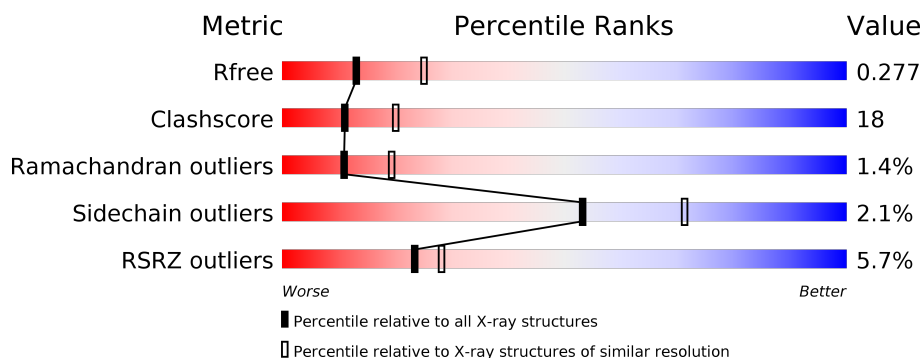
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>35%</div> <div>..</div> </div> </div>
1	N	446	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>36%</div> <div>..</div> </div> </div>
2	B	441	<div> <div>5%</div> <div> <div></div> <div>54%</div> <div>39%</div> <div>• 5%</div> </div> </div>
2	O	441	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>38%</div> <div>• •</div> </div> </div>
3	C	380	<div> <div></div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>
3	P	380	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>•</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PEE	N	3008	-	X	-	-
12	UNL	C	2046	-	-	-	X
12	UNL	P	3013	-	-	-	X
12	UNL	P	3014	-	-	-	X
12	UNL	P	3046	-	-	-	X
17	BOG	D	2091	-	-	-	X
17	BOG	P	2010	-	-	-	X
17	BOG	Q	3091	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32703 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	1
			3440	2155	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
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, 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
			1512	952	262	292	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	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	78	Total	C	N	O	0	0	0
			654	428	116	110			

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

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

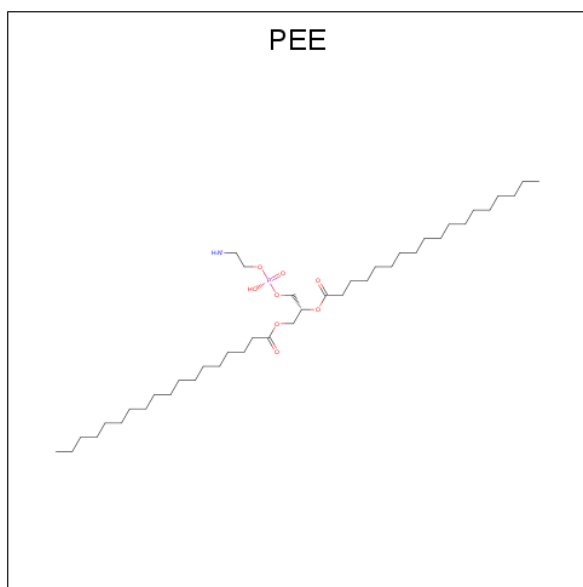
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			288	172	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

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

- Molecule 11 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
11	C	1	Total	C	O	P		0	0
			21	12	8	1			
11	N	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

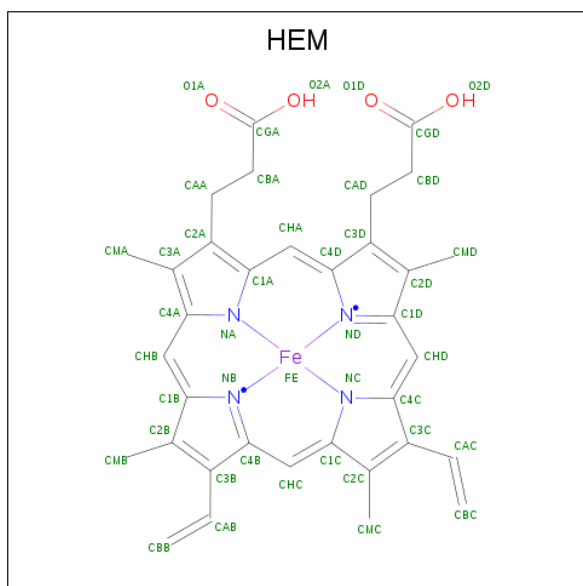
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	P	5	Total 7 7	0	0

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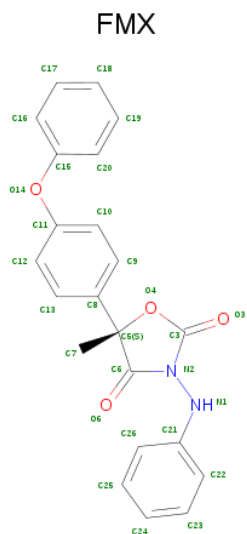
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	Q	1	Total	O	0	0
			1	1		
12	A	1	Total	O	0	0
			1	1		
12	C	3	Total	O	0	0
			5	5		
12	E	1	Total	O	0	0
			2	2		

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



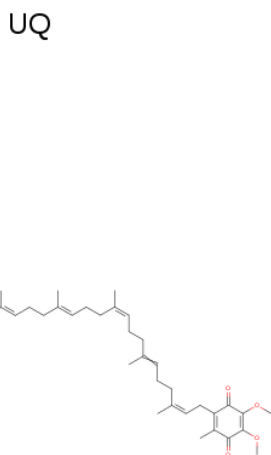
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 14 is FAMOXADONE (three-letter code: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total 28	C 22	N 2	O 4	0	0
14	P	1	Total 28	C 22	N 2	O 4	0	0

- Molecule 15 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



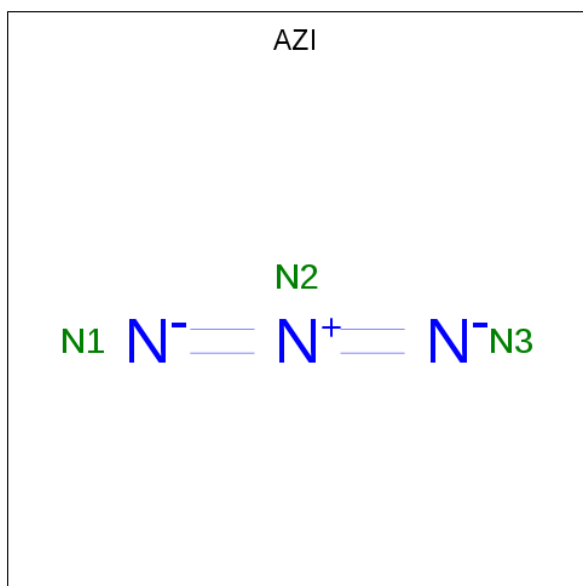
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			19	15	4		

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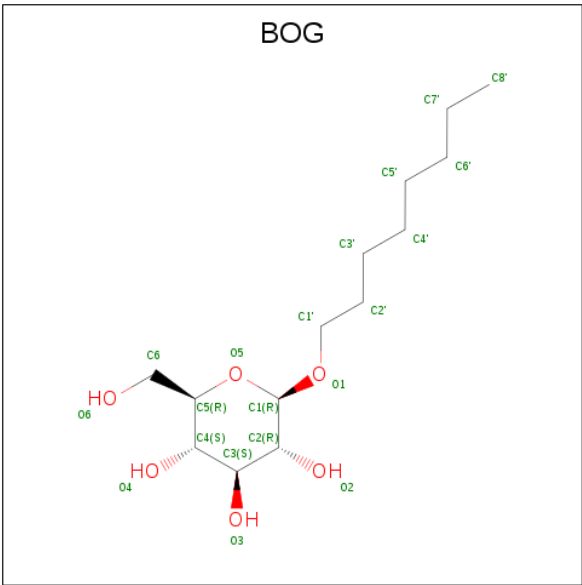
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 16 is AZIDE ION (three-letter code: AZI) (formula: N₃).



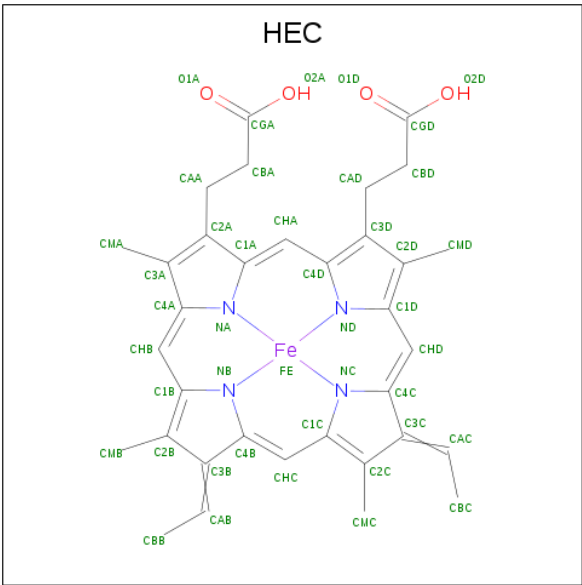
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	N	0	0
			3	3		
16	P	1	Total	N	0	0
			3	3		

- Molecule 17 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



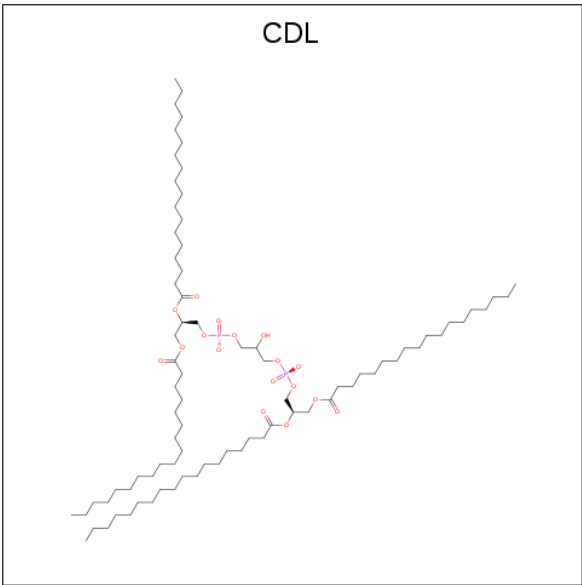
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			12	10	2		
17	D	1	Total	C	O	0	0
			20	14	6		
17	D	1	Total	C	O	0	0
			20	14	6		
17	P	1	Total	C	O	0	0
			19	13	6		
17	Q	1	Total	C	O	0	0
			20	14	6		
17	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 18 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



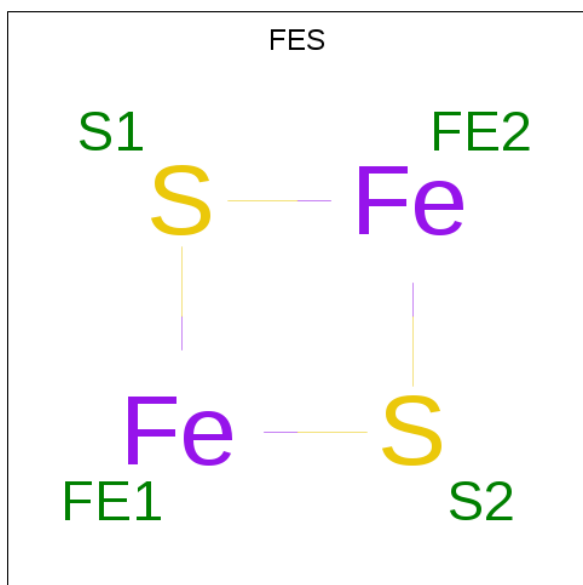
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	O	P	0	0
			42	23	17	2		
19	G	1	Total	C	O	P	0	0
			40	21	17	2		

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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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		

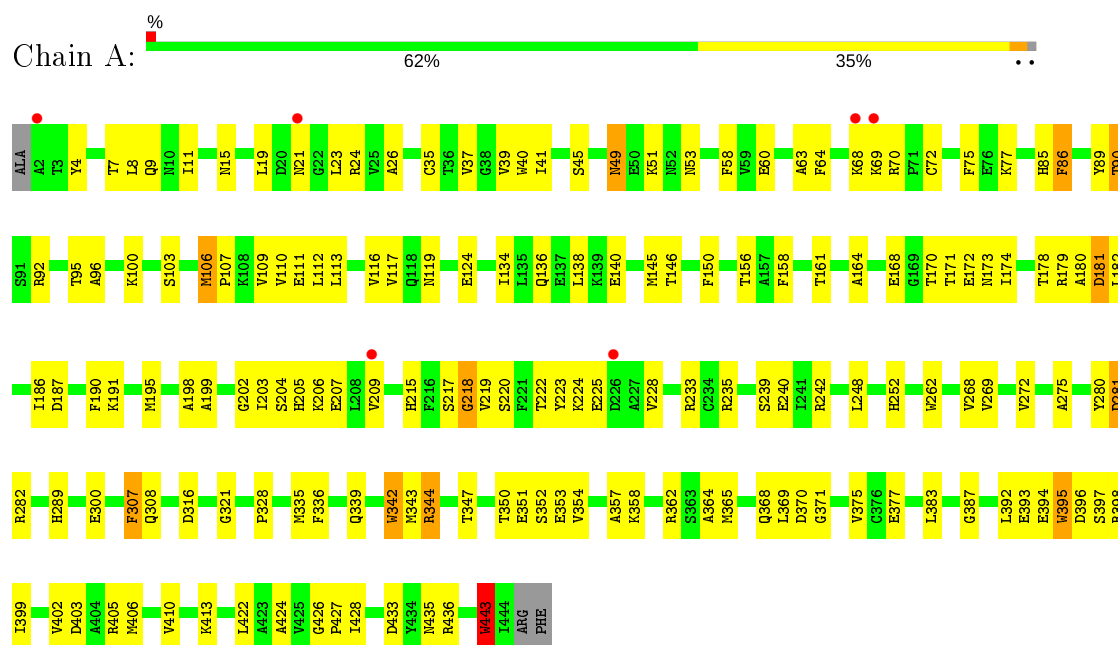
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	O	0	0
			2	2		
21	C	9	Total	O	0	0
			9	9		
21	E	1	Total	O	0	0
			1	1		
21	P	12	Total	O	0	0
			12	12		
21	R	4	Total	O	0	0
			4	4		

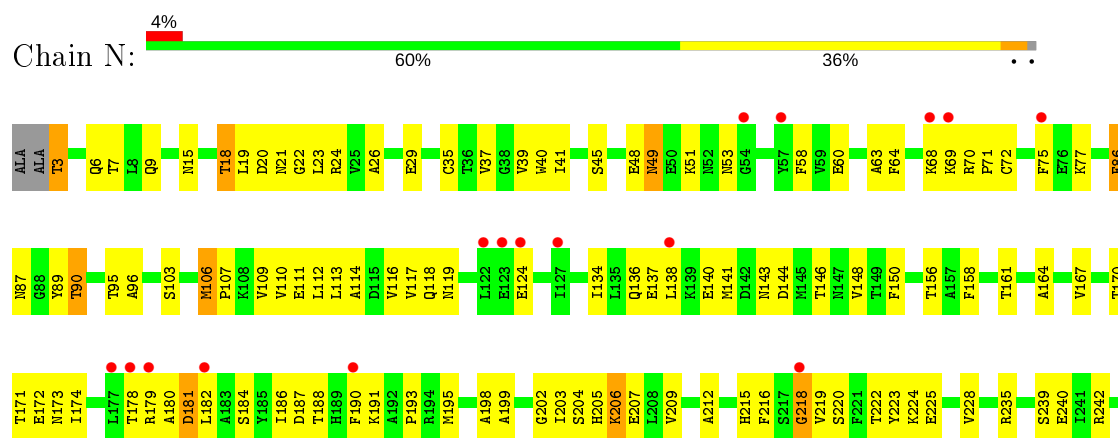
3 Residue-property plots [i](#)

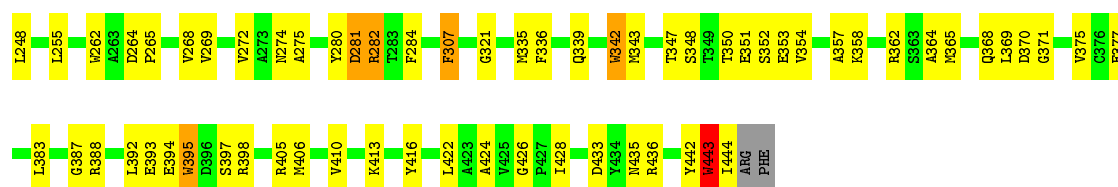
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

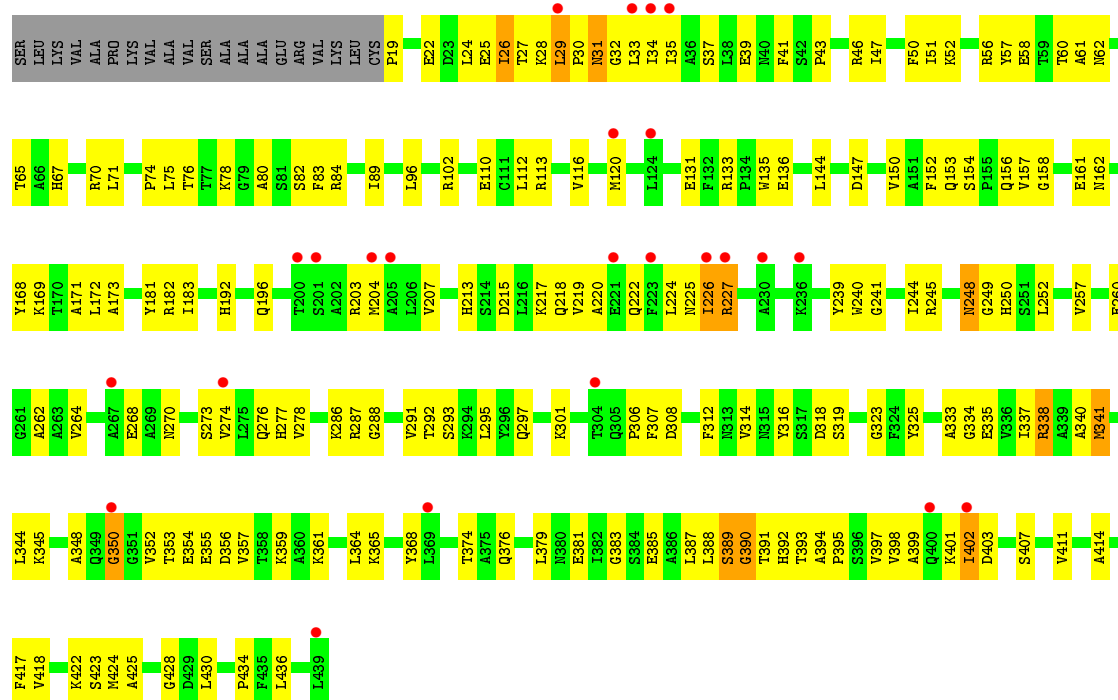


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

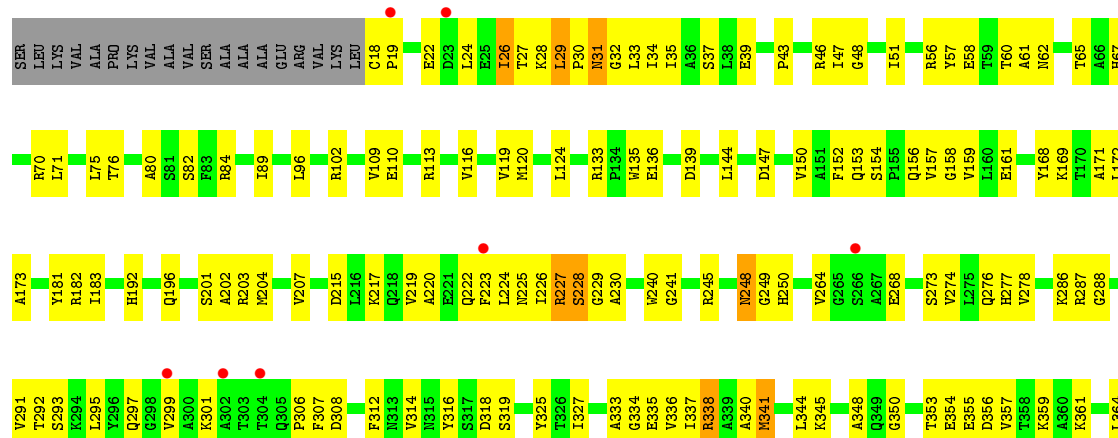




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

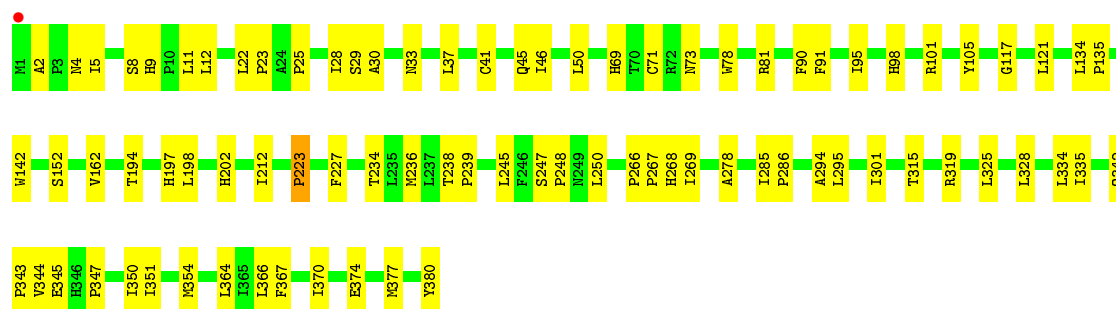


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

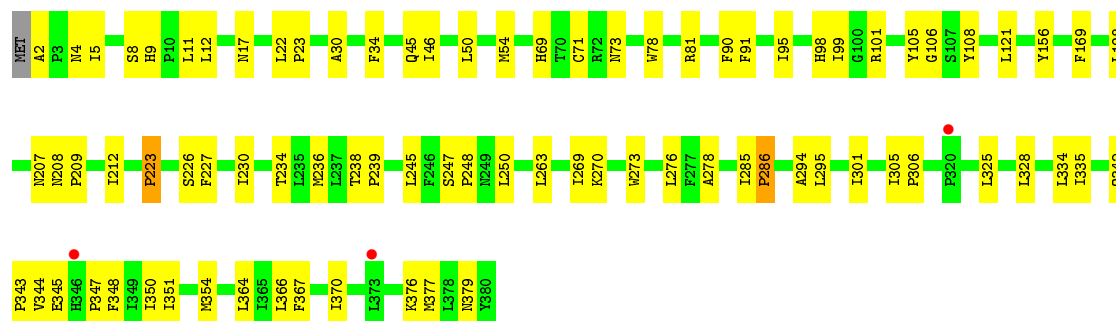
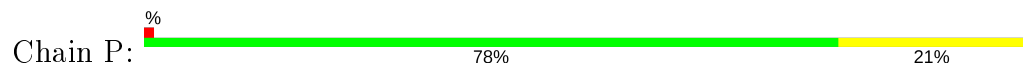




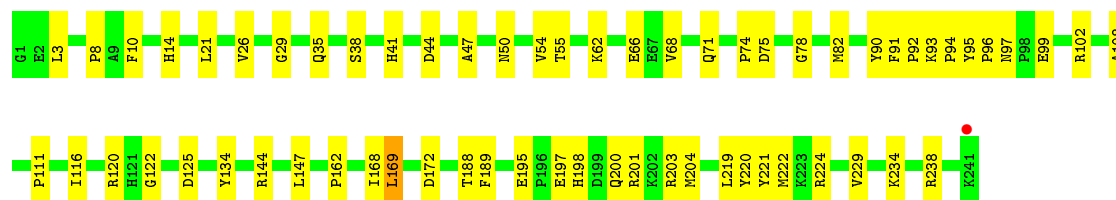
• Molecule 3: CYTOCHROME B



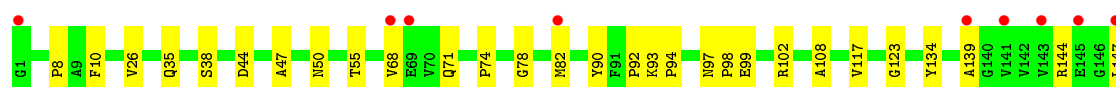
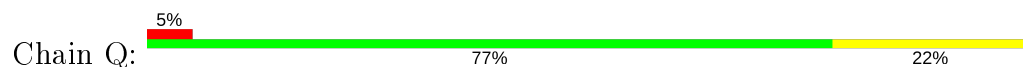
• Molecule 3: CYTOCHROME B



• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

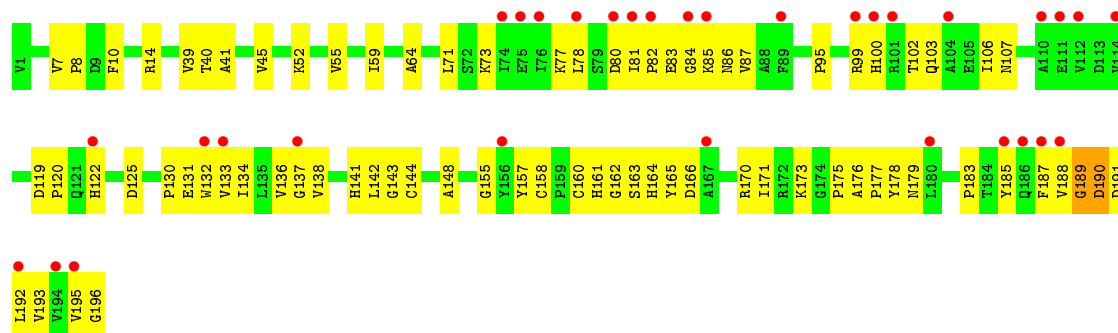


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

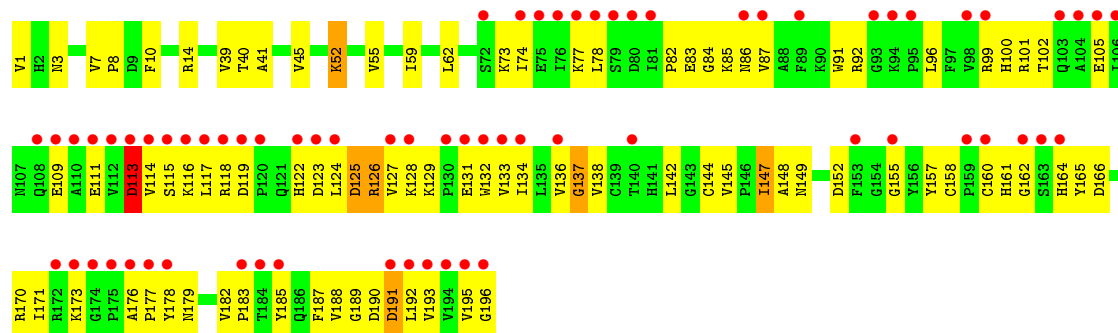




- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, 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



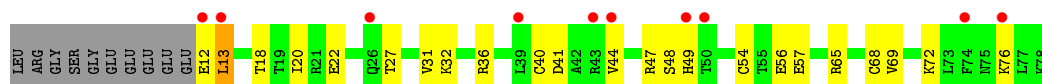
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



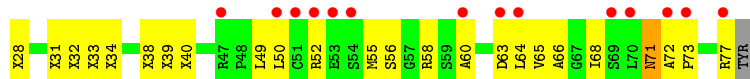
- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

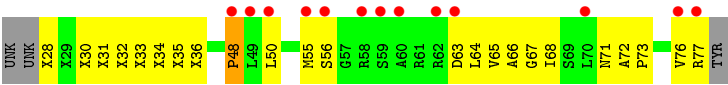


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

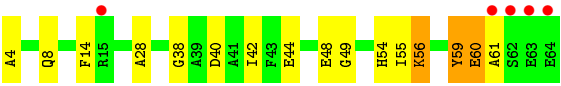


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

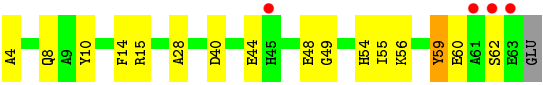




● Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



● 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	171.89Å 181.69Å 240.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.66 – 2.76 58.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.66-2.76) 96.6 (58.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.286 0.247 , 0.277	Depositor DCC
R_{free} test set	3886 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32703	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: AZI, FMX, CDL, UQ, FES, HEC, PEE, UNL, HEM, BOG

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	0.43	0/3511	0.63	0/4757
1	N	0.42	0/3508	0.63	0/4753
2	B	0.36	0/3196	0.59	0/4334
2	O	0.38	0/3202	0.62	1/4343 (0.0%)
3	C	0.51	0/3119	0.65	0/4270
3	P	0.45	0/3114	0.63	0/4263
4	D	0.46	0/1956	0.63	0/2658
4	Q	0.38	0/1956	0.60	0/2658
5	E	0.37	0/1547	0.60	1/2103 (0.0%)
5	R	0.35	0/1545	0.57	0/2098
6	F	0.53	0/911	0.66	0/1219
6	S	0.40	0/911	0.60	0/1219
7	G	0.49	0/698	0.67	0/946
7	T	0.44	0/676	0.64	0/918
8	H	0.44	0/582	0.60	0/779
8	U	0.31	0/561	0.54	0/751
9	I	0.35	0/218	0.62	0/293
9	V	0.35	0/218	0.59	0/293
10	J	0.42	0/508	0.59	0/682
10	W	0.43	0/490	0.56	0/660
All	All	0.42	0/32427	0.62	2/43997 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	227	ARG	N-CA-C	5.49	125.83	111.00
5	E	143	GLY	N-CA-C	5.23	126.18	113.10

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	3440	0	3353	141	0
1	N	3437	0	3349	154	0
2	B	3141	0	3142	195	0
2	O	3147	0	3146	180	0
3	C	3017	0	3063	78	0
3	P	3012	0	3058	77	0
4	D	1898	0	1846	50	0
4	Q	1898	0	1846	47	0
5	E	1513	0	1478	64	0
5	R	1512	0	1476	84	0
6	F	891	0	893	14	0
6	S	891	0	893	25	0
7	G	676	0	659	27	0
7	T	654	0	641	25	0
8	H	574	0	548	13	0
8	U	553	0	535	18	0
9	I	288	0	253	41	0
9	V	278	0	253	30	0
10	J	497	0	490	14	0
10	W	479	0	478	11	0
11	A	50	0	77	0	0
11	C	69	0	83	0	0
11	N	55	0	77	0	0
11	P	48	0	70	0	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	E	2	0	0	0	0
12	P	7	0	0	0	0
12	Q	1	0	0	0	0
13	C	86	0	60	8	0
13	P	86	0	60	7	0
14	C	28	0	18	2	0
14	P	28	0	18	2	0
15	C	19	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	19	0	17	3	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0
17	C	12	0	18	0	0
17	D	40	0	56	3	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	4	0
18	Q	43	0	30	2	0
19	D	42	0	28	2	0
19	G	40	0	24	2	0
19	Q	42	0	28	3	0
19	T	40	0	24	1	0
20	E	4	0	0	1	0
20	R	4	0	0	1	0
21	A	2	0	0	0	0
21	C	9	0	0	2	0
21	E	1	0	0	0	0
21	P	12	0	0	2	0
21	R	4	0	0	0	0
All	All	32703	0	32215	1170	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 18.

