



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:17 PM BST

PDB ID : 3L73
Title : Cytochrome BC1 complex from chicken with triazolone inhibitor
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 3.04 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

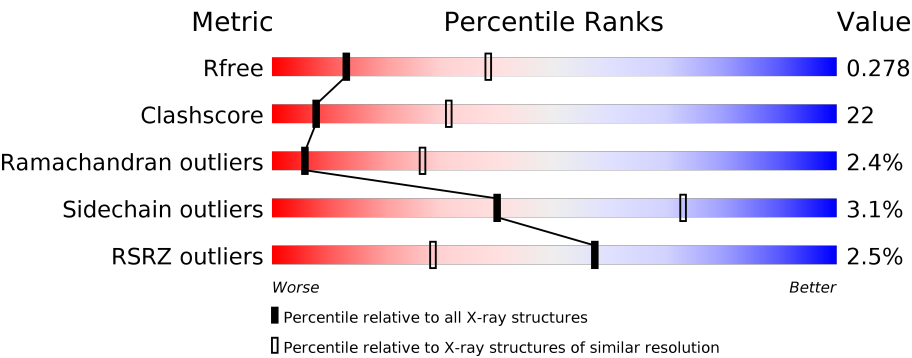
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	
1	N	446	
2	B	441	
2	O	441	
3	C	380	
3	P	380	

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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	P	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
14	UQ	P	3002	-	-	-	X
18	BOG	D	2091	-	-	-	X
18	BOG	P	2010	-	-	-	X
18	BOG	Q	3091	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32645 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 1.

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

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 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
			1509	950	263	290	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

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

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

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

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

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

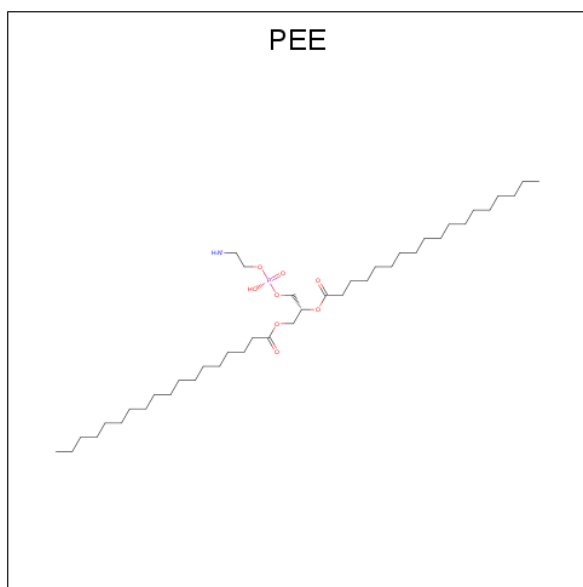
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

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

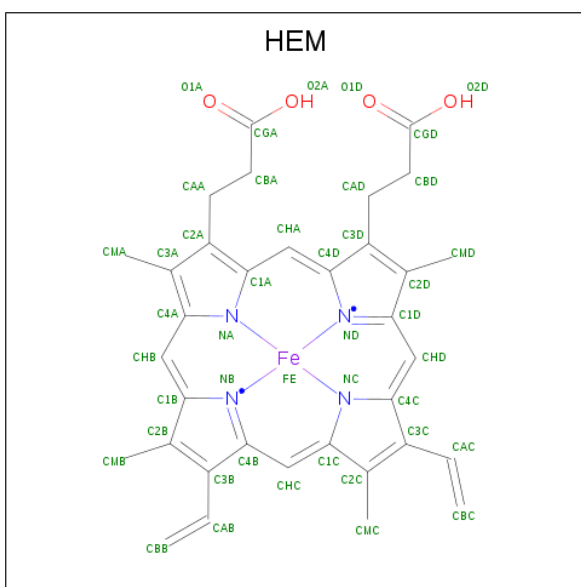
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

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



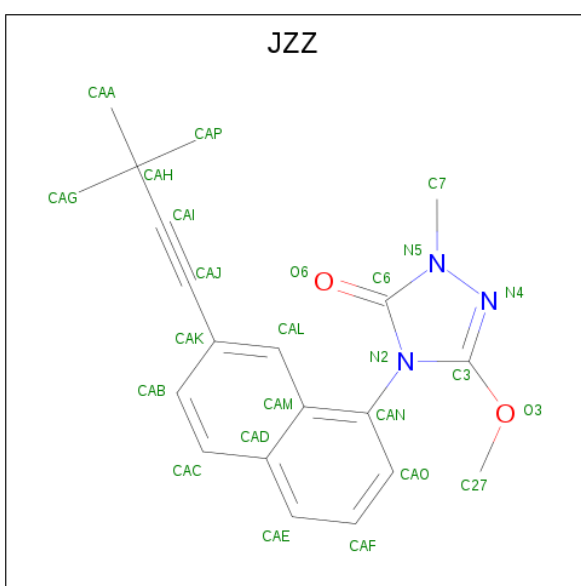
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			21	12	8	1		
11	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	E	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	P	1	Total	O	P		0	0
			5	4	1			
11	R	1	Total	C	N	O	P	0
			50	40	1	8	1	

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



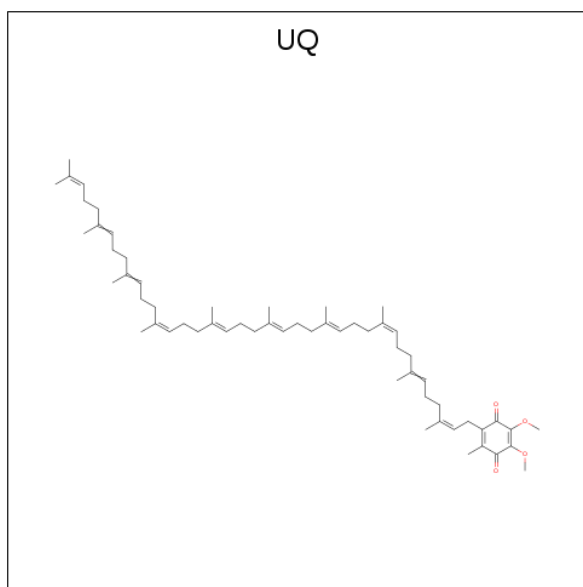
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is 4-[7-(3,3-dimethylbut-1-yn-1-yl)naphthalen-1-yl]-5-methoxy-2-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one (three-letter code: JZZ) (formula: C₂₀H₂₁N₃O₂).



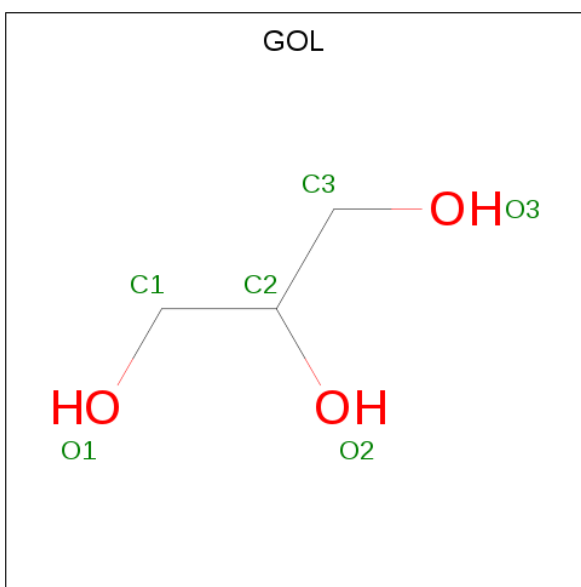
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			25	20	3	2		
13	P	1	Total	C	N	O	0	0
			25	20	3	2		

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



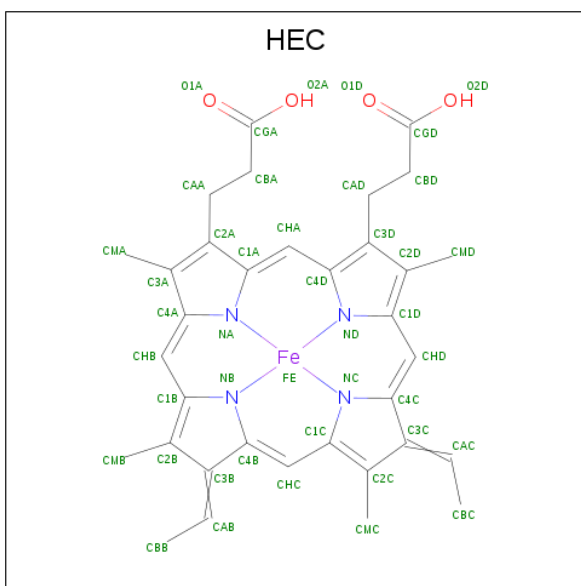
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



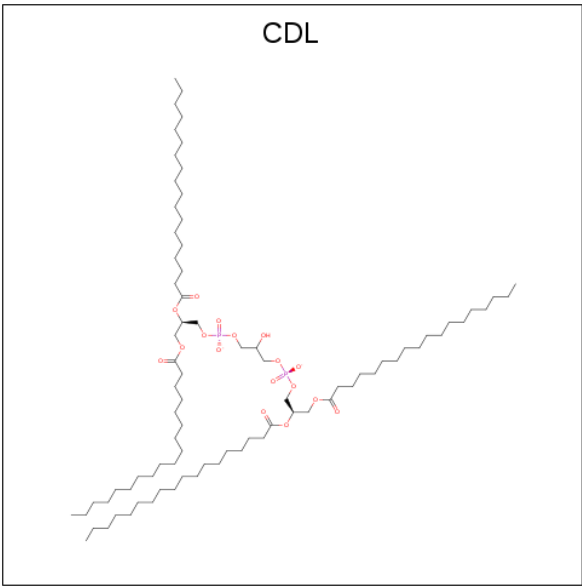
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total 6	C 3	O 3	0	0
15	P	1	Total 6	C 3	O 3	0	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



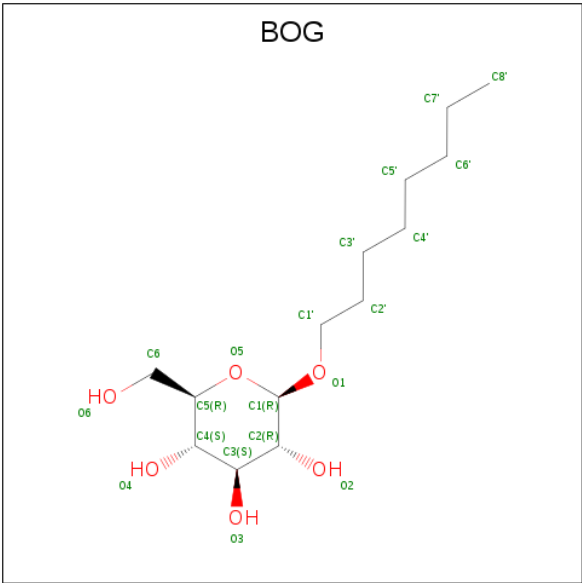
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



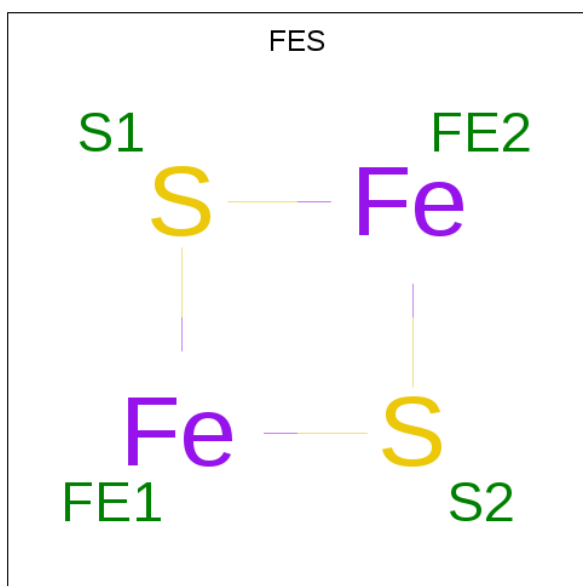
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

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



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 20 is water.

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

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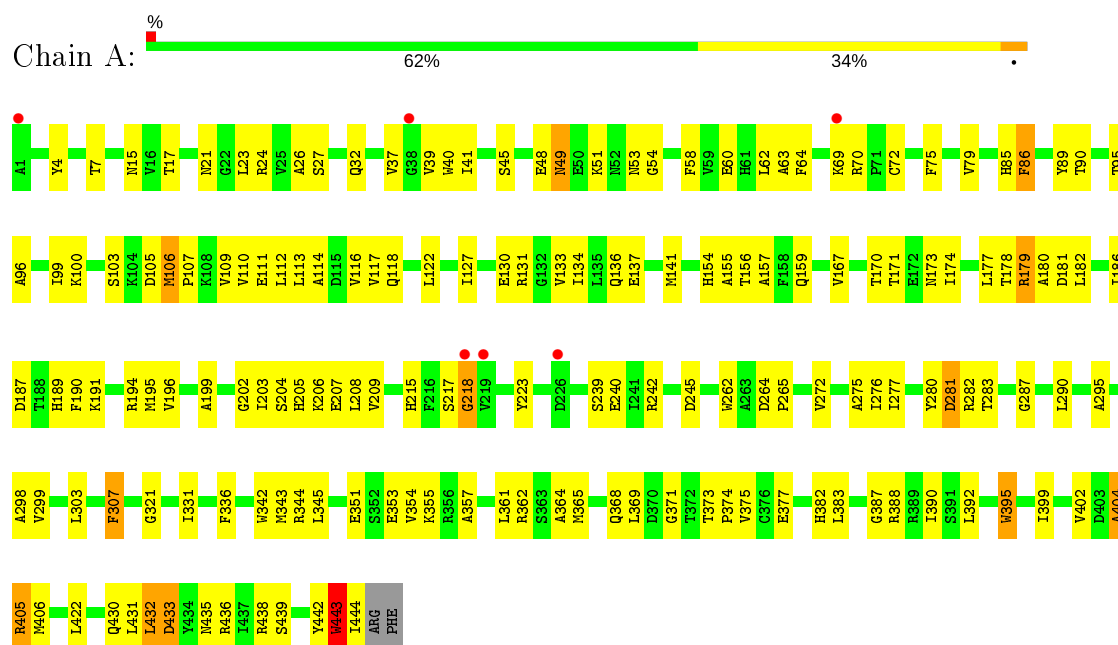
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	R	1	Total	O	0	0
			1	1		

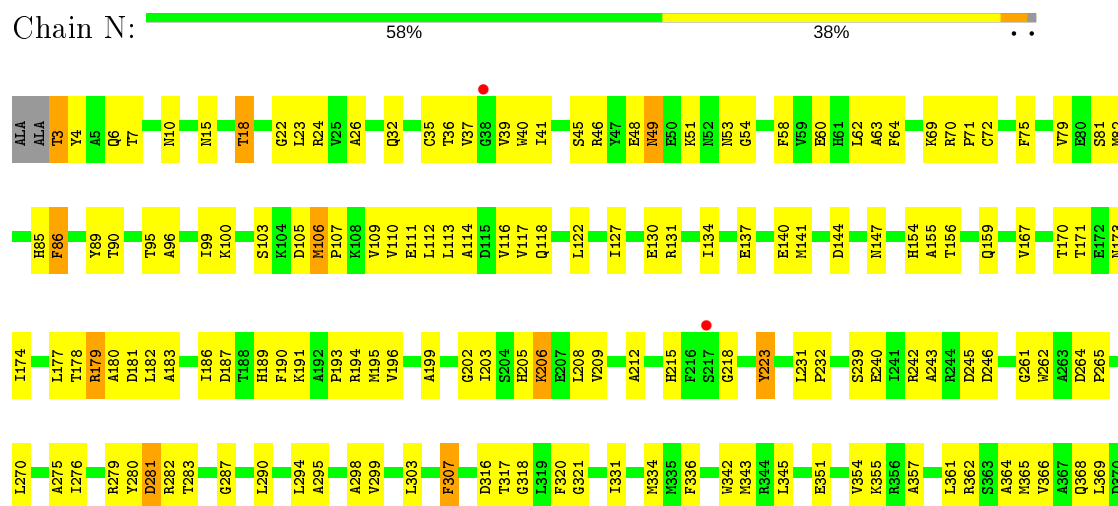
3 Residue-property plots

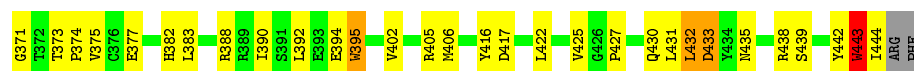
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

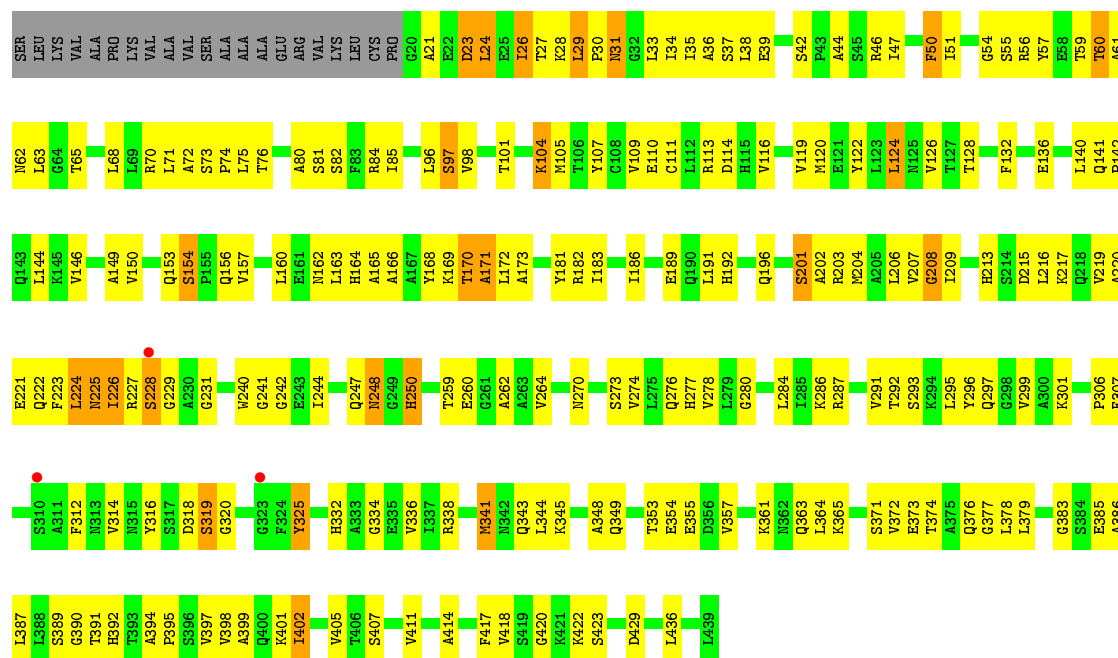


• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

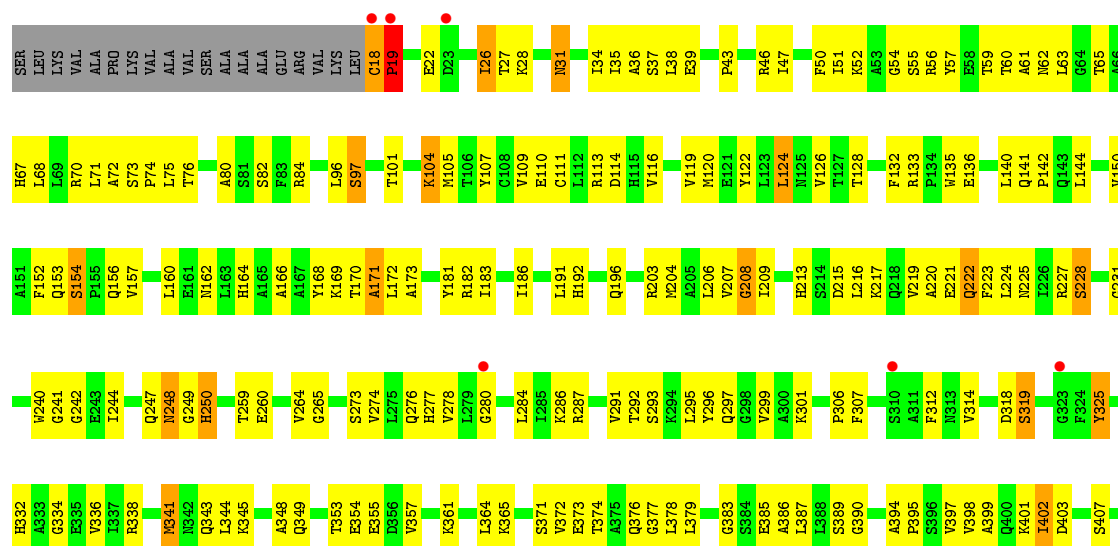




• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

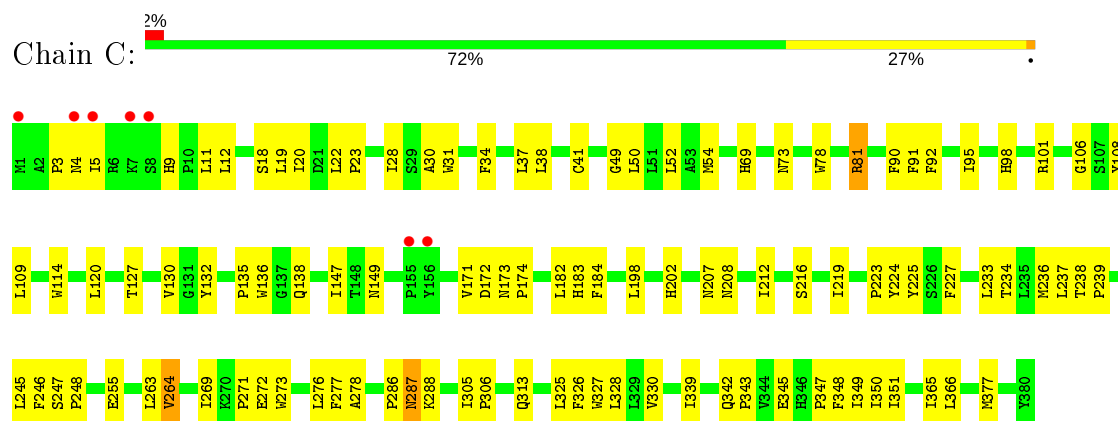


• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

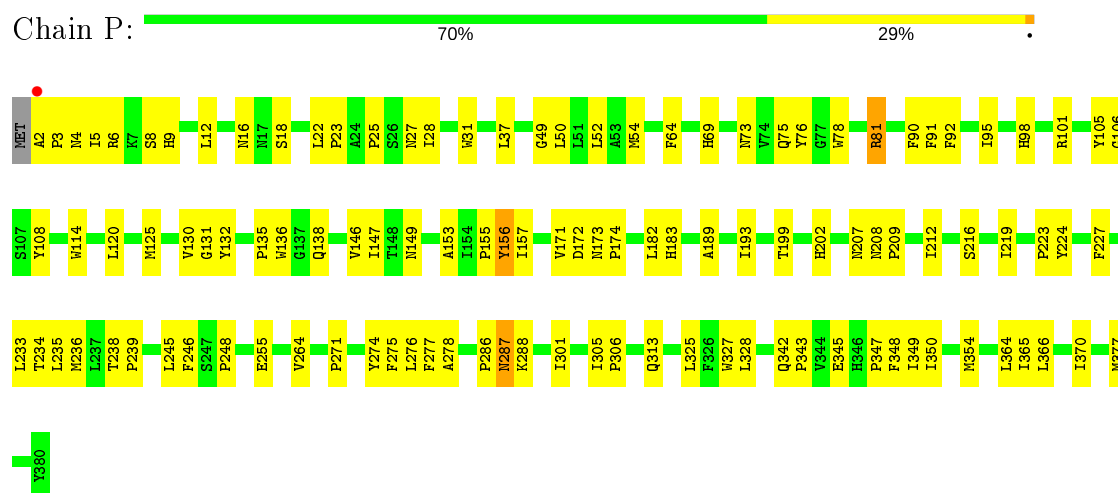




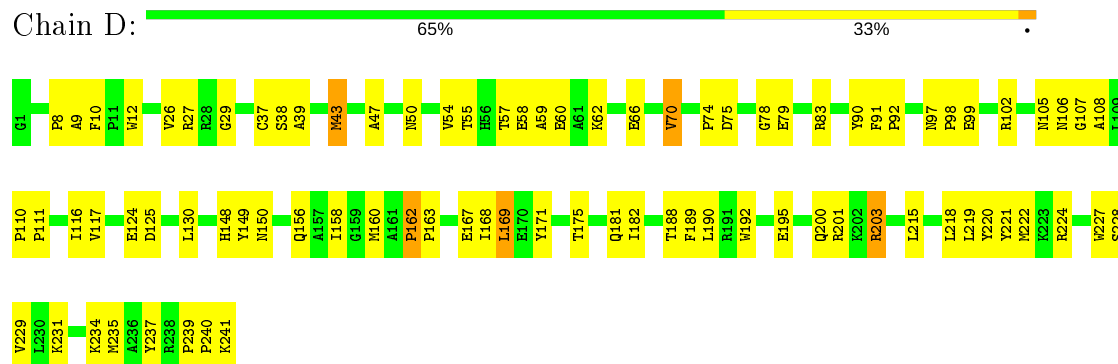
• Molecule 3: CYTOCHROME B



• Molecule 3: CYTOCHROME B

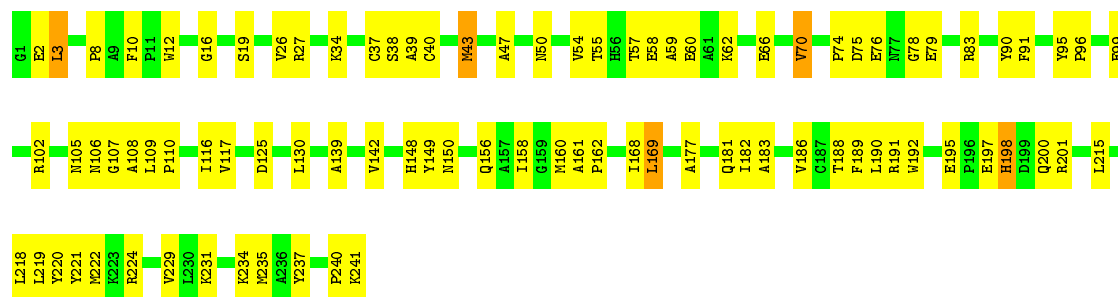


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

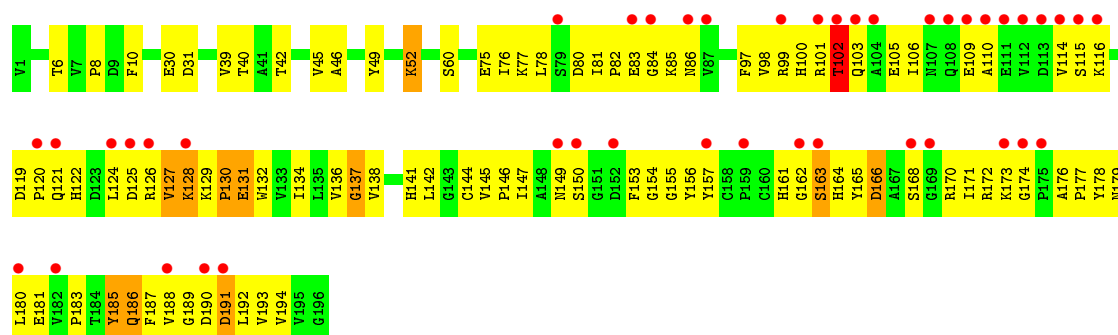


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

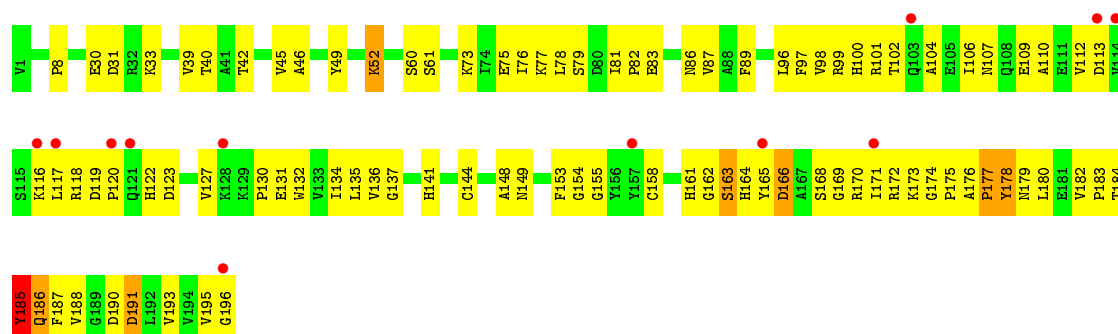




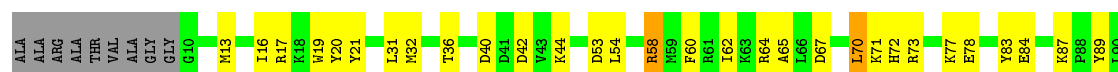
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



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



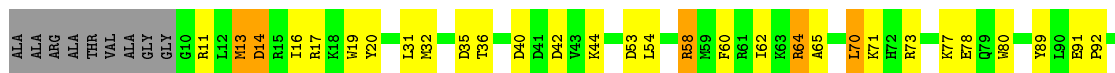
- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN





- Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S: 61% 26% 5% 8%



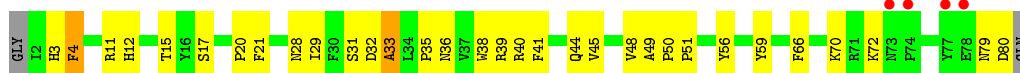
- Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G: 59% 37%



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

Chain T: 5% 58% 37%



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

Chain H: 3% 68% 22% 9%

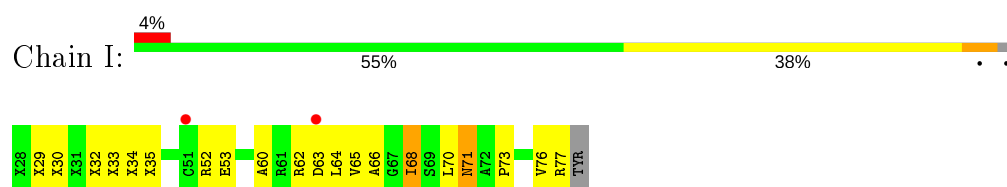


- Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

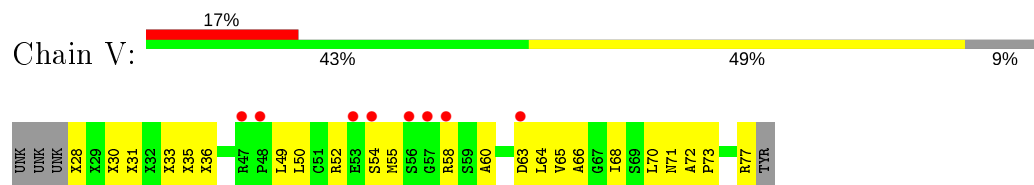
Chain U: 5% 53% 30% 13%



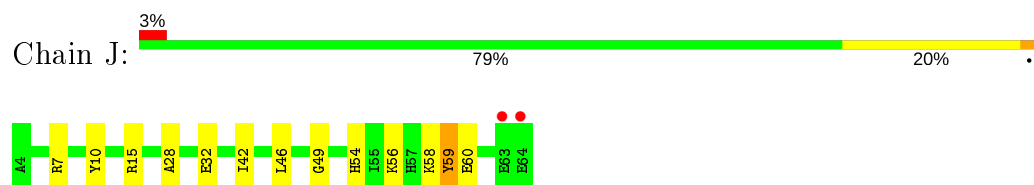
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



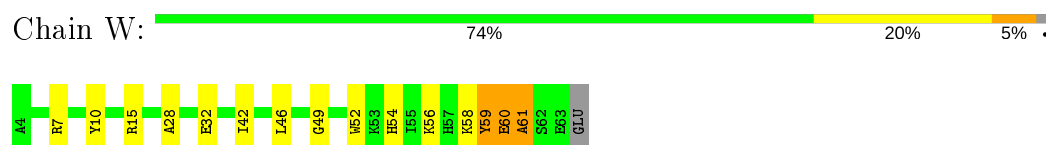
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



• 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	171.50Å 182.93Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 3.04 24.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.97-3.04) 99.5 (24.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.293 0.246 , 0.278	Depositor DCC
R_{free} test set	3273 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32645	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: GOL, CDL, UQ, JZZ, HEC, PEE, BOG, HEM, FES

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	0.46	0/3518	0.68	0/4767
1	N	0.44	0/3508	0.66	0/4753
2	B	0.41	0/3187	0.65	0/4321
2	O	0.42	0/3202	0.66	0/4343
3	C	0.54	0/3119	0.70	0/4270
3	P	0.49	0/3114	0.66	0/4263
4	D	0.49	0/1956	0.67	0/2658
4	Q	0.41	0/1956	0.63	0/2658
5	E	0.39	0/1547	0.60	0/2103
5	R	0.40	0/1543	0.60	0/2098
6	F	0.55	0/911	0.68	0/1219
6	S	0.45	0/911	0.64	0/1219
7	G	0.52	0/694	0.69	0/941
7	T	0.46	0/684	0.66	0/929
8	H	0.44	0/582	0.64	0/779
8	U	0.35	0/561	0.61	0/751
9	I	0.44	0/218	0.59	0/293
9	V	0.39	0/218	0.60	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/490	0.61	0/660
All	All	0.46	0/32427	0.66	0/44000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	135	0
1	N	3437	0	3349	164	0
2	B	3133	0	3130	212	0
2	O	3147	0	3146	208	0
3	C	3017	0	3063	91	0
3	P	3012	0	3058	95	0
4	D	1898	0	1846	75	0
4	Q	1898	0	1846	76	0
5	E	1513	0	1478	108	0
5	R	1509	0	1474	103	0
6	F	891	0	893	24	0
6	S	891	0	893	29	0
7	G	672	0	653	32	0
7	T	662	0	645	33	0
8	H	574	0	548	19	0
8	U	553	0	535	26	0
9	I	287	0	249	28	0
9	V	277	0	250	32	0
10	J	497	0	490	16	0
10	W	479	0	478	21	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	P	54	0	72	4	0
11	R	50	0	77	1	0
12	C	86	0	60	6	0
12	P	86	0	60	5	0
13	C	25	0	21	2	0
13	P	25	0	21	6	0
14	C	19	0	17	4	0
14	P	19	0	17	5	0
15	C	6	0	8	1	0
15	P	6	0	8	1	0
16	D	43	0	30	1	0
16	Q	43	0	30	2	0
17	D	42	0	28	3	0
17	G	40	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	42	0	28	1	0
17	T	40	0	24	5	0
18	D	33	0	39	2	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	0	0
20	R	1	0	0	0	0
All	All	32645	0	32162	1407	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 22.

