



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:14 PM EDT

PDB ID : 1PP9 / pdb_00001pp9
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2003-06-16
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

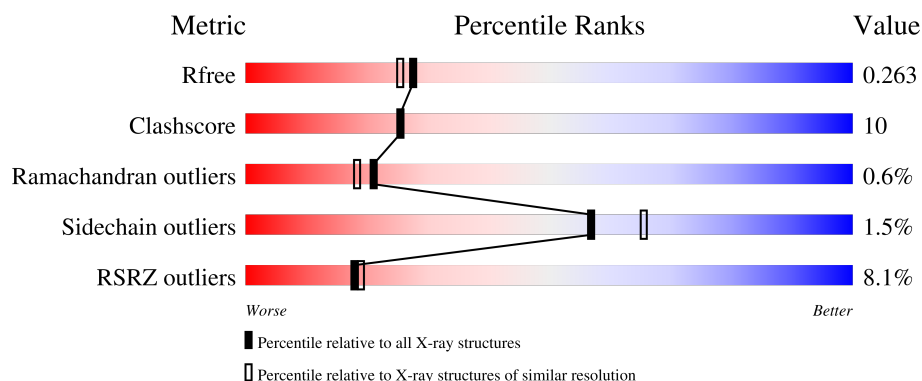
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



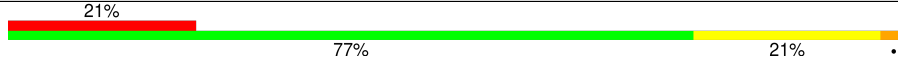
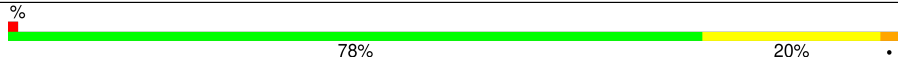
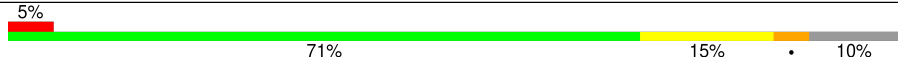
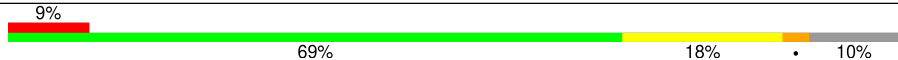
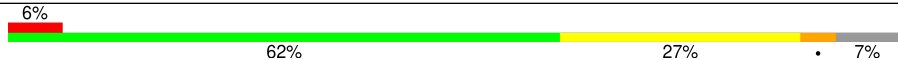
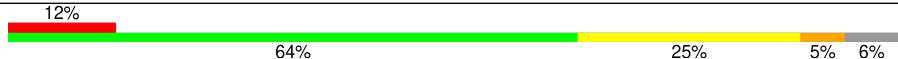
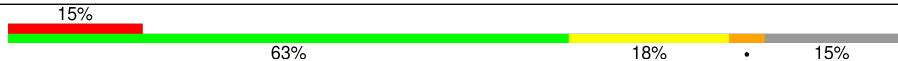
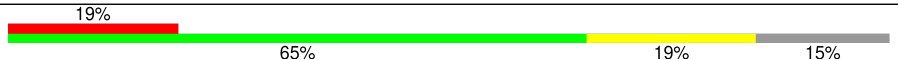
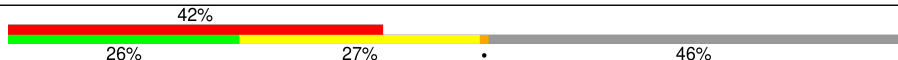
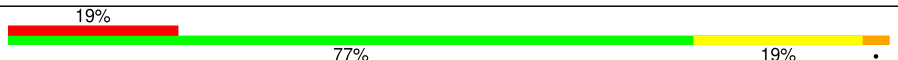
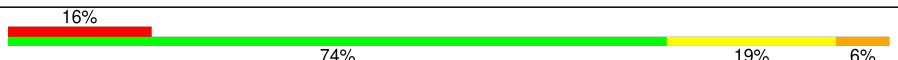
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	446	6% 76% 21% ..
1	N	446	4% 80% 18% ..
2	B	439	6% 77% 19% ..
2	O	439	8% 79% 16% ..
3	C	379	2% 79% 16% ..

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Mol	Chain	Length	Quality of chain
3	P	379	
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	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

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
12	AZI	A	4005	-	X	-	-
12	AZI	C	2014	-	X	-	-
12	AZI	D	4004	-	X	-	-
12	AZI	P	3014	-	X	-	-
13	PEE	C	2012	-	X	-	-
13	PEE	N	3012	-	X	-	-
14	PO4	B	3010	-	X	-	-
14	PO4	O	2010	-	X	-	-
15	GOL	B	2013	-	-	-	X
19	HEC	D	501	X	-	-	-
19	HEC	Q	501	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33959 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			
1	N	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3177	1996	562	612	7			
2	O	424	Total	C	N	O	S	0	0	0
			3180	1998	562	613	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2931	1968	455	490	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

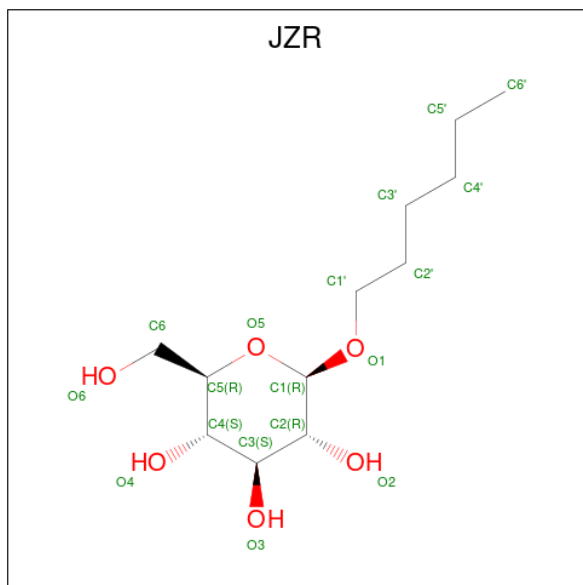
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

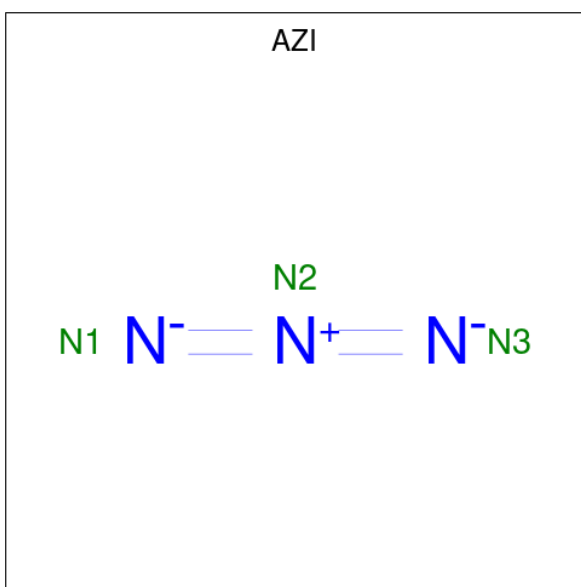
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			507	333	88	86			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: C₁₂H₂₄O₆).



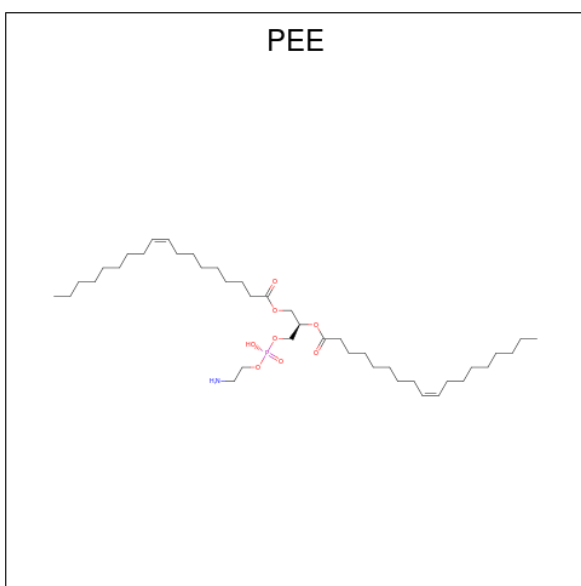
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is AZIDE ION (CCD ID: AZI) (formula: N₃).



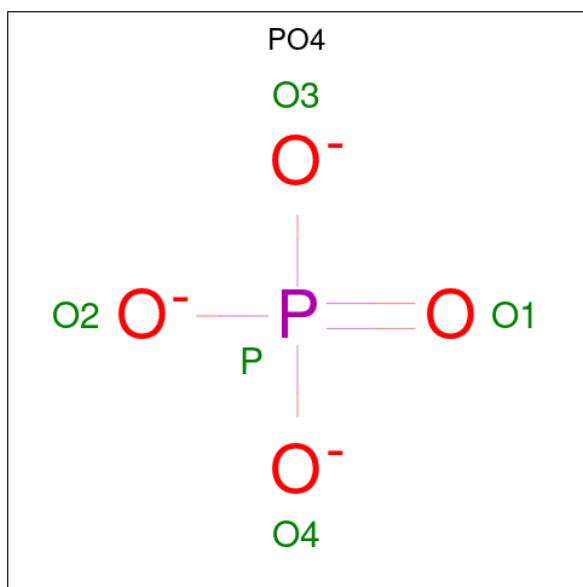
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total N 3 3	0	0
12	C	1	Total N 3 3	0	0
12	D	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



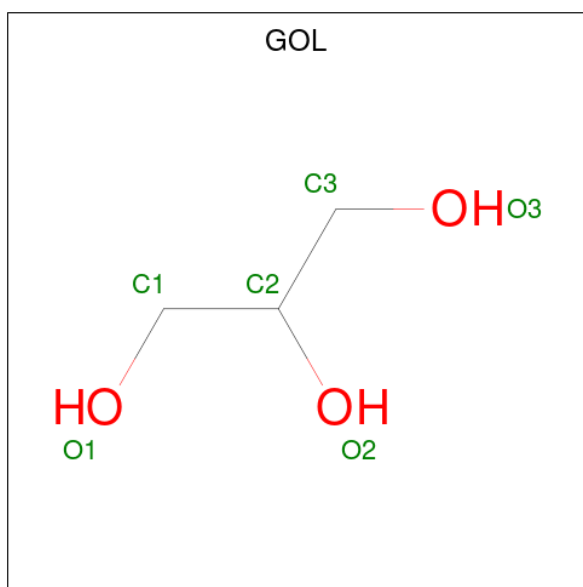
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	O			0	0
			6	3	3				
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	C	1	Total	O	P			0	0
			5	4	1				
13	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
13	G	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	N	1	Total	O	P			0	0
			5	4	1				
13	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
13	T	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



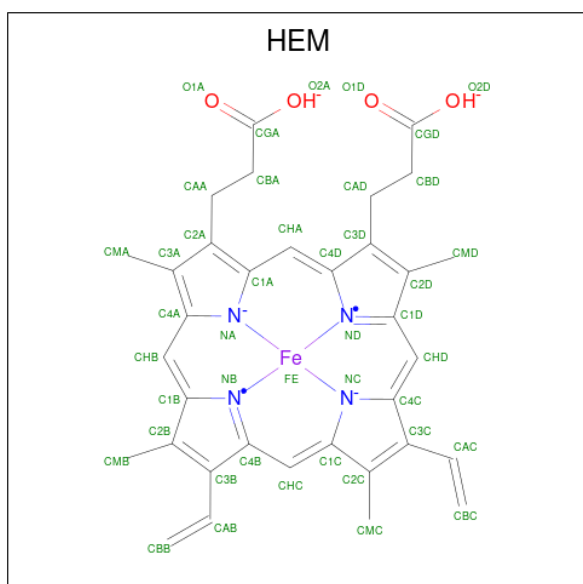
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	O	P	0	0
			5	4	1		
14	O	1	Total	O	P	0	0
			5	4	1		

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



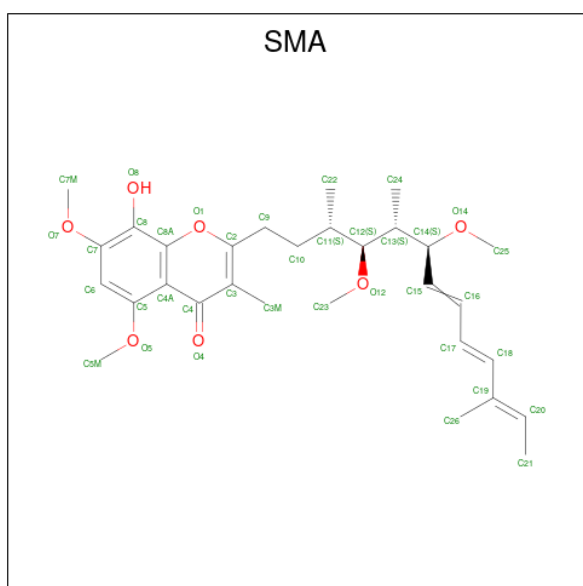
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			6	3	3		
15	C	1	Total	C	O	0	0
			6	3	3		
15	O	1	Total	C	O	0	0
			6	3	3		
15	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



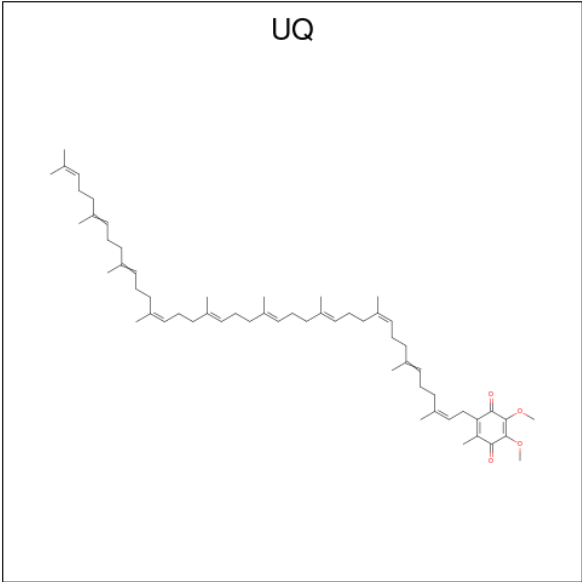
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 17 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



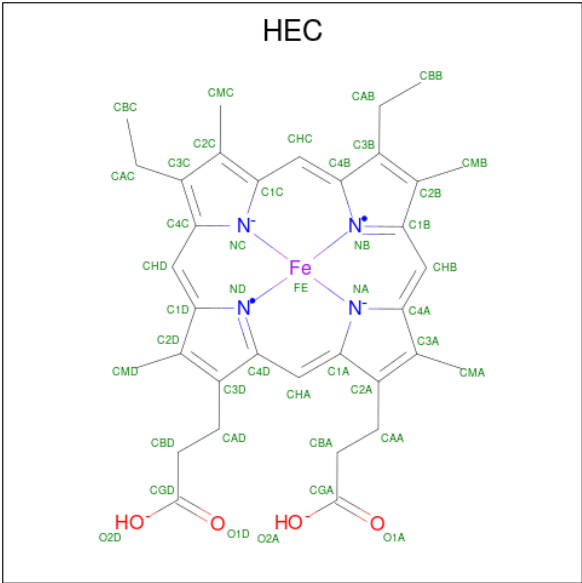
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	1	Total	C O		
			37	30 7	0	0
17	P	1	Total	C O		
			37	30 7	0	0

- Molecule 18 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$).



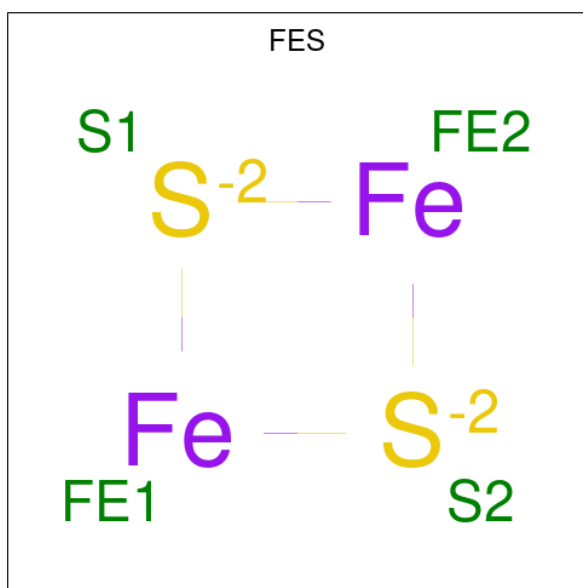
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			14	10	4		
18	P	1	Total	C	O	0	0
			14	10	4		

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



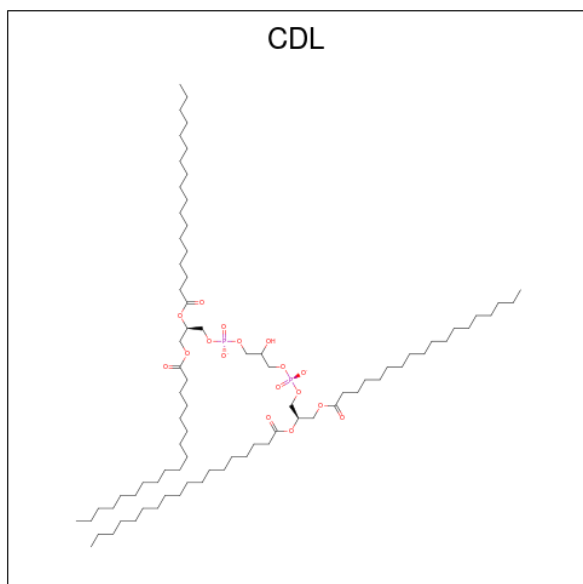
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



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

- Molecule 21 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	G	1	Total	C	O	P	0	0
			50	31	17	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	G	1	Total	C	O	P	0	0
			44	25	17	2		
21	Q	1	Total	C	O	P	0	0
			50	31	17	2		
21	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	187	Total	O	0	0
			187	187		
22	B	149	Total	O	0	0
			149	149		
22	C	125	Total	O	0	0
			125	125		
22	D	118	Total	O	0	0
			118	118		
22	E	54	Total	O	0	0
			54	54		
22	F	57	Total	O	0	0
			57	57		
22	G	24	Total	O	0	0
			24	24		
22	H	14	Total	O	0	0
			14	14		
22	I	16	Total	O	0	0
			16	16		
22	J	5	Total	O	0	0
			5	5		
22	N	134	Total	O	0	0
			134	134		
22	O	130	Total	O	0	0
			130	130		
22	P	122	Total	O	0	0
			122	122		
22	Q	109	Total	O	0	0
			109	109		
22	R	64	Total	O	0	0
			64	64		
22	S	73	Total	O	0	0
			73	73		

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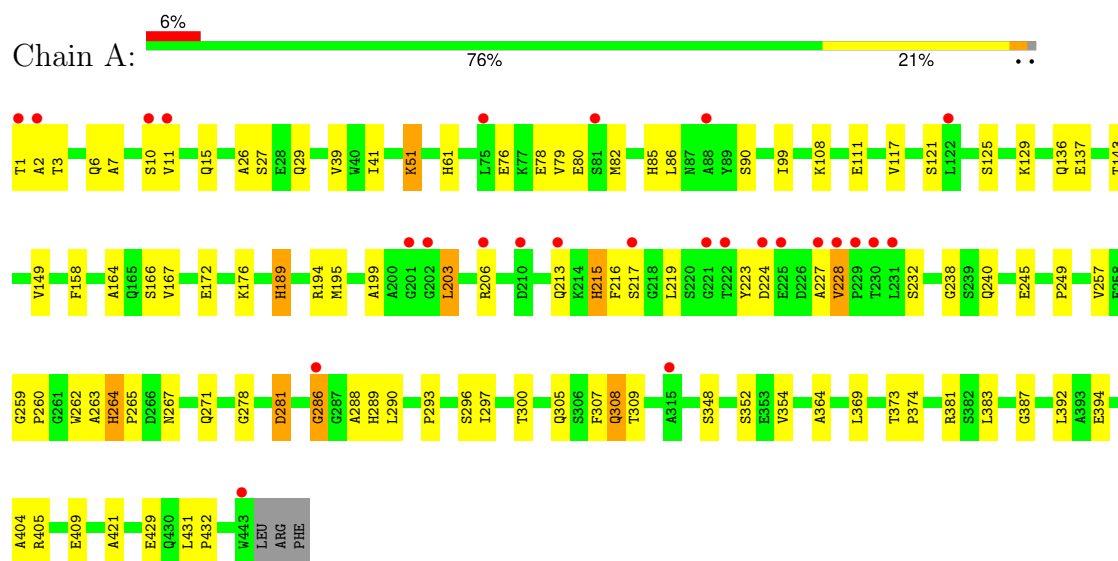
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	T	21	Total 21	O 21	0	0
22	U	16	Total 16	O 16	0	0
22	V	10	Total 10	O 10	0	0
22	W	9	Total 9	O 9	0	0

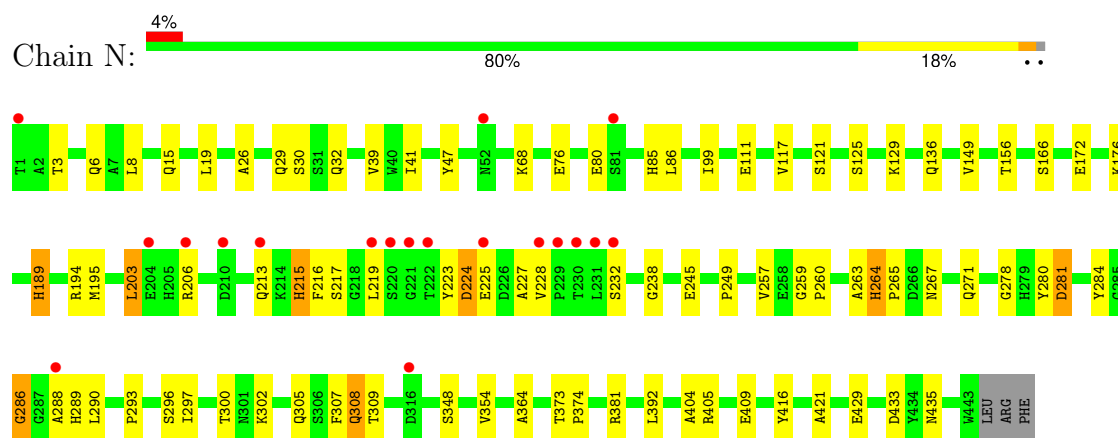
3 Residue-property plots [i](#)

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

- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

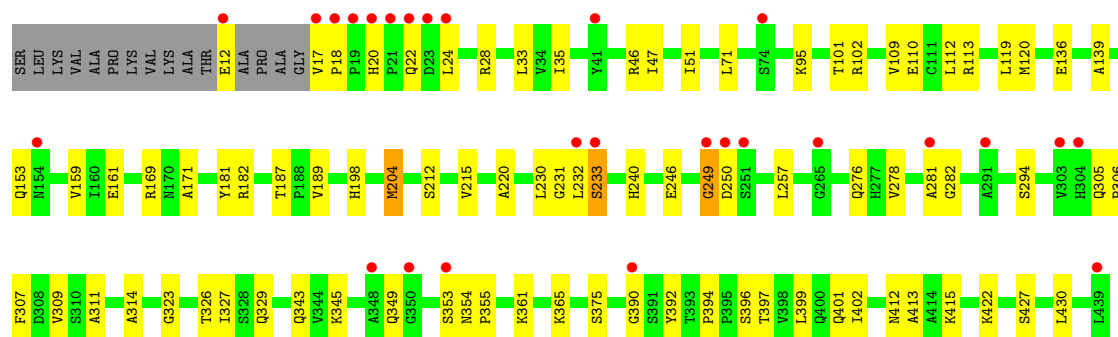


- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

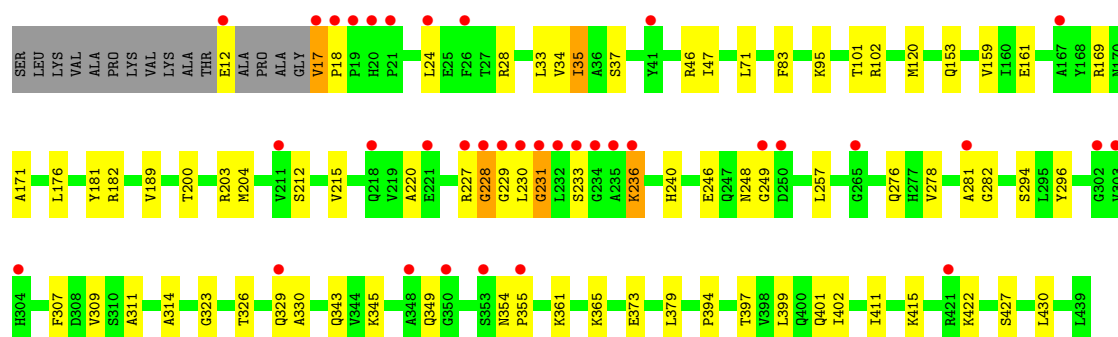
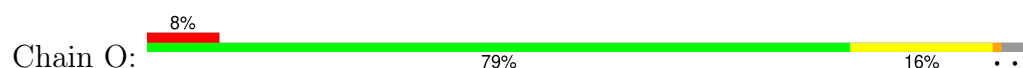


- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

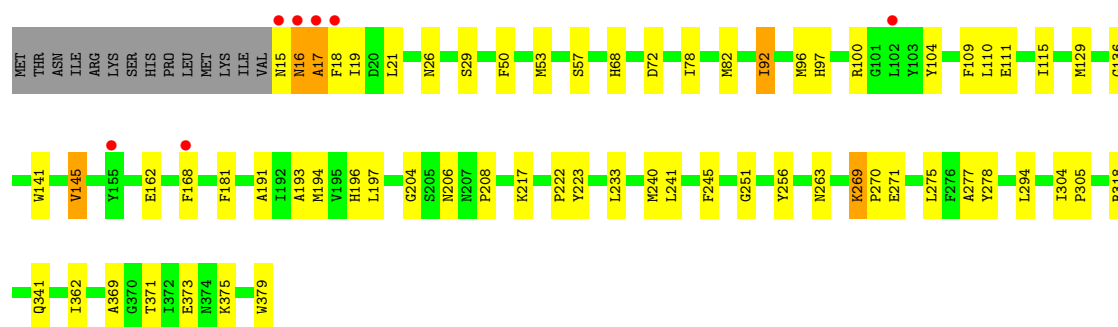
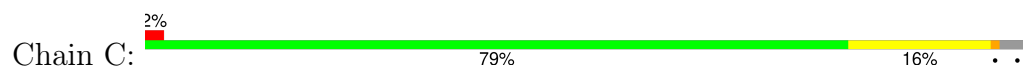




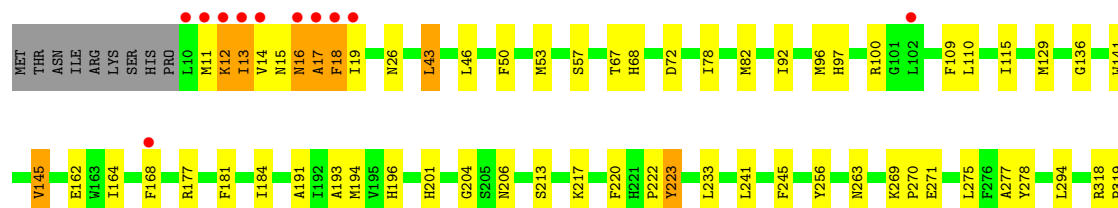
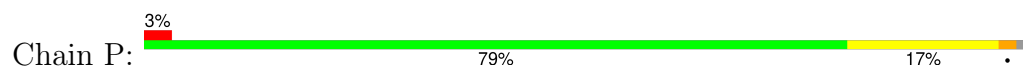
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial



- Molecule 3: Cytochrome b

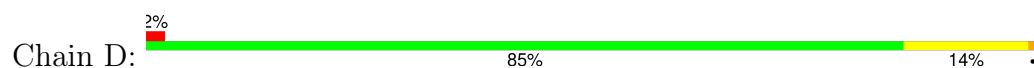


- Molecule 3: Cytochrome b

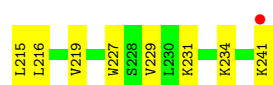
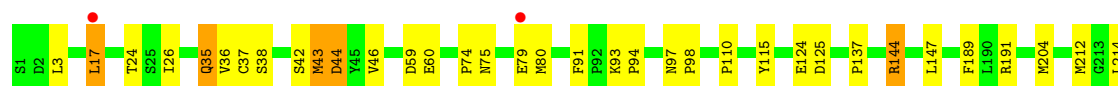
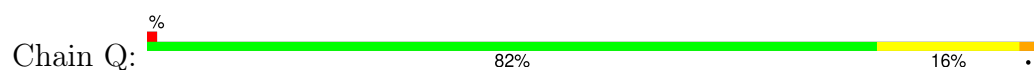




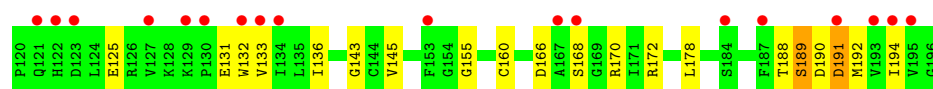
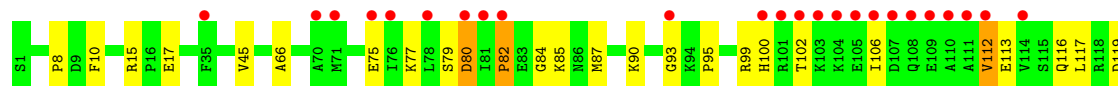
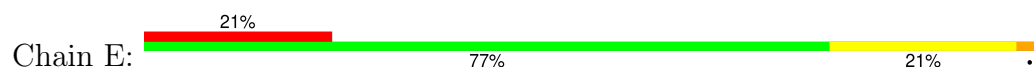
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



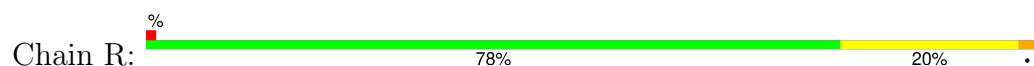
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

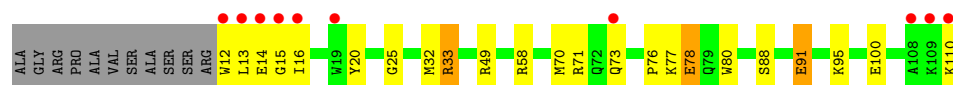


- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein





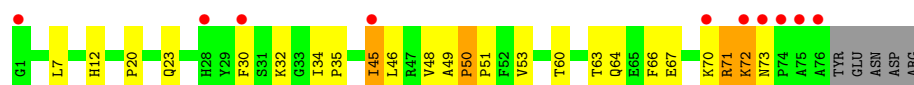
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



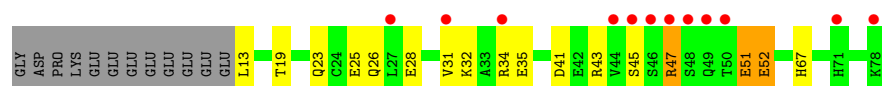
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



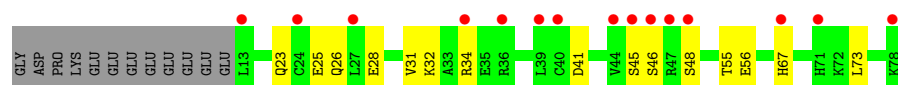
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C



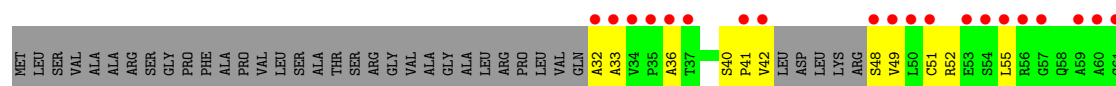
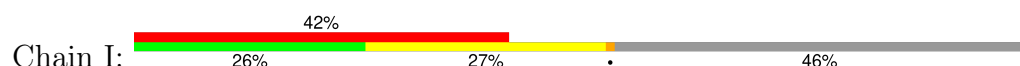
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

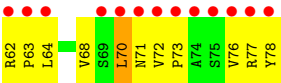


- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

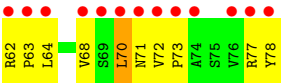
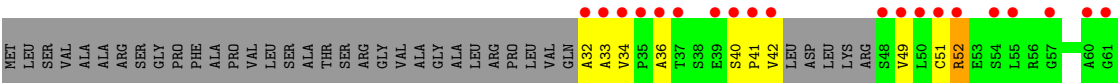
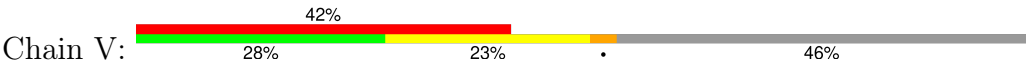


- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

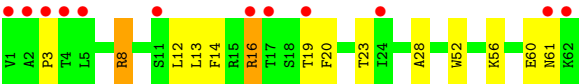
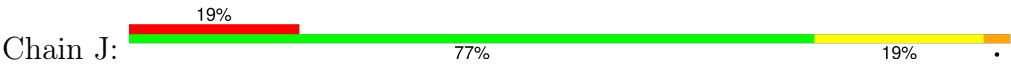




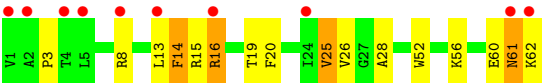
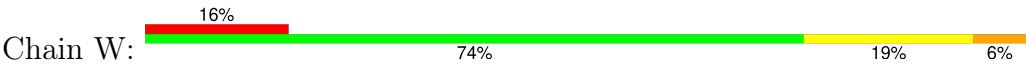
● Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial



● Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein



● Molecule 10: Ubiquinol-cytochrome C reductase complex 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	139.12Å 171.06Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.10 24.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.98-2.10) 97.3 (24.98-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.287 0.242 , 0.263	Depositor DCC
R_{free} test set	15323 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33959	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UQ, PO4, JZR, SMA, FES, AZI, CDL, GOL, HEC, HEM, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/3472	1.03	23/4714 (0.5%)
1	N	0.43	0/3472	1.01	21/4714 (0.4%)
2	B	0.42	0/3235	0.99	20/4387 (0.5%)
2	O	0.42	0/3239	1.01	18/4393 (0.4%)
3	C	0.49	0/2986	1.04	25/4089 (0.6%)
3	P	0.47	0/3024	1.02	24/4137 (0.6%)
4	D	0.45	0/1978	1.02	7/2684 (0.3%)
4	Q	0.44	0/1978	1.04	12/2684 (0.4%)
5	E	0.40	0/1553	1.00	9/2100 (0.4%)
5	R	0.44	0/1553	1.02	12/2100 (0.6%)
6	F	0.40	0/878	0.96	7/1175 (0.6%)
6	S	0.41	0/878	0.98	6/1175 (0.5%)
7	G	0.39	0/642	1.01	7/869 (0.8%)
7	T	0.42	0/647	1.02	7/876 (0.8%)
8	H	0.39	0/544	0.93	2/729 (0.3%)
8	U	0.39	0/544	0.89	2/729 (0.3%)
9	I	0.48	0/285	1.14	3/384 (0.8%)
9	V	0.48	0/285	1.24	4/384 (1.0%)
10	J	0.41	0/520	0.94	0/699
10	W	0.42	0/520	0.94	1/699 (0.1%)
All	All	0.44	0/32233	1.01	210/43721 (0.5%)

There are no bond length outliers.