All (1170) 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)
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.04	1.10
1:A:344:ARG:HB2	1:A:344:ARG:NH1	1.69	1.08
1:N:178:THR:HG22	1:N:180:ALA:H	1.18	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.13	1.07
1:A:178:THR:HG22	1:A:180:ALA:H	1.20	1.04
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.01
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.59	1.00
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.00
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.00
1:N:206:LYS:H	1:N:206:LYS:HD2	1.28	0.98
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.45	0.97
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.44	0.97
1:A:343:MET:O	1:A:347:THR:HG22	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.47	0.96
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.44	0.95
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.14	0.95
2:B:27:THR:HG22	2:B:28:LYS:H	1.29	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.46	0.94
1:N:343:MET:O	1:N:347:THR:HG22	1.64	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.18	0.92
1:N:206:LYS:H	1:N:206:LYS:CD	1.83	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.50	0.91
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.90
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.35	0.89
9:I:64:LEU:HD12	9:I:77:ARG:O	1.73	0.88
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.72	0.88
2:O:27:THR:HG22	2:O:28:LYS:H	1.36	0.88
2:O:376:GLN:HE22	9:V:77:ARG:HH22	1.23	0.86
1:A:178:THR:HB	1:A:181:ASP:OD1	1.76	0.86
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.39	0.85
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.57	0.85
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.12	0.84
1:A:281:ASP:CG	9:I:33:UNK:HB1	1.98	0.83
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.44	0.82
1:N:49:ASN:HD22	1:N:51:LYS:H	1.26	0.82
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.82
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.60	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
1:N:178:THR:HB	1:N:181:ASP:OD1	1.81	0.81
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.44	0.80
2:B:27:THR:HG22	2:B:28:LYS:N	1.96	0.80
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.11	0.80
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.63	0.80
3:C:69:HIS:CD2	3:C:73:ASN:HD22	1.99	0.80
1:N:178:THR:HG22	1:N:180:ALA:N	1.95	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.23	0.78
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.65	0.78
1:N:350:THR:HG22	1:N:352:SER:H	1.49	0.78
2:B:338:ARG:HB2	2:B:338:ARG:HH11	1.48	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
9:I:71:ASN:HD22	9:I:71:ASN:H	1.27	0.78
2:O:31:ASN:ND2	2:O:33:LEU:H	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.97	0.77
1:A:350:THR:HG22	1:A:352:SER:H	1.49	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.81	0.77
1:N:49:ASN:ND2	1:N:51:LYS:H	1.81	0.77
1:A:362:ARG:O	1:A:365:MET:HG2	1.84	0.77
2:B:31:ASN:ND2	2:B:33:LEU:H	1.81	0.77
1:N:22:GLY:O	1:N:193:PRO:HA	1.85	0.77
2:O:248:ASN:HD22	2:O:248:ASN:C	1.88	0.77
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.32	0.77
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.66	0.77
5:R:190:ASP:O	5:R:191:ASP:HB2	1.85	0.77
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.48	0.76
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.65	0.76
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.65	0.76
2:B:248:ASN:HD22	2:B:248:ASN:C	1.88	0.76
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.67	0.76
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.08	0.76
9:I:32:UNK:N	9:I:73:PRO:HG2	1.99	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.84	0.76
1:N:362:ARG:O	1:N:365:MET:HG2	1.85	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.67	0.76
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
2:O:27:THR:HG22	2:O:28:LYS:N	2.01	0.75
1:A:49:ASN:HD22	1:A:51:LYS:H	1.34	0.75
1:N:19:LEU:O	1:N:21:ASN:N	2.19	0.75
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.50	0.75
1:A:344:ARG:HH11	1:A:344:ARG:CB	1.94	0.75
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.21	0.74
3:P:269:ILE:HG23	14:P:3001:FMX:H231	1.68	0.74
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.74
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.70	0.74
2:B:76:THR:HG22	2:B:82:SER:N	1.98	0.74
2:B:264:VAL:HG23	2:B:316:TYR:C	2.08	0.74
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.70	0.74
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.70	0.73
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.69	0.73
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.70	0.73
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.73
1:N:205:HIS:HB3	1:N:206:LYS:NZ	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.73
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.73
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.70	0.73
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.88	0.73
3:P:101:ARG:C	3:P:101:ARG:HD2	2.10	0.73
9:I:71:ASN:N	9:I:71:ASN:HD22	1.87	0.72
2:B:47:ILE:HD13	2:B:120:MET:CE	2.19	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.52	0.72
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.55	0.72
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.71	0.72
2:B:227:ARG:NE	2:B:227:ARG:HA	2.05	0.72
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.72
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.72	0.72
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.20	0.71
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.72	0.71
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.24	0.71
7:G:48:VAL:O	7:G:51:PRO:HD2	1.89	0.71
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.71	0.71
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.05	0.71
1:A:49:ASN:ND2	1:A:51:LYS:H	1.89	0.71
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.55	0.70
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.04	0.70
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.73	0.70
5:R:10:PHE:O	5:R:14:ARG:HG3	1.91	0.70
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.06	0.70
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.91	0.69
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.56	0.69
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.74	0.69
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.75	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.06	0.69
1:N:282:ARG:HH21	9:V:36:UNK:CB	2.05	0.69
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.57	0.69
8:U:47:ARG:HG3	8:U:49:HIS:H	1.58	0.69
3:C:245:LEU:O	4:D:201:ARG:HD2	1.92	0.69
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.75	0.68
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.76	0.68
2:B:389:SER:O	2:B:391:THR:HG23	1.92	0.68
1:N:9:GLN:HG2	1:N:393:GLU:OE2	1.93	0.68
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.59	0.68
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.75	0.68
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.75	0.68
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.76	0.68
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.75	0.68
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.68
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.08	0.68
2:B:113:ARG:O	2:B:116:VAL:HG23	1.93	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.29	0.68
1:A:103:SER:HB3	1:A:202:GLY:O	1.94	0.68
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.76	0.67
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.76	0.67
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.60	0.67
2:O:297:GLN:O	2:O:301:LYS:HG3	1.93	0.67
8:H:18:THR:O	8:H:22:GLU:HG3	1.96	0.66
1:N:178:THR:CG2	1:N:180:ALA:H	2.04	0.66
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.94	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
1:A:350:THR:HB	1:A:353:GLU:HG3	1.77	0.66
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.29	0.66
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.59	0.66
2:B:297:GLN:O	2:B:301:LYS:HG3	1.95	0.66
4:D:222:MET:HE1	5:E:40:THR:HG23	1.77	0.66
4:D:204:MET:HG2	17:D:2009:BOG:H5	1.78	0.66
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.95	0.66
7:T:48:VAL:O	7:T:51:PRO:HD2	1.95	0.66
9:V:34:UNK:N	9:V:35:UNK:N	2.44	0.66
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.26	0.65
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.78	0.65
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.96	0.65
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.88	0.65
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.78	0.65
1:A:178:THR:CG2	1:A:180:ALA:H	2.04	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.10	0.65
2:B:27:THR:CG2	2:B:28:LYS:H	2.05	0.65
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.79	0.65
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.78	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.97	0.64
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.79	0.64
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.78	0.64
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.61	0.64
2:O:43:PRO:O	2:O:113:ARG:HG3	1.97	0.64
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.80	0.64
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.32	0.64
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.10	0.64
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.78	0.64
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.80	0.64
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.80	0.64
3:P:9:HIS:HD2	3:P:12:LEU:H	1.43	0.64
2:O:338:ARG:NH1	2:O:338:ARG:HB2	2.12	0.64
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.13	0.64
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.64
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.79	0.64
1:A:7:THR:HG21	2:B:113:ARG:CD	2.27	0.64
3:C:344:VAL:O	3:C:345:GLU:HG3	1.98	0.64
2:O:389:SER:O	2:O:391:THR:HG23	1.97	0.64
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.79	0.63
3:C:101:ARG:C	3:C:101:ARG:HD2	2.18	0.63
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.42	0.63
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.63
1:N:350:THR:HB	1:N:353:GLU:HG3	1.79	0.63
1:A:170:THR:HG22	1:A:171:THR:N	2.12	0.63
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.34	0.63
5:R:122:HIS:O	5:R:125:ASP:HB2	1.99	0.63
1:A:9:GLN:HG2	1:A:393:GLU:OE2	1.97	0.63
2:B:43:PRO:O	2:B:113:ARG:HG3	1.98	0.63
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.61	0.63
3:P:247:SER:OG	3:P:250:LEU:HB2	1.99	0.63
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.64	0.63
3:P:350:ILE:O	3:P:354:MET:HG2	1.99	0.63
10:J:40:ASP:O	10:J:44:GLU:HG3	1.99	0.63
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.33	0.63
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.81	0.63
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.80	0.62
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.81	0.62
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.62
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.62
1:N:187:ASP:O	1:N:191:LYS:HE3	1.98	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.81	0.62
2:B:192:HIS:O	2:B:196:GLN:HG3	1.99	0.62
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.80	0.62
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.63	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
1:N:170:THR:HG22	1:N:171:THR:N	2.15	0.62
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.62
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.00	0.62
9:I:71:ASN:N	9:I:71:ASN:ND2	2.48	0.62
2:O:31:ASN:HD22	2:O:32:GLY:N	1.98	0.62
2:O:338:ARG:CB	2:O:338:ARG:HH11	2.12	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.80	0.62
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.80	0.61
2:B:31:ASN:HD22	2:B:32:GLY:N	1.98	0.61
10:W:40:ASP:O	10:W:44:GLU:HG3	2.00	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.83	0.61
2:O:203:ARG:HD2	2:O:230:ALA:O	1.99	0.61
1:N:112:LEU:O	1:N:116:VAL:HG23	2.01	0.61
7:T:41:PHE:O	7:T:45:VAL:HG23	2.00	0.61
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.83	0.61
2:O:31:ASN:HD22	2:O:31:ASN:C	2.05	0.61
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.35	0.60
1:A:15:ASN:O	1:A:26:ALA:HA	2.01	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.01	0.60
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.01	0.60
3:C:269:ILE:HG23	14:C:2001:FMX:H231	1.82	0.60
2:O:381:GLU:OE1	2:O:381:GLU:HA	2.01	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.83	0.60
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.83	0.60
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.83	0.60
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.02	0.60
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.35	0.60
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.60
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.65	0.60
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.65	0.60
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.83	0.60
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.35	0.60
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:O	2:B:292:THR:HG22	2.01	0.60
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.15	0.60
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.17	0.60
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.37	0.60
2:B:31:ASN:HD22	2:B:31:ASN:C	2.04	0.59
1:N:103:SER:HB3	1:N:202:GLY:O	2.02	0.59
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.84	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.02	0.59
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.42	0.59
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.59
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.59
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.84	0.59
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.33	0.59
1:N:410:VAL:O	1:N:413:LYS:HB3	2.02	0.59
1:A:187:ASP:O	1:A:191:LYS:HE3	2.02	0.59
1:A:49:ASN:HD22	1:A:51:LYS:N	2.01	0.59
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.84	0.59
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.85	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.03	0.59
5:R:147:ILE:HG22	5:R:148:ALA:N	2.18	0.59
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.43	0.59
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.84	0.59
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.43	0.59
7:G:71:ARG:NH1	8:H:56:GLU:OE1	2.33	0.59
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.16	0.59
8:H:65:ARG:O	8:H:69:VAL:HG23	2.03	0.59
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.17	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.03	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
2:B:226:ILE:O	2:B:226:ILE:HG23	2.03	0.58
1:N:21:ASN:HB2	1:N:218:GLY:O	2.04	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
8:U:47:ARG:HD3	8:U:48:SER:H	1.68	0.58
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.33	0.58
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.04	0.58
2:O:150:VAL:O	2:O:153:GLN:HG3	2.04	0.58
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.86	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.86	0.58
1:A:350:THR:HG22	1:A:352:SER:N	2.18	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.58
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.38	0.58
1:A:272:VAL:O	1:A:275:ALA:HB3	2.04	0.57
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.86	0.57
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.86	0.57
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.57
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.70	0.57
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.84	0.57
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.57
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.57
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.18	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
2:B:422:LYS:O	2:B:436:LEU:HD21	2.05	0.57
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.57
2:O:361:LYS:O	2:O:365:LYS:HG3	2.03	0.57
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.86	0.57
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.19	0.57
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.39	0.57
2:O:308:ASP:OD2	9:V:55:MET:O	2.21	0.57
10:W:4:ALA:O	10:W:8:GLN:HG3	2.04	0.57
2:O:273:SER:O	2:O:276:GLN:HB3	2.04	0.57
2:B:52:LYS:HE2	2:B:388:LEU:HD23	1.86	0.57
2:O:154:SER:O	2:O:157:VAL:HG12	2.04	0.57
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.86	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.57
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.88	0.56
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.56
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.53	0.56
3:P:101:ARG:O	3:P:101:ARG:HD2	2.06	0.56
2:B:338:ARG:CB	2:B:338:ARG:HH11	2.18	0.56
9:I:49:LEU:O	9:I:50:LEU:HD23	2.05	0.56
5:R:126:ARG:HB3	5:R:182:VAL:HG21	1.87	0.56
2:B:353:THR:HB	2:B:356:ASP:CG	2.25	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.26	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.88	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.87	0.56
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.71	0.56
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.20	0.56
1:N:383:LEU:O	1:N:387:GLY:HA2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:49:ASN:C	1:N:49:ASN:HD22	2.09	0.56
2:O:308:ASP:OD2	9:V:56:SER:HA	2.06	0.56
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.04	0.56
1:N:394:GLU:O	1:N:397:SER:HB3	2.06	0.56
2:O:376:GLN:NE2	9:V:77:ARG:NH2	2.47	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.86	0.56
5:E:83:GLU:HG2	5:E:102:THR:HA	1.88	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
2:B:273:SER:O	2:B:276:GLN:HB3	2.06	0.56
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.87	0.56
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.06	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.04	0.56
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.69	0.56
1:N:49:ASN:HD22	1:N:51:LYS:N	1.98	0.56
2:O:306:PRO:HG2	9:V:50:LEU:O	2.06	0.56
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.87	0.56
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.71	0.55
4:D:47:ALA:N	4:D:50:ASN:HD22	1.98	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.88	0.55
2:O:341:MET:CE	2:O:417:PHE:HE2	2.18	0.55
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.40	0.55
5:R:115:SER:O	5:R:116:LYS:HG2	2.05	0.55
5:R:126:ARG:H	5:R:126:ARG:HD3	1.71	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.89	0.55
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.47	0.55
3:C:344:VAL:O	3:C:344:VAL:HG23	2.07	0.55
8:H:40:CYS:O	8:H:44:VAL:HG23	2.06	0.55
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.89	0.55
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.06	0.55
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.55
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.07	0.55
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.07	0.55
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.55
2:O:402:ILE:HD13	2:O:402:ILE:C	2.26	0.55
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.42	0.55
8:U:18:THR:O	8:U:22:GLU:HG3	2.05	0.55
2:B:156:GLN:HE22	9:I:77:ARG:C	2.09	0.55
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.18	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.37	0.55
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ALA:HA	4:D:90:TYR:HA	1.89	0.55
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.07	0.55
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
2:B:248:ASN:ND2	2:B:248:ASN:C	2.60	0.54
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.54
2:O:353:THR:HG22	2:O:354:GLU:N	2.22	0.54
3:P:198:LEU:HD21	13:P:502:HEM:HMA3	1.89	0.54
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.42	0.54
1:A:106:MET:O	1:A:106:MET:HE2	2.07	0.54
2:B:26:ILE:O	2:B:26:ILE:HG12	2.07	0.54
5:E:10:PHE:O	5:E:14:ARG:HG3	2.07	0.54
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.89	0.54
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.90	0.54
2:O:202:ALA:HB3	2:O:229:GLY:O	2.07	0.54
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.70	0.54
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.96	0.54
2:B:60:THR:CG2	2:B:61:ALA:N	2.71	0.54
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.41	0.54
5:R:190:ASP:O	5:R:191:ASP:CB	2.55	0.54
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.89	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.43	0.54
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.42	0.54
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.41	0.54
1:N:191:LYS:C	1:N:195:MET:HE2	2.28	0.54
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.54
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.89	0.54
1:A:383:LEU:O	1:A:387:GLY:HA2	2.08	0.54
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.42	0.54
2:B:227:ARG:HE	2:B:227:ARG:HA	1.72	0.54
2:B:361:LYS:O	2:B:365:LYS:HG3	2.08	0.54
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.07	0.54
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.89	0.54
4:Q:241:LYS:OXT	4:Q:241:LYS:HG3	2.07	0.54
5:E:171:ILE:HG12	5:E:176:ALA:O	2.08	0.54
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.54
3:P:286:PRO:HA	21:P:1285:HOH:O	2.08	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
2:B:353:THR:HG22	2:B:354:GLU:N	2.23	0.54
3:C:198:LEU:HD21	13:C:502:HEM:HMA3	1.90	0.54
1:N:350:THR:HG22	1:N:352:SER:N	2.19	0.54
2:O:156:GLN:HE22	9:V:77:ARG:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.48	0.54
1:N:206:LYS:N	1:N:206:LYS:HD2	2.11	0.53
2:B:399:ALA:O	2:B:402:ILE:HG22	2.09	0.53
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.23	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.89	0.53
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.36	0.53
2:B:407:SER:O	2:B:411:VAL:HG23	2.09	0.53
1:N:106:MET:HE2	1:N:106:MET:O	2.09	0.53
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.43	0.53
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.44	0.53
2:O:60:THR:CG2	2:O:61:ALA:N	2.71	0.53
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.44	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.53
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.43	0.53
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.53
2:O:26:ILE:O	2:O:26:ILE:HG12	2.07	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.53
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.90	0.53
9:V:31:UNK:C	9:V:73:PRO:HG2	2.38	0.53
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.09	0.53
2:O:388:LEU:O	2:O:389:SER:HB3	2.09	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.27	0.53
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.09	0.53
1:A:394:GLU:O	1:A:397:SER:HB3	2.09	0.53
1:A:49:ASN:C	1:A:49:ASN:HD22	2.11	0.53
2:B:31:ASN:ND2	2:B:31:ASN:C	2.63	0.53
1:N:347:THR:HG21	1:N:444:ILE:C	2.27	0.53
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.09	0.53
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.53
2:B:157:VAL:HG13	2:B:158:GLY:N	2.24	0.53
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.44	0.53
2:O:353:THR:HB	2:O:356:ASP:CG	2.28	0.52
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.52
8:U:65:ARG:O	8:U:69:VAL:HG23	2.10	0.52
2:O:393:THR:HG23	2:O:397:VAL:HB	1.90	0.52
1:A:219:VAL:HG12	1:A:220:SER:N	2.24	0.52
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.09	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.75	0.52
2:B:393:THR:HG23	2:B:397:VAL:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.44	0.52
1:N:146:THR:O	1:N:150:PHE:HD1	1.92	0.52
1:N:21:ASN:CB	1:N:219:VAL:HA	2.39	0.52
1:N:443:TRP:O	1:N:444:ILE:CB	2.56	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.77	0.52
2:O:33:LEU:HD22	2:O:224:LEU:HD12	1.92	0.52
3:P:34:PHE:HB2	21:P:381:HOH:O	2.09	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.57	0.52
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.74	0.52
2:O:225:ASN:O	2:O:226:ILE:C	2.47	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.90	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
1:A:106:MET:N	1:A:107:PRO:HD2	2.25	0.52
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.52
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.38	0.52
4:Q:38:SER:O	4:Q:94:PRO:HG3	2.09	0.52
2:B:388:LEU:O	2:B:389:SER:HB3	2.10	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.91	0.52
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.92	0.52
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.09	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.42	0.52
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.10	0.52
5:E:103:GLN:O	5:E:107:ASN:ND2	2.43	0.52
5:E:73:LYS:HB3	5:E:195:VAL:O	2.10	0.52
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.45	0.52
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.52
3:P:344:VAL:O	3:P:345:GLU:HG3	2.10	0.52
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.52
5:R:114:VAL:HG13	5:R:122:HIS:HD2	1.75	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.51
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.51
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.92	0.51
3:C:269:ILE:CG2	14:C:2001:FMX:H231	2.40	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.92	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.45	0.51
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:27:THR:HG21	2:O:217:LYS:HE3	1.93	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.40	0.51
2:B:248:ASN:HD22	2:B:249:GLY:N	2.07	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.92	0.51
4:D:71:GLN:HG3	4:D:82:MET:HE2	1.91	0.51
5:E:155:GLY:HA3	5:E:166:ASP:C	2.31	0.51
5:R:101:ARG:CZ	5:R:133:VAL:HB	2.41	0.51
10:J:49:GLY:N	10:J:54:HIS:ND1	2.58	0.51
1:N:191:LYS:CA	1:N:195:MET:HE2	2.41	0.51
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.46	0.51
5:R:52:LYS:HD3	5:R:52:LYS:C	2.30	0.51
1:A:307:PHE:C	1:A:307:PHE:CD1	2.83	0.51
1:A:351:GLU:O	1:A:354:VAL:HG22	2.10	0.51
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.45	0.51
1:N:106:MET:N	1:N:107:PRO:HD2	2.25	0.51
1:A:146:THR:O	1:A:150:PHE:HD1	1.93	0.51
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.11	0.51
8:H:27:THR:O	8:H:31:VAL:HG23	2.11	0.51
1:N:268:VAL:O	1:N:272:VAL:HG23	2.10	0.51
2:O:62:ASN:O	2:O:65:THR:HG22	2.10	0.51
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.11	0.51
3:P:269:ILE:O	3:P:269:ILE:HG22	2.09	0.51
3:P:376:LYS:O	6:S:17:ARG:NH1	2.44	0.51
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.41	0.51
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.92	0.51
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.92	0.51
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.11	0.51
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.45	0.51
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.92	0.51
18:D:501:HEC:HMC1	18:D:501:HEC:HBC3	1.93	0.51
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.93	0.51
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.93	0.51
1:A:23:LEU:HD23	1:A:24:ARG:N	2.25	0.50
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.92	0.50
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.40	0.50
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.76	0.50
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.92	0.50
5:R:114:VAL:HG13	5:R:122:HIS:CD2	2.47	0.50
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.93	0.50
2:B:24:LEU:HD12	2:B:37:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:TYR:O	3:C:315:THR:HG22	2.11	0.50
4:D:38:SER:O	4:D:94:PRO:HG3	2.12	0.50
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.93	0.50
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:333:ALA:O	2:B:337:ILE:HG13	2.12	0.50
5:E:83:GLU:HA	5:E:100:HIS:CG	2.46	0.50
2:O:248:ASN:HD22	2:O:249:GLY:N	2.09	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.42	0.50
4:D:41:HIS:HE1	4:D:111:PRO:HD2	1.76	0.50
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.94	0.50
4:D:71:GLN:HE21	4:D:82:MET:CE	2.25	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.46	0.50
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.93	0.50
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.46	0.50
2:B:264:VAL:HG23	2:B:316:TYR:O	2.11	0.50
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.42	0.50
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.12	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.27	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.11	0.50
3:C:285:ILE:CD1	3:C:294:ALA:HB2	2.42	0.50
5:E:163:SER:OG	5:E:175:PRO:HD2	2.12	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.44	0.50
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.76	0.50
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.47	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.49
1:A:242:ARG:O	7:G:14:ILE:HA	2.11	0.49
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.47	0.49
6:S:11:ARG:O	6:S:15:ARG:HG3	2.12	0.49
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.27	0.49
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.49
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.11	0.49
3:C:350:ILE:O	3:C:354:MET:HG2	2.11	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.12	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.41	0.49
1:A:268:VAL:O	1:A:272:VAL:HG23	2.12	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
1:N:161:THR:HG21	1:N:235:ARG:H	1.77	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.13	0.49
9:V:30:UNK:HG3	9:V:31:UNK:N	2.27	0.49
1:A:191:LYS:N	1:A:195:MET:HE2	2.28	0.49
2:B:156:GLN:NE2	9:I:77:ARG:C	2.66	0.49
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.47	0.49
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.47	0.49
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.94	0.49
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.28	0.49
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.95	0.49
9:V:65:VAL:HG12	9:V:66:ALA:N	2.27	0.49
1:A:358:LYS:HE3	1:A:399:ILE:O	2.13	0.49
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.49
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.49
8:U:12:GLU:O	8:U:13:LEU:HB2	2.12	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.11	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.13	0.49
10:J:4:ALA:O	10:J:8:GLN:HG3	2.13	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.95	0.49
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.33	0.49
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.95	0.49
4:D:220:TYR:O	4:D:224:ARG:HG2	2.12	0.49
15:P:3002:UQ:HM51	15:P:3002:UQ:C8	2.43	0.49
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.28	0.49
5:E:102:THR:O	5:E:106:ILE:HG13	2.13	0.49
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.48	0.49
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.95	0.48
2:B:318:ASP:O	2:B:319:SER:HB2	2.11	0.48
2:B:60:THR:HG23	2:B:61:ALA:N	2.28	0.48
13:C:502:HEM:HBD1	21:C:386:HOH:O	2.11	0.48
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.45	0.48
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.95	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.94	0.48
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.94	0.48
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.93	0.48
4:D:54:VAL:HG22	17:D:2091:BOG:H5'2	1.96	0.48
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.43	0.48
1:N:53:ASN:H	1:N:173:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:116:VAL:HG23	2.13	0.48
3:C:9:HIS:CD2	3:C:11:LEU:H	2.31	0.48
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.47	0.48
5:R:155:GLY:HA3	5:R:166:ASP:C	2.33	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.41	0.48
10:J:55:ILE:HG22	10:J:59:TYR:CE1	2.44	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.77	0.48
2:O:60:THR:HG23	2:O:61:ALA:N	2.28	0.48
5:R:161:HIS:HB2	20:R:501:FES:S1	2.53	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.96	0.48
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.48
3:C:247:SER:OG	3:C:250:LEU:HB2	2.13	0.48
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.27	0.48
3:P:269:ILE:CG2	14:P:3001:FMX:H231	2.42	0.48
6:S:12:LEU:HB3	6:S:13:MET:HE1	1.95	0.48
8:U:65:ARG:O	8:U:68:CYS:HB3	2.13	0.48
1:A:370:ASP:O	2:B:374:THR:HG22	2.14	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.13	0.48
5:E:161:HIS:HB2	20:E:501:FES:S1	2.53	0.48
3:P:5:ILE:CG2	3:P:12:LEU:HD12	2.44	0.48
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.95	0.48
2:B:257:VAL:O	2:B:323:GLY:HA3	2.14	0.48
2:B:26:ILE:HA	2:B:35:ILE:O	2.13	0.48
2:B:424:MET:HG2	2:B:425:ALA:N	2.29	0.48
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.29	0.48
1:A:280:TYR:CG	1:A:281:ASP:N	2.82	0.48
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.34	0.48
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.78	0.48
2:O:147:ASP:O	2:O:150:VAL:HG22	2.14	0.48
2:O:24:LEU:HD12	2:O:37:SER:O	2.13	0.48
4:Q:238:ARG:HD2	7:T:14:ILE:HD12	1.96	0.48
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.77	0.48
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.14	0.47
3:C:45:GLN:HB3	13:C:501:HEM:HAB	1.95	0.47
1:N:219:VAL:HG12	1:N:220:SER:N	2.28	0.47
2:O:307:PHE:CD1	2:O:308:ASP:N	2.82	0.47
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.82	0.47
4:Q:71:GLN:HG3	4:Q:82:MET:HE2	1.96	0.47
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.15	0.47
3:C:344:VAL:C	3:C:345:GLU:HG3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47
5:E:133:VAL:HG13	5:E:133:VAL:O	2.14	0.47
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.29	0.47
9:I:64:LEU:HA	9:I:77:ARG:O	2.14	0.47
1:N:272:VAL:O	1:N:275:ALA:HB3	2.14	0.47
2:O:58:GLU:HG2	2:O:65:THR:HG22	1.95	0.47
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	1.96	0.47
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.29	0.47
1:A:191:LYS:CA	1:A:195:MET:HE2	2.44	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.29	0.47
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.94	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.96	0.47
1:N:209:VAL:O	1:N:212:ALA:HB3	2.15	0.47
1:N:21:ASN:HB2	1:N:219:VAL:HA	1.96	0.47
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.45	0.47
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.95	0.47
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.47
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.44	0.47
1:A:371:GLY:O	1:A:375:VAL:HG23	2.14	0.47
4:D:222:MET:CE	5:E:40:THR:HG23	2.43	0.47
1:N:124:GLU:OE1	1:N:179:ARG:HG3	2.15	0.47
1:N:23:LEU:HD23	1:N:24:ARG:N	2.29	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.15	0.47
3:C:5:ILE:CG2	3:C:12:LEU:HD12	2.45	0.47
6:F:109:LYS:O	6:F:110:LYS:HB2	2.14	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.15	0.47
2:O:57:TYR:N	2:O:57:TYR:CD1	2.83	0.47
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.50	0.47
6:S:12:LEU:HB3	6:S:13:MET:CE	2.45	0.47
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.47
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.96	0.47
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.14	0.47
2:B:345:LYS:O	2:B:348:ALA:N	2.48	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.29	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.15	0.47
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.95	0.47
2:O:31:ASN:ND2	2:O:31:ASN:C	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.47
2:O:159:VAL:HG21	2:O:325:TYR:HE1	1.80	0.47
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.44	0.47
6:S:94:LEU:O	6:S:98:ILE:HG13	2.15	0.47
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.97	0.47
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.32	0.47
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.97	0.47
3:C:69:HIS:HD2	3:C:73:ASN:ND2	2.08	0.47
3:P:247:SER:N	3:P:248:PRO:HD3	2.30	0.47
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.30	0.47
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.97	0.46
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.45	0.46
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.97	0.46
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.46
5:E:190:ASP:CG	5:E:191:ASP:H	2.19	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.80	0.46
2:O:264:VAL:HG23	2:O:316:TYR:C	2.36	0.46
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.14	0.46
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.51	0.46
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.82	0.46
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.97	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.97	0.46
2:O:345:LYS:O	2:O:348:ALA:N	2.48	0.46
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.16	0.46
5:R:147:ILE:HG13	5:R:157:TYR:O	2.16	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.46
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.80	0.46
2:O:286:LYS:C	2:O:288:GLY:H	2.19	0.46
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.96	0.46
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.97	0.46
6:F:40:ASP:O	6:F:44:LYS:HG3	2.15	0.46
1:N:53:ASN:N	1:N:173:ASN:ND2	2.63	0.46
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.44	0.46
1:A:63:ALA:O	1:A:116:VAL:HG13	2.16	0.46
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.16	0.46
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.30	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
10:J:59:TYR:O	10:J:61:ALA:N	2.45	0.46
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ARG:O	3:C:101:ARG:HD2	2.16	0.46
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.15	0.46
2:O:353:THR:CG2	2:O:354:GLU:N	2.79	0.46
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.98	0.46
1:A:45:SER:OG	1:A:92:ARG:HA	2.16	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.16	0.46
5:E:189:GLY:O	5:E:192:LEU:N	2.48	0.46
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.46
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.46	0.46
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.98	0.46
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.46
2:B:62:ASN:O	2:B:65:THR:HG22	2.16	0.46
1:N:178:THR:CG2	1:N:179:ARG:N	2.79	0.46
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.98	0.46
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.64	0.46
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.46
8:H:11:GLU:H	8:H:11:GLU:CD	2.19	0.46
1:N:184:SER:O	1:N:188:THR:OG1	2.28	0.46
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.46
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.51	0.46
3:P:347:PRO:O	3:P:351:ILE:HG13	2.16	0.46
4:D:3:LEU:HD11	7:G:72:LYS:CE	2.46	0.46
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.46	0.46
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.46
2:O:26:ILE:HA	2:O:35:ILE:O	2.16	0.45
1:A:124:GLU:OE1	1:A:179:ARG:HG3	2.16	0.45
2:B:19:PRO:O	2:B:41:PHE:HE1	1.98	0.45
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.52	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
2:O:31:ASN:HD22	2:O:33:LEU:H	1.61	0.45
2:O:76:THR:HG23	2:O:136:GLU:CD	2.36	0.45
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.49	0.45
5:R:113:ASP:HB3	5:R:116:LYS:HG3	1.99	0.45
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.51	0.45
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.44	0.45
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.98	0.45
1:N:350:THR:HG22	1:N:351:GLU:N	2.31	0.45
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.46	0.45
3:P:45:GLN:HB3	13:P:501:HEM:HAB	1.99	0.45
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HD2	1:A:119:ASN:HB3	1.98	0.45
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.84	0.45
1:N:106:MET:C	1:N:106:MET:HE2	2.36	0.45
1:N:191:LYS:N	1:N:195:MET:HE2	2.31	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.85	0.45
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.52	0.45
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.45
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.30	0.45
3:P:270:LYS:O	3:P:270:LYS:HG3	2.16	0.45
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.99	0.45
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.34	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.98	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.33	0.45
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.45
3:C:50:LEU:HD23	13:C:501:HEM:HBC1	1.98	0.45
5:R:73:LYS:HB3	5:R:195:VAL:O	2.16	0.45
1:A:136:GLN:O	1:A:140:GLU:HG3	2.17	0.45
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.17	0.45
2:B:46:ARG:HE	2:B:376:GLN:HA	1.81	0.45
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.17	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
3:P:69:HIS:HD2	3:P:73:ASN:ND2	2.11	0.45
5:R:55:VAL:O	5:R:59:ILE:HG12	2.17	0.45
5:R:99:ARG:NH2	5:R:149:ASN:OD1	2.49	0.45
2:O:327:ILE:HG22	9:V:55:MET:CE	2.47	0.45
2:O:156:GLN:NE2	9:V:77:ARG:C	2.69	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.47	0.45
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.98	0.45
1:N:206:LYS:CE	1:N:206:LYS:H	2.27	0.45
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.45
2:O:215:ASP:O	2:O:219:VAL:HG23	2.17	0.45
2:O:222:GLN:HG2	2:O:222:GLN:O	2.17	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.17	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.00	0.45
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.45
2:O:157:VAL:HG13	2:O:158:GLY:N	2.31	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:334:LEU:HA	3:P:334:LEU:HD23	1.75	0.45
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.47	0.44
5:E:84:GLY:N	5:E:100:HIS:O	2.45	0.44
2:O:222:GLN:O	2:O:223:PHE:HD2	2.00	0.44
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.18	0.44
4:Q:71:GLN:HE21	4:Q:82:MET:CE	2.30	0.44
8:U:47:ARG:CD	8:U:48:SER:H	2.30	0.44
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.44
2:B:215:ASP:O	2:B:219:VAL:HG23	2.16	0.44
5:E:85:LYS:HG2	5:E:86:ASN:N	2.33	0.44
2:B:308:ASP:OD2	9:I:55:MET:O	2.36	0.44
1:N:158:PHE:O	1:N:164:ALA:HB2	2.16	0.44
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.47	0.44
10:W:60:GLU:CD	10:W:60:GLU:C	2.76	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.77	0.44
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.44
3:P:350:ILE:HG23	3:P:351:ILE:N	2.32	0.44
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.53	0.44
3:P:377:MET:HE1	6:S:19:TRP:HZ3	1.82	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.18	0.44
1:A:156:THR:HA	5:E:7:VAL:HG21	2.00	0.44
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.65	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
3:P:285:ILE:CD1	3:P:294:ALA:HB2	2.46	0.44
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.44
5:R:41:ALA:O	5:R:45:VAL:HG23	2.18	0.44
8:U:40:CYS:O	8:U:44:VAL:HG23	2.17	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
1:A:350:THR:HG22	1:A:351:GLU:N	2.33	0.44
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.18	0.44
2:B:157:VAL:CG1	2:B:158:GLY:N	2.80	0.44
2:B:353:THR:CG2	2:B:354:GLU:N	2.81	0.44
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.53	0.44
2:B:57:TYR:CD1	2:B:57:TYR:N	2.86	0.44
3:C:347:PRO:O	3:C:350:ILE:HG22	2.17	0.44
3:P:344:VAL:O	3:P:344:VAL:HG23	2.17	0.44
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.99	0.44
9:V:65:VAL:O	9:V:76:VAL:HG23	2.16	0.44
2:B:218:GLN:O	2:B:222:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.47	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
1:A:23:LEU:C	1:A:23:LEU:HD23	2.38	0.44
2:B:286:LYS:C	2:B:288:GLY:H	2.21	0.44
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.86	0.44
5:E:52:LYS:C	5:E:52:LYS:HD3	2.38	0.44
10:J:60:GLU:O	10:J:61:ALA:HB3	2.18	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
2:O:18:CYS:HA	2:O:19:PRO:HD2	1.74	0.44
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.99	0.44
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.00	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.33	0.44
2:B:116:VAL:O	2:B:120:MET:HB2	2.18	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.42	0.44
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.51	0.44
5:E:55:VAL:O	5:E:59:ILE:HG12	2.18	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.90	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44
1:N:95:THR:HG22	1:N:96:ALA:N	2.33	0.44
5:R:117:LEU:O	5:R:118:ARG:C	2.56	0.44
5:R:128:LYS:O	5:R:129:LYS:HG3	2.18	0.44
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.99	0.44
9:V:28:UNK:HA	9:V:72:ALA:HB2	2.00	0.44
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.32	0.43
2:B:89:ILE:HD13	2:B:96:LEU:HB2	2.00	0.43
4:D:116:ILE:HG12	18:D:501:HEC:HMA3	1.99	0.43
1:N:223:TYR:OH	1:N:224:LYS:HE3	2.17	0.43
2:O:47:ILE:HG22	2:O:48:GLY:N	2.33	0.43
5:R:147:ILE:HG22	5:R:148:ALA:H	1.81	0.43
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.46	0.43
2:B:71:LEU:O	2:B:74:PRO:HD2	2.18	0.43
5:E:136:VAL:O	5:E:138:VAL:N	2.47	0.43
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.18	0.43
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.98	0.43
2:O:76:THR:HG22	2:O:82:SER:N	2.17	0.43
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.00	0.43
7:T:36:ASN:O	7:T:40:ARG:HG3	2.18	0.43
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.43
1:A:95:THR:HG22	1:A:96:ALA:N	2.33	0.43
5:R:109:GLU:C	5:R:111:GLU:H	2.22	0.43
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:HB2	1:A:100:LYS:HB2	2.00	0.43
2:B:368:TYR:HE1	2:B:381:GLU:OE2	2.02	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.47	0.43
2:B:385:GLU:C	2:B:387:LEU:H	2.22	0.43
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
6:F:71:LYS:O	6:F:72:HIS:HB2	2.19	0.43
9:I:64:LEU:HD12	9:I:77:ARG:C	2.37	0.43
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.48	0.43
18:Q:501:HEC:HBC3	18:Q:501:HEC:HMC1	2.00	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.48	0.43
5:R:133:VAL:HG13	5:R:133:VAL:O	2.18	0.43
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.43
1:A:240:GLU:HA	1:A:422:LEU:O	2.18	0.43
2:B:295:LEU:HD11	2:B:340:ALA:HB1	2.01	0.43
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.48	0.43
9:I:71:ASN:H	9:I:71:ASN:ND2	2.02	0.43
1:N:19:LEU:C	1:N:21:ASN:H	2.22	0.43
1:N:284:PHE:CE2	9:V:71:ASN:O	2.71	0.43
3:C:152:SER:HB3	3:C:162:VAL:HG21	2.00	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.57	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.43
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.49	0.43
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.01	0.43
5:R:84:GLY:N	5:R:100:HIS:O	2.52	0.43
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.02	0.43
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.54	0.43
8:H:32:LYS:O	8:H:36:ARG:HG3	2.19	0.43
1:N:248:LEU:HD12	1:N:426:GLY:HA2	2.01	0.43
3:C:25:PRO:HB2	3:C:28:ILE:HG23	2.00	0.43
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.54	0.43
5:E:191:ASP:OD1	5:E:191:ASP:O	2.37	0.43
1:N:37:VAL:HG22	1:N:109:VAL:HG11	2.01	0.43
2:O:397:VAL:O	2:O:401:LYS:HG2	2.18	0.43
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.18	0.43
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.33	0.43
18:Q:501:HEC:HMB1	18:Q:501:HEC:HBB3	2.01	0.43
9:I:38:UNK:C	9:I:40:UNK:N	2.80	0.43
1:N:137:GLU:O	1:N:141:MET:HG3	2.19	0.43
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.19	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:137:GLY:O	5:R:145:VAL:HG22	2.19	0.43
5:R:74:ILE:HD11	5:R:96:LEU:HD23	2.01	0.43
1:A:182:LEU:O	1:A:186:ILE:HG13	2.19	0.42
1:A:191:LYS:C	1:A:195:MET:HE2	2.39	0.42
2:B:58:GLU:HG2	2:B:65:THR:HG22	2.00	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.54	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.80	0.42
1:N:49:ASN:C	1:N:49:ASN:ND2	2.72	0.42
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.47	0.42
5:R:124:LEU:HA	5:R:127:VAL:HG22	2.01	0.42
5:R:165:TYR:HA	5:R:170:ARG:O	2.18	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
1:A:64:PHE:CE2	1:A:86:PHE:CE1	3.07	0.42
2:B:273:SER:HB3	2:B:364:LEU:HD21	2.02	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.85	0.42
5:E:77:LYS:CE	5:E:80:ASP:OD2	2.65	0.42
2:O:156:GLN:O	2:O:159:VAL:HG22	2.19	0.42
2:O:31:ASN:HD21	2:O:33:LEU:H	1.61	0.42
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.19	0.42
5:R:171:ILE:O	5:R:171:ILE:HG23	2.18	0.42
9:V:67:GLY:O	9:V:68:ILE:HD13	2.20	0.42
1:A:106:MET:C	1:A:106:MET:HE2	2.39	0.42
1:A:178:THR:CG2	1:A:179:ARG:N	2.81	0.42
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.85	0.42
3:C:269:ILE:HG22	3:C:269:ILE:O	2.19	0.42
5:E:164:HIS:HB2	5:E:173:LYS:HB3	2.01	0.42
2:O:89:ILE:HD13	2:O:96:LEU:HB2	2.00	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
3:C:334:LEU:HA	3:C:334:LEU:HD23	1.86	0.42
6:F:84:GLU:CD	6:F:84:GLU:H	2.22	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.20	0.42
1:N:350:THR:CG2	1:N:351:GLU:N	2.83	0.42
1:N:398:ARG:HH11	1:N:398:ARG:CG	2.25	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.42
1:N:140:GLU:HG3	9:V:50:LEU:HD12	2.02	0.42
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.42
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.50	0.42
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.42
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:ARG:HA	4:D:108:ALA:O	2.19	0.42
4:D:122:GLY:O	4:D:125:ASP:HB2	2.18	0.42
1:N:206:LYS:N	1:N:206:LYS:CD	2.63	0.42
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.50	0.42
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.54	0.42
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.00	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.85	0.42
7:G:71:ARG:HD3	8:H:56:GLU:CD	2.39	0.42
2:O:31:ASN:HD21	2:O:33:LEU:CB	2.33	0.42
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.42
2:O:424:MET:HG2	2:O:425:ALA:N	2.34	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42
5:R:164:HIS:HB2	5:R:173:LYS:HB3	2.02	0.42
1:N:239:SER:HB2	7:T:17:SER:O	2.20	0.42
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.85	0.42
3:C:194:THR:O	3:C:197:HIS:HB3	2.20	0.42
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.55	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.20	0.42
2:O:295:LEU:HD11	2:O:340:ALA:HB1	2.01	0.42
1:N:370:ASP:O	2:O:374:THR:HG22	2.20	0.42
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.01	0.42
5:E:189:GLY:O	5:E:190:ASP:C	2.58	0.42
3:C:335:ILE:HD13	7:G:58:LEU:HD23	2.01	0.42
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.42
2:O:157:VAL:CG1	2:O:158:GLY:N	2.82	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
2:O:201:SER:OG	2:O:228:SER:HA	2.20	0.42
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.01	0.42
5:E:71:LEU:HD11	3:P:169:PHE:CE1	2.55	0.42
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.02	0.42
5:R:131:GLU:CD	5:R:131:GLU:H	2.22	0.42
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.20	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.02	0.42
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.55	0.42
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.55	0.42
4:D:54:VAL:HG12	4:D:55:THR:HG23	2.02	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
2:O:299:VAL:HG11	2:O:336:VAL:HG13	2.00	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:ARG:HB3	5:R:105:GLU:HB2	2.02	0.42
6:S:13:MET:HB3	6:S:17:ARG:HE	1.84	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.76	0.42
2:B:389:SER:O	2:B:390:GLY:C	2.58	0.42
3:C:377:MET:HE1	6:F:20:TYR:HD1	1.85	0.42
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.42
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.50	0.42
2:O:318:ASP:O	2:O:319:SER:HB2	2.20	0.42
2:O:414:ALA:O	2:O:418:VAL:HG23	2.20	0.42
8:U:32:LYS:O	8:U:36:ARG:HG3	2.20	0.42
1:A:26:ALA:O	1:A:198:ALA:HA	2.20	0.41
1:A:281:ASP:C	1:A:281:ASP:OD1	2.58	0.41
4:D:195:GLU:HG3	4:D:198:HIS:HB2	2.02	0.41
1:N:274:ASN:HA	1:N:274:ASN:HD22	1.65	0.41
2:O:31:ASN:HD21	2:O:33:LEU:HB3	1.85	0.41
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.48	0.41
3:P:207:ASN:ND2	3:P:208:ASN:H	2.18	0.41
3:P:345:GLU:O	3:P:348:PHE:HB2	2.19	0.41
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.85	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.41
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.34	0.41
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.50	0.41
2:B:31:ASN:HD21	2:B:33:LEU:H	1.60	0.41
18:D:501:HEC:HBB3	18:D:501:HEC:HMB1	2.01	0.41
10:J:14:PHE:CD2	10:J:14:PHE:N	2.87	0.41
10:J:38:GLY:O	10:J:42:ILE:HG13	2.20	0.41
2:O:102:ARG:HH22	2:O:161:GLU:HA	1.86	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.29	0.41
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.49	0.41
1:N:242:ARG:O	7:T:14:ILE:HA	2.20	0.41
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.56	0.41
1:A:170:THR:HG22	1:A:171:THR:H	1.83	0.41
1:A:217:SER:O	1:A:218:GLY:C	2.58	0.41
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.20	0.41
5:E:132:TRP:CB	5:E:187:PHE:HZ	2.33	0.41
8:H:11:GLU:O	8:H:12:GLU:HB2	2.20	0.41
9:I:55:MET:O	9:I:58:ARG:HG2	2.20	0.41
1:N:68:LYS:HD2	1:N:119:ASN:HB3	2.02	0.41
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.85	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.21	0.41
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.41
2:B:337:ILE:HD12	2:B:434:PRO:HD2	2.01	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.41
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.20	0.41
2:O:225:ASN:O	2:O:227:ARG:N	2.53	0.41
2:O:248:ASN:HD22	2:O:250:HIS:H	1.68	0.41
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.19	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.36	0.41
1:A:168:GLU:H	1:A:168:GLU:CD	2.23	0.41
2:B:389:SER:O	2:B:391:THR:N	2.54	0.41
3:C:101:ARG:CD	3:C:101:ARG:C	2.88	0.41
2:O:368:TYR:HE1	2:O:381:GLU:OE2	2.03	0.41
3:P:156:TYR:CD2	3:P:156:TYR:N	2.88	0.41
3:P:273:TRP:HA	3:P:276:LEU:HD12	2.02	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
6:S:84:GLU:H	6:S:84:GLU:CD	2.24	0.41
1:A:77:LYS:HE3	2:B:359:LYS:HZ1	1.85	0.41
1:A:362:ARG:HB2	2:B:112:LEU:HD11	2.03	0.41
2:B:224:LEU:HD23	2:B:224:LEU:HA	1.90	0.41
5:E:171:ILE:HG23	5:E:171:ILE:O	2.21	0.41
5:E:77:LYS:HE2	5:E:80:ASP:CG	2.39	0.41
2:B:307:PHE:H	9:I:52:ARG:HG2	1.86	0.41
1:N:358:LYS:O	1:N:362:ARG:HG3	2.21	0.41
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.86	0.41
3:P:226:SER:O	3:P:230:ILE:HG13	2.20	0.41
1:A:106:MET:HE1	1:A:107:PRO:HA	2.03	0.41
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.85	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.56	0.41
2:B:50:PHE:C	2:B:51:ILE:HG13	2.40	0.41
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.50	0.41
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.92	0.41
1:N:45:SER:HA	1:N:48:GLU:HG3	2.03	0.41
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.20	0.41
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.83	0.41
9:V:32:UNK:O	9:V:33:UNK:C	2.68	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.55	0.41
4:D:14:HIS:HB3	4:D:21:LEU:HA	2.03	0.41
10:J:56:LYS:O	10:J:60:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.86	0.41
3:P:54:MET:SD	5:R:62:LEU:HD21	2.61	0.41
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.41
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.03	0.41
3:C:37:LEU:CD1	3:C:236:MET:HG3	2.51	0.41
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.80	0.41
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.41
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.50	0.41
6:S:71:LYS:O	6:S:72:HIS:HB2	2.20	0.41
6:S:77:LYS:O	6:S:77:LYS:HG2	2.21	0.41
1:A:402:VAL:HG22	1:A:406:MET:HE2	2.03	0.41
5:E:106:ILE:HG21	5:E:130:PRO:HB3	2.02	0.41
5:E:193:VAL:HG13	5:E:193:VAL:O	2.21	0.41
1:N:182:LEU:O	1:N:186:ILE:HG13	2.21	0.41
1:N:280:TYR:CG	1:N:281:ASP:N	2.89	0.41
1:A:106:MET:CE	1:A:107:PRO:HA	2.50	0.40
3:C:2:ALA:HB3	3:C:8:SER:HB3	2.02	0.40
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.04	0.40
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.21	0.40
1:N:387:GLY:O	1:N:388:ARG:HB3	2.20	0.40
5:R:193:VAL:HG13	5:R:193:VAL:O	2.20	0.40
1:A:49:ASN:ND2	1:A:49:ASN:C	2.73	0.40
2:B:350:GLY:C	2:B:352:VAL:H	2.23	0.40
2:B:46:ARG:HG3	2:B:110:GLU:HG2	2.04	0.40
3:C:30:ALA:O	3:C:33:ASN:HB2	2.20	0.40
3:C:347:PRO:O	3:C:351:ILE:HG13	2.20	0.40
1:N:371:GLY:O	1:N:375:VAL:HG23	2.21	0.40
2:O:268:GLU:HG2	2:O:268:GLU:O	2.21	0.40
8:U:12:GLU:HG2	8:U:13:LEU:N	2.36	0.40
8:H:65:ARG:O	8:H:68:CYS:HB3	2.22	0.40
1:N:26:ALA:O	1:N:198:ALA:HA	2.22	0.40
2:O:109:VAL:HG21	2:O:119:VAL:CG1	2.51	0.40
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.04	0.40
3:C:29:SER:HB2	19:G:2004:CDL:OB4	2.21	0.40
10:W:14:PHE:CD2	10:W:14:PHE:N	2.84	0.40
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.21	0.40
1:A:350:THR:CG2	1:A:351:GLU:N	2.84	0.40
1:A:364:ALA:O	1:A:368:GLN:HG3	2.21	0.40
1:A:7:THR:O	1:A:11:ILE:HG13	2.22	0.40
3:C:134:LEU:N	3:C:135:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.03	0.40
5:E:78:LEU:HD13	5:E:132:TRP:CE2	2.56	0.40
1:N:144:ASP:O	1:N:148:VAL:HG23	2.21	0.40
1:N:364:ALA:O	1:N:368:GLN:HG3	2.21	0.40
2:O:124:LEU:HD21	2:O:223:PHE:HB3	2.04	0.40
2:O:399:ALA:HA	2:O:402:ILE:CG2	2.52	0.40
3:P:69:HIS:CD2	3:P:73:ASN:ND2	2.81	0.40
3:P:98:HIS:HD2	13:P:502:HEM:C1C	2.40	0.40
5:R:116:LYS:O	5:R:117:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	415 (94%)	21 (5%)	5 (1%)	14	25
1	N	440/446 (99%)	413 (94%)	21 (5%)	6 (1%)	11	19
2	B	419/441 (95%)	370 (88%)	40 (10%)	9 (2%)	7	12
2	O	420/441 (95%)	374 (89%)	38 (9%)	8 (2%)	8	14
3	C	378/380 (100%)	363 (96%)	14 (4%)	1 (0%)	41	60
3	P	377/380 (99%)	361 (96%)	15 (4%)	1 (0%)	41	60
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	34	53
5	E	194/196 (99%)	174 (90%)	13 (7%)	7 (4%)	3	5
5	R	192/196 (98%)	163 (85%)	22 (12%)	7 (4%)	3	5
6	F	99/110 (90%)	94 (95%)	4 (4%)	1 (1%)	15	27
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	76/81 (94%)	69 (91%)	7 (9%)	0	100	100
8	H	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	10	18
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	10	18
9	I	29/47 (62%)	25 (86%)	4 (14%)	0	100	100
9	V	29/47 (62%)	25 (86%)	3 (10%)	1 (3%)	3	5
10	J	59/61 (97%)	54 (92%)	3 (5%)	2 (3%)	3	5
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3	5
All	All	4000/4160 (96%)	3688 (92%)	258 (6%)	54 (1%)	11	19