All (1407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.21	1.16
9:V:35:UNK:HG3	9:V:36:UNK:H	1.22	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.04
2:O:353:THR:HG22	2:O:355:GLU:H	1.21	1.04
2:O:76:THR:HG22	2:O:82:SER:H	1.22	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.44	0.99
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.26	0.98
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.27	0.97
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.48	0.95
2:B:76:THR:HG22	2:B:82:SER:H	1.32	0.94
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.34	0.93
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.84	0.92
4:D:47:ALA:H	4:D:50:ASN:HD22	1.13	0.91
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.16	0.91
1:A:178:THR:HG22	1:A:180:ALA:H	1.36	0.91
1:N:178:THR:HG22	1:N:180:ALA:H	1.36	0.91
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.01	0.91
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.52	0.89
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.54	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
5:E:127:VAL:HG12	5:E:128:LYS:H	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.89	0.86
2:O:154:SER:O	2:O:157:VAL:HG12	1.75	0.86
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.57	0.86
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.11	0.86
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.76	0.85
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.42	0.85
2:B:154:SER:O	2:B:157:VAL:HG12	1.77	0.85
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.59	0.85
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.85
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.12	0.84
7:G:41:PHE:O	7:G:45:VAL:HG23	1.79	0.83
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.13	0.83
2:B:341:MET:HE2	2:B:341:MET:HA	1.58	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.83
3:C:9:HIS:HD2	3:C:12:LEU:H	1.24	0.83
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.60	0.82
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.60	0.82
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.61	0.82
2:B:47:ILE:HD13	2:B:120:MET:CE	2.10	0.82
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.61	0.82
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.80	0.82
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.63	0.81
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.63	0.81
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.62	0.80
1:N:170:THR:HG22	1:N:171:THR:H	1.47	0.80
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.62	0.80
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.17	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.64	0.79
9:I:70:LEU:HD23	9:I:71:ASN:H	1.45	0.79
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
4:D:57:THR:HB	4:D:60:GLU:HG3	1.65	0.79
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.18	0.78
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.19	0.78
2:O:219:VAL:O	2:O:223:PHE:HB2	1.84	0.78
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.66	0.78
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.66	0.77
1:N:187:ASP:O	1:N:191:LYS:HE3	1.85	0.77
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.67	0.77
2:O:27:THR:HG22	2:O:28:LYS:N	2.00	0.77
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.66	0.77
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.77
1:N:112:LEU:O	1:N:116:VAL:HG23	1.84	0.77
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.85	0.77
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.66	0.77
2:O:422:LYS:O	2:O:436:LEU:HD21	1.82	0.77
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.48	0.76
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.66	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.50	0.76
1:A:295:ALA:O	1:A:299:VAL:HG23	1.86	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.65	0.76
1:A:103:SER:HB3	1:A:202:GLY:O	1.87	0.75
1:N:10:ASN:HD21	2:O:18:CYS:N	1.83	0.75
1:N:295:ALA:O	1:N:299:VAL:HG23	1.85	0.75
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.75
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.52	0.75
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.69	0.75
2:O:221:GLU:HG3	2:O:222:GLN:H	1.50	0.75
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.69	0.74
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.02	0.74
1:N:105:ASP:O	1:N:109:VAL:HG23	1.87	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.86	0.74
2:B:422:LYS:O	2:B:436:LEU:HD21	1.87	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.74
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.87	0.74
1:A:178:THR:HB	1:A:181:ASP:OD1	1.87	0.73
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.51	0.73
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.89	0.73
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.73
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.70	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.07	0.73
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.71	0.72
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.71	0.72
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.54	0.72
2:B:38:LEU:HD12	2:B:39:GLU:N	2.05	0.72
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.19	0.72
2:O:338:ARG:NH1	2:O:338:ARG:HG3	1.98	0.72
2:O:192:HIS:O	2:O:196:GLN:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.71	0.72
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.25	0.72
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.70	0.72
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.72	0.72
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.90	0.72
2:B:122:TYR:O	2:B:126:VAL:HG23	1.90	0.72
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.71	0.71
1:N:170:THR:HG22	1:N:171:THR:N	2.05	0.71
2:B:31:ASN:N	2:B:31:ASN:HD22	1.88	0.71
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.20	0.71
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.71
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.71	0.71
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.53	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.71
10:W:60:GLU:HG2	10:W:60:GLU:O	1.89	0.71
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.72	0.70
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.19	0.70
2:O:361:LYS:O	2:O:365:LYS:HG3	1.92	0.70
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.04	0.70
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.56	0.70
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.70
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.55	0.70
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.21	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.70
3:P:238:THR:HB	3:P:239:PRO:HD3	1.73	0.70
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.70
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.70
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.74	0.70
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.70
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.74	0.70
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.57	0.69
2:O:156:GLN:HE22	9:V:77:ARG:C	1.95	0.69
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.07	0.69
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.74	0.69
5:E:190:ASP:C	5:E:192:LEU:H	1.95	0.69
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.75	0.69
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.74	0.69
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.58	0.69
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.57	0.69
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HA	9:I:52:ARG:CG	2.22	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.74	0.69
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.75	0.68
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.73	0.68
1:A:187:ASP:O	1:A:191:LYS:HE3	1.93	0.68
2:B:150:VAL:O	2:B:153:GLN:HG3	1.94	0.68
1:N:178:THR:HB	1:N:181:ASP:OD1	1.93	0.68
2:B:164:HIS:O	2:B:173:ALA:HA	1.94	0.68
1:N:178:THR:HG22	1:N:179:ARG:N	2.09	0.68
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.28	0.68
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.59	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
2:B:202:ALA:HB3	2:B:229:GLY:O	1.94	0.68
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.58	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.68
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.75	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.68
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.76	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.94	0.68
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.74	0.68
1:A:112:LEU:O	1:A:116:VAL:HG23	1.93	0.68
2:O:248:ASN:HD22	2:O:248:ASN:C	1.97	0.68
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.75	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.94	0.68
2:O:341:MET:CE	2:O:417:PHE:HE2	2.06	0.67
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.29	0.67
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.76	0.67
1:A:343:MET:HB3	1:A:444:ILE:HA	1.75	0.67
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.77	0.67
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.75	0.67
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.59	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
1:A:137:GLU:O	1:A:141:MET:HG3	1.95	0.67
2:B:341:MET:CE	2:B:417:PHE:HE2	2.08	0.67
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.41	0.67
3:C:238:THR:HB	3:C:239:PRO:HD3	1.75	0.67
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.22	0.67
1:A:178:THR:HG22	1:A:179:ARG:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
1:N:371:GLY:O	1:N:375:VAL:HG23	1.96	0.66
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.35	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
2:O:122:TYR:O	2:O:126:VAL:HG23	1.94	0.66
2:B:318:ASP:O	2:B:319:SER:HB2	1.96	0.66
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.78	0.66
8:H:28:GLU:O	8:H:32:LYS:HG3	1.96	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.66
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.66
1:A:105:ASP:O	1:A:109:VAL:HG23	1.96	0.66
9:V:70:LEU:HD23	9:V:71:ASN:N	2.12	0.66
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.29	0.65
1:N:182:LEU:O	1:N:186:ILE:HG13	1.96	0.65
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.96	0.65
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.11	0.65
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.31	0.65
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.78	0.65
8:U:28:GLU:O	8:U:32:LYS:HG3	1.96	0.65
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.76	0.65
1:N:106:MET:O	1:N:110:VAL:HG23	1.96	0.65
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.31	0.65
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.32	0.65
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.12	0.65
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.32	0.65
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.12	0.65
5:E:109:GLU:OE2	5:E:153:PHE:HB3	1.95	0.65
9:V:64:LEU:HD12	9:V:77:ARG:O	1.97	0.65
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.78	0.65
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.32	0.65
8:U:18:THR:O	8:U:22:GLU:HG3	1.95	0.65
2:B:27:THR:HG22	2:B:28:LYS:H	1.61	0.64
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.64
2:O:318:ASP:O	2:O:319:SER:HB2	1.98	0.64
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.78	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.32	0.64
9:V:35:UNK:HG3	9:V:36:UNK:N	2.04	0.64
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.32	0.64
2:B:215:ASP:O	2:B:219:VAL:HG23	1.97	0.64
5:E:155:GLY:HA3	5:E:166:ASP:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:103:SER:HB3	1:N:202:GLY:O	1.97	0.64
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.79	0.64
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.78	0.64
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.64
7:T:79:ASN:O	7:T:80:ASP:HB2	1.98	0.64
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.33	0.64
7:G:29:ILE:O	7:G:33:ALA:HB3	1.98	0.64
5:R:169:GLY:O	5:R:179:ASN:HB3	1.97	0.64
3:P:147:ILE:HD11	13:P:3001:JZZ:CAB	2.27	0.64
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.33	0.64
16:Q:501:HEC:HMB1	16:Q:501:HEC:HBB3	1.80	0.64
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.33	0.63
5:E:163:SER:HA	5:E:174:GLY:HA3	1.80	0.63
2:O:38:LEU:HD12	2:O:39:GLU:N	2.13	0.63
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.63	0.63
1:A:106:MET:HE2	1:A:107:PRO:HA	1.80	0.63
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.29	0.63
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.33	0.63
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.63	0.63
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.27	0.63
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.63
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.14	0.63
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.32	0.63
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.63
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.63
2:O:31:ASN:N	2:O:31:ASN:HD22	1.97	0.63
6:S:95:LYS:O	6:S:99:ARG:HG3	1.99	0.63
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.34	0.62
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.64	0.62
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.63	0.62
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.63	0.62
1:A:371:GLY:O	1:A:375:VAL:HG23	1.98	0.62
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.34	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.99	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
1:N:45:SER:HA	1:N:48:GLU:HG3	1.81	0.62
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.80	0.62
2:O:150:VAL:O	2:O:153:GLN:HG3	1.99	0.62
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.34	0.62
1:A:388:ARG:NH2	1:A:390:ILE:HG12	2.14	0.62
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:382:HIS:HB3	1:N:388:ARG:O	1.99	0.62
1:N:178:THR:CG2	1:N:179:ARG:N	2.63	0.62
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.81	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.30	0.62
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.82	0.62
3:P:199:THR:HA	18:P:2010:BOG:O1	2.00	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.30	0.62
1:N:137:GLU:O	1:N:141:MET:HG3	1.99	0.61
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.61
2:B:248:ASN:HD22	2:B:248:ASN:C	2.03	0.61
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.15	0.61
9:I:34:UNK:HG3	9:I:35:UNK:N	2.14	0.61
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.36	0.61
2:B:192:HIS:O	2:B:196:GLN:HG3	2.00	0.61
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.80	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.65	0.61
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.65	0.61
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.81	0.61
2:B:31:ASN:N	2:B:31:ASN:ND2	2.49	0.61
1:N:7:THR:HG21	2:O:113:ARG:CD	2.30	0.61
2:O:62:ASN:O	2:O:65:THR:HG22	2.00	0.61
5:R:155:GLY:HA3	5:R:166:ASP:O	2.00	0.61
8:U:36:ARG:NH1	8:U:36:ARG:HB3	2.16	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.35	0.61
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.82	0.61
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.82	0.61
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.27	0.61
1:A:178:THR:CG2	1:A:179:ARG:N	2.64	0.61
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.46	0.61
3:P:92:PHE:O	3:P:95:ILE:HG22	2.01	0.61
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.48	0.61
2:B:292:THR:O	2:B:292:THR:HG22	2.01	0.60
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.82	0.60
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.82	0.60
5:R:165:TYR:HA	5:R:170:ARG:O	2.01	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
2:O:156:GLN:NE2	9:V:77:ARG:C	2.54	0.60
2:B:31:ASN:ND2	2:B:31:ASN:H	1.99	0.60
3:C:147:ILE:HD11	13:C:2001:JZZ:CAB	2.30	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60
2:O:215:ASP:O	2:O:219:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.83	0.60
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.30	0.60
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.17	0.60
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.83	0.60
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.01	0.60
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.02	0.60
2:B:372:VAL:O	2:B:372:VAL:HG12	2.01	0.60
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.84	0.60
3:P:52:LEU:HD13	12:P:501:HEM:HBD1	1.84	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.02	0.60
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.37	0.60
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.84	0.60
4:D:222:MET:HE1	5:E:40:THR:HG23	1.84	0.60
2:O:164:HIS:O	2:O:173:ALA:HA	2.02	0.60
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.60
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.82	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.05	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.60
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.67	0.60
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.27	0.60
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.60
5:E:84:GLY:N	5:E:102:THR:HG23	2.17	0.60
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.01	0.60
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.60
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.66	0.60
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.67	0.60
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.36	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.02	0.59
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.84	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.18	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.84	0.59
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.36	0.59
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.59
3:C:101:ARG:C	3:C:101:ARG:HD2	2.22	0.59
1:N:388:ARG:NH2	1:N:390:ILE:HG12	2.17	0.59
2:O:170:THR:O	2:O:172:LEU:N	2.36	0.59
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.84	0.59
1:A:182:LEU:O	1:A:186:ILE:HG13	2.03	0.59
1:N:90:THR:O	1:N:167:VAL:HG11	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
1:A:106:MET:O	1:A:110:VAL:HG23	2.03	0.59
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.66	0.59
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.31	0.59
8:H:27:THR:O	8:H:31:VAL:HG23	2.03	0.59
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.84	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.18	0.59
9:I:29:UNK:O	9:I:30:UNK:HB2	2.02	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.85	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.68	0.59
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.84	0.59
9:V:70:LEU:HD23	9:V:71:ASN:H	1.67	0.59
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.68	0.58
2:O:372:VAL:O	2:O:372:VAL:HG12	2.03	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.02	0.58
2:O:27:THR:CG2	2:O:28:LYS:H	2.15	0.58
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.86	0.58
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.85	0.58
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.23	0.58
2:B:169:LYS:O	2:B:170:THR:HG23	2.02	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.84	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.58
1:N:361:LEU:O	1:N:364:ALA:HB3	2.03	0.58
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.38	0.58
9:V:49:LEU:HD22	9:V:54:SER:O	2.04	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.85	0.58
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.86	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.03	0.58
5:E:84:GLY:N	5:E:100:HIS:O	2.36	0.58
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
1:A:7:THR:HG21	2:B:113:ARG:CD	2.33	0.58
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.58
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.86	0.58
5:E:165:TYR:HA	5:E:170:ARG:O	2.03	0.58
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.69	0.58
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.85	0.58
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.69	0.58
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.58
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.86	0.57
2:B:26:ILE:O	2:B:26:ILE:HG12	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.84	0.57
1:N:15:ASN:O	1:N:26:ALA:HA	2.05	0.57
2:O:417:PHE:O	2:O:422:LYS:HE3	2.04	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
4:D:57:THR:HG22	4:D:58:GLU:N	2.19	0.57
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.35	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.05	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.57
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.86	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.19	0.57
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.86	0.57
5:E:189:GLY:O	5:E:192:LEU:N	2.38	0.57
2:O:52:LYS:O	2:O:203:ARG:NH2	2.23	0.57
2:B:28:LYS:O	2:B:29:LEU:O	2.22	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.57
1:A:95:THR:HG22	1:A:96:ALA:N	2.20	0.57
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.40	0.57
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.85	0.57
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.84	0.57
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.86	0.57
3:C:92:PHE:O	3:C:95:ILE:HG22	2.04	0.56
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.05	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.19	0.56
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.30	0.56
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.40	0.56
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.40	0.56
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.71	0.56
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.19	0.56
2:B:189:GLU:OE1	2:B:189:GLU:N	2.39	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.70	0.56
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.86	0.56
1:N:362:ARG:O	1:N:365:MET:HG2	2.05	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.06	0.56
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.86	0.56
5:E:106:ILE:C	5:E:110:ALA:HB3	2.26	0.56
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.88	0.56
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:106:ILE:O	5:R:109:GLU:HB3	2.06	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.41	0.56
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.05	0.56
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.38	0.56
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.88	0.56
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.87	0.56
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.36	0.56
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.69	0.56
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.88	0.56
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.36	0.56
2:B:312:PHE:HE1	9:I:62:ARG:O	1.89	0.56
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.33	0.56
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.41	0.56
5:R:185:TYR:O	5:R:186:GLN:HB3	2.06	0.56
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	1.88	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.44	0.55
1:N:281:ASP:O	1:N:283:THR:N	2.39	0.55
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.55
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.71	0.55
2:O:150:VAL:HA	2:O:153:GLN:HG3	1.88	0.55
5:R:79:SER:OG	5:R:191:ASP:HB2	2.06	0.55
2:B:374:THR:HG22	2:B:376:GLN:H	1.71	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.87	0.55
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.88	0.55
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.41	0.55
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.20	0.55
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.55
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.41	0.55
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.55
2:B:225:ASN:O	2:B:227:ARG:N	2.40	0.55
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.37	0.55
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.89	0.55
4:D:37:CYS:C	4:D:39:ALA:H	2.10	0.55
1:N:205:HIS:O	1:N:208:LEU:HB3	2.06	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.41	0.55
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.55
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.55
1:A:191:LYS:CA	1:A:195:MET:HE2	2.37	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.07	0.55
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.89	0.55
2:O:345:LYS:O	2:O:349:GLN:HG3	2.07	0.55
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.22	0.55
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.27	0.55
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.55
2:O:264:VAL:HG12	2:O:265:GLY:N	2.22	0.55
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.88	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.37	0.54
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.89	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.07	0.54
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.74	0.54
4:D:47:ALA:HA	4:D:90:TYR:HA	1.88	0.54
5:E:77:LYS:HG3	5:E:191:ASP:O	2.06	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
2:B:374:THR:HB	2:B:377:GLY:H	1.72	0.54
1:N:317:THR:HG23	1:N:318:GLY:N	2.23	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.08	0.54
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.86	0.54
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	1.89	0.54
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.54
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.54
1:A:430:GLN:HG3	7:G:4:PHE:O	2.08	0.54
1:A:280:TYR:CG	1:A:281:ASP:N	2.76	0.54
7:G:36:ASN:O	7:G:40:ARG:HG3	2.08	0.54
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.89	0.54
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.71	0.54
2:O:332:HIS:O	2:O:336:VAL:HG23	2.07	0.54
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.90	0.54
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.90	0.54
1:N:156:THR:HA	1:N:159:GLN:HB3	1.90	0.54
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.90	0.54
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.22	0.54
1:A:272:VAL:O	1:A:275:ALA:HB3	2.09	0.53
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.08	0.53
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.71	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.08	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:HH22	1:A:390:ILE:HG12	1.73	0.53
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.43	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53
2:O:217:LYS:O	2:O:221:GLU:HG2	2.09	0.53
2:O:402:ILE:HD13	2:O:402:ILE:C	2.29	0.53
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.89	0.53
1:A:191:LYS:N	1:A:195:MET:HE2	2.22	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.73	0.53
5:R:52:LYS:HD3	5:R:52:LYS:C	2.29	0.53
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.53
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.91	0.53
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.43	0.53
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.41	0.53
1:N:430:GLN:HG3	7:T:4:PHE:O	2.08	0.53
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.90	0.53
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.53
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.91	0.53
1:N:22:GLY:O	1:N:193:PRO:HA	2.07	0.53
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.53
5:R:170:ARG:HA	5:R:179:ASN:CB	2.38	0.53
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.44	0.53
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.72	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.23	0.53
5:E:52:LYS:C	5:E:52:LYS:HD3	2.29	0.53
6:F:40:ASP:O	6:F:44:LYS:HG3	2.09	0.53
1:N:131:ARG:NH2	1:N:177:LEU:O	2.41	0.53
1:N:186:ILE:HG23	1:N:190:PHE:HD1	1.74	0.53
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.53
1:A:90:THR:O	1:A:167:VAL:HG11	2.09	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.07	0.53
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.53
3:C:130:VAL:HG23	3:C:183:HIS:HB2	1.91	0.53
3:C:326:PHE:O	3:C:330:VAL:HG23	2.09	0.53
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.89	0.53
4:Q:2:GLU:O	4:Q:3:LEU:O	2.27	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.53
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.44	0.53
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:173:ASN:N	3:P:174:PRO:HD2	2.24	0.53
6:S:40:ASP:O	6:S:44:LYS:HG3	2.09	0.52
7:T:36:ASN:O	7:T:40:ARG:HG3	2.09	0.52
2:O:295:LEU:O	2:O:299:VAL:HG23	2.09	0.52
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.26	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
3:C:236:MET:O	3:C:239:PRO:HD2	2.08	0.52
5:E:187:PHE:C	5:E:189:GLY:N	2.63	0.52
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.91	0.52
1:A:130:GLU:O	1:A:134:ILE:HG13	2.10	0.52
2:B:156:GLN:HE22	9:I:77:ARG:C	2.13	0.52
2:B:96:LEU:HD12	2:B:97:SER:N	2.25	0.52
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.90	0.52
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.42	0.52
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.39	0.52
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.10	0.52
5:E:75:GLU:HA	5:E:193:VAL:O	2.09	0.52
1:N:354:VAL:HG23	1:N:355:LYS:N	2.25	0.52
2:O:225:ASN:O	2:O:227:ARG:HG3	2.09	0.52
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.25	0.52
1:A:204:SER:HB3	1:A:207:GLU:HG3	1.92	0.52
2:B:50:PHE:CD1	2:B:50:PHE:N	2.77	0.52
3:C:345:GLU:C	3:C:349:ILE:HG13	2.30	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.52
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.91	0.52
2:B:297:GLN:O	2:B:301:LYS:HG3	2.09	0.52
1:N:106:MET:HE2	1:N:107:PRO:HA	1.91	0.52
10:W:49:GLY:N	10:W:54:HIS:ND1	2.58	0.52
5:E:136:VAL:O	5:E:138:VAL:N	2.41	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.52
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.52
5:E:147:ILE:HG22	5:E:149:ASN:H	1.74	0.52
6:S:91:GLU:CG	6:S:95:LYS:HE3	2.37	0.52
8:U:36:ARG:CZ	8:U:36:ARG:HB3	2.40	0.52
1:A:75:PHE:O	1:A:79:VAL:HG23	2.10	0.52
2:B:27:THR:CG2	2:B:28:LYS:N	2.73	0.51
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.76	0.51
2:O:397:VAL:O	2:O:401:LYS:HG2	2.10	0.51
5:R:131:GLU:N	5:R:131:GLU:OE1	2.40	0.51
2:B:207:VAL:HG12	2:B:208:GLY:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.92	0.51
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.39	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.40	0.51
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.23	0.51
3:P:9:HIS:CD2	3:P:12:LEU:H	2.16	0.51
5:R:141:HIS:HB3	19:R:501:FES:S2	2.50	0.51
5:R:186:GLN:O	5:R:193:VAL:HG23	2.10	0.51
2:B:28:LYS:HG3	2:B:34:ILE:HG12	1.91	0.51
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.92	0.51
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.92	0.51
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.40	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.09	0.51
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.25	0.51
3:C:245:LEU:O	4:D:201:ARG:HD2	2.10	0.51
2:O:221:GLU:C	2:O:223:PHE:H	2.13	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.75	0.51
5:E:190:ASP:C	5:E:192:LEU:N	2.63	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.26	0.51
3:C:207:ASN:ND2	3:C:208:ASN:H	2.08	0.51
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.92	0.51
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.11	0.51
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.10	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.46	0.51
5:E:185:TYR:O	5:E:186:GLN:HB3	2.09	0.51
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.51
2:B:307:PHE:H	9:I:52:ARG:HG2	1.74	0.51
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.76	0.51
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.51
10:J:10:TYR:HE2	10:J:15:ARG:HD2	1.74	0.51
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.51
3:C:347:PRO:O	3:C:350:ILE:HG22	2.11	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.93	0.51
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.93	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.46	0.51
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.42	0.50
2:O:31:ASN:ND2	2:O:31:ASN:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:295:LEU:O	2:B:299:VAL:HG23	2.11	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.27	0.50
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.94	0.50
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.24	0.50
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.50
2:B:150:VAL:HA	2:B:153:GLN:HG3	1.92	0.50
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.94	0.50
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.50
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.50
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.50
1:A:223:TYR:HD2	1:A:223:TYR:H	1.59	0.50
1:A:354:VAL:HG23	1:A:355:LYS:N	2.26	0.50
12:C:502:HEM:HMB1	12:C:502:HEM:HBB2	1.92	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.50
5:E:189:GLY:O	5:E:192:LEU:O	2.29	0.50
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.92	0.50
2:O:57:TYR:N	2:O:57:TYR:CD1	2.79	0.50
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.94	0.50
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.46	0.50
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.15	0.50
10:W:7:ARG:HH11	10:W:7:ARG:CB	2.25	0.50
3:C:132:TYR:O	3:C:135:PRO:HD2	2.12	0.50
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.50
4:D:57:THR:HG22	4:D:59:ALA:N	2.23	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.24	0.50
2:O:124:LEU:HD23	2:O:124:LEU:C	2.32	0.50
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.50
5:R:163:SER:H	5:R:175:PRO:HD2	1.76	0.50
1:A:45:SER:HA	1:A:48:GLU:HG3	1.92	0.50
3:C:52:LEU:HD13	12:C:501:HEM:HBD1	1.94	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
1:N:223:TYR:HD2	1:N:223:TYR:H	1.58	0.50
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.75	0.50
1:N:439:SER:HA	1:N:442:TYR:CE2	2.46	0.50
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.59	0.50
9:V:31:UNK:C	9:V:73:PRO:HG2	2.41	0.50
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.12	0.50
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:CD	1:A:54:GLY:H	2.15	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
5:E:121:GLN:CB	5:E:170:ARG:HD3	2.40	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.47	0.50
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.94	0.50
1:A:89:TYR:O	1:A:95:THR:HG23	2.12	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.12	0.49
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.47	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
3:P:223:PRO:O	3:P:227:PHE:HD2	1.94	0.49
3:C:286:PRO:O	3:C:287:ASN:CB	2.60	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.44	0.49
3:P:50:LEU:O	3:P:54:MET:HG3	2.12	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.93	0.49
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.47	0.49
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.75	0.49
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.47	0.49
1:A:382:HIS:HB3	1:A:388:ARG:O	2.12	0.49
5:E:76:ILE:O	5:E:193:VAL:HG12	2.13	0.49
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.94	0.49
2:O:26:ILE:O	2:O:26:ILE:HG12	2.11	0.49
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.41	0.49
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.27	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.12	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.42	0.49
2:O:222:GLN:HG2	2:O:222:GLN:O	2.12	0.49
2:O:280:GLY:HA3	2:O:293:SER:OG	2.12	0.49
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.28	0.49
2:O:353:THR:HG22	2:O:354:GLU:N	2.28	0.49
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.93	0.49
3:P:49:GLY:C	12:P:501:HEM:HAC	2.33	0.49
1:N:191:LYS:C	1:N:195:MET:HE2	2.33	0.49
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.47	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
2:B:338:ARG:CG	2:B:338:ARG:NH1	2.74	0.49
2:B:402:ILE:HD13	2:B:402:ILE:C	2.32	0.49
5:E:122:HIS:O	5:E:125:ASP:HB2	2.11	0.49
1:N:364:ALA:O	1:N:368:GLN:HG3	2.12	0.49
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:147:ILE:HD11	13:P:3001:JZZ:HAB	1.95	0.49
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.78	0.49
4:D:102:ARG:HA	4:D:108:ALA:O	2.12	0.49
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.47	0.49
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.13	0.49
8:U:27:THR:HG22	8:U:29:LYS:H	1.77	0.49
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.49
2:B:385:GLU:O	2:B:387:LEU:N	2.46	0.49
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.43	0.49
5:E:147:ILE:O	5:E:156:TYR:HA	2.13	0.49
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.53	0.49
4:Q:148:HIS:CD2	4:Q:148:HIS:N	2.81	0.49
1:A:23:LEU:HD23	1:A:24:ARG:N	2.28	0.48
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.48	0.48
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.47	0.48
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.94	0.48
3:P:347:PRO:O	3:P:350:ILE:HG22	2.13	0.48
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.48
6:S:70:LEU:HD12	6:S:70:LEU:C	2.33	0.48
2:B:59:THR:O	2:B:61:ALA:N	2.45	0.48
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.48
3:P:155:PRO:O	3:P:156:TYR:HB2	2.13	0.48
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.48
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.77	0.48
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.28	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.95	0.48
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.48
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.17	0.48
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.96	0.48
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.48
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.48
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.96	0.48
5:R:161:HIS:HB2	19:R:501:FES:S1	2.53	0.48
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.48
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.78	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
5:R:82:PRO:O	5:R:100:HIS:HB3	2.13	0.48
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.28	0.48
2:B:27:THR:CG2	2:B:28:LYS:H	2.26	0.48
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.79	0.48
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:37:CYS:C	4:Q:39:ALA:H	2.17	0.48
5:R:166:ASP:OD1	5:R:168:SER:N	2.45	0.48
1:A:133:VAL:O	1:A:136:GLN:HB2	2.14	0.48
4:D:220:TYR:O	4:D:224:ARG:HG2	2.13	0.48
1:N:351:GLU:O	1:N:354:VAL:HG22	2.12	0.48
2:O:221:GLU:O	2:O:223:PHE:N	2.46	0.48
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.48
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.29	0.48
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.48
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.48
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.96	0.48
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.48
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.44	0.48
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.29	0.48
6:S:13:MET:O	6:S:17:ARG:HG3	2.14	0.48
5:E:97:PHE:O	5:E:134:ILE:HA	2.13	0.48
1:N:32:GLN:HE22	2:O:373:GLU:HA	1.79	0.48
2:O:54:GLY:C	2:O:56:ARG:H	2.17	0.48
5:R:75:GLU:HA	5:R:193:VAL:O	2.14	0.48
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.14	0.48
1:N:402:VAL:HA	1:N:406:MET:CE	2.44	0.48
1:N:45:SER:HA	1:N:48:GLU:CG	2.44	0.48
2:O:338:ARG:O	2:O:341:MET:HB2	2.14	0.48
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.48	0.48
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.28	0.48
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.96	0.48
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.13	0.48
4:D:239:PRO:C	4:D:241:LYS:H	2.17	0.48
6:F:53:ASP:OD1	6:F:54:LEU:N	2.46	0.48
7:G:28:ASN:HB3	7:G:31:SER:OG	2.14	0.48
1:N:240:GLU:HA	1:N:422:LEU:O	2.14	0.48
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.95	0.48
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.79	0.48
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.48
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.95	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.14	0.47
2:B:206:LEU:CD2	2:B:220:ALA:HB2	2.43	0.47
3:C:49:GLY:C	12:C:501:HEM:HAC	2.34	0.47
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:71:ASN:HD22	9:I:71:ASN:H	1.61	0.47
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.96	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.96	0.47
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.49	0.47
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.45	0.47
1:A:287:GLY:O	1:A:290:LEU:HG	2.14	0.47
1:A:362:ARG:O	1:A:365:MET:HG2	2.14	0.47
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.47
2:B:124:LEU:CD1	2:B:223:PHE:HB3	2.42	0.47
2:B:262:ALA:O	2:B:320:GLY:HA3	2.14	0.47
2:B:332:HIS:O	2:B:336:VAL:HG23	2.13	0.47
3:C:50:LEU:O	3:C:54:MET:HG3	2.15	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.47
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.44	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.14	0.47
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.96	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.77	0.47
1:A:205:HIS:O	1:A:208:LEU:HB3	2.15	0.47
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.14	0.47
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.96	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.15	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.40	0.47
1:N:36:THR:HG21	1:N:373:THR:HA	1.96	0.47
1:N:90:THR:O	1:N:90:THR:HG23	2.15	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.47
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.47
7:T:56:TYR:O	7:T:59:TYR:HB3	2.14	0.47
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.17	0.47
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.47
1:A:402:VAL:HA	1:A:406:MET:CE	2.44	0.47
2:B:207:VAL:HG12	2:B:208:GLY:N	2.29	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.95	0.47
1:A:281:ASP:O	1:A:283:THR:N	2.47	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.47
2:B:353:THR:HG22	2:B:354:GLU:N	2.29	0.47
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.14	0.47
1:N:154:HIS:O	1:N:156:THR:N	2.48	0.47
1:N:388:ARG:HH22	1:N:390:ILE:HG12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.50	0.47
6:F:16:ILE:O	6:F:19:TRP:HB3	2.14	0.47
3:P:275:PHE:CG	13:P:3001:JZZ:HAGB	2.50	0.47
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.97	0.47
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.77	0.47
9:V:64:LEU:HD12	9:V:77:ARG:C	2.35	0.47
2:B:264:VAL:HG23	2:B:316:TYR:C	2.35	0.47
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.97	0.47
8:U:32:LYS:O	8:U:36:ARG:HG3	2.15	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.44	0.47
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.47
10:J:59:TYR:CD1	10:J:59:TYR:N	2.82	0.47
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.43	0.47
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.45	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.78	0.47
8:H:50:THR:O	8:H:50:THR:HG23	2.14	0.47
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.95	0.47
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.50	0.47
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.96	0.47
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.50	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.72	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.15	0.47
2:B:338:ARG:O	2:B:341:MET:HB2	2.15	0.46
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.45	0.46
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.82	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.50	0.46
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.47	0.46
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.97	0.46
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.30	0.46
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.50	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.97	0.46
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.50	0.46
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.96	0.46
5:E:191:ASP:N	5:E:191:ASP:OD2	2.48	0.46
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.14	0.46
12:P:502:HEM:HBB2	12:P:502:HEM:CMB	2.45	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.45	0.46
2:B:42:SER:C	2:B:44:ALA:H	2.19	0.46
8:U:22:GLU:O	8:U:26:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.30	0.46
4:D:235:MET:HB3	7:G:15:THR:HG22	1.97	0.46
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.77	0.46
5:R:186:GLN:NE2	5:R:187:PHE:O	2.48	0.46
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.50	0.46
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.46
3:C:286:PRO:O	3:C:287:ASN:HB2	2.15	0.46
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.45	0.46
5:E:106:ILE:O	5:E:106:ILE:HG22	2.15	0.46
4:Q:222:MET:HE1	5:R:40:THR:HG23	1.97	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.50	0.46
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.45	0.46
5:E:161:HIS:HB2	19:E:501:FES:S1	2.56	0.46
8:H:27:THR:HG22	8:H:29:LYS:H	1.81	0.46
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.97	0.46
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.98	0.46
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.15	0.46
10:W:60:GLU:O	10:W:61:ALA:HB2	2.14	0.46
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.97	0.46
7:G:65:GLU:O	7:G:69:LEU:HG	2.16	0.46
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.46
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.46
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.16	0.46
10:W:56:LYS:O	10:W:60:GLU:HB3	2.15	0.46
1:A:156:THR:HA	1:A:159:GLN:HB3	1.97	0.46
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.31	0.46
2:B:54:GLY:C	2:B:56:ARG:H	2.18	0.46
3:C:245:LEU:O	4:D:201:ARG:CD	2.64	0.46
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.79	0.46
5:E:144:CYS:HB2	19:E:501:FES:S2	2.56	0.46
1:N:294:LEU:HD11	1:N:334:MET:CE	2.45	0.46
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.96	0.46
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.46	0.46
2:O:207:VAL:HG12	2:O:208:GLY:H	1.81	0.46
2:O:334:GLY:O	2:O:338:ARG:HG2	2.15	0.46
5:R:97:PHE:O	5:R:134:ILE:HA	2.16	0.46
5:R:118:ARG:NH1	5:R:174:GLY:O	2.48	0.46
1:A:114:ALA:O	1:A:118:GLN:HB2	2.16	0.46
2:B:274:VAL:O	2:B:278:VAL:HG23	2.16	0.46
3:C:269:ILE:HG22	3:C:269:ILE:O	2.16	0.46
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:245:LEU:O	4:Q:201:ARG:CD	2.64	0.46
4:Q:43:MET:HE3	4:Q:91:PHE:CE2	2.51	0.46
10:W:59:TYR:N	10:W:59:TYR:CD1	2.83	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
2:O:385:GLU:O	2:O:387:LEU:N	2.48	0.46
5:R:177:PRO:HG2	5:R:178:TYR:HD1	1.81	0.46
5:R:185:TYR:HD2	5:R:185:TYR:N	2.14	0.46
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
4:D:227:TRP:O	4:D:228:SER:C	2.52	0.45
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.45
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.45
2:O:31:ASN:H	2:O:31:ASN:ND2	2.13	0.45
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.97	0.45
2:B:140:LEU:C	2:B:142:PRO:HD2	2.36	0.45
2:B:24:LEU:HD12	2:B:37:SER:O	2.16	0.45
16:D:501:HEC:HBB3	16:D:501:HEC:HMB1	1.97	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.12	0.45
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.96	0.45
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.97	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.16	0.45
1:N:180:ALA:O	1:N:183:ALA:HB3	2.16	0.45
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.52	0.45
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.51	0.45
1:A:106:MET:N	1:A:107:PRO:HD2	2.32	0.45
2:B:81:SER:O	2:B:85:ILE:HG13	2.17	0.45
3:C:31:TRP:CH2	17:G:2004:CDL:H512	2.51	0.45
8:H:58:LEU:O	8:H:58:LEU:HD12	2.15	0.45
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.41	0.45
2:O:227:ARG:HB3	2:O:228:SER:H	1.47	0.45
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.31	0.45
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.32	0.45
2:B:395:PRO:O	2:B:398:VAL:HG12	2.17	0.45
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.79	0.45
2:O:162:ASN:O	2:O:244:ILE:HD12	2.17	0.45
2:O:67:HIS:O	2:O:70:ARG:HB3	2.17	0.45
3:P:101:ARG:O	3:P:101:ARG:HD2	2.16	0.45
3:P:286:PRO:O	3:P:287:ASN:CB	2.64	0.45
5:R:134:ILE:HD12	5:R:185:TYR:HE1	1.80	0.45
1:A:170:THR:CG2	1:A:171:THR:N	2.79	0.45
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.98	0.45
2:O:76:THR:CG2	2:O:82:SER:H	2.10	0.45
5:R:163:SER:OG	5:R:176:ALA:HB2	2.17	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.35	0.45
9:I:65:VAL:HG12	9:I:66:ALA:N	2.31	0.45
1:N:48:GLU:CD	1:N:54:GLY:H	2.21	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.81	0.45
3:P:275:PHE:CD2	13:P:3001:JZZ:HAGB	2.52	0.45
3:P:81:ARG:O	3:P:81:ARG:HD3	2.17	0.45
5:R:107:ASN:C	5:R:109:GLU:N	2.70	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
7:T:40:ARG:CB	17:T:3004:CDL:HA32	2.45	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
4:D:169:LEU:CD2	4:D:182:ILE:HD11	2.47	0.45
5:E:171:ILE:HG12	5:E:176:ALA:O	2.16	0.45
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.45
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.45
3:P:350:ILE:O	3:P:354:MET:HG2	2.16	0.45
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.52	0.45
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.98	0.45
1:A:307:PHE:C	1:A:307:PHE:CD1	2.90	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.52	0.45
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.51	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.99	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.46	0.45
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.45
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.52	0.45
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.97	0.45
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.57	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.17	0.45
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.37	0.45
5:R:185:TYR:CD2	5:R:185:TYR:N	2.85	0.45
1:A:106:MET:CE	1:A:110:VAL:HG21	2.47	0.44
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.44
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.41	0.44
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.52	0.44
1:N:53:ASN:N	1:N:173:ASN:HD22	2.14	0.44
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.99	0.44
3:P:246:PHE:C	3:P:248:PRO:HD3	2.37	0.44
4:Q:40:CYS:SG	16:Q:501:HEC:HMC1	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.98	0.44
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.44
2:B:38:LEU:HD12	2:B:38:LEU:C	2.36	0.44
4:D:200:GLN:HB2	18:D:2091:BOG:H3	1.99	0.44
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.46	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.00	0.44
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.99	0.44
3:P:75:GLN:HB2	5:R:61:SER:HA	1.98	0.44
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.53	0.44
2:B:31:ASN:HD22	2:B:31:ASN:H	1.58	0.44
3:C:127:THR:O	3:C:130:VAL:HG22	2.18	0.44
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.44
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.99	0.44
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.80	0.44
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.99	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.43	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	1.99	0.44
3:P:271:PRO:HG2	3:P:276:LEU:HD23	2.00	0.44
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.52	0.44
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.00	0.44
3:C:147:ILE:HD11	13:C:2001:JZZ:HAB	1.98	0.44
1:N:191:LYS:CA	1:N:195:MET:HE2	2.47	0.44
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.99	0.44
2:O:297:GLN:O	2:O:301:LYS:HG3	2.17	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.33	0.44
5:R:184:THR:O	5:R:185:TYR:HB3	2.17	0.44
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.52	0.44
5:R:76:ILE:HD12	5:R:98:VAL:HG21	2.00	0.44
1:N:239:SER:HB2	7:T:17:SER:O	2.17	0.44
1:A:53:ASN:N	1:A:173:ASN:ND2	2.65	0.44
3:C:138:GLN:HB2	3:C:255:GLU:O	2.18	0.44
5:E:150:SER:OG	5:E:157:TYR:HB3	2.18	0.44
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.30	0.44
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.47	0.44
2:O:374:THR:HB	2:O:377:GLY:H	1.81	0.44
4:Q:234:LYS:HD2	5:R:8:PRO:HB2	2.00	0.44
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.16	0.44
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.44
1:N:402:VAL:HG22	1:N:406:MET:HE1	2.00	0.44
1:N:85:HIS:HB2	1:N:100:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.53	0.44
1:A:21:ASN:N	1:A:21:ASN:OD1	2.47	0.44
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.82	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.47	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.48	0.44
2:B:24:LEU:O	2:B:24:LEU:HG	2.17	0.44
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.00	0.44
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.48	0.44
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.44
1:N:383:LEU:HD23	1:N:388:ARG:HA	1.98	0.44
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.98	0.44
8:U:12:GLU:HG2	8:U:13:LEU:N	2.33	0.44
5:E:155:GLY:HA3	5:E:166:ASP:C	2.38	0.44
2:O:407:SER:O	2:O:411:VAL:HG23	2.17	0.44
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.33	0.44
1:A:53:ASN:N	1:A:173:ASN:HD22	2.16	0.44
1:A:373:THR:HB	1:A:374:PRO:CD	2.47	0.44
5:E:178:TYR:H	5:E:178:TYR:HD1	1.66	0.44
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.26	0.44
2:B:124:LEU:C	2:B:124:LEU:HD23	2.38	0.43
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.99	0.43
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.18	0.43
3:C:34:PHE:HB2	20:C:381:HOH:O	2.18	0.43
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.33	0.43
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.53	0.43
1:N:170:THR:CG2	1:N:171:THR:H	2.23	0.43
10:W:56:LYS:HB3	10:W:56:LYS:HE2	1.63	0.43
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.00	0.43
3:C:246:PHE:C	3:C:248:PRO:HD3	2.37	0.43
3:C:263:LEU:O	3:C:264:VAL:CG2	2.66	0.43
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.18	0.43
2:O:59:THR:O	2:O:61:ALA:N	2.51	0.43
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.34	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.18	0.43
2:B:407:SER:O	2:B:411:VAL:HG23	2.18	0.43
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.53	0.43
3:C:30:ALA:HB1	17:D:2003:CDL:H111	1.99	0.43
5:E:115:SER:CB	5:E:116:LYS:HD2	2.49	0.43
6:F:32:MET:HE3	6:F:87:LYS:HE2	2.00	0.43
3:P:189:ALA:O	3:P:193:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:207:ASN:ND2	3:P:208:ASN:H	2.16	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43
4:Q:109:LEU:HD12	4:Q:110:PRO:HD2	1.99	0.43
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
2:B:76:THR:CG2	2:B:82:SER:H	2.16	0.43
4:D:37:CYS:C	4:D:39:ALA:N	2.72	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.50	0.43
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.43
5:E:187:PHE:O	5:E:189:GLY:N	2.50	0.43
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.43
1:N:206:LYS:N	1:N:206:LYS:HD3	2.34	0.43
5:R:116:LYS:O	5:R:117:LEU:HD23	2.19	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.49	0.43
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.43
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.82	0.43
4:Q:43:MET:HE3	4:Q:91:PHE:HE2	1.84	0.43
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.48	0.43
2:B:104:LYS:C	2:B:104:LYS:HD2	2.39	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.45	0.43
3:C:277:PHE:CG	3:C:278:ALA:N	2.86	0.43
17:D:2003:CDL:HB22	7:G:40:ARG:HH21	1.84	0.43
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.93	0.43
2:O:54:GLY:O	2:O:56:ARG:N	2.51	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
3:C:350:ILE:HG23	3:C:351:ILE:N	2.33	0.43
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.01	0.43
5:E:171:ILE:HG23	5:E:171:ILE:O	2.18	0.43
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.43
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.53	0.43
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.18	0.43
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.43
2:O:306:PRO:HA	9:V:52:ARG:CG	2.48	0.43
1:A:277:ILE:HD11	1:A:345:LEU:HD11	2.01	0.43
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.43
1:N:394:GLU:O	1:N:395:TRP:C	2.57	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	2.01	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.84	0.43
2:B:166:ALA:HB1	2:B:242:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:ND2	2:B:248:ASN:C	2.71	0.43
5:E:129:LYS:HB2	5:E:132:TRP:HB2	2.01	0.43
9:I:70:LEU:CD2	9:I:71:ASN:N	2.79	0.43
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.40	0.43
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.88	0.43
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.83	0.43
4:D:171:TYR:CD1	4:D:175:THR:HB	2.54	0.43
3:P:101:ARG:CD	3:P:101:ARG:C	2.83	0.43
3:P:156:TYR:CD2	3:P:156:TYR:N	2.87	0.43
5:R:162:GLY:O	5:R:163:SER:C	2.56	0.43
1:A:275:ALA:HB3	1:A:357:ALA:HB1	2.00	0.42
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.42
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.84	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.01	0.42
5:E:75:GLU:HB3	5:E:194:VAL:HG22	2.00	0.42
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.37	0.42
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.42
2:O:54:GLY:C	2:O:56:ARG:N	2.72	0.42
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.19	0.42
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.01	0.42
1:A:382:HIS:HE1	1:A:390:ILE:HB	1.85	0.42
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.76	0.42
3:C:272:GLU:O	3:C:273:TRP:C	2.56	0.42
5:E:52:LYS:CD	5:E:52:LYS:C	2.88	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.19	0.42
1:N:402:VAL:HG13	1:N:406:MET:HE2	2.01	0.42
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.19	0.42
3:P:130:VAL:HG23	3:P:183:HIS:HB2	2.01	0.42
3:P:125:MET:CE	13:P:3001:JZZ:HAGA	2.49	0.42
8:U:73:LEU:O	8:U:73:LEU:HD12	2.19	0.42
2:O:160:LEU:HB2	9:V:64:LEU:HD22	2.01	0.42
1:A:245:ASP:OD1	7:G:11:ARG:NE	2.47	0.42
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.19	0.42
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.01	0.42
5:E:166:ASP:OD1	5:E:168:SER:N	2.45	0.42
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.42
2:O:50:PHE:CD1	2:O:50:PHE:N	2.88	0.42
6:S:60:PHE:O	6:S:64:ARG:HB2	2.19	0.42
9:V:65:VAL:HG12	9:V:66:ALA:N	2.33	0.42
1:A:178:THR:CG2	1:A:179:ARG:H	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.54	0.42
8:H:43:ARG:NH1	8:H:43:ARG:HG2	2.34	0.42
1:N:106:MET:CG	1:N:203:ILE:HD13	2.46	0.42
1:N:287:GLY:O	1:N:290:LEU:HG	2.19	0.42
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.42
2:O:68:LEU:HD23	2:O:186:ILE:HG21	2.00	0.42
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.84	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.67	0.42
1:A:369:LEU:HD11	1:A:392:LEU:HD21	2.02	0.42
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.54	0.42
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.54	0.42
3:C:365:ILE:HG22	3:C:366:LEU:HD23	2.01	0.42
4:D:218:LEU:HD11	5:E:42:THR:HG22	2.01	0.42
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.02	0.42
1:N:369:LEU:HD11	1:N:392:LEU:HD21	2.00	0.42
1:N:95:THR:HG22	1:N:96:ALA:N	2.34	0.42
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.80	0.42
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.54	0.42
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.42
1:A:156:THR:HG23	1:A:157:ALA:N	2.35	0.42
1:A:361:LEU:O	1:A:364:ALA:HB3	2.19	0.42
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.01	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
2:B:334:GLY:O	2:B:338:ARG:HG2	2.20	0.42
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.55	0.42
3:C:182:LEU:HD23	3:C:182:LEU:HA	1.86	0.42
5:E:127:VAL:O	5:E:128:LYS:HB2	2.20	0.42
1:N:382:HIS:HE1	1:N:390:ILE:HB	1.84	0.42
1:N:89:TYR:O	1:N:95:THR:HG23	2.20	0.42
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.84	0.42
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.54	0.42
3:P:345:GLU:C	3:P:349:ILE:HG13	2.38	0.42
3:P:92:PHE:HA	3:P:95:ILE:HG22	2.02	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42
5:R:81:ILE:HG12	5:R:87:VAL:CG2	2.49	0.42
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.00	0.42
2:B:50:PHE:HD1	2:B:50:PHE:N	2.18	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.31	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.87	0.42
3:P:286:PRO:O	3:P:287:ASN:HB2	2.19	0.42
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.81	0.42
3:C:37:LEU:HD21	3:C:233:LEU:HA	2.01	0.42
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.34	0.42
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.20	0.42
5:E:149:ASN:HD22	5:E:149:ASN:N	2.17	0.42
7:G:80:ASP:O	7:G:81:GLN:C	2.58	0.42
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.54	0.42
1:N:417:ASP:O	1:N:438:ARG:NH2	2.53	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.54	0.42
7:T:48:VAL:O	7:T:51:PRO:HD2	2.19	0.42
9:V:52:ARG:HG3	9:V:52:ARG:NH1	2.33	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.68	0.42
10:W:60:GLU:CG	10:W:60:GLU:O	2.65	0.42
2:B:59:THR:C	2:B:61:ALA:N	2.71	0.42
2:B:76:THR:HG23	2:B:82:SER:HB2	2.02	0.42
4:D:150:ASN:O	4:D:156:GLN:HA	2.20	0.42
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.42
1:N:113:LEU:O	1:N:116:VAL:N	2.49	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.73	0.42
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.23	0.42
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.84	0.42
5:R:83:GLU:CD	5:R:102:THR:HA	2.39	0.42
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.20	0.42
2:B:385:GLU:HB3	2:B:391:THR:O	2.20	0.42
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.49	0.42
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.42
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.35	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.60	0.42
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.82	0.42
1:A:154:HIS:O	1:A:156:THR:N	2.53	0.41
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.02	0.41
2:B:206:LEU:HG	2:B:206:LEU:O	2.20	0.41
3:C:19:LEU:C	3:C:20:ILE:HG13	2.41	0.41
3:P:132:TYR:HD2	13:P:3001:JZZ:H27A	1.85	0.41
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.41
3:P:75:GLN:O	3:P:76:TYR:HB2	2.20	0.41
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.49	0.41
5:R:76:ILE:HB	5:R:193:VAL:CG1	2.50	0.41
8:U:52:GLU:HG2	8:U:53:GLN:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:42:ILE:HG22	10:W:46:LEU:HD12	2.02	0.41
1:A:27:SER:HA	1:A:199:ALA:O	2.20	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.38	0.41
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.54	0.41
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.54	0.41
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.56	0.41
7:G:56:TYR:O	7:G:59:TYR:HB3	2.20	0.41
2:B:287:ARG:HB3	9:I:53:GLU:HG3	2.02	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.20	0.41
3:P:235:LEU:HD23	3:P:235:LEU:HA	1.84	0.41
2:B:163:LEU:C	2:B:165:ALA:N	2.74	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.01	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.53	0.41
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.02	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.03	0.41
3:P:31:TRP:CH2	17:T:3004:CDL:H512	2.54	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.20	0.41
7:T:35:PRO:O	7:T:38:TRP:HB3	2.19	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.41
3:C:339:ILE:HA	3:C:339:ILE:HD13	1.92	0.41
4:D:169:LEU:HD22	4:D:182:ILE:HD11	2.02	0.41
5:E:178:TYR:CD1	5:E:178:TYR:N	2.89	0.41
6:F:84:GLU:CD	6:F:84:GLU:H	2.23	0.41
8:H:43:ARG:HH11	8:H:43:ARG:HG2	1.86	0.41
1:N:402:VAL:HG22	1:N:406:MET:HE2	2.00	0.41
1:N:79:VAL:O	1:N:82:MET:HG2	2.20	0.41
2:O:206:LEU:O	2:O:206:LEU:HG	2.19	0.41
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.89	0.41
5:R:73:LYS:HB3	5:R:196:GLY:O	2.20	0.41
8:U:65:ARG:O	8:U:68:CYS:HB3	2.20	0.41
2:B:153:GLN:NE2	9:I:34:UNK:HB1	2.35	0.41
2:B:59:THR:HG22	2:B:60:THR:N	2.35	0.41
1:N:114:ALA:O	1:N:118:GLN:HB2	2.20	0.41
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.41
1:N:402:VAL:HA	1:N:406:MET:HE1	2.02	0.41
3:P:146:VAL:HG12	3:P:147:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:16:GLY:N	4:Q:19:SER:OG	2.54	0.41
5:R:171:ILE:N	5:R:179:ASN:OD1	2.46	0.41
4:Q:218:LEU:HD11	5:R:42:THR:HG22	2.01	0.41
2:B:128:THR:O	2:B:226:ILE:HD11	2.20	0.41
2:B:153:GLN:HE22	9:I:34:UNK:HB1	1.85	0.41
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.49	0.41
3:C:101:ARG:CD	3:C:101:ARG:C	2.89	0.41
4:D:9:ALA:HA	4:D:125:ASP:OD1	2.20	0.41
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.41
1:N:106:MET:HE1	1:N:208:LEU:HA	2.02	0.41
1:N:154:HIS:C	1:N:156:THR:N	2.74	0.41
1:N:373:THR:HB	1:N:374:PRO:CD	2.51	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.51	0.41
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.56	0.41
5:R:171:ILE:HB	5:R:178:TYR:O	2.20	0.41
1:A:133:VAL:O	1:A:137:GLU:HG3	2.20	0.41
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.41
2:B:146:VAL:O	2:B:149:ALA:N	2.53	0.41
2:B:223:PHE:O	2:B:225:ASN:N	2.54	0.41
3:C:172:ASP:HB3	3:C:174:PRO:HD2	2.02	0.41
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.41
4:D:239:PRO:HG2	4:D:241:LYS:HB2	2.02	0.41
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.41	0.41
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.50	0.41
2:O:18:CYS:CB	2:O:19:PRO:CD	2.93	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.35	0.41
6:S:32:MET:O	6:S:35:ASP:HB2	2.20	0.41
1:A:240:GLU:HA	1:A:422:LEU:O	2.21	0.41
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.41
2:B:207:VAL:HG21	2:B:383:GLY:HA3	2.03	0.41
4:D:158:ILE:HG12	4:D:160:MET:H	1.85	0.41
4:D:169:LEU:HD23	4:D:169:LEU:C	2.40	0.41
6:F:31:LEU:HD21	6:F:65:ALA:HB2	2.03	0.41
2:O:43:PRO:O	2:O:113:ARG:HG3	2.20	0.41
2:O:207:VAL:HG12	2:O:208:GLY:N	2.36	0.41
5:R:130:PRO:C	5:R:132:TRP:H	2.24	0.41
1:A:439:SER:HA	1:A:442:TYR:CE2	2.56	0.41
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.41
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.69	0.41
6:F:70:LEU:HD12	6:F:70:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:71:LYS:O	6:F:72:HIS:HB2	2.21	0.41
6:F:21:TYR:CG	6:F:83:TYR:HD1	2.39	0.41
2:O:59:THR:C	2:O:61:ALA:N	2.73	0.41
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.89	0.41
4:Q:34:LYS:HG2	4:Q:34:LYS:O	2.20	0.41
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.01	0.41
10:W:52:TRP:O	10:W:56:LYS:HB2	2.20	0.41
1:A:32:GLN:HE22	2:B:373:GLU:HA	1.85	0.41
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.20	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.86	0.41
3:C:287:ASN:O	3:C:288:LYS:C	2.58	0.41
4:D:239:PRO:C	4:D:241:LYS:N	2.74	0.41
7:G:34:LEU:HB2	7:G:35:PRO:HD3	2.03	0.41
4:Q:169:LEU:HD23	4:Q:169:LEU:O	2.20	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.51	0.41
2:B:35:ILE:HD11	2:B:220:ALA:HB3	2.03	0.41
2:B:73:SER:N	2:B:74:PRO:HD2	2.36	0.41
3:C:223:PRO:O	3:C:227:PHE:HD2	2.04	0.41
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.54	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.21	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.68	0.41
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.21	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.41
1:A:134:ILE:HG21	1:A:174:ILE:HD13	2.02	0.40
2:B:292:THR:CG2	2:B:292:THR:O	2.68	0.40
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.40
2:O:341:MET:HA	2:O:341:MET:HE2	2.02	0.40
2:O:38:LEU:HD12	2:O:38:LEU:C	2.41	0.40
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.40
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.87	0.40
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.24	0.40
2:B:84:ARG:HG3	6:S:107:TRP:CZ3	2.56	0.40
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.56	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.84	0.40
11:E:2005:PEE:H13	11:E:2005:PEE:H8	2.03	0.40
1:N:373:THR:N	1:N:374:PRO:HD2	2.36	0.40
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.38	0.40
4:Q:197:GLU:O	4:Q:198:HIS:C	2.59	0.40
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.36	0.40
5:R:171:ILE:HG12	5:R:176:ALA:O	2.21	0.40
11:R:3005:PEE:H13	11:R:3005:PEE:H8	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:O	1:A:399:ILE:HG13	2.20	0.40
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.57	0.40
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.03	0.40
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.40
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.40
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.80	0.40
3:P:64:PHE:CE1	15:P:3011:GOL:H12	2.56	0.40
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.50	0.40
2:B:325:TYR:CD2	2:B:325:TYR:C	2.95	0.40
3:C:98:HIS:CE1	12:C:502:HEM:NA	2.89	0.40
4:D:102:ARG:HB3	4:D:107:GLY:HA2	2.02	0.40
5:E:10:PHE:CB	7:G:18:LEU:HD11	2.51	0.40
7:G:40:ARG:CB	17:G:2004:CDL:HA32	2.52	0.40
7:G:35:PRO:O	7:G:38:TRP:HB3	2.22	0.40
1:N:246:ASP:HA	1:N:427:PRO:HB3	2.03	0.40
2:O:104:LYS:HD2	2:O:104:LYS:C	2.42	0.40
2:O:181:TYR:CD1	2:O:182:ARG:HG3	2.55	0.40
3:P:182:LEU:HA	3:P:182:LEU:HD23	1.85	0.40
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.04	0.40
5:R:171:ILE:O	5:R:171:ILE:HG23	2.22	0.40
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.83	0.40
1:A:63:ALA:O	1:A:116:VAL:HG13	2.21	0.40
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.40
3:C:101:ARG:O	3:C:101:ARG:HD2	2.21	0.40
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.57	0.40
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.54	0.40
5:E:125:ASP:C	5:E:126:ARG:HG3	2.42	0.40
5:E:126:ARG:O	5:E:127:VAL:CG2	2.69	0.40
1:N:23:LEU:HD23	1:N:24:ARG:N	2.37	0.40
1:N:342:TRP:O	1:N:345:LEU:HB2	2.21	0.40
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.40
8:U:52:GLU:CG	8:U:53:GLN:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/446 (99%)	388 (88%)	46 (10%)	8 (2%)	8	34
1	N	440/446 (99%)	386 (88%)	45 (10%)	9 (2%)	7	31
2	B	418/441 (95%)	342 (82%)	56 (13%)	20 (5%)	2	12
2	O	420/441 (95%)	355 (84%)	51 (12%)	14 (3%)	4	19
3	C	378/380 (100%)	347 (92%)	28 (7%)	3 (1%)	19	54
3	P	377/380 (99%)	345 (92%)	26 (7%)	6 (2%)	9	37
4	D	239/241 (99%)	215 (90%)	22 (9%)	2 (1%)	19	54
4	Q	239/241 (99%)	213 (89%)	22 (9%)	4 (2%)	9	35
5	E	194/196 (99%)	150 (77%)	31 (16%)	13 (7%)	1	6
5	R	194/196 (99%)	156 (80%)	26 (13%)	12 (6%)	1	7
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100	100
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100	100
7	G	78/81 (96%)	68 (87%)	9 (12%)	1 (1%)	12	42
7	T	77/81 (95%)	66 (86%)	10 (13%)	1 (1%)	12	42
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100	100
8	U	65/77 (84%)	59 (91%)	4 (6%)	2 (3%)	4	20
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	3	18
9	V	29/47 (62%)	25 (86%)	4 (14%)	0	100	100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
10	W	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	35
All	All	4002/4160 (96%)	3500 (88%)	405 (10%)	97 (2%)	6	26