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	228	GLY	N-CA-C	-14.09	95.71	115.30
4	Q	36	VAL	N-CA-C	10.69	120.75	111.56
1	A	223	TYR	N-CA-C	-9.07	100.53	111.69
5	R	143	GLY	N-CA-C	8.72	127.36	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	40	SER	CA-C-N	8.35	130.28	119.84
9	I	40	SER	C-N-CA	8.35	130.28	119.84
9	V	40	SER	CA-C-N	8.16	130.03	119.84
9	V	40	SER	C-N-CA	8.16	130.03	119.84
5	E	15	ARG	N-CA-C	-8.15	98.84	110.08
5	E	143	GLY	N-CA-C	8.13	126.54	115.32
7	G	49	ALA	N-CA-C	7.93	123.53	112.75
3	C	318	ARG	CA-C-N	7.90	127.46	119.24
3	C	318	ARG	C-N-CA	7.90	127.46	119.24
3	C	19	ILE	N-CA-C	7.72	118.26	110.23
7	T	49	ALA	N-CA-C	7.70	123.22	112.75
9	V	34	VAL	N-CA-C	7.70	115.54	107.76
3	P	318	ARG	CA-C-N	7.65	127.20	119.24
3	P	318	ARG	C-N-CA	7.65	127.20	119.24
1	A	260	PRO	N-CA-C	7.65	123.59	113.57
1	A	286	GLY	N-CA-C	7.55	121.26	112.50
5	R	15	ARG	N-CA-C	-7.48	99.75	110.08
1	A	259	GLY	CA-C-N	7.46	127.10	119.19
1	A	259	GLY	C-N-CA	7.46	127.10	119.19
2	B	305	GLN	N-CA-C	-7.45	101.37	110.31
1	N	223	TYR	N-CA-C	-7.33	102.46	111.40
3	P	223	TYR	N-CA-C	7.26	118.84	111.07
3	P	26	ASN	N-CA-C	7.14	121.31	112.59
5	R	125	GLU	N-CA-C	-7.11	104.64	113.38
5	E	168	SER	N-CA-C	-7.09	104.50	113.72
2	O	249	GLY	N-CA-C	7.08	124.94	115.59
3	P	19	ILE	N-CA-C	7.07	117.58	110.23
1	A	11	VAL	N-CA-C	7.02	115.83	108.95
3	C	26	ASN	N-CA-C	7.01	121.92	112.88
3	C	206	ASN	N-CA-C	-6.99	99.52	110.36
1	N	260	PRO	N-CA-C	6.95	122.67	113.57
3	C	110	LEU	N-CA-C	6.94	119.44	111.11
5	R	168	SER	N-CA-C	-6.93	104.71	113.72
3	C	223	TYR	N-CA-C	6.90	119.39	111.11
1	N	121	SER	N-CA-C	6.89	118.44	111.07
2	B	249	GLY	N-CA-C	6.88	124.16	115.42
1	A	309	THR	N-CA-C	-6.84	100.67	110.59
3	P	110	LEU	N-CA-C	6.84	119.31	111.11
3	P	206	ASN	N-CA-C	-6.82	99.78	110.36
1	A	305	GLN	N-CA-C	-6.77	104.03	112.90
7	T	48	VAL	N-CA-C	6.76	117.38	110.82
3	P	241	LEU	N-CA-C	-6.72	104.04	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	278	VAL	N-CA-C	-6.71	104.23	110.53
1	N	286	GLY	N-CA-C	6.70	120.75	112.64
3	C	109	PHE	N-CA-C	-6.69	96.91	108.56
6	F	25	GLY	N-CA-C	6.68	124.92	115.30
3	P	136	GLY	N-CA-C	-6.68	103.42	112.57
4	D	215	LEU	N-CA-C	6.67	118.55	111.28
7	T	50	PRO	N-CA-C	6.61	118.76	110.70
3	C	57	SER	N-CA-C	6.58	120.92	113.02
2	O	282	GLY	CA-C-N	6.57	126.54	119.78
2	O	282	GLY	C-N-CA	6.57	126.54	119.78
4	Q	24	THR	N-CA-C	-6.54	104.23	111.36
10	W	14	PHE	N-CA-C	6.54	120.47	112.23
3	C	269	LYS	CA-C-N	6.52	126.47	120.21
3	C	269	LYS	C-N-CA	6.52	126.47	120.21
5	E	125	GLU	N-CA-C	-6.46	105.39	113.28
4	D	44	ASP	N-CA-C	6.45	120.25	112.38
2	O	422	LYS	N-CA-C	6.45	120.07	110.52
2	O	101	THR	N-CA-C	-6.45	100.02	109.18
3	P	72	ASP	N-CA-C	6.44	122.22	113.97
7	G	50	PRO	N-CA-C	6.41	118.52	110.70
3	P	204	GLY	N-CA-C	-6.40	101.95	112.83
4	Q	215	LEU	N-CA-C	6.38	118.23	111.28
1	N	309	THR	N-CA-C	-6.38	101.34	110.59
2	B	101	THR	N-CA-C	-6.37	100.14	109.18
5	E	136	ILE	N-CA-C	-6.36	99.13	108.54
1	N	238	GLY	N-CA-C	-6.36	101.05	110.97
1	N	348	SER	N-CA-C	6.34	122.12	112.54
3	P	109	PHE	N-CA-C	-6.34	97.53	108.56
6	S	32	MET	N-CA-C	-6.33	99.89	109.95
4	D	24	THR	N-CA-C	-6.29	104.53	111.82
3	C	72	ASP	N-CA-C	6.25	121.97	113.97
1	N	278	GLY	N-CA-C	6.25	123.65	112.02
1	A	121	SER	N-CA-C	6.22	117.73	111.07
1	N	421	ALA	N-CA-C	-6.22	99.06	109.07
2	B	282	GLY	CA-C-N	6.22	126.19	119.78
2	B	282	GLY	C-N-CA	6.22	126.19	119.78
3	C	136	GLY	N-CA-C	-6.21	103.10	112.41
3	C	241	LEU	N-CA-C	-6.18	104.62	111.36
1	N	305	GLN	N-CA-C	-6.17	104.82	112.90
1	A	249	PRO	N-CA-C	6.17	121.98	113.65
1	A	348	SER	N-CA-C	6.17	121.85	112.54
2	B	204	MET	N-CA-C	6.13	119.54	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	SER	N-CA-C	-6.13	102.62	110.53
5	R	136	ILE	N-CA-C	-6.13	98.85	108.23
1	A	278	GLY	N-CA-C	6.12	123.41	112.02
3	C	275	LEU	N-CA-C	6.12	117.94	111.28
4	Q	44	ASP	N-CA-C	6.09	119.81	112.38
1	N	249	PRO	N-CA-C	6.05	121.50	113.57
2	B	233	SER	N-CA-C	6.05	118.33	110.53
2	B	422	LYS	N-CA-C	5.96	119.23	110.59
4	Q	216	LEU	CA-C-N	-5.95	112.88	119.19
4	Q	216	LEU	C-N-CA	-5.95	112.88	119.19
3	P	271	GLU	N-CA-C	-5.92	102.29	110.35
3	P	57	SER	N-CA-C	5.90	120.10	113.02
4	Q	125	ASP	N-CA-C	-5.90	104.93	111.36
3	C	204	GLY	N-CA-C	-5.90	101.96	112.58
5	E	178	LEU	N-CA-C	5.89	118.65	109.52
1	N	166	SER	N-CA-C	-5.88	102.94	110.53
7	T	53	VAL	N-CA-C	-5.88	104.78	110.72
4	D	36	VAL	N-CA-C	5.86	121.54	109.34
1	A	262	TRP	N-CA-C	5.86	120.97	111.37
6	S	25	GLY	N-CA-C	5.84	123.70	115.30
8	H	52	GLU	N-CA-C	5.82	118.27	110.35
1	N	264	HIS	CA-C-N	5.82	125.68	119.28
1	N	264	HIS	C-N-CA	5.82	125.68	119.28
4	D	37	CYS	N-CA-C	5.80	118.55	111.82
4	D	113	LEU	N-CA-C	5.79	120.47	113.17
1	A	264	HIS	CA-C-N	5.79	125.65	119.28
1	A	264	HIS	C-N-CA	5.79	125.65	119.28
2	O	17	VAL	CA-C-N	5.78	126.33	120.38
2	O	17	VAL	C-N-CA	5.78	126.33	120.38
6	S	14	GLU	N-CA-C	-5.77	104.96	112.23
1	A	189	HIS	N-CA-C	5.75	120.43	113.41
3	P	184	ILE	N-CA-C	5.75	119.14	111.44
3	P	263	ASN	N-CA-C	5.74	118.00	108.13
5	R	178	LEU	N-CA-C	5.73	118.41	109.52
2	O	153	GLN	N-CA-C	-5.72	105.80	112.89
2	B	430	LEU	N-CA-C	5.71	119.33	112.93
3	C	115	ILE	N-CA-C	-5.69	104.98	110.72
3	C	271	GLU	N-CA-C	-5.68	102.62	110.35
8	U	67	HIS	N-CA-C	-5.67	105.09	111.28
7	G	53	VAL	N-CA-C	-5.67	104.99	110.72
3	P	82	MET	N-CA-C	-5.67	105.18	111.36
7	T	23	GLN	N-CA-C	5.67	118.03	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	26	ILE	N-CA-C	-5.67	105.20	110.53
7	T	12	HIS	N-CA-C	5.66	119.49	112.24
1	A	263	ALA	N-CA-C	5.65	119.91	113.19
3	C	145	VAL	N-CA-C	5.63	115.76	110.30
4	D	125	ASP	N-CA-C	-5.62	105.23	111.36
1	A	238	GLY	N-CA-C	-5.61	102.22	110.97
3	C	82	MET	N-CA-C	-5.59	105.27	111.36
2	O	394	PRO	CA-C-N	5.59	125.05	119.24
2	O	394	PRO	C-N-CA	5.59	125.05	119.24
2	B	394	PRO	CA-C-N	5.58	125.04	119.24
2	B	394	PRO	C-N-CA	5.58	125.04	119.24
1	N	259	GLY	CA-C-N	5.57	125.10	119.19
1	N	259	GLY	C-N-CA	5.57	125.10	119.19
1	N	257	VAL	N-CA-C	-5.55	101.41	109.29
3	C	17	ALA	N-CA-C	-5.55	98.99	110.80
5	E	119	ASP	CA-C-N	5.54	126.76	119.84
5	E	119	ASP	C-N-CA	5.54	126.76	119.84
3	C	263	ASN	N-CA-C	5.53	117.64	108.13
1	N	232	SER	N-CA-C	-5.51	102.97	110.36
3	C	362	ILE	N-CA-C	5.50	115.70	110.53
5	R	119	ASP	CA-C-N	5.48	126.33	119.98
5	R	119	ASP	C-N-CA	5.48	126.33	119.98
3	P	269	LYS	CA-C-N	5.47	125.46	120.21
3	P	269	LYS	C-N-CA	5.47	125.46	120.21
3	C	256	TYR	N-CA-C	-5.46	106.20	112.92
7	G	23	GLN	N-CA-C	5.45	117.69	109.41
1	N	189	HIS	N-CA-C	5.43	120.77	114.04
1	A	257	VAL	N-CA-C	-5.43	101.58	109.29
3	P	145	VAL	N-CA-C	5.43	115.56	110.30
9	V	49	VAL	N-CA-C	5.43	116.12	108.36
3	C	92	ILE	N-CA-C	-5.42	105.22	110.42
7	G	48	VAL	N-CA-C	5.40	116.47	111.45
3	P	365	LEU	N-CA-C	5.39	116.84	111.07
6	F	76	PRO	N-CA-C	-5.39	102.73	111.14
1	A	215	HIS	N-CA-C	5.38	120.86	113.97
6	S	91	GLU	CA-C-N	-5.37	113.37	119.28
6	S	91	GLU	C-N-CA	-5.37	113.37	119.28
1	A	421	ALA	N-CA-C	-5.34	100.47	109.07
5	E	66	ALA	N-CA-C	5.33	117.78	111.33
5	R	191	ASP	N-CA-C	-5.33	99.69	108.49
1	N	215	HIS	N-CA-C	5.32	120.78	113.97
6	S	76	PRO	N-CA-C	-5.32	102.84	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	73	LEU	N-CA-C	5.31	120.08	111.37
2	B	278	VAL	N-CA-C	-5.30	105.37	110.72
5	R	122	HIS	N-CA-C	-5.29	102.65	110.48
3	P	256	TYR	N-CA-C	-5.29	106.42	112.92
4	Q	37	CYS	N-CA-C	5.27	118.87	112.23
2	O	330	ALA	N-CA-C	5.26	117.70	111.33
2	B	198	HIS	N-CA-C	5.26	121.09	114.31
2	O	176	LEU	N-CA-C	-5.25	106.82	113.18
7	G	12	HIS	N-CA-C	5.25	118.96	112.24
1	A	232	SER	N-CA-C	-5.22	103.56	110.40
3	P	115	ILE	N-CA-C	-5.22	105.45	110.72
2	B	413	ALA	N-CA-C	-5.19	105.62	111.28
5	R	66	ALA	N-CA-C	5.18	117.59	111.33
7	G	5	GLY	N-CA-C	-5.17	107.86	114.37
2	B	159	VAL	N-CA-C	5.17	115.38	110.42
2	O	430	LEU	N-CA-C	5.15	119.28	113.15
2	B	329	GLN	N-CA-C	-5.15	103.24	110.50
6	F	13	LEU	N-CA-C	-5.15	104.74	111.02
2	B	112	LEU	N-CA-C	-5.15	103.25	110.50
4	Q	137	PRO	CA-C-N	-5.15	115.27	120.21
4	Q	137	PRO	C-N-CA	-5.15	115.27	120.21
2	O	159	VAL	N-CA-C	5.13	115.34	110.42
9	I	49	VAL	N-CA-C	5.12	115.68	108.36
2	B	311	ALA	N-CA-C	-5.11	103.30	110.50
7	T	71	ARG	N-CA-C	5.10	121.67	110.80
2	O	329	GLN	N-CA-C	-5.08	102.75	110.28
2	B	187	THR	N-CA-C	5.08	117.06	110.40
6	F	24	ALA	N-CA-C	-5.07	105.75	111.28
1	N	263	ALA	N-CA-C	5.07	119.22	113.19
2	B	153	GLN	N-CA-C	-5.05	106.63	112.89
8	H	67	HIS	N-CA-C	-5.04	105.78	111.28
3	P	275	LEU	N-CA-C	5.04	116.78	111.28
6	F	32	MET	N-CA-C	-5.03	102.07	110.17
4	Q	38	SER	N-CA-C	5.02	118.51	112.38
5	R	85	LYS	N-CA-C	5.02	117.99	109.76
6	F	91	GLU	CA-C-N	-5.01	113.77	119.28
6	F	91	GLU	C-N-CA	-5.01	113.77	119.28
2	O	311	ALA	N-CA-C	-5.00	103.45	110.50