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	226	ILE
2	B	227	ARG
2	B	389	SER
5	E	188	VAL
5	E	190	ASP
1	N	20	ASP
1	N	282	ARG
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
5	R	137	GLY
5	R	189	GLY
8	U	13	LEU
1	A	72	CYS
1	N	72	CYS
1	N	262	TRP
9	V	48	PRO
1	A	262	TRP

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Mol	Chain	Res	Type
2	B	220	ALA
5	E	64	ALA
5	E	120	PRO
5	E	141	HIS
8	H	12	GLU
10	J	56	LYS
2	O	350	GLY
5	R	152	ASP
10	W	62	SER
1	A	443	TRP
7	G	33	ALA
10	J	60	GLU
1	N	443	TRP
2	O	220	ALA
2	O	390	GLY
4	Q	177	ALA
10	W	56	LYS
2	B	29	LEU
6	F	77	LYS
3	P	286	PRO
5	E	189	GLY
2	B	350	GLY
5	R	8	PRO
3	C	286	PRO
2	O	29	LEU
5	R	147	ILE

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%)	351 (96%)	14 (4%)	33	53
1	N	365/368 (99%)	348 (95%)	17 (5%)	26	45
2	B	332/347 (96%)	327 (98%)	5 (2%)	65	78
2	O	333/347 (96%)	327 (98%)	6 (2%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	328/329 (100%)	325 (99%)	3 (1%)	78	87
3	P	328/329 (100%)	325 (99%)	3 (1%)	78	87
4	D	200/200 (100%)	198 (99%)	2 (1%)	76	85
4	Q	200/200 (100%)	197 (98%)	3 (2%)	65	78
5	E	166/166 (100%)	166 (100%)	0	100	100
5	R	165/166 (99%)	160 (97%)	5 (3%)	41	61
6	F	93/96 (97%)	91 (98%)	2 (2%)	52	70
6	S	93/96 (97%)	91 (98%)	2 (2%)	52	70
7	G	71/71 (100%)	70 (99%)	1 (1%)	67	79
7	T	69/71 (97%)	67 (97%)	2 (3%)	42	62
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	78
8	U	63/71 (89%)	62 (98%)	1 (2%)	62	77
9	I	23/26 (88%)	22 (96%)	1 (4%)	29	48
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	72
10	W	47/49 (96%)	46 (98%)	1 (2%)	53	71
All	All	3378/3446 (98%)	3308 (98%)	70 (2%)	53	71

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	90	THR
1	A	106	MET
1	A	181	ASP
1	A	281	ASP
1	A	307	PHE
1	A	308	GLN
1	A	342	TRP
1	A	344	ARG
1	A	395	TRP
1	A	405	ARG
1	A	443	TRP
2	B	31	ASN

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Mol	Chain	Res	Type
2	B	248	ASN
2	B	338	ARG
2	B	341	MET
2	B	402	ILE
3	C	91	PHE
3	C	223	PRO
3	C	367	PHE
4	D	169	LEU
4	D	172	ASP
6	F	58	ARG
6	F	70	LEU
7	G	27	PRO
8	H	72	LYS
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	29	GLU
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	90	THR
1	N	106	MET
1	N	181	ASP
1	N	206	LYS
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	348	SER
1	N	395	TRP
1	N	405	ARG
1	N	443	TRP
2	O	31	ASN
2	O	139	ASP
2	O	248	ASN
2	O	338	ARG
2	O	341	MET
2	O	402	ILE
3	P	91	PHE
3	P	223	PRO
3	P	367	PHE
4	Q	169	LEU

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Mol	Chain	Res	Type
4	Q	172	ASP
4	Q	241	LYS
5	R	52	LYS
5	R	113	ASP
5	R	125	ASP
5	R	126	ARG
5	R	187	PHE
6	S	58	ARG
6	S	70	LEU
7	T	2	ILE
7	T	27	PRO
8	U	72	LYS
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	126	GLN
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	342	GLN
3	C	346	HIS
4	D	35	GLN
4	D	50	ASN

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Mol	Chain	Res	Type
4	D	71	GLN
4	D	148	HIS
4	D	200	GLN
5	E	3	ASN
5	E	57	GLN
5	E	86	ASN
5	E	103	GLN
5	E	107	ASN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	79	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	126	GLN
1	N	143	ASN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	305	GLN
2	O	329	GLN
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN

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Mol	Chain	Res	Type
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
6	S	56	ASN
6	S	79	GLN
7	T	23	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS
10	W	8	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 11 are unknown - leaving 30 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	$\# Z > 2$
13	HEM	C	501	3	27,50,50	2.00	6 (22%)	17,82,82	1.66	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BOG	D	2091	-	20,20,20	1.12	2 (10%)	25,25,25	1.02	1 (4%)
17	BOG	Q	3091	-	20,20,20	1.12	2 (10%)	25,25,25	0.87	1 (4%)
17	BOG	C	3010	-	11,11,20	1.07	2 (18%)	10,11,25	0.98	1 (10%)
20	FES	E	501	5	0,4,4	0.00	-	-	-	-
11	PEE	P	3007	-	47,47,50	1.24	5 (10%)	50,52,55	0.88	4 (8%)
14	FMX	P	3001	-	29,31,31	0.98	1 (3%)	34,44,44	1.01	2 (5%)
20	FES	R	501	5	0,4,4	0.00	-	-	-	-
16	AZI	P	3011	-	0,2,2	0.00	-	0,1,1	0.00	-
19	CDL	D	2003	-	41,41,99	1.17	0	47,53,111	1.04	4 (8%)
15	UQ	C	2002	-	19,19,63	2.59	10 (52%)	23,26,79	1.03	2 (8%)
11	PEE	A	2005	-	49,49,50	1.36	9 (18%)	52,54,55	0.92	5 (9%)
16	AZI	C	2011	-	0,2,2	0.00	-	0,1,1	0.00	-
17	BOG	P	2010	-	18,18,20	1.07	3 (16%)	22,22,25	0.56	0
18	HEC	Q	501	4	26,50,50	2.25	3 (11%)	18,82,82	1.56	4 (22%)
13	HEM	P	502	3	27,50,50	1.71	5 (18%)	17,82,82	1.72	4 (23%)
17	BOG	Q	3009	-	20,20,20	0.96	1 (5%)	25,25,25	0.85	1 (4%)
11	PEE	N	3005	-	49,49,50	1.34	9 (18%)	52,54,55	0.91	5 (9%)
13	HEM	C	502	3	27,50,50	2.09	7 (25%)	17,82,82	1.71	4 (23%)
19	CDL	T	3004	-	39,39,99	1.19	3 (7%)	45,51,111	1.04	1 (2%)
13	HEM	P	501	3	27,50,50	1.73	6 (22%)	17,82,82	1.32	4 (23%)
19	CDL	G	2004	-	39,39,99	1.20	3 (7%)	45,51,111	1.03	3 (6%)
18	HEC	D	501	4	26,50,50	1.89	3 (11%)	18,82,82	1.34	3 (16%)
11	PEE	C	2007	-	47,47,50	1.21	6 (12%)	50,52,55	0.91	5 (10%)
17	BOG	D	2009	-	20,20,20	1.02	2 (10%)	25,25,25	0.88	2 (8%)
19	CDL	Q	3003	-	41,41,99	1.18	2 (4%)	47,53,111	1.05	3 (6%)
11	PEE	C	2008	-	20,20,50	1.65	5 (25%)	23,25,55	0.65	0
11	PEE	N	3008	-	4,4,50	3.64	4 (100%)	6,6,55	0.54	0
14	FMX	C	2001	-	29,31,31	1.07	1 (3%)	34,44,44	1.04	2 (5%)
15	UQ	P	3002	-	19,19,63	2.47	10 (52%)	23,26,79	1.09	2 (8%)

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
13	HEM	C	501	3	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BOG	D	2091	-	-	6/11/31/31	0/1/1/1
17	BOG	Q	3091	-	-	5/11/31/31	0/1/1/1
17	BOG	C	3010	-	-	4/9/9/31	-
20	FES	E	501	5	-	-	0/1/1/1
11	PEE	P	3007	-	-	24/51/51/54	-
14	FMX	P	3001	-	-	3/14/33/33	0/4/4/4
20	FES	R	501	5	-	-	0/1/1/1
19	CDL	D	2003	-	-	25/51/51/110	-
15	UQ	C	2002	-	-	2/11/35/87	0/1/1/1
11	PEE	A	2005	-	-	32/53/53/54	-
17	BOG	Q	3009	-	-	6/11/31/31	0/1/1/1
17	BOG	P	2010	-	-	1/6/26/31	0/1/1/1
18	HEC	Q	501	4	-	2/6/54/54	-
13	HEM	P	502	3	-	2/6/54/54	-
11	PEE	N	3005	-	-	32/53/53/54	-
13	HEM	C	502	3	-	2/6/54/54	-
19	CDL	T	3004	-	-	24/49/49/110	-
13	HEM	P	501	3	-	0/6/54/54	-
19	CDL	G	2004	-	-	23/49/49/110	-
18	HEC	D	501	4	-	3/6/54/54	-
11	PEE	C	2007	-	-	24/51/51/54	-
17	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
19	CDL	Q	3003	-	-	23/51/51/110	-
11	PEE	C	2008	-	-	11/24/24/54	-
14	FMX	C	2001	-	-	4/14/33/33	0/4/4/4
15	UQ	P	3002	-	-	2/11/35/87	0/1/1/1