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	433	ASP
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA

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Mol	Chain	Res	Type
2	B	226	ILE
2	B	228	SER
2	B	231	GLY
3	C	287	ASN
5	E	80	ASP
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
1	N	282	ARG
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
8	U	49	HIS
10	W	61	ALA
1	A	72	CYS
1	A	218	GLY
2	B	224	LEU
2	B	371	SER
2	B	386	ALA
4	D	38	SER
5	E	130	PRO
5	E	163	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	222	GLN
2	O	231	GLY
2	O	371	SER
2	O	386	ALA
5	R	137	GLY
5	R	154	GLY
5	R	163	SER
5	R	185	TYR
8	U	52	GLU
1	A	155	ALA
1	A	262	TRP
2	B	60	THR
2	B	221	GLU

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Mol	Chain	Res	Type
2	B	222	GLN
5	E	137	GLY
5	E	166	ASP
1	N	72	CYS
1	N	155	ALA
2	O	319	SER
4	Q	38	SER
4	Q	177	ALA
5	R	127	VAL
5	R	186	GLN
5	R	191	ASP
2	B	55	SER
2	B	389	SER
2	B	420	GLY
1	N	81	SER
1	N	443	TRP
2	O	19	PRO
2	O	55	SER
2	O	60	THR
3	P	156	TYR
3	P	274	TYR
4	Q	198	HIS
5	R	166	ASP
5	R	190	ASP
7	T	33	ALA
1	A	443	TRP
2	B	201	SER
5	E	120	PRO
5	E	154	GLY
5	E	186	GLN
7	G	33	ALA
1	N	206	LYS
2	O	389	SER
3	P	3	PRO
5	R	113	ASP
1	A	404	ALA
2	B	319	SER
3	C	3	PRO
5	R	120	PRO
3	C	264	VAL
3	P	157	ILE
2	B	208	GLY

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Mol	Chain	Res	Type
2	O	208	GLY
3	P	264	VAL
4	D	162	PRO
9	I	76	VAL
2	O	420	GLY
5	R	177	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	354 (97%)	11 (3%)	41	73
1	N	365/368 (99%)	351 (96%)	14 (4%)	33	67
2	B	331/347 (95%)	315 (95%)	16 (5%)	25	60
2	O	333/347 (96%)	319 (96%)	14 (4%)	30	64
3	C	328/329 (100%)	323 (98%)	5 (2%)	65	86
3	P	328/329 (100%)	324 (99%)	4 (1%)	71	89
4	D	200/200 (100%)	195 (98%)	5 (2%)	47	77
4	Q	200/200 (100%)	196 (98%)	4 (2%)	55	81
5	E	166/166 (100%)	160 (96%)	6 (4%)	35	68
5	R	165/166 (99%)	161 (98%)	4 (2%)	49	78
6	F	93/96 (97%)	89 (96%)	4 (4%)	29	63
6	S	93/96 (97%)	87 (94%)	6 (6%)	17	47
7	G	71/71 (100%)	70 (99%)	1 (1%)	67	86
7	T	70/71 (99%)	69 (99%)	1 (1%)	67	86
8	H	65/71 (92%)	64 (98%)	1 (2%)	65	86
8	U	63/71 (89%)	61 (97%)	2 (3%)	39	72
9	I	23/26 (88%)	21 (91%)	2 (9%)	10	34
9	V	23/26 (88%)	21 (91%)	2 (9%)	10	34
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	W	47/49 (96%)	45 (96%)	2 (4%)	29	63
All	All	3378/3446 (98%)	3273 (97%)	105 (3%)	40	73

All (105) 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	106	MET
1	A	179	ARG
1	A	281	ASP
1	A	307	PHE
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	50	PHE
2	B	97	SER
2	B	104	LYS
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	296	TYR
2	B	325	TYR
2	B	341	MET
2	B	343	GLN
2	B	402	ILE
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	184	PHE
3	C	216	SER
4	D	43	MET
4	D	70	VAL
4	D	130	LEU
4	D	169	LEU