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	3403	0	3302	69	0
1	N	3403	0	3302	55	0
2	B	3177	0	3152	67	0
2	O	3180	0	3156	58	0
3	C	2892	0	2938	43	0
3	P	2931	0	2989	60	0
4	D	1919	0	1868	32	0
4	Q	1919	0	1868	40	0
5	E	1519	0	1503	31	0
5	R	1519	0	1503	26	0
6	F	861	0	854	14	0
6	S	861	0	854	21	0
7	G	621	0	626	17	0
7	T	626	0	631	24	0
8	H	539	0	524	14	0
8	U	539	0	524	11	0
9	I	285	0	288	38	0
9	V	285	0	288	32	0
10	J	507	0	513	23	0
10	W	507	0	513	27	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	S	18	0	24	8	0
12	A	3	0	0	0	0
12	C	3	0	0	0	0
12	D	3	0	0	0	0
12	P	3	0	0	0	0
13	A	6	0	5	0	0
13	C	54	0	72	3	0
13	D	51	0	82	4	0
13	G	49	0	72	0	0
13	N	5	0	0	0	0
13	P	49	0	72	3	0
13	Q	51	0	82	11	0
13	T	49	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	B	5	0	0	0	0
14	O	5	0	0	0	0
15	B	6	0	8	0	0
15	C	6	0	8	0	0
15	O	6	0	8	0	0
15	P	6	0	8	0	0
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	1	0
17	P	37	0	42	2	0
18	C	14	0	9	3	0
18	P	14	0	9	5	0
19	D	43	0	30	0	0
19	Q	43	0	30	1	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	G	94	0	76	5	0
21	Q	50	0	44	0	0
21	T	49	0	42	0	0
22	A	187	0	0	8	0
22	B	149	0	0	2	0
22	C	125	0	0	4	0
22	D	118	0	0	2	0
22	E	54	0	0	2	0
22	F	57	0	0	3	0
22	G	24	0	0	1	0
22	H	14	0	0	0	0
22	I	16	0	0	1	0
22	J	5	0	0	0	0
22	N	134	0	0	1	0
22	O	130	0	0	1	0
22	P	122	0	0	6	0
22	Q	109	0	0	1	0
22	R	64	0	0	0	0
22	S	73	0	0	2	0
22	T	21	0	0	1	0
22	U	16	0	0	1	0
22	V	10	0	0	1	0
22	W	9	0	0	0	0
All	All	33959	0	32273	622	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 10.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.20	1.12
2:B:12:GLU:HG2	2:B:17:VAL:H	1.15	1.09
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.34	1.08
7:T:45:ILE:HG22	7:T:46:LEU:HD22	1.31	1.04
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.19	1.04
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.37	1.04
2:O:200:THR:HB	2:O:229:GLY:HA2	1.36	1.04
3:P:43:LEU:HD21	13:Q:3006:PEE:H30	1.40	1.01
5:E:166:ASP:HA	22:E:541:HOH:O	1.59	1.01
4:Q:74:PRO:HG3	4:Q:80:MET:HE1	1.40	0.99
4:D:74:PRO:HG3	4:D:80:MET:HE1	1.47	0.96
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.29	0.95
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.00	0.94
1:A:136:GLN:HE21	9:I:51:CYS:HB3	1.34	0.91
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.71	0.91
6:S:13:LEU:HD12	6:S:16:ILE:HD11	1.52	0.91
6:F:104:ARG:HH11	11:F:3011:JZR:H6	1.36	0.91
1:A:293:PRO:O	1:A:297:ILE:HG12	1.71	0.90
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.06	0.90
1:N:136:GLN:HE21	9:V:51:CYS:HB3	1.37	0.89
9:V:64:LEU:HD12	9:V:77:ARG:O	1.73	0.88
9:I:32:ALA:N	9:I:72:VAL:HG23	1.88	0.88
2:O:229:GLY:C	2:O:231:GLY:H	1.76	0.88
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.56	0.87
1:A:1:THR:HG21	2:B:212:SER:HB3	1.55	0.86
9:V:52:ARG:HH11	9:V:52:ARG:HB3	1.40	0.86
2:B:12:GLU:HG2	2:B:17:VAL:N	1.90	0.85
2:O:236:LYS:H	2:O:236:LYS:HD2	1.42	0.84
2:O:95:LYS:CB	9:V:32:ALA:HB2	2.06	0.84
1:N:293:PRO:O	1:N:297:ILE:HG12	1.78	0.83
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.57	0.83
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.59	0.83
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.61	0.83
3:P:12:LYS:HE2	3:P:16:ASN:H	1.42	0.82
9:V:52:ARG:HB3	9:V:52:ARG:NH1	1.94	0.82
10:J:16:ARG:HB2	10:J:19:THR:HG22	1.58	0.82
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.81
1:N:29:GLN:HB3	2:O:12:GLU:O	1.80	0.80
4:D:212:MET:HE2	13:D:2006:PEE:H54	1.63	0.80
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.62	0.80
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.17	0.80
2:O:200:THR:CB	2:O:229:GLY:HA2	2.11	0.79
1:A:1:THR:HG21	2:B:212:SER:CB	2.13	0.78
10:J:16:ARG:NH1	10:J:19:THR:HG21	1.99	0.78
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.18	0.78
9:I:32:ALA:N	9:I:71:ASN:HB3	1.99	0.77
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.65	0.77
10:W:13:LEU:O	10:W:19:THR:HG23	1.84	0.76
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.65	0.76
10:W:3:PRO:HB2	10:W:8:ARG:NH1	2.01	0.76
3:P:43:LEU:HD21	13:Q:3006:PEE:C19	2.17	0.75
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.22	0.74
9:I:32:ALA:N	9:I:71:ASN:CB	2.51	0.74
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.69	0.74
10:W:16:ARG:HH11	10:W:19:THR:HG21	1.54	0.73
3:P:78:ILE:CD1	4:Q:204:MET:HE1	2.18	0.73
1:A:3:THR:OG1	1:A:6:GLN:HG3	1.88	0.73
8:U:28:GLU:O	8:U:31:VAL:HG22	1.89	0.73
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.69	0.72
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.71	0.72
8:H:43:ARG:O	8:H:47:ARG:HD2	1.89	0.72
6:F:13:LEU:O	6:F:16:ILE:HG12	1.89	0.72
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.70	0.72
10:J:16:ARG:HB2	10:J:16:ARG:HH11	1.55	0.72
3:C:129:MET:CE	3:C:181:PHE:HD2	2.02	0.71
2:O:229:GLY:C	2:O:231:GLY:N	2.47	0.71
5:E:113:GLU:HB3	5:E:116:GLN:HE21	1.55	0.71
5:E:113:GLU:HB3	5:E:116:GLN:NE2	2.05	0.71
10:J:13:LEU:O	10:J:19:THR:HG23	1.90	0.71
4:Q:35:GLN:HG3	22:Q:3086:HOH:O	1.91	0.71
4:Q:212:MET:HE2	13:Q:3006:PEE:H54	1.74	0.70
4:Q:74:PRO:CG	4:Q:80:MET:HE1	2.20	0.69
8:H:28:GLU:O	8:H:31:VAL:HG22	1.92	0.69
1:A:352:SER:HB3	6:S:110:LYS:CD	2.23	0.69
2:B:231:GLY:N	2:B:233:SER:H	1.90	0.69
3:P:68:HIS:HD2	22:P:3131:HOH:O	1.75	0.69
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.69
4:Q:75:ASN:HD21	4:Q:79:GLU:HG2	1.58	0.69
1:A:136:GLN:HE21	9:I:51:CYS:CB	2.04	0.68
3:P:78:ILE:HD12	4:Q:204:MET:HE1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:4185:HOH:O	9:I:73:PRO:HG3	1.94	0.68
1:N:29:GLN:HG3	1:N:203:LEU:O	1.94	0.68
2:B:353:SER:HB3	2:B:355:PRO:HD2	1.76	0.68
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.23	0.68
5:R:79:SER:HB3	5:R:191:ASP:OD1	1.93	0.68
3:C:78:ILE:CD1	4:D:204:MET:HE1	2.23	0.68
2:B:95:LYS:HD3	2:B:110:GLU:OE2	1.94	0.68
7:T:71:ARG:HH11	7:T:72:LYS:HZ2	1.40	0.67
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.76	0.67
4:D:204:MET:HE3	13:D:2006:PEE:C10	2.24	0.67
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.76	0.67
6:S:100:GLU:HB3	11:S:2011:JZR:H6A	1.76	0.67
10:W:16:ARG:NH1	10:W:19:THR:HG21	2.10	0.67
1:N:32:GLN:OE1	2:O:373:GLU:HB2	1.94	0.67
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.76	0.67
1:A:2:ALA:O	2:B:113:ARG:NE	2.28	0.66
3:C:191:ALA:HA	3:C:194:MET:HE2	1.78	0.66
10:W:8:ARG:HG2	10:W:8:ARG:HH11	1.60	0.65
2:O:227:ARG:C	2:O:229:GLY:N	2.50	0.65
5:R:190:ASP:HB2	5:R:192:MET:HG2	1.79	0.65
7:G:60:THR:O	7:G:64:GLN:HG3	1.95	0.65
10:J:16:ARG:HB2	10:J:19:THR:CG2	2.26	0.65
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.78	0.65
4:Q:110:PRO:HG3	19:Q:501:HEC:HMD2	1.79	0.65
4:Q:204:MET:HE3	13:Q:3006:PEE:C10	2.27	0.65
6:S:13:LEU:HA	6:S:16:ILE:HG12	1.78	0.65
3:P:96:MET:CE	13:P:3007:PEE:H27	2.27	0.64
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.79	0.64
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.78	0.64
1:N:136:GLN:NE2	9:V:51:CYS:HB3	2.11	0.64
2:B:231:GLY:N	2:B:232:LEU:N	2.46	0.64
3:P:96:MET:HE1	13:P:3007:PEE:H27	1.80	0.64
7:T:60:THR:O	7:T:64:GLN:HG3	1.98	0.64
10:J:16:ARG:HH11	10:J:16:ARG:CB	2.10	0.64
4:Q:74:PRO:HG3	4:Q:80:MET:CE	2.22	0.64
8:H:25:GLU:HG2	8:H:34:ARG:HH22	1.62	0.64
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.12	0.63
2:O:236:LYS:H	2:O:236:LYS:CD	2.07	0.63
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.26	0.63
2:O:227:ARG:C	2:O:229:GLY:H	2.02	0.63
3:C:50:PHE:HA	3:C:53:MET:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:28:LYS:HE3	22:F:4052:HOH:O	1.98	0.63
4:Q:75:ASN:ND2	4:Q:79:GLU:HG2	2.13	0.63
4:D:74:PRO:HG3	4:D:80:MET:CE	2.27	0.63
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.80	0.62
5:E:113:GLU:CB	5:E:116:GLN:HE21	2.12	0.62
4:D:74:PRO:CG	4:D:80:MET:HE1	2.26	0.62
10:J:14:PHE:HA	10:J:20:PHE:HD2	1.64	0.62
3:P:191:ALA:HA	3:P:194:MET:HE2	1.80	0.62
10:J:16:ARG:HH11	10:J:16:ARG:CG	2.12	0.62
9:V:32:ALA:N	9:V:71:ASN:CB	2.63	0.62
2:B:397:THR:O	2:B:401:GLN:HG3	2.00	0.62
2:O:296:TYR:OH	9:V:52:ARG:NE	2.33	0.62
3:C:29:SER:HB2	21:G:2004:CDL:HA31	1.82	0.62
2:B:412:ASN:HA	2:B:415:LYS:HD2	1.80	0.61
10:J:3:PRO:HD2	10:J:8:ARG:CZ	2.30	0.61
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.83	0.61
2:O:397:THR:O	2:O:401:GLN:HG3	2.01	0.61
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.15	0.61
1:A:29:GLN:HG3	1:A:203:LEU:O	2.00	0.61
9:V:32:ALA:N	9:V:71:ASN:HB2	2.15	0.61
2:O:35:ILE:N	2:O:35:ILE:HD12	2.16	0.60
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.01	0.60
2:O:203:ARG:HH12	2:O:233:SER:HA	1.65	0.60
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.84	0.60
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.31	0.60
1:N:308:GLN:HG2	22:N:3026:HOH:O	2.01	0.60
3:P:14:VAL:O	3:P:18:PHE:HB3	2.01	0.60
7:T:71:ARG:HH11	7:T:72:LYS:NZ	1.99	0.60
1:N:86:LEU:HD13	1:N:99:ILE:HG12	1.82	0.60
5:E:85:LYS:NZ	5:E:87:MET:SD	2.75	0.60
1:N:216:PHE:HD2	1:N:219:LEU:HD22	1.67	0.59
3:P:129:MET:CE	3:P:181:PHE:HD2	2.08	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.33	0.59
2:B:412:ASN:HD22	2:B:415:LYS:HD2	1.67	0.59
3:P:43:LEU:HD21	13:Q:3006:PEE:C20	2.33	0.59
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.84	0.59
1:A:296:SER:O	1:A:300:THR:HG23	2.02	0.59
7:G:40:ARG:HB3	21:G:2004:CDL:HB32	1.85	0.59
7:G:45:ILE:HG22	7:G:46:LEU:HD12	1.85	0.59
10:J:3:PRO:HD2	10:J:8:ARG:NH2	2.18	0.59
2:B:354:ASN:N	2:B:355:PRO:CD	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.84	0.59
7:T:66:PHE:CZ	7:T:70:LYS:HD2	2.38	0.58
3:C:96:MET:CE	13:C:2007:PEE:H27	2.34	0.58
2:B:189:VAL:HG23	22:B:3089:HOH:O	2.03	0.58
5:E:77:LYS:HE3	5:E:79:SER:OG	2.03	0.58
10:W:56:LYS:HG2	10:W:60:GLU:CD	2.28	0.58
2:B:309:VAL:HG23	2:B:326:THR:HG22	1.85	0.58
1:N:8:LEU:HD22	1:N:392:LEU:HB3	1.84	0.58
3:P:100:ARG:HD2	3:P:100:ARG:C	2.28	0.58
1:A:289:HIS:HE1	11:S:2011:JZR:H1'A	1.69	0.58
2:B:20:HIS:HB2	2:B:22:GLN:HG3	1.84	0.58
10:J:12:LEU:O	10:J:13:LEU:HD23	2.04	0.58
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.58
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.86	0.58
1:N:30:SER:HA	2:O:18:PRO:HG3	1.85	0.58
1:N:286:GLY:HA3	1:N:290:LEU:HD21	1.85	0.58
2:B:139:ALA:HB3	11:S:2011:JZR:H5'	1.86	0.57
10:W:8:ARG:HH11	10:W:8:ARG:CG	2.18	0.57
1:A:136:GLN:NE2	9:I:51:CYS:CB	2.67	0.57
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.84	0.57
6:F:82:LYS:HE3	22:F:4032:HOH:O	2.04	0.57
1:N:373:THR:HB	1:N:374:PRO:HD3	1.86	0.57
9:V:62:ARG:O	9:V:78:TYR:HB3	2.05	0.57
2:O:47:ILE:CG2	2:O:120:MET:HE1	2.25	0.57
10:J:3:PRO:HB2	10:J:8:ARG:HD3	1.86	0.56
1:A:51:LYS:NZ	1:A:51:LYS:H	2.03	0.56
10:W:25:VAL:HG12	10:W:26:VAL:N	2.20	0.56
2:B:95:LYS:CG	9:I:32:ALA:HB2	2.35	0.56
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.36	0.56
3:C:78:ILE:HD12	4:D:204:MET:HE1	1.86	0.56
9:I:32:ALA:N	9:I:71:ASN:HB2	2.19	0.56
8:H:25:GLU:CG	8:H:34:ARG:HH22	2.19	0.56
3:P:50:PHE:HA	3:P:53:MET:HE3	1.88	0.56
5:E:190:ASP:O	5:E:192:MET:HG2	2.05	0.56
7:T:30:PHE:O	7:T:34:ILE:HG12	2.06	0.56
8:U:25:GLU:HG2	8:U:34:ARG:HH22	1.71	0.56
1:A:227:ALA:O	1:A:228:VAL:C	2.49	0.56
3:P:319:PRO:HD2	22:P:3113:HOH:O	2.05	0.55
7:G:63:THR:O	7:G:67:GLU:HG2	2.06	0.55
4:Q:231:LYS:HD3	6:S:70:MET:HE3	1.87	0.55
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:PHE:O	7:G:34:ILE:HG12	2.06	0.55
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.89	0.55
5:E:189:SER:C	5:E:190:ASP:OD1	2.49	0.55
11:F:3011:JZR:H6A	2:O:83:PHE:HB2	1.89	0.55
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.28	0.55
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
4:Q:241:LYS:OXT	4:Q:241:LYS:HD3	2.06	0.55
9:I:62:ARG:O	9:I:78:TYR:HB3	2.07	0.55
2:B:12:GLU:CG	2:B:17:VAL:H	2.04	0.55
1:N:136:GLN:HE21	9:V:51:CYS:CB	2.15	0.55
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.37	0.55
3:C:96:MET:HE2	3:C:96:MET:HA	1.89	0.55
1:N:364:ALA:HB2	9:V:33:ALA:HB1	1.89	0.55
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.41	0.54
3:C:341:GLN:NE2	22:C:2099:HOH:O	2.39	0.54
5:R:77:LYS:HE3	5:R:79:SER:OG	2.07	0.54
6:F:63:LYS:HE2	22:G:1280:HOH:O	2.06	0.54
7:T:63:THR:O	7:T:67:GLU:HG2	2.07	0.54
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.89	0.54
3:P:12:LYS:HA	3:P:12:LYS:CE	2.37	0.54
1:A:216:PHE:HD2	1:A:219:LEU:HD22	1.71	0.54
6:S:78:GLU:CD	6:S:78:GLU:H	2.16	0.54
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.06	0.54
7:T:45:ILE:HG22	7:T:46:LEU:CD2	2.22	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.07	0.54
2:B:12:GLU:O	2:B:18:PRO:HD3	2.08	0.54
2:O:411:ILE:O	2:O:415:LYS:HG3	2.08	0.54
5:R:191:ASP:OD2	5:R:191:ASP:N	2.40	0.54
1:A:41:ILE:HG12	1:A:195:MET:HG2	1.89	0.53
3:C:15:ASN:O	3:C:16:ASN:C	2.50	0.53
1:A:51:LYS:HB2	1:A:51:LYS:HZ2	1.72	0.53
2:B:306:PRO:HA	9:I:52:ARG:HE	1.74	0.53
3:P:43:LEU:HD21	13:Q:3006:PEE:H31	1.89	0.53
4:Q:59:ASP:OD2	10:W:62:LYS:CB	2.52	0.53
5:R:188:THR:HG21	5:R:194:ILE:CD1	2.37	0.53
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.74	0.53
2:B:294:SER:OG	2:B:343:GLN:NE2	2.42	0.53
4:D:166:ASN:HB3	8:H:13:LEU:HD23	1.91	0.53
2:O:229:GLY:O	2:O:230:LEU:HB2	2.07	0.53
3:P:220:PHE:HE1	18:P:3002:UQ:CM2	2.22	0.53
10:W:56:LYS:O	10:W:60:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:71:ARG:HD3	7:T:72:LYS:HZ3	1.74	0.53
9:V:32:ALA:N	9:V:71:ASN:HB3	2.24	0.53
2:B:353:SER:CB	2:B:355:PRO:HD2	2.38	0.52
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.31	0.52
5:E:90:LYS:CE	5:E:93:GLY:HA2	2.40	0.52
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.91	0.52
9:I:72:VAL:HG13	9:I:73:PRO:HD2	1.92	0.52
2:O:95:LYS:HG3	9:V:32:ALA:N	2.24	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.40	0.52
10:W:61:ASN:C	10:W:62:LYS:HG3	2.35	0.52
6:F:78:GLU:H	6:F:78:GLU:CD	2.16	0.52
8:H:41:ASP:O	8:H:45:SER:HB2	2.09	0.52
2:B:314:ALA:HA	9:I:63:PRO:HD3	1.90	0.52
4:D:234:LYS:HD3	5:E:8:PRO:HB2	1.91	0.52
10:J:13:LEU:HB3	10:J:23:THR:OG1	2.10	0.52
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.09	0.52
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.91	0.52
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.92	0.52
2:O:189:VAL:HG23	22:O:3052:HOH:O	2.10	0.52
1:A:289:HIS:HE1	11:S:2011:JZR:C1'	2.23	0.52
1:N:30:SER:CA	2:O:18:PRO:HG3	2.39	0.52
3:C:100:ARG:HD2	3:C:100:ARG:C	2.35	0.52
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.44	0.52
3:P:14:VAL:C	3:P:15:ASN:CA	2.83	0.52
4:D:34:LYS:HE3	22:D:4097:HOH:O	2.09	0.52
9:V:72:VAL:HG13	9:V:73:PRO:HD2	1.91	0.52
1:A:51:LYS:H	1:A:51:LYS:HZ2	1.56	0.52
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.91	0.52
5:E:102:THR:O	5:E:106:ILE:HG13	2.09	0.52
3:P:12:LYS:CE	3:P:15:ASN:HB3	2.39	0.52
3:P:220:PHE:HE1	18:P:3002:UQ:HM22	1.74	0.52
3:P:162:GLU:OE2	3:P:168:PHE:HD1	1.93	0.51
6:S:88:SER:OG	6:S:91:GLU:HB2	2.09	0.51
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.44	0.51
6:S:71:ARG:O	6:S:73:GLN:HG3	2.10	0.51
3:P:12:LYS:HE3	3:P:12:LYS:CA	2.36	0.51
10:W:52:TRP:O	10:W:56:LYS:HB2	2.11	0.51
1:N:206:ARG:HG3	1:N:206:ARG:HH11	1.75	0.51
5:R:77:LYS:HD3	5:R:80:ASP:OD2	2.10	0.51
2:B:33:LEU:CD2	2:B:220:ALA:HB1	2.41	0.51
16:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.46	0.51
1:N:39:VAL:HG11	1:N:195:MET:HE3	1.92	0.51
2:O:294:SER:OG	2:O:343:GLN:NE2	2.44	0.51
2:O:309:VAL:HG23	2:O:326:THR:HG22	1.93	0.51
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.59	0.51
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.76	0.51
7:G:40:ARG:CB	21:G:2004:CDL:HB32	2.41	0.51
1:N:68:LYS:HE3	1:N:68:LYS:HA	1.93	0.51
3:P:96:MET:HE2	3:P:96:MET:HA	1.93	0.51
6:S:12:TRP:O	6:S:16:ILE:N	2.36	0.51
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.33	0.51
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.75	0.51
8:U:25:GLU:CG	8:U:34:ARG:HH22	2.24	0.51
3:C:369:ALA:O	3:C:373:GLU:HG3	2.11	0.50
1:N:213:GLN:O	1:N:217:SER:OG	2.25	0.50
5:R:188:THR:HG21	5:R:194:ILE:HD12	1.91	0.50
1:A:308:GLN:HG2	22:A:4140:HOH:O	2.10	0.50
7:T:71:ARG:HB2	7:T:72:LYS:HD3	1.93	0.50
3:C:68:HIS:HD2	22:C:2126:HOH:O	1.95	0.50
1:N:136:GLN:NE2	9:V:51:CYS:CB	2.72	0.50
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.42	0.50
2:B:35:ILE:N	2:B:35:ILE:HD12	2.27	0.50
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.75	0.50
3:P:245:PHE:CG	4:Q:17:LEU:HD13	2.47	0.50
5:R:129:LYS:HG3	5:R:187:PHE:CE1	2.47	0.50
6:F:88:SER:OG	6:F:91:GLU:HB2	2.12	0.50
11:F:3011:JZR:H4	1:N:289:HIS:CE1	2.47	0.50
1:A:373:THR:HB	1:A:374:PRO:HD3	1.92	0.50
2:O:229:GLY:O	2:O:231:GLY:N	2.44	0.50
3:P:15:ASN:O	3:P:17:ALA:N	2.44	0.50
4:Q:124:GLU:OE2	4:Q:191:ARG:CD	2.60	0.50
1:A:90:SER:HB3	22:A:4116:HOH:O	2.11	0.50
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.42	0.50
2:O:200:THR:O	2:O:204:MET:HG3	2.12	0.50
5:R:80:ASP:O	5:R:82:PRO:HD3	2.12	0.50
1:A:289:HIS:CE1	11:S:2011:JZR:H1'A	2.47	0.50
7:G:66:PHE:CZ	7:G:70:LYS:HD2	2.47	0.50
1:N:125:SER:O	1:N:129:LYS:HG3	2.11	0.50
1:A:125:SER:O	1:A:129:LYS:HG3	2.12	0.49
2:B:47:ILE:CG2	2:B:120:MET:HE1	2.23	0.49
2:O:354:ASN:N	2:O:355:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:ILE:O	3:P:177:ARG:HD2	2.12	0.49
13:Q:3006:PEE:H56	5:R:50:ALA:CB	2.42	0.49
9:V:32:ALA:HA	9:V:71:ASN:HD22	1.77	0.49
3:C:96:MET:HE1	13:C:2007:PEE:H27	1.93	0.49
10:W:3:PRO:HB2	10:W:8:ARG:HH11	1.74	0.49
5:E:82:PRO:O	5:E:100:HIS:HB3	2.12	0.49
1:A:364:ALA:HB2	9:I:33:ALA:HB1	1.95	0.49
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.94	0.49
1:N:405:ARG:O	1:N:409:GLU:HG3	2.13	0.49
1:A:172:GLU:HG3	1:A:176:LYS:HE3	1.95	0.49
8:H:28:GLU:O	8:H:32:LYS:HG2	2.13	0.49
1:N:227:ALA:O	1:N:228:VAL:HB	2.13	0.49
1:N:264:HIS:ND1	1:N:265:PRO:HD2	2.28	0.49
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.48	0.49
3:P:191:ALA:HA	3:P:194:MET:CE	2.43	0.48
6:S:100:GLU:OE1	11:S:2011:JZR:H4	2.13	0.48
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.94	0.48
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.95	0.48
3:C:251:GLY:HA3	22:C:2091:HOH:O	2.13	0.48
3:C:371:THR:O	3:C:375:LYS:HG2	2.13	0.48
10:J:16:ARG:NH1	10:J:16:ARG:CG	2.75	0.48
5:R:79:SER:CB	5:R:191:ASP:OD1	2.61	0.48
6:S:13:LEU:HB3	22:S:2070:HOH:O	2.13	0.48
1:A:143:THR:OG1	9:I:48:SER:HB3	2.13	0.48
3:C:97:HIS:CD2	16:C:502:HEM:NC	2.81	0.48
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.39	0.48
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.48	0.48
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.29	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.49	0.48
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.96	0.48
3:C:379:TRP:CE3	6:F:33:ARG:HD3	2.47	0.48
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.42	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.49	0.48
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.14	0.48
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.49	0.48
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.49	0.48
4:Q:3:LEU:HD12	8:U:55:THR:HG22	1.96	0.48
5:E:155:GLY:N	22:E:541:HOH:O	2.46	0.47
2:O:354:ASN:HB3	2:O:355:PRO:HD3	1.96	0.47
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:ALA:HA	3:C:194:MET:CE	2.43	0.47
10:J:16:ARG:CB	10:J:19:THR:HG22	2.38	0.47
10:J:16:ARG:O	10:J:19:THR:HG22	2.14	0.47
10:W:8:ARG:NH1	10:W:8:ARG:CG	2.75	0.47
1:A:213:GLN:HG2	22:A:4055:HOH:O	2.15	0.47
2:B:212:SER:OG	2:B:215:VAL:HG23	2.15	0.47
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.44	0.47
7:G:32:LYS:C	7:G:35:PRO:HD2	2.39	0.47
3:P:14:VAL:O	3:P:15:ASN:O	2.32	0.47
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.14	0.47
4:D:239:PRO:HG2	4:D:241:LYS:HZ3	1.79	0.47
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.47
1:N:296:SER:O	1:N:300:THR:HG23	2.14	0.47
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.96	0.47
2:O:361:LYS:HE2	2:O:402:ILE:O	2.14	0.47
1:A:167:VAL:HG13	22:A:4111:HOH:O	2.15	0.47
2:B:246:GLU:O	2:B:427:SER:HA	2.15	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.14	0.47
3:P:193:ALA:O	3:P:196:HIS:HB3	2.15	0.47
2:B:396:SER:HB3	22:B:3031:HOH:O	2.14	0.47
3:C:96:MET:HE2	13:C:2007:PEE:H27	1.96	0.47
1:N:111:GLU:HG3	1:N:215:HIS:CE1	2.50	0.47
7:T:46:LEU:HD23	22:T:3018:HOH:O	2.13	0.47
8:U:28:GLU:O	8:U:32:LYS:HG2	2.15	0.47
1:A:394:GLU:HA	11:A:4002:JZR:H2	1.96	0.47
3:C:162:GLU:OE2	3:C:168:PHE:HD1	1.98	0.47
2:O:17:VAL:HG13	2:O:18:PRO:HD2	1.96	0.47
4:Q:234:LYS:HD3	5:R:8:PRO:HB2	1.95	0.47
2:B:95:LYS:HE3	9:I:72:VAL:HG21	1.97	0.47
2:B:257:LEU:O	2:B:323:GLY:HA3	2.15	0.47
5:E:79:SER:HB3	5:E:191:ASP:OD2	2.15	0.47
1:N:172:GLU:HG3	1:N:176:LYS:HE3	1.96	0.47
3:P:97:HIS:CD2	16:P:502:HEM:NC	2.83	0.47
7:T:46:LEU:HD22	7:T:46:LEU:N	2.30	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.95	0.47
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.97	0.47
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.63	0.46
3:P:361:LEU:O	3:P:366:MET:HG3	2.15	0.46
16:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.15	0.46
7:T:32:LYS:C	7:T:35:PRO:HD2	2.40	0.46
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.15	0.46
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.45	0.46
3:P:375:LYS:HD2	3:P:375:LYS:N	2.29	0.46
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.81	0.46
2:B:46:ARG:HD2	2:B:375:SER:OG	2.14	0.46
3:C:245:PHE:CG	4:D:17:LEU:HD13	2.50	0.46
3:P:92:ILE:O	3:P:96:MET:HG2	2.16	0.46
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.95	0.46
8:H:31:VAL:HG23	8:H:32:LYS:N	2.30	0.46
10:J:16:ARG:HH12	10:J:19:THR:HG21	1.76	0.46
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.46
1:N:47:TYR:HB3	1:N:189:HIS:CE1	2.51	0.46
1:N:281:ASP:C	1:N:281:ASP:OD1	2.58	0.46
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.45	0.46
22:P:3113:HOH:O	6:S:20:TYR:HE1	1.99	0.46
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.74	0.46
22:A:4072:HOH:O	6:S:110:LYS:HD2	2.15	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
3:C:233:LEU:HD11	4:D:219:VAL:HG21	1.98	0.46
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.96	0.46
5:E:85:LYS:HZ3	5:E:87:MET:HA	1.80	0.46
13:Q:3006:PEE:H56	5:R:50:ALA:HB1	1.98	0.46
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.46	0.46
1:A:29:GLN:HB3	2:B:12:GLU:O	2.16	0.46
9:I:70:LEU:HB3	22:I:1016:HOH:O	2.16	0.46
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.16	0.46
1:A:15:GLN:O	1:A:26:ALA:HA	2.16	0.46
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.51	0.46
9:I:36:ALA:CB	9:I:73:PRO:HB2	2.46	0.46
2:O:34:VAL:C	2:O:35:ILE:HD12	2.41	0.46
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.45	0.45
3:C:193:ALA:O	3:C:196:HIS:HB3	2.16	0.45
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.98	0.45
8:U:31:VAL:HG23	8:U:32:LYS:N	2.30	0.45
9:V:36:ALA:CB	9:V:73:PRO:HB2	2.46	0.45
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.82	0.45
7:G:40:ARG:NH2	21:G:2004:CDL:HB31	2.32	0.45
3:P:43:LEU:CD2	13:Q:3006:PEE:H30	2.29	0.45
8:U:41:ASP:O	8:U:45:SER:HB2	2.15	0.45
2:O:71:LEU:CD2	9:V:68:VAL:HG21	2.43	0.45
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:62:ARG:HB3	9:V:63:PRO:HD2	1.99	0.45
10:W:16:ARG:O	10:W:19:THR:HG22	2.17	0.45
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.51	0.45
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.52	0.45
1:A:85:HIS:O	1:A:99:ILE:HA	2.16	0.45
1:A:213:GLN:O	1:A:217:SER:OG	2.30	0.45
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.99	0.45
10:J:16:ARG:NH1	10:J:16:ARG:HG3	2.32	0.45
7:T:71:ARG:NH1	7:T:72:LYS:HZ2	2.12	0.45
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.46	0.45
3:C:92:ILE:O	3:C:96:MET:HG2	2.17	0.44
1:N:19:LEU:HD22	1:N:213:GLN:HG3	1.99	0.44
3:P:12:LYS:HE2	3:P:16:ASN:HB2	1.99	0.44
3:P:13:ILE:HG22	3:P:13:ILE:O	2.17	0.44
3:P:213:SER:OG	3:P:217:LYS:NZ	2.42	0.44
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.80	0.44
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.98	0.44
2:B:28:ARG:HH21	2:B:390:GLY:HA3	1.81	0.44
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.99	0.44
7:G:38:LEU:HB3	7:G:42:ARG:NH1	2.32	0.44
8:H:51:GLU:HG3	8:H:52:GLU:N	2.32	0.44
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.47	0.44
8:H:31:VAL:O	8:H:35:GLU:HG3	2.17	0.44
9:I:76:VAL:HG13	9:I:76:VAL:O	2.16	0.44
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	2.18	0.44
4:Q:144:ARG:HG3	4:Q:147:LEU:HD12	1.98	0.44
7:T:71:ARG:NH1	7:T:72:LYS:HD2	2.31	0.44
3:P:96:MET:HE2	13:P:3007:PEE:H27	1.98	0.44
6:S:110:LYS:O	6:S:110:LYS:HG3	2.17	0.44
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.98	0.44
3:P:270:PRO:HG2	3:P:278:TYR:CG	2.53	0.44
7:G:40:ARG:CZ	21:G:2004:CDL:HB31	2.47	0.44
5:R:75:GLU:HG2	5:R:194:ILE:HG12	2.00	0.44
1:A:39:VAL:HG11	1:A:195:MET:HE3	1.98	0.44
2:B:230:LEU:HB3	2:B:233:SER:OG	2.18	0.44
3:C:197:LEU:HD21	16:C:502:HEM:HMA1	2.00	0.44
18:P:3002:UQ:HM31	22:P:3116:HOH:O	2.17	0.44
6:S:58:ARG:HD3	22:S:2031:HOH:O	2.18	0.44
1:N:307:PHE:CD1	1:N:307:PHE:C	2.95	0.43
16:C:501:HEM:HMC1	16:C:501:HEM:HBC2	2.00	0.43
4:Q:42:SER:HB3	4:Q:94:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:117:LEU:HD13	5:R:170:ARG:HD2	2.00	0.43
6:S:49:ARG:HH22	11:S:2011:JZR:H4	1.83	0.43
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.45	0.43
2:B:361:LYS:HE2	2:B:402:ILE:O	2.18	0.43
2:O:314:ALA:HA	9:V:63:PRO:HD3	2.00	0.43
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.53	0.43
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.33	0.43
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.54	0.43
8:H:19:THR:O	8:H:23:GLN:HG3	2.19	0.43
1:N:288:ALA:HB2	1:N:300:THR:HG22	2.01	0.43
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.17	0.43
1:A:27:SER:HA	1:A:199:ALA:O	2.18	0.43
1:N:15:GLN:O	1:N:26:ALA:HA	2.18	0.43
3:P:369:ALA:O	3:P:373:GLU:HG3	2.19	0.43
1:A:307:PHE:CD1	1:A:307:PHE:C	2.96	0.43
3:C:68:HIS:HE1	22:C:2049:HOH:O	2.01	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
2:B:136:GLU:HG2	11:S:2011:JZR:H2'	2.00	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
22:D:4077:HOH:O	6:F:71:ARG:HD3	2.18	0.43
5:E:112:VAL:HG22	5:E:172:ARG:NH2	2.34	0.43
5:E:188:THR:C	5:E:189:SER:O	2.60	0.43
2:O:228:GLY:O	2:O:231:GLY:HA2	2.18	0.43
1:A:79:VAL:HA	1:A:82:MET:HE3	2.01	0.43
16:C:501:HEM:O2D	16:C:501:HEM:O2A	2.37	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43
9:I:36:ALA:HB2	9:I:73:PRO:CD	2.40	0.43
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.62	0.43
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.72	0.43
1:A:383:LEU:O	1:A:387:GLY:HA2	2.18	0.43
9:I:64:LEU:CD1	9:I:78:TYR:C	2.92	0.43
1:N:224:ASP:OD1	1:N:227:ALA:HB2	2.18	0.43
2:O:345:LYS:O	2:O:349:GLN:HG3	2.19	0.43
4:D:43:MET:HE1	4:D:189:PHE:CE2	2.54	0.43
5:E:75:GLU:HG2	5:E:194:ILE:HG12	2.00	0.43
1:N:416:TYR:HB3	10:W:15:ARG:NH2	2.33	0.43
1:A:381:ARG:HG2	22:A:4120:HOH:O	2.19	0.42
2:B:181:TYR:CE1	2:B:182:ARG:HG2	2.54	0.42
7:G:48:VAL:O	7:G:51:PRO:HD2	2.19	0.42
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.19	0.42
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:LYS:HA	3:C:270:PRO:HD3	1.81	0.42
9:I:77:ARG:O	9:I:78:TYR:HB2	2.19	0.42
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.54	0.42
1:A:240:GLN:NE2	22:A:4184:HOH:O	2.51	0.42
3:P:67:THR:HB	4:Q:115:TYR:OH	2.20	0.42
3:P:68:HIS:HE1	22:P:3053:HOH:O	2.03	0.42
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.84	0.42
4:D:204:MET:HE3	13:D:2006:PEE:O4	2.19	0.42
5:E:189:SER:O	5:E:190:ASP:C	2.63	0.42
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.35	0.42
8:U:23:GLN:O	8:U:26:GLN:HG2	2.20	0.42
1:A:78:GLU:OE2	1:A:108:LYS:HD2	2.20	0.42
1:A:158:PHE:O	1:A:164:ALA:HB2	2.20	0.42
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.54	0.42
1:N:286:GLY:HA3	1:N:290:LEU:CD2	2.47	0.42
3:C:111:GLU:H	3:C:111:GLU:CD	2.28	0.42
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.01	0.42
1:A:267:ASN:O	1:A:271:GLN:HG2	2.20	0.42
3:P:320:LEU:HG	22:P:3113:HOH:O	2.19	0.42
7:T:71:ARG:HB2	7:T:72:LYS:H	1.66	0.42
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.85	0.42
3:P:46:LEU:HD11	13:Q:3006:PEE:H81	2.01	0.42
4:Q:75:ASN:HD21	4:Q:79:GLU:CG	2.30	0.42
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.42
1:N:267:ASN:O	1:N:271:GLN:HG2	2.19	0.42
2:O:17:VAL:HA	2:O:18:PRO:HD3	1.85	0.42
2:O:257:LEU:O	2:O:323:GLY:HA3	2.19	0.42
2:O:307:PHE:CD1	2:O:307:PHE:C	2.98	0.42
3:C:240:MET:HE2	13:D:2006:PEE:H17	2.02	0.41
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.49	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.56	0.41
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
2:O:203:ARG:HH12	2:O:233:SER:CA	2.32	0.41
2:O:212:SER:OG	2:O:215:VAL:HG23	2.20	0.41
2:B:307:PHE:CD1	2:B:307:PHE:C	2.96	0.41
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.03	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.41
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.68	0.41
2:O:102:ARG:HH22	2:O:161:GLU:CD	2.27	0.41
2:O:246:GLU:O	2:O:427:SER:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:O	2:B:47:ILE:HD13	2.21	0.41
9:I:36:ALA:HB3	9:I:73:PRO:HB2	2.02	0.41
1:N:302:LYS:HA	1:N:302:LYS:HD3	1.93	0.41
2:B:412:ASN:HA	2:B:412:ASN:HD22	1.67	0.41
8:H:31:VAL:CG2	8:H:32:LYS:N	2.83	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
1:A:7:ALA:O	1:A:10:SER:OG	2.38	0.41
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.28	0.41
5:E:84:GLY:N	5:E:100:HIS:O	2.54	0.41
5:E:160:CYS:HB3	17:P:3001:SMA:H4	2.03	0.41
4:Q:204:MET:HE3	13:Q:3006:PEE:O4	2.19	0.41
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.03	0.41
1:A:264:HIS:ND1	1:A:265:PRO:HD2	2.36	0.41
2:B:249:GLY:O	2:B:250:ASP:C	2.64	0.41
6:F:63:LYS:HG3	22:F:4045:HOH:O	2.20	0.41
8:H:51:GLU:HG3	8:H:52:GLU:H	1.86	0.41
4:Q:124:GLU:OE2	4:Q:191:ARG:HD3	2.21	0.41
6:S:12:TRP:O	6:S:15:GLY:N	2.53	0.41
10:W:16:ARG:NH1	10:W:16:ARG:HG3	2.36	0.41
6:F:101:ARG:O	6:F:105:GLU:HG3	2.21	0.41
8:H:23:GLN:O	8:H:26:GLN:HG2	2.20	0.41
1:N:85:HIS:O	1:N:99:ILE:HA	2.20	0.41
9:V:64:LEU:CD1	9:V:78:TYR:C	2.93	0.41
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.44	0.41
10:J:14:PHE:N	10:J:14:PHE:CD1	2.87	0.41
2:O:47:ILE:HG13	2:O:120:MET:CE	2.51	0.41
1:A:288:ALA:HB2	1:A:300:THR:HG22	2.02	0.41
1:A:405:ARG:O	1:A:409:GLU:HG3	2.20	0.41
9:I:62:ARG:HB3	9:I:63:PRO:HD2	2.02	0.41
3:P:162:GLU:OE2	3:P:168:PHE:CD1	2.73	0.41
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.41	0.40
5:E:80:ASP:O	5:E:82:PRO:HD3	2.21	0.40
1:N:19:LEU:CD2	1:N:213:GLN:HG3	2.51	0.40
1:A:281:ASP:OD1	1:A:281:ASP:C	2.63	0.40
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.76	0.40
3:P:223:TYR:HB3	4:Q:227:TRP:CZ2	2.56	0.40
4:Q:214:LEU:HA	13:T:3005:PEE:H58	2.03	0.40
9:V:62:ARG:HB2	9:V:78:TYR:CG	2.56	0.40
2:B:47:ILE:HG13	2:B:120:MET:CE	2.52	0.40
4:D:223:LYS:C	4:D:223:LYS:HD3	2.47	0.40
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:113:GLU:OE2	5:R:115:SER:OG	2.33	0.40
9:V:70:LEU:HB3	22:V:1017:HOH:O	2.22	0.40
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.75	0.40
3:C:21:LEU:HD21	18:C:2002:UQ:CM3	2.52	0.40
1:N:225:GLU:C	1:N:227:ALA:H	2.30	0.40
16:P:501:HEM:HMC1	16:P:501:HEM:HBC2	2.02	0.40
8:U:23:GLN:CD	22:U:1583:HOH:O	2.64	0.40
10:W:14:PHE:CD1	10:W:14:PHE:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	24	22
1	N	441/446 (99%)	425 (96%)	15 (3%)	1 (0%)	43	44
2	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	43	44
2	O	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	24	22
3	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	16	12
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	9	5
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	183 (94%)	7 (4%)	4 (2%)	5	2
5	R	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	24	22
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
7	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	9	5
8	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
8	U	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	7	4
9	I	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	4	1
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	4	1
10	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	3
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
All	All	3980/4220 (94%)	3851 (97%)	104 (3%)	25 (1%)	21	18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	16	ASN
3	C	17	ALA
9	I	41	PRO
10	J	61	ASN
1	N	224	ASP
3	P	17	ALA
7	T	72	LYS
9	V	41	PRO
10	W	61	ASN
2	B	171	ALA
5	E	112	VAL
2	O	171	ALA
2	O	231	GLY
3	P	16	ASN
8	U	48	SER
5	R	189	SER
1	A	228	VAL
3	C	18	PHE
5	E	189	SER
5	E	191	ASP
3	P	11	MET
3	P	18	PHE
5	E	82	PRO
3	P	13	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/370 (98%)	358 (98%)	6 (2%)	55	64
1	N	364/370 (98%)	359 (99%)	5 (1%)	59	67
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	332/343 (97%)	330 (99%)	2 (1%)	78	86
3	C	312/327 (95%)	311 (100%)	1 (0%)	86	91
3	P	316/327 (97%)	313 (99%)	3 (1%)	70	78
4	D	206/206 (100%)	202 (98%)	4 (2%)	50	58
4	Q	206/206 (100%)	202 (98%)	4 (2%)	50	58
5	E	168/168 (100%)	166 (99%)	2 (1%)	63	72
5	R	168/168 (100%)	164 (98%)	4 (2%)	43	49
6	F	90/98 (92%)	87 (97%)	3 (3%)	33	37
6	S	90/98 (92%)	87 (97%)	3 (3%)	33	37
7	G	66/71 (93%)	65 (98%)	1 (2%)	57	65
7	T	66/71 (93%)	64 (97%)	2 (3%)	36	41
8	H	63/74 (85%)	61 (97%)	2 (3%)	34	38
8	U	63/74 (85%)	62 (98%)	1 (2%)	55	64
9	I	28/60 (47%)	26 (93%)	2 (7%)	13	11
9	V	28/60 (47%)	25 (89%)	3 (11%)	6	4
10	J	51/52 (98%)	49 (96%)	2 (4%)	28	31
10	W	51/52 (98%)	49 (96%)	2 (4%)	28	31
All	All	3364/3538 (95%)	3312 (98%)	52 (2%)	57	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	149	VAL
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	245	GLU
1	A	281	ASP
1	A	308	GLN
3	C	222	PRO
4	D	17	LEU
4	D	43	MET
4	D	76	GLU
4	D	144	ARG
5	E	17	GLU
5	E	80	ASP
6	F	33	ARG
6	F	78	GLU
6	F	95	LYS
7	G	45	ILE
8	H	47	ARG
8	H	51	GLU
9	I	42	VAL
9	I	70	LEU
10	J	8	ARG
10	J	16	ARG
1	N	149	VAL
1	N	203	LEU
1	N	245	GLU
1	N	281	ASP
1	N	308	GLN
2	O	35	ILE
2	O	236	LYS
3	P	12	LYS
3	P	43	LEU
3	P	222	PRO
4	Q	17	LEU
4	Q	35	GLN
4	Q	43	MET
4	Q	144	ARG
5	R	17	GLU
5	R	113	GLU
5	R	128	LYS
5	R	190	ASP
6	S	33	ARG
6	S	78	GLU
6	S	95	LYS
7	T	45	ILE