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	C3B-C2B	-7.53	1.32	1.40
18	Q	501	HEC	C3C-C2C	-6.64	1.33	1.40
18	D	501	HEC	C3B-C2B	-6.58	1.33	1.40
13	C	501	HEM	C3B-CAB	-5.61	1.36	1.47
15	P	3002	UQ	C7-C6	5.39	1.60	1.51
15	C	2002	UQ	C7-C6	5.09	1.59	1.51
15	C	2002	UQ	C6-C5	4.99	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	C3B-CAB	-4.94	1.37	1.47
11	N	3008	PEE	P-O1P	4.93	1.62	1.50
15	P	3002	UQ	C6-C5	4.74	1.43	1.35
13	C	502	HEM	C4D-C3D	4.71	1.53	1.42
13	P	501	HEM	C3B-CAB	-4.71	1.38	1.47
18	D	501	HEC	C3C-C2C	-4.41	1.36	1.40
13	P	502	HEM	CBB-CAB	4.05	1.56	1.29
13	C	501	HEM	C3C-C2C	-3.81	1.35	1.40
13	C	502	HEM	CBB-CAB	3.79	1.54	1.29
15	C	2002	UQ	C6-C1	3.79	1.57	1.46
13	C	501	HEM	C3C-CAC	-3.73	1.40	1.47
13	C	502	HEM	C3C-CAC	-3.60	1.40	1.47
15	P	3002	UQ	C6-C1	3.58	1.56	1.46
13	P	502	HEM	CBC-CAC	3.55	1.52	1.29
11	N	3008	PEE	P-O4P	3.53	1.65	1.54
13	C	501	HEM	CBC-CAC	3.51	1.52	1.29
13	P	502	HEM	C4D-C3D	3.51	1.50	1.42
13	C	502	HEM	CBC-CAC	3.43	1.52	1.29
13	P	502	HEM	C3B-CAB	-3.42	1.41	1.47
11	C	2008	PEE	O3-C30	3.26	1.42	1.33
11	A	2005	PEE	O2-C10	3.23	1.43	1.34
13	P	501	HEM	CBC-CAC	3.21	1.50	1.29
13	P	501	HEM	CBB-CAB	3.21	1.50	1.29
15	C	2002	UQ	O3-C3	3.20	1.44	1.36
11	N	3008	PEE	P-O3P	3.19	1.64	1.54
11	N	3005	PEE	O2-C10	3.15	1.43	1.34
11	A	2005	PEE	P-O1P	3.08	1.61	1.50
11	N	3005	PEE	P-O1P	3.05	1.61	1.50
11	P	3007	PEE	C22-C21	-3.02	1.34	1.51
11	N	3005	PEE	C19-C18	-3.01	1.34	1.51
11	A	2005	PEE	C19-C18	-3.00	1.34	1.51
11	P	3007	PEE	C19-C18	-2.99	1.34	1.51
11	C	2007	PEE	C19-C18	-2.97	1.34	1.51
11	C	2008	PEE	O2-C10	2.97	1.42	1.34
15	C	2002	UQ	CM5-C5	2.96	1.57	1.50
13	C	502	HEM	C4A-NA	2.96	1.42	1.36
11	P	3007	PEE	O3-C30	2.95	1.42	1.33
11	C	2007	PEE	P-O1P	2.95	1.61	1.50
11	N	3005	PEE	C22-C21	-2.94	1.35	1.51
11	P	3007	PEE	P-O1P	2.91	1.61	1.50
11	C	2007	PEE	C22-C21	-2.90	1.35	1.51
15	C	2002	UQ	C2-C1	2.90	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	CBB-CAB	2.89	1.48	1.29
11	A	2005	PEE	O3-C30	2.88	1.41	1.33
11	A	2005	PEE	C22-C21	-2.84	1.35	1.51
15	P	3002	UQ	O3-C3	2.80	1.43	1.36
13	P	502	HEM	C3C-CAC	-2.80	1.42	1.47
13	C	502	HEM	C3C-C2C	-2.77	1.36	1.40
15	C	2002	UQ	O2-C2	2.74	1.43	1.36
11	C	2008	PEE	P-O1P	2.74	1.60	1.50
13	P	501	HEM	C3C-CAC	-2.70	1.42	1.47
11	N	3005	PEE	O3-C30	2.68	1.41	1.33
14	C	2001	FMX	C6-N2	-2.68	1.34	1.38
11	P	3007	PEE	O2-C10	2.67	1.41	1.34
11	C	2007	PEE	O3-C30	2.64	1.41	1.33
15	P	3002	UQ	CM5-C5	2.60	1.56	1.50
15	P	3002	UQ	C7-C8	2.53	1.54	1.50
15	P	3002	UQ	C2-C1	2.50	1.56	1.48
15	C	2002	UQ	C5-C4	2.48	1.56	1.47
17	D	2091	BOG	O5-C1	2.48	1.48	1.41
11	N	3008	PEE	P-O2P	2.44	1.61	1.54
17	C	3010	BOG	C2-C1	2.43	1.57	1.50
17	Q	3091	BOG	C4-C5	2.42	1.58	1.53
17	Q	3091	BOG	O5-C1	2.40	1.48	1.41
18	Q	501	HEC	C1C-CHC	-2.40	1.34	1.41
11	A	2005	PEE	C31-C30	2.39	1.57	1.50
17	C	3010	BOG	O5-C1	2.39	1.45	1.40
15	P	3002	UQ	O2-C2	2.37	1.42	1.36
17	D	2091	BOG	C4-C5	2.37	1.58	1.53
15	C	2002	UQ	C3-C4	2.35	1.55	1.48
17	D	2009	BOG	O5-C1	2.35	1.47	1.41
15	P	3002	UQ	C5-C4	2.34	1.55	1.47
19	T	3004	CDL	O1-C1	2.34	1.50	1.43
11	C	2007	PEE	O2-C10	2.33	1.40	1.34
13	P	501	HEM	C4A-NA	2.31	1.40	1.36
11	N	3005	PEE	C1-C2	2.30	1.57	1.50
13	C	501	HEM	C4D-C3D	2.28	1.47	1.42
11	N	3005	PEE	C3-C2	2.26	1.57	1.50
19	T	3004	CDL	CA3-CA4	2.25	1.57	1.50
11	A	2005	PEE	C3-C2	2.24	1.57	1.50
15	P	3002	UQ	C3-C4	2.22	1.55	1.48
11	N	3005	PEE	C11-C10	2.20	1.57	1.50
15	C	2002	UQ	C7-C8	2.20	1.53	1.50
11	A	2005	PEE	C11-C10	2.20	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	2004	CDL	O1-C1	2.19	1.49	1.43
17	P	2010	BOG	C4-C5	2.17	1.57	1.53
11	N	3005	PEE	C31-C30	2.15	1.57	1.50
19	Q	3003	CDL	O1-C1	2.14	1.49	1.43
11	A	2005	PEE	C1-C2	2.14	1.57	1.50
17	Q	3009	BOG	O5-C1	2.13	1.47	1.41
13	P	501	HEM	C3C-C2C	-2.12	1.37	1.40
11	C	2007	PEE	C3-C2	2.12	1.57	1.50
11	C	2008	PEE	C3-C2	2.11	1.57	1.50
11	C	2008	PEE	C1-C2	2.11	1.57	1.50
19	T	3004	CDL	OA8-CA6	-2.10	1.40	1.45
14	P	3001	FMX	C26-C21	2.08	1.42	1.39
19	G	2004	CDL	CA3-CA4	2.05	1.57	1.50
19	G	2004	CDL	OA6-CA5	2.04	1.40	1.34
19	Q	3003	CDL	OA2-CA2	-2.04	1.36	1.44
17	P	2010	BOG	O5-C1	2.02	1.48	1.42
17	D	2009	BOG	C1-C2	2.02	1.58	1.52
17	P	2010	BOG	C1-C2	2.02	1.57	1.52
18	D	501	HEC	CAA-C2A	-2.02	1.48	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	CBD-CAD-C3D	4.38	120.55	112.48
17	D	2091	BOG	C1'-O1-C1	4.15	120.72	113.84
14	P	3001	FMX	C21-N1-N2	3.93	123.80	116.23
14	C	2001	FMX	C21-N1-N2	3.90	123.73	116.23
13	P	502	HEM	C4C-C3C-C2C	-3.87	104.20	106.90
18	Q	501	HEC	CBA-CAA-C2A	3.65	119.20	112.48
13	C	502	HEM	C4C-C3C-C2C	-3.46	104.48	106.90
17	Q	3091	BOG	C1'-O1-C1	3.07	118.92	113.84
19	T	3004	CDL	CB4-OB6-CB5	-3.00	110.41	117.79
18	D	501	HEC	CBA-CAA-C2A	2.99	117.99	112.48
15	P	3002	UQ	C8-C7-C6	2.99	120.10	112.05
18	D	501	HEC	CAA-C2A-C3A	-2.97	118.72	127.25
17	Q	3009	BOG	C1'-O1-C1	2.97	118.76	113.84
17	D	2009	BOG	C1'-O1-C1	2.95	118.73	113.84
19	G	2004	CDL	CB4-OB6-CB5	-2.95	110.54	117.79
13	P	502	HEM	CBA-CAA-C2A	2.85	117.74	112.49
18	Q	501	HEC	CAA-C2A-C3A	-2.82	119.15	127.25
11	P	3007	PEE	C20-C19-C18	2.81	128.68	114.42
11	A	2005	PEE	C20-C19-C18	2.74	128.32	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	2007	PEE	C20-C19-C18	2.73	128.30	114.42
11	N	3005	PEE	C20-C19-C18	2.72	128.24	114.42
13	P	502	HEM	CMB-C2B-C3B	2.71	129.75	124.68
13	C	502	HEM	CMC-C2C-C3C	2.71	129.75	124.68
15	C	2002	UQ	C8-C7-C6	2.71	119.34	112.05
11	C	2007	PEE	C19-C18-C17	2.67	127.97	114.42
13	C	501	HEM	C4A-C3A-C2A	-2.65	105.15	107.00
13	C	502	HEM	C3B-C4B-NB	2.59	112.56	109.21
11	A	2005	PEE	C19-C18-C17	2.58	127.50	114.42
11	P	3007	PEE	C19-C18-C17	2.58	127.50	114.42
13	P	501	HEM	CBD-CAD-C3D	2.56	117.20	112.48
11	N	3005	PEE	C19-C18-C17	2.56	127.42	114.42
11	N	3005	PEE	C22-C21-C20	2.53	127.28	114.42
11	C	2007	PEE	C22-C21-C20	2.51	127.19	114.42
19	D	2003	CDL	CB4-OB6-CB5	-2.51	111.60	117.79
11	A	2005	PEE	C22-C21-C20	2.51	127.15	114.42
11	P	3007	PEE	C22-C21-C20	2.48	127.03	114.42
17	C	3010	BOG	C1'-O1-C1	2.46	119.40	114.00
19	Q	3003	CDL	CB4-OB6-CB5	-2.45	111.75	117.79
11	A	2005	PEE	C23-C22-C21	2.45	126.87	114.42
18	D	501	HEC	CBD-CAD-C3D	2.42	116.96	112.49
14	C	2001	FMX	C15-O14-C11	-2.42	113.15	118.80
15	P	3002	UQ	C7-C6-C1	-2.41	115.57	118.48
11	N	3005	PEE	C23-C22-C21	2.40	126.59	114.42
11	C	2007	PEE	C23-C22-C21	2.39	126.55	114.42
13	C	501	HEM	CAD-C3D-C2D	-2.38	120.41	127.25
13	P	501	HEM	CMB-C2B-C3B	2.35	129.07	124.68
11	P	3007	PEE	C23-C22-C21	2.30	126.09	114.42
13	C	502	HEM	CBA-CAA-C2A	2.28	116.69	112.49
19	Q	3003	CDL	CA4-OA6-CA5	-2.26	112.23	117.79
13	P	501	HEM	C4A-C3A-C2A	-2.26	105.43	107.00
19	D	2003	CDL	CA6-OA8-CA7	-2.24	111.46	117.10
18	Q	501	HEC	CMC-C2C-C3C	-2.24	123.19	125.82
18	Q	501	HEC	CBD-CAD-C3D	2.21	116.56	112.49
19	Q	3003	CDL	CA6-OA8-CA7	-2.19	111.59	117.10
17	D	2009	BOG	O1-C1-C2	2.17	111.69	108.30
13	C	501	HEM	CMB-C2B-C3B	2.14	128.69	124.68
14	P	3001	FMX	C15-O14-C11	-2.14	113.79	118.80
13	P	502	HEM	C3B-C4B-NB	2.14	111.97	109.21
15	C	2002	UQ	C7-C6-C1	-2.13	115.92	118.48
11	C	2007	PEE	O3-C3-C2	2.10	114.55	108.43
11	N	3005	PEE	O3-C3-C2	2.09	114.52	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	2004	CDL	CA4-OA6-CA5	-2.07	112.69	117.79
19	D	2003	CDL	CA6-CA4-CA3	-2.05	106.93	111.79
19	D	2003	CDL	CA4-OA6-CA5	-2.05	112.75	117.79
13	P	501	HEM	C4C-C3C-C2C	-2.03	105.48	106.90
19	G	2004	CDL	CB6-CB4-CB3	-2.02	107.00	111.79
11	A	2005	PEE	O3-C3-C2	2.02	114.31	108.43

There are no chirality outliers.

All (264) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	D	2091	BOG	O5-C1-O1-C1'
17	Q	3091	BOG	C2-C1-O1-C1'
17	Q	3091	BOG	O5-C1-O1-C1'
17	C	3010	BOG	C2'-C1'-O1-C1
11	A	2005	PEE	O4P-C4-C5-N
11	A	2005	PEE	C11-C10-O2-C2
11	A	2005	PEE	C4-O4P-P-O1P
11	A	2005	PEE	C4-O4P-P-O2P
18	Q	501	HEC	C1A-C2A-CAA-CBA
18	Q	501	HEC	C3A-C2A-CAA-CBA
13	P	502	HEM	C2D-C3D-CAD-CBD
13	P	502	HEM	C4D-C3D-CAD-CBD
11	N	3005	PEE	O4P-C4-C5-N
11	N	3005	PEE	C11-C10-O2-C2
11	N	3005	PEE	C4-O4P-P-O1P
11	N	3005	PEE	C4-O4P-P-O2P
13	C	502	HEM	C2D-C3D-CAD-CBD
13	C	502	HEM	C4D-C3D-CAD-CBD
19	T	3004	CDL	O1-C1-CA2-OA2
19	T	3004	CDL	CB3-OB5-PB2-OB3
19	G	2004	CDL	CB3-OB5-PB2-OB3
18	D	501	HEC	C1A-C2A-CAA-CBA
18	D	501	HEC	C3A-C2A-CAA-CBA
18	D	501	HEC	C4D-C3D-CAD-CBD
19	Q	3003	CDL	CB2-C1-CA2-OA2
19	Q	3003	CDL	CA2-OA2-PA1-OA3
19	Q	3003	CDL	CA2-OA2-PA1-OA4
19	Q	3003	CDL	CA2-OA2-PA1-OA5
19	Q	3003	CDL	CB2-OB2-PB2-OB3
19	Q	3003	CDL	CB2-OB2-PB2-OB5
11	P	3007	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
15	C	2002	UQ	C1-C6-C7-C8
11	C	2008	PEE	C1-O3P-P-O1P
11	C	2008	PEE	C1-O3P-P-O4P
19	D	2003	CDL	CB2-C1-CA2-OA2
19	D	2003	CDL	CA2-OA2-PA1-OA3
19	D	2003	CDL	CA2-OA2-PA1-OA4
19	D	2003	CDL	CA2-OA2-PA1-OA5
19	D	2003	CDL	CB2-OB2-PB2-OB3
19	D	2003	CDL	CB2-OB2-PB2-OB5
15	P	3002	UQ	C1-C6-C7-C8
15	P	3002	UQ	C5-C6-C7-C8
11	N	3005	PEE	O5-C30-O3-C3
11	A	2005	PEE	O5-C30-O3-C3
19	T	3004	CDL	OB9-CB7-OB8-CB6
19	G	2004	CDL	OB9-CB7-OB8-CB6
19	D	2003	CDL	C31-CA7-OA8-CA6
11	A	2005	PEE	O4-C10-O2-C2
11	N	3005	PEE	O4-C10-O2-C2
11	A	2005	PEE	C31-C30-O3-C3
11	N	3005	PEE	C31-C30-O3-C3
19	Q	3003	CDL	C31-CA7-OA8-CA6
19	T	3004	CDL	C71-CB7-OB8-CB6
19	G	2004	CDL	C71-CB7-OB8-CB6
17	D	2009	BOG	C4-C5-C6-O6
19	G	2004	CDL	O1-C1-CA2-OA2
19	Q	3003	CDL	O1-C1-CA2-OA2
19	D	2003	CDL	O1-C1-CA2-OA2
19	T	3004	CDL	C51-CB5-OB6-CB4
19	G	2004	CDL	C51-CB5-OB6-CB4
17	D	2009	BOG	O5-C5-C6-O6
19	D	2003	CDL	OA9-CA7-OA8-CA6
19	T	3004	CDL	CB2-C1-CA2-OA2
19	G	2004	CDL	CB2-C1-CA2-OA2
19	T	3004	CDL	OB7-CB5-OB6-CB4
19	Q	3003	CDL	C71-CB7-OB8-CB6
19	D	2003	CDL	C71-CB7-OB8-CB6
19	Q	3003	CDL	OA9-CA7-OA8-CA6
19	G	2004	CDL	OB7-CB5-OB6-CB4
19	Q	3003	CDL	CB7-C71-C72-C73
19	D	2003	CDL	CB7-C71-C72-C73
19	Q	3003	CDL	OB9-CB7-OB8-CB6
19	D	2003	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
17	Q	3009	BOG	O5-C1-O1-C1'
17	Q	3009	BOG	O1-C1'-C2'-C3'
17	D	2091	BOG	O5-C5-C6-O6
17	D	2091	BOG	C4-C5-C6-O6
11	A	2005	PEE	C4-O4P-P-O3P
11	N	3005	PEE	C4-O4P-P-O3P
11	C	2008	PEE	C31-C30-O3-C3
11	N	3005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C10-C11-C12-C13
11	C	2007	PEE	C39-C40-C41-C42
11	A	2005	PEE	C14-C15-C16-C17
11	A	2005	PEE	C19-C20-C21-C22
11	N	3005	PEE	C19-C20-C21-C22
11	P	3007	PEE	C39-C40-C41-C42
19	T	3004	CDL	OA7-CA5-OA6-CA4
11	A	2005	PEE	C16-C17-C18-C19
17	P	2010	BOG	C3'-C4'-C5'-C6'
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C17-C18-C19-C20
11	N	3005	PEE	C14-C15-C16-C17
11	N	3005	PEE	C16-C17-C18-C19
17	Q	3009	BOG	C2-C1-O1-C1'
11	A	2005	PEE	C30-C31-C32-C33
11	N	3005	PEE	C18-C19-C20-C21
11	C	2007	PEE	C21-C22-C23-C24
11	P	3007	PEE	C36-C37-C38-C39
11	P	3007	PEE	C40-C41-C42-C43
19	T	3004	CDL	C11-CA5-OA6-CA4
19	G	2004	CDL	C11-CA5-OA6-CA4
11	C	2007	PEE	C36-C37-C38-C39
11	P	3007	PEE	C21-C22-C23-C24
11	C	2007	PEE	C10-C11-C12-C13
17	C	3010	BOG	C3'-C4'-C5'-C6'
11	A	2005	PEE	C18-C19-C20-C21
11	C	2007	PEE	C40-C41-C42-C43
11	N	3005	PEE	C40-C41-C42-C43
11	C	2007	PEE	C34-C35-C36-C37
11	C	2007	PEE	O4P-C4-C5-N
11	N	3005	PEE	C33-C34-C35-C36
11	A	2005	PEE	C40-C41-C42-C43
11	N	3005	PEE	C37-C38-C39-C40
17	D	2091	BOG	C2'-C1'-O1-C1

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Mol	Chain	Res	Type	Atoms
11	A	2005	PEE	C33-C34-C35-C36
11	P	3007	PEE	C12-C13-C14-C15
11	P	3007	PEE	C34-C35-C36-C37
11	A	2005	PEE	C11-C12-C13-C14
11	A	2005	PEE	C37-C38-C39-C40
11	N	3005	PEE	C11-C12-C13-C14
11	P	3007	PEE	C37-C38-C39-C40
11	C	2008	PEE	C11-C10-O2-C2
17	Q	3009	BOG	C2'-C3'-C4'-C5'
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C11-C12-C13-C14
11	P	3007	PEE	C14-C15-C16-C17
19	T	3004	CDL	CB5-C51-C52-C53
19	G	2004	CDL	CB5-C51-C52-C53
11	C	2008	PEE	O5-C30-O3-C3
19	G	2004	CDL	OA7-CA5-OA6-CA4
11	P	3007	PEE	C18-C19-C20-C21
11	C	2007	PEE	C14-C15-C16-C17
11	A	2005	PEE	C10-C11-C12-C13
11	N	3005	PEE	C10-C11-C12-C13
11	C	2007	PEE	C18-C19-C20-C21
11	C	2007	PEE	C11-C12-C13-C14
11	A	2005	PEE	C35-C36-C37-C38
11	C	2008	PEE	O4-C10-O2-C2
17	C	3010	BOG	C4'-C5'-C6'-C7'
11	C	2007	PEE	C12-C13-C14-C15
17	D	2009	BOG	C3'-C4'-C5'-C6'
11	N	3005	PEE	C35-C36-C37-C38
17	D	2009	BOG	C2'-C3'-C4'-C5'
11	P	3007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C15-C16-C17-C18
19	T	3004	CDL	CB3-OB5-PB2-OB2
19	G	2004	CDL	CB3-OB5-PB2-OB2
11	A	2005	PEE	O3P-C1-C2-C3
11	N	3005	PEE	O3P-C1-C2-C3
11	C	2008	PEE	O3P-C1-C2-C3
11	P	3007	PEE	C32-C33-C34-C35
11	A	2005	PEE	C20-C21-C22-C23
19	T	3004	CDL	CA3-CA4-CA6-OA8
15	C	2002	UQ	C5-C6-C7-C8
11	N	3005	PEE	C20-C21-C22-C23
19	T	3004	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
11	C	2007	PEE	C35-C36-C37-C38
19	Q	3003	CDL	C71-C72-C73-C74
19	D	2003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C32-C33-C34-C35
11	P	3007	PEE	C35-C36-C37-C38
19	G	2004	CDL	C31-CA7-OA8-CA6
11	P	3007	PEE	C16-C17-C18-C19
11	A	2005	PEE	C12-C13-C14-C15
11	C	2007	PEE	C16-C17-C18-C19
19	G	2004	CDL	CA3-CA4-CA6-OA8
17	Q	3091	BOG	C3'-C4'-C5'-C6'
19	T	3004	CDL	OA6-CA4-CA6-OA8
19	Q	3003	CDL	OA6-CA4-CA6-OA8
19	D	2003	CDL	OA6-CA4-CA6-OA8
17	D	2091	BOG	C1'-C2'-C3'-C4'
11	N	3005	PEE	C12-C13-C14-C15
11	P	3007	PEE	C43-C44-C45-C46
11	N	3005	PEE	C42-C43-C44-C45
11	C	2007	PEE	C43-C44-C45-C46
11	C	2008	PEE	O3P-C1-C2-O2
19	D	2003	CDL	OB5-CB3-CB4-OB6
19	G	2004	CDL	OA6-CA4-CA6-OA8
11	A	2005	PEE	C42-C43-C44-C45
11	N	3005	PEE	C24-C25-C26-C27
19	D	2003	CDL	CB5-C51-C52-C53
11	A	2005	PEE	C24-C25-C26-C27
17	Q	3009	BOG	C1'-C2'-C3'-C4'
19	G	2004	CDL	CA3-OA5-PA1-OA2
11	A	2005	PEE	C21-C22-C23-C24
19	T	3004	CDL	CA3-OA5-PA1-OA4
19	T	3004	CDL	CB2-OB2-PB2-OB3
19	T	3004	CDL	CB3-OB5-PB2-OB4
19	G	2004	CDL	CA3-OA5-PA1-OA4
19	G	2004	CDL	CB2-OB2-PB2-OB3
19	G	2004	CDL	CB3-OB5-PB2-OB4
11	C	2007	PEE	C33-C34-C35-C36
11	A	2005	PEE	O3P-C1-C2-O2
11	N	3005	PEE	O3P-C1-C2-O2
19	Q	3003	CDL	OB5-CB3-CB4-OB6
11	P	3007	PEE	C33-C34-C35-C36
14	P	3001	FMX	O4-C5-C8-C9
14	P	3001	FMX	O4-C5-C8-C13

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Mol	Chain	Res	Type	Atoms
19	T	3004	CDL	OA9-CA7-OA8-CA6
14	C	2001	FMX	O4-C5-C8-C9
14	C	2001	FMX	O4-C5-C8-C13
19	Q	3003	CDL	CB5-C51-C52-C53
11	N	3005	PEE	C22-C23-C24-C25
11	N	3005	PEE	C17-C18-C19-C20
11	A	2005	PEE	C43-C44-C45-C46
11	A	2005	PEE	C17-C18-C19-C20
17	C	3010	BOG	C1'-C2'-C3'-C4'
11	N	3005	PEE	C21-C22-C23-C24
19	T	3004	CDL	OB6-CB4-CB6-OB8
19	T	3004	CDL	CA2-OA2-PA1-OA5
19	T	3004	CDL	CA3-OA5-PA1-OA2
19	G	2004	CDL	CA2-OA2-PA1-OA5
11	P	3007	PEE	C20-C21-C22-C23
19	Q	3003	CDL	CA3-CA4-CA6-OA8
19	D	2003	CDL	CA3-CA4-CA6-OA8
19	G	2004	CDL	C1-CB2-OB2-PB2
11	A	2005	PEE	C22-C23-C24-C25
19	Q	3003	CDL	OB7-CB5-OB6-CB4
19	T	3004	CDL	OB5-CB3-CB4-OB6
11	N	3005	PEE	C43-C44-C45-C46
19	D	2003	CDL	OB7-CB5-OB6-CB4
19	G	2004	CDL	OB6-CB4-CB6-OB8
19	G	2004	CDL	OA9-CA7-OA8-CA6
17	Q	3091	BOG	C2'-C3'-C4'-C5'
11	N	3005	PEE	C15-C16-C17-C18
11	C	2007	PEE	C20-C21-C22-C23
19	Q	3003	CDL	CA3-OA5-PA1-OA2
19	T	3004	CDL	C1-CB2-OB2-PB2
19	G	2004	CDL	OB5-CB3-CB4-OB6
17	Q	3091	BOG	O1-C1'-C2'-C3'
19	D	2003	CDL	C52-C51-CB5-OB6
19	Q	3003	CDL	C51-CB5-OB6-CB4
11	A	2005	PEE	C15-C16-C17-C18
19	Q	3003	CDL	C52-C51-CB5-OB6
19	D	2003	CDL	OB5-CB3-CB4-CB6
11	C	2008	PEE	O3-C30-C31-C32
11	P	3007	PEE	O3-C30-C31-C32
19	D	2003	CDL	C51-CB5-OB6-CB4
19	D	2003	CDL	CA3-OA5-PA1-OA2
11	C	2008	PEE	O5-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
11	P	3007	PEE	O2-C10-C11-C12
11	N	3005	PEE	C1-C2-O2-C10
17	Q	3009	BOG	C4'-C5'-C6'-C7'
11	C	2007	PEE	O2-C10-C11-C12
11	C	2007	PEE	O3-C30-C31-C32
11	N	3005	PEE	C39-C40-C41-C42
19	Q	3003	CDL	OB5-CB3-CB4-CB6
11	P	3007	PEE	O5-C30-C31-C32
11	P	3007	PEE	O4-C10-C11-C12
19	D	2003	CDL	C12-C11-CA5-OA7
19	T	3004	CDL	CB3-CB4-CB6-OB8
11	C	2007	PEE	O5-C30-C31-C32
11	C	2007	PEE	O4-C10-C11-C12
14	P	3001	FMX	C6-C5-C8-C9
11	A	2005	PEE	C1-C2-O2-C10
14	C	2001	FMX	C6-C5-C8-C9
14	C	2001	FMX	C6-C5-C8-C13
19	D	2003	CDL	C72-C71-CB7-OB8
17	D	2091	BOG	C2'-C3'-C4'-C5'
11	C	2008	PEE	O2-C10-C11-C12
11	A	2005	PEE	C39-C40-C41-C42
19	Q	3003	CDL	C12-C11-CA5-OA6
19	D	2003	CDL	C12-C11-CA5-OA6

There are no ring outliers.