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Mol	Chain	Res	Type
4	D	203	ARG
5	E	6	THR
5	E	52	LYS
5	E	60	SER
5	E	102	THR
5	E	131	GLU
5	E	185	TYR
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	78	GLU
7	G	4	PHE
8	H	21	ARG
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	179	ARG
1	N	223	TYR
1	N	281	ASP
1	N	307	PHE
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	31	ASN
2	O	97	SER
2	O	104	LYS
2	O	124	LEU
2	O	154	SER
2	O	248	ASN
2	O	250	HIS
2	O	296	TYR
2	O	325	TYR
2	O	341	MET

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Mol	Chain	Res	Type
2	O	343	GLN
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	149	ASN
3	P	216	SER
4	Q	43	MET
4	Q	70	VAL
4	Q	130	LEU
4	Q	169	LEU
5	R	52	LYS
5	R	60	SER
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	14	ASP
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
6	S	78	GLU
7	T	4	PHE
8	U	21	ARG
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
10	W	59	TYR
10	W	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	HIS
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN

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Mol	Chain	Res	Type
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS

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Mol	Chain	Res	Type
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
4	Q	200	GLN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

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](#)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	HEM	P	501	3	27,50,50	2.02	8 (29%)	17,82,82	1.65	4 (23%)
11	PEE	P	3008	-	4,4,50	3.64	4 (100%)	6,6,55	0.61	0
16	HEC	Q	501	4	26,50,50	2.42	4 (15%)	18,82,82	1.22	3 (16%)
14	UQ	C	2002	-	19,19,63	2.79	10 (52%)	23,26,79	1.33	3 (13%)
11	PEE	R	3005	-	49,49,50	1.50	10 (20%)	52,54,55	1.00	5 (9%)
13	JZZ	P	3001	-	22,27,27	2.56	3 (13%)	27,40,40	2.05	2 (7%)
19	FES	R	501	5	0,4,4	0.00	-	-	-	-
17	CDL	G	2004	-	39,39,99	1.22	2 (5%)	45,51,111	1.08	4 (8%)
16	HEC	D	501	4	26,50,50	2.93	5 (19%)	18,82,82	1.01	2 (11%)
11	PEE	C	2007	-	48,48,50	1.34	7 (14%)	51,53,55	0.93	5 (9%)
17	CDL	T	3004	-	39,39,99	1.22	2 (5%)	45,51,111	1.09	4 (8%)
18	BOG	Q	3091	-	13,13,20	1.51	3 (23%)	18,18,25	1.17	2 (11%)
14	UQ	P	3002	-	19,19,63	2.67	10 (52%)	23,26,79	1.33	3 (13%)
18	BOG	D	2009	-	20,20,20	1.00	2 (10%)	25,25,25	0.86	2 (8%)
15	GOL	P	3011	-	5,5,5	1.30	0	5,5,5	0.53	0
18	BOG	D	2091	-	13,13,20	1.37	2 (15%)	18,18,25	1.09	2 (11%)
12	HEM	C	502	3	27,50,50	2.44	10 (37%)	17,82,82	1.31	2 (11%)
12	HEM	P	502	3	27,50,50	2.01	7 (25%)	17,82,82	1.47	4 (23%)
11	PEE	P	3007	-	48,48,50	1.31	7 (14%)	51,53,55	0.90	4 (7%)
15	GOL	C	2011	-	5,5,5	1.43	0	5,5,5	0.66	0
12	HEM	C	501	3	27,50,50	1.78	5 (18%)	17,82,82	1.89	4 (23%)
18	BOG	P	2010	-	12,12,20	1.46	3 (25%)	17,17,25	0.67	0
17	CDL	D	2003	-	41,41,99	1.22	4 (9%)	47,53,111	0.98	2 (4%)
18	BOG	Q	3009	-	20,20,20	0.98	1 (5%)	25,25,25	0.90	1 (4%)
11	PEE	A	2008	-	20,20,50	1.89	6 (30%)	23,25,55	0.67	0
11	PEE	E	2005	-	49,49,50	1.48	9 (18%)	52,54,55	1.00	5 (9%)
17	CDL	Q	3003	-	41,41,99	1.21	3 (7%)	47,53,111	1.02	2 (4%)
19	FES	E	501	5	0,4,4	0.00	-	-	-	-
13	JZZ	C	2001	-	22,27,27	2.48	3 (13%)	27,40,40	1.95	2 (7%)

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
12	HEM	P	501	3	-	1/6/54/54	-
16	HEC	Q	501	4	-	2/6/54/54	-
14	UQ	C	2002	-	-	4/11/35/87	0/1/1/1
11	PEE	R	3005	-	-	29/53/53/54	-
13	JZZ	P	3001	-	-	2/10/12/12	0/3/3/3
19	FES	R	501	5	-	-	0/1/1/1
17	CDL	G	2004	-	-	19/49/49/110	-
16	HEC	D	501	4	-	2/6/54/54	-
11	PEE	C	2007	-	-	21/52/52/54	-
17	CDL	T	3004	-	-	19/49/49/110	-
18	BOG	Q	3091	-	-	4/4/24/31	0/1/1/1
14	UQ	P	3002	-	-	4/11/35/87	0/1/1/1
18	BOG	D	2009	-	-	4/11/31/31	0/1/1/1
15	GOL	P	3011	-	-	4/4/4/4	-
18	BOG	D	2091	-	-	2/4/24/31	0/1/1/1
12	HEM	C	502	3	-	0/6/54/54	-
12	HEM	P	502	3	-	0/6/54/54	-
11	PEE	P	3007	-	-	24/52/52/54	-
15	GOL	C	2011	-	-	4/4/4/4	-
12	HEM	C	501	3	-	1/6/54/54	-
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
17	CDL	D	2003	-	-	23/51/51/110	-
18	BOG	Q	3009	-	-	4/11/31/31	0/1/1/1
11	PEE	A	2008	-	-	11/24/24/54	-
11	PEE	E	2005	-	-	30/53/53/54	-
17	CDL	Q	3003	-	-	26/51/51/110	-
19	FES	E	501	5	-	-	0/1/1/1
13	JZZ	C	2001	-	-	0/10/12/12	0/3/3/3

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	JZZ	CAN-N2	-10.70	1.33	1.45
13	C	2001	JZZ	CAN-N2	-10.37	1.33	1.45
16	D	501	HEC	C3B-C2B	-9.63	1.30	1.40
16	D	501	HEC	C3C-C2C	-9.29	1.31	1.40
16	Q	501	HEC	C3B-C2B	-8.30	1.32	1.40
16	Q	501	HEC	C3C-C2C	-7.32	1.33	1.40
12	C	502	HEM	C3C-C2C	-6.62	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	2002	UQ	C7-C6	5.83	1.60	1.51
14	P	3002	UQ	C7-C6	5.76	1.60	1.51
12	C	502	HEM	C3C-CAC	-5.29	1.37	1.47
14	C	2002	UQ	C6-C5	5.21	1.44	1.35
12	P	502	HEM	C3C-CAC	-4.99	1.37	1.47
11	P	3008	PEE	P-O1P	4.93	1.62	1.50
14	P	3002	UQ	C6-C5	4.75	1.43	1.35
12	P	501	HEM	C3B-CAB	-4.57	1.38	1.47
12	P	502	HEM	C3B-CAB	-4.55	1.38	1.47
12	C	502	HEM	C3B-CAB	-4.27	1.39	1.47
12	C	501	HEM	C3B-CAB	-4.17	1.39	1.47
12	C	501	HEM	CBC-CAC	4.14	1.56	1.29
12	P	501	HEM	C3C-CAC	-3.98	1.39	1.47
11	R	3005	PEE	O2-C10	3.92	1.45	1.34
12	P	501	HEM	C3B-C2B	-3.76	1.35	1.40
14	C	2002	UQ	C6-C1	3.74	1.57	1.46
14	P	3002	UQ	C6-C1	3.69	1.57	1.46
12	P	501	HEM	CBC-CAC	3.64	1.53	1.29
12	C	502	HEM	CBB-CAB	3.63	1.53	1.29
11	E	2005	PEE	O3-C30	3.57	1.43	1.33
11	E	2005	PEE	O2-C10	3.56	1.44	1.34
14	P	3002	UQ	O3-C3	3.51	1.45	1.36
11	C	2007	PEE	O3-C30	3.49	1.43	1.33
11	P	3008	PEE	P-O4P	3.47	1.65	1.54
16	D	501	HEC	C4A-C3A	3.44	1.50	1.42
12	P	502	HEM	CBB-CAB	3.38	1.51	1.29
12	P	501	HEM	CBB-CAB	3.37	1.51	1.29
12	C	502	HEM	C4D-C3D	3.36	1.50	1.42
11	P	3008	PEE	P-O3P	3.36	1.64	1.54
11	P	3007	PEE	O3-C30	3.35	1.43	1.33
11	A	2008	PEE	O2-C10	3.32	1.43	1.34
14	C	2002	UQ	O3-C3	3.30	1.44	1.36
11	R	3005	PEE	O3-C30	3.29	1.42	1.33
12	P	502	HEM	C3B-C2B	-3.26	1.35	1.40
11	A	2008	PEE	O3-C30	3.20	1.42	1.33
12	C	501	HEM	CBB-CAB	3.19	1.50	1.29
12	C	501	HEM	C3C-CAC	-3.18	1.41	1.47
11	R	3005	PEE	P-O1P	3.17	1.62	1.50
11	A	2008	PEE	P-O1P	3.13	1.62	1.50
11	E	2005	PEE	P-O1P	3.05	1.61	1.50
11	E	2005	PEE	C19-C18	-3.05	1.34	1.51
12	C	502	HEM	C1C-C2C	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3007	PEE	O2-C10	3.04	1.42	1.34
14	P	3002	UQ	C7-C8	3.04	1.55	1.50
12	P	502	HEM	CBC-CAC	3.03	1.49	1.29
14	C	2002	UQ	C2-C1	3.02	1.57	1.48
11	P	3007	PEE	C22-C21	-3.01	1.34	1.51
11	C	2007	PEE	P-O1P	2.97	1.61	1.50
14	C	2002	UQ	C7-C8	2.96	1.54	1.50
16	D	501	HEC	C1A-C2A	2.94	1.49	1.42
11	R	3005	PEE	C19-C18	-2.92	1.35	1.51
14	C	2002	UQ	CM5-C5	2.86	1.56	1.50
14	C	2002	UQ	O2-C2	2.84	1.43	1.36
16	D	501	HEC	C1D-CHD	-2.83	1.33	1.41
13	P	3001	JZZ	CAJ-CAI	2.81	1.23	1.19
11	C	2007	PEE	O2-C10	2.81	1.42	1.34
11	P	3007	PEE	P-O1P	2.79	1.60	1.50
11	P	3007	PEE	C19-C18	-2.79	1.35	1.51
11	R	3005	PEE	C11-C10	2.78	1.58	1.50
11	E	2005	PEE	C22-C21	-2.76	1.36	1.51
11	C	2007	PEE	C22-C21	-2.76	1.36	1.51
11	A	2008	PEE	C1-C2	2.76	1.59	1.50
11	R	3005	PEE	C22-C21	-2.76	1.36	1.51
18	Q	3091	BOG	O5-C1	2.74	1.48	1.41
14	C	2002	UQ	C5-C4	2.73	1.57	1.47
11	E	2005	PEE	C3-C2	2.73	1.59	1.50
14	P	3002	UQ	C2-C1	2.72	1.56	1.48
11	C	2007	PEE	C19-C18	-2.70	1.36	1.51
12	P	502	HEM	C4D-C3D	2.61	1.48	1.42
11	E	2005	PEE	C31-C30	2.60	1.58	1.50
18	P	2010	BOG	C4-C5	2.59	1.58	1.53
12	C	502	HEM	CBC-CAC	2.58	1.46	1.29
14	P	3002	UQ	C5-C4	2.57	1.56	1.47
13	C	2001	JZZ	CAJ-CAI	2.55	1.22	1.19
18	D	2091	BOG	C4-C5	2.53	1.58	1.53
18	Q	3091	BOG	C4-C5	2.53	1.58	1.53
11	R	3005	PEE	C3-C2	2.52	1.58	1.50
14	P	3002	UQ	CM5-C5	2.51	1.56	1.50
14	C	2002	UQ	C3-C4	2.49	1.56	1.48
14	P	3002	UQ	C3-C4	2.49	1.56	1.48
14	P	3002	UQ	O2-C2	2.49	1.42	1.36
11	R	3005	PEE	C1-C2	2.46	1.58	1.50
11	E	2005	PEE	C11-C10	2.44	1.57	1.50
11	A	2008	PEE	C3-C2	2.44	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	3005	PEE	C31-C30	2.41	1.57	1.50
18	D	2091	BOG	O5-C1	2.38	1.47	1.41
18	Q	3009	BOG	O5-C1	2.38	1.47	1.41
18	D	2009	BOG	O5-C1	2.36	1.47	1.41
12	C	502	HEM	C4A-CHB	-2.35	1.34	1.41
18	P	2010	BOG	C1-C2	2.35	1.57	1.52
11	P	3008	PEE	P-O2P	2.34	1.61	1.54
11	R	3005	PEE	O2-C2	2.33	1.52	1.46
12	C	501	HEM	C1B-C2B	2.33	1.47	1.42
17	G	2004	CDL	CB3-CB4	2.31	1.57	1.50
17	Q	3003	CDL	O1-C1	2.29	1.50	1.43
12	C	502	HEM	C1B-C2B	2.28	1.47	1.42
11	E	2005	PEE	C1-C2	2.28	1.57	1.50
11	C	2007	PEE	C31-C30	2.25	1.57	1.50
11	A	2008	PEE	C11-C10	2.24	1.57	1.50
11	C	2007	PEE	C3-C2	2.24	1.57	1.50
17	T	3004	CDL	O1-C1	2.24	1.50	1.43
12	C	502	HEM	C1D-ND	2.23	1.40	1.36
17	D	2003	CDL	O1-C1	2.23	1.50	1.43
13	P	3001	JZZ	CAN-CAM	-2.22	1.39	1.43
17	T	3004	CDL	CB3-CB4	2.22	1.57	1.50
17	Q	3003	CDL	CA3-CA4	2.21	1.57	1.50
12	P	501	HEM	C4D-C3D	2.21	1.47	1.42
18	D	2009	BOG	C1-C2	2.20	1.58	1.52
16	Q	501	HEC	C4D-CHA	-2.19	1.34	1.41
16	Q	501	HEC	C1A-C2A	2.19	1.47	1.42
11	P	3007	PEE	C31-C30	2.15	1.57	1.50
17	D	2003	CDL	OA6-CA5	2.14	1.40	1.34
18	Q	3091	BOG	O5-C5	2.12	1.49	1.44
18	P	2010	BOG	C4-C3	2.11	1.57	1.52
17	G	2004	CDL	O1-C1	2.09	1.49	1.43
12	P	502	HEM	C1D-ND	2.08	1.40	1.36
13	C	2001	JZZ	CAN-CAM	-2.05	1.39	1.43
17	Q	3003	CDL	OB2-CB2	-2.03	1.36	1.44
17	D	2003	CDL	CA3-CA4	2.03	1.56	1.50
12	P	501	HEM	C1D-ND	2.02	1.40	1.36
11	P	3007	PEE	C3-C2	2.01	1.56	1.50
12	P	501	HEM	C1D-CHD	-2.01	1.35	1.41
17	D	2003	CDL	OB2-CB2	-2.00	1.37	1.44

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	3001	JZZ	C27-O3-C3	-9.44	108.90	117.50
13	C	2001	JZZ	C27-O3-C3	-8.62	109.64	117.50
12	C	501	HEM	CMA-C3A-C4A	-4.10	122.16	128.46
14	C	2002	UQ	C8-C7-C6	3.91	122.58	112.05
14	P	3002	UQ	C8-C7-C6	3.91	122.58	112.05
18	Q	3091	BOG	C1'-O1-C1	3.80	119.14	113.27
12	C	501	HEM	CMA-C3A-C2A	3.48	131.50	124.94
18	Q	3009	BOG	C1'-O1-C1	3.43	119.53	113.84
12	C	501	HEM	C4C-C3C-C2C	-3.43	104.50	106.90
17	T	3004	CDL	CB4-OB6-CB5	-3.33	109.60	117.79
18	D	2091	BOG	C1'-O1-C1	3.30	118.37	113.27
12	P	501	HEM	C4C-C3C-C2C	-3.28	104.61	106.90
12	C	502	HEM	C4A-C3A-C2A	-3.26	104.73	107.00
12	P	501	HEM	C4A-C3A-C2A	-3.20	104.77	107.00
14	C	2002	UQ	C7-C6-C1	-3.20	114.63	118.48
17	G	2004	CDL	CB4-OB6-CB5	-3.09	110.18	117.79
12	P	502	HEM	C4A-C3A-C2A	-3.04	104.88	107.00
14	P	3002	UQ	C7-C6-C1	-2.96	114.91	118.48
18	D	2009	BOG	C1'-O1-C1	2.90	118.66	113.84
11	C	2007	PEE	C20-C19-C18	2.86	128.93	114.42
11	P	3007	PEE	C20-C19-C18	2.83	128.80	114.42
13	C	2001	JZZ	CAL-CAM-CAN	-2.83	119.23	124.66
13	P	3001	JZZ	CAL-CAM-CAN	-2.75	119.37	124.66
12	C	502	HEM	CMB-C2B-C3B	2.70	129.74	124.68
11	R	3005	PEE	C20-C19-C18	2.69	128.10	114.42
11	R	3005	PEE	C19-C18-C17	2.68	128.04	114.42
11	E	2005	PEE	C20-C19-C18	2.67	127.97	114.42
11	R	3005	PEE	C22-C21-C20	2.66	127.92	114.42
11	E	2005	PEE	C19-C18-C17	2.64	127.85	114.42
11	E	2005	PEE	C22-C21-C20	2.64	127.81	114.42
12	P	501	HEM	C3B-C4B-NB	2.63	112.61	109.21
11	C	2007	PEE	C19-C18-C17	2.61	127.68	114.42
17	G	2004	CDL	CA4-OA6-CA5	-2.55	111.51	117.79
11	C	2007	PEE	C22-C21-C20	2.55	127.35	114.42
11	C	2007	PEE	C23-C22-C21	2.54	127.32	114.42
16	Q	501	HEC	CAA-C2A-C3A	-2.52	120.00	127.25
11	P	3007	PEE	C19-C18-C17	2.52	127.22	114.42
18	D	2091	BOG	O1-C1-C2	2.49	111.07	108.15
18	Q	3091	BOG	O1-C1-C2	2.48	111.06	108.15
11	E	2005	PEE	C23-C22-C21	2.48	127.02	114.42
11	R	3005	PEE	C23-C22-C21	2.46	126.89	114.42
16	Q	501	HEC	CMB-C2B-C3B	-2.45	122.94	125.82
11	E	2005	PEE	O3-C3-C2	2.41	115.46	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	3004	CDL	CA4-OA6-CA5	-2.41	111.85	117.79
11	P	3007	PEE	C23-C22-C21	2.41	126.66	114.42
17	T	3004	CDL	CA6-CA4-CA3	-2.39	106.14	111.79
11	P	3007	PEE	C22-C21-C20	2.38	126.50	114.42
16	D	501	HEC	CAA-C2A-C3A	-2.37	120.44	127.25
12	C	501	HEM	C3B-C4B-NB	2.34	112.24	109.21
11	R	3005	PEE	O3-C3-C2	2.32	115.19	108.43
12	P	502	HEM	CMB-C2B-C3B	2.27	128.92	124.68
17	D	2003	CDL	CB4-OB6-CB5	-2.20	112.38	117.79
18	D	2009	BOG	O1-C1-C2	2.20	111.73	108.30
17	D	2003	CDL	CA6-CA4-CA3	-2.19	106.61	111.79
16	D	501	HEC	CMC-C2C-C3C	-2.19	123.25	125.82
12	P	502	HEM	C4C-C3C-C2C	-2.19	105.37	106.90
11	C	2007	PEE	O3-C3-C2	2.16	114.72	108.43
17	G	2004	CDL	CA6-CA4-CA3	-2.15	106.69	111.79
17	Q	3003	CDL	CB4-OB6-CB5	-2.15	112.51	117.79
17	Q	3003	CDL	CA6-CA4-CA3	-2.15	106.71	111.79
12	P	501	HEM	CMA-C3A-C2A	2.14	128.97	124.94
17	T	3004	CDL	OB6-CB4-CB3	2.13	116.12	108.40
14	P	3002	UQ	C10-C9-C8	-2.13	118.22	123.68
12	P	502	HEM	C1D-C2D-C3D	2.12	108.47	107.00
14	C	2002	UQ	C10-C9-C8	-2.10	118.29	123.68
17	G	2004	CDL	OB6-CB4-CB3	2.02	115.70	108.40
16	Q	501	HEC	CBA-CAA-C2A	2.01	116.18	112.48

There are no chirality outliers.

All (240) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	501	HEC	C1A-C2A-CAA-CBA
16	Q	501	HEC	C3A-C2A-CAA-CBA
14	C	2002	UQ	C1-C6-C7-C8
14	C	2002	UQ	C5-C6-C7-C8
14	C	2002	UQ	C12-C11-C9-C8
11	R	3005	PEE	C11-C10-O2-C2
11	R	3005	PEE	C4-O4P-P-O1P
11	R	3005	PEE	C4-O4P-P-O2P
17	G	2004	CDL	CA3-OA5-PA1-OA3
17	G	2004	CDL	CA3-OA5-PA1-OA4
17	G	2004	CDL	CB3-OB5-PB2-OB3
17	G	2004	CDL	CB3-OB5-PB2-OB4
17	G	2004	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
16	D	501	HEC	C1A-C2A-CAA-CBA
16	D	501	HEC	C3A-C2A-CAA-CBA
11	C	2007	PEE	C4-O4P-P-O3P
17	T	3004	CDL	O1-C1-CA2-OA2
17	T	3004	CDL	CA3-OA5-PA1-OA4
17	T	3004	CDL	CB3-OB5-PB2-OB3
17	T	3004	CDL	CB3-OB5-PB2-OB4
17	T	3004	CDL	C51-CB5-OB6-CB4
18	Q	3091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	O5-C1-O1-C1'
14	P	3002	UQ	C1-C6-C7-C8
14	P	3002	UQ	C5-C6-C7-C8
14	P	3002	UQ	C12-C11-C9-C8
18	D	2009	BOG	C2-C1-O1-C1'
18	D	2009	BOG	O5-C1-O1-C1'
15	P	3011	GOL	C1-C2-C3-O3
11	P	3007	PEE	C4-O4P-P-O3P
15	C	2011	GOL	O1-C1-C2-C3
15	C	2011	GOL	C1-C2-C3-O3
17	D	2003	CDL	CA2-OA2-PA1-OA5
18	Q	3009	BOG	C2-C1-O1-C1'
18	Q	3009	BOG	O5-C1-O1-C1'
11	E	2005	PEE	C11-C10-O2-C2
11	E	2005	PEE	C4-O4P-P-O1P
11	E	2005	PEE	C4-O4P-P-O2P
17	Q	3003	CDL	CA2-OA2-PA1-OA5
11	R	3005	PEE	O5-C30-O3-C3
17	G	2004	CDL	OB9-CB7-OB8-CB6
17	T	3004	CDL	OB9-CB7-OB8-CB6
17	G	2004	CDL	OA9-CA7-OA8-CA6
17	T	3004	CDL	OA9-CA7-OA8-CA6
11	E	2005	PEE	O5-C30-O3-C3
17	G	2004	CDL	C31-CA7-OA8-CA6
17	T	3004	CDL	C31-CA7-OA8-CA6
11	R	3005	PEE	O4-C10-O2-C2
17	G	2004	CDL	OB7-CB5-OB6-CB4
17	T	3004	CDL	OB7-CB5-OB6-CB4
11	E	2005	PEE	O4-C10-O2-C2
11	R	3005	PEE	C31-C30-O3-C3
17	G	2004	CDL	C71-CB7-OB8-CB6
17	T	3004	CDL	C71-CB7-OB8-CB6
17	D	2003	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
17	Q	3003	CDL	C31-CA7-OA8-CA6
11	A	2008	PEE	C31-C30-O3-C3
11	E	2005	PEE	C31-C30-O3-C3
11	A	2008	PEE	O5-C30-O3-C3
17	G	2004	CDL	O1-C1-CA2-OA2
18	Q	3091	BOG	O5-C5-C6-O6
18	D	2091	BOG	C2-C1-O1-C1'
18	Q	3091	BOG	C4-C5-C6-O6
17	D	2003	CDL	O1-C1-CA2-OA2
17	Q	3003	CDL	O1-C1-CA2-OA2
18	D	2091	BOG	O5-C1-O1-C1'
17	D	2003	CDL	OA9-CA7-OA8-CA6
17	Q	3003	CDL	OA9-CA7-OA8-CA6
17	Q	3003	CDL	CB7-C71-C72-C73
17	D	2003	CDL	CB7-C71-C72-C73
17	G	2004	CDL	C11-CA5-OA6-CA4
17	T	3004	CDL	C11-CA5-OA6-CA4
11	R	3005	PEE	C4-O4P-P-O3P
17	G	2004	CDL	CA3-OA5-PA1-OA2
17	G	2004	CDL	CB3-OB5-PB2-OB2
17	T	3004	CDL	CB3-OB5-PB2-OB2
17	D	2003	CDL	CB2-OB2-PB2-OB5
17	D	2003	CDL	CB3-OB5-PB2-OB2
11	E	2005	PEE	C4-O4P-P-O3P
17	Q	3003	CDL	CB2-OB2-PB2-OB5
17	Q	3003	CDL	CB3-OB5-PB2-OB2
17	D	2003	CDL	C71-CB7-OB8-CB6
17	G	2004	CDL	CB2-C1-CA2-OA2
17	T	3004	CDL	CB2-C1-CA2-OA2
17	G	2004	CDL	OA7-CA5-OA6-CA4
17	T	3004	CDL	OA7-CA5-OA6-CA4
17	Q	3003	CDL	C71-CB7-OB8-CB6
18	Q	3009	BOG	O1-C1'-C2'-C3'
11	C	2007	PEE	C18-C19-C20-C21
11	C	2007	PEE	C36-C37-C38-C39
11	C	2007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C35-C36-C37-C38
11	P	3007	PEE	C36-C37-C38-C39
11	R	3005	PEE	C16-C17-C18-C19
11	E	2005	PEE	C18-C19-C20-C21
11	C	2007	PEE	C10-C11-C12-C13
11	R	3005	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	E	2005	PEE	C36-C37-C38-C39
11	C	2007	PEE	C17-C18-C19-C20
11	P	3007	PEE	C18-C19-C20-C21
11	E	2005	PEE	C16-C17-C18-C19
11	R	3005	PEE	C36-C37-C38-C39
11	P	3007	PEE	C17-C18-C19-C20
17	D	2003	CDL	OB9-CB7-OB8-CB6
18	D	2009	BOG	O1-C1'-C2'-C3'
17	D	2003	CDL	C51-CB5-OB6-CB4
17	Q	3003	CDL	C51-CB5-OB6-CB4
11	R	3005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C10-C11-C12-C13
17	Q	3003	CDL	OB9-CB7-OB8-CB6
11	R	3005	PEE	C34-C35-C36-C37
11	E	2005	PEE	C23-C24-C25-C26
11	E	2005	PEE	C34-C35-C36-C37
17	D	2003	CDL	OB7-CB5-OB6-CB4
11	R	3005	PEE	C23-C24-C25-C26
11	R	3005	PEE	C41-C42-C43-C44
15	P	3011	GOL	O2-C2-C3-O3
15	C	2011	GOL	O2-C2-C3-O3
17	D	2003	CDL	CB5-C51-C52-C53
17	Q	3003	CDL	CB5-C51-C52-C53
11	E	2005	PEE	C41-C42-C43-C44
17	Q	3003	CDL	OB7-CB5-OB6-CB4
18	Q	3009	BOG	C1'-C2'-C3'-C4'
11	E	2005	PEE	C30-C31-C32-C33
11	P	3007	PEE	C20-C21-C22-C23
11	C	2007	PEE	C31-C32-C33-C34
18	D	2009	BOG	C1'-C2'-C3'-C4'
11	C	2007	PEE	C39-C40-C41-C42
11	P	3007	PEE	C31-C32-C33-C34
11	E	2005	PEE	C11-C12-C13-C14
11	E	2005	PEE	C35-C36-C37-C38
11	R	3005	PEE	C35-C36-C37-C38
11	P	3007	PEE	C40-C41-C42-C43
11	A	2008	PEE	C11-C10-O2-C2
11	R	3005	PEE	C11-C12-C13-C14
11	C	2007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C11-C12-C13-C14
11	C	2007	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
11	A	2008	PEE	O4-C10-O2-C2
11	R	3005	PEE	O3P-C1-C2-C3
11	A	2008	PEE	O3P-C1-C2-C3
11	E	2005	PEE	O3P-C1-C2-C3
11	P	3007	PEE	C37-C38-C39-C40
11	P	3007	PEE	C16-C17-C18-C19
11	C	2007	PEE	C20-C21-C22-C23
11	P	3007	PEE	C39-C40-C41-C42
11	C	2007	PEE	C43-C44-C45-C46
11	P	3007	PEE	C43-C44-C45-C46
15	C	2011	GOL	O1-C1-C2-O2
17	G	2004	CDL	CB5-C51-C52-C53
17	T	3004	CDL	CB5-C51-C52-C53
11	P	3007	PEE	C33-C34-C35-C36
11	C	2007	PEE	C16-C17-C18-C19
11	C	2007	PEE	C33-C34-C35-C36
11	A	2008	PEE	O2-C2-C3-O3
11	R	3005	PEE	C20-C21-C22-C23
17	Q	3003	CDL	C71-C72-C73-C74
11	P	3007	PEE	C15-C16-C17-C18
11	C	2007	PEE	C15-C16-C17-C18
17	D	2003	CDL	OB5-CB3-CB4-CB6
17	Q	3003	CDL	OB5-CB3-CB4-CB6
11	E	2005	PEE	C19-C20-C21-C22
17	D	2003	CDL	C71-C72-C73-C74
11	C	2007	PEE	C34-C35-C36-C37
11	E	2005	PEE	C20-C21-C22-C23
11	R	3005	PEE	C19-C20-C21-C22
11	R	3005	PEE	C39-C40-C41-C42
11	E	2005	PEE	C21-C22-C23-C24
17	T	3004	CDL	CA3-OA5-PA1-OA2
17	D	2003	CDL	CA3-OA5-PA1-OA2
17	Q	3003	CDL	CA3-OA5-PA1-OA2
11	E	2005	PEE	C39-C40-C41-C42
11	R	3005	PEE	C21-C22-C23-C24
17	D	2003	CDL	OA6-CA4-CA6-OA8
17	Q	3003	CDL	OA6-CA4-CA6-OA8
11	P	3007	PEE	C42-C43-C44-C45
14	C	2002	UQ	C12-C11-C9-C10
14	P	3002	UQ	C12-C11-C9-C10
11	P	3007	PEE	C34-C35-C36-C37
11	R	3005	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
17	D	2003	CDL	OB5-CB3-CB4-OB6
17	Q	3003	CDL	OB5-CB3-CB4-OB6
15	P	3011	GOL	O1-C1-C2-O2
11	A	2008	PEE	C10-C11-C12-C13
17	T	3004	CDL	CA3-OA5-PA1-OA3
17	D	2003	CDL	CA2-OA2-PA1-OA4
17	D	2003	CDL	CB2-OB2-PB2-OB4
17	D	2003	CDL	CB3-OB5-PB2-OB4
17	Q	3003	CDL	CA2-OA2-PA1-OA4
17	Q	3003	CDL	CB2-OB2-PB2-OB4
17	Q	3003	CDL	CB3-OB5-PB2-OB4
11	R	3005	PEE	O4P-C4-C5-N
11	C	2007	PEE	C42-C43-C44-C45
13	P	3001	JZZ	CAP-CAH-CAI-CAJ
11	A	2008	PEE	O3P-C1-C2-O2
11	E	2005	PEE	O3P-C1-C2-O2
11	R	3005	PEE	C12-C13-C14-C15
11	E	2005	PEE	C12-C13-C14-C15
11	P	3007	PEE	C13-C14-C15-C16
11	R	3005	PEE	C22-C23-C24-C25
11	C	2007	PEE	C13-C14-C15-C16
11	P	3007	PEE	C14-C15-C16-C17
11	R	3005	PEE	C14-C15-C16-C17
17	T	3004	CDL	C1-CB2-OB2-PB2
11	E	2005	PEE	C14-C15-C16-C17
11	R	3005	PEE	C38-C39-C40-C41
12	P	501	HEM	C3D-CAD-CBD-CGD
12	C	501	HEM	C3D-CAD-CBD-CGD
11	R	3005	PEE	C1-C2-O2-C10
11	E	2005	PEE	C1-C2-O2-C10
11	A	2008	PEE	O3-C30-C31-C32
17	Q	3003	CDL	C12-C11-CA5-OA6
11	E	2005	PEE	C22-C23-C24-C25
11	E	2005	PEE	C38-C39-C40-C41
11	R	3005	PEE	C43-C44-C45-C46
17	Q	3003	CDL	CA3-CA4-CA6-OA8
11	E	2005	PEE	C43-C44-C45-C46
17	G	2004	CDL	C1-CB2-OB2-PB2
11	P	3007	PEE	O2-C10-C11-C12
11	A	2008	PEE	O5-C30-C31-C32
11	C	2007	PEE	O2-C10-C11-C12
17	G	2004	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
17	T	3004	CDL	OB5-CB3-CB4-OB6
11	P	3007	PEE	C12-C13-C14-C15
17	Q	3003	CDL	C72-C71-CB7-OB8
17	D	2003	CDL	C72-C71-CB7-OB8
11	C	2007	PEE	O4-C10-C11-C12
15	P	3011	GOL	O1-C1-C2-C3
11	P	3007	PEE	O4-C10-C11-C12
11	A	2008	PEE	C1-C2-C3-O3
11	P	3007	PEE	O4-C10-O2-C2
17	Q	3003	CDL	CA3-OA5-PA1-OA4
17	Q	3003	CDL	CB3-OB5-PB2-OB3
17	D	2003	CDL	C72-C71-CB7-OB9
17	Q	3003	CDL	C72-C71-CB7-OB9
11	E	2005	PEE	C10-C11-C12-C13
11	E	2005	PEE	O4P-C4-C5-N
13	P	3001	JZZ	CAA-CAH-CAI-CAJ
17	D	2003	CDL	C12-C11-CA5-OA6

There are no ring outliers.