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Mol	Chain	Res	Type
7	T	73	ASN
8	U	46	SER
9	V	42	VAL
9	V	52	ARG
9	V	70	LEU
10	W	16	ARG
10	W	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	61	HIS
1	A	136	GLN
1	A	165	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
1	A	308	GLN
2	B	22	GLN
2	B	343	GLN
2	B	401	GLN
2	B	412	ASN
2	B	429	ASN
3	C	15	ASN
3	C	68	HIS
3	C	159	ASN
3	C	312	GLN
4	D	106	ASN
4	D	121	HIS
4	D	156	GLN
5	E	116	GLN
7	G	73	ASN
10	J	37	GLN
1	N	53	ASN
1	N	61	HIS
1	N	136	GLN
1	N	139	GLN
1	N	165	GLN
1	N	213	GLN
1	N	271	GLN
2	O	22	GLN

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Mol	Chain	Res	Type
2	O	305	GLN
2	O	343	GLN
2	O	401	GLN
2	O	412	ASN
3	P	68	HIS
3	P	159	ASN
4	Q	106	ASN
4	Q	121	HIS
4	Q	225	HIS
5	R	149	ASN
6	S	73	GLN
7	T	28	HIS
8	U	23	GLN
9	V	71	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 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
15	GOL	P	3009	-	5,5,5	1.40	1 (20%)	5,5,5	0.62	0
11	JZR	S	2011	-	18,18,18	1.84	3 (16%)	23,23,23	0.78	0
16	HEM	P	501	3	50,50,50	1.65	6 (12%)	67,82,82	1.21	7 (10%)
12	AZI	P	3014	-	2,2,2	5.19	2 (100%)	0,1,1	-	-
13	PEE	G	2005	-	48,48,50	1.37	7 (14%)	51,53,55	0.76	2 (3%)
12	AZI	C	2014	-	2,2,2	4.50	2 (100%)	0,1,1	-	-
11	JZR	C	2008	-	18,18,18	1.82	6 (33%)	23,23,23	0.70	0
20	FES	E	501	5	0,4,4	-	-	-	-	-
21	CDL	G	2004	-	43,43,99	1.14	2 (4%)	49,55,111	1.23	4 (8%)
15	GOL	C	2009	-	5,5,5	1.37	1 (20%)	5,5,5	0.65	0
19	HEC	D	501	4	50,50,50	1.03	2 (4%)	68,82,82	1.27	6 (8%)
13	PEE	D	2006	-	50,50,50	1.37	6 (12%)	53,55,55	0.79	2 (3%)
15	GOL	O	3013	-	5,5,5	1.33	0	5,5,5	0.71	0
16	HEM	C	502	3	50,50,50	1.62	8 (16%)	67,82,82	1.67	13 (19%)
21	CDL	G	2003	-	49,49,99	1.10	2 (4%)	55,61,111	1.11	4 (7%)
16	HEM	C	501	3	50,50,50	1.77	8 (16%)	67,82,82	1.70	18 (26%)
13	PEE	C	2012	-	4,4,50	3.35	4 (100%)	6,6,55	0.61	0
17	SMA	C	2001	-	38,38,38	1.43	7 (18%)	47,52,52	1.08	3 (6%)
12	AZI	A	4005	-	2,2,2	3.93	2 (100%)	0,1,1	-	-
13	PEE	T	3005	-	48,48,50	1.41	7 (14%)	51,53,55	0.75	3 (5%)
14	PO4	O	2010	-	4,4,4	1.38	0	6,6,6	5.99	5 (83%)
17	SMA	P	3001	-	38,38,38	1.59	10 (26%)	47,52,52	1.12	4 (8%)
20	FES	R	501	5	0,4,4	-	-	-	-	-
14	PO4	B	3010	-	4,4,4	1.37	1 (25%)	6,6,6	6.01	5 (83%)
13	PEE	N	3012	-	4,4,50	3.16	4 (100%)	6,6,55	0.62	0
21	CDL	T	3004	-	48,48,99	1.15	4 (8%)	54,60,111	1.13	2 (3%)
13	PEE	P	3007	-	48,48,50	1.36	5 (10%)	51,53,55	0.73	2 (3%)
11	JZR	P	3008	-	18,18,18	1.83	6 (33%)	23,23,23	0.69	0
11	JZR	F	4001	-	18,18,18	1.80	5 (27%)	23,23,23	0.67	0
13	PEE	A	4003	-	5,5,50	1.35	0	5,5,55	0.65	0
13	PEE	Q	3006	-	50,50,50	1.35	5 (10%)	53,55,55	0.78	2 (3%)
12	AZI	D	4004	-	2,2,2	3.85	2 (100%)	0,1,1	-	-
11	JZR	A	4002	-	18,18,18	1.91	5 (27%)	23,23,23	0.77	1 (4%)
13	PEE	C	2007	-	48,48,50	1.31	5 (10%)	51,53,55	0.75	2 (3%)
16	HEM	P	502	3	50,50,50	1.83	12 (24%)	67,82,82	1.38	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	UQ	P	3002	-	14,14,63	2.11	8 (57%)	20,20,79	0.42	0
11	JZR	F	3011	-	18,18,18	1.91	4 (22%)	23,23,23	0.73	0
19	HEC	Q	501	4	50,50,50	1.11	3 (6%)	68,82,82	1.26	6 (8%)
21	CDL	Q	3003	-	49,49,99	1.10	3 (6%)	55,61,111	1.17	4 (7%)
15	GOL	B	2013	-	5,5,5	1.34	0	5,5,5	0.65	0
18	UQ	C	2002	-	14,14,63	2.31	8 (57%)	20,20,79	0.54	0

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
15	GOL	P	3009	-	-	2/4/4/4	-
11	JZR	S	2011	-	-	6/9/29/29	0/1/1/1
16	HEM	P	501	3	-	4/14/54/54	-
13	PEE	G	2005	-	-	25/52/52/54	-
11	JZR	C	2008	-	-	4/9/29/29	0/1/1/1
20	FES	E	501	5	-	-	0/1/1/1
21	CDL	G	2004	-	-	35/52/52/110	-
15	GOL	C	2009	-	-	0/4/4/4	-
19	HEC	D	501	4	1/1/3/7	7/14/54/54	-
13	PEE	D	2006	-	-	17/54/54/54	-
15	GOL	O	3013	-	-	2/4/4/4	-
16	HEM	C	502	3	-	4/14/54/54	-
21	CDL	G	2003	-	-	26/58/58/110	-
16	HEM	C	501	3	-	4/14/54/54	-
17	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
13	PEE	T	3005	-	-	26/52/52/54	-
17	SMA	P	3001	-	-	2/34/34/34	0/2/2/2
20	FES	R	501	5	-	-	0/1/1/1
21	CDL	T	3004	-	-	21/57/57/110	-
13	PEE	P	3007	-	-	16/52/52/54	-
11	JZR	P	3008	-	-	3/9/29/29	0/1/1/1
11	JZR	F	4001	-	-	5/9/29/29	0/1/1/1
13	PEE	A	4003	-	-	4/4/4/54	-
13	PEE	Q	3006	-	-	17/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	JZR	A	4002	-	-	5/9/29/29	0/1/1/1
13	PEE	C	2007	-	-	16/52/52/54	-
16	HEM	P	502	3	-	4/14/54/54	-
18	UQ	P	3002	-	-	2/4/28/87	0/1/1/1
11	JZR	F	3011	-	-	4/9/29/29	0/1/1/1
19	HEC	Q	501	4	1/1/3/7	8/14/54/54	-
21	CDL	Q	3003	-	-	37/58/58/110	-
15	GOL	B	2013	-	-	4/4/4/4	-
18	UQ	C	2002	-	-	0/4/28/87	0/1/1/1

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	502	HEM	CBB-CAB	5.53	1.57	1.30
12	P	3014	AZI	N1-N2	-5.51	1.11	1.23
16	P	501	HEM	CBB-CAB	5.46	1.56	1.30
11	F	3011	JZR	O1-C1	5.15	1.48	1.40
11	S	2011	JZR	O1-C1	5.04	1.48	1.40
12	C	2014	AZI	N1-N2	-5.03	1.12	1.23
11	A	4002	JZR	O1-C1	5.03	1.48	1.40
16	C	501	HEM	CBB-CAB	5.01	1.54	1.30
16	C	501	HEM	CBC-CAC	4.92	1.54	1.30
16	C	502	HEM	CBB-CAB	4.88	1.53	1.30
12	P	3014	AZI	N3-N2	-4.84	1.13	1.23
16	C	502	HEM	CBC-CAC	4.79	1.53	1.30
11	P	3008	JZR	O1-C1	4.74	1.48	1.40
11	C	2008	JZR	O1-C1	4.71	1.48	1.40
11	F	4001	JZR	O1-C1	4.66	1.48	1.40
13	C	2012	PEE	P-O1P	4.62	1.61	1.50
16	P	502	HEM	CBC-CAC	4.59	1.52	1.30
16	P	501	HEM	CBC-CAC	4.50	1.52	1.30
13	N	3012	PEE	P-O1P	4.30	1.60	1.50
12	A	4005	AZI	N1-N2	-4.26	1.14	1.23
13	P	3007	PEE	C39-C38	4.23	1.55	1.31
13	C	2007	PEE	C39-C38	4.20	1.55	1.31
13	Q	3006	PEE	C39-C38	4.18	1.55	1.31
13	D	2006	PEE	C39-C38	4.17	1.55	1.31
16	P	501	HEM	CAB-C3B	-4.15	1.36	1.47
16	C	501	HEM	CAC-C3C	-4.15	1.36	1.47
13	T	3005	PEE	C39-C38	4.15	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	4004	AZI	N1-N2	-4.10	1.14	1.23
13	G	2005	PEE	C39-C38	4.01	1.54	1.31
12	C	2014	AZI	N3-N2	-3.90	1.15	1.23
17	P	3001	SMA	C6-C5	3.77	1.45	1.38
16	P	501	HEM	CAC-C3C	-3.76	1.37	1.47
16	C	502	HEM	CAC-C3C	-3.75	1.37	1.47
19	Q	501	HEC	C4B-C3B	3.72	1.51	1.45
16	P	502	HEM	CAB-C3B	-3.68	1.37	1.47
16	P	502	HEM	CAC-C3C	-3.68	1.37	1.47
11	S	2011	JZR	O5-C1	3.64	1.51	1.41
12	D	4004	AZI	N3-N2	-3.59	1.15	1.23
12	A	4005	AZI	N3-N2	-3.57	1.15	1.23
13	G	2005	PEE	C21-C22	-3.50	1.34	1.51
13	T	3005	PEE	C21-C22	-3.49	1.34	1.51
13	Q	3006	PEE	C21-C22	-3.48	1.34	1.51
16	C	501	HEM	CAB-C3B	-3.48	1.38	1.47
11	F	3011	JZR	O5-C1	3.47	1.50	1.41
13	D	2006	PEE	C21-C22	-3.40	1.34	1.51
16	C	501	HEM	C4D-C3D	3.39	1.50	1.45
13	P	3007	PEE	C21-C22	-3.39	1.34	1.51
17	P	3001	SMA	C6-C7	3.36	1.44	1.38
13	D	2006	PEE	O3-C30	3.36	1.43	1.33
13	P	3007	PEE	P-O1P	3.31	1.62	1.50
13	C	2007	PEE	C21-C22	-3.31	1.35	1.51
18	C	2002	UQ	O3-C3	3.30	1.44	1.36
11	A	4002	JZR	O5-C1	3.29	1.50	1.41
17	C	2001	SMA	C4A-C5	3.27	1.46	1.40
13	P	3007	PEE	O3-C30	3.20	1.42	1.33
17	C	2001	SMA	C6-C7	3.19	1.44	1.38
11	F	4001	JZR	O5-C1	3.18	1.50	1.41
13	Q	3006	PEE	P-O1P	3.16	1.61	1.50
13	D	2006	PEE	P-O1P	3.15	1.61	1.50
13	T	3005	PEE	P-O1P	3.14	1.61	1.50
11	C	2008	JZR	O5-C1	3.14	1.49	1.41
11	P	3008	JZR	O5-C1	3.14	1.49	1.41
13	C	2012	PEE	P-O4P	3.13	1.63	1.54
18	P	3002	UQ	C7-C6	3.12	1.57	1.50
17	P	3001	SMA	O1-C2	3.11	1.40	1.36
17	C	2001	SMA	C6-C5	3.11	1.44	1.38
18	C	2002	UQ	C7-C6	3.11	1.57	1.50
13	C	2007	PEE	O3-C30	3.08	1.42	1.33
13	G	2005	PEE	P-O1P	3.05	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	3001	SMA	C20-C19	3.05	1.35	1.33
18	C	2002	UQ	C3-C4	3.05	1.57	1.48
18	C	2002	UQ	C2-C1	3.03	1.57	1.48
13	Q	3006	PEE	O3-C30	3.03	1.42	1.33
13	N	3012	PEE	P-O4P	2.99	1.63	1.54
18	C	2002	UQ	O2-C2	2.98	1.44	1.36
13	C	2007	PEE	P-O1P	2.97	1.61	1.50
17	P	3001	SMA	C4A-C5	2.95	1.45	1.40
16	P	502	HEM	CMC-C2C	2.94	1.56	1.50
18	C	2002	UQ	CM5-C5	2.93	1.56	1.50
13	C	2012	PEE	P-O3P	2.93	1.63	1.54
13	T	3005	PEE	O3-C30	2.93	1.41	1.33
18	P	3002	UQ	CM5-C5	2.88	1.56	1.50
13	N	3012	PEE	P-O3P	2.87	1.63	1.54
16	C	502	HEM	FE-NB	2.84	2.03	1.94
13	G	2005	PEE	O2-C10	2.82	1.42	1.34
13	D	2006	PEE	O2-C10	2.80	1.42	1.34
13	Q	3006	PEE	O2-C10	2.79	1.42	1.34
13	T	3005	PEE	O2-C10	2.78	1.42	1.34
17	C	2001	SMA	C7-C8	2.77	1.44	1.40
13	G	2005	PEE	O3-C30	2.74	1.41	1.33
13	P	3007	PEE	O2-C10	2.72	1.42	1.34
16	P	501	HEM	C4D-C3D	2.71	1.49	1.45
13	C	2007	PEE	O2-C10	2.70	1.41	1.34
21	G	2004	CDL	O1-C1	2.67	1.51	1.43
18	P	3002	UQ	O2-C2	2.64	1.43	1.36
11	P	3008	JZR	C4-C5	2.63	1.58	1.53
18	P	3002	UQ	O3-C3	2.62	1.43	1.36
18	P	3002	UQ	C2-C1	2.62	1.56	1.48
18	P	3002	UQ	C6-C1	2.59	1.56	1.47
17	P	3001	SMA	C7-C8	2.58	1.44	1.40
11	A	4002	JZR	C4-C5	2.55	1.58	1.53
16	C	502	HEM	C3B-C4B	2.53	1.49	1.44
21	T	3004	CDL	O1-C1	2.52	1.50	1.43
17	P	3001	SMA	C3-C2	2.51	1.39	1.34
17	C	2001	SMA	C20-C19	2.50	1.35	1.33
11	C	2008	JZR	C4-C5	2.50	1.58	1.53
11	S	2011	JZR	O5-C5	2.49	1.50	1.44
21	T	3004	CDL	OB8-CB6	-2.48	1.39	1.45
18	C	2002	UQ	C6-C1	2.47	1.55	1.47
16	P	502	HEM	C4A-C3A	2.46	1.48	1.43
16	P	502	HEM	C1B-C2B	2.45	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	501	HEM	C1A-C2A	2.45	1.49	1.44
18	P	3002	UQ	C5-C4	2.43	1.55	1.47
16	C	501	HEM	C4C-NC	-2.43	1.35	1.39
16	P	502	HEM	C3C-C2C	2.41	1.42	1.37
21	T	3004	CDL	OA8-CA6	-2.40	1.39	1.45
18	C	2002	UQ	C5-C4	2.40	1.55	1.47
16	P	501	HEM	C4A-C3A	2.39	1.48	1.43
16	C	502	HEM	C1D-C2D	2.39	1.49	1.44
18	P	3002	UQ	C3-C4	2.38	1.55	1.48
11	F	4001	JZR	C4-C5	2.38	1.58	1.53
21	Q	3003	CDL	O1-C1	2.38	1.50	1.43
16	P	502	HEM	CHC-C1C	-2.35	1.33	1.38
11	A	4002	JZR	O5-C5	2.34	1.50	1.44
17	C	2001	SMA	C3-C2	2.34	1.39	1.34
11	F	3011	JZR	C4-C5	2.32	1.58	1.53
16	C	502	HEM	C4D-C3D	2.32	1.49	1.45
16	P	502	HEM	C1A-C2A	2.31	1.49	1.44
21	G	2003	CDL	O1-C1	2.30	1.50	1.43
11	F	3011	JZR	O5-C5	2.29	1.50	1.44
13	C	2012	PEE	P-O2P	2.26	1.61	1.54
21	T	3004	CDL	CB3-CB4	2.25	1.57	1.50
16	P	502	HEM	FE-NC	2.24	2.02	1.95
16	P	502	HEM	C1D-C2D	2.21	1.49	1.44
19	D	501	HEC	C4C-C3C	2.20	1.49	1.44
17	P	3001	SMA	C8-C8A	2.15	1.43	1.39
19	Q	501	HEC	C1C-C2C	2.13	1.48	1.43
21	Q	3003	CDL	OA8-CA6	-2.11	1.40	1.45
17	P	3001	SMA	C4A-C4	2.11	1.52	1.46
17	C	2001	SMA	O1-C2	2.11	1.39	1.36
11	C	2008	JZR	O5-C5	2.11	1.49	1.44
13	D	2006	PEE	C31-C30	2.11	1.56	1.50
16	C	501	HEM	C1C-C2C	2.10	1.49	1.45
19	Q	501	HEC	C1C-NC	-2.10	1.35	1.39
21	G	2004	CDL	OA8-CA6	-2.09	1.40	1.45
11	P	3008	JZR	O5-C5	2.09	1.49	1.44
21	Q	3003	CDL	OB8-CB6	-2.09	1.40	1.45
11	F	4001	JZR	O5-C5	2.09	1.49	1.44
19	D	501	HEC	C1A-C2A	2.08	1.48	1.45
13	N	3012	PEE	P-O2P	2.07	1.60	1.54
11	F	4001	JZR	C1-C2	2.07	1.58	1.52
13	T	3005	PEE	C31-C30	2.05	1.56	1.50
15	P	3009	GOL	O2-C2	2.04	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	2003	CDL	OB8-CB6	-2.04	1.40	1.45
15	C	2009	GOL	O2-C2	2.04	1.49	1.43
11	P	3008	JZR	C1-C2	2.04	1.58	1.52
14	B	3010	PO4	P-O1	2.04	1.55	1.50
13	G	2005	PEE	C3-C2	2.04	1.57	1.50
11	C	2008	JZR	C1-C2	2.04	1.58	1.52
11	A	4002	JZR	C1-C2	2.02	1.58	1.52
17	P	3001	SMA	C4A-C8A	2.02	1.45	1.40
16	C	502	HEM	FE-ND	2.02	2.01	1.94
11	C	2008	JZR	C4-C3	2.02	1.57	1.52
13	T	3005	PEE	C3-C2	2.01	1.57	1.50
11	P	3008	JZR	C4-C3	2.00	1.57	1.52
13	G	2005	PEE	C1-C2	2.00	1.57	1.50

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	3010	PO4	O4-P-O1	-8.40	81.24	110.95
14	O	2010	PO4	O4-P-O1	-8.34	81.46	110.95
14	O	2010	PO4	O4-P-O2	-7.98	83.09	107.91
14	B	3010	PO4	O4-P-O2	-7.89	83.37	107.91
14	O	2010	PO4	O4-P-O3	-7.29	85.24	107.91
14	B	3010	PO4	O4-P-O3	-7.27	85.29	107.91
16	C	502	HEM	C3B-C4B-NB	6.76	114.33	109.47
14	B	3010	PO4	O2-P-O1	4.89	128.24	110.95
16	C	501	HEM	C3B-C4B-NB	4.67	112.82	109.47
14	O	2010	PO4	O2-P-O1	4.66	127.43	110.95
17	P	3001	SMA	C9-C10-C11	-4.56	105.94	114.46
21	G	2004	CDL	CB4-OB6-CB5	-4.54	109.83	117.85
16	C	501	HEM	C2D-C1D-ND	4.42	115.01	109.90
16	C	502	HEM	C4B-C3B-C2B	-4.24	103.38	107.28
17	C	2001	SMA	C9-C10-C11	-4.13	106.74	114.46
19	D	501	HEC	CAB-C3B-C4B	-4.08	119.48	124.79
21	Q	3003	CDL	CA4-OA6-CA5	-3.97	110.83	117.85
21	T	3004	CDL	CB4-OB6-CB5	-3.97	110.84	117.85
16	C	502	HEM	CHD-C1D-ND	-3.91	120.21	124.42
16	P	502	HEM	CHC-C1C-NC	-3.90	120.21	124.45
19	Q	501	HEC	CAC-C3C-C2C	3.84	132.97	126.89
21	G	2003	CDL	CA4-OA6-CA5	-3.72	111.28	117.85
16	C	502	HEM	CHC-C4B-NB	-3.65	120.50	124.42
19	D	501	HEC	CAC-C3C-C2C	3.63	132.63	126.89
16	C	501	HEM	CHD-C1D-ND	-3.62	120.53	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	501	HEM	CHC-C1C-NC	-3.49	120.66	124.45
19	Q	501	HEC	CHC-C4B-NB	-3.45	120.09	124.37
16	C	501	HEM	C4A-C3A-C2A	-3.39	102.93	106.82
21	T	3004	CDL	CA4-OA6-CA5	-3.08	110.42	117.80
16	P	502	HEM	C2A-C1A-NA	3.05	113.54	110.15
16	C	502	HEM	C1B-NB-C4B	-3.03	101.62	105.21
16	P	502	HEM	CHD-C4C-NC	-3.01	121.17	124.45
16	C	501	HEM	CMA-C3A-C4A	3.01	130.01	125.42
16	C	502	HEM	CBD-CAD-C3D	-2.99	104.27	112.53
21	Q	3003	CDL	CB6-CB4-CB3	-2.97	104.86	111.78
16	C	501	HEM	C1D-C2D-C3D	-2.90	103.93	106.98
16	C	501	HEM	CHD-C4C-C3C	-2.88	120.36	125.21
16	C	501	HEM	C4D-ND-C1D	-2.84	101.84	105.21
17	P	3001	SMA	C4A-C4-C3	-2.82	114.62	118.78
21	G	2003	CDL	CB4-OB6-CB5	-2.77	111.16	117.80
13	D	2006	PEE	C22-C21-C20	2.76	127.13	113.86
21	G	2004	CDL	CA6-CA4-CA3	-2.75	105.37	111.78
13	P	3007	PEE	C22-C21-C20	2.73	126.99	113.86
13	C	2007	PEE	C22-C21-C20	2.72	126.95	113.86
14	O	2010	PO4	O3-P-O2	2.72	116.38	107.91
13	G	2005	PEE	C22-C21-C20	2.69	126.78	113.86
13	T	3005	PEE	C22-C21-C20	2.69	126.77	113.86
16	C	501	HEM	C4B-C3B-C2B	-2.67	104.83	107.28
21	Q	3003	CDL	CB4-OB6-CB5	-2.67	111.41	117.80
14	B	3010	PO4	O3-P-O2	2.65	116.17	107.91
16	C	502	HEM	C2D-C1D-ND	2.65	112.96	109.90
17	C	2001	SMA	C4A-C4-C3	-2.65	114.88	118.78
13	Q	3006	PEE	C22-C21-C20	2.60	126.36	113.86
16	P	502	HEM	CMA-C3A-C4A	-2.59	121.48	125.42
16	C	502	HEM	CHB-C1B-NB	-2.54	121.22	124.37
17	P	3001	SMA	O1-C2-C3	2.54	124.05	121.81
19	D	501	HEC	CAC-C3C-C4C	-2.52	121.44	124.91
16	P	502	HEM	CMD-C2D-C1D	2.51	128.96	125.03
16	C	502	HEM	C2B-C1B-NB	2.48	112.69	109.84
13	C	2007	PEE	C21-C22-C23	2.47	126.88	114.37
13	P	3007	PEE	C21-C22-C23	2.46	126.80	114.37
16	C	502	HEM	C4D-ND-C1D	-2.42	102.34	105.21
16	C	501	HEM	C3C-C2C-C1C	-2.40	104.77	107.05
21	G	2003	CDL	CB6-CB4-CB3	-2.38	106.23	111.78
19	Q	501	HEC	CAB-C3B-C2B	2.34	131.85	127.56
13	G	2005	PEE	C21-C22-C23	2.33	126.14	114.37
16	P	502	HEM	CMA-C3A-C2A	2.33	130.56	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	501	HEC	CAC-C3C-C4C	-2.32	121.72	124.91
13	T	3005	PEE	C21-C22-C23	2.30	126.00	114.37
16	C	501	HEM	CHA-C4D-ND	-2.25	121.58	124.37
16	P	502	HEM	C4A-NA-C1A	-2.25	102.16	105.82
21	G	2004	CDL	CA4-OA6-CA5	-2.25	112.42	117.80
11	A	4002	JZR	C1'-O1-C1	2.24	117.51	113.68
16	P	501	HEM	CAD-C3D-C4D	2.23	128.59	124.70
13	D	2006	PEE	C21-C22-C23	2.23	125.63	114.37
21	Q	3003	CDL	CA6-OA8-CA7	-2.23	111.59	117.08
13	Q	3006	PEE	C21-C22-C23	2.22	125.58	114.37
16	C	501	HEM	C1A-C2A-C3A	2.21	110.29	106.87
16	C	501	HEM	C3A-C4A-NA	2.21	113.68	110.14
16	C	501	HEM	C3B-C2B-C1B	2.21	108.07	106.41
16	C	502	HEM	CHA-C4D-ND	-2.19	121.66	124.37
16	P	501	HEM	CHD-C4C-NC	-2.18	122.08	124.45
19	D	501	HEC	CAB-C3B-C2B	2.18	131.56	127.56
16	C	501	HEM	CMC-C2C-C1C	2.17	128.55	124.73
16	P	501	HEM	CMD-C2D-C1D	2.16	128.41	125.03
19	D	501	HEC	C3A-C4A-NA	2.16	113.63	109.64
19	Q	501	HEC	CHC-C4B-C3B	2.15	129.19	125.23
16	C	502	HEM	CHB-C4A-C3A	-2.15	121.19	127.43
16	P	501	HEM	C4C-NC-C1C	-2.14	102.33	105.82
21	G	2003	CDL	CA6-OA8-CA7	-2.12	111.85	117.08
13	T	3005	PEE	O3-C3-C2	2.11	114.49	108.40
16	P	501	HEM	CAC-C3C-C4C	-2.11	119.78	124.82
19	D	501	HEC	C2B-C1B-NB	2.11	112.34	109.90
21	G	2004	CDL	CB6-CB4-CB3	-2.11	106.88	111.78
16	C	502	HEM	CMA-C3A-C2A	2.11	130.09	125.62
17	C	2001	SMA	O1-C2-C3	2.10	123.66	121.81
16	C	501	HEM	CHC-C4B-NB	-2.08	122.19	124.42
16	P	502	HEM	CAD-C3D-C4D	2.07	128.30	124.70
16	C	501	HEM	CAA-C2A-C3A	-2.05	122.48	127.07
16	C	501	HEM	CHD-C4C-NC	2.04	126.67	124.45
16	P	501	HEM	C4A-C3A-C2A	-2.04	104.48	106.82
16	P	502	HEM	C1A-C2A-C3A	-2.03	103.73	106.87
17	P	3001	SMA	O1-C2-C9	-2.02	105.83	110.12
16	P	502	HEM	C4C-NC-C1C	-2.02	102.53	105.82
19	Q	501	HEC	C1D-ND-C4D	-2.01	102.83	105.21