20 monomers are involved in 48 short contacts:

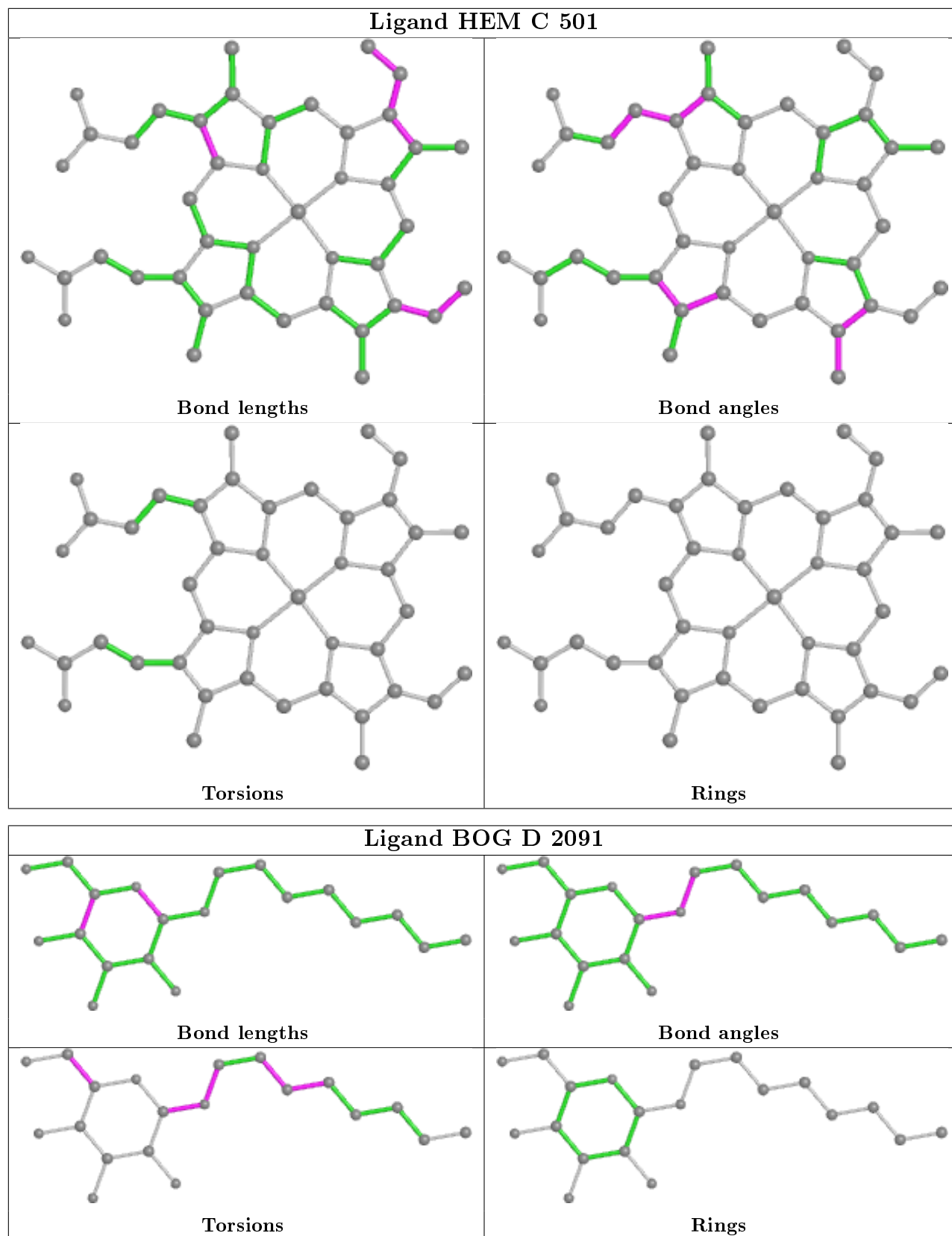
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	501	HEM	4	0
17	D	2091	BOG	2	0
17	Q	3091	BOG	1	0
20	E	501	FES	1	0
14	P	3001	FMX	2	0
20	R	501	FES	1	0
19	D	2003	CDL	2	0
15	C	2002	UQ	5	0
17	P	2010	BOG	1	0
18	Q	501	HEC	2	0
13	P	502	HEM	4	0
13	C	502	HEM	4	0
19	T	3004	CDL	1	0
13	P	501	HEM	3	0

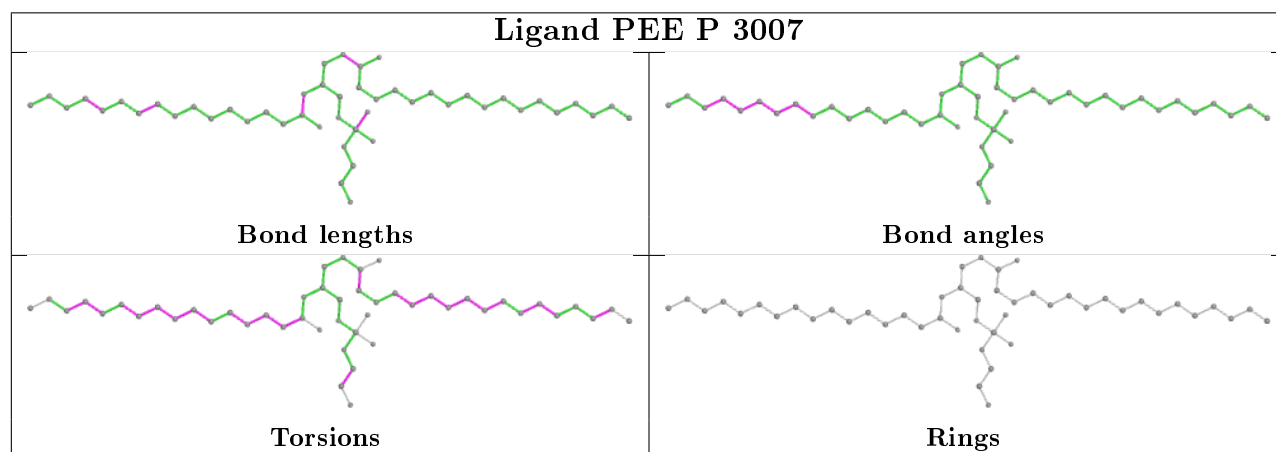
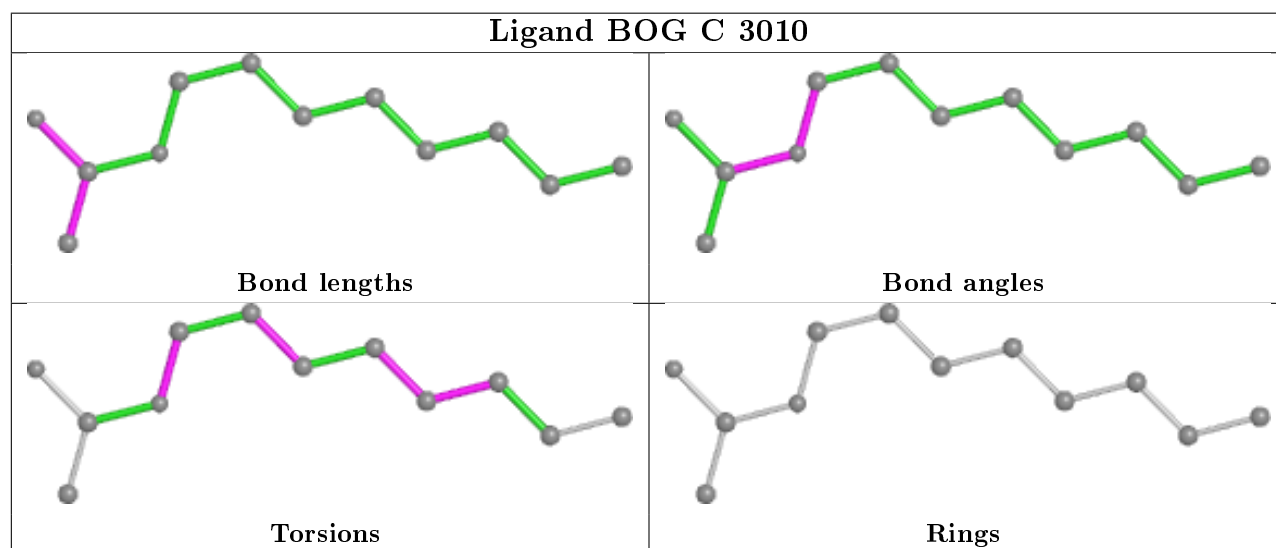
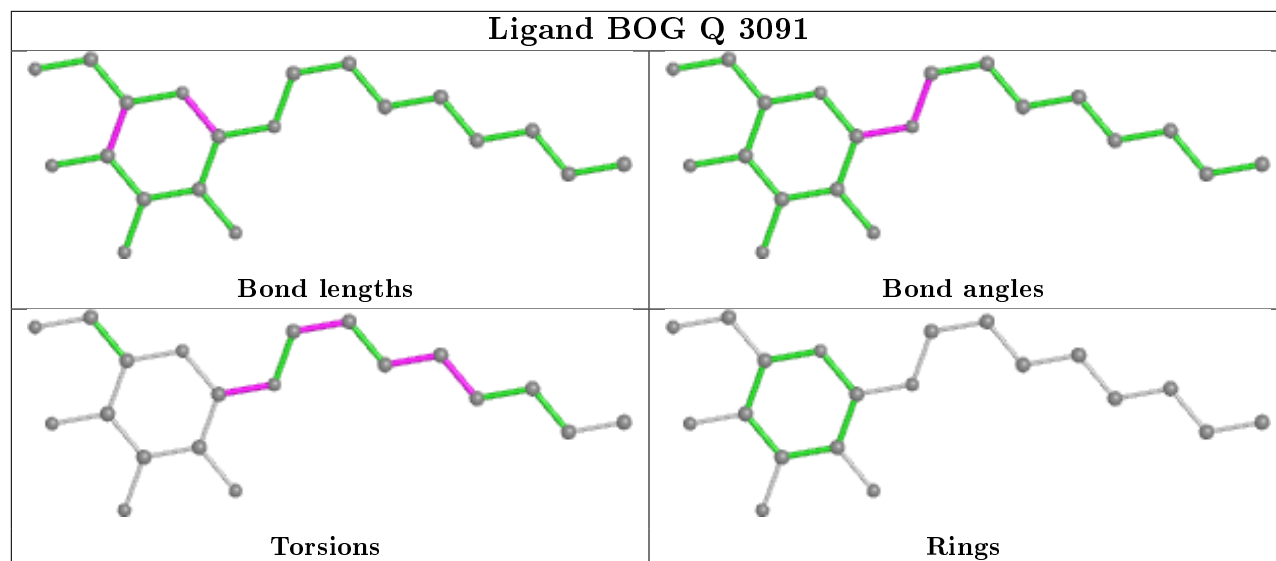
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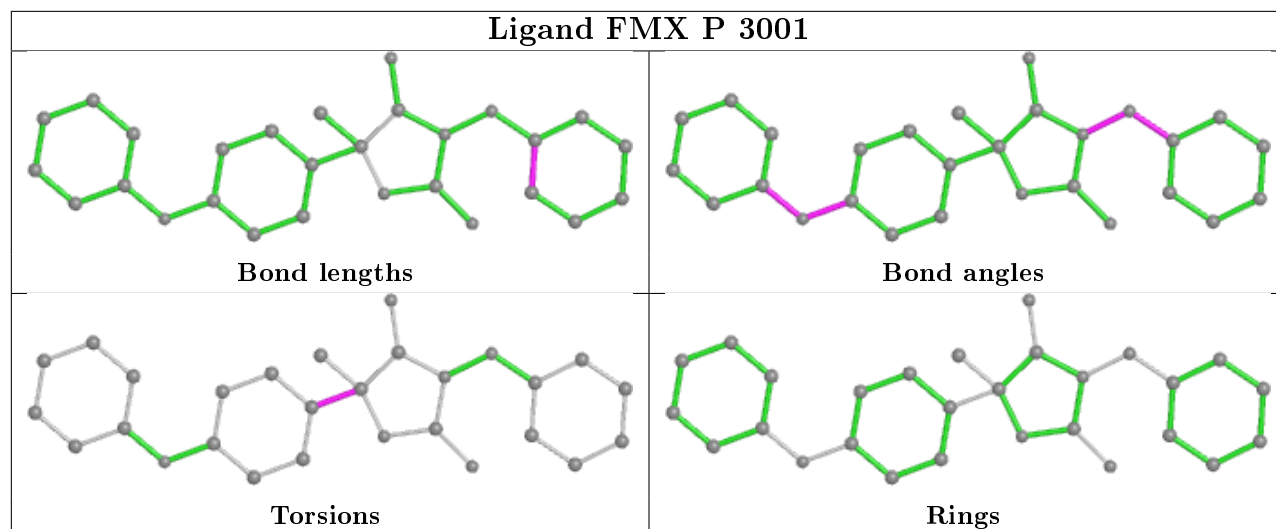
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	2004	CDL	2	0
18	D	501	HEC	4	0
17	D	2009	BOG	1	0
19	Q	3003	CDL	3	0
14	C	2001	FMX	2	0
15	P	3002	UQ	3	0

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.

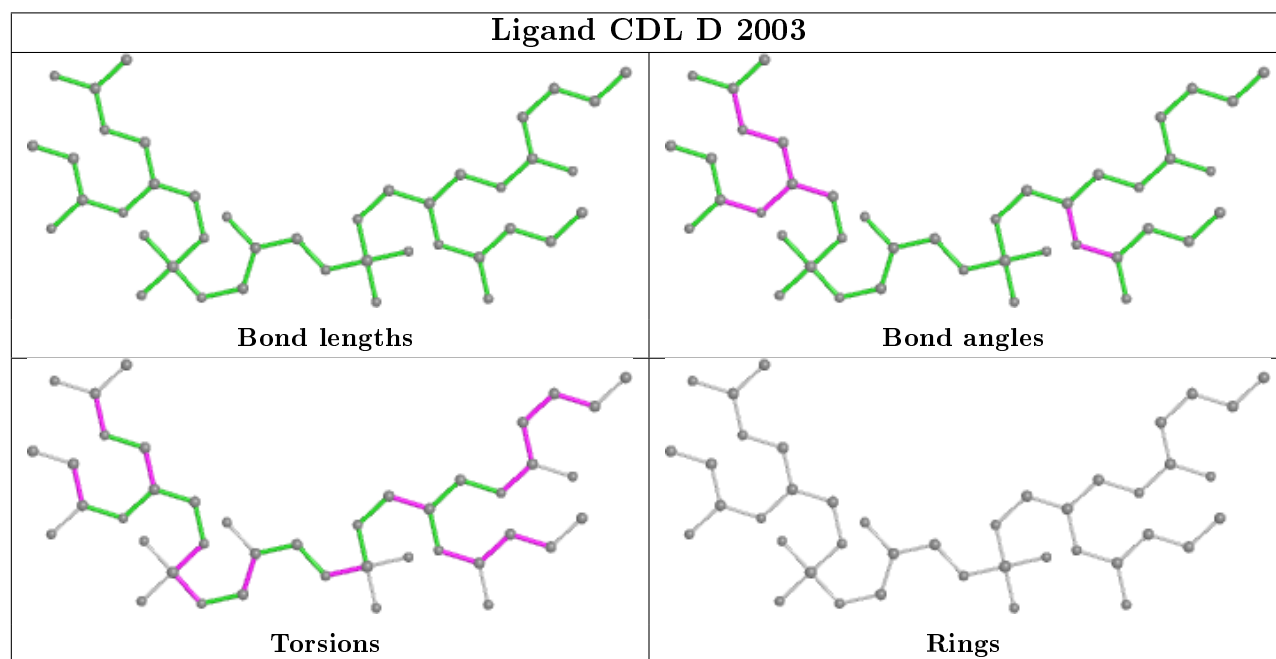


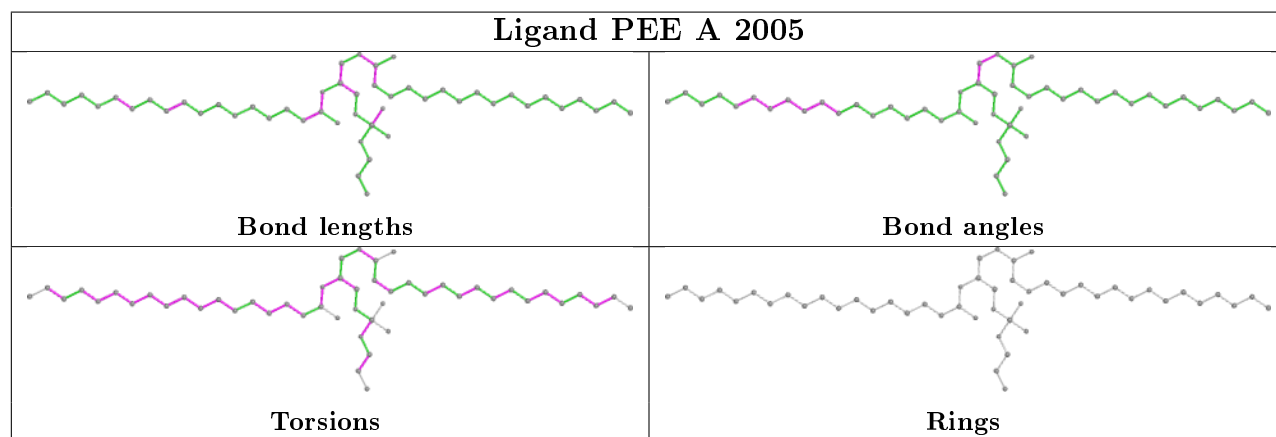
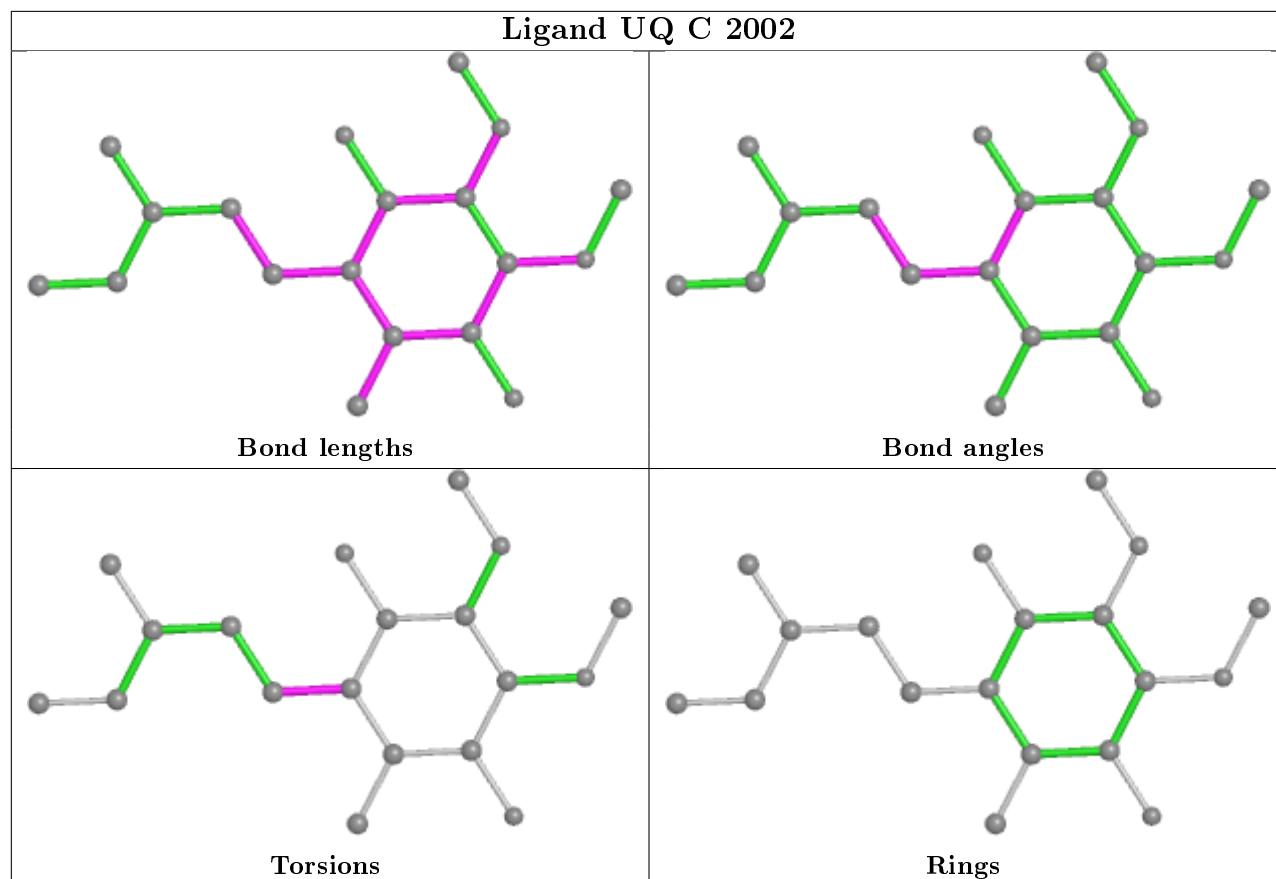


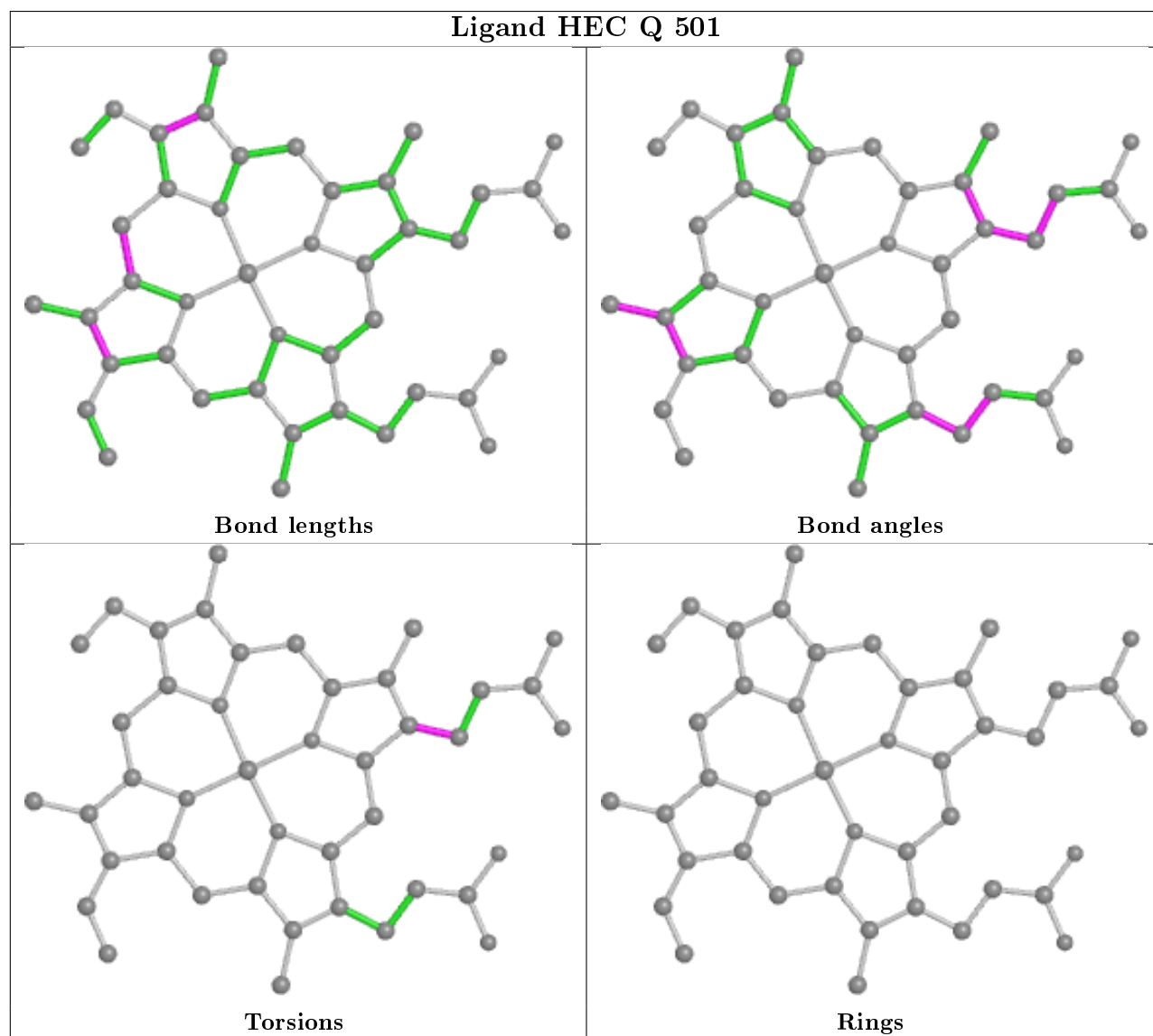
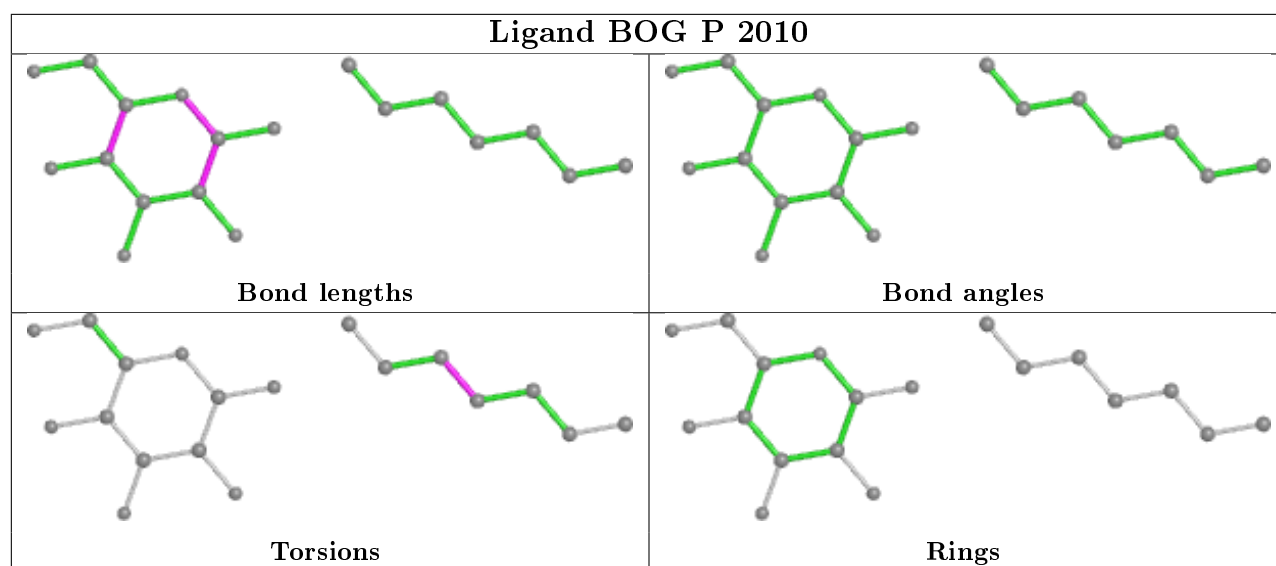
Ligand FMX P 3001

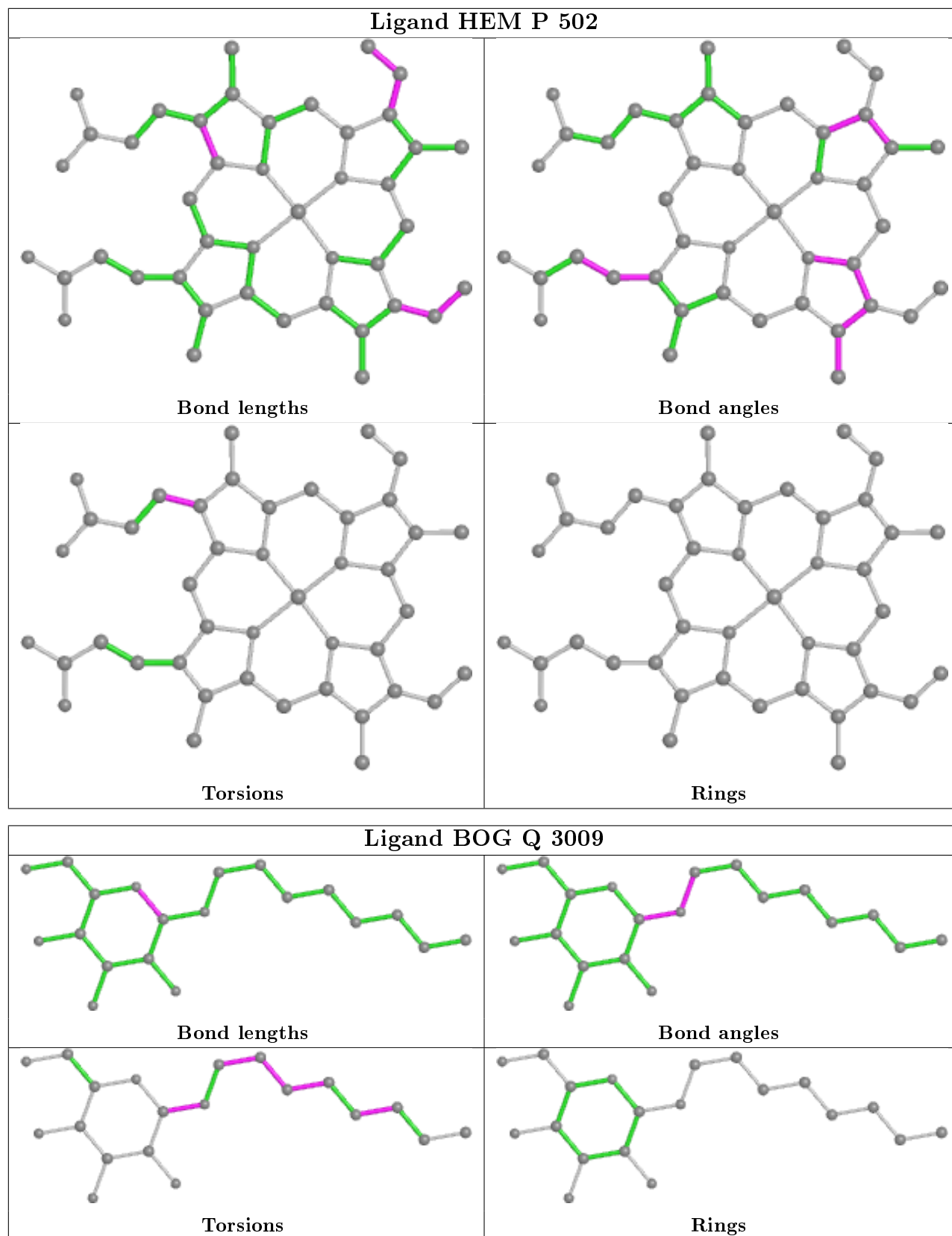


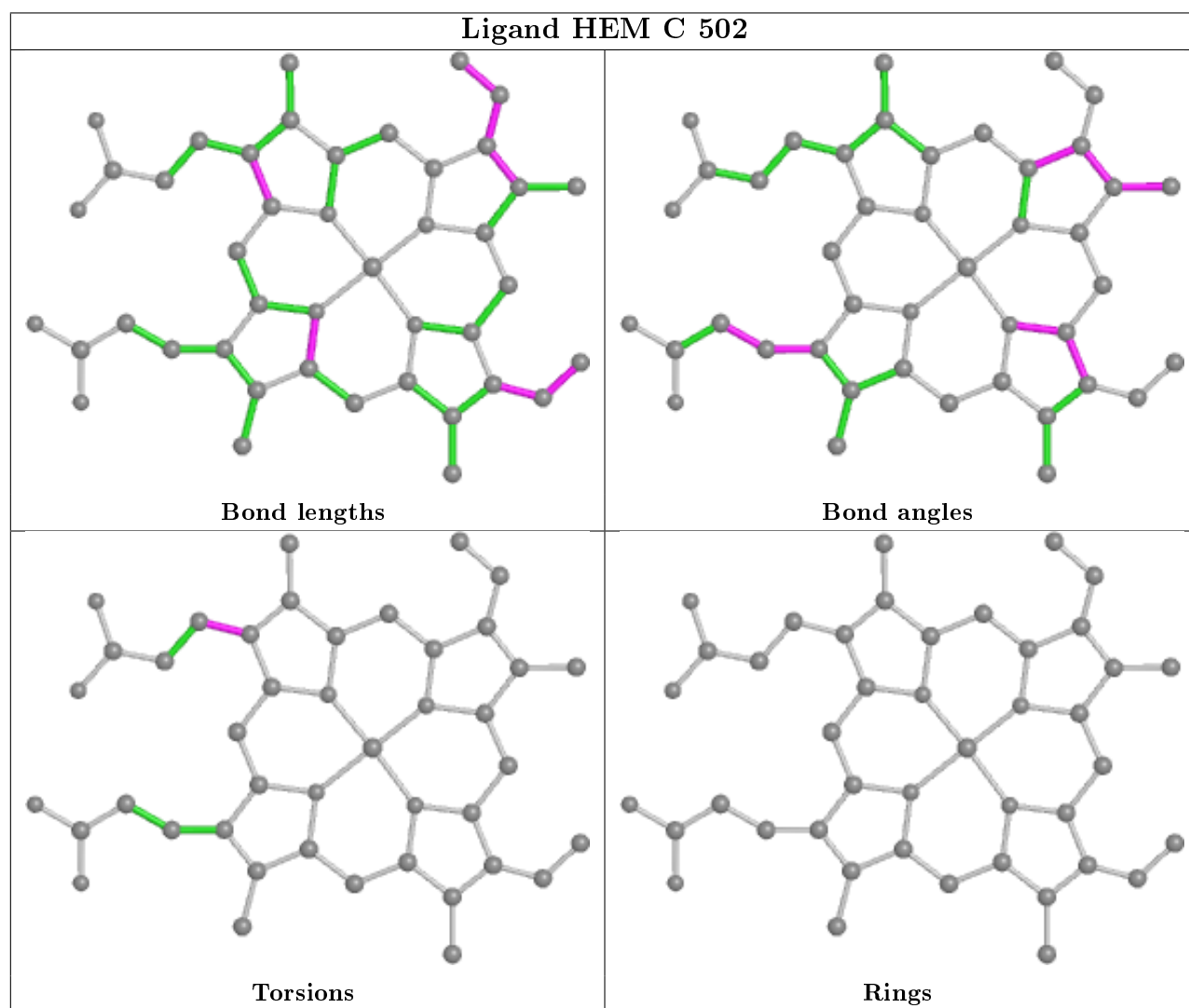
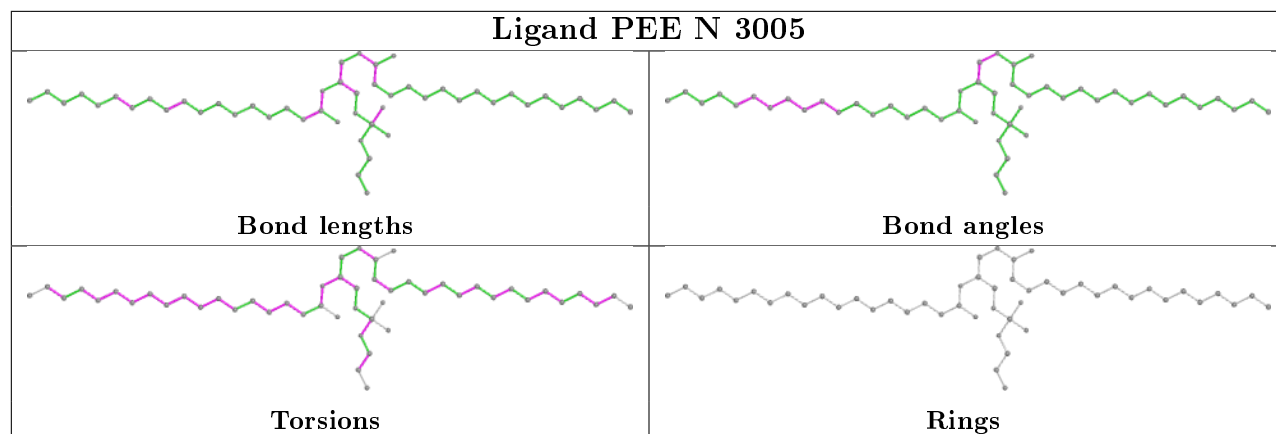
Ligand CDL D 2003