25 monomers are involved in 63 short contacts:

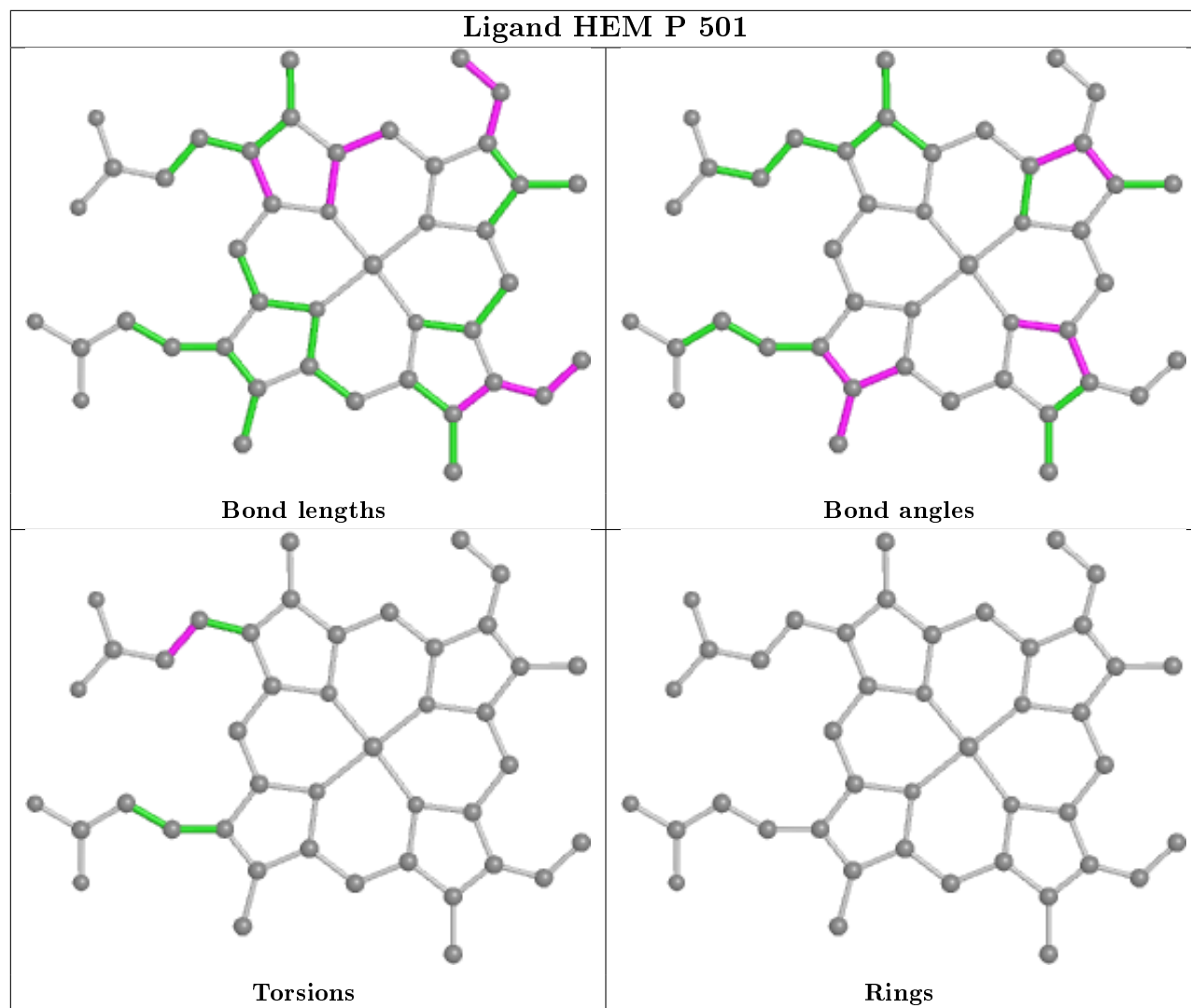
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	P	501	HEM	2	0
16	Q	501	HEC	2	0
14	C	2002	UQ	4	0
11	R	3005	PEE	1	0
13	P	3001	JZZ	6	0
19	R	501	FES	2	0
17	G	2004	CDL	5	0
16	D	501	HEC	1	0
11	C	2007	PEE	4	0
17	T	3004	CDL	5	0
18	Q	3091	BOG	1	0
14	P	3002	UQ	5	0
15	P	3011	GOL	1	0
18	D	2091	BOG	2	0
12	C	502	HEM	4	0
12	P	502	HEM	3	0
11	P	3007	PEE	4	0
15	C	2011	GOL	1	0
12	C	501	HEM	2	0
18	P	2010	BOG	1	0

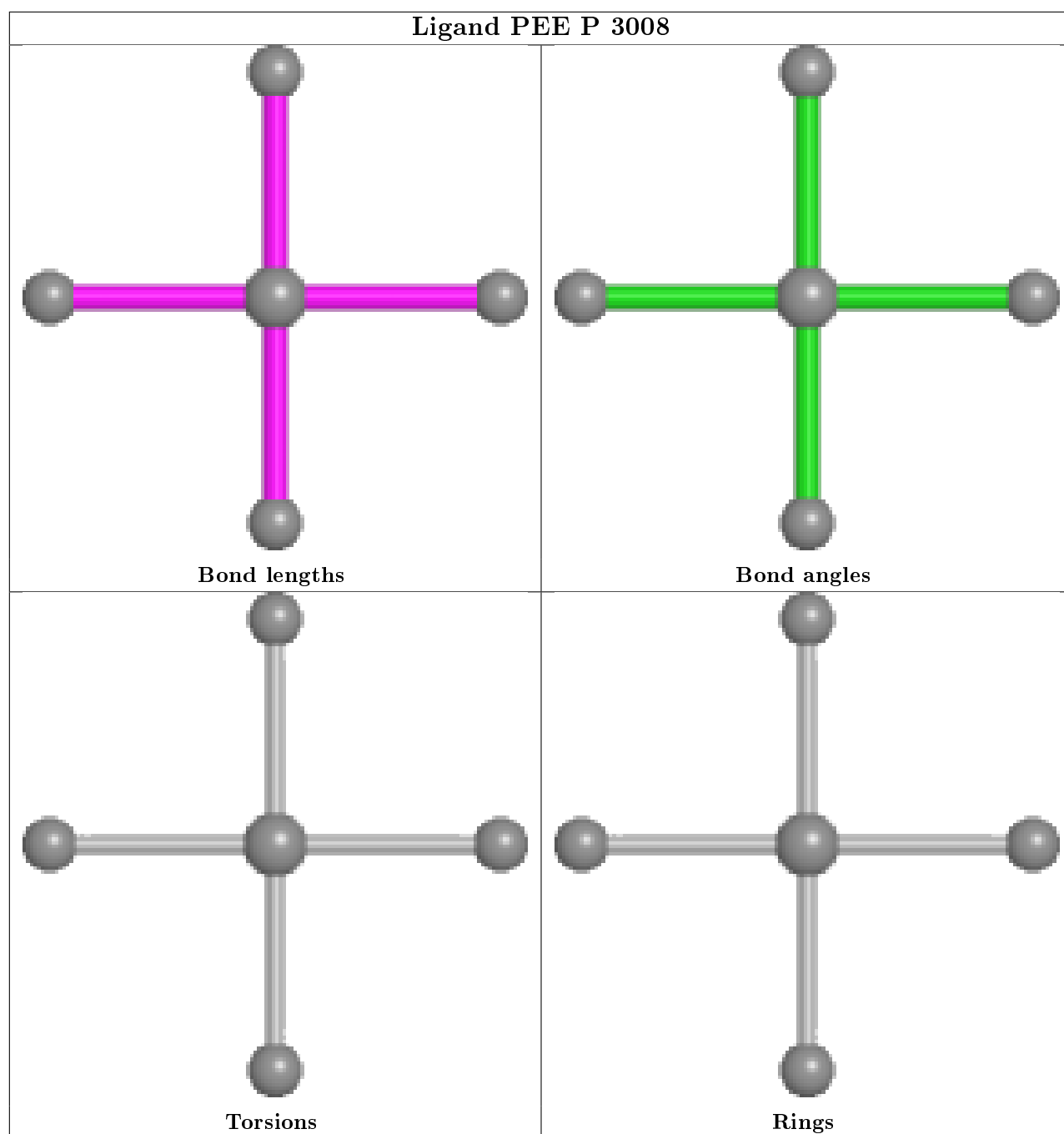
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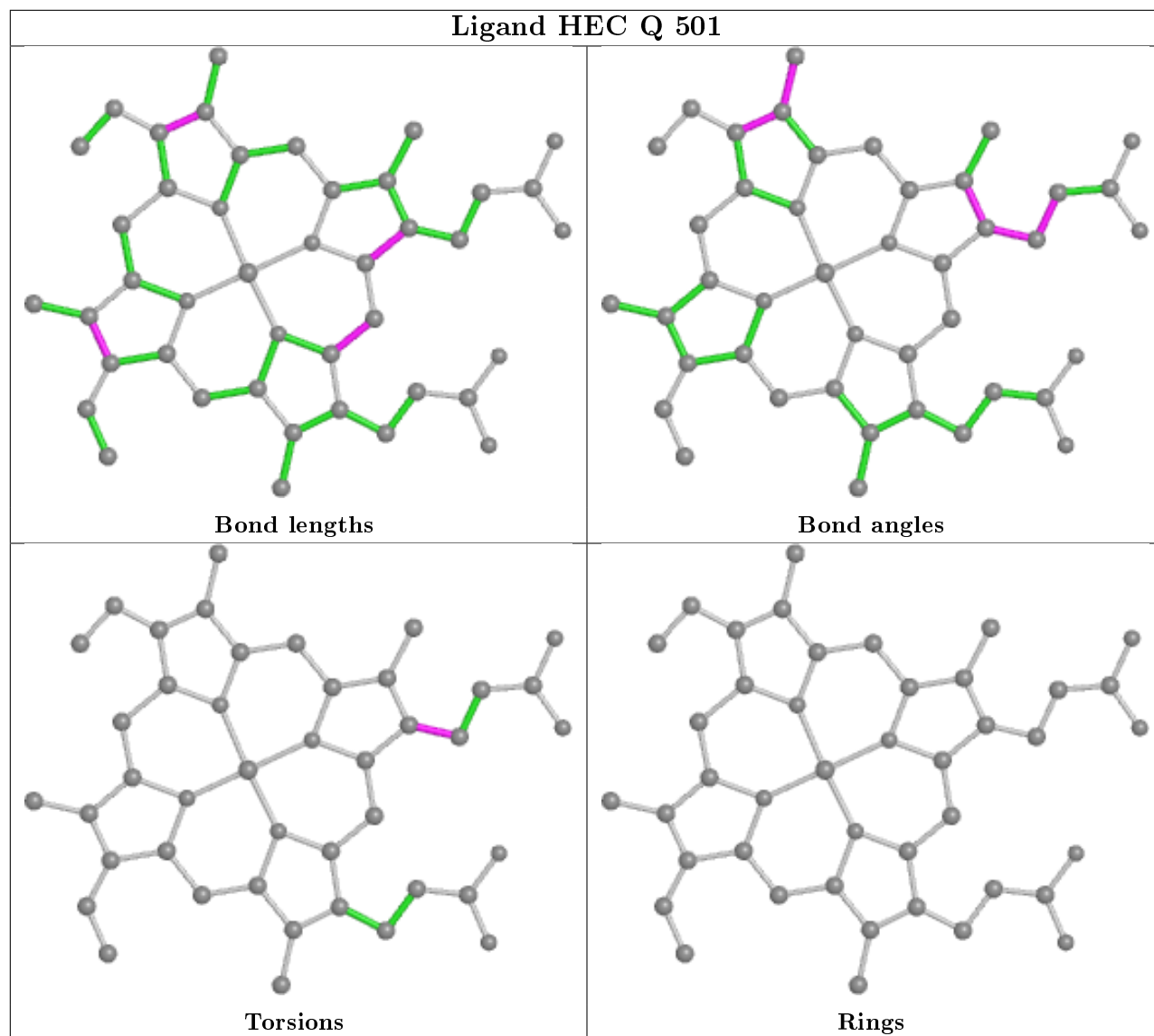
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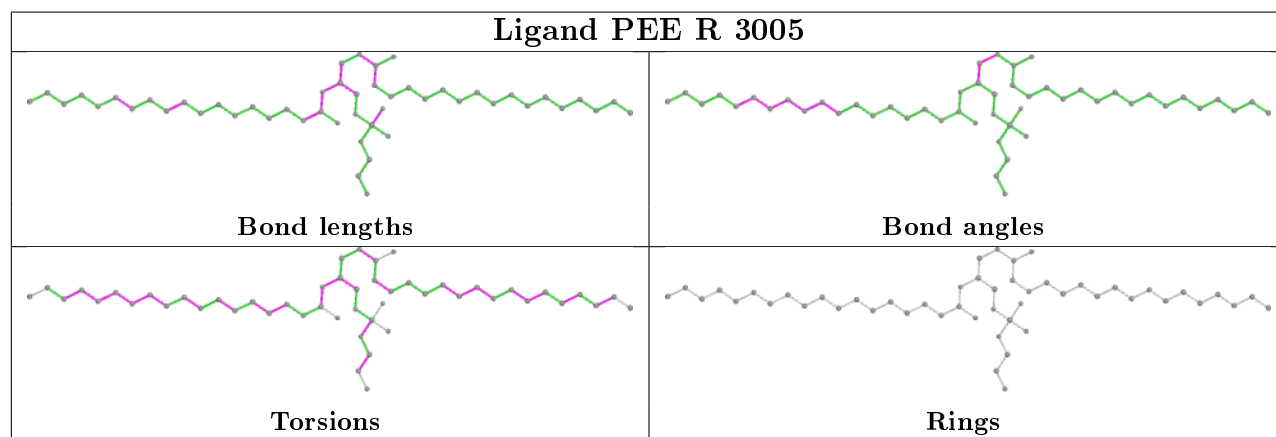
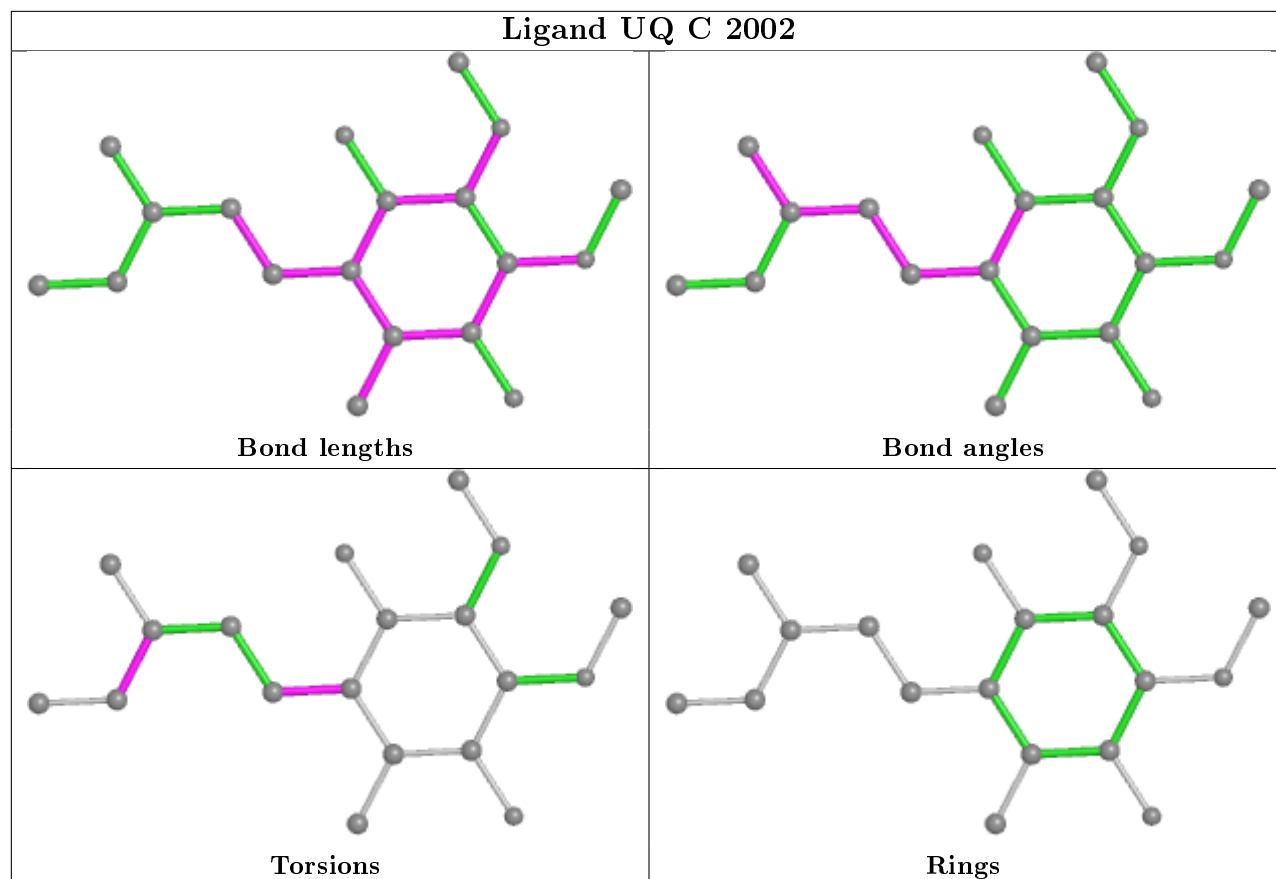
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	2003	CDL	3	0
11	E	2005	PEE	1	0
17	Q	3003	CDL	1	0
19	E	501	FES	2	0
13	C	2001	JZZ	2	0

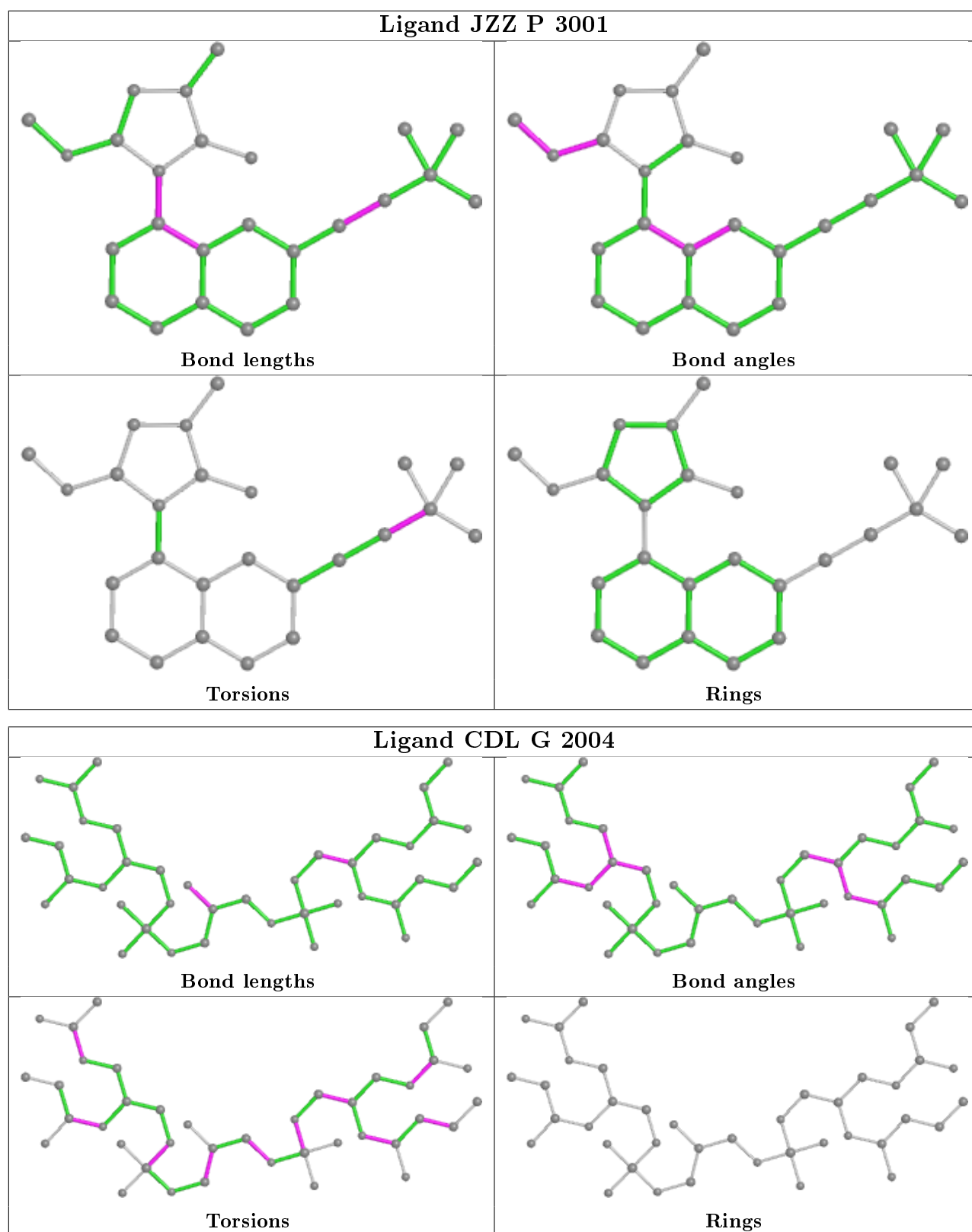
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

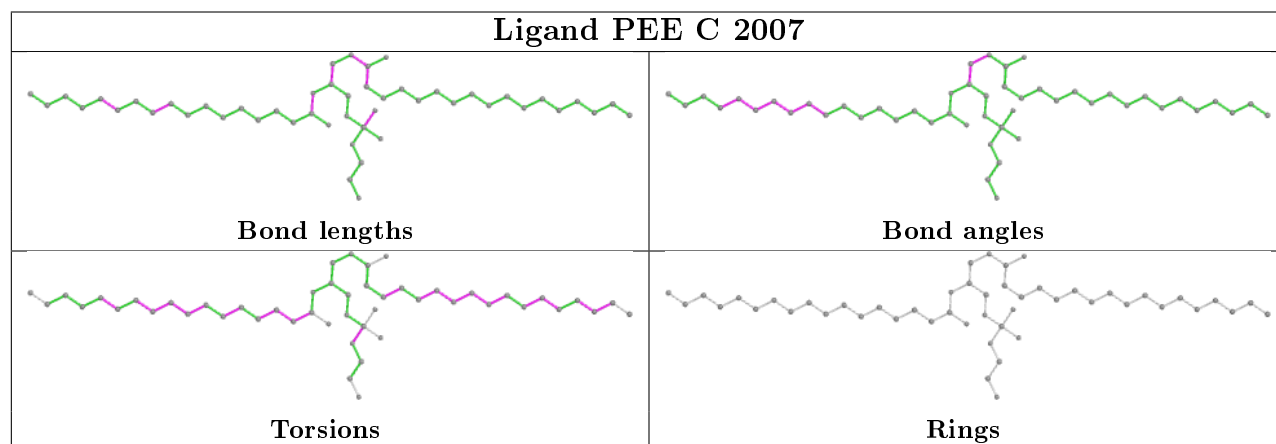
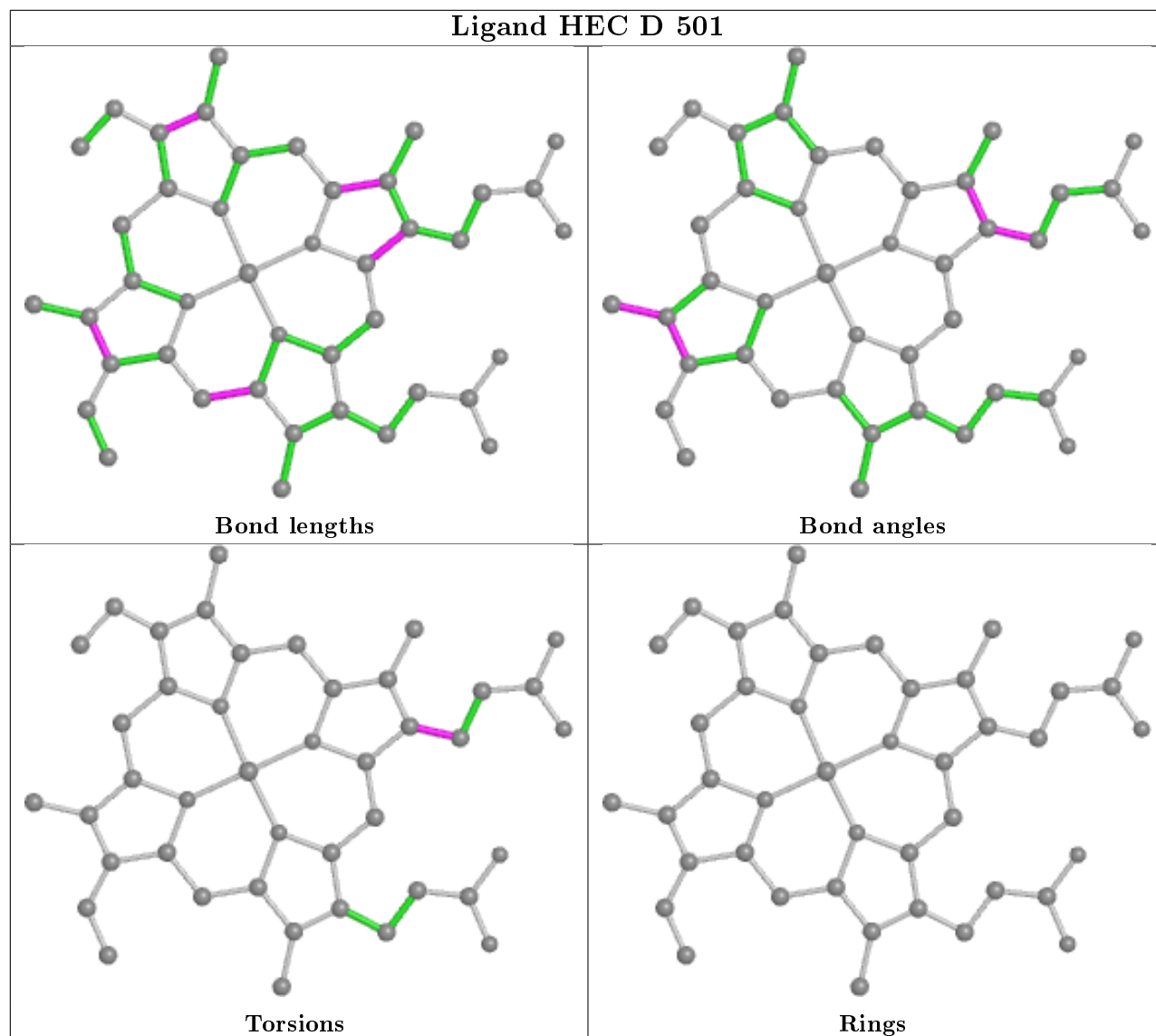