All (2) chirality outliers are listed below:

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

All (312) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	4003	PEE	O3P-C1-C2-C3
13	G	2005	PEE	C1-O3P-P-O1P
13	T	3005	PEE	C11-C10-O2-C2
13	T	3005	PEE	O4-C10-O2-C2
13	T	3005	PEE	C4-O4P-P-O3P
13	T	3005	PEE	C4-O4P-P-O2P
13	T	3005	PEE	C4-O4P-P-O1P
13	T	3005	PEE	O4P-C4-C5-N
15	B	2013	GOL	O1-C1-C2-C3
15	B	2013	GOL	C1-C2-C3-O3
15	P	3009	GOL	O1-C1-C2-C3
17	C	2001	SMA	C3-C2-C9-C10
17	C	2001	SMA	O1-C2-C9-C10
17	P	3001	SMA	C3-C2-C9-C10
17	P	3001	SMA	O1-C2-C9-C10
21	G	2003	CDL	C11-CA5-OA6-CA4
21	G	2003	CDL	CB2-OB2-PB2-OB3
21	G	2003	CDL	CB2-OB2-PB2-OB5
21	G	2003	CDL	OB5-CB3-CB4-OB6
21	G	2004	CDL	CA2-C1-CB2-OB2
21	G	2004	CDL	CA2-OA2-PA1-OA3
21	G	2004	CDL	CA2-OA2-PA1-OA4
21	G	2004	CDL	CA2-OA2-PA1-OA5
21	G	2004	CDL	CA3-OA5-PA1-OA2
21	G	2004	CDL	CA3-OA5-PA1-OA3
21	G	2004	CDL	CA3-OA5-PA1-OA4
21	G	2004	CDL	OA7-CA5-OA6-CA4
21	G	2004	CDL	CB2-OB2-PB2-OB5
21	G	2004	CDL	CB3-OB5-PB2-OB2
21	G	2004	CDL	CB3-OB5-PB2-OB3
21	G	2004	CDL	CB3-OB5-PB2-OB4
21	Q	3003	CDL	CA2-OA2-PA1-OA3
21	Q	3003	CDL	CA2-OA2-PA1-OA4
21	Q	3003	CDL	CA2-OA2-PA1-OA5
21	Q	3003	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
21	Q	3003	CDL	CA3-OA5-PA1-OA3
21	Q	3003	CDL	CB2-OB2-PB2-OB3
21	Q	3003	CDL	CB2-OB2-PB2-OB4
21	Q	3003	CDL	CB2-OB2-PB2-OB5
21	Q	3003	CDL	CB3-OB5-PB2-OB2
21	Q	3003	CDL	CB3-OB5-PB2-OB3
21	Q	3003	CDL	CB3-OB5-PB2-OB4
21	Q	3003	CDL	OB6-CB4-CB6-OB8
21	T	3004	CDL	CA2-C1-CB2-OB2
21	T	3004	CDL	CB2-OB2-PB2-OB4
21	T	3004	CDL	CB2-OB2-PB2-OB5
21	T	3004	CDL	CB3-OB5-PB2-OB3
21	G	2003	CDL	OA7-CA5-OA6-CA4
21	G	2004	CDL	C51-CB5-OB6-CB4
21	Q	3003	CDL	C11-CA5-OA6-CA4
21	T	3004	CDL	C51-CB5-OB6-CB4
21	G	2003	CDL	C31-CA7-OA8-CA6
21	Q	3003	CDL	OA7-CA5-OA6-CA4
21	T	3004	CDL	OB7-CB5-OB6-CB4
21	Q	3003	CDL	C31-CA7-OA8-CA6
19	Q	501	HEC	C4C-C3C-CAC-CBC
21	T	3004	CDL	C31-CA7-OA8-CA6
21	G	2004	CDL	OB7-CB5-OB6-CB4
21	G	2004	CDL	C11-CA5-OA6-CA4
21	G	2003	CDL	OA9-CA7-OA8-CA6
21	G	2003	CDL	C71-CB7-OB8-CB6
21	Q	3003	CDL	OA9-CA7-OA8-CA6
21	T	3004	CDL	OA9-CA7-OA8-CA6
11	C	2008	JZR	O5-C5-C6-O6
21	G	2004	CDL	O1-C1-CB2-OB2
21	T	3004	CDL	O1-C1-CB2-OB2
13	G	2005	PEE	C31-C30-O3-C3
21	G	2003	CDL	OB9-CB7-OB8-CB6
11	F	3011	JZR	O5-C5-C6-O6
13	G	2005	PEE	O5-C30-O3-C3
21	Q	3003	CDL	CB2-C1-CA2-OA2
21	Q	3003	CDL	O1-C1-CA2-OA2
11	C	2008	JZR	C4-C5-C6-O6
11	S	2011	JZR	C4-C5-C6-O6
21	T	3004	CDL	C11-CA5-OA6-CA4
13	T	3005	PEE	C31-C30-O3-C3
19	Q	501	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
11	P	3008	JZR	O1-C1'-C2'-C3'
13	G	2005	PEE	C30-C31-C32-C33
13	P	3007	PEE	C10-C11-C12-C13
11	F	3011	JZR	C4-C5-C6-O6
11	F	4001	JZR	O1-C1'-C2'-C3'
13	C	2007	PEE	C10-C11-C12-C13
21	Q	3003	CDL	CB5-C51-C52-C53
21	Q	3003	CDL	CB7-C71-C72-C73
21	G	2003	CDL	O1-C1-CA2-OA2
13	T	3005	PEE	C37-C38-C39-C40
13	T	3005	PEE	O5-C30-O3-C3
13	T	3005	PEE	C10-C11-C12-C13
21	T	3004	CDL	OA7-CA5-OA6-CA4
21	G	2003	CDL	CB2-C1-CA2-OA2
19	D	501	HEC	C4C-C3C-CAC-CBC
13	D	2006	PEE	C17-C18-C19-C20
13	Q	3006	PEE	C37-C38-C39-C40
11	S	2011	JZR	O5-C5-C6-O6
15	O	3013	GOL	C1-C2-C3-O3
21	G	2003	CDL	C51-CB5-OB6-CB4
11	C	2008	JZR	C2'-C3'-C4'-C5'
13	D	2006	PEE	C37-C38-C39-C40
13	G	2005	PEE	C37-C38-C39-C40
13	Q	3006	PEE	C17-C18-C19-C20
13	P	3007	PEE	C34-C35-C36-C37
13	C	2007	PEE	C34-C35-C36-C37
13	D	2006	PEE	C13-C14-C15-C16
21	T	3004	CDL	C31-C32-C33-C34
13	A	4003	PEE	O3P-C1-C2-O2
15	B	2013	GOL	O1-C1-C2-O2
15	B	2013	GOL	O2-C2-C3-O3
15	O	3013	GOL	O2-C2-C3-O3
21	T	3004	CDL	CA7-C31-C32-C33
13	G	2005	PEE	C21-C22-C23-C24
13	G	2005	PEE	C11-C10-O2-C2
11	A	4002	JZR	C2'-C3'-C4'-C5'
13	Q	3006	PEE	C13-C14-C15-C16
21	Q	3003	CDL	C77-C78-C79-C80
11	C	2008	JZR	C1'-C2'-C3'-C4'
13	P	3007	PEE	C41-C42-C43-C44
13	C	2007	PEE	C41-C42-C43-C44
21	G	2004	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
13	C	2007	PEE	C21-C22-C23-C24
13	G	2005	PEE	C22-C23-C24-C25
13	G	2005	PEE	C12-C13-C14-C15
13	P	3007	PEE	C12-C13-C14-C15
13	P	3007	PEE	C42-C43-C44-C45
13	Q	3006	PEE	C42-C43-C44-C45
13	D	2006	PEE	C42-C43-C44-C45
21	Q	3003	CDL	C78-C79-C80-C81
13	C	2007	PEE	C17-C18-C19-C20
13	P	3007	PEE	C17-C18-C19-C20
13	C	2007	PEE	C42-C43-C44-C45
13	G	2005	PEE	O4-C10-O2-C2
13	P	3007	PEE	C21-C22-C23-C24
13	T	3005	PEE	C11-C12-C13-C14
13	G	2005	PEE	C40-C41-C42-C43
21	G	2003	CDL	OB7-CB5-OB6-CB4
13	G	2005	PEE	C35-C36-C37-C38
13	T	3005	PEE	C21-C22-C23-C24
11	A	4002	JZR	O1-C1'-C2'-C3'
21	Q	3003	CDL	C76-C77-C78-C79
21	Q	3003	CDL	C71-C72-C73-C74
21	Q	3003	CDL	C73-C74-C75-C76
21	T	3004	CDL	C13-C14-C15-C16
13	D	2006	PEE	C35-C36-C37-C38
13	C	2007	PEE	C12-C13-C14-C15
13	T	3005	PEE	C41-C42-C43-C44
13	G	2005	PEE	C33-C34-C35-C36
21	G	2004	CDL	O1-C1-CA2-OA2
21	G	2004	CDL	C31-CA7-OA8-CA6
13	D	2006	PEE	C22-C23-C24-C25
15	P	3009	GOL	O1-C1-C2-O2
13	P	3007	PEE	C31-C32-C33-C34
13	G	2005	PEE	C39-C40-C41-C42
13	P	3007	PEE	C15-C16-C17-C18
13	Q	3006	PEE	C35-C36-C37-C38
13	T	3005	PEE	C15-C16-C17-C18
13	T	3005	PEE	C39-C40-C41-C42
21	G	2004	CDL	OA5-CA3-CA4-CA6
13	G	2005	PEE	C42-C43-C44-C45
13	C	2007	PEE	C22-C23-C24-C25
19	D	501	HEC	C2C-C3C-CAC-CBC
13	G	2005	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
13	T	3005	PEE	C1-C2-C3-O3
21	G	2003	CDL	CB3-CB4-CB6-OB8
21	Q	3003	CDL	CB3-CB4-CB6-OB8
21	T	3004	CDL	CA3-CA4-CA6-OA8
13	D	2006	PEE	C15-C16-C17-C18
13	Q	3006	PEE	C15-C16-C17-C18
13	C	2007	PEE	C31-C32-C33-C34
13	Q	3006	PEE	C22-C23-C24-C25
21	G	2004	CDL	C31-C32-C33-C34
21	G	2004	CDL	OA9-CA7-OA8-CA6
11	S	2011	JZR	O1-C1'-C2'-C3'
21	Q	3003	CDL	C72-C73-C74-C75
13	C	2007	PEE	C39-C40-C41-C42
13	P	3007	PEE	C39-C40-C41-C42
13	P	3007	PEE	C20-C21-C22-C23
13	P	3007	PEE	C32-C33-C34-C35
13	C	2007	PEE	C32-C33-C34-C35
21	G	2004	CDL	OA6-CA4-CA6-OA8
21	G	2003	CDL	C73-C74-C75-C76
13	G	2005	PEE	C15-C16-C17-C18
11	S	2011	JZR	C2'-C3'-C4'-C5'
13	P	3007	PEE	C22-C23-C24-C25
13	T	3005	PEE	C17-C18-C19-C20
13	T	3005	PEE	C33-C34-C35-C36
21	T	3004	CDL	C14-C15-C16-C17
11	F	4001	JZR	C4-C5-C6-O6
13	D	2006	PEE	C43-C44-C45-C46
21	Q	3003	CDL	C79-C80-C81-C82
21	G	2003	CDL	OB5-CB3-CB4-CB6
21	Q	3003	CDL	OB5-CB3-CB4-CB6
11	A	4002	JZR	C3'-C4'-C5'-C6'
13	Q	3006	PEE	C43-C44-C45-C46
11	F	4001	JZR	C1'-C2'-C3'-C4'
11	P	3008	JZR	C1'-C2'-C3'-C4'
21	Q	3003	CDL	C75-C76-C77-C78
13	T	3005	PEE	O3P-C1-C2-O2
21	T	3004	CDL	OB5-CB3-CB4-OB6
11	A	4002	JZR	C4-C5-C6-O6
13	G	2005	PEE	C34-C35-C36-C37
13	C	2007	PEE	C15-C16-C17-C18
11	A	4002	JZR	O5-C5-C6-O6
21	G	2004	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
21	T	3004	CDL	OB5-CB3-CB4-CB6
21	G	2004	CDL	C71-CB7-OB8-CB6
13	P	3007	PEE	C18-C19-C20-C21
13	Q	3006	PEE	C34-C35-C36-C37
13	G	2005	PEE	C43-C44-C45-C46
13	A	4003	PEE	C1-C2-C3-O3
21	G	2004	CDL	OA5-CA3-CA4-OA6
21	Q	3003	CDL	OB5-CB3-CB4-OB6
21	G	2004	CDL	CA3-CA4-CA6-OA8
13	G	2005	PEE	C5-C4-O4P-P
13	C	2007	PEE	C20-C21-C22-C23
13	D	2006	PEE	C40-C41-C42-C43
13	T	3005	PEE	O2-C2-C3-O3
21	G	2003	CDL	OB6-CB4-CB6-OB8
13	D	2006	PEE	C34-C35-C36-C37
13	D	2006	PEE	C23-C24-C25-C26
21	G	2003	CDL	C72-C73-C74-C75
11	S	2011	JZR	C1'-C2'-C3'-C4'
19	Q	501	HEC	C4B-C3B-CAB-CBB
13	C	2007	PEE	C18-C19-C20-C21
13	T	3005	PEE	O3P-C1-C2-C3
21	Q	3003	CDL	C74-C75-C76-C77
13	P	3007	PEE	C43-C44-C45-C46
13	T	3005	PEE	C12-C13-C14-C15
13	Q	3006	PEE	C23-C24-C25-C26
13	Q	3006	PEE	C40-C41-C42-C43
21	G	2003	CDL	C71-C72-C73-C74
13	G	2005	PEE	O2-C2-C3-O3
21	T	3004	CDL	OA6-CA4-CA6-OA8
21	G	2004	CDL	CB3-CB4-CB6-OB8
13	C	2007	PEE	C43-C44-C45-C46
13	C	2007	PEE	C4-O4P-P-O1P
21	G	2003	CDL	CB2-OB2-PB2-OB4
21	G	2004	CDL	CB2-OB2-PB2-OB3
21	T	3004	CDL	CB2-OB2-PB2-OB3
21	G	2003	CDL	CB7-C71-C72-C73
13	D	2006	PEE	C16-C17-C18-C19
13	T	3005	PEE	C18-C19-C20-C21
11	F	4001	JZR	O5-C5-C6-O6
13	D	2006	PEE	C31-C32-C33-C34
13	G	2005	PEE	C14-C15-C16-C17
13	D	2006	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
16	P	502	HEM	CAA-CBA-CGA-O1A
16	C	501	HEM	CAA-CBA-CGA-O1A
16	C	501	HEM	CAD-CBD-CGD-O1D
16	C	502	HEM	CAA-CBA-CGA-O2A
16	P	502	HEM	CAA-CBA-CGA-O2A
21	G	2003	CDL	OA5-CA3-CA4-OA6
21	G	2004	CDL	C12-C11-CA5-OA6
16	C	502	HEM	CAA-CBA-CGA-O1A
21	G	2004	CDL	OB5-CB3-CB4-CB6
19	Q	501	HEC	C2B-C3B-CAB-CBB
16	C	501	HEM	CAA-CBA-CGA-O2A
16	P	501	HEM	CAD-CBD-CGD-O1D
21	T	3004	CDL	C12-C13-C14-C15
21	Q	3003	CDL	C51-C52-C53-C54
21	G	2004	CDL	OB9-CB7-OB8-CB6
16	C	501	HEM	CAD-CBD-CGD-O2D
16	P	501	HEM	CAD-CBD-CGD-O2D
21	G	2003	CDL	C78-C79-C80-C81
18	P	3002	UQ	C4-C3-O3-CM3
13	Q	3006	PEE	C16-C17-C18-C19
13	G	2005	PEE	C11-C12-C13-C14
13	D	2006	PEE	C36-C37-C38-C39
11	F	4001	JZR	C2'-C3'-C4'-C5'
19	D	501	HEC	CAA-CBA-CGA-O2A
16	P	502	HEM	CAD-CBD-CGD-O2D
13	D	2006	PEE	C39-C40-C41-C42
13	P	3007	PEE	C19-C20-C21-C22
21	G	2003	CDL	C76-C77-C78-C79
13	D	2006	PEE	C20-C21-C22-C23
13	Q	3006	PEE	C36-C37-C38-C39
13	T	3005	PEE	C36-C37-C38-C39
13	G	2005	PEE	C17-C18-C19-C20
13	Q	3006	PEE	C32-C33-C34-C35
13	Q	3006	PEE	C31-C32-C33-C34
19	D	501	HEC	CAA-CBA-CGA-O1A
16	P	502	HEM	CAD-CBD-CGD-O1D
13	A	4003	PEE	O2-C2-C3-O3
16	P	501	HEM	CAA-CBA-CGA-O1A
11	F	3011	JZR	C2'-C3'-C4'-C5'
21	G	2003	CDL	OA5-CA3-CA4-CA6
16	P	501	HEM	CAA-CBA-CGA-O2A
19	Q	501	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	P	3008	JZR	C2'-C3'-C4'-C5'
13	T	3005	PEE	O2-C10-C11-C12
11	S	2011	JZR	C3'-C4'-C5'-C6'
21	G	2003	CDL	C51-C52-C53-C54
19	D	501	HEC	CAD-CBD-CGD-O1D
21	Q	3003	CDL	C72-C71-CB7-OB8
16	C	502	HEM	CAD-CBD-CGD-O2D
19	Q	501	HEC	CAD-CBD-CGD-O1D
11	F	3011	JZR	O1-C1'-C2'-C3'
19	Q	501	HEC	CAD-CBD-CGD-O2D
21	G	2004	CDL	C32-C31-CA7-OA8
19	Q	501	HEC	CAA-CBA-CGA-O1A
18	P	3002	UQ	C2-C3-O3-CM3
13	Q	3006	PEE	C11-C12-C13-C14
19	D	501	HEC	C4B-C3B-CAB-CBB
13	G	2005	PEE	C10-C11-C12-C13
16	C	502	HEM	CAD-CBD-CGD-O1D
19	D	501	HEC	CAD-CBD-CGD-O2D
21	Q	3003	CDL	OB9-CB7-OB8-CB6
21	G	2004	CDL	C12-C11-CA5-OA7
13	T	3005	PEE	O4-C10-C11-C12
21	G	2004	CDL	C32-C31-CA7-OA9
21	Q	3003	CDL	C72-C71-CB7-OB9
21	Q	3003	CDL	C52-C51-CB5-OB6
13	Q	3006	PEE	C41-C42-C43-C44

There are no ring outliers.

18 monomers are involved in 57 short contacts:

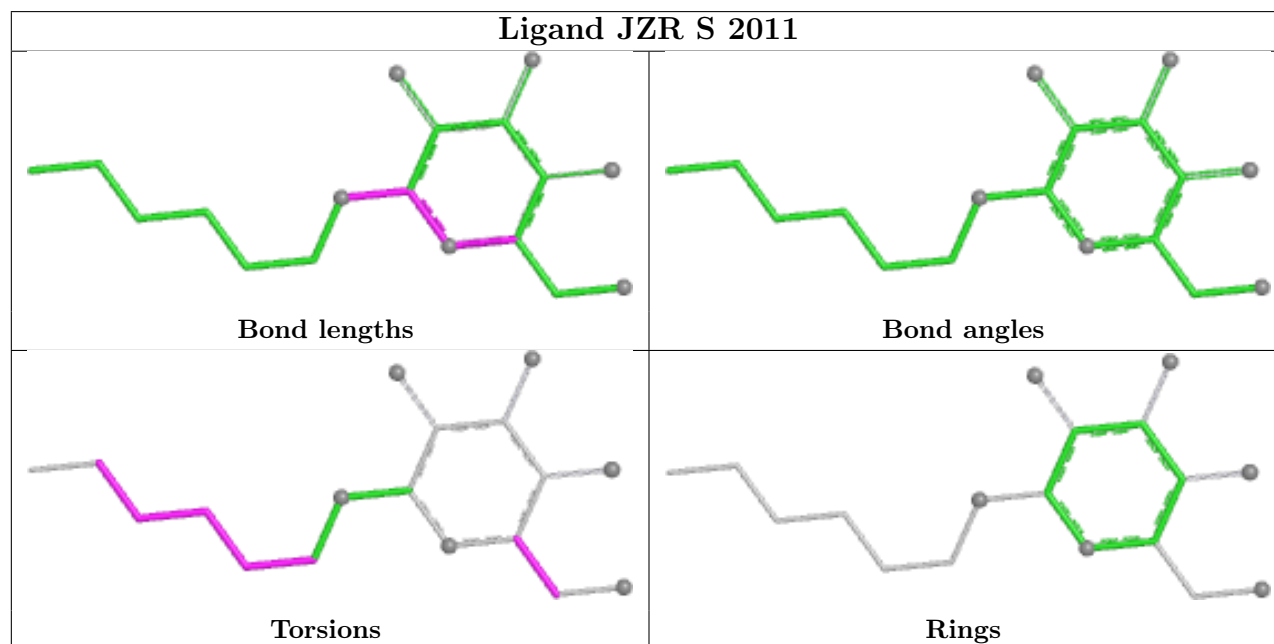
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	2011	JZR	8	0
16	P	501	HEM	1	0
21	G	2004	CDL	5	0
13	D	2006	PEE	4	0
16	C	502	HEM	3	0
16	C	501	HEM	2	0
17	C	2001	SMA	1	0
13	T	3005	PEE	1	0
17	P	3001	SMA	2	0
13	P	3007	PEE	3	0
13	Q	3006	PEE	11	0
11	A	4002	JZR	1	0

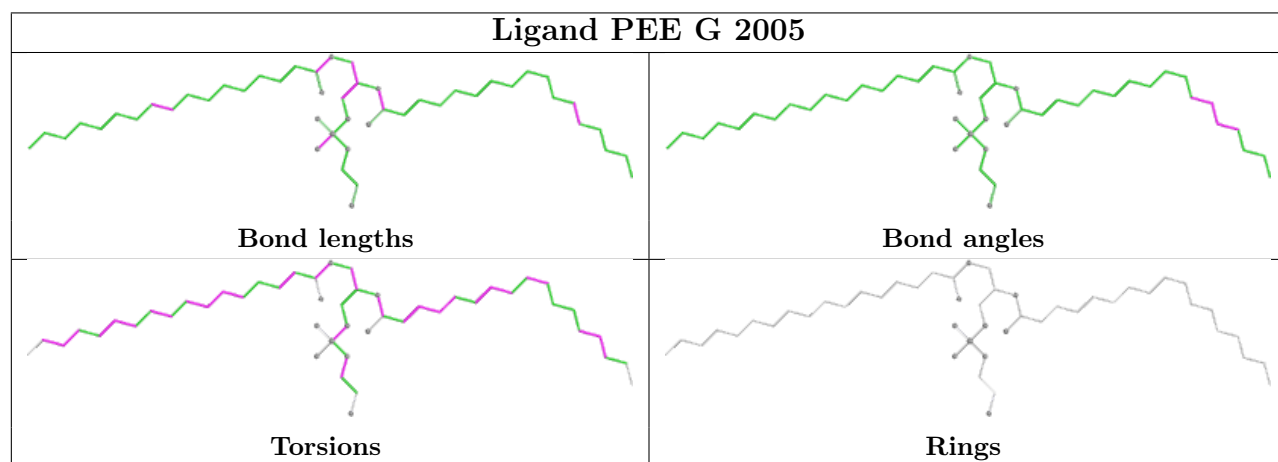
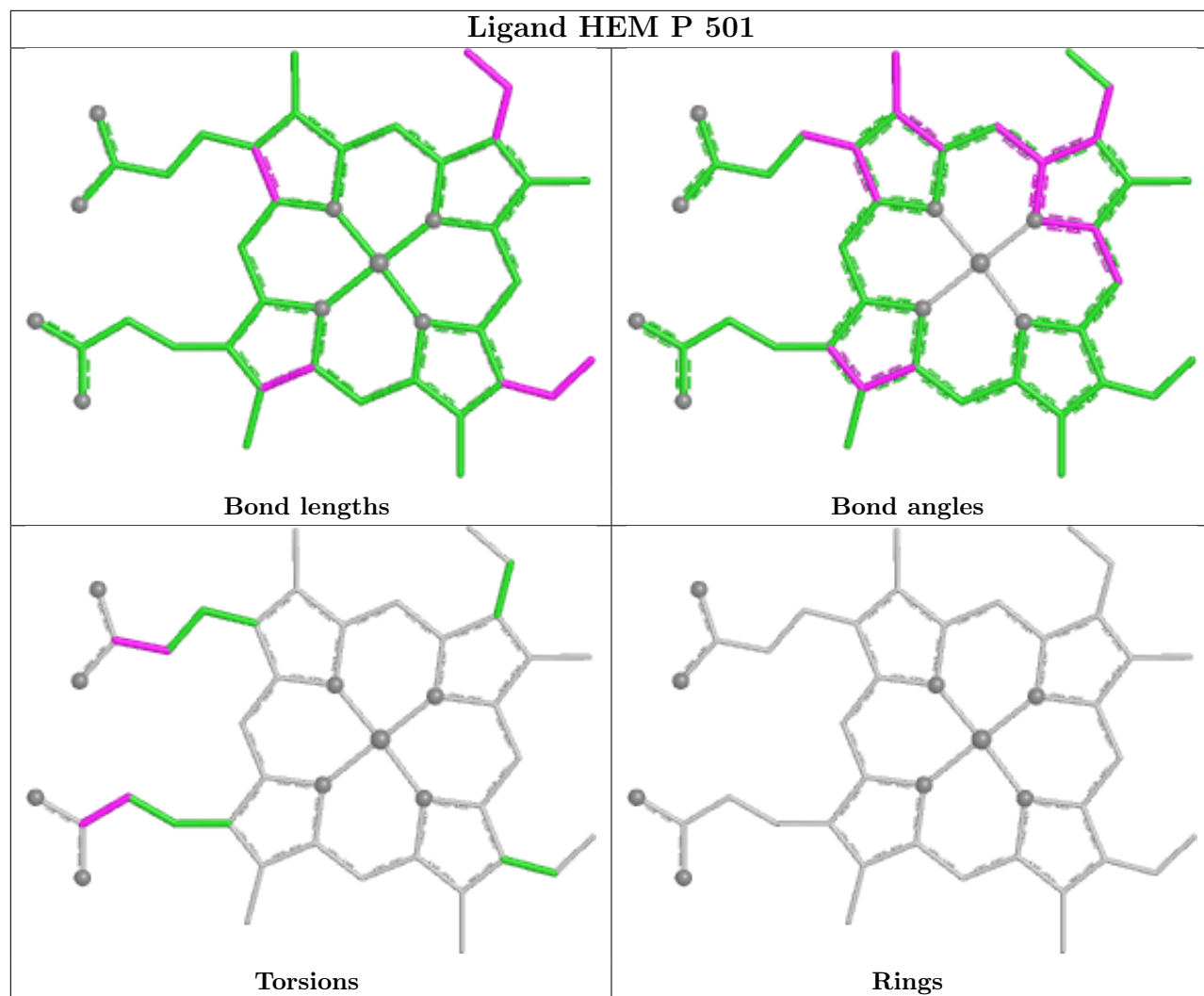
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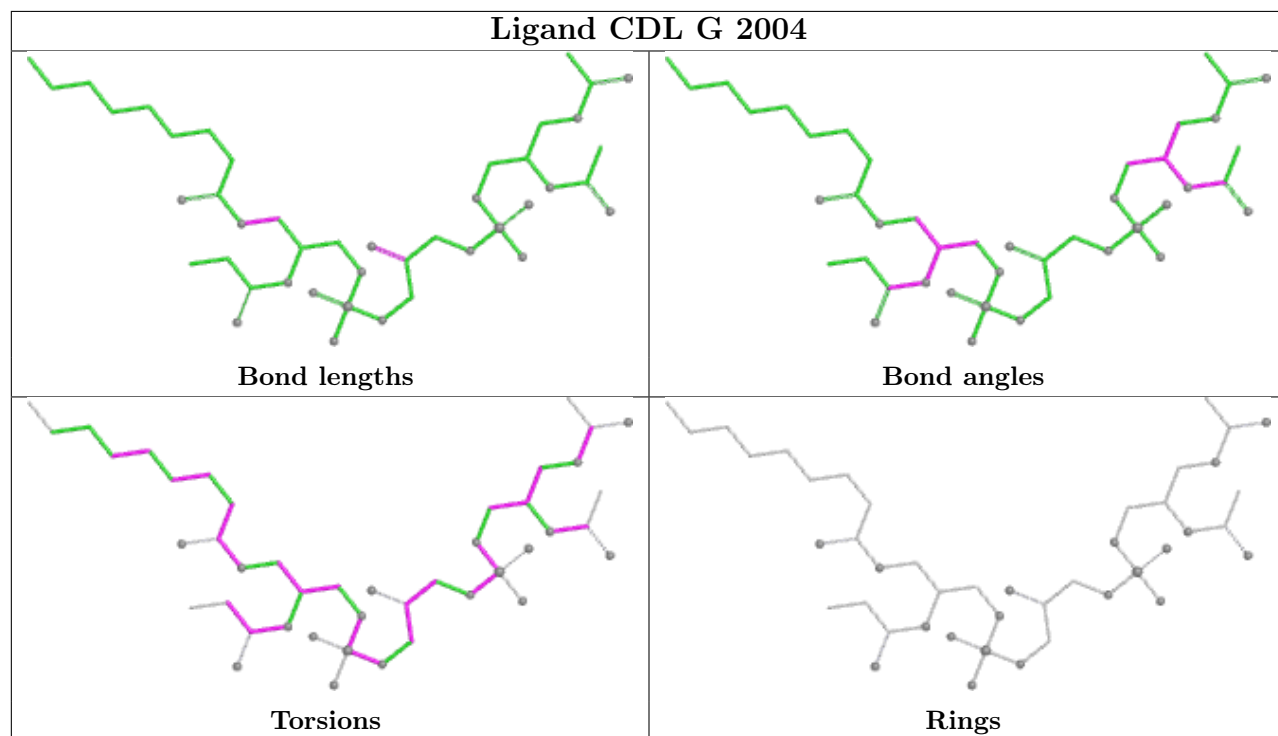
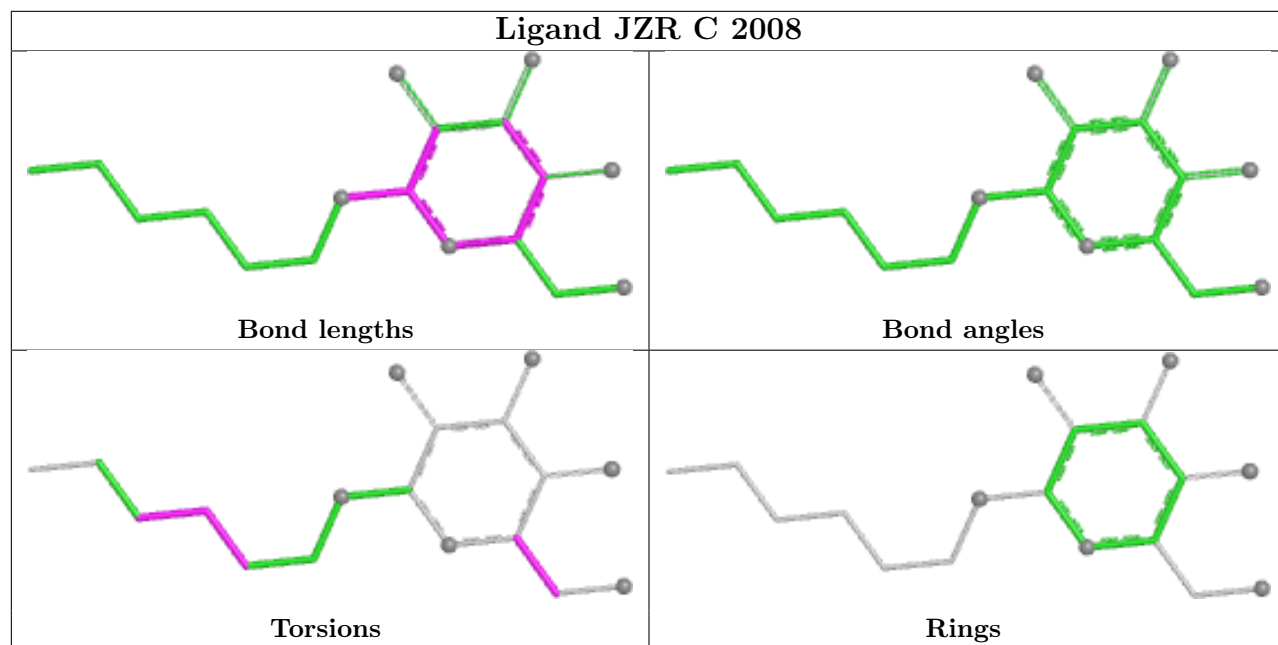
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2007	PEE	3	0
16	P	502	HEM	2	0
18	P	3002	UQ	5	0
11	F	3011	JZR	3	0
19	Q	501	HEC	1	0
18	C	2002	UQ	3	0