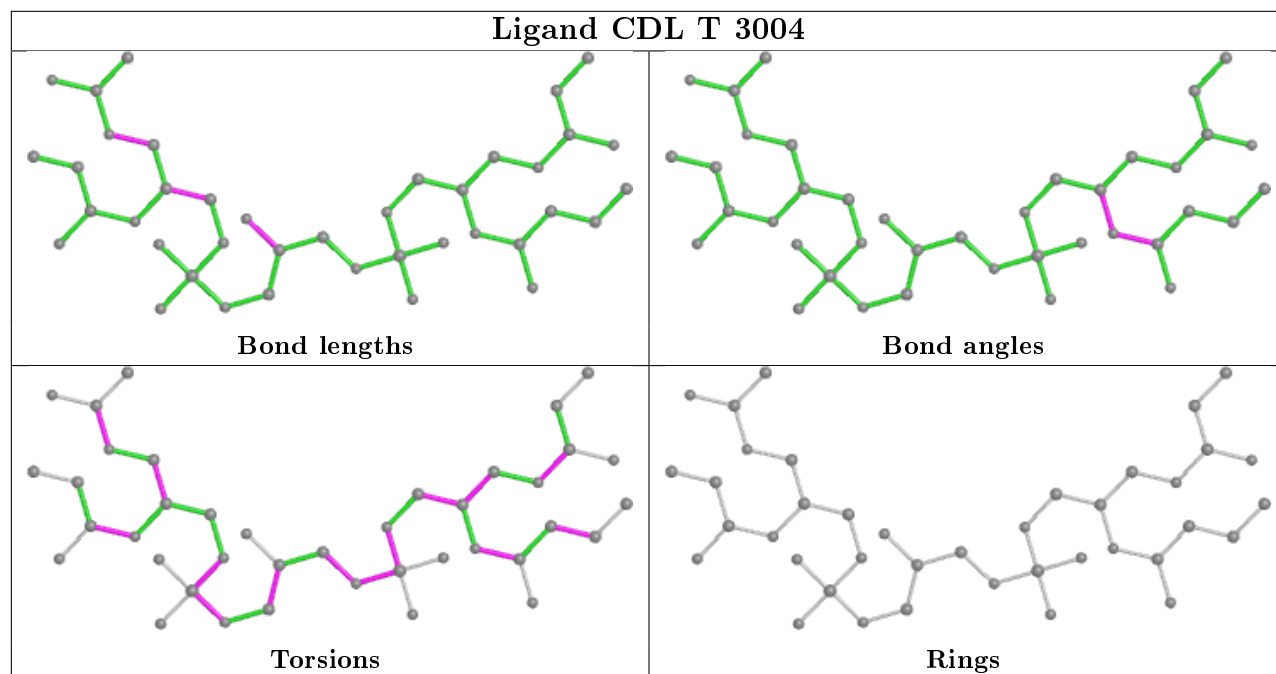




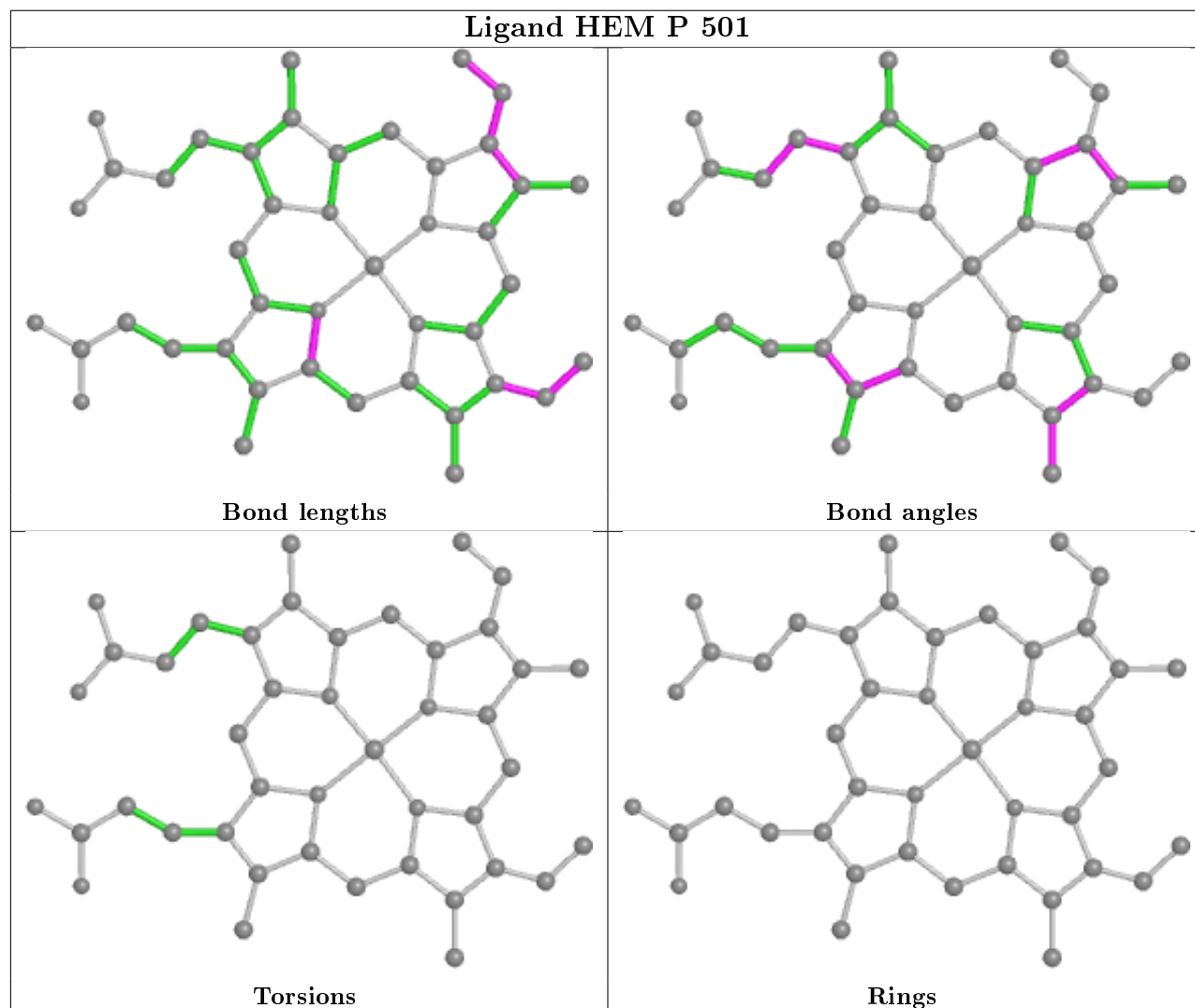


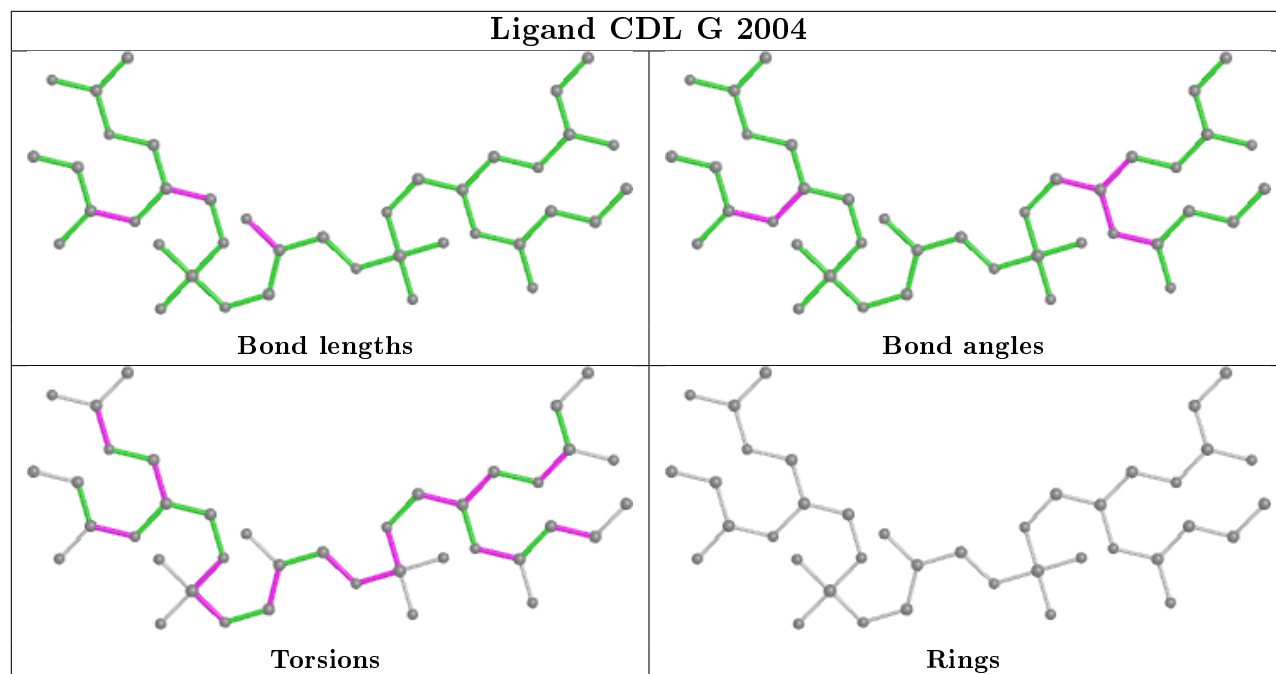


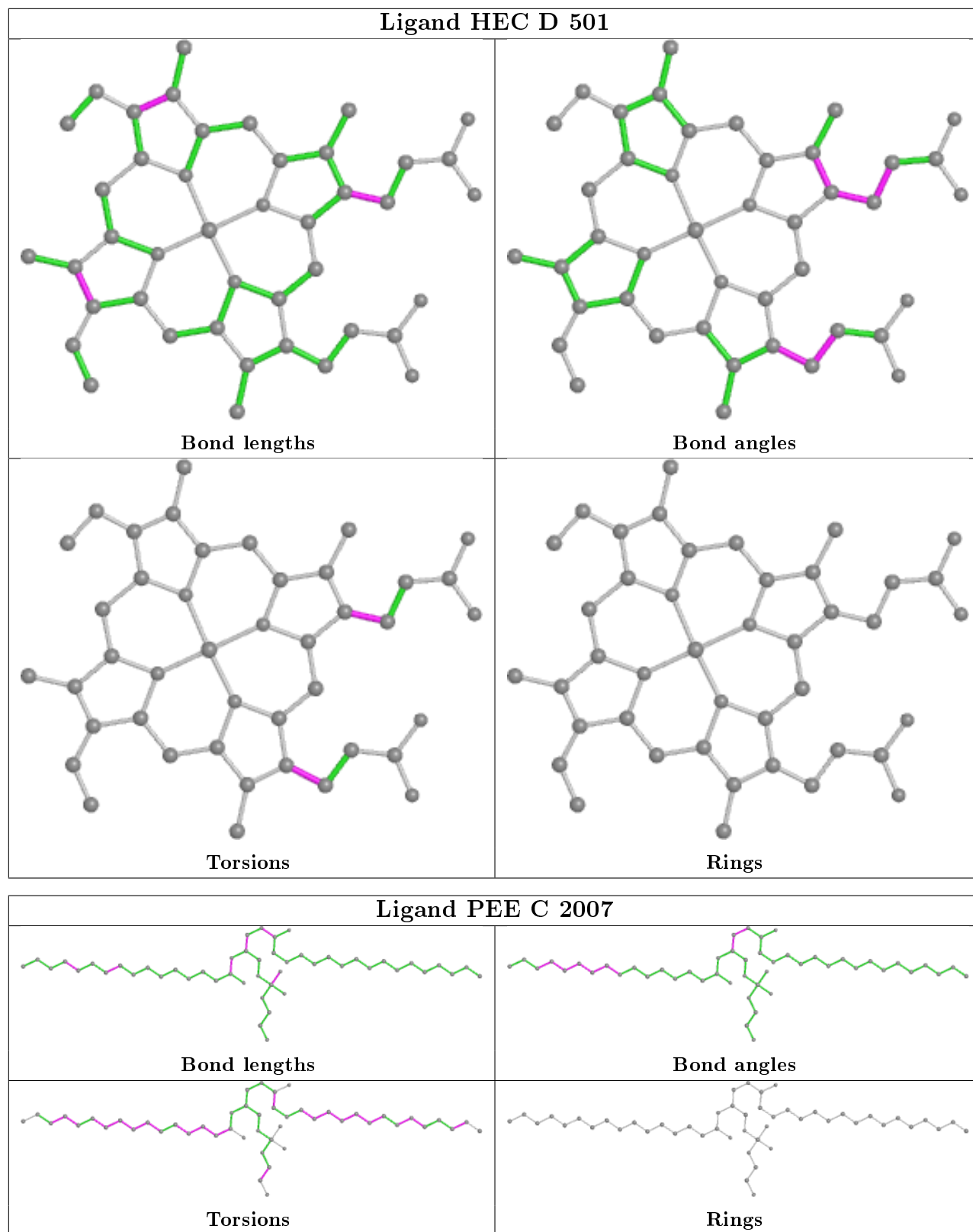
Ligand CDL T 3004

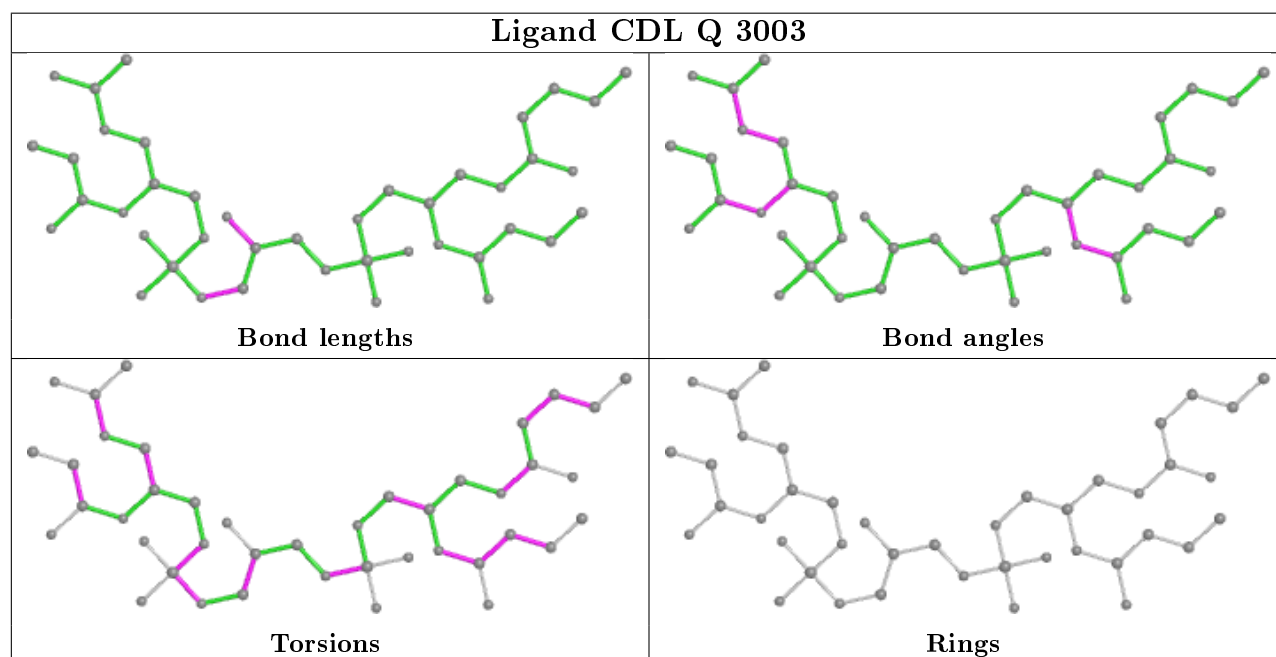
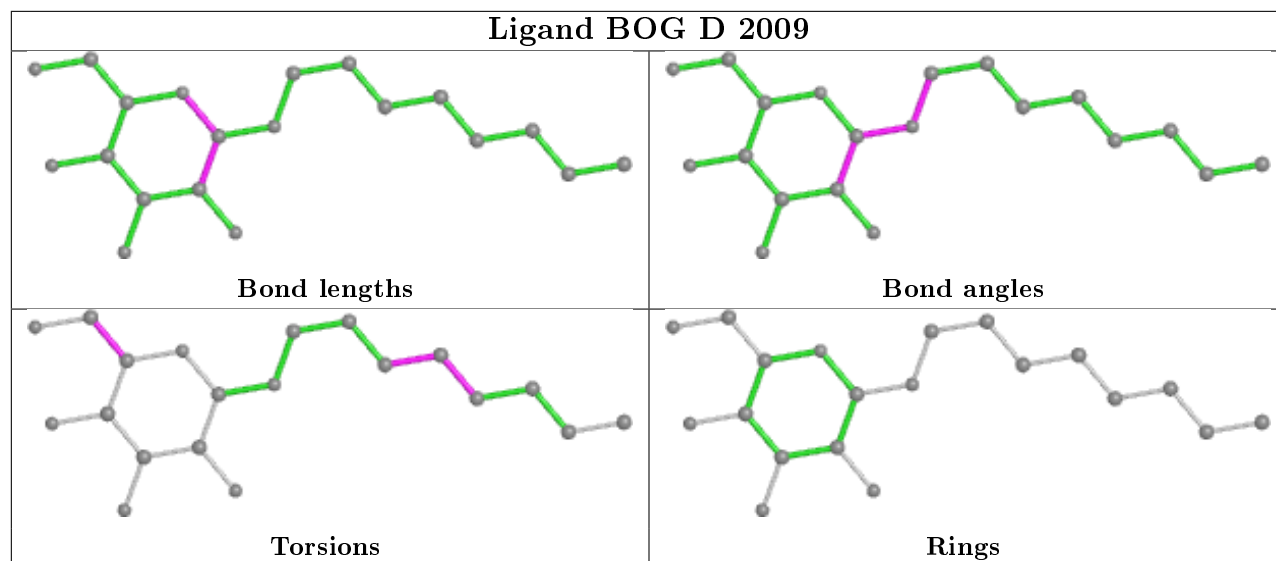