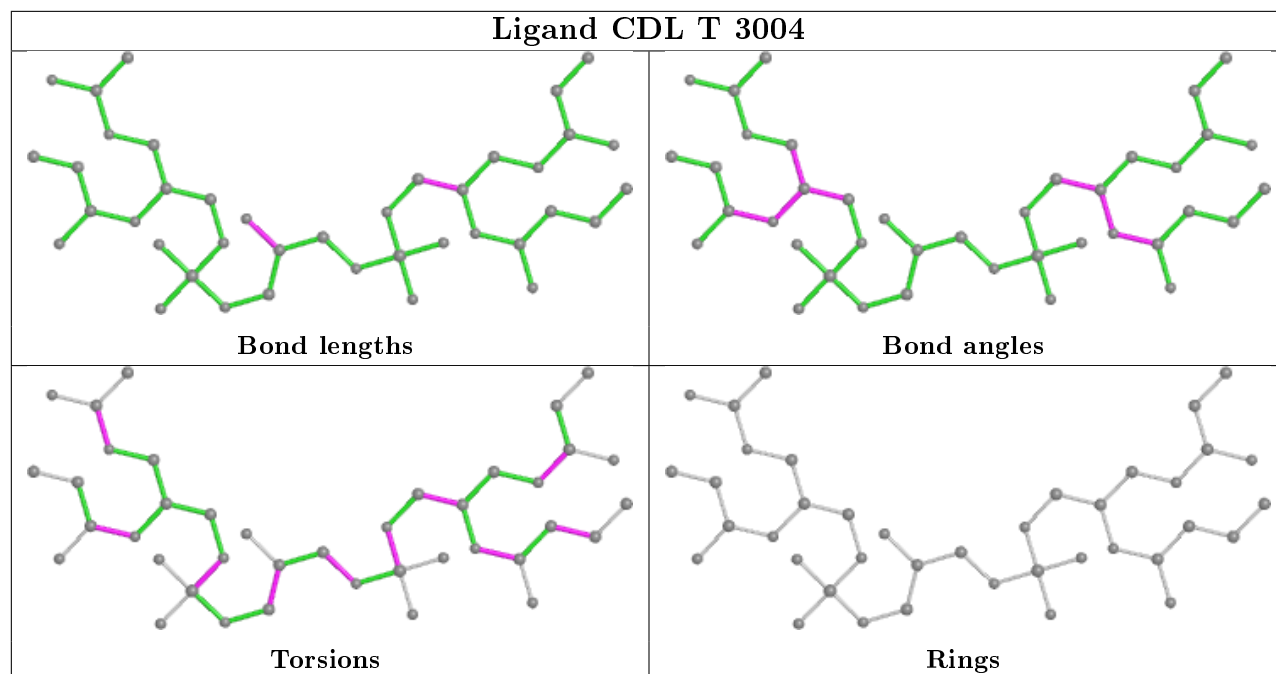




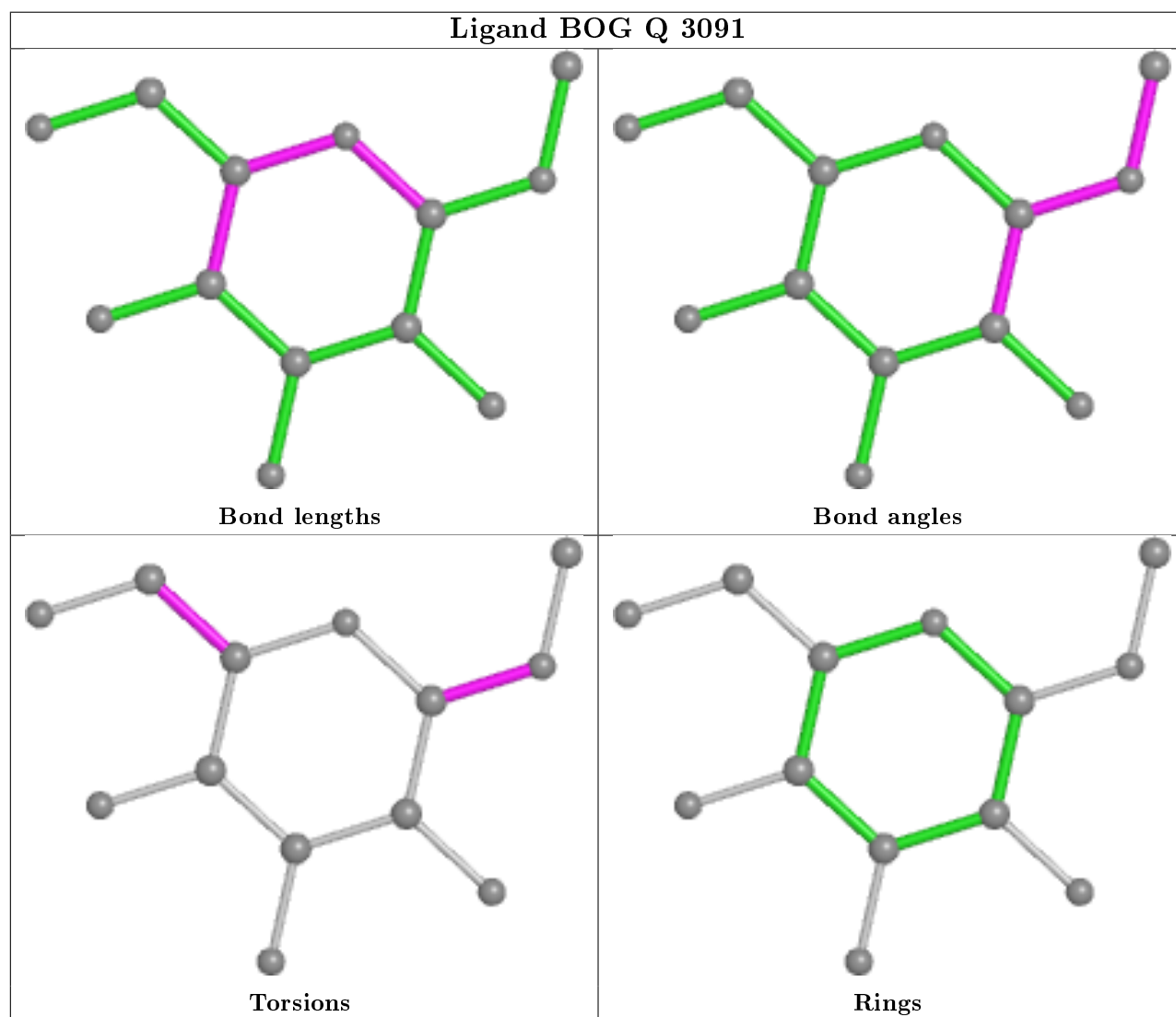


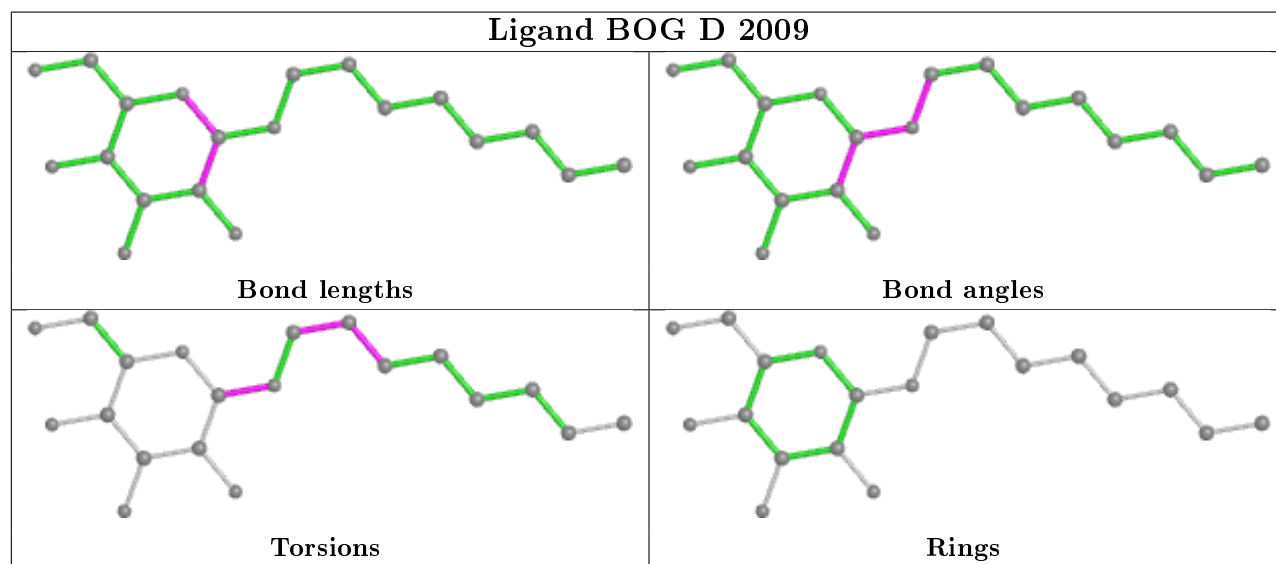
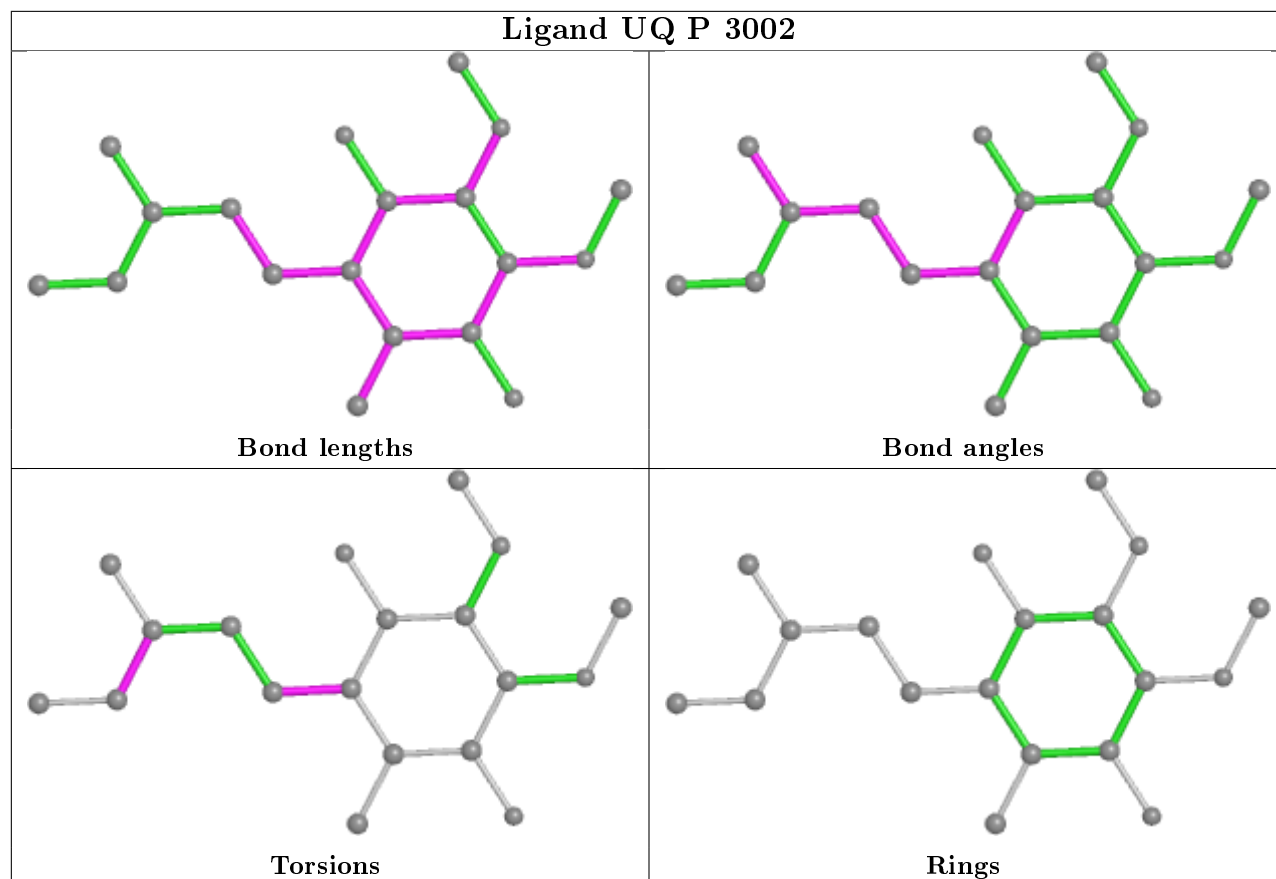


Ligand CDL T 3004

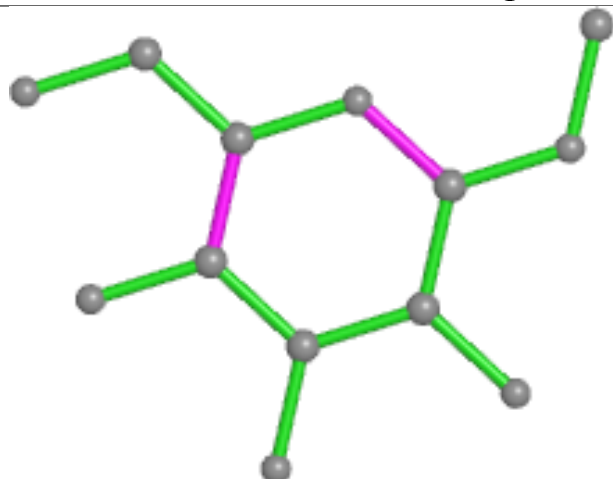


Ligand BOG Q 3091

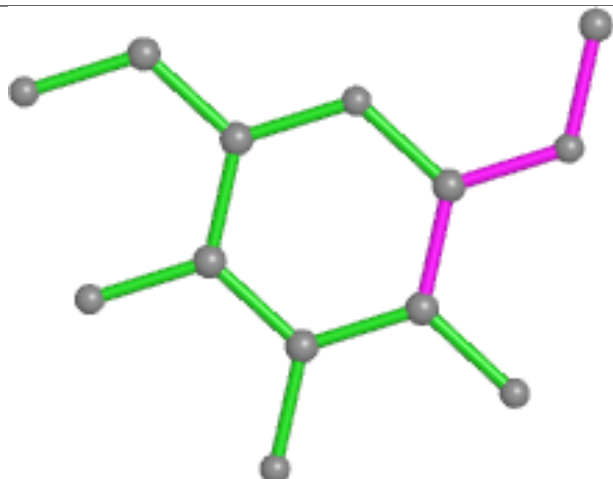




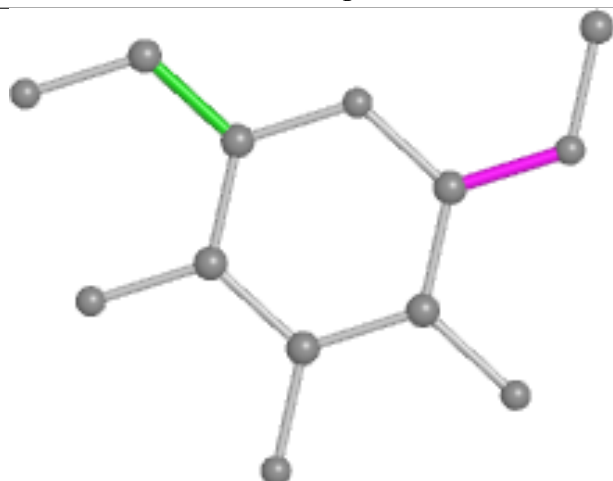
Ligand BOG D 2091



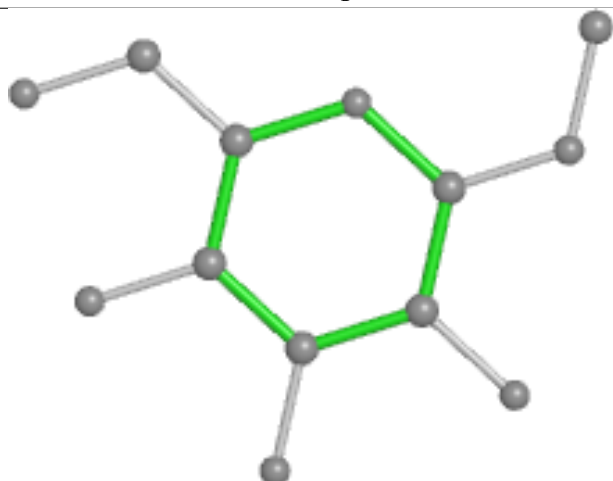
Bond lengths



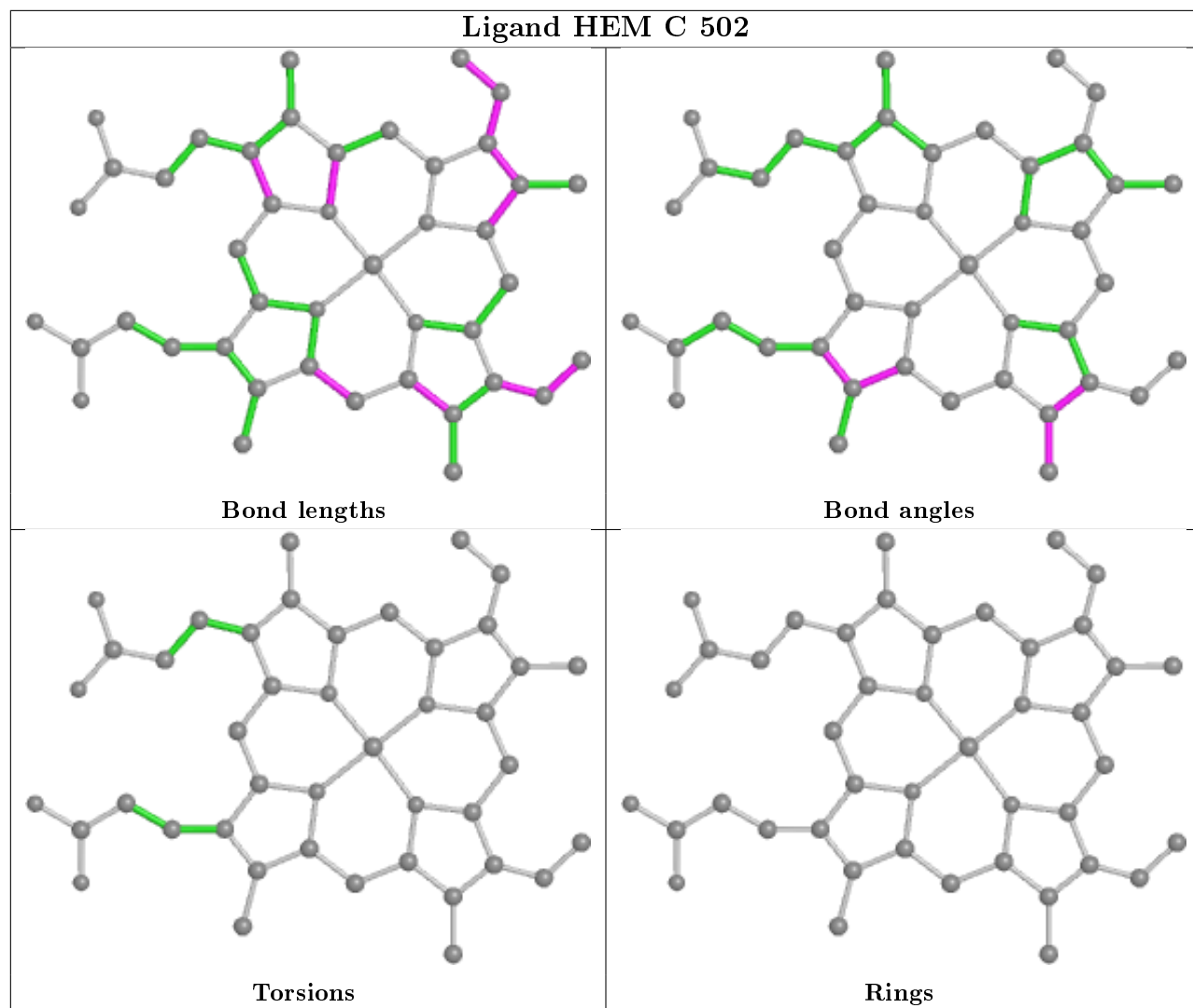
Bond angles

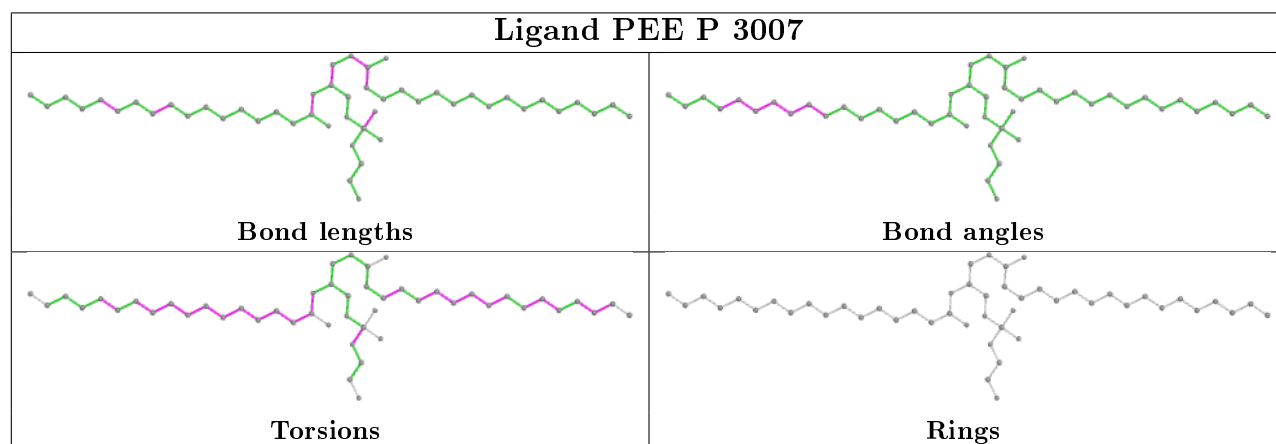
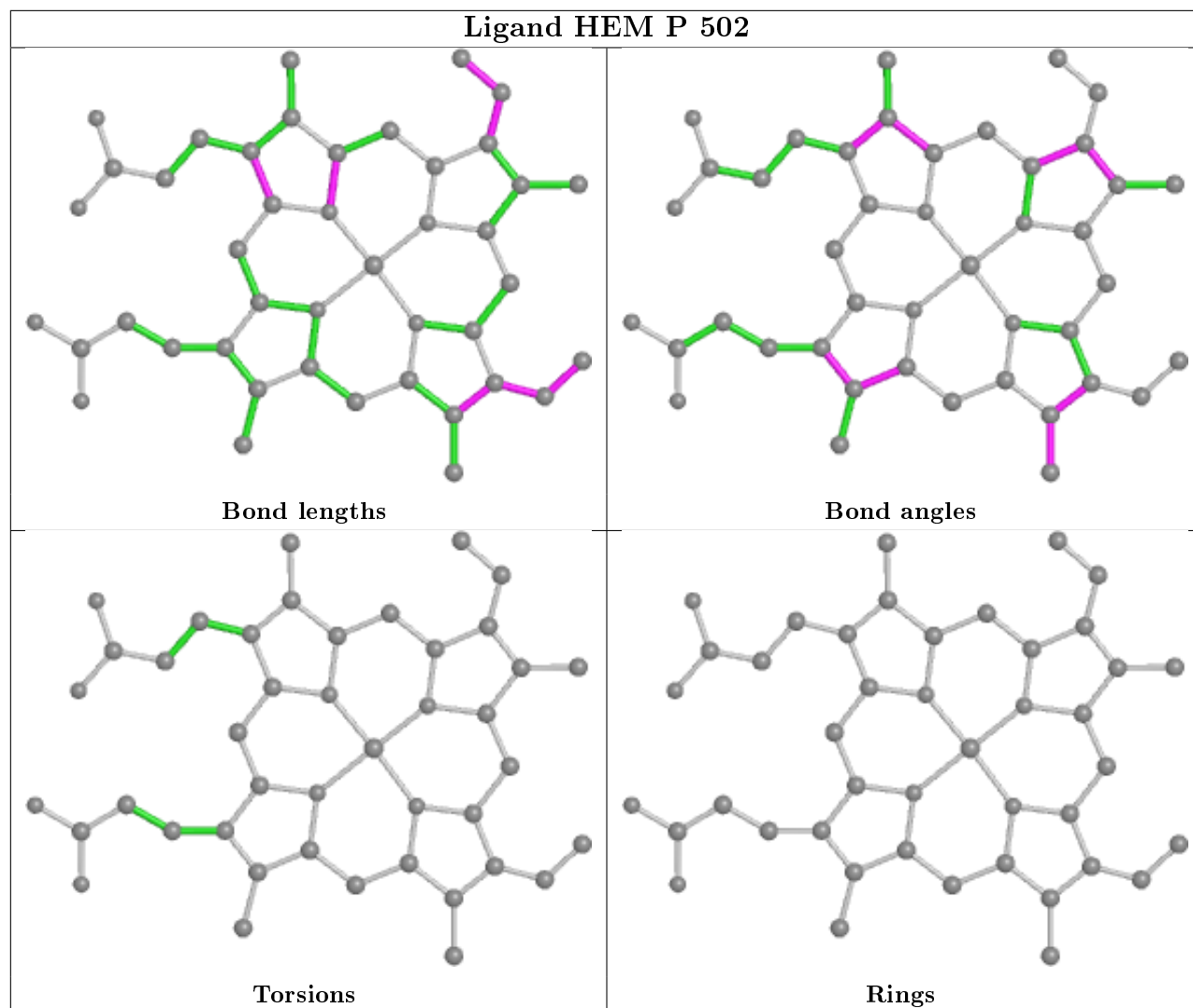


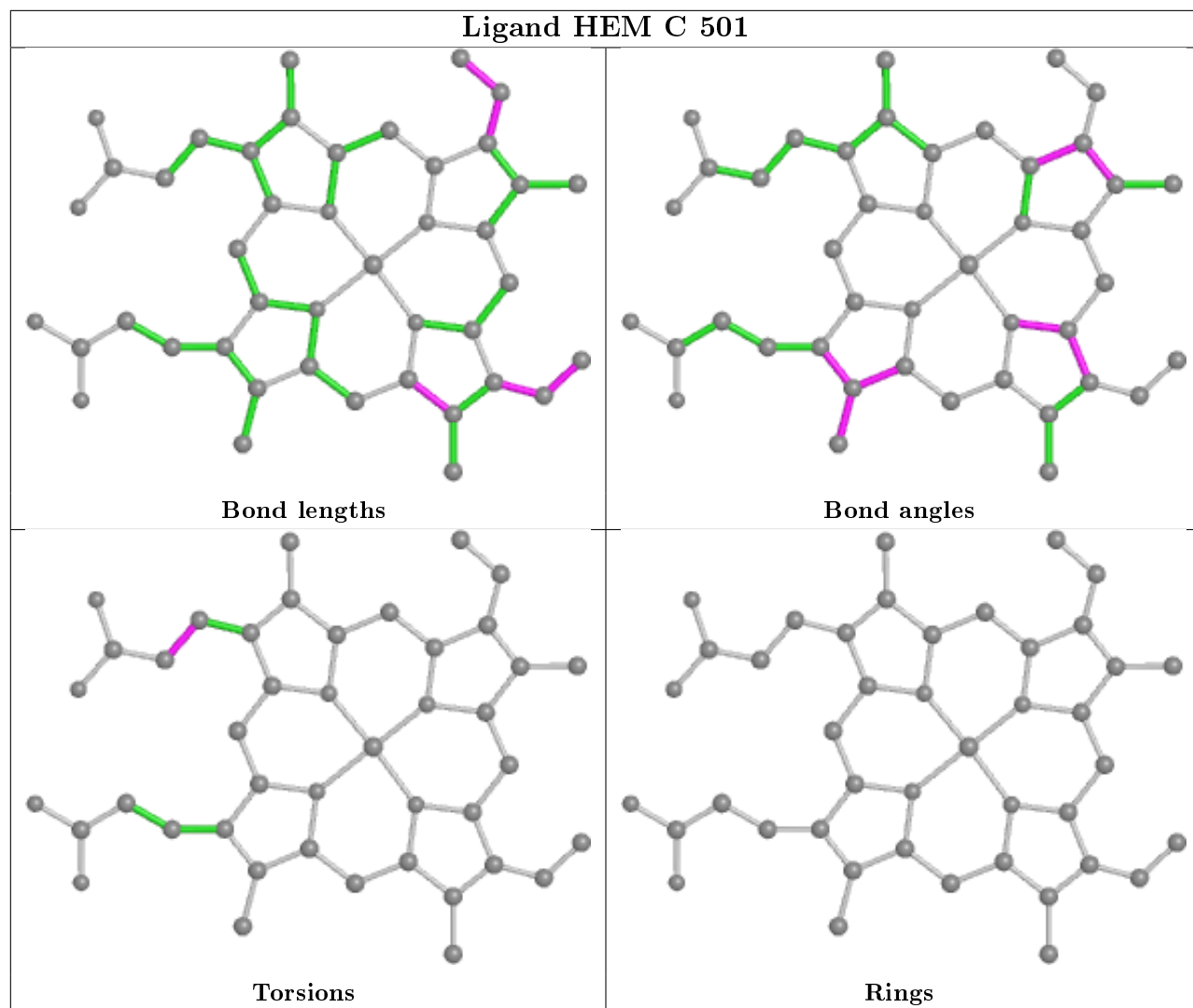
Torsions



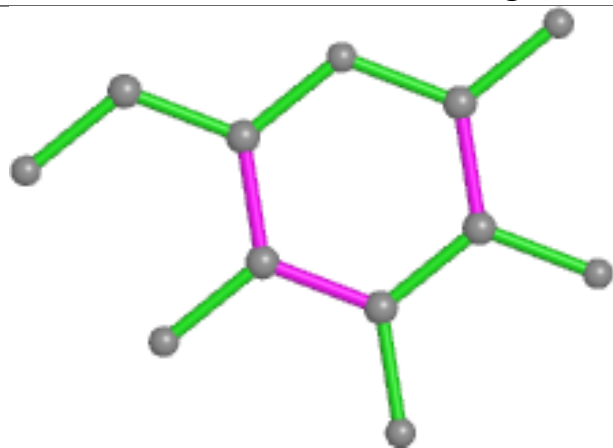
Rings



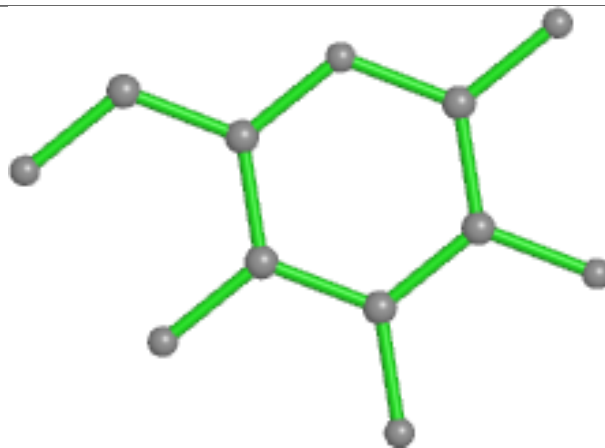




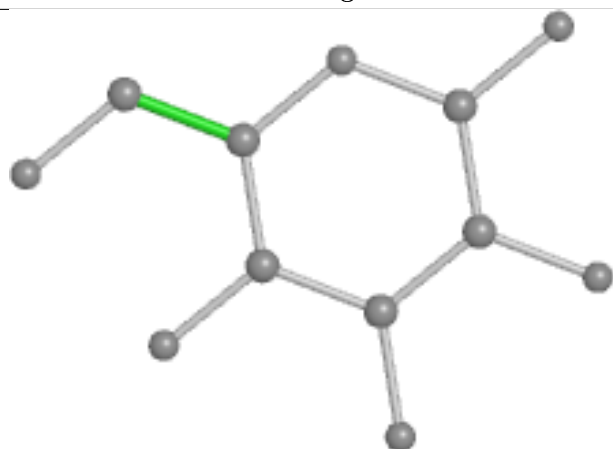
Ligand BOG P 2010



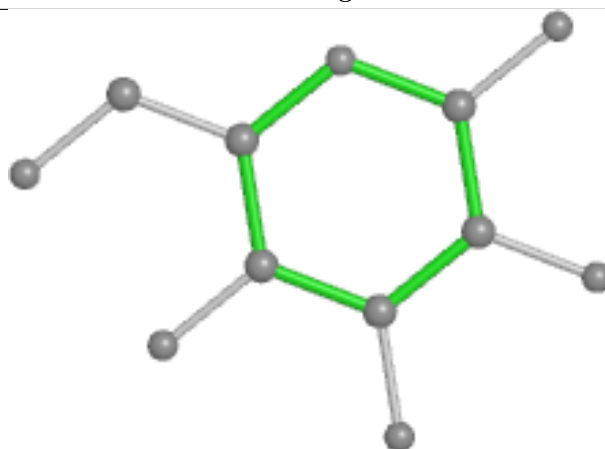
Bond lengths



Bond angles

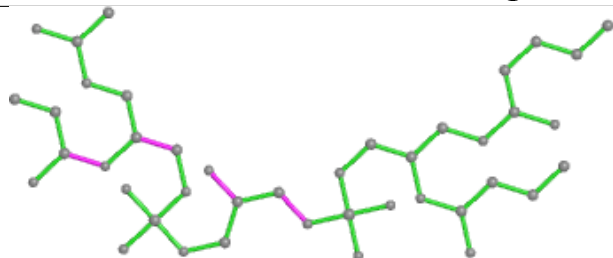


Torsions

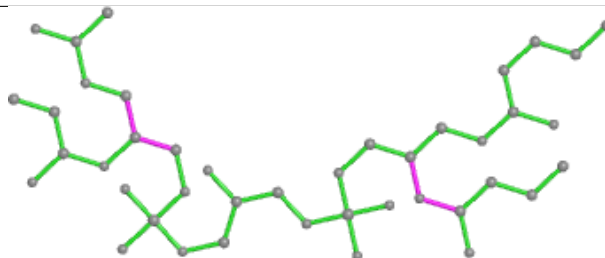


Rings

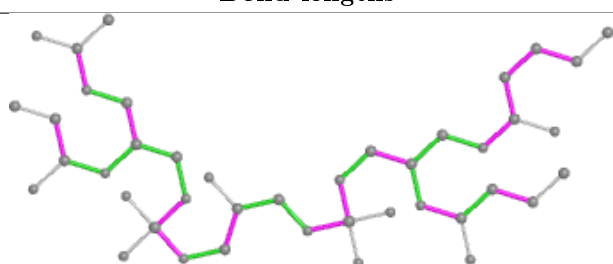
Ligand CDL D 2003



Bond lengths



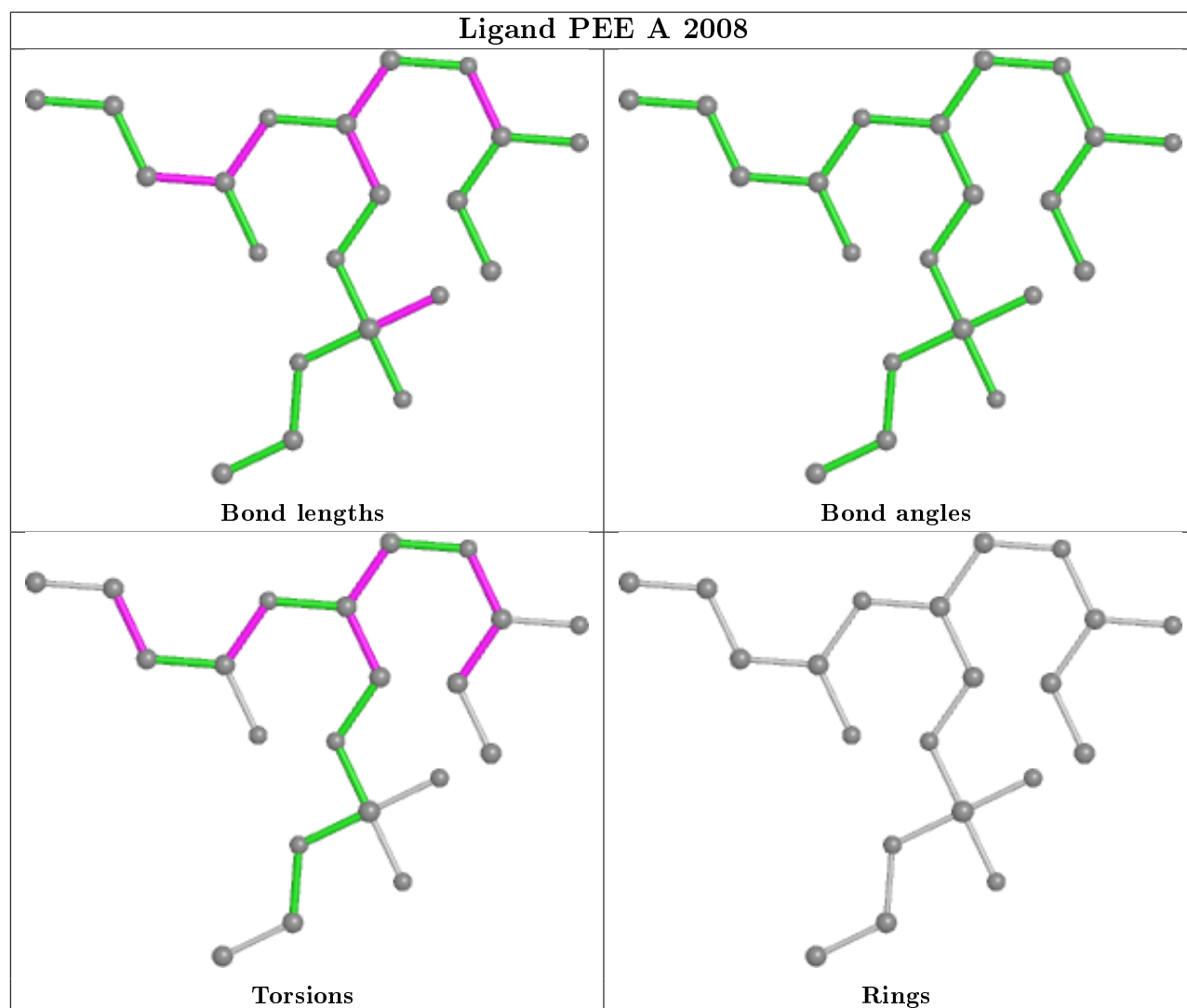
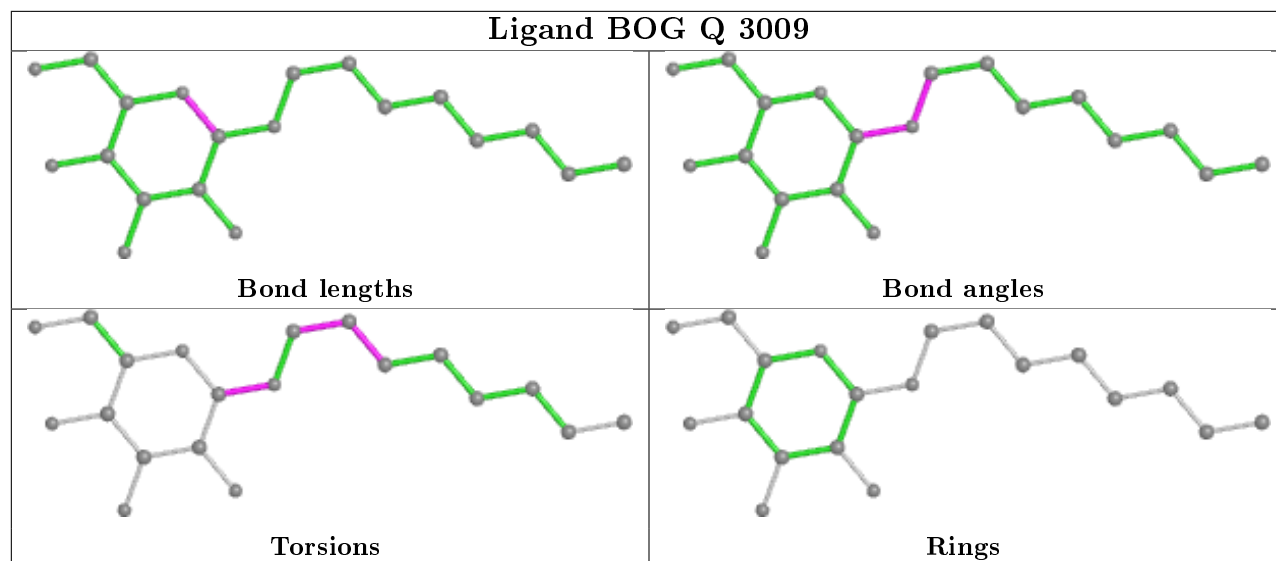
Bond angles