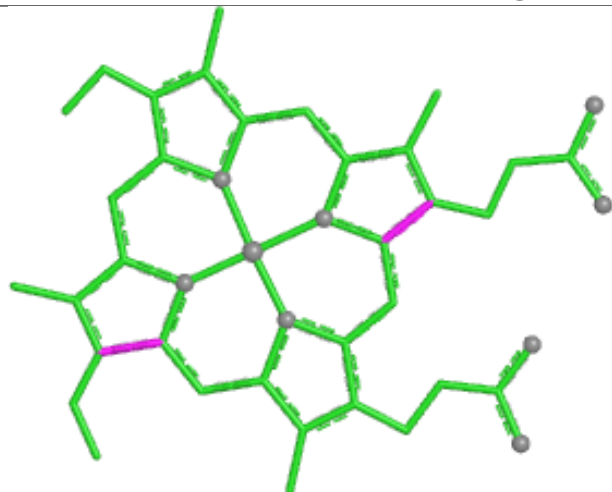
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



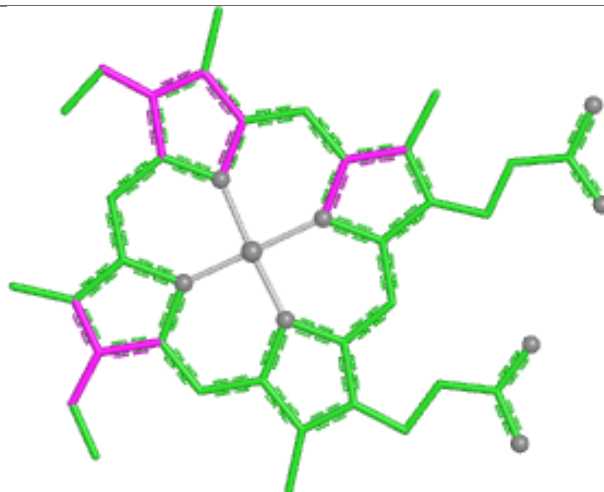




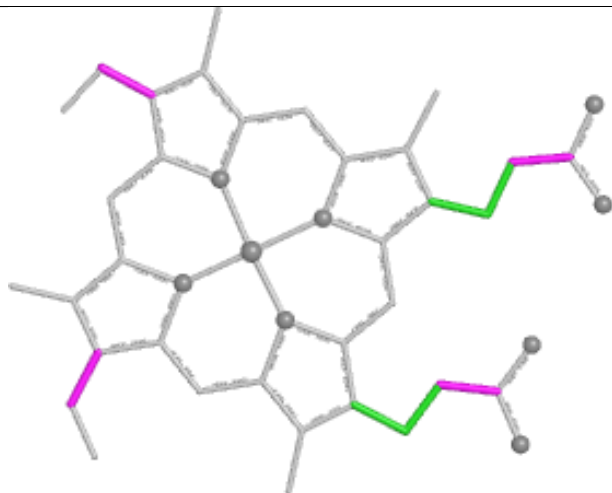
Ligand HEC D 501



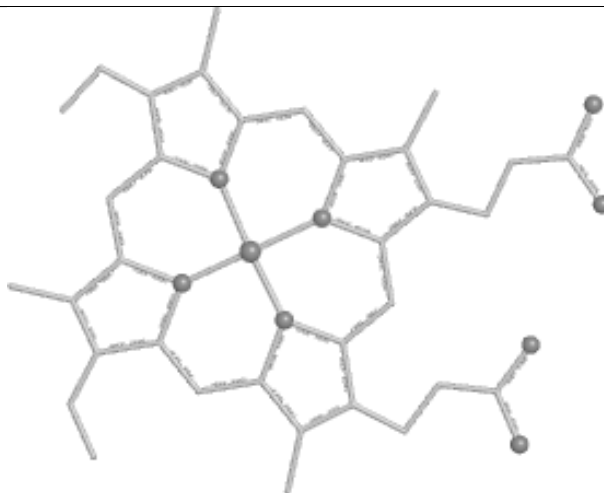
Bond lengths



Bond angles

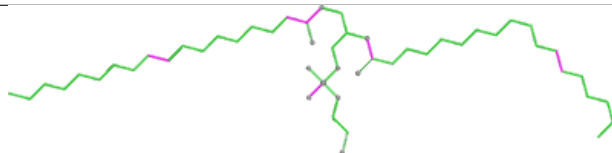


Torsions

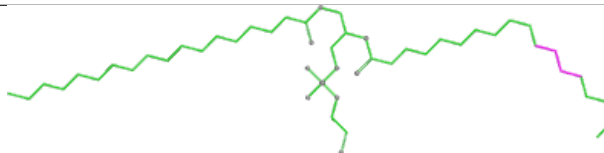


Rings

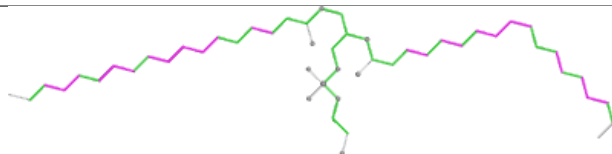
Ligand PEE D 2006



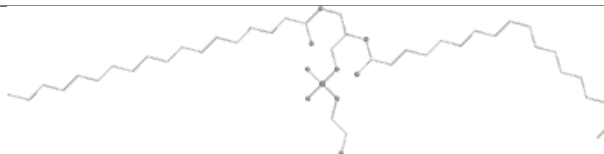
Bond lengths



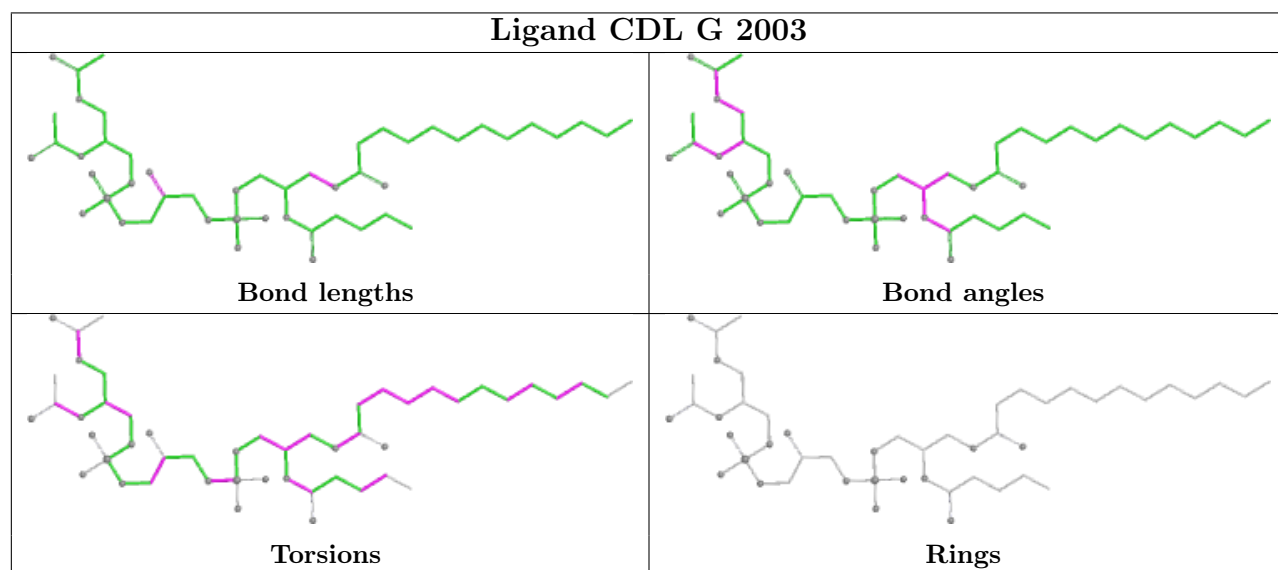
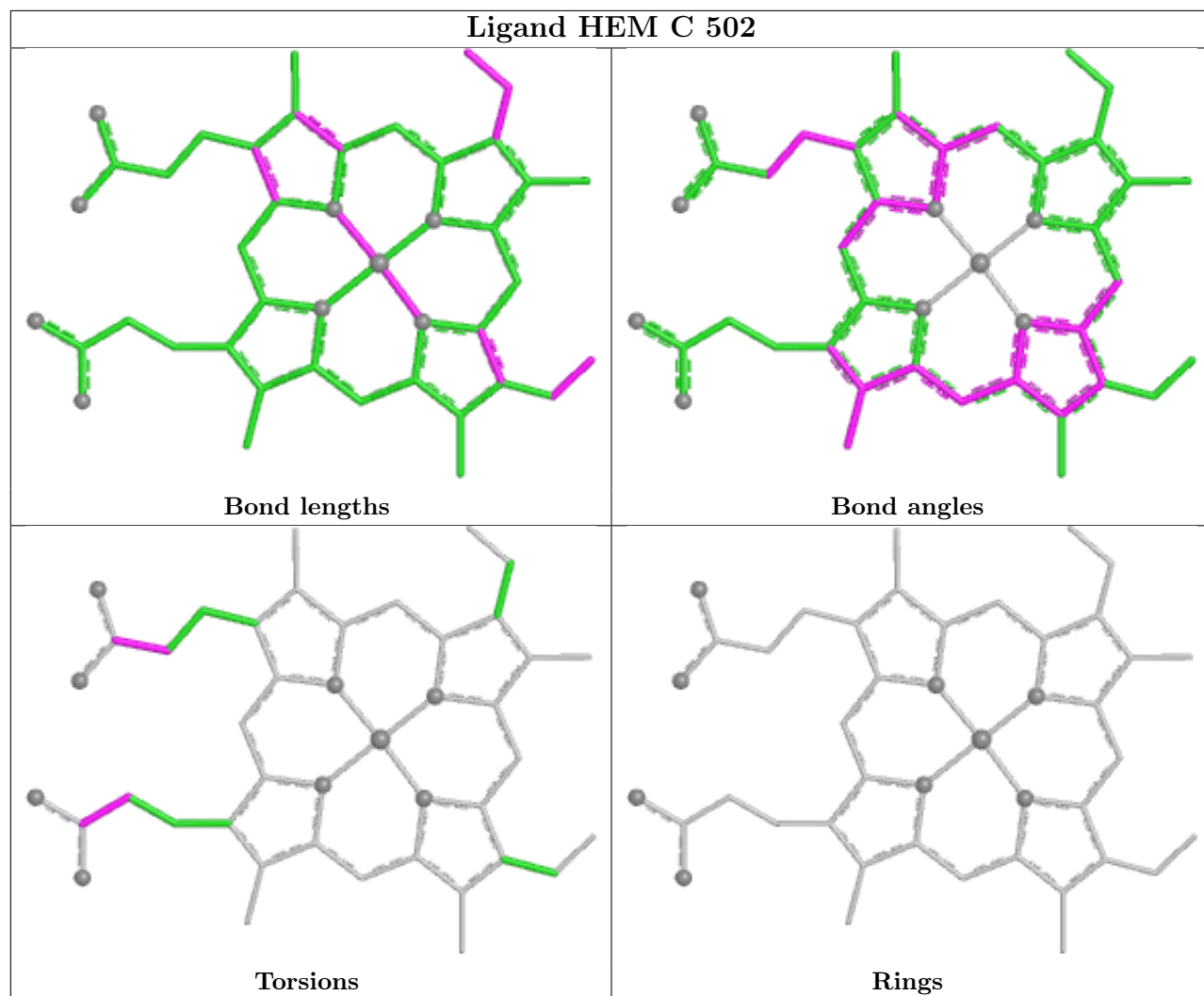
Bond angles