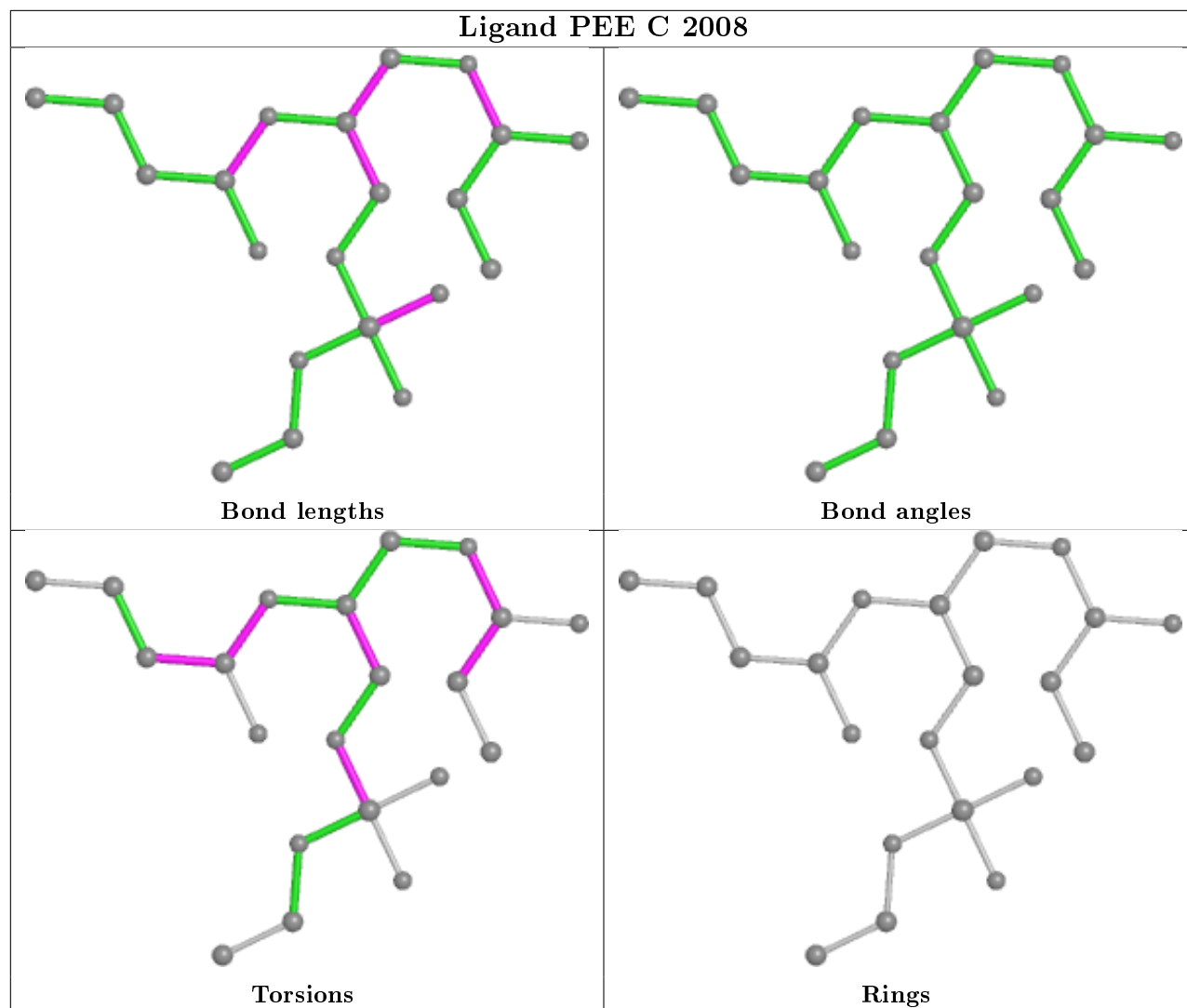
Ligand HEM P 501

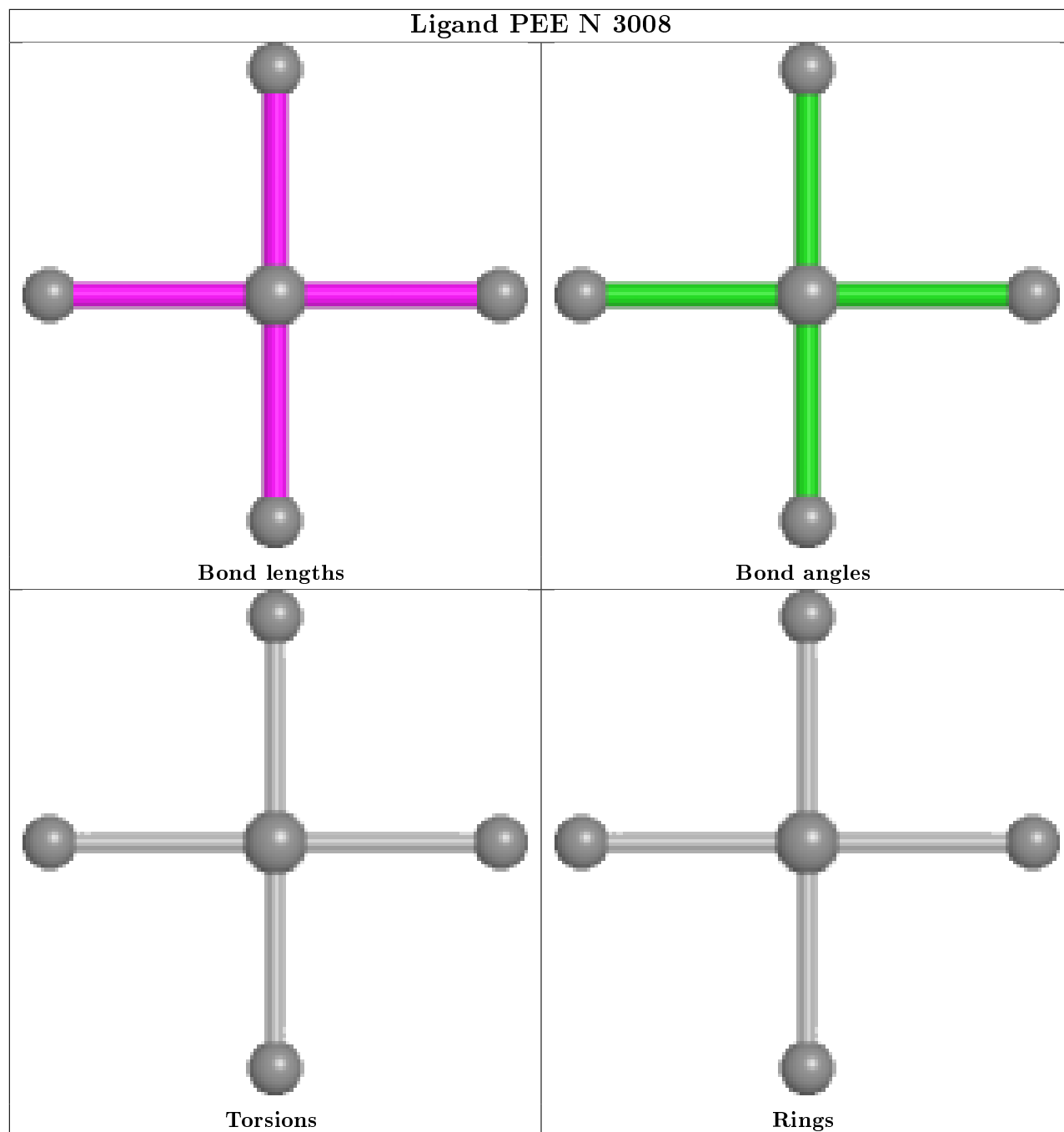


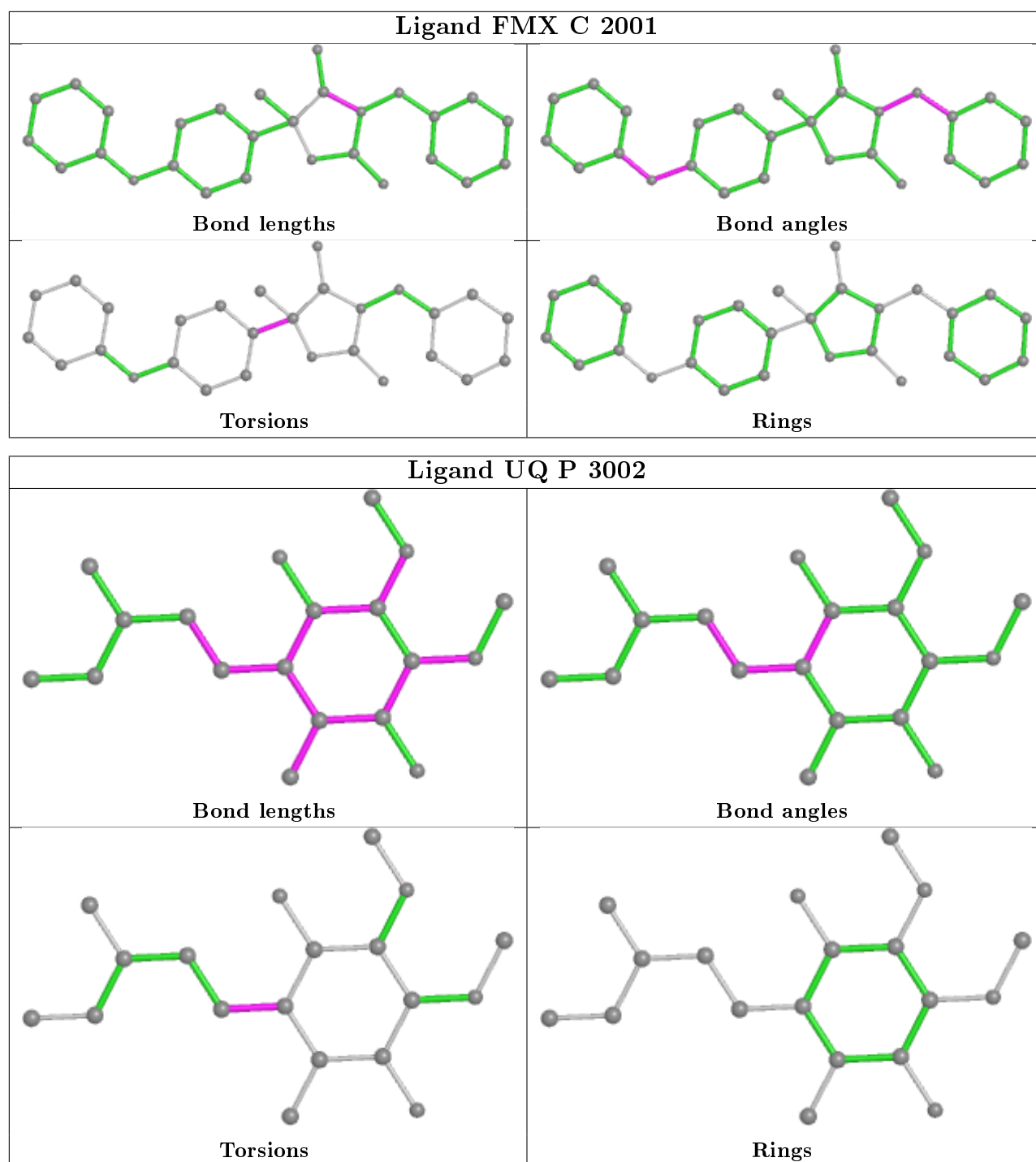












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.03	6 (1%) 75 82	29, 57, 82, 98	0
1	N	442/446 (99%)	0.24	16 (3%) 42 51	33, 64, 89, 98	0
2	B	421/441 (95%)	0.36	24 (5%) 23 28	44, 74, 109, 137	0
2	O	422/441 (95%)	0.15	9 (2%) 63 72	32, 69, 100, 114	0
3	C	380/380 (100%)	0.02	1 (0%) 94 96	18, 33, 63, 102	0
3	P	379/380 (99%)	0.17	3 (0%) 86 90	26, 56, 76, 85	0
4	D	241/241 (100%)	-0.15	1 (0%) 92 95	25, 36, 70, 88	0
4	Q	241/241 (100%)	0.17	11 (4%) 32 39	39, 65, 91, 114	0
5	E	196/196 (100%)	0.78	32 (16%) 1 1	33, 80, 112, 120	0
5	R	196/196 (100%)	1.77	69 (35%) 0 0	32, 102, 153, 158	0
6	F	101/110 (91%)	-0.34	0 100 100	19, 35, 54, 85	0
6	S	101/110 (91%)	0.29	2 (1%) 65 73	52, 65, 106, 131	0
7	G	81/81 (100%)	0.01	1 (1%) 79 85	28, 46, 82, 97	0
7	T	78/81 (96%)	0.75	7 (8%) 9 11	43, 77, 139, 156	0
8	H	70/77 (90%)	0.02	3 (4%) 35 42	34, 51, 75, 115	0
8	U	67/77 (87%)	1.11	10 (14%) 2 2	87, 108, 130, 134	0
9	I	31/47 (65%)	2.18	14 (45%) 0 0	80, 102, 120, 121	0
9	V	31/47 (65%)	2.09	13 (41%) 0 0	65, 105, 136, 138	0
10	J	61/61 (100%)	0.29	5 (8%) 11 14	40, 53, 85, 124	0
10	W	60/61 (98%)	0.87	4 (6%) 17 21	52, 70, 96, 105	0
All	All	4042/4160 (97%)	0.31	231 (5%) 23 28	18, 61, 109, 158	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	W	63	GLU	12.1
5	R	195	VAL	9.2
10	W	62	SER	8.7
5	R	193	VAL	8.3
5	R	133	VAL	8.2
5	R	114	VAL	8.0
5	R	80	ASP	7.5
5	R	127	VAL	7.3
2	B	226	ILE	7.0
5	R	87	VAL	6.7
7	T	77	TYR	6.5
5	R	130	PRO	6.5
5	R	132	TRP	6.4
9	V	63	ASP	6.3
5	R	194	VAL	6.3
5	R	112	VAL	6.2
5	R	116	LYS	6.0
8	H	9	GLU	5.9
7	T	78	GLU	5.9
5	R	115	SER	5.9
5	R	176	ALA	5.7
9	V	77	ARG	5.6
5	R	192	LEU	5.5
3	C	1	MET	5.4
5	R	191	ASP	5.3
5	R	93	GLY	5.3
5	R	79	SER	5.3
10	W	61	ALA	5.2
5	R	184	THR	5.1
5	R	185	TYR	5.1
5	R	117	LEU	5.1
10	J	63	GLU	4.9
5	E	111	GLU	4.8
4	Q	139	ALA	4.8
5	R	104	ALA	4.8
5	R	113	ASP	4.7
5	R	118	ARG	4.7
7	T	75	ALA	4.6
5	R	98	VAL	4.6
5	R	175	PRO	4.6
5	R	109	GLU	4.6
10	J	61	ALA	4.5
8	U	49	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	402	ILE	4.4
9	I	51	CYS	4.3
6	S	11	ARG	4.2
1	A	69	LYS	4.2
9	I	63	ASP	4.2
5	R	136	VAL	4.2
2	B	33	LEU	4.2
5	E	112	VAL	4.1
5	R	172	ARG	4.1
10	J	64	GLU	4.0
8	H	10	GLU	4.0
5	E	133	VAL	4.0
5	R	120	PRO	3.9
5	R	174	GLY	3.9
2	O	19	PRO	3.9
1	N	182	LEU	3.9
9	I	77	ARG	3.9
8	U	44	VAL	3.9
7	T	79	ASN	3.9
5	R	183	PRO	3.8
5	R	94	LYS	3.8
5	R	99	ARG	3.8
5	R	119	ASP	3.8
9	I	47	ARG	3.8
5	E	89	PHE	3.8
10	J	62	SER	3.8
6	S	15	ARG	3.7
9	I	53	GLU	3.7
7	G	1	GLY	3.7
8	U	26	GLN	3.6
5	E	132	TRP	3.6
5	R	74	ILE	3.6
5	R	177	PRO	3.6
5	E	81	ILE	3.6
5	R	81	ILE	3.6
8	U	50	THR	3.6
9	V	55	MET	3.5
1	N	124	GLU	3.5
9	V	70	LEU	3.5
5	R	153	PHE	3.5
5	E	85	LYS	3.5
9	V	49	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
5	R	164	HIS	3.4
5	R	163	SER	3.4
5	E	80	ASP	3.4
5	E	114	VAL	3.4
9	I	50	LEU	3.3
9	I	52	ARG	3.3
7	T	74	PRO	3.3
2	B	236	LYS	3.3
1	A	2	ALA	3.3
2	B	29	LEU	3.3
2	O	299	VAL	3.3
5	R	173	LYS	3.3
5	E	195	VAL	3.2
5	E	186	GLN	3.2
8	U	13	LEU	3.2
1	N	179	ARG	3.2
1	N	75	PHE	3.2
2	O	304	THR	3.2
5	E	188	VAL	3.2
5	R	131	GLU	3.1
5	R	111	GLU	3.1
4	Q	180	SER	3.1
9	I	70	LEU	3.1
5	R	103	GLN	3.1
5	R	122	HIS	3.1
4	Q	145	GLU	3.1
1	N	54	GLY	3.1
5	R	89	PHE	3.1
5	R	162	GLY	3.0
5	E	122	HIS	3.0
5	R	108	GLN	3.0
5	R	128	LYS	3.0
5	R	160	CYS	3.0
9	V	62	ARG	3.0
4	Q	143	VAL	3.0
5	R	134	ILE	2.9
9	V	59	SER	2.9
5	E	167	ALA	2.9
5	R	72	SER	2.9
9	V	76	VAL	2.9
5	R	178	TYR	2.9
5	E	76	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	346	HIS	2.8
5	E	101	ARG	2.8
2	B	369	LEU	2.8
5	R	155	GLY	2.8
5	E	100	HIS	2.7
2	B	350	GLY	2.7
5	R	76	ILE	2.7
5	R	124	LEU	2.7
2	B	223	PHE	2.7
5	E	185	TYR	2.7
5	E	82	PRO	2.7
2	B	230	ALA	2.6
9	I	60	ALA	2.6
5	R	95	PRO	2.6
5	R	105	GLU	2.6
5	E	78	LEU	2.6
9	V	50	LEU	2.6
5	R	78	LEU	2.6
5	R	123	ASP	2.6
5	R	140	THR	2.6
2	B	439	LEU	2.6
1	N	190	PHE	2.6
8	U	76	LYS	2.6
2	B	124	LEU	2.5
8	H	71	HIS	2.5
4	Q	147	LEU	2.5
2	B	120	MET	2.5
5	R	86	ASN	2.5
9	I	64	LEU	2.5
1	A	226	ASP	2.5
1	A	68	LYS	2.4
5	E	110	ALA	2.4
5	E	194	VAL	2.4
2	B	204	MET	2.4
5	E	74	ILE	2.4
2	B	200	THR	2.4
4	D	241	LYS	2.4
4	Q	141	VAL	2.4
1	N	123	GLU	2.4
1	N	218	GLY	2.4
5	E	137	GLY	2.3
5	R	196	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	34	ILE	2.3
7	T	72	LYS	2.3
1	N	178	THR	2.3
2	B	205	ALA	2.3
1	A	209	VAL	2.3
2	O	23	ASP	2.3
9	I	73	PRO	2.3
2	O	302	ALA	2.3
3	P	373	LEU	2.3
1	N	177	LEU	2.3
2	O	368	TYR	2.3
1	N	127	ILE	2.3
9	V	58	ARG	2.3
1	N	69	LYS	2.3
1	N	57	TYR	2.3
5	E	99	ARG	2.3
2	O	266	SER	2.2
9	V	56	SER	2.2
9	I	72	ALA	2.2
5	R	106	ILE	2.2
5	R	159	PRO	2.2
9	V	48	PRO	2.2
2	B	201	SER	2.2
4	Q	69	GLU	2.2
5	E	104	ALA	2.2
4	Q	68	VAL	2.2
1	N	122	LEU	2.2
2	B	267	ALA	2.2
2	O	223	PHE	2.2
8	U	12	GLU	2.1
2	B	274	VAL	2.1
5	E	192	LEU	2.1
3	P	320	PRO	2.1
2	B	400	GLN	2.1
1	N	68	LYS	2.1
8	U	39	LEU	2.1
5	E	75	GLU	2.1
5	E	156	TYR	2.1
5	R	77	LYS	2.1
9	I	54	SER	2.1
9	V	60	ALA	2.1
2	B	304	THR	2.1

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Mol	Chain	Res	Type	RSRZ
8	U	43	ARG	2.1
9	I	69	SER	2.1
10	J	15	ARG	2.1
2	B	221	GLU	2.1
5	E	84	GLY	2.1
1	N	138	LEU	2.1
1	A	21	ASN	2.0
5	R	75	GLU	2.0
5	R	110	ALA	2.0
4	Q	82	MET	2.0
10	W	45	HIS	2.0
2	B	35	ILE	2.0
7	T	38	TRP	2.0
2	O	387	LEU	2.0
5	E	180	LEU	2.0
4	Q	167	GLU	2.0
4	Q	1	GLY	2.0
5	E	187	PHE	2.0
8	U	74	PHE	2.0
2	B	227	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
17	BOG	D	2091	20/20	0.22	0.71	171,182,183,184	0
17	BOG	Q	3091	20/20	0.32	0.80	172,179,180,180	0
12	UNL	P	3048	2/-	0.41	0.28	93,93,93,95	0

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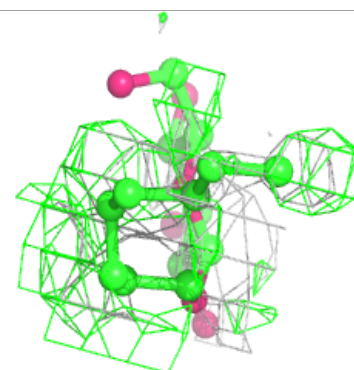
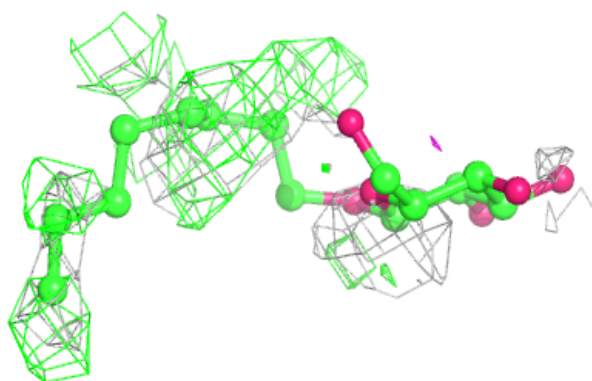
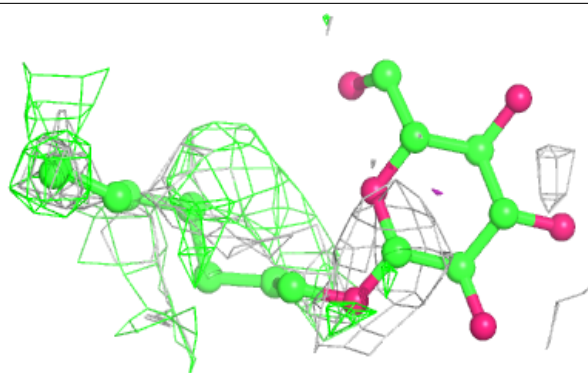
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
17	BOG	P	2010	19/20	0.53	0.48	97,177,178,178	0
12	UNL	P	3013	1/-	0.62	0.48	72,72,72,72	0
12	UNL	P	3046	2/-	0.68	0.75	85,85,85,86	0
15	UQ	P	3002	19/63	0.75	0.40	132,136,138,138	0
15	UQ	C	2002	19/63	0.76	0.36	80,84,86,86	0
12	UNL	C	2046	2/-	0.78	0.47	78,78,78,80	0
12	UNL	P	3014	1/-	0.79	0.43	55,55,55,55	0
16	AZI	C	2011	3/3	0.81	0.48	62,62,63,64	0
11	PEE	A	2005	50/51	0.83	0.30	74,85,89,90	0
11	PEE	N	3005	50/51	0.83	0.30	64,92,98,98	0
12	UNL	E	2012	2/-	0.83	0.32	51,51,51,51	0
19	CDL	Q	3003	42/100	0.83	0.26	114,118,123,124	0
19	CDL	T	3004	40/100	0.84	0.23	85,89,100,101	0
12	UNL	P	3047	1/-	0.84	0.30	45,45,45,45	0
12	UNL	A	3015	1/-	0.84	0.29	45,45,45,45	0
12	UNL	Q	3012	1/-	0.86	0.32	33,33,33,33	0
19	CDL	D	2003	42/100	0.86	0.20	60,75,87,88	0
17	BOG	Q	3009	20/20	0.87	0.22	69,80,83,84	0
11	PEE	C	2008	21/51	0.88	0.23	89,103,110,111	0
16	AZI	P	3011	3/3	0.91	0.44	66,66,68,68	0
14	FMX	P	3001	28/28	0.91	0.21	55,65,70,71	0
11	PEE	P	3007	48/51	0.91	0.28	71,83,98,100	0
17	BOG	C	3010	12/20	0.92	0.29	78,81,83,84	0
19	CDL	G	2004	40/100	0.92	0.21	48,63,77,78	0
17	BOG	D	2009	20/20	0.93	0.19	47,57,61,61	0
14	FMX	C	2001	28/28	0.93	0.21	31,49,61,62	0
12	UNL	C	2048	2/-	0.93	0.24	41,41,41,45	0
11	PEE	N	3008	5/51	0.94	0.14	74,74,75,76	0
11	PEE	C	2007	48/51	0.95	0.22	33,49,72,72	0
12	UNL	C	2047	1/-	0.96	0.37	28,28,28,28	0
18	HEC	Q	501	43/43	0.96	0.18	40,49,58,60	0
20	FES	R	501	4/4	0.98	0.10	85,85,86,86	0
13	HEM	P	502	43/43	0.98	0.16	32,38,50,56	0
20	FES	E	501	4/4	0.98	0.11	72,73,74,74	0
13	HEM	P	501	43/43	0.98	0.20	37,41,52,56	0
13	HEM	C	501	43/43	0.98	0.21	17,27,37,40	0
18	HEC	D	501	43/43	0.98	0.17	14,25,29,32	0
13	HEM	C	502	43/43	0.99	0.17	15,20,28,32	0

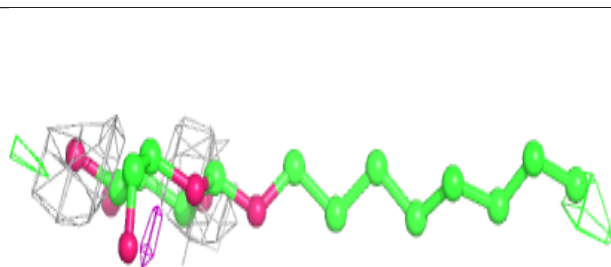
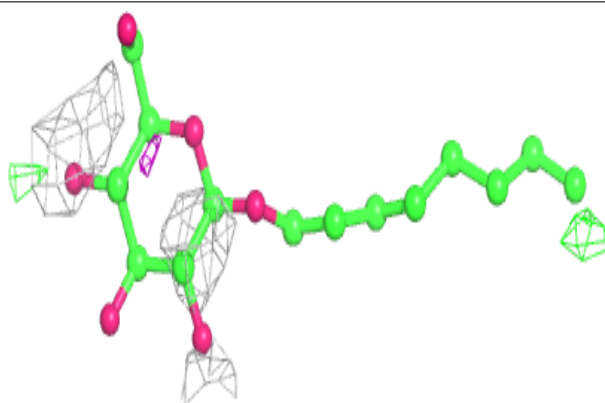
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG D 2091:

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

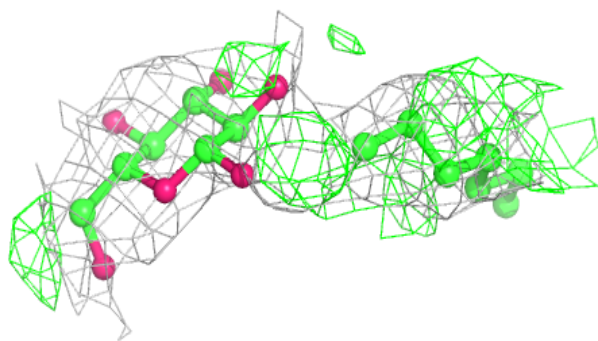
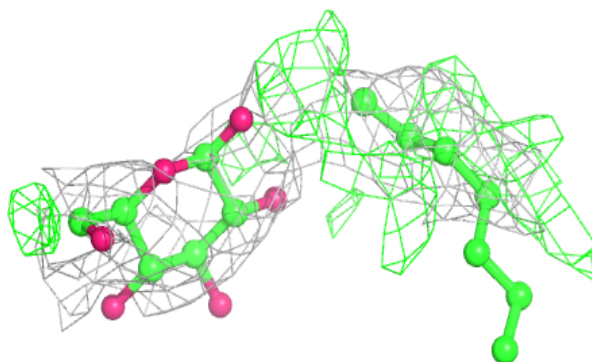
**Electron density around BOG Q 3091:**

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

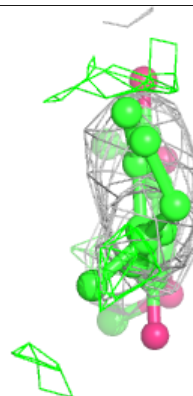
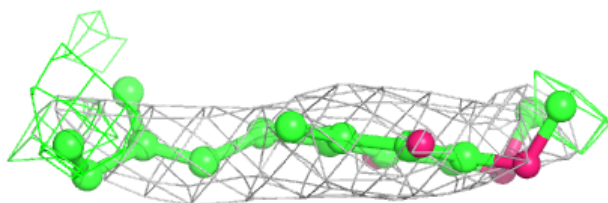
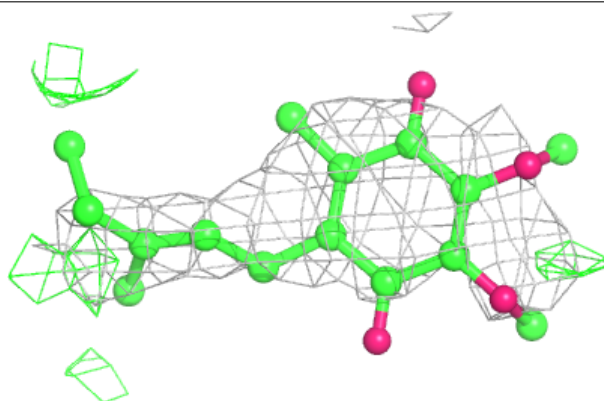


Electron density around BOG P 2010:

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

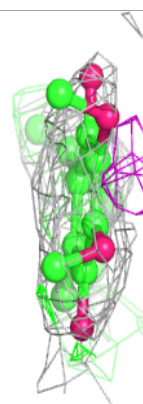
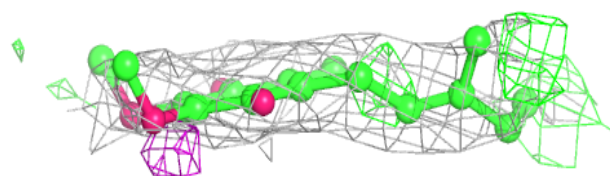
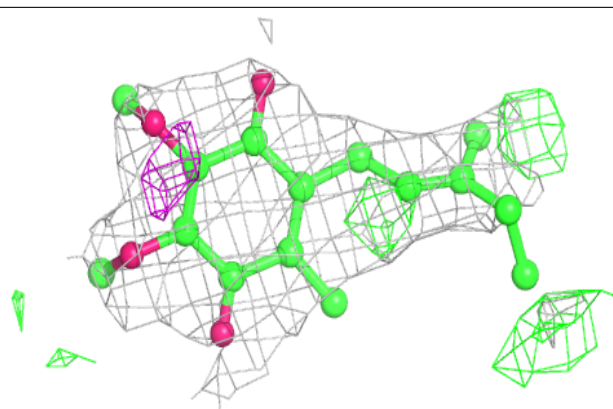
**Electron density around UQ P 3002:**

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

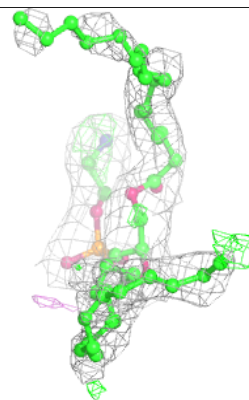
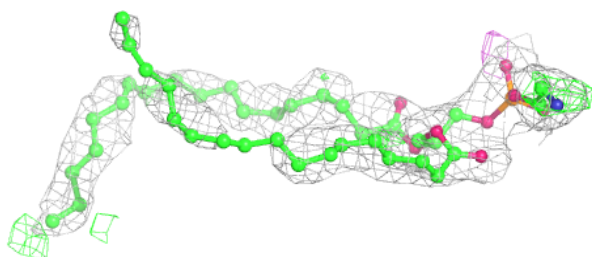
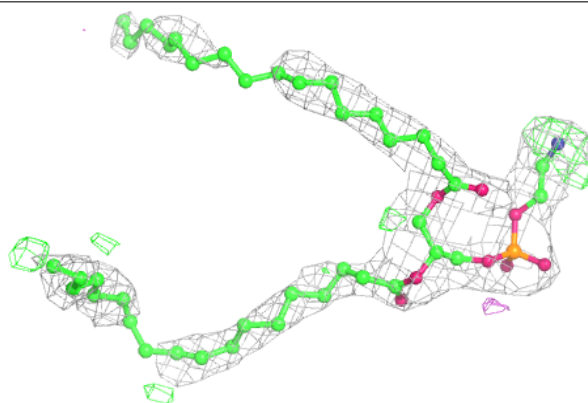


Electron density around UQ C 2002:

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

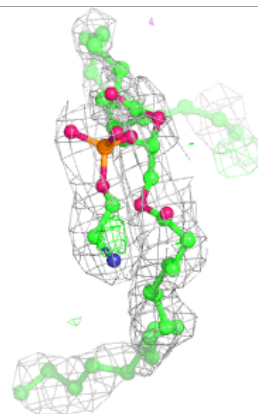
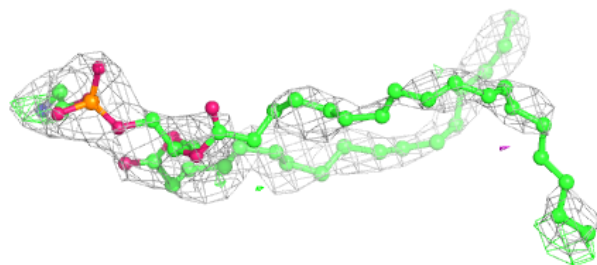
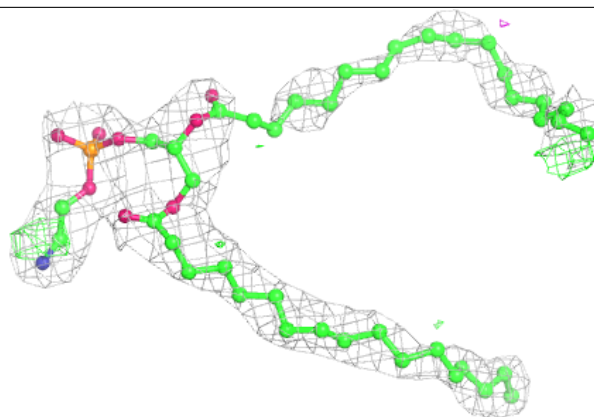
**Electron density around PEE A 2005:**

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



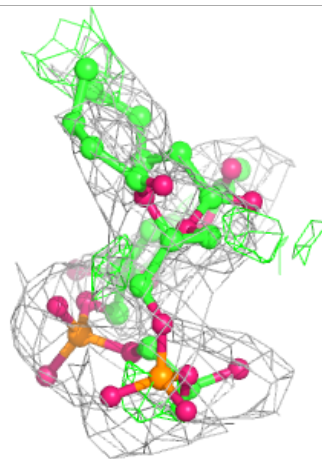
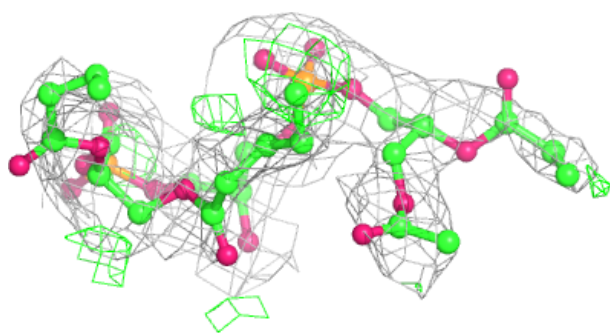
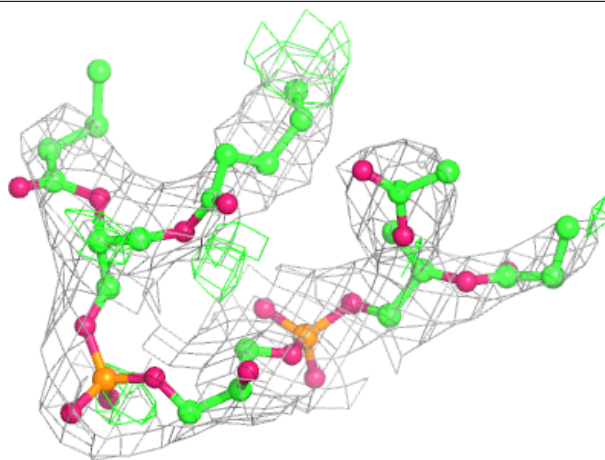
Electron density around PEE N 3005:

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



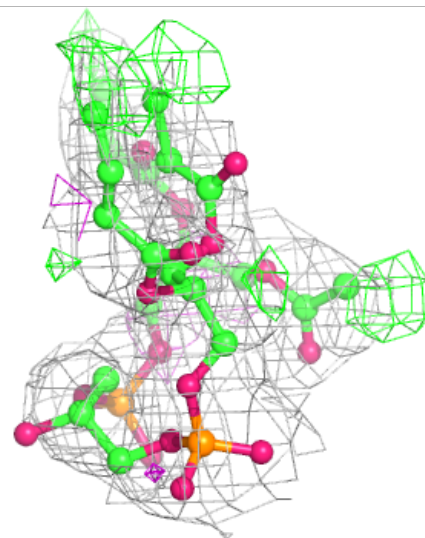
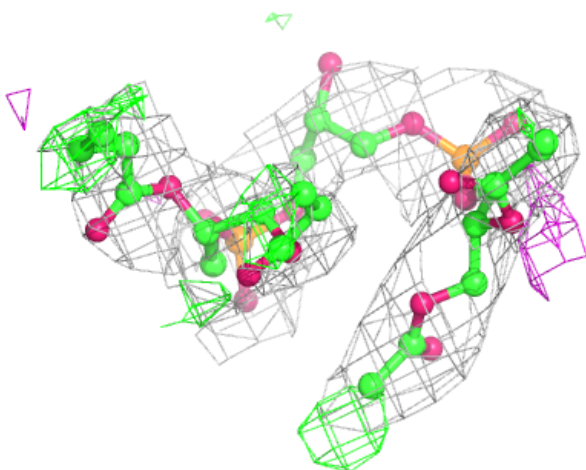
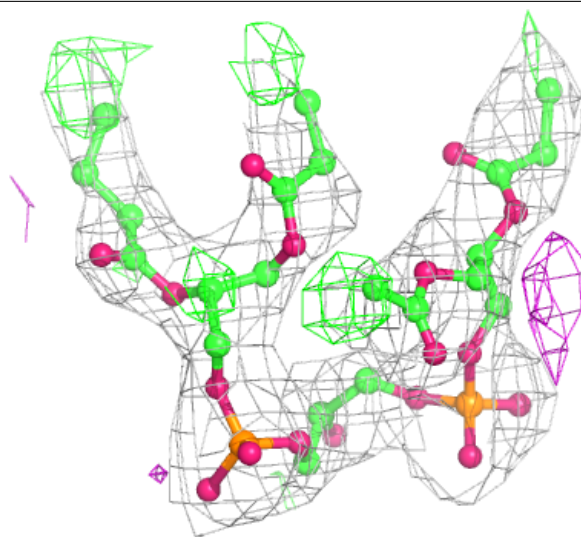
Electron density around CDL Q 3003:

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



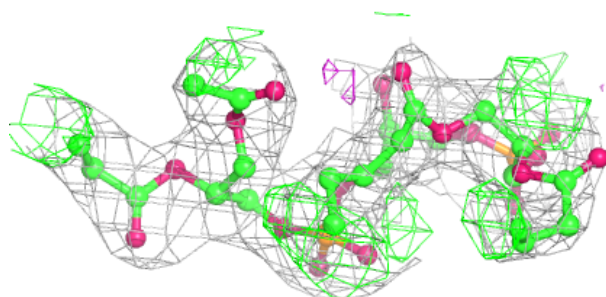
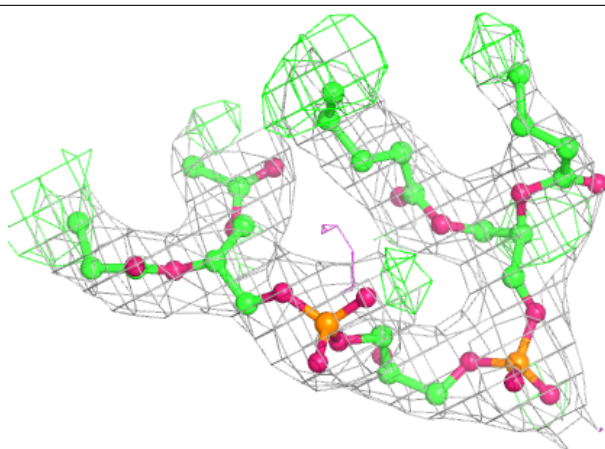
Electron density around CDL T 3004:

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

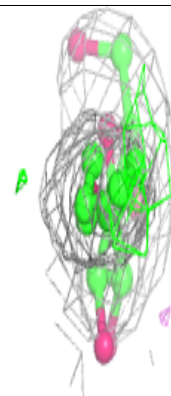
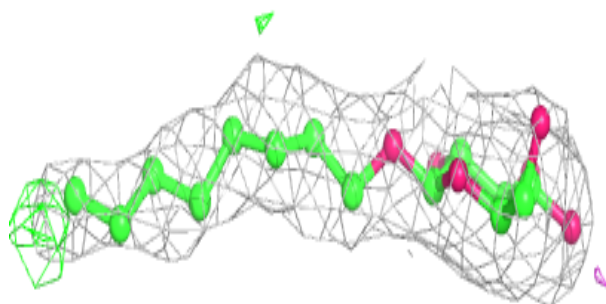
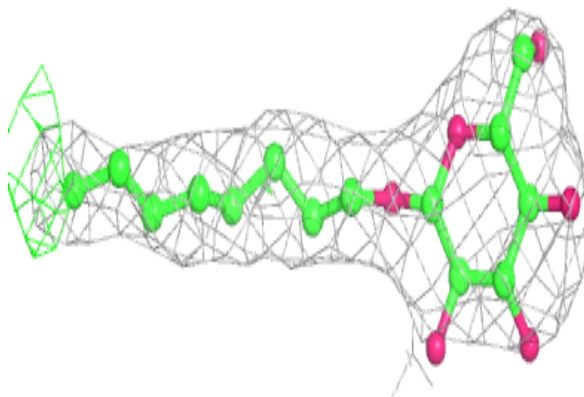


Electron density around CDL D 2003:

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

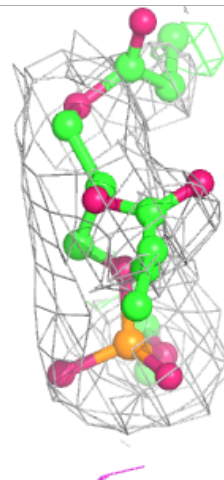
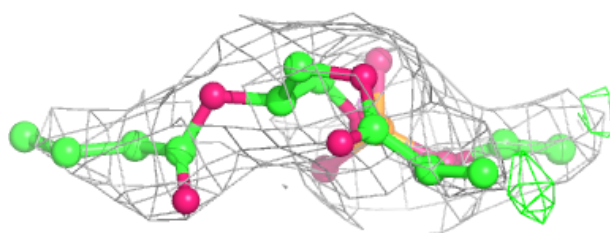
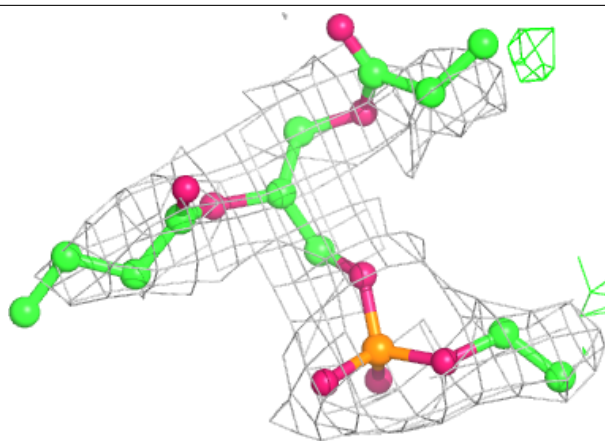
**Electron density around BOG Q 3009:**

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



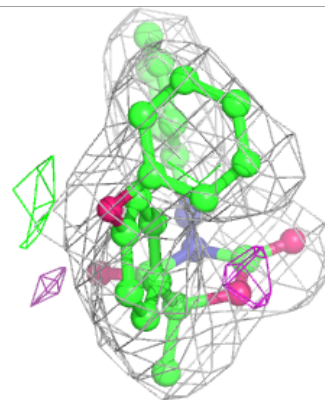
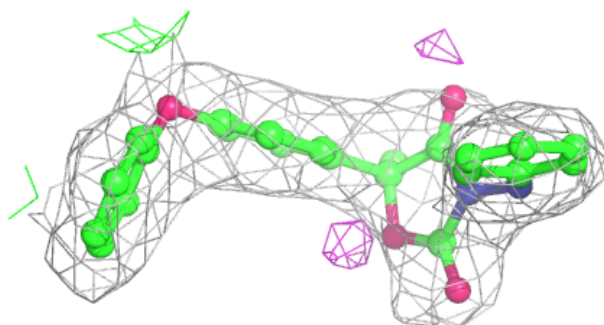
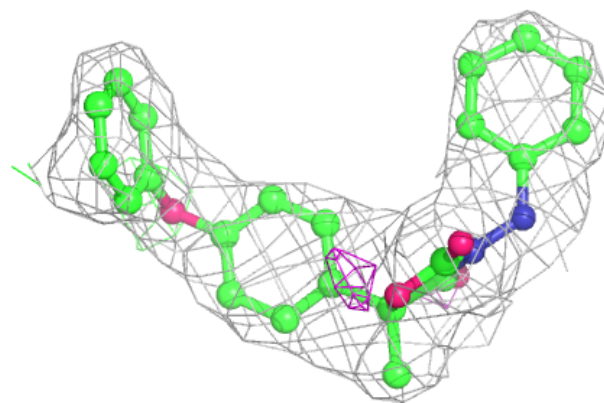
Electron density around PEE C 2008:

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

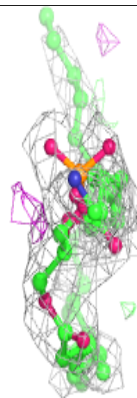
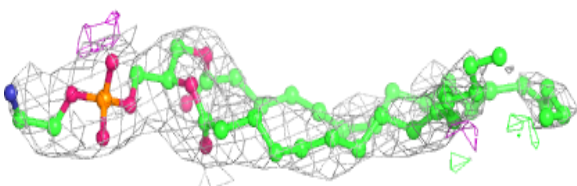
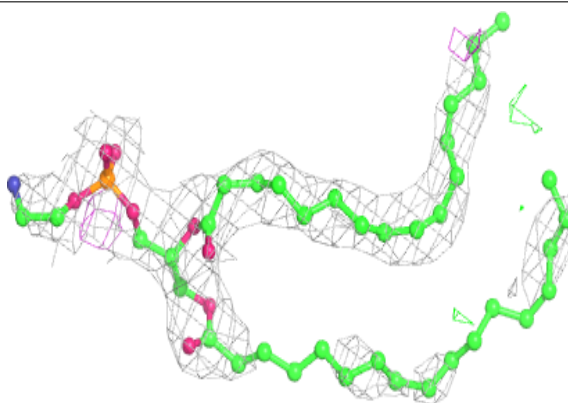


Electron density around FMX P 3001:

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

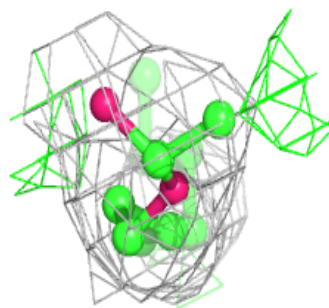
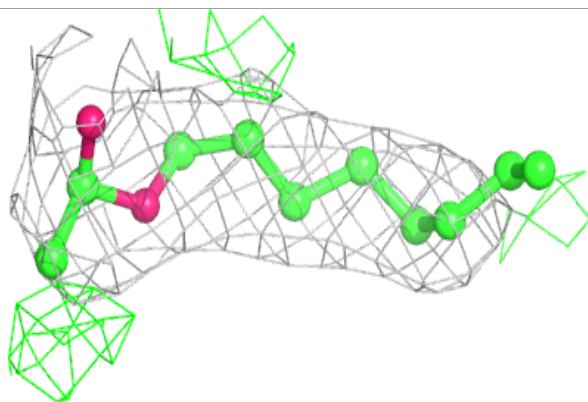
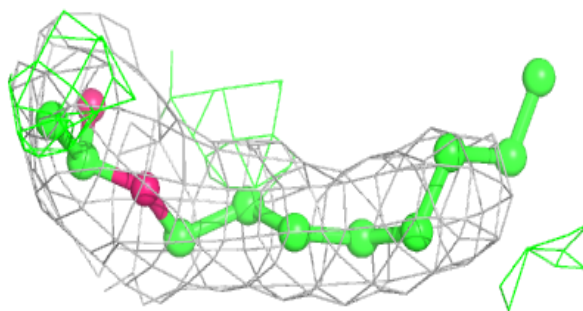
**Electron density around PEE P 3007:**

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



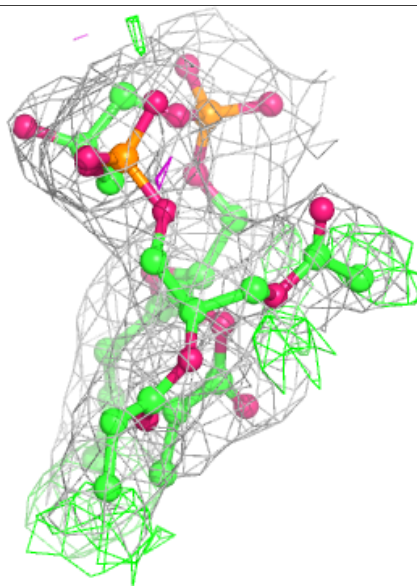
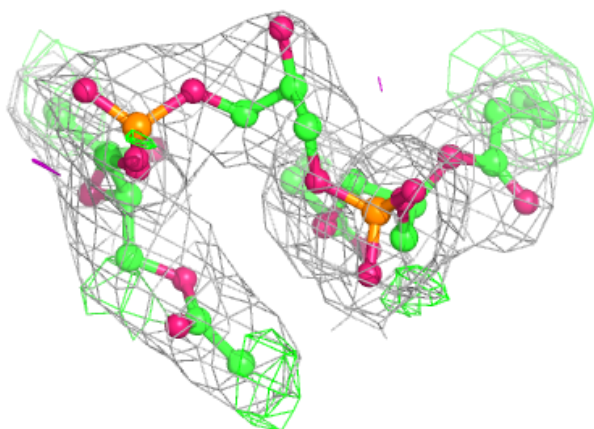
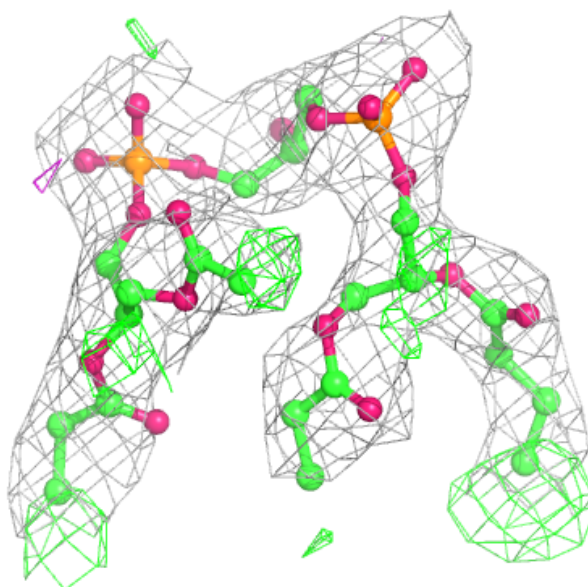
Electron density around BOG C 3010:

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



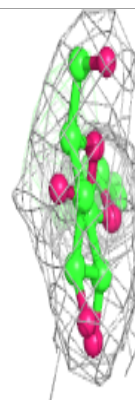
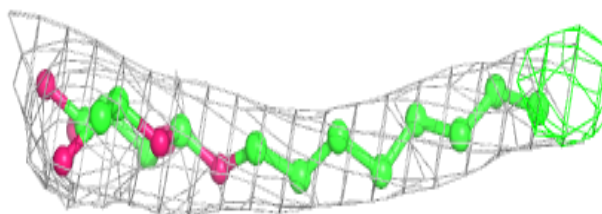
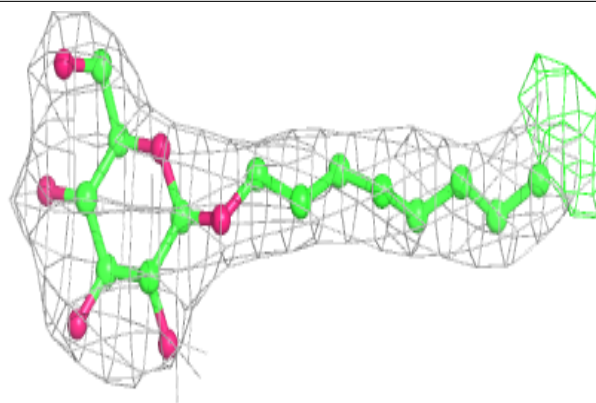
Electron density around CDL G 2004:

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

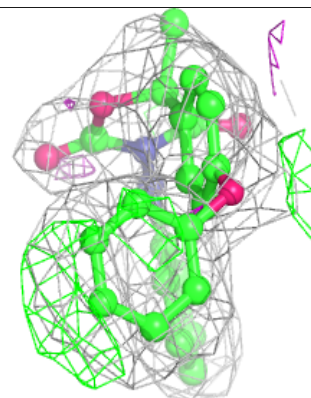
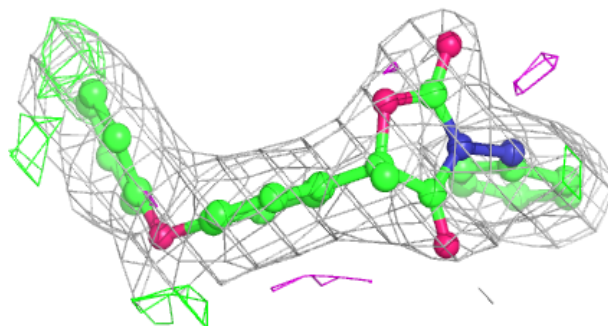
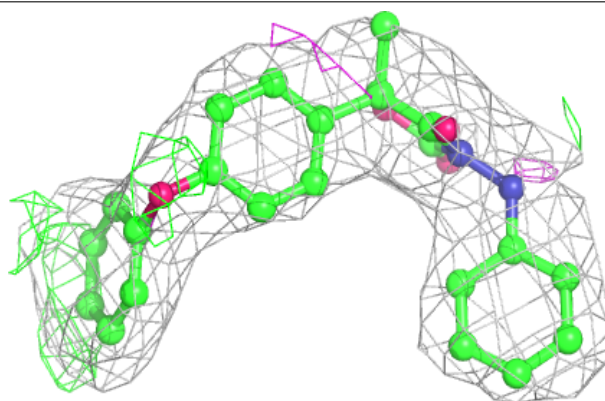


Electron density around BOG D 2009:

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

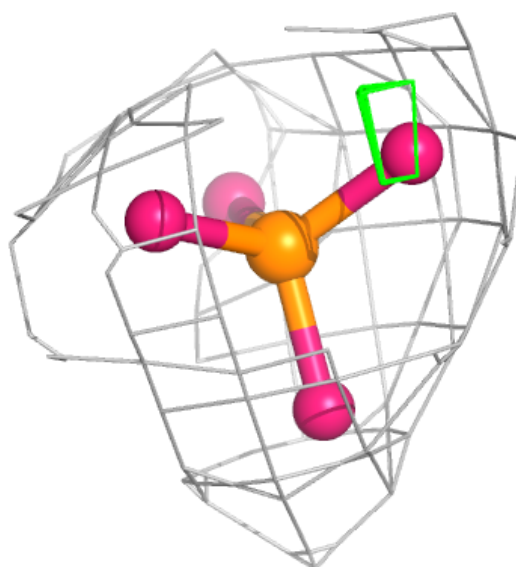
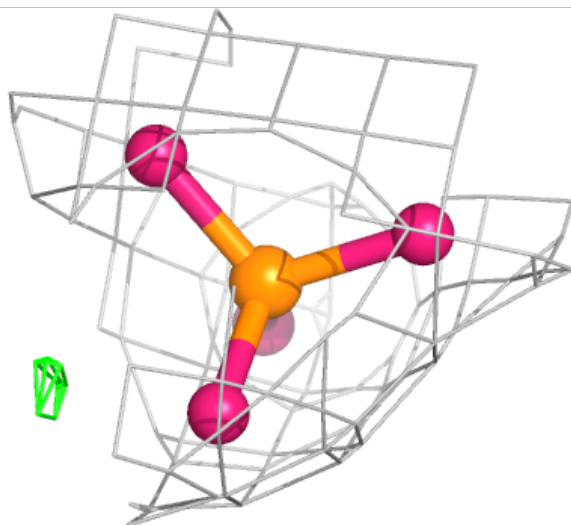
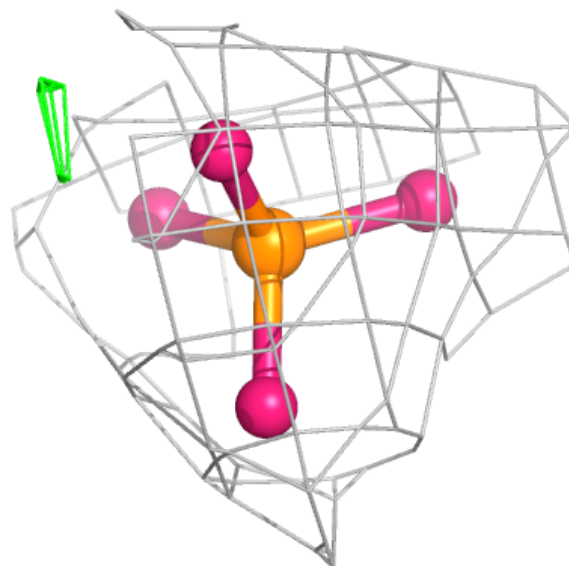
**Electron density around FMX C 2001:**

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



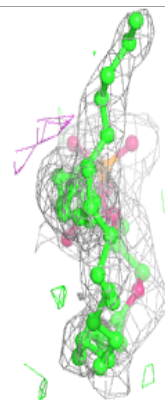
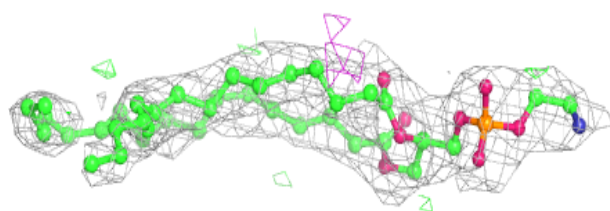
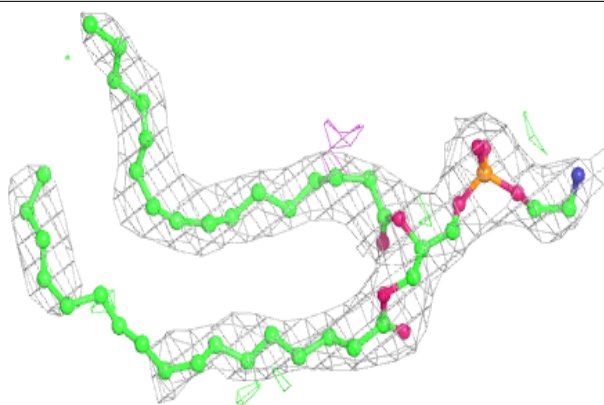
Electron density around PEE N 3008:

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and green (positive)

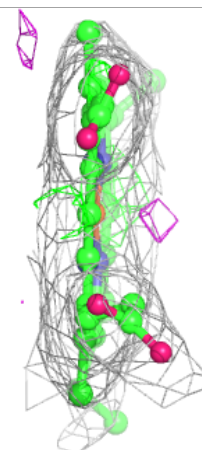
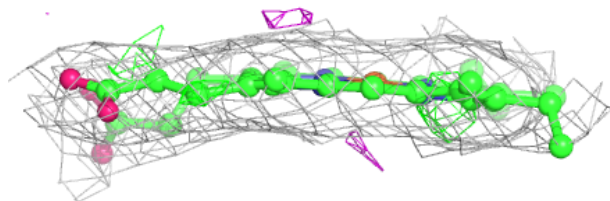
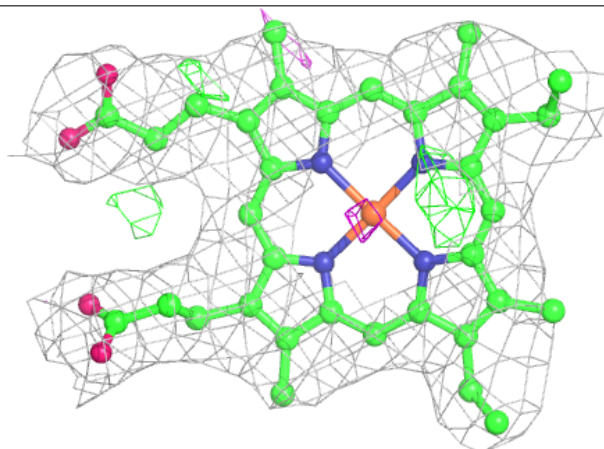


Electron density around PEE C 2007:

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

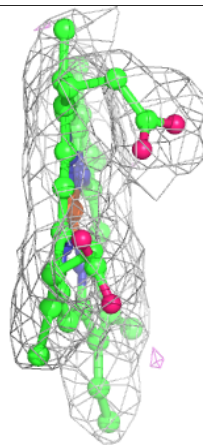
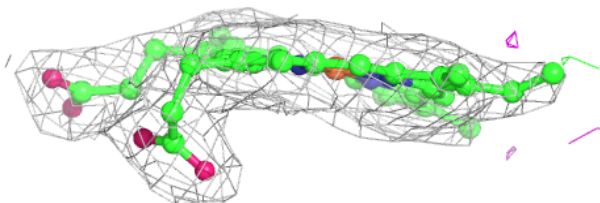
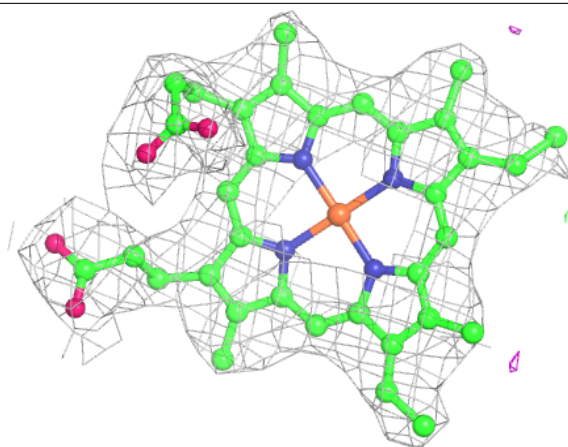
**Electron density around HEC Q 501:**

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



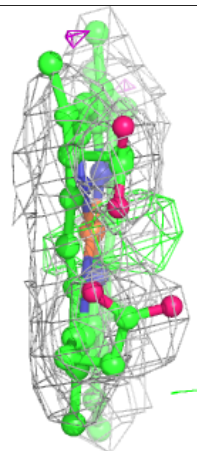
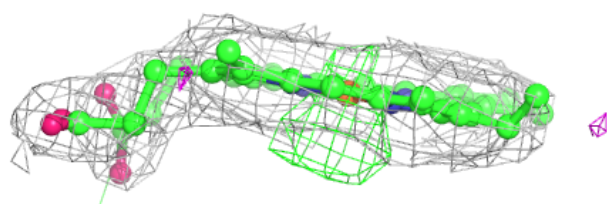
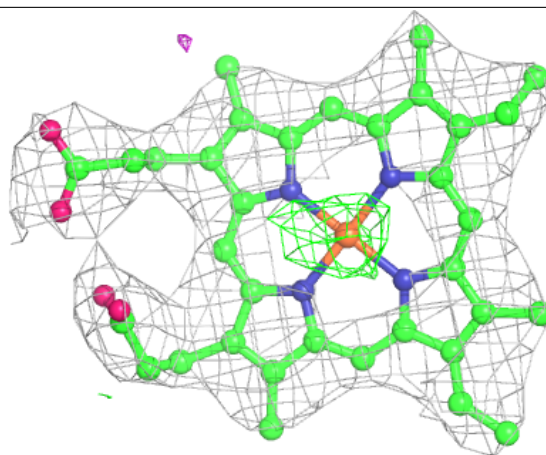
Electron density around HEM P 502:

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



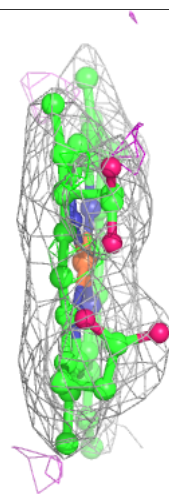
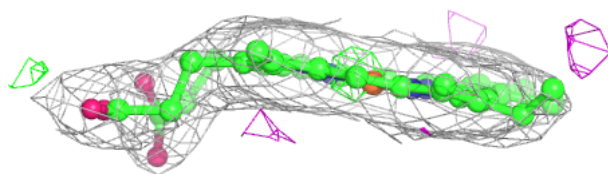
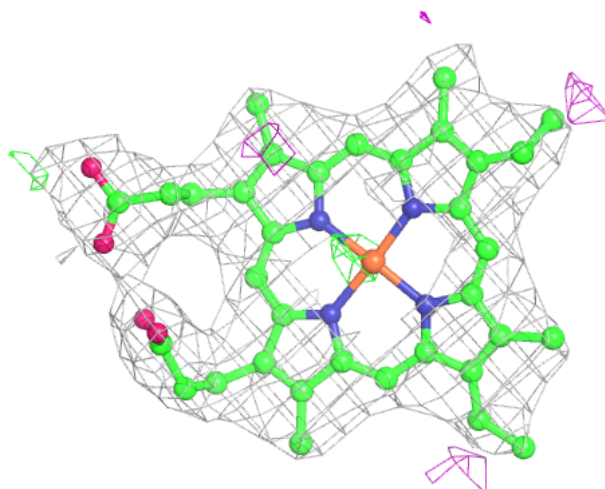
Electron density around HEM P 501:

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



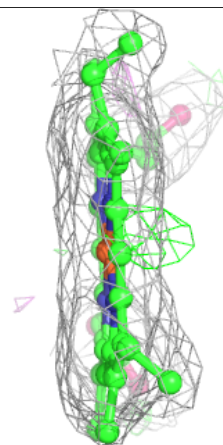
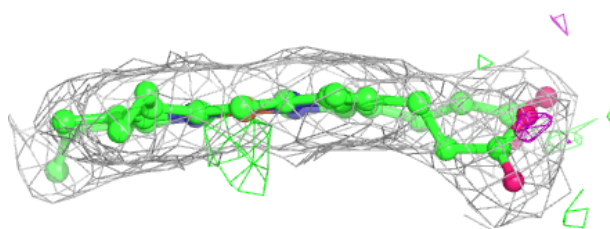
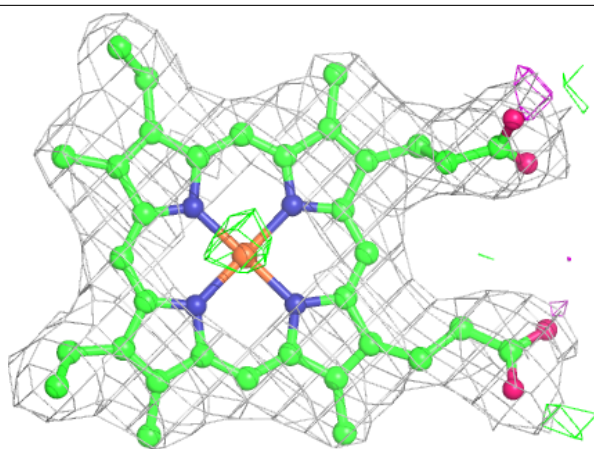
Electron density around HEM C 501:

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



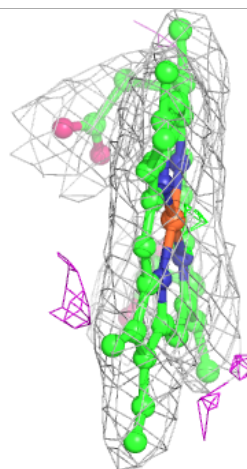
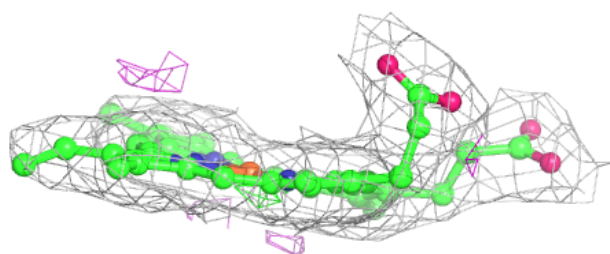
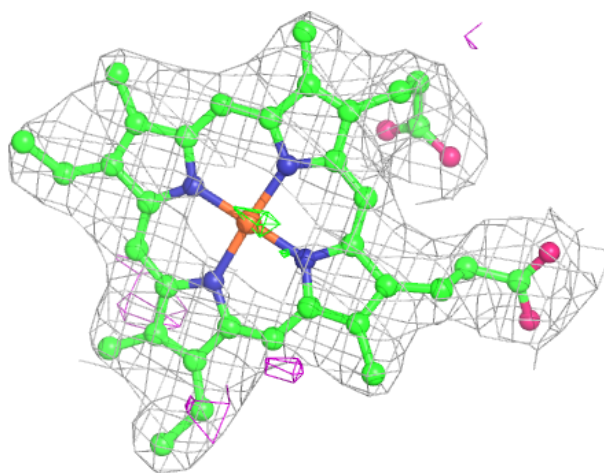
Electron density around HEC D 501:

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



Electron density around HEM C 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.