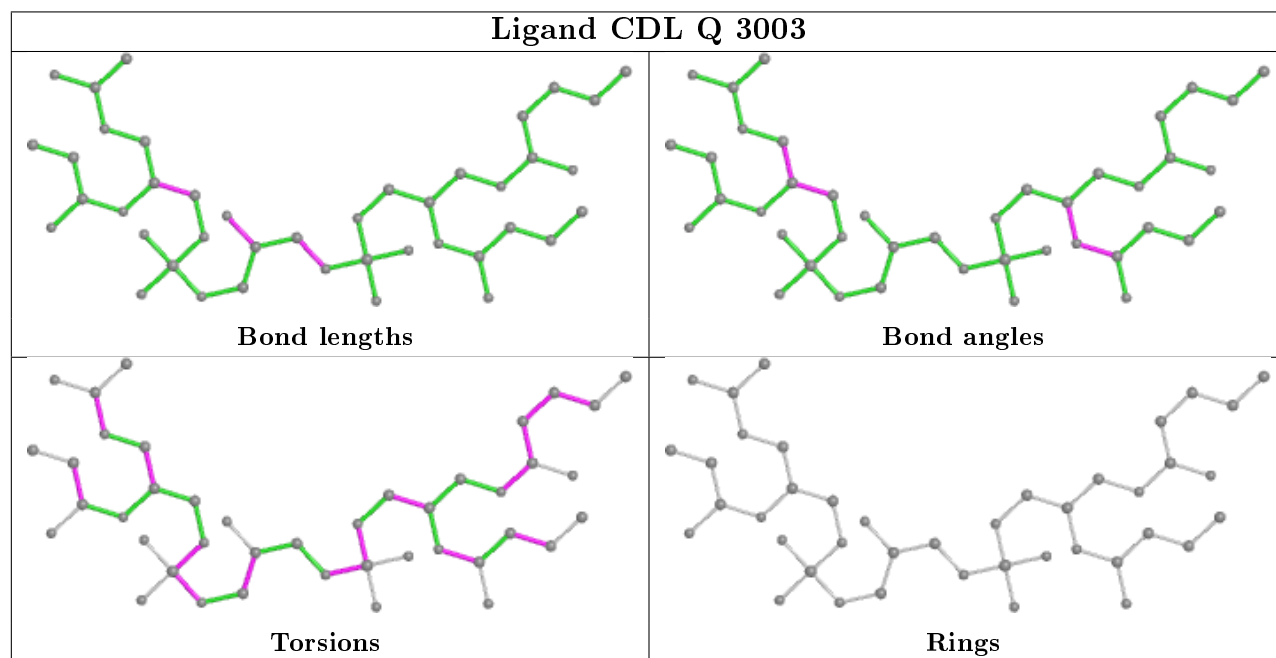
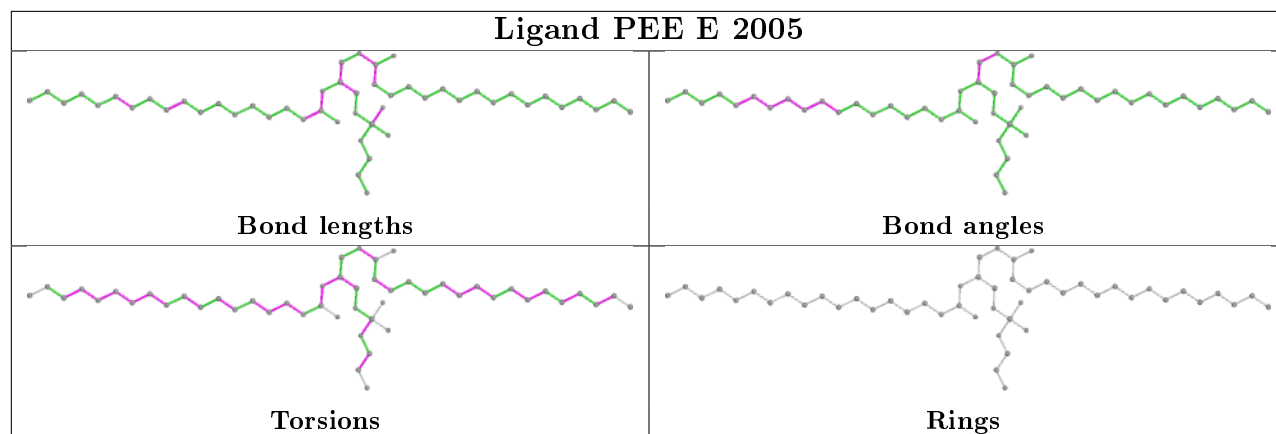


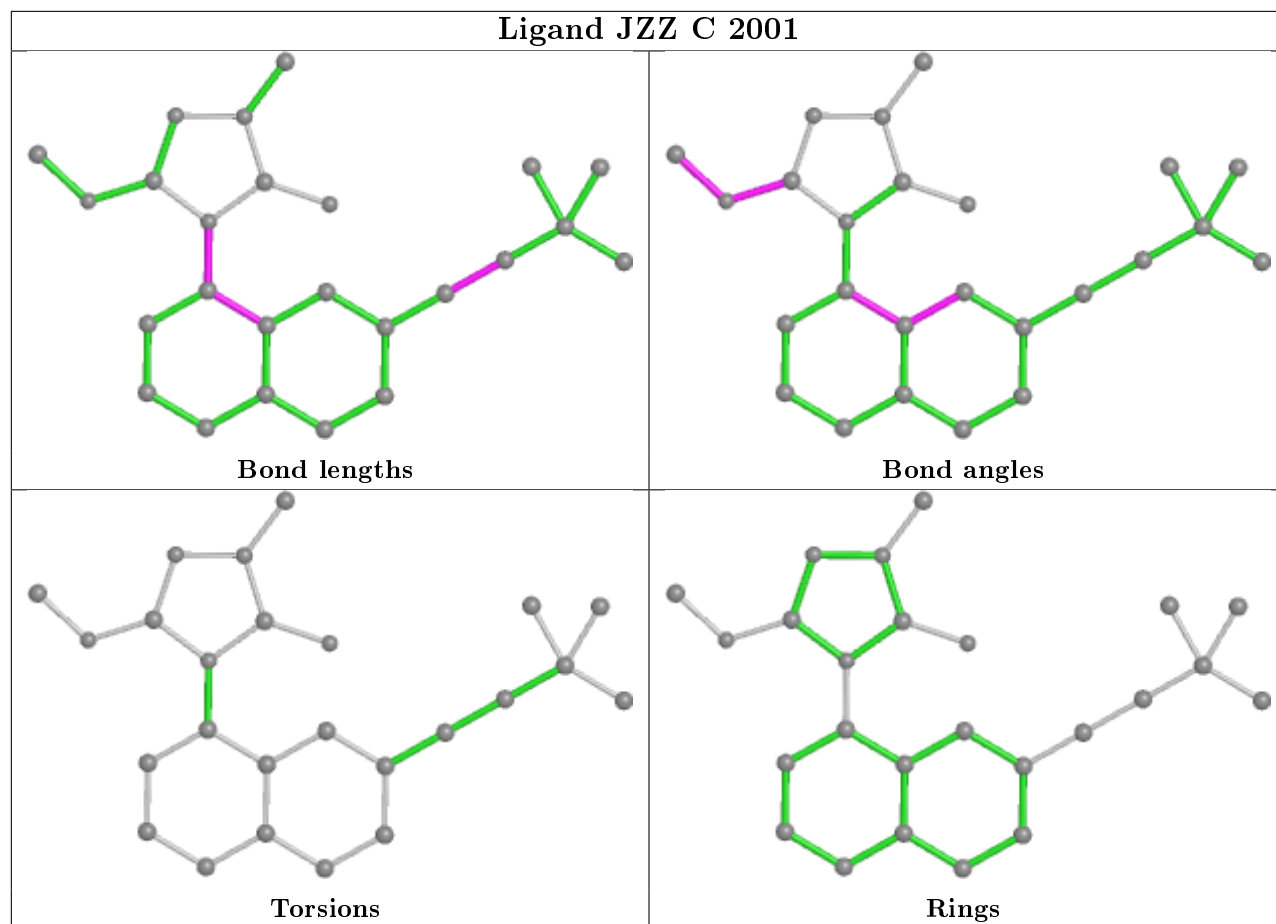
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/446 (99%)	-0.43	6 (1%) 75 49	49, 78, 110, 121	0
1	N	442/446 (99%)	-0.33	2 (0%) 91 75	55, 88, 114, 124	0
2	B	420/441 (95%)	-0.29	3 (0%) 87 69	66, 97, 130, 152	0
2	O	422/441 (95%)	-0.25	6 (1%) 75 49	52, 92, 124, 143	0
3	C	380/380 (100%)	-0.60	7 (1%) 68 40	30, 51, 98, 137	0
3	P	379/380 (99%)	-0.56	1 (0%) 94 83	39, 75, 106, 134	0
4	D	241/241 (100%)	-0.57	0 100 100	42, 56, 102, 124	0
4	Q	241/241 (100%)	-0.27	0 100 100	64, 88, 119, 136	0
5	E	196/196 (100%)	0.81	43 (21%) 0 0	47, 154, 185, 192	124 (63%)
5	R	196/196 (100%)	0.04	12 (6%) 21 7	60, 109, 155, 165	0
6	F	101/110 (91%)	-0.75	0 100 100	41, 59, 76, 111	0
6	S	101/110 (91%)	-0.33	0 100 100	65, 84, 122, 139	0
7	G	80/81 (98%)	-0.42	0 100 100	46, 64, 114, 128	0
7	T	79/81 (97%)	0.03	4 (5%) 28 10	62, 96, 159, 169	0
8	H	70/77 (90%)	-0.47	2 (2%) 51 23	50, 77, 102, 138	0
8	U	67/77 (87%)	0.07	4 (5%) 21 7	101, 131, 147, 150	0
9	I	31/47 (65%)	0.61	2 (6%) 18 5	90, 127, 152, 153	0
9	V	31/47 (65%)	1.26	8 (25%) 0 0	93, 128, 156, 160	0
10	J	61/61 (100%)	-0.56	2 (3%) 46 20	59, 72, 116, 156	0
10	W	60/61 (98%)	-0.35	0 100 100	71, 85, 121, 131	0
All	All	4042/4160 (97%)	-0.30	102 (2%) 57 28	30, 83, 141, 192	124 (3%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	9.0
5	E	157	TYR	8.5
5	E	168	SER	8.1
9	V	63	ASP	6.8
5	E	112	VAL	6.2
5	E	107	ASN	6.1
5	E	173	LYS	5.7
5	E	114	VAL	5.4
5	E	109	GLU	5.0
9	V	54	SER	5.0
5	E	174	GLY	4.9
9	V	56	SER	4.8
5	E	103	GLN	4.8
9	I	63	ASP	4.7
5	E	111	GLU	4.6
5	E	102	THR	4.6
5	E	115	SER	4.5
3	C	4	ASN	4.5
5	E	169	GLY	4.2
3	C	155	PRO	4.1
10	J	64	GLU	4.1
5	E	190	ASP	4.0
5	E	163	SER	4.0
9	V	47	ARG	4.0
5	E	108	GLN	3.9
5	R	121	GLN	3.9
7	T	78	GLU	3.8
5	E	152	ASP	3.7
5	E	159	PRO	3.7
5	E	188	VAL	3.6
5	R	157	TYR	3.6
1	A	1	ALA	3.5
1	A	218	GLY	3.5
7	T	73	ASN	3.4
5	E	149	ASN	3.4
5	E	110	ALA	3.3
5	E	104	ALA	3.3
8	U	12	GLU	3.3
5	R	196	GLY	3.3
8	U	49	HIS	3.3
9	V	53	GLU	3.3
8	U	13	LEU	3.3
1	N	38	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	84	GLY	3.2
2	O	323	GLY	3.2
5	E	124	LEU	3.2
5	E	126	ARG	3.1
5	E	83	GLU	3.1
1	A	226	ASP	3.1
2	O	19	PRO	3.1
5	E	86	ASN	3.1
5	E	125	ASP	3.1
1	N	217	SER	3.0
5	E	121	GLN	3.0
2	O	310	SER	2.9
9	V	58	ARG	2.9
9	V	57	GLY	2.9
5	E	120	PRO	2.9
5	R	165	TYR	2.9
5	E	175	PRO	2.8
9	V	48	PRO	2.8
3	C	7	LYS	2.8
8	U	50	THR	2.8
2	B	228	SER	2.7
5	R	171	ILE	2.7
5	E	150	SER	2.6
5	E	116	LYS	2.6
7	T	77	TYR	2.6
1	A	219	VAL	2.6
9	I	51	CYS	2.6
5	E	162	GLY	2.5
7	T	74	PRO	2.5
2	B	310	SER	2.5
3	C	5	ILE	2.5
10	J	63	GLU	2.5
1	A	69	LYS	2.5
8	H	10	GLU	2.4
1	A	38	GLY	2.4
2	O	23	ASP	2.3
3	C	156	TYR	2.3
5	R	114	VAL	2.3
8	H	71	HIS	2.3
5	E	99	ARG	2.3
5	R	128	LYS	2.3
5	R	117	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	8	SER	2.2
2	O	18	CYS	2.2
2	O	280	GLY	2.2
5	E	101	ARG	2.2
3	C	1	MET	2.1
5	R	113	ASP	2.1
5	E	79	SER	2.1
2	B	323	GLY	2.1
5	R	116	LYS	2.1
5	E	182	VAL	2.1
5	E	191	ASP	2.0
5	R	103	GLN	2.0
5	E	87	VAL	2.0
5	E	180	LEU	2.0
3	P	2	ALA	2.0
5	E	128	LYS	2.0
5	R	120	PRO	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(\AA^2)	Q<0.9
18	BOG	Q	3091	13/20	0.23	0.76	201,204,205,205	0
18	BOG	D	2091	13/20	0.24	0.90	215,217,218,218	0
18	BOG	P	2010	12/20	0.53	0.56	149,151,153,154	0
11	PEE	A	2008	21/51	0.64	0.30	139,142,145,145	0
11	PEE	R	3005	50/51	0.68	0.45	94,113,121,122	0
17	CDL	Q	3003	42/100	0.75	0.32	127,135,146,147	0

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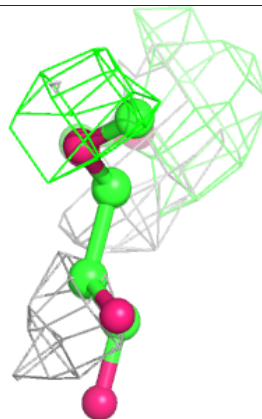
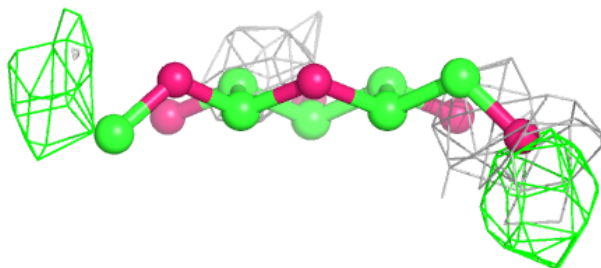
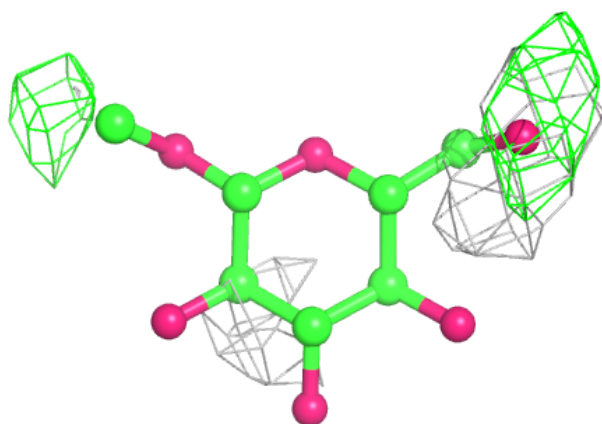
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	UQ	P	3002	19/63	0.77	0.46	134,141,143,143	0
11	PEE	E	2005	50/51	0.83	0.36	88,101,111,112	0
17	CDL	D	2003	42/100	0.84	0.25	94,105,109,110	0
11	PEE	P	3007	49/51	0.85	0.30	85,95,107,108	0
17	CDL	T	3004	40/100	0.86	0.25	104,109,120,121	0
15	GOL	P	3011	6/6	0.87	0.32	90,91,93,95	0
11	PEE	C	2007	49/51	0.88	0.28	53,73,95,96	0
14	UQ	C	2002	19/63	0.88	0.30	95,99,101,102	0
11	PEE	P	3008	5/51	0.88	0.17	108,109,110,110	0
17	CDL	G	2004	40/100	0.89	0.26	72,83,101,103	0
15	GOL	C	2011	6/6	0.91	0.24	90,90,91,91	0
18	BOG	Q	3009	20/20	0.93	0.23	86,92,94,95	0
18	BOG	D	2009	20/20	0.94	0.17	58,73,76,76	0
13	JZZ	P	3001	25/25	0.95	0.22	74,76,79,80	0
19	FES	E	501	4/4	0.95	0.13	162,162,163,163	4
16	HEC	Q	501	43/43	0.96	0.20	71,75,83,84	0
13	JZZ	C	2001	25/25	0.96	0.16	45,49,51,51	0
12	HEM	P	501	43/43	0.97	0.22	51,55,62,67	0
12	HEM	C	501	43/43	0.97	0.21	30,42,53,55	0
12	HEM	P	502	43/43	0.98	0.19	42,52,65,70	0
16	HEC	D	501	43/43	0.98	0.16	39,45,50,56	0
19	FES	R	501	4/4	0.98	0.06	100,101,102,102	0
12	HEM	C	502	43/43	0.98	0.19	31,37,47,52	0

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

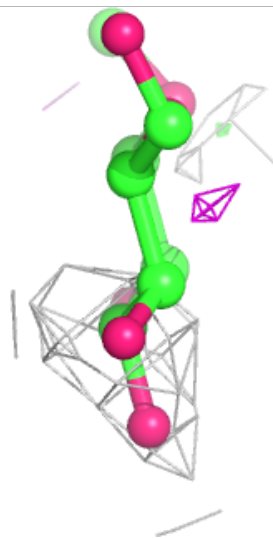
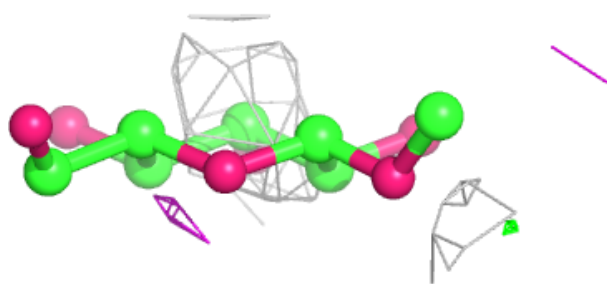
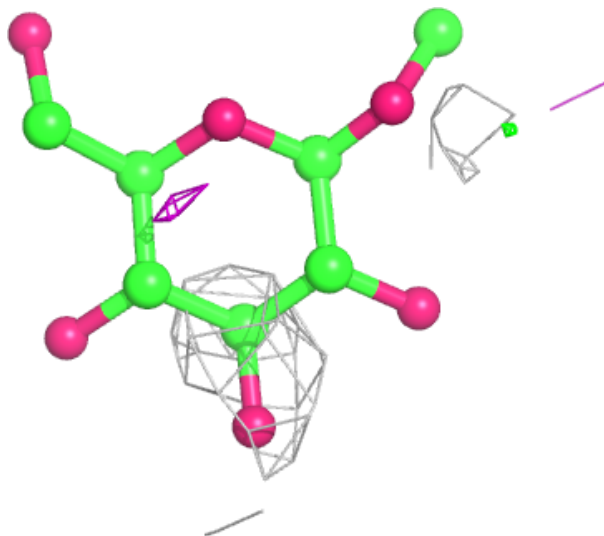
Electron density around BOG Q 3091:

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



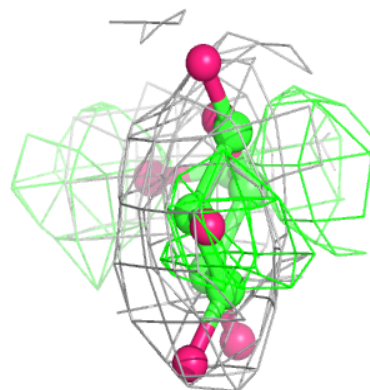
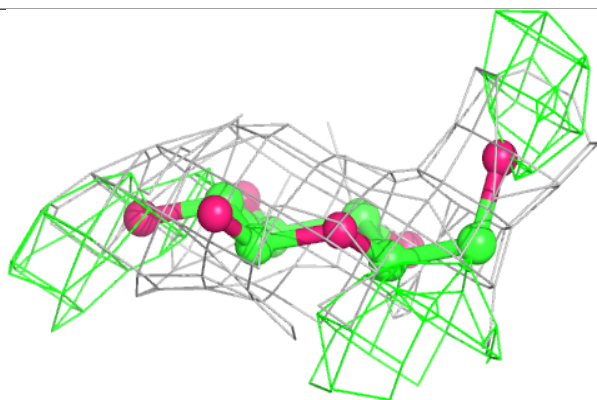
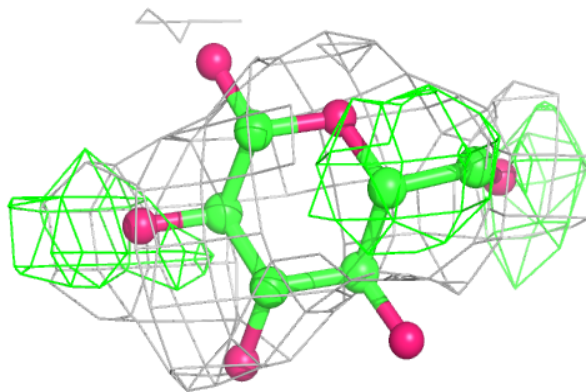
Electron density around BOG D 2091:

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



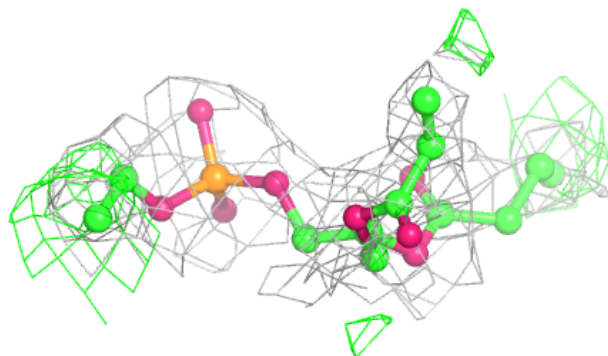
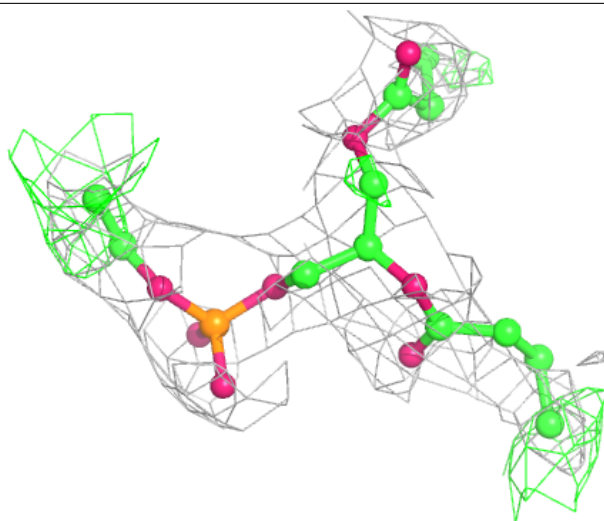
Electron density around BOG P 2010:

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



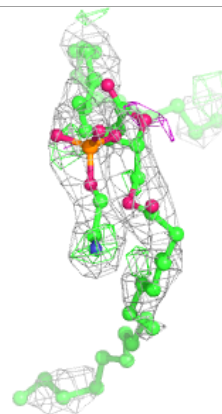
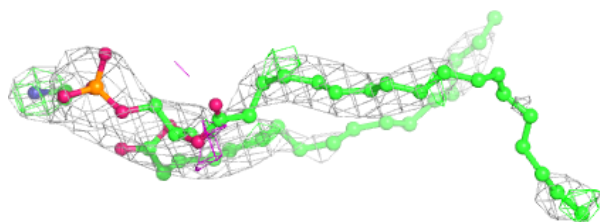
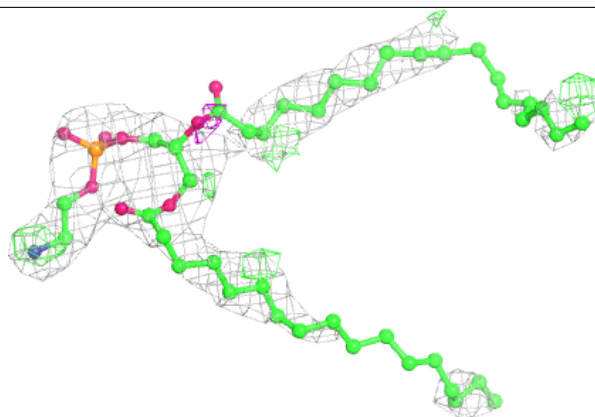
Electron density around PEE A 2008:

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

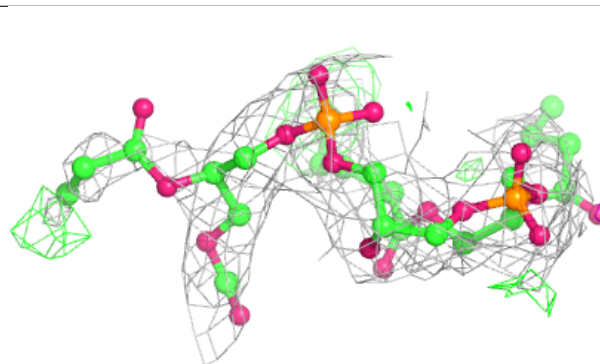
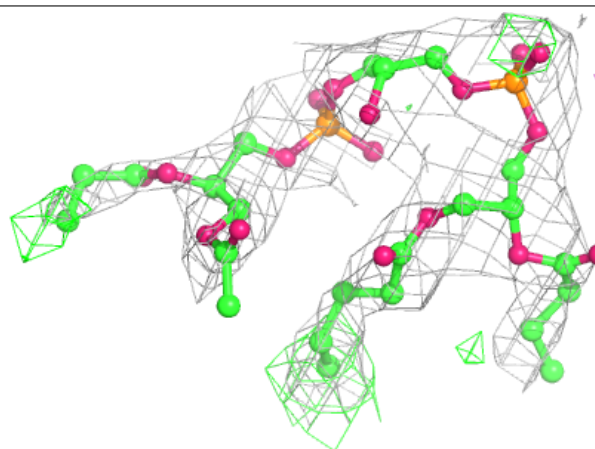


Electron density around PEE R 3005:

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

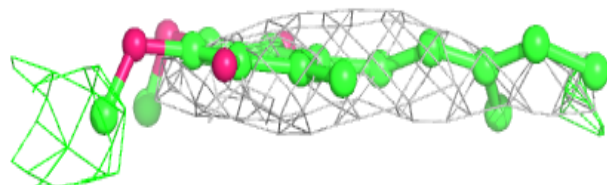
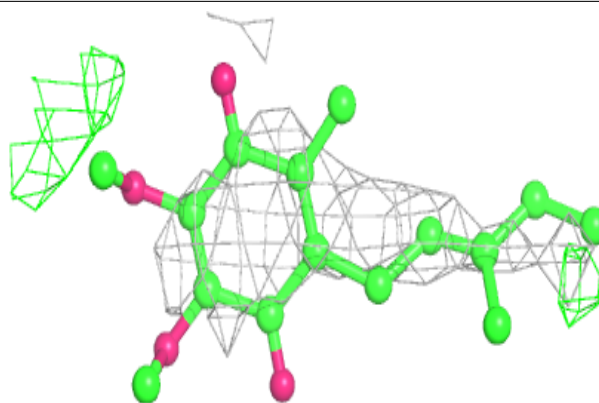
**Electron density around CDL Q 3003:**

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

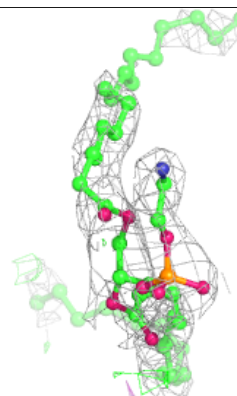
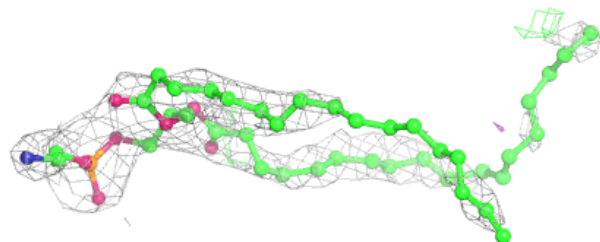
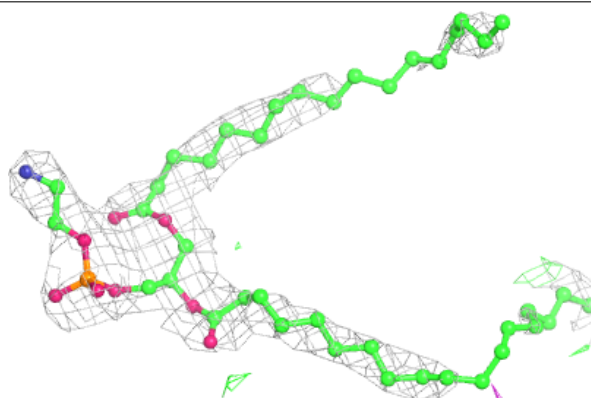


Electron density around UQ P 3002:

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

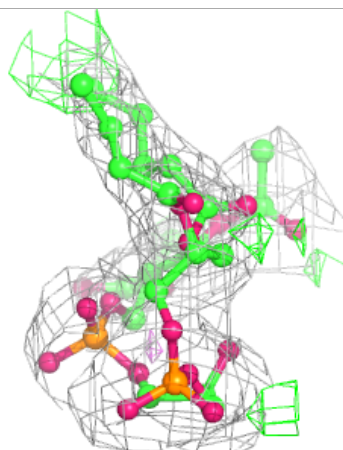
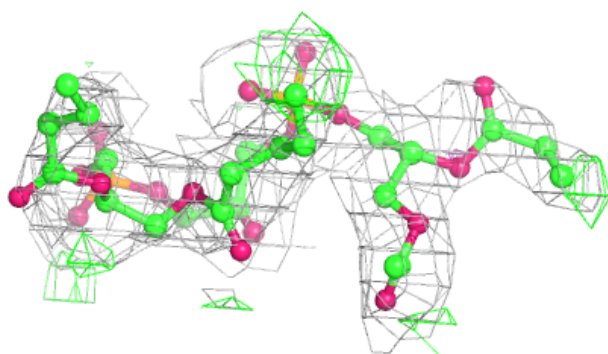
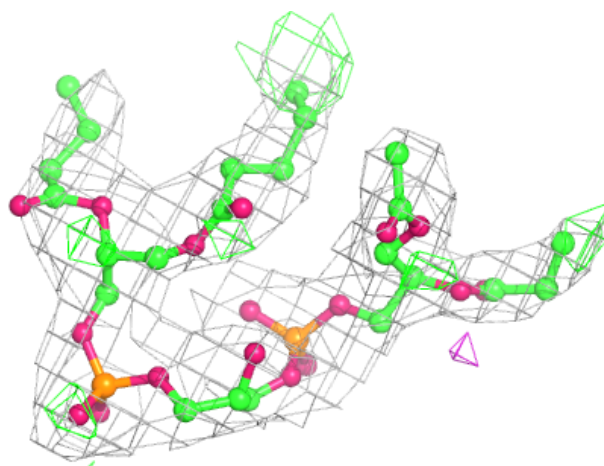
**Electron density around PEE E 2005:**