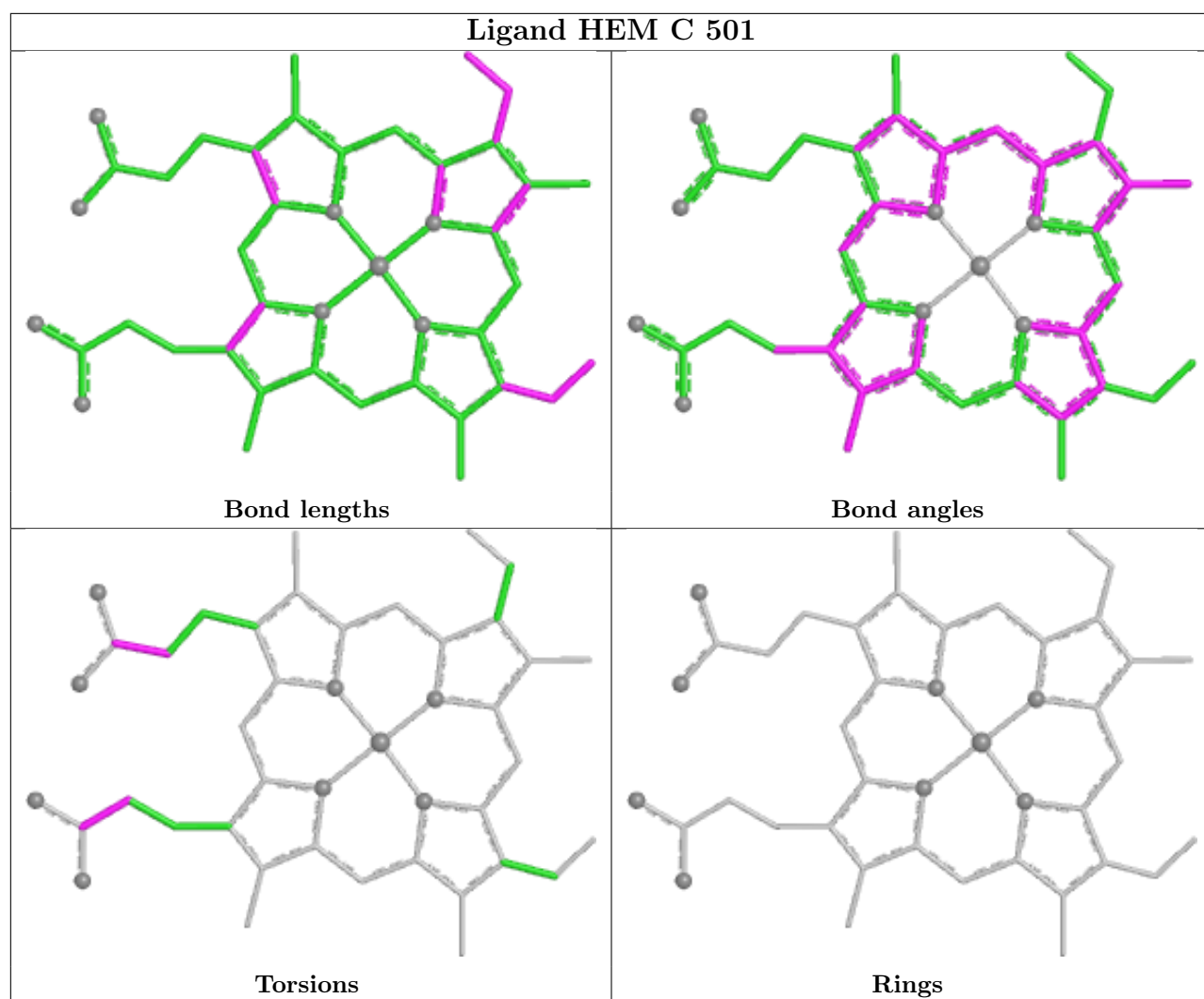


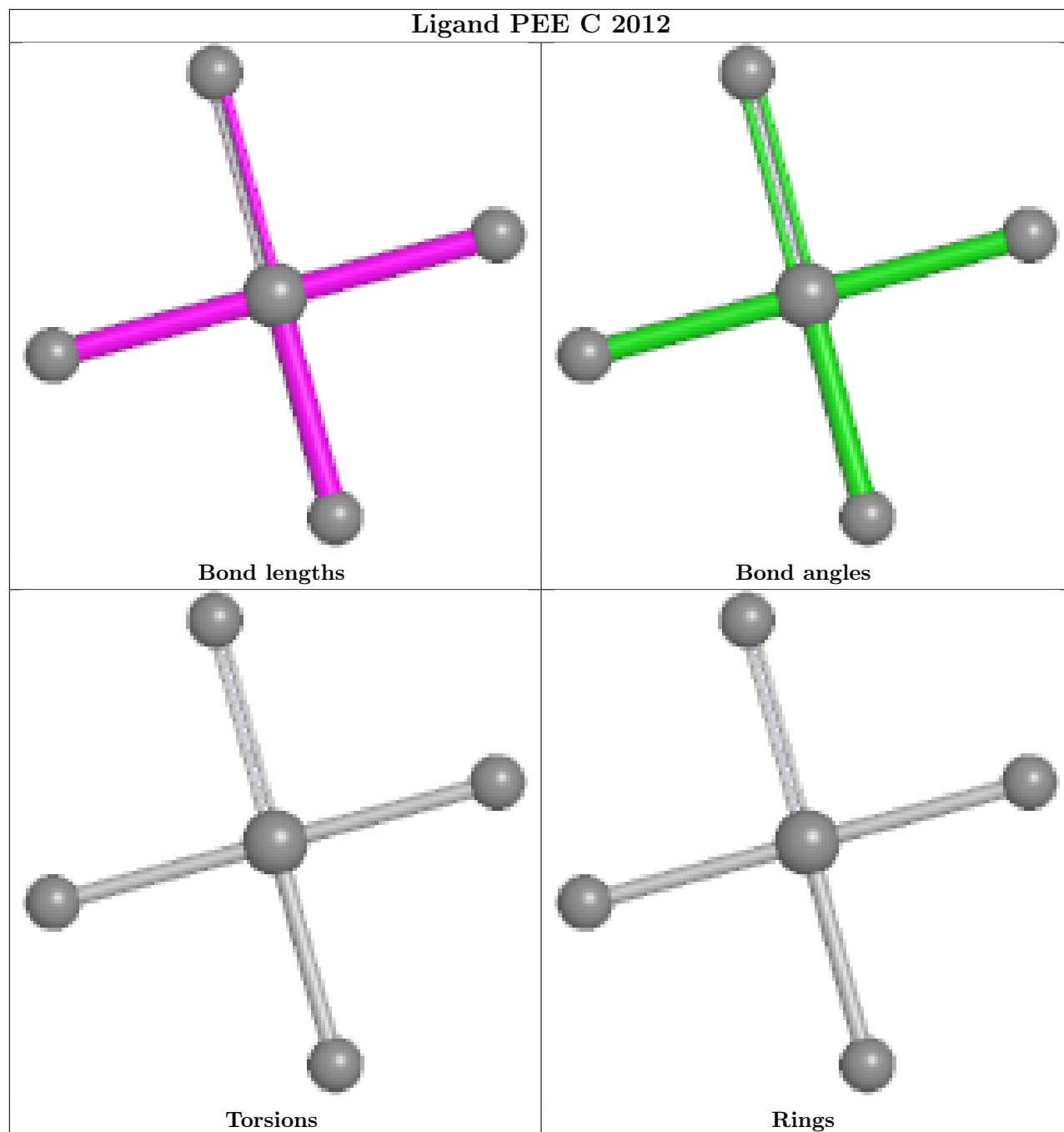
Torsions

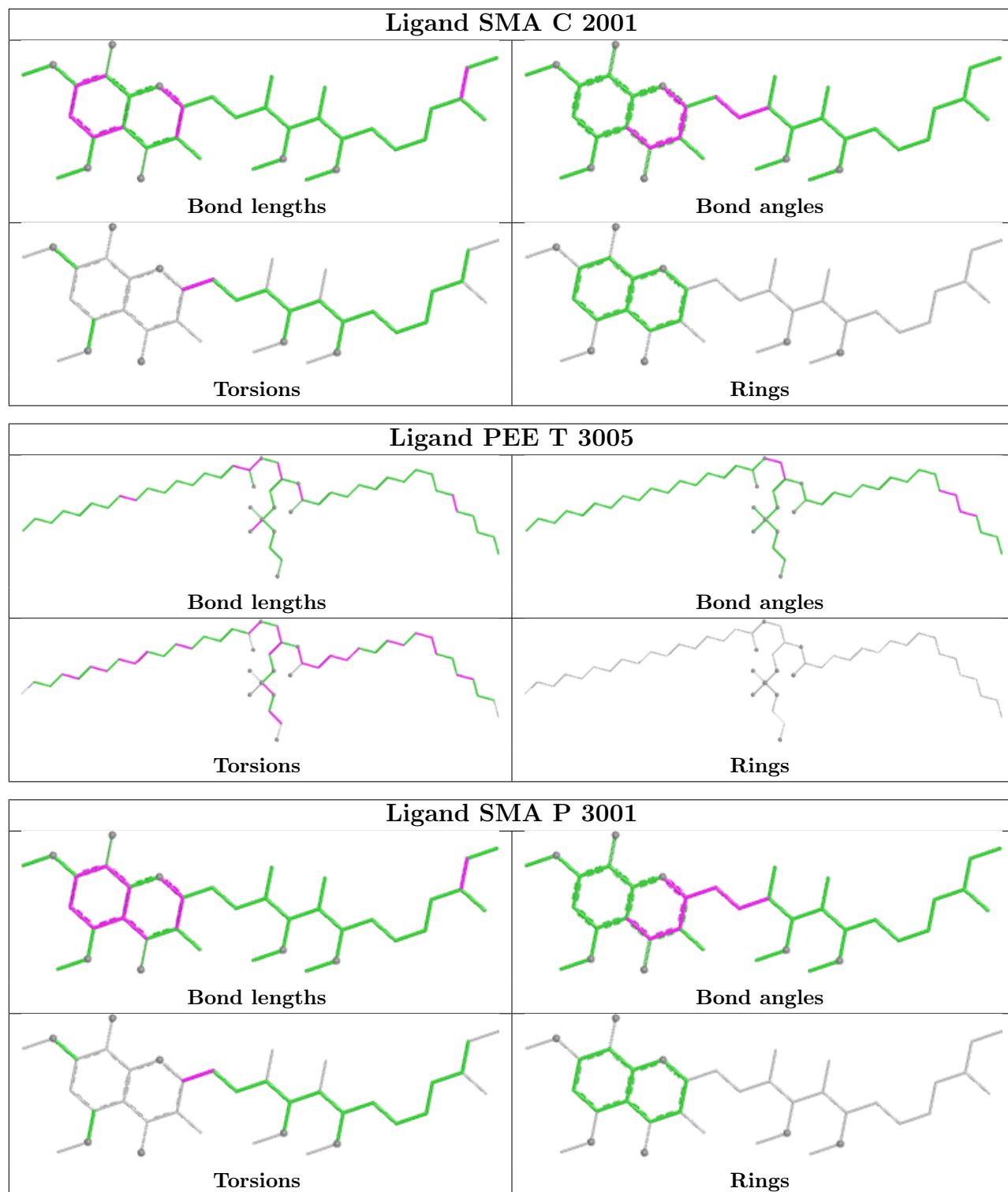


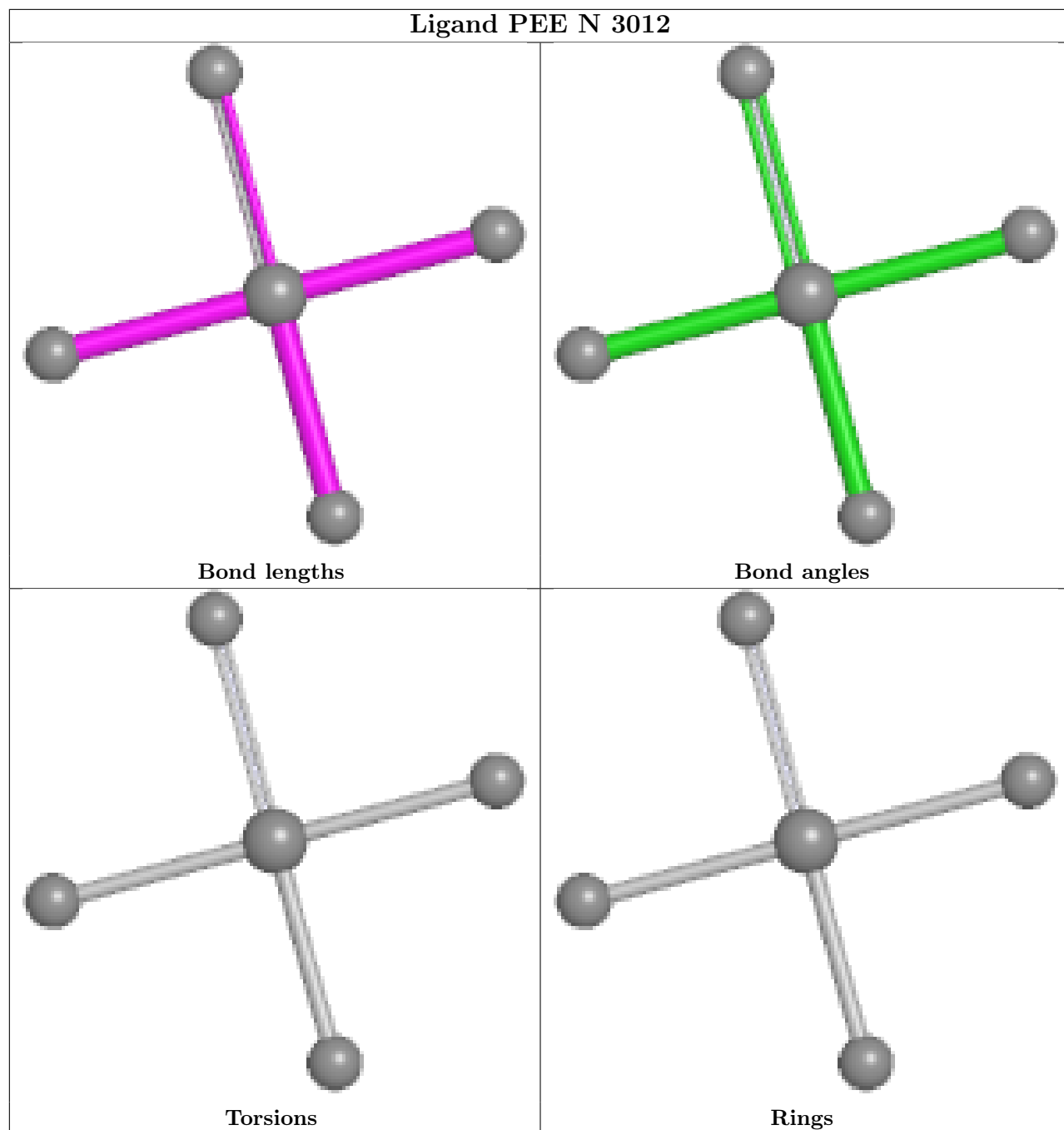
Rings

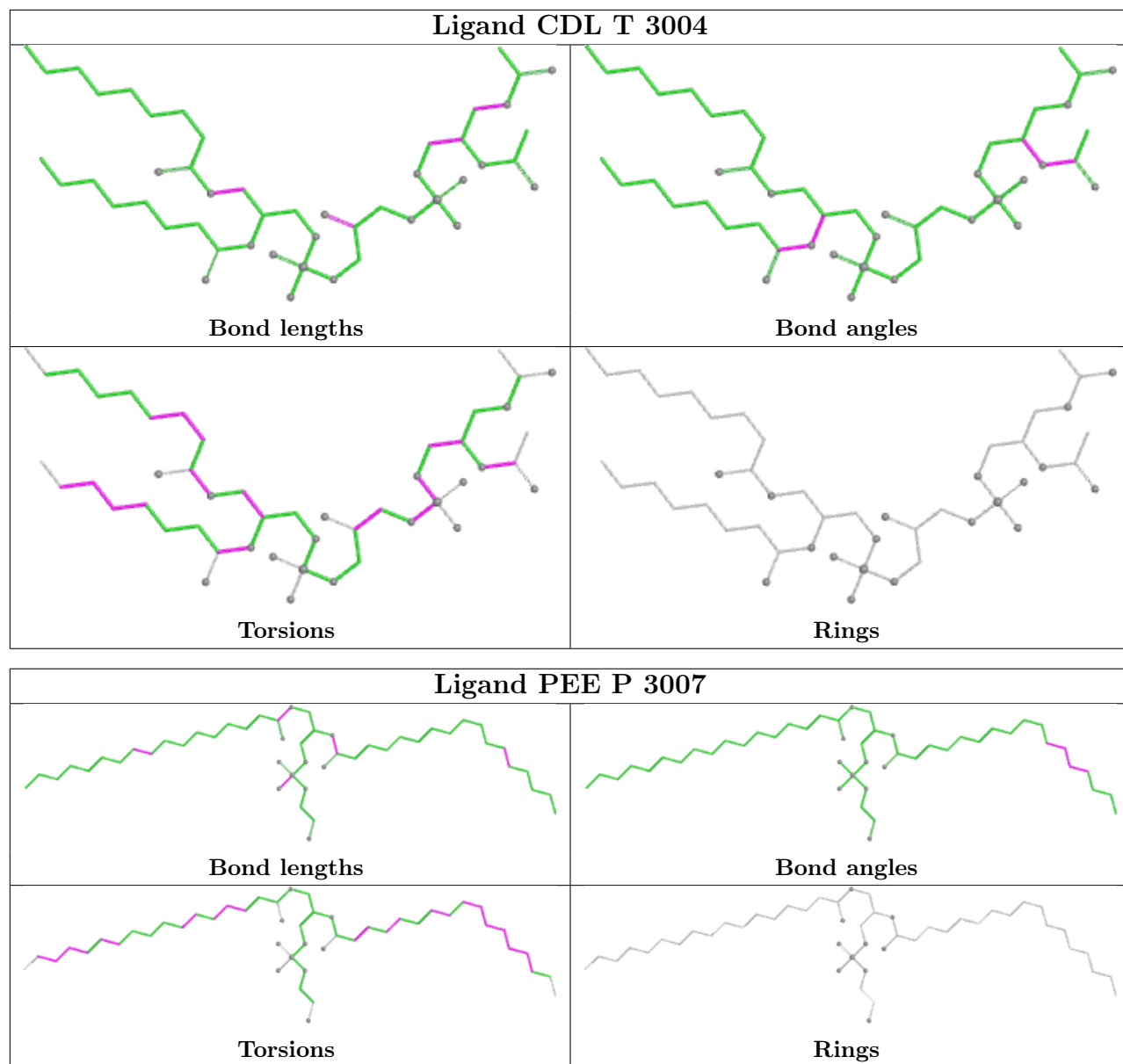


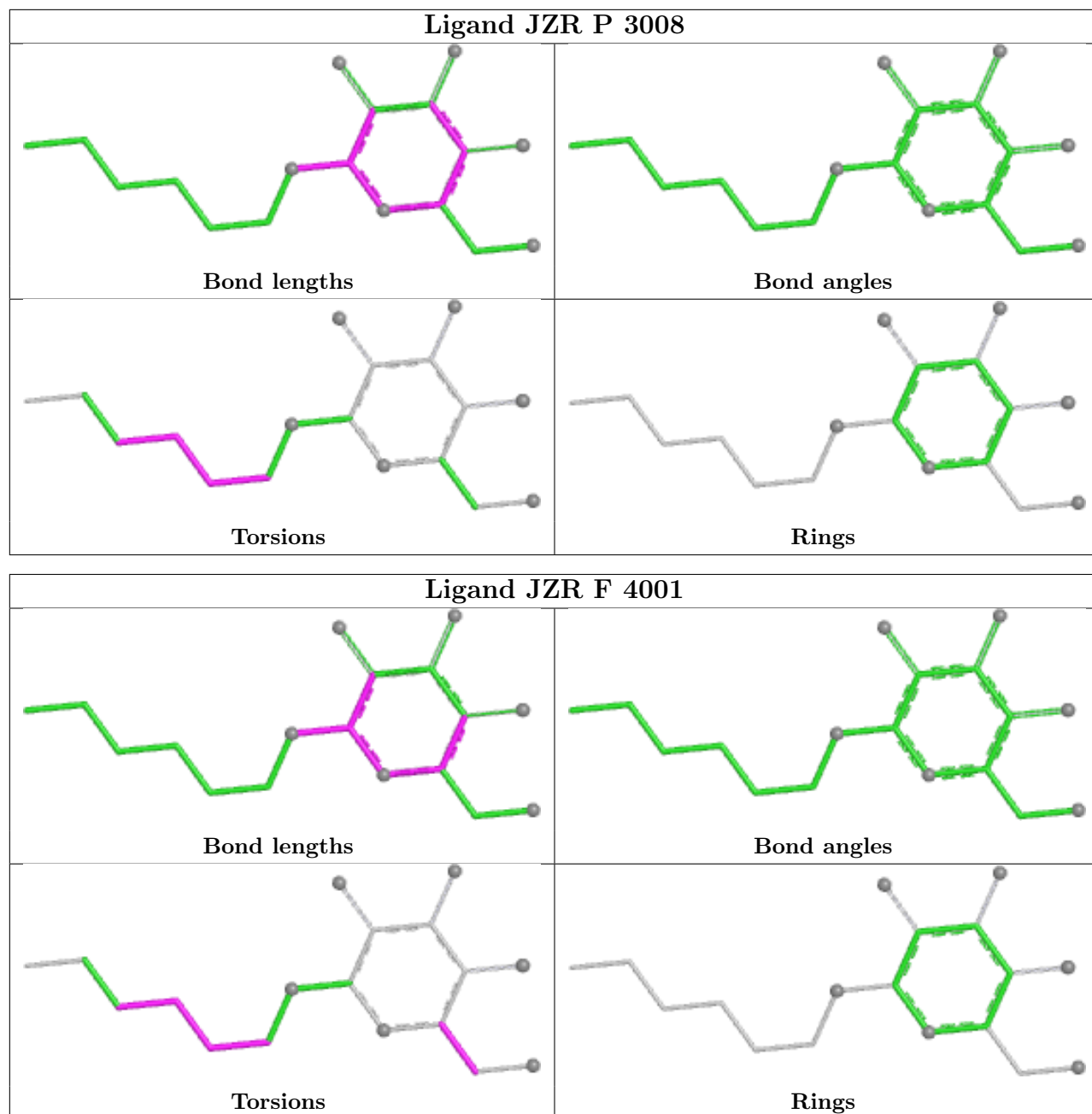


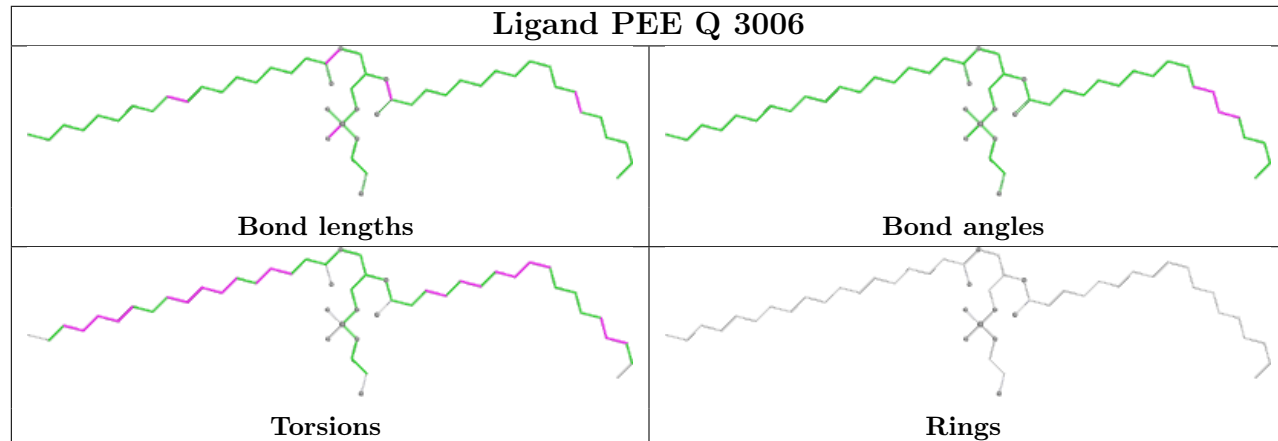
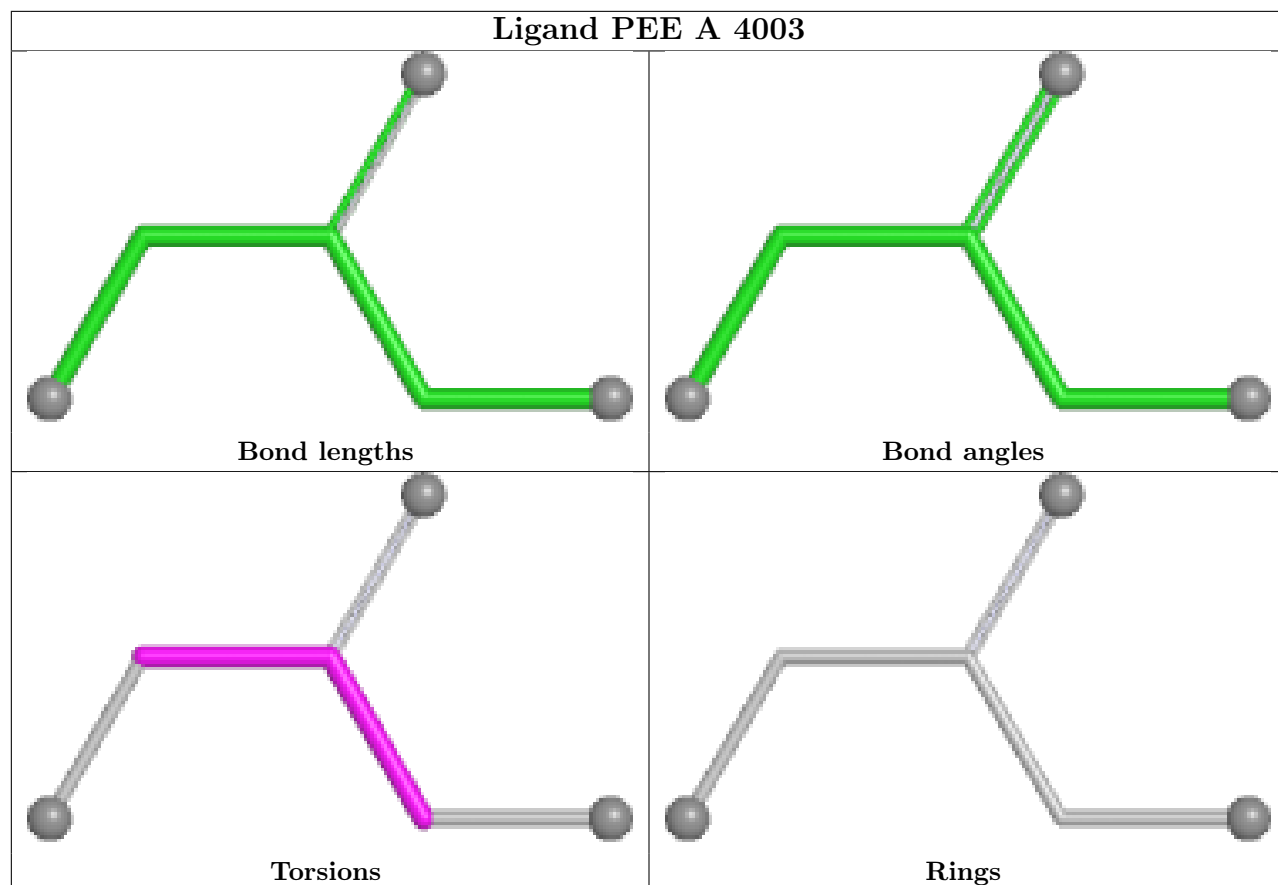


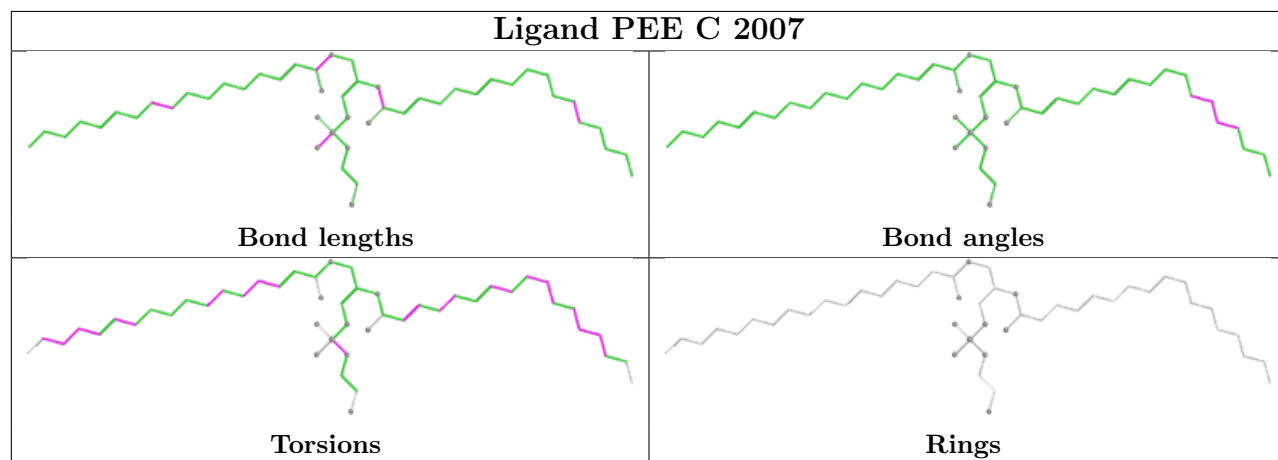
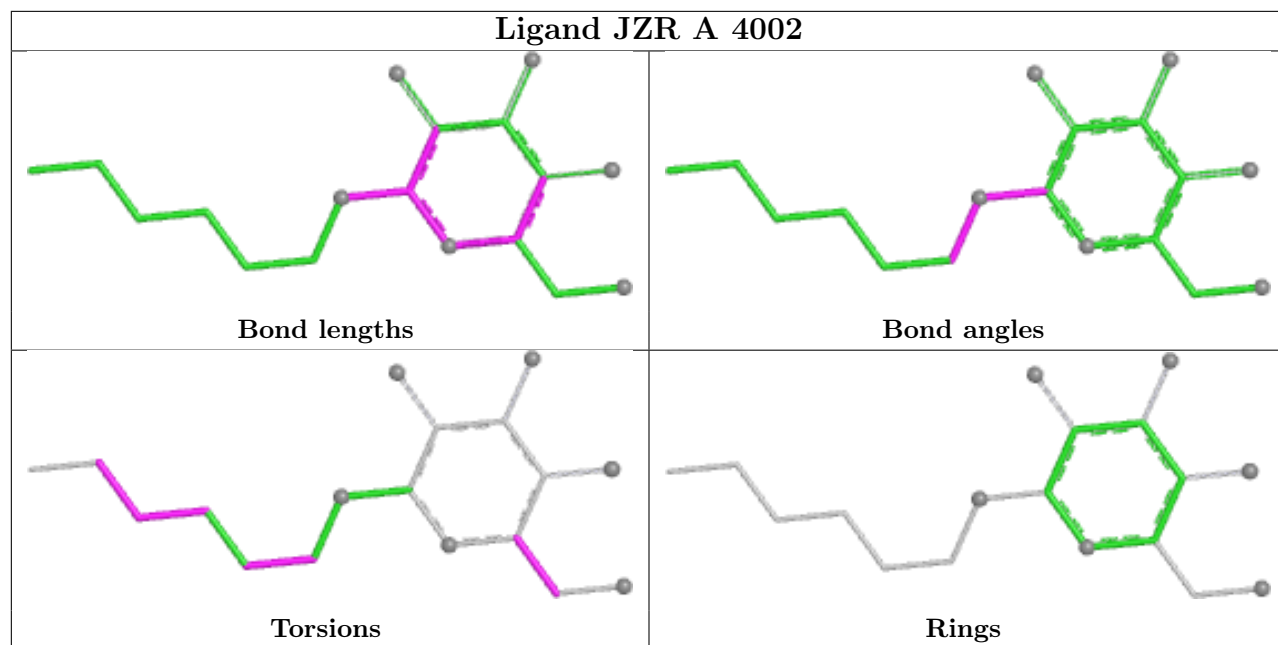


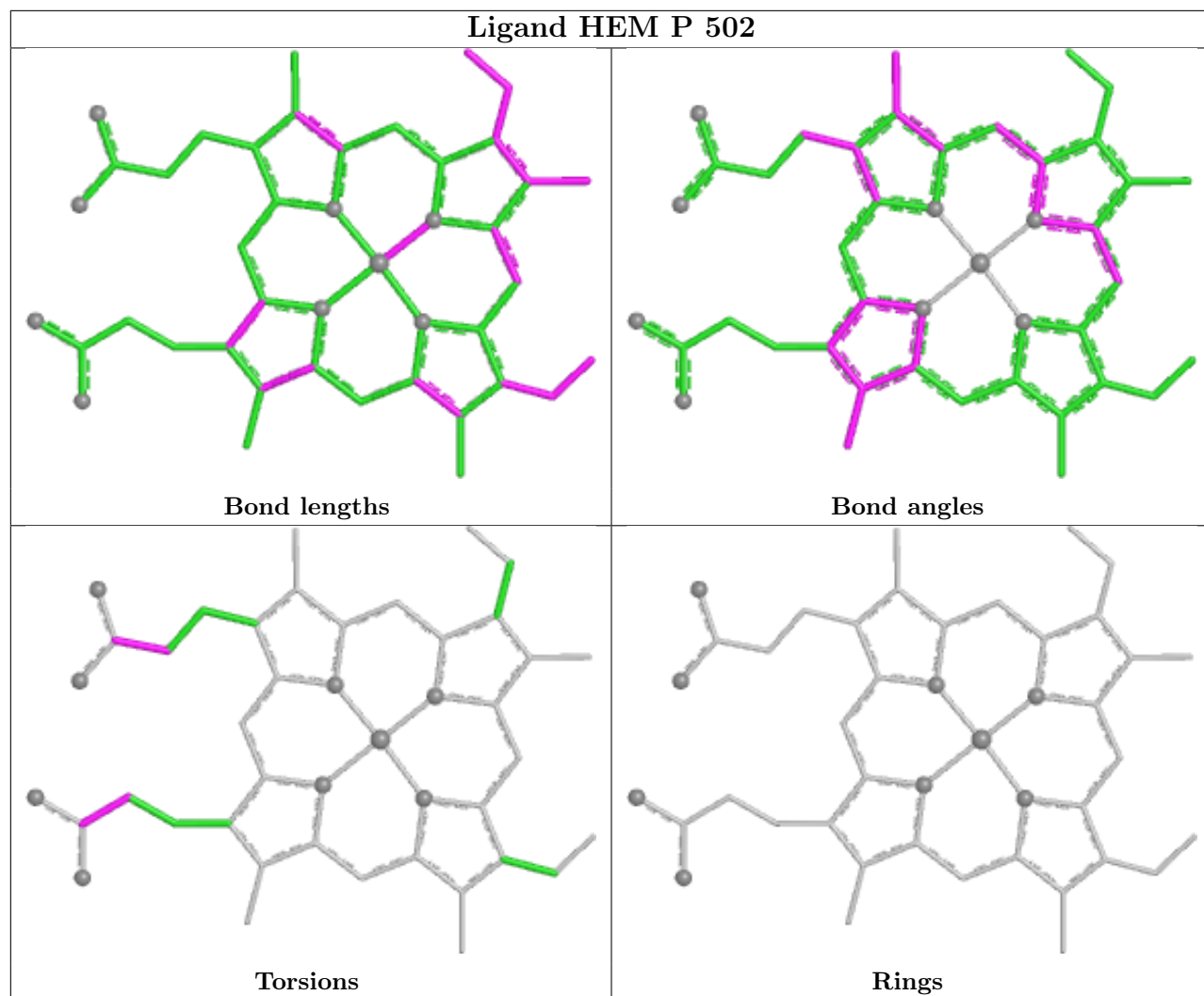




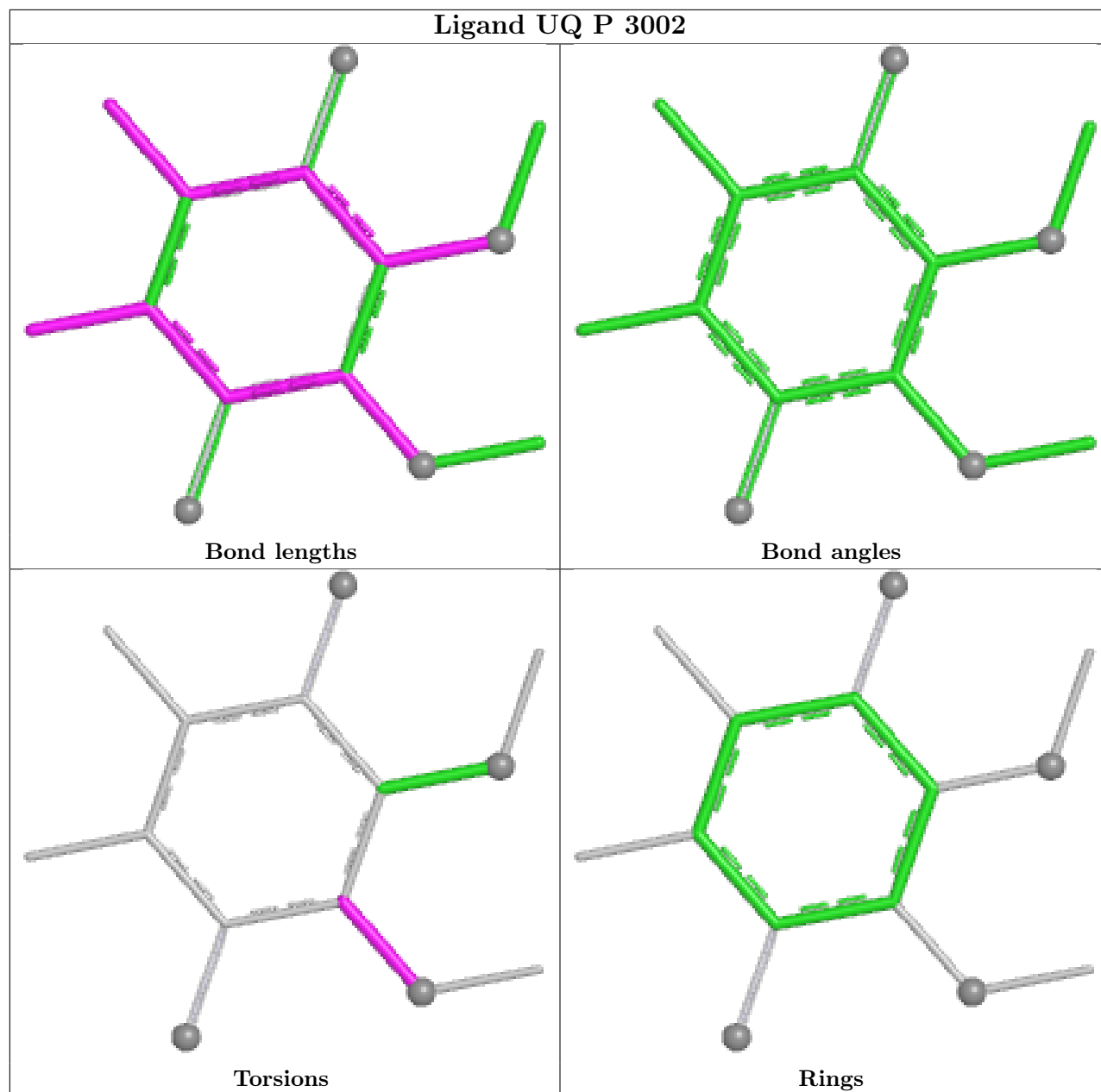


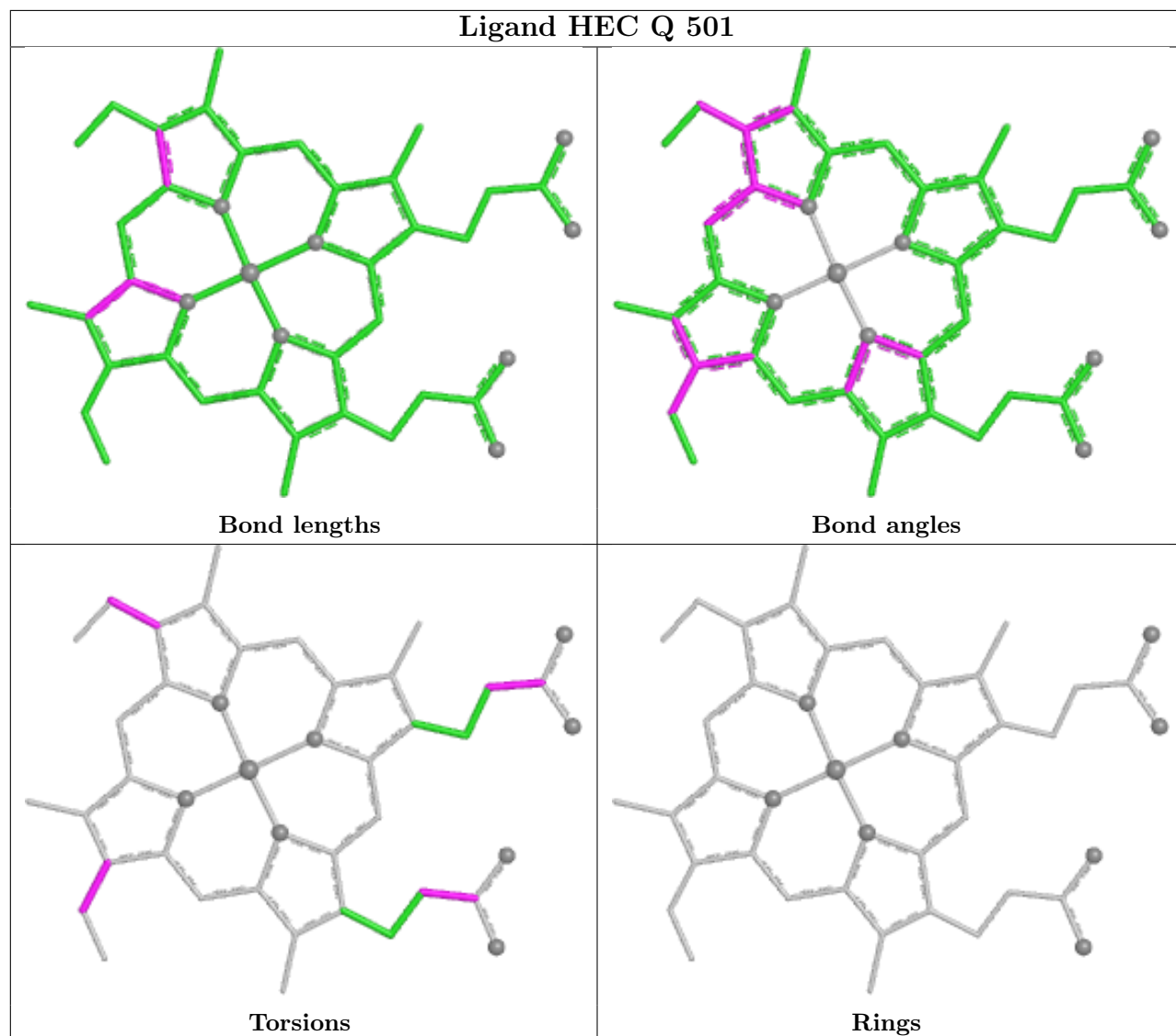
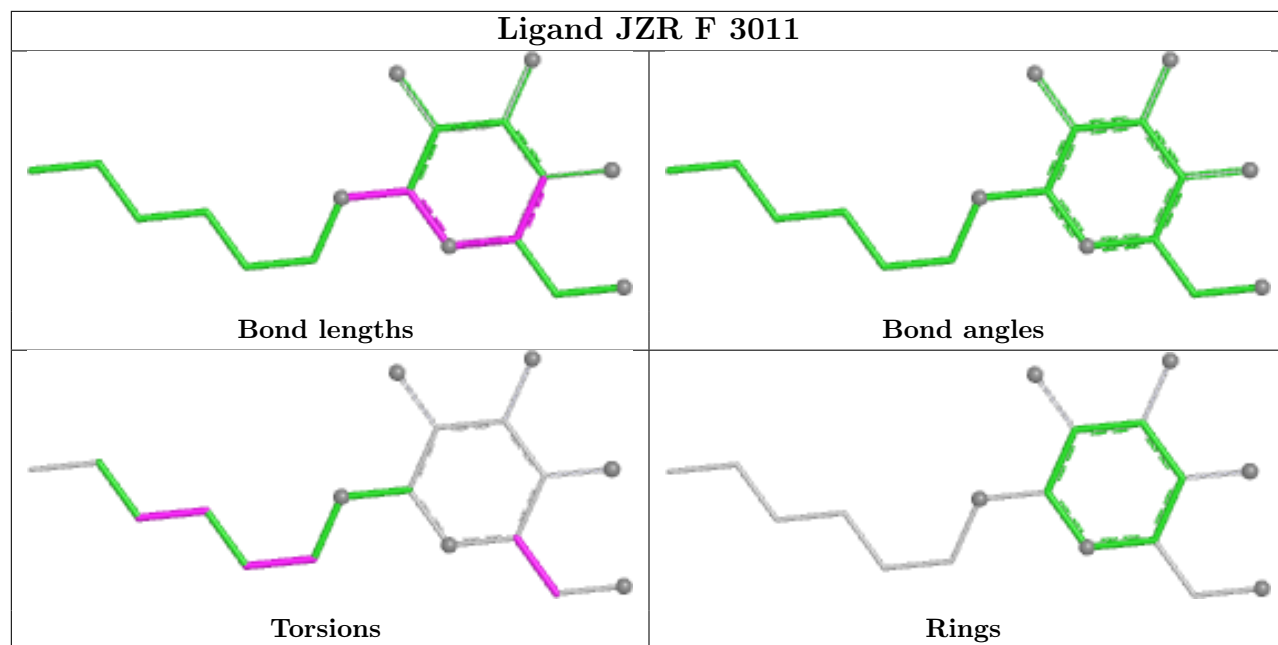


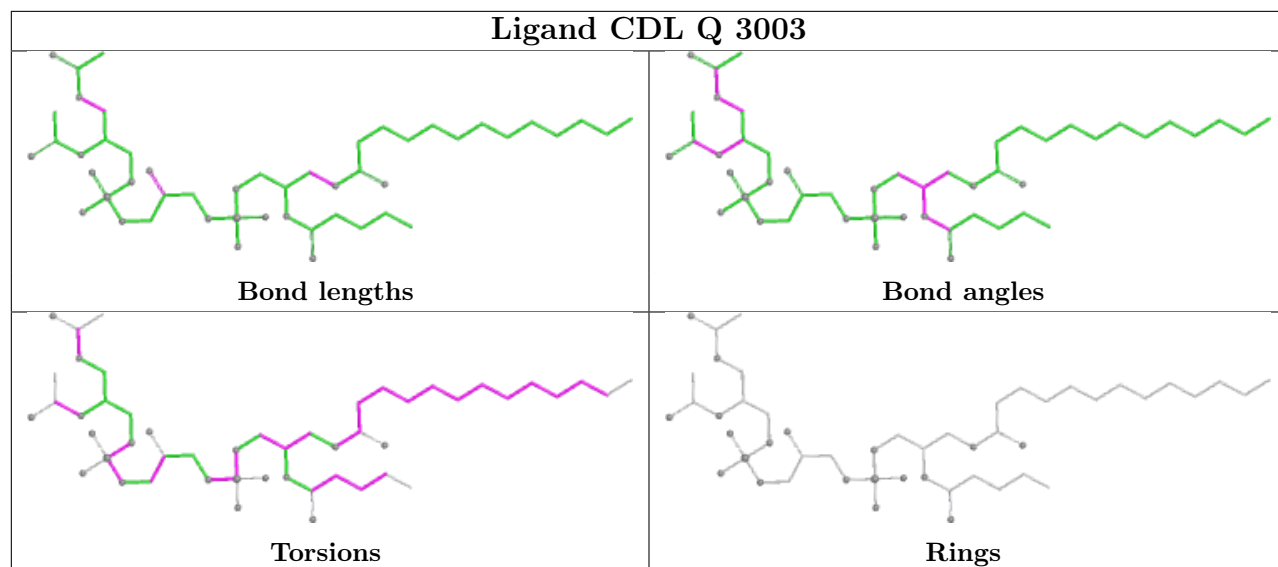


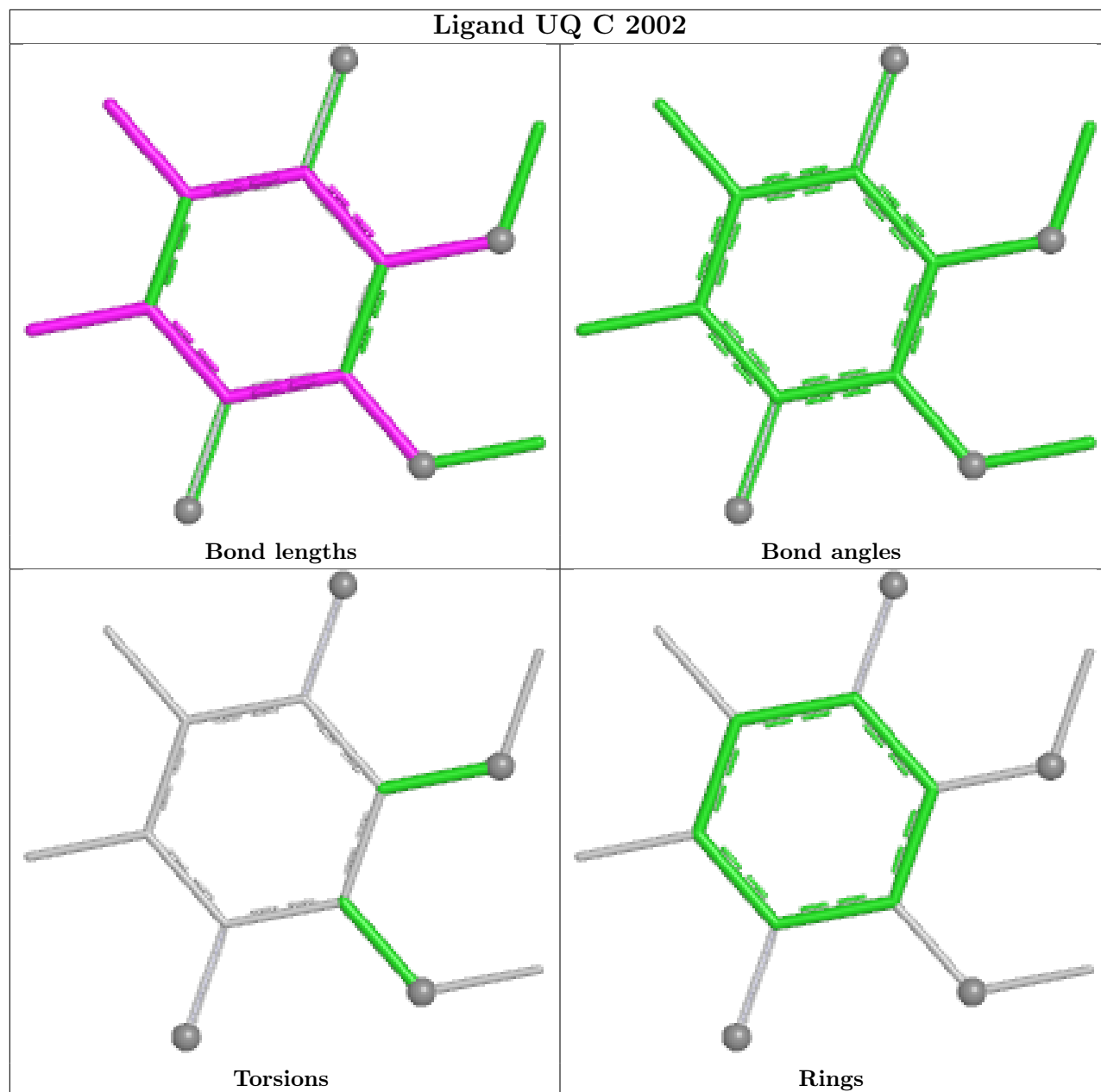


Ligand UQ P 3002









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	442/446 (99%)	0.55	26 (5%)	28 30	27, 43, 65, 115	1 (0%)
1	N	442/446 (99%)	0.60	19 (4%)	40 41	28, 43, 63, 128	1 (0%)
2	B	424/439 (96%)	0.64	27 (6%)	25 27	29, 45, 67, 132	0
2	O	424/439 (96%)	0.80	36 (8%)	16 17	33, 47, 73, 162	0
3	C	365/379 (96%)	0.15	7 (1%)	66 69	25, 34, 47, 106	0
3	P	370/379 (97%)	0.23	12 (3%)	50 53	26, 34, 52, 165	0
4	D	241/241 (100%)	0.27	6 (2%)	58 61	28, 39, 59, 80	0
4	Q	241/241 (100%)	0.26	3 (1%)	76 78	28, 38, 59, 81	0
5	E	196/196 (100%)	1.21	42 (21%)	2 2	29, 54, 96, 117	0
5	R	196/196 (100%)	0.51	2 (1%)	79 81	29, 43, 61, 85	0
6	F	99/110 (90%)	0.51	5 (5%)	33 35	29, 44, 70, 80	0
6	S	99/110 (90%)	0.53	10 (10%)	12 13	28, 39, 79, 109	0
7	G	75/81 (92%)	0.90	5 (6%)	24 25	31, 50, 72, 80	0
7	T	76/81 (93%)	1.09	10 (13%)	7 7	30, 50, 97, 117	0
8	H	66/78 (84%)	1.26	12 (18%)	3 3	40, 55, 87, 101	0
8	U	66/78 (84%)	1.18	15 (22%)	2 2	40, 54, 79, 89	0
9	I	42/78 (53%)	3.56	33 (78%)	0 0	40, 75, 88, 93	0
9	V	42/78 (53%)	3.26	33 (78%)	0 0	45, 72, 92, 97	0
10	J	62/62 (100%)	1.23	12 (19%)	3 3	35, 60, 85, 116	0
10	W	62/62 (100%)	1.16	10 (16%)	4 5	34, 51, 80, 111	0
All	All	4030/4220 (95%)	0.64	325 (8%)	18 19	25, 42, 76, 165	2 (0%)

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	222	THR	12.6
1	A	222	THR	11.1
7	T	1	GLY	9.1
3	P	13	ILE	8.6
9	I	63	PRO	8.4
2	O	19	PRO	7.5
6	S	12	TRP	7.4
9	I	78	TYR	7.4
3	P	10	LEU	7.4
7	G	1	GLY	7.3
2	O	12	GLU	7.2
9	I	72	VAL	7.1
10	J	1	VAL	7.1
9	V	78	TYR	6.9
2	O	232	LEU	6.8
9	V	32	ALA	6.6
9	V	42	VAL	6.6
3	P	14	VAL	6.4
9	I	76	VAL	6.3
6	S	13	LEU	6.2
2	O	17	VAL	6.1
6	F	12	TRP	6.1
9	I	70	LEU	6.0
2	B	233	SER	5.9
2	B	41	TYR	5.9
3	C	17	ALA	5.8
9	V	34	VAL	5.8
9	V	48	SER	5.7
2	B	12	GLU	5.6
3	P	18	PHE	5.5
9	I	61	GLY	5.4
9	I	60	ALA	5.4
2	B	232	LEU	5.4
9	I	71	ASN	5.2
10	W	61	ASN	5.2
9	I	48	SER	5.2
1	N	228	VAL	5.1
9	I	73	PRO	5.1
2	O	230	LEU	5.1
9	V	70	LEU	5.0
9	V	33	ALA	5.0
2	O	229	GLY	4.9
9	I	34	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	N	221	GLY	4.8
2	B	17	VAL	4.8
9	I	42	VAL	4.8
7	T	75	ALA	4.8
9	V	35	PRO	4.7
9	I	32	ALA	4.7
9	V	76	VAL	4.6
1	A	1	THR	4.6
10	W	62	LYS	4.6
2	O	21	PRO	4.6
9	I	50	LEU	4.6
2	O	233	SER	4.6
5	E	106	ILE	4.5
1	N	229	PRO	4.5
1	A	2	ALA	4.5
7	T	76	ALA	4.5
2	O	18	PRO	4.4
9	V	63	PRO	4.4
10	J	61	ASN	4.4
6	S	14	GLU	4.3
10	W	1	VAL	4.3
9	I	49	VAL	4.2
6	S	16	ILE	4.2
2	B	18	PRO	4.2
9	V	50	LEU	4.2
9	I	77	ARG	4.1
2	O	228	GLY	4.1
9	V	49	VAL	4.1
2	B	19	PRO	4.1
9	V	62	ARG	4.1
10	J	2	ALA	4.0
1	A	221	GLY	4.0
9	I	59	ALA	4.0
5	E	71	MET	4.0
9	I	35	PRO	3.9
3	C	18	PHE	3.9
8	H	47	ARG	3.9
5	E	111	ALA	3.9
1	A	228	VAL	3.8
1	N	220	SER	3.8
10	W	2	ALA	3.8
9	I	62	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	187	PHE	3.8
5	E	194	ILE	3.7
5	E	70	ALA	3.7
9	V	41	PRO	3.7
1	A	443	TRP	3.7
2	O	231	GLY	3.7
5	E	110	ALA	3.7
5	E	191	ASP	3.6
1	A	227	ALA	3.6
9	I	55	LEU	3.6
7	T	73	ASN	3.6
8	H	48	SER	3.6
5	E	81	ILE	3.6
9	V	72	VAL	3.5
3	P	16	ASN	3.5
5	E	104	LYS	3.5
5	E	193	VAL	3.5
3	P	17	ALA	3.5
1	A	75	LEU	3.5
5	E	133	VAL	3.5
7	T	72	LYS	3.5
2	O	20	HIS	3.4
2	O	303	VAL	3.4
1	N	210	ASP	3.4
9	V	36	ALA	3.4
5	E	112	VAL	3.3
1	N	225	GLU	3.3
9	V	39	GLU	3.3
1	N	213	GLN	3.3
2	O	234	GLY	3.3
9	I	57	GLY	3.3
5	E	153	PHE	3.3
2	O	41	TYR	3.2
8	H	45	SER	3.2
9	V	37	THR	3.2
2	B	20	HIS	3.2
9	V	55	LEU	3.2
2	O	26	PHE	3.2
10	J	3	PRO	3.2
5	E	195	VAL	3.2
5	E	132	TRP	3.1
9	V	52	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	GLU	3.1
5	E	102	THR	3.1
5	E	114	VAL	3.1
9	V	74	ALA	3.1
1	N	231	LEU	3.1
6	S	110	LYS	3.1
10	J	62	LYS	3.1
1	A	286	GLY	3.1
6	S	15	GLY	3.1
9	V	77	ARG	3.1
5	E	76	ILE	3.1
2	B	353	SER	3.1
9	I	41	PRO	3.1
1	A	224	ASP	3.0
9	I	74	ALA	3.0
9	I	64	LEU	3.0
1	A	81	SER	3.0
3	P	19	ILE	3.0
10	J	24	ILE	3.0
10	W	16	ARG	3.0
5	E	108	GLN	3.0
2	O	353	SER	3.0
8	H	46	SER	3.0
4	D	144	ARG	2.9
5	E	105	GLU	2.9
3	P	102	LEU	2.9
8	H	50	THR	2.9
5	E	130	PRO	2.9
7	T	74	PRO	2.9
7	G	30	PHE	2.9
7	T	30	PHE	2.9
6	F	18	LYS	2.9
8	H	78	LYS	2.9
1	N	1	THR	2.9
8	U	34	ARG	2.9
3	C	15	ASN	2.9
2	O	249	GLY	2.9
8	H	44	VAL	2.8
9	I	69	SER	2.8
2	B	23	ASP	2.8
8	H	27	LEU	2.8
5	E	134	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	52	ASN	2.8
1	A	210	ASP	2.8
5	E	75	GLU	2.8
2	B	249	GLY	2.8
2	B	250	ASP	2.7
2	O	350	GLY	2.7
1	N	230	THR	2.7
9	V	61	GLY	2.7
2	B	303	VAL	2.7
1	N	232	SER	2.7
5	E	129	LYS	2.7
2	B	281	ALA	2.7
7	G	75	ALA	2.7
3	C	102	LEU	2.7
2	O	355	PRO	2.7
2	O	24	LEU	2.6
8	U	27	LEU	2.6
8	U	71	HIS	2.6
9	I	75	SER	2.6
9	V	40	SER	2.6
9	I	51	CYS	2.6
2	O	265	GLY	2.6
9	V	71	ASN	2.6
9	V	73	PRO	2.6
2	O	236	LYS	2.6
7	T	70	LYS	2.6
5	E	127	VAL	2.6
1	A	202	GLY	2.6
9	I	37	THR	2.6
5	E	82	PRO	2.6
8	H	49	GLN	2.6
9	V	68	VAL	2.6
3	C	16	ASN	2.6
2	B	291	ALA	2.6
4	D	2	ASP	2.6
5	E	123	ASP	2.6
1	N	81	SER	2.6
2	B	251	SER	2.6
4	Q	17	LEU	2.6
6	S	19	TRP	2.6
1	N	288	ALA	2.5
7	T	28	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	206	ARG	2.5
8	H	34	ARG	2.5
9	V	60	ALA	2.5
9	V	64	LEU	2.5
8	U	45	SER	2.5
10	J	4	THR	2.5
2	O	235	ALA	2.5
5	E	93	GLY	2.5
2	O	250	ASP	2.4
3	P	12	LYS	2.4
5	E	103	LYS	2.4
9	I	56	ARG	2.4
10	W	8	ARG	2.4
3	P	11	MET	2.4
1	N	219	LEU	2.4
6	S	73	GLN	2.4
2	O	211	VAL	2.4
10	J	11	SER	2.4
5	R	35	PHE	2.4
8	U	47	ARG	2.4
2	B	304	HIS	2.4
7	G	28	HIS	2.4
2	B	439	LEU	2.3
1	N	316	ASP	2.3
5	E	168	SER	2.3
4	D	17	LEU	2.3
5	R	69	LEU	2.3
9	V	57	GLY	2.3
5	E	101	ARG	2.3
2	B	74	SER	2.3
5	E	122	HIS	2.3
7	T	45	ILE	2.3
8	H	71	HIS	2.3
1	A	230	THR	2.3
2	B	21	PRO	2.3
10	J	19	THR	2.3
2	O	348	ALA	2.3
10	J	16	ARG	2.3
4	Q	79	GLU	2.3
5	E	35	PHE	2.3
5	E	109	GLU	2.3
9	I	54	SER	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	121	GLN	2.3
2	O	227	ARG	2.3
2	O	421	ARG	2.3
1	A	315	ALA	2.3
2	B	348	ALA	2.3
5	E	107	ASP	2.3
6	S	108	ALA	2.3
4	D	143	LEU	2.3
8	U	39	LEU	2.3
4	D	145	GLU	2.2
9	V	54	SER	2.2
10	W	24	ILE	2.2
8	H	31	VAL	2.2
8	U	44	VAL	2.2
8	U	36	ARG	2.2
8	U	78	LYS	2.2
1	A	122	LEU	2.2
5	E	100	HIS	2.2
1	A	206	ARG	2.2
2	O	302	GLY	2.2
9	V	51	CYS	2.2
1	A	213	GLN	2.2
3	C	155	TYR	2.2
5	E	184	SER	2.2
5	E	80	ASP	2.2
1	A	11	VAL	2.2
2	O	167	ALA	2.2
2	O	281	ALA	2.2
2	O	329	GLN	2.2
8	U	67	HIS	2.2
4	Q	241	LYS	2.2
2	B	350	GLY	2.1
7	G	3	GLN	2.1
6	S	109	LYS	2.1
4	D	45	TYR	2.1
2	O	221	GLU	2.1
10	J	17	THR	2.1
6	F	19	TRP	2.1
1	A	217	SER	2.1
2	B	24	LEU	2.1
8	U	24	CYS	2.1
8	U	48	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	22	GLN	2.1
10	W	4	THR	2.1
1	A	88	ALA	2.1
5	E	167	ALA	2.1
3	P	320	LEU	2.1
9	V	69	SER	2.1
10	W	5	LEU	2.1
10	W	13	LEU	2.1
2	B	154	ASN	2.1
1	A	229	PRO	2.1
2	O	304	HIS	2.1
2	B	265	GLY	2.1
3	C	168	PHE	2.1
1	A	10	SER	2.1
8	U	46	SER	2.1
1	A	231	LEU	2.0
2	O	218	GLN	2.0
6	F	87	LYS	2.0
2	B	390	GLY	2.0
1	N	204	GLU	2.0
3	P	168	PHE	2.0
6	F	78	GLU	2.0
9	I	53	GLU	2.0
9	I	33	ALA	2.0
9	I	36	ALA	2.0
5	E	78	LEU	2.0
8	U	13	LEU	2.0
10	J	5	LEU	2.0
8	U	40	CYS	2.0
1	A	201	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	JZR	A	4002	18/18	0.42	0.39	130,143,145,145	0
12	AZI	P	3014	3/3	0.42	0.34	54,54,55,61	0
14	PO4	B	3010	5/5	0.58	0.16	99,100,100,100	0
11	JZR	F	3011	18/18	0.59	0.34	114,118,122,122	0
11	JZR	S	2011	18/18	0.60	0.32	73,86,91,91	0
15	GOL	O	3013	6/6	0.63	0.35	112,115,116,116	0
13	PEE	N	3012	5/51	0.64	0.15	94,94,94,96	0
12	AZI	D	4004	3/3	0.64	0.28	69,69,72,73	0
12	AZI	C	2014	3/3	0.64	0.27	53,53,57,59	0
18	UQ	C	2002	14/63	0.65	0.31	74,78,80,82	0
15	GOL	B	2013	6/6	0.66	0.44	145,148,148,149	0
13	PEE	C	2012	5/51	0.67	0.18	116,116,116,116	0
11	JZR	F	4001	18/18	0.68	0.31	168,171,173,173	0
11	JZR	C	2008	18/18	0.69	0.28	109,112,116,116	0
13	PEE	A	4003	6/51	0.69	0.23	110,111,112,113	0
13	PEE	T	3005	49/51	0.71	0.35	96,121,136,136	0
13	PEE	G	2005	49/51	0.73	0.34	105,123,129,129	0
18	UQ	P	3002	14/63	0.73	0.35	90,93,97,97	0
15	GOL	C	2009	6/6	0.75	0.33	56,59,63,67	0
14	PO4	O	2010	5/5	0.75	0.14	106,106,107,108	0
11	JZR	P	3008	18/18	0.76	0.25	100,102,107,109	0
21	CDL	G	2003	50/100	0.77	0.23	62,96,113,113	0
15	GOL	P	3009	6/6	0.80	0.26	59,65,67,68	0
12	AZI	A	4005	3/3	0.80	0.30	72,72,73,74	0
21	CDL	Q	3003	50/100	0.80	0.18	55,78,90,92	0
21	CDL	G	2004	44/100	0.81	0.21	62,79,105,107	0
13	PEE	D	2006	51/51	0.83	0.21	52,66,94,95	0
13	PEE	Q	3006	51/51	0.84	0.19	45,59,83,83	0
21	CDL	T	3004	49/100	0.86	0.18	54,69,98,101	0
13	PEE	C	2007	49/51	0.88	0.16	39,53,68,69	0
13	PEE	P	3007	49/51	0.91	0.14	35,54,62,63	0
17	SMA	C	2001	37/37	0.94	0.08	25,30,32,38	0
17	SMA	P	3001	37/37	0.94	0.08	24,32,37,37	0
19	HEC	Q	501	43/43	0.97	0.07	32,35,36,37	0
20	FES	E	501	4/4	0.97	0.05	34,35,37,37	0
16	HEM	C	502	43/43	0.98	0.06	22,26,31,33	0
16	HEM	P	501	43/43	0.98	0.07	25,29,37,42	0

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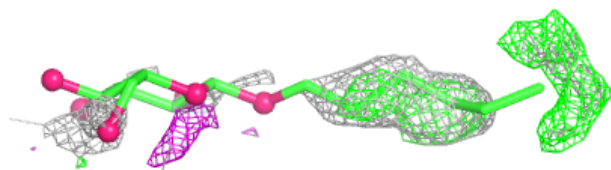
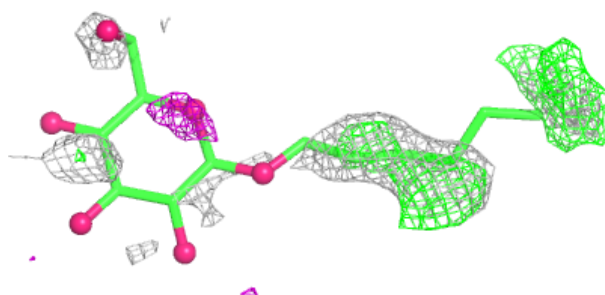
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	HEM	P	502	43/43	0.98	0.07	24,27,32,37	0
19	HEC	D	501	43/43	0.98	0.07	29,33,36,38	0
16	HEM	C	501	43/43	0.98	0.06	21,26,33,37	0
20	FES	R	501	4/4	0.99	0.04	31,31,33,33	0

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.

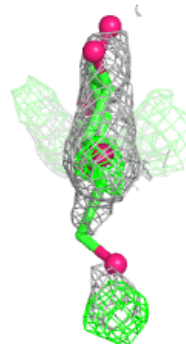
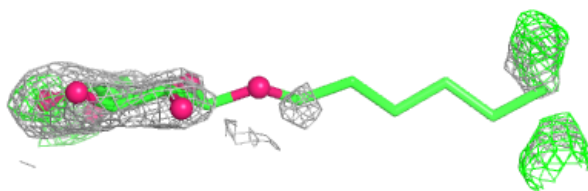
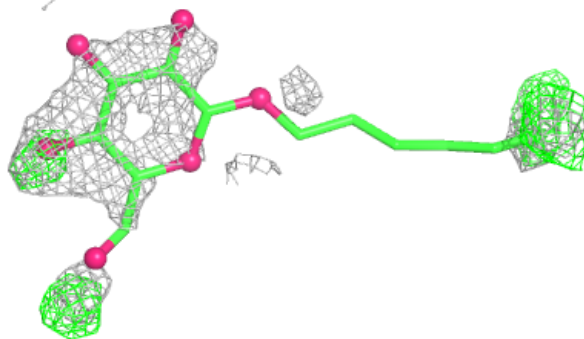
Electron density around JZR A 4002:

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

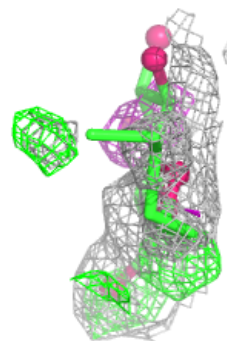
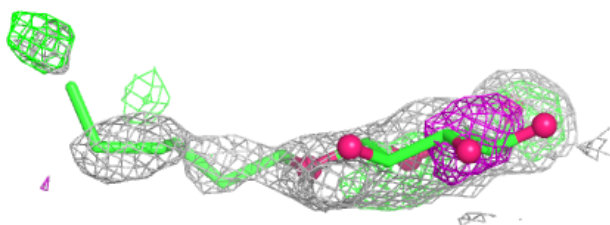
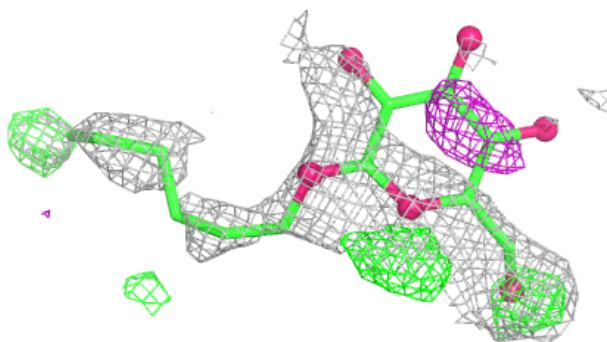


Electron density around JZR F 3011:

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

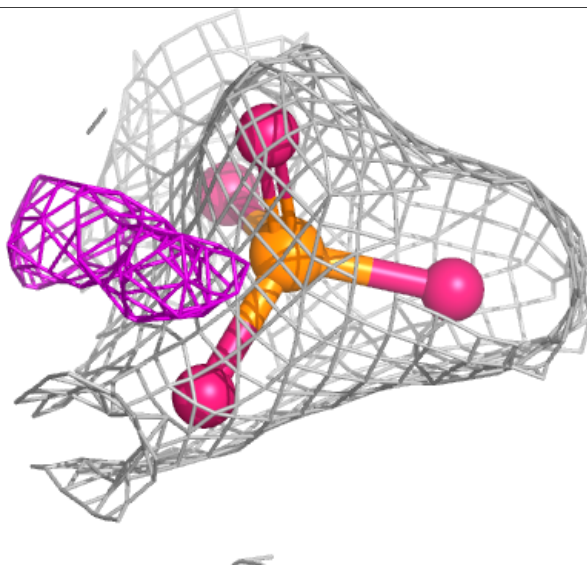
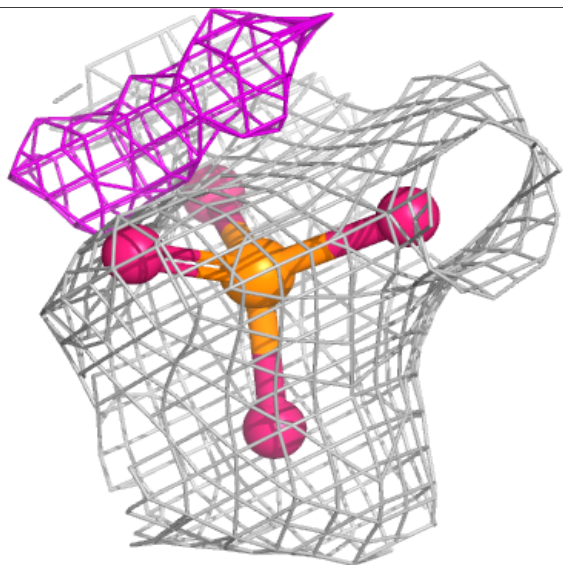
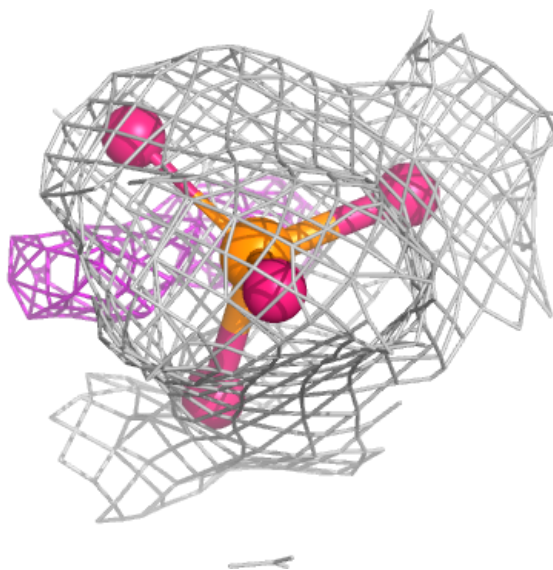
**Electron density around JZR S 2011:**

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



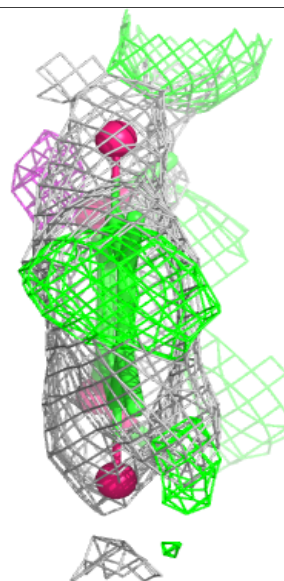
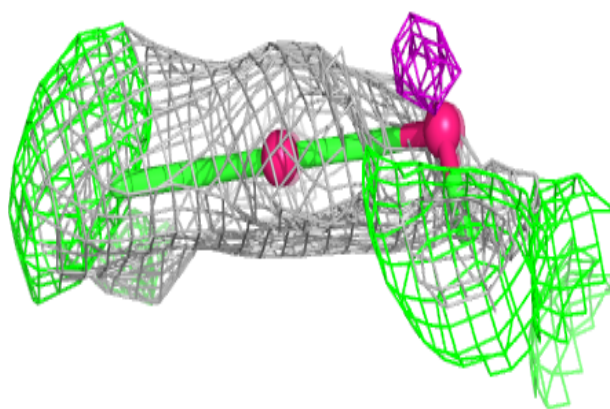
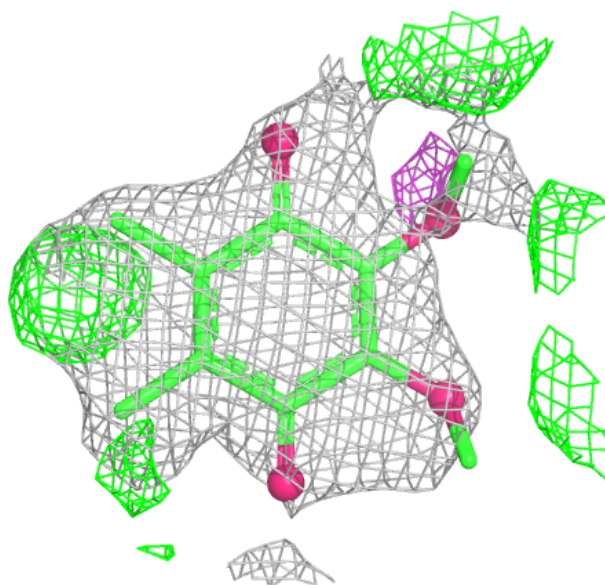
Electron density around PEE N 3012:

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



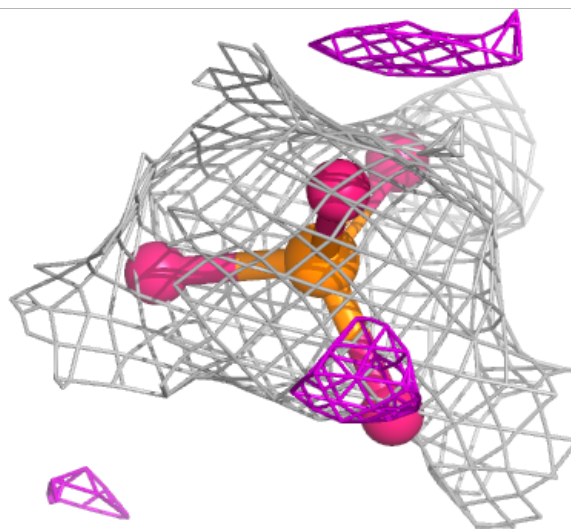
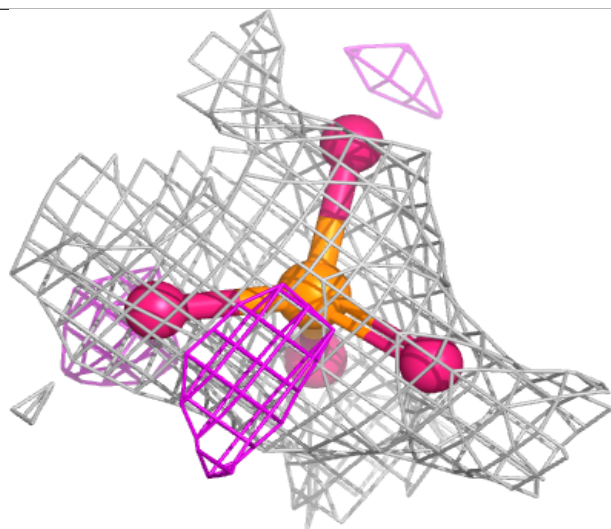