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



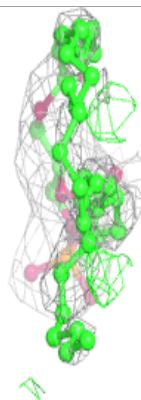
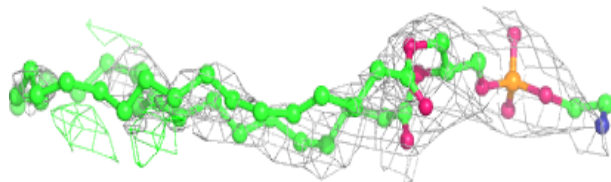
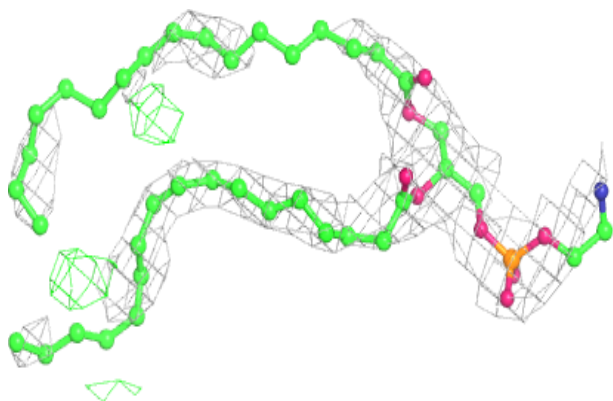
Electron density around CDL D 2003:

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



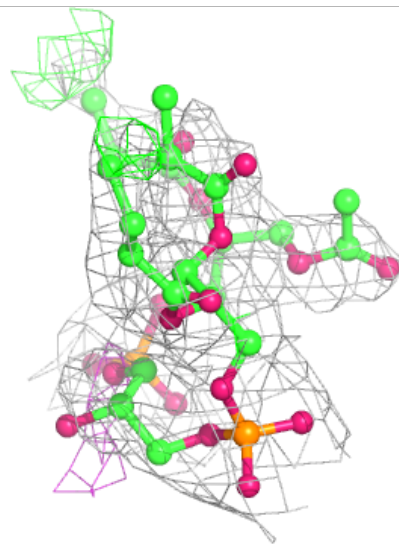
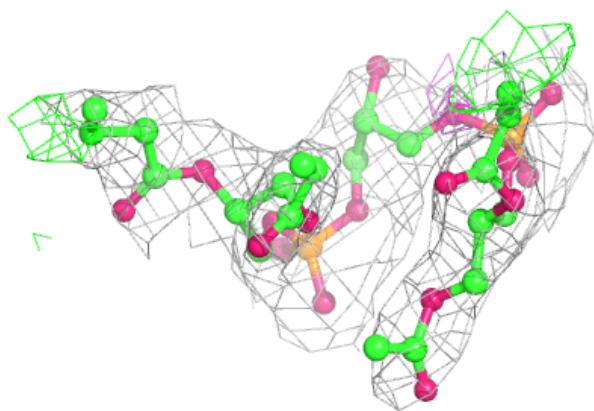
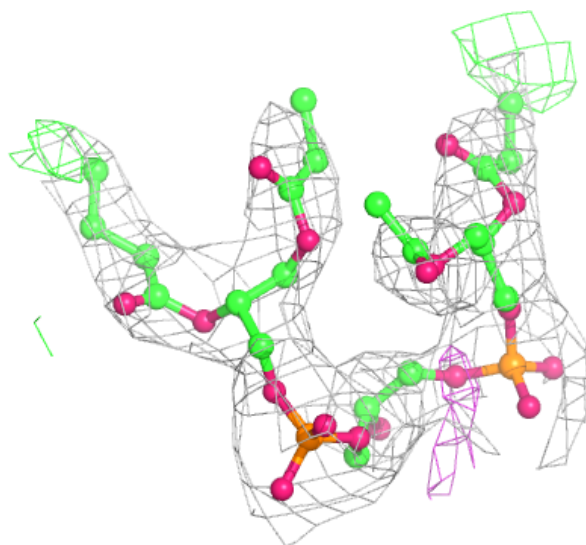
Electron density around PEE P 3007:

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



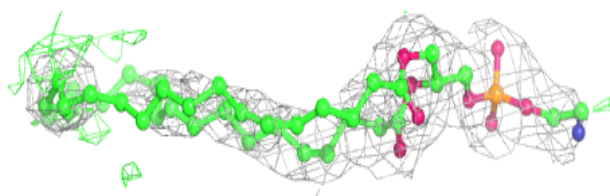
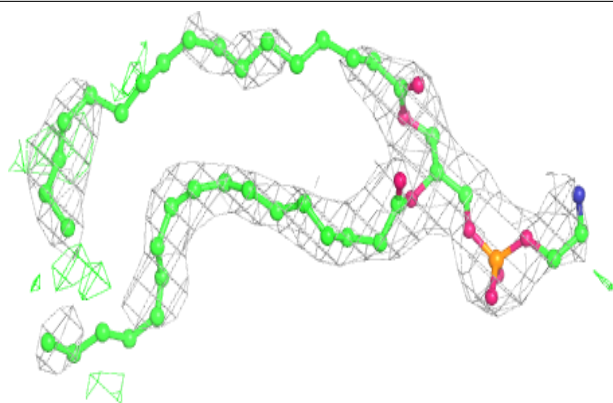
Electron density around CDL T 3004:

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

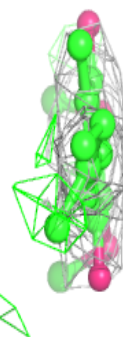
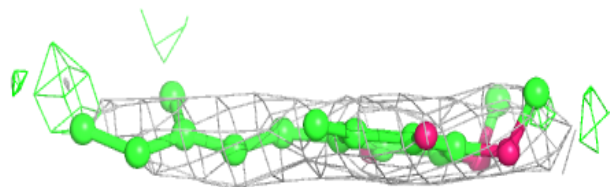
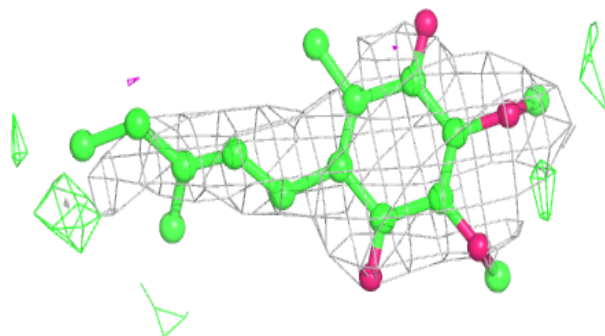


Electron density around PEE C 2007:

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

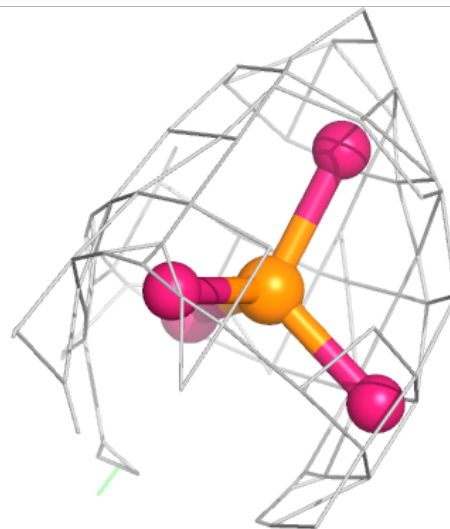
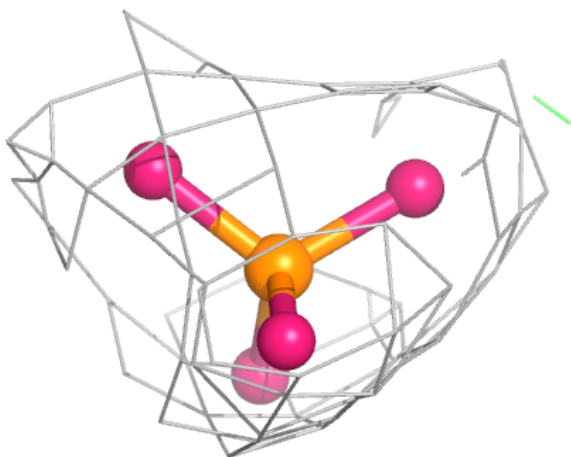
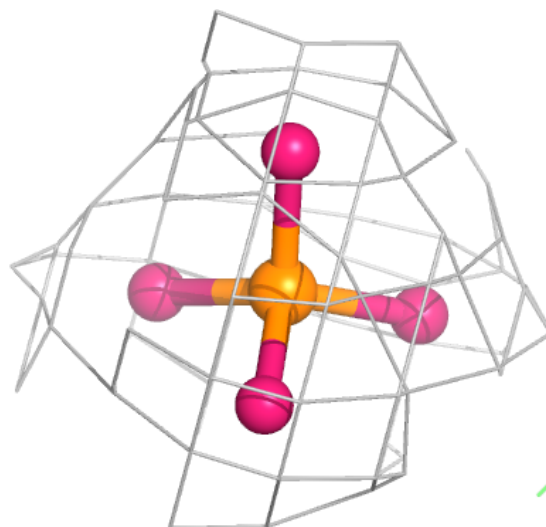
**Electron density around UQ C 2002:**

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



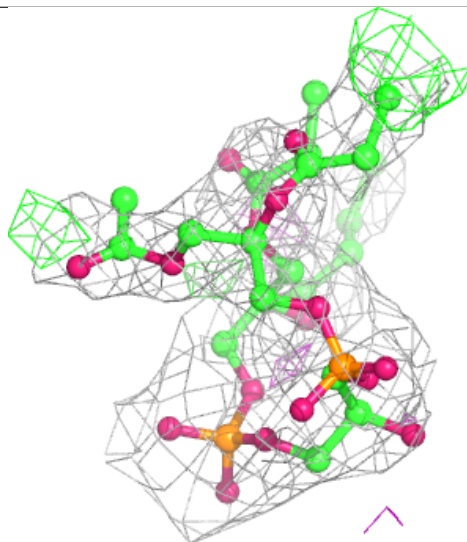
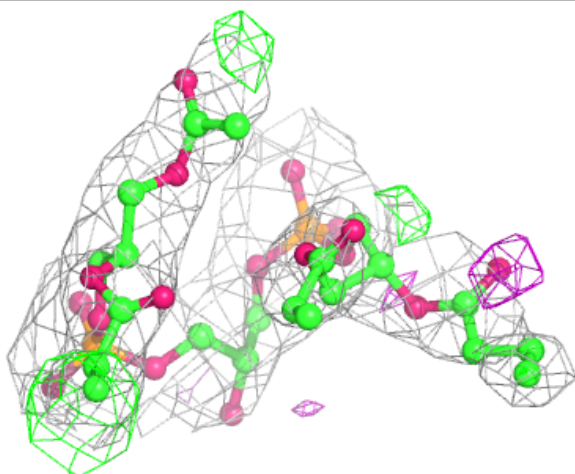
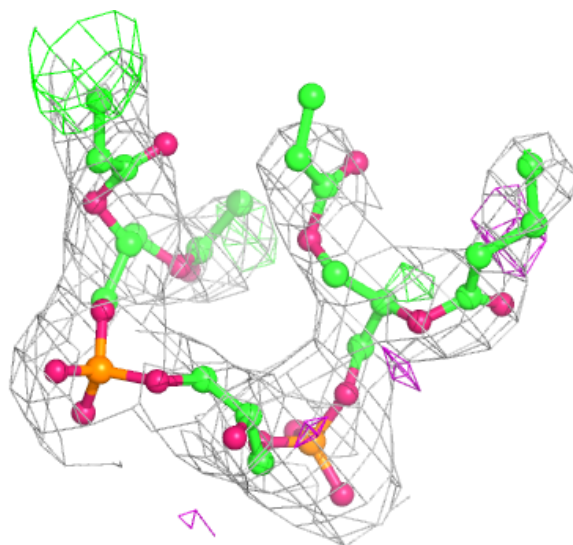
Electron density around PEE P 3008:

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



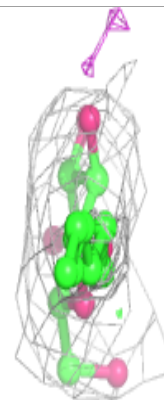
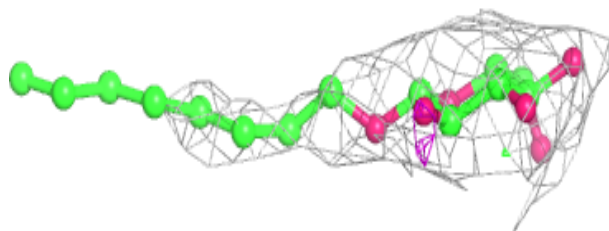
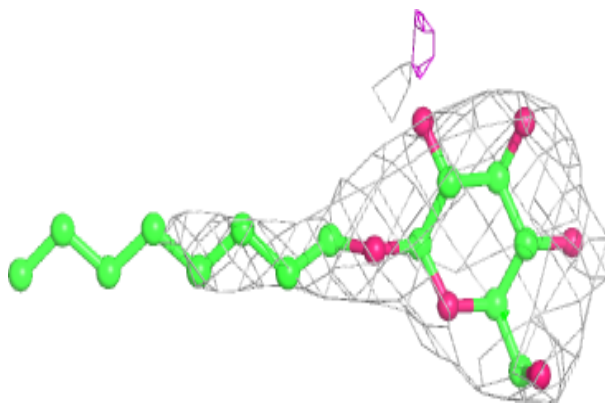
Electron density around CDL G 2004:

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

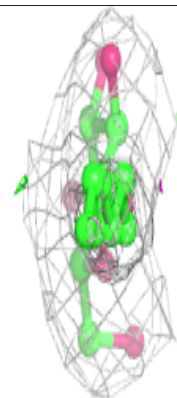
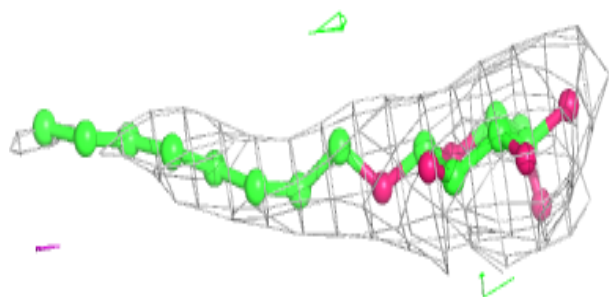
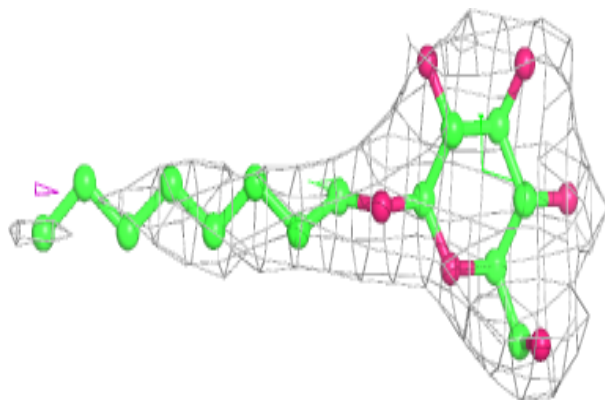


Electron density around BOG Q 3009:

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

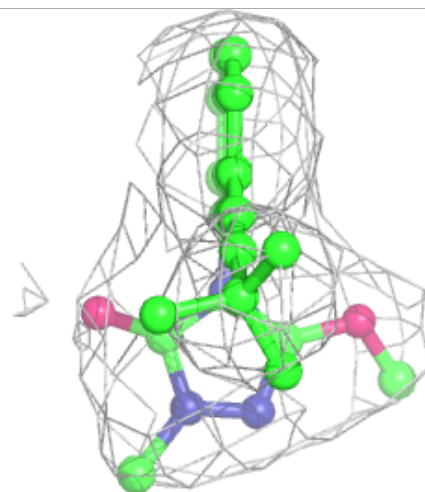
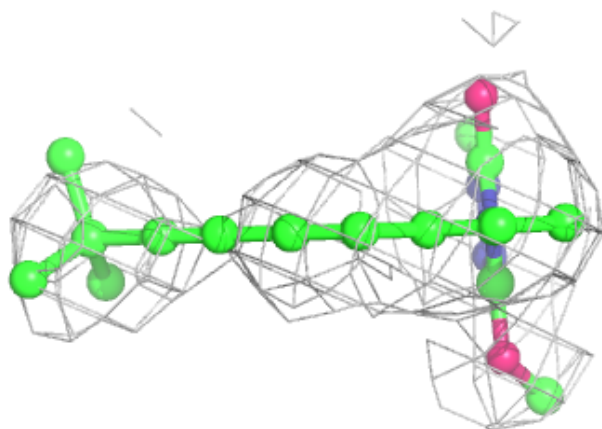
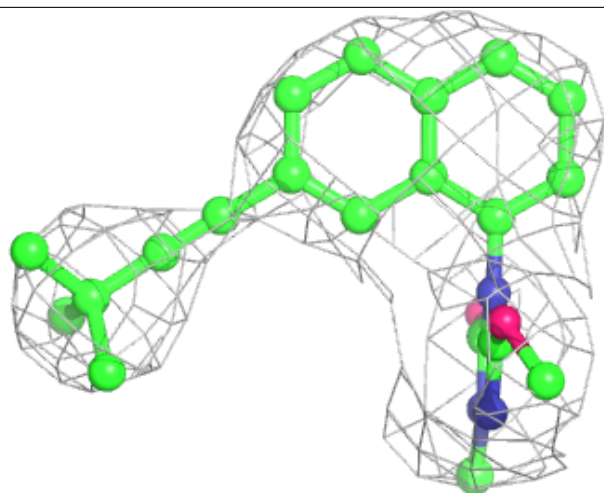
**Electron density around BOG D 2009:**

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



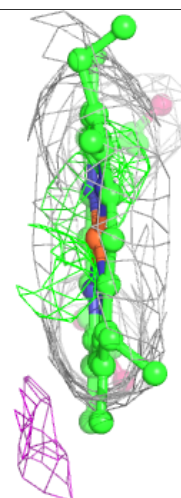
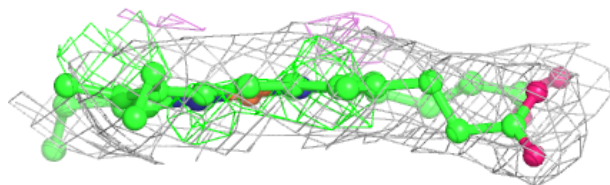
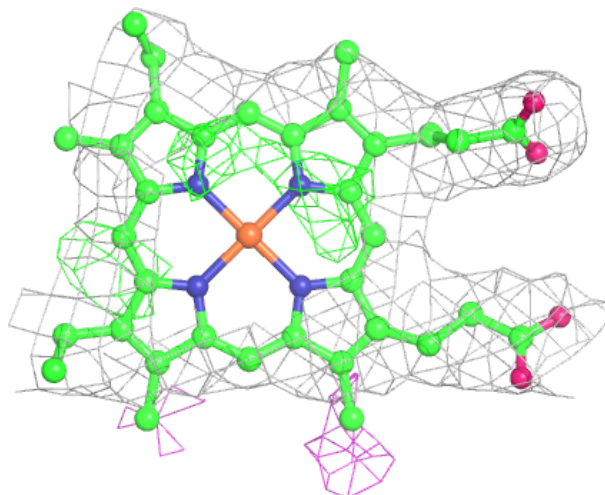
Electron density around JZZ P 3001:

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



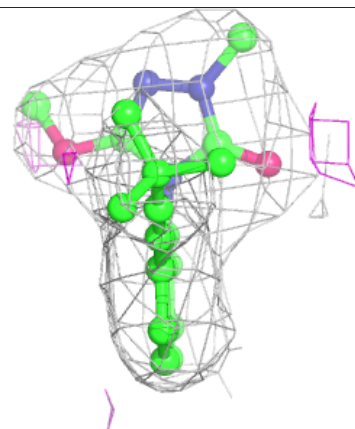
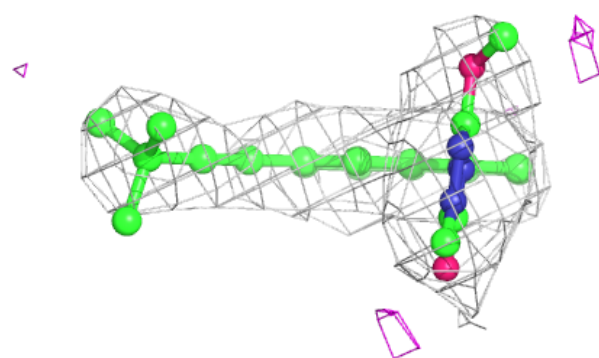
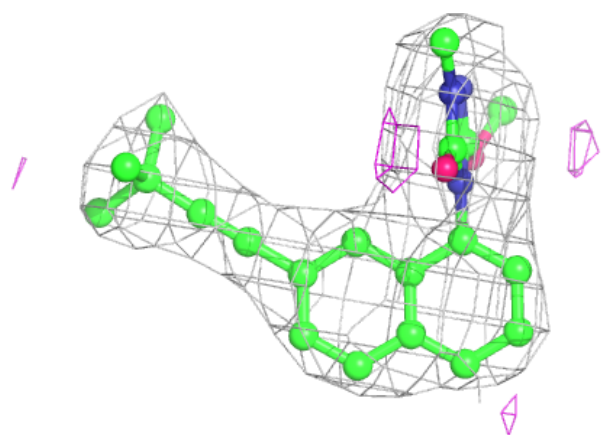
Electron density around HEC Q 501:

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



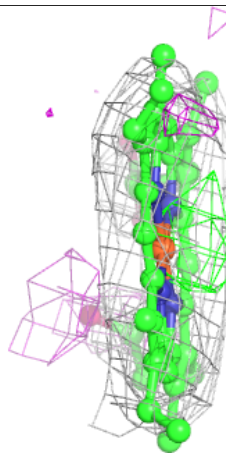
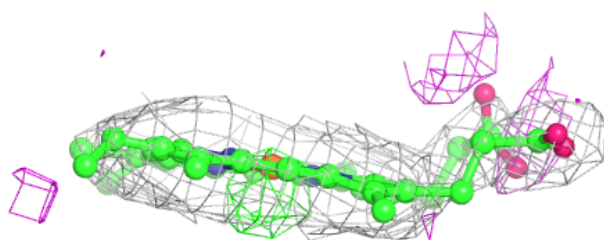
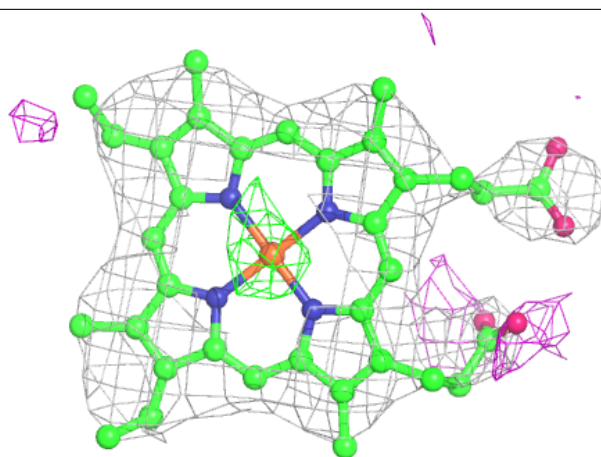
Electron density around JZZ C 2001:

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



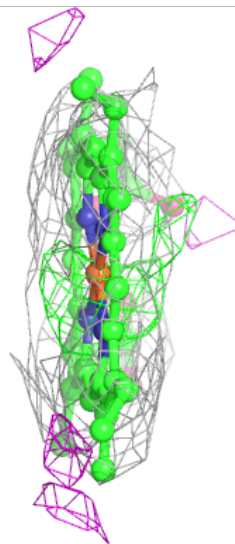
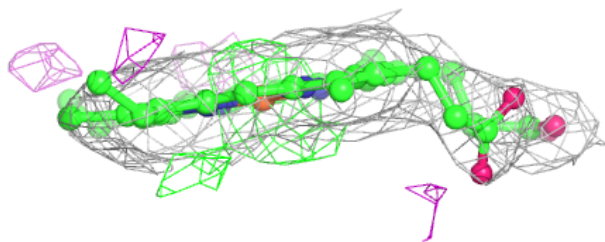
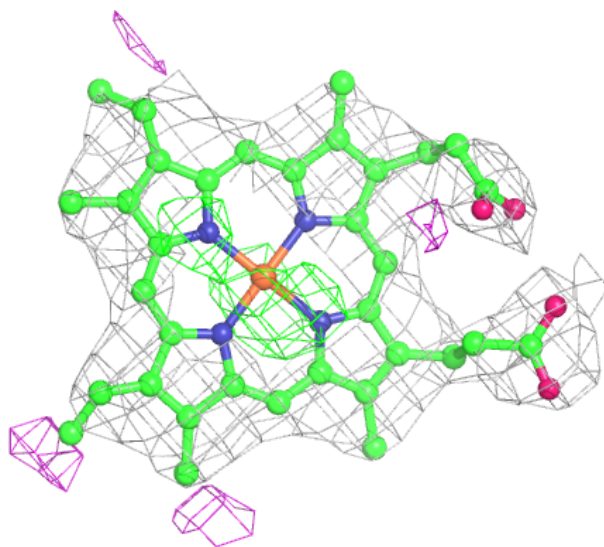
Electron density around HEM P 501:

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



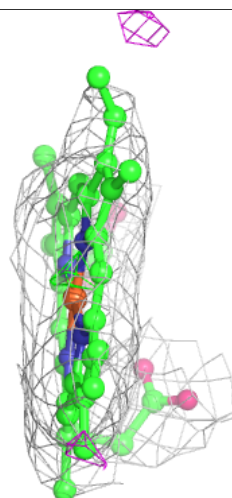
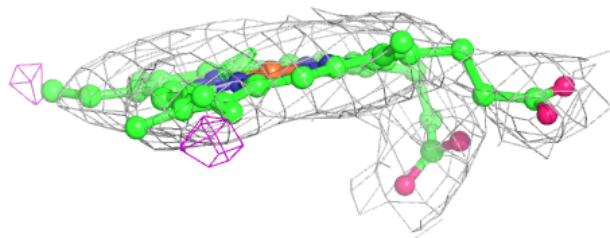
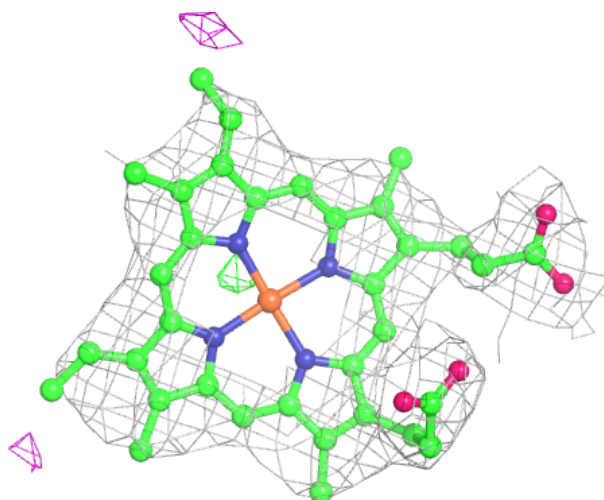
Electron density around HEM C 501:

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



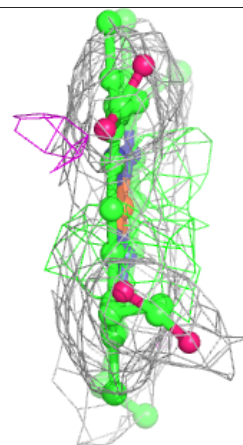
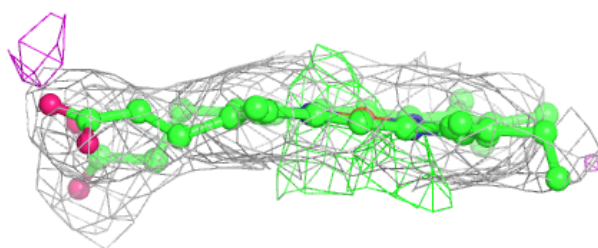
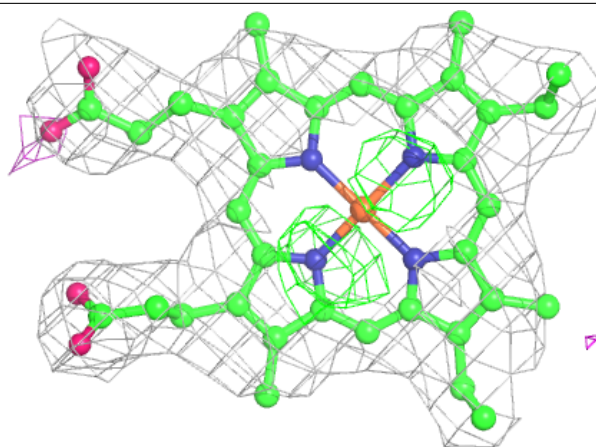
Electron density around HEM P 502:

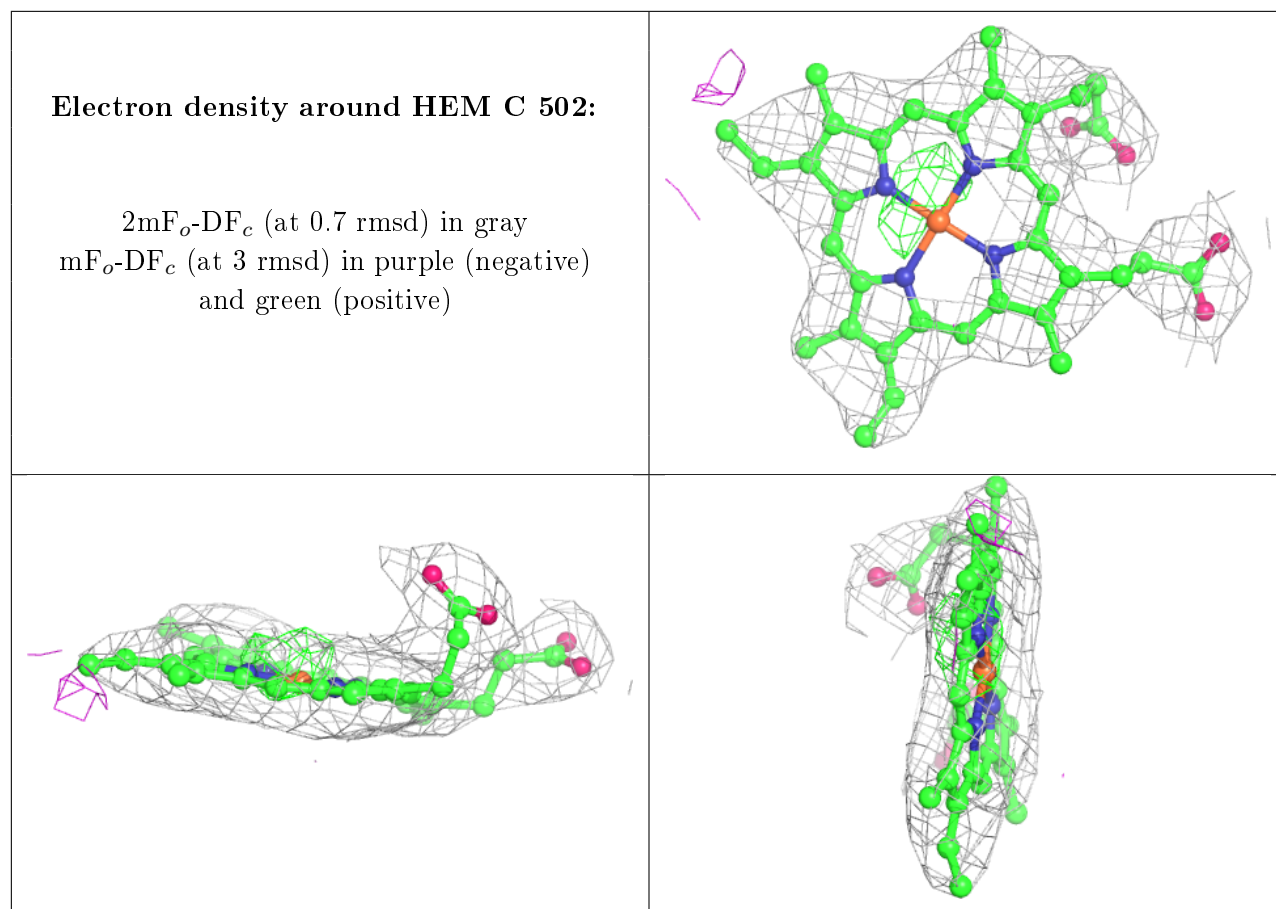
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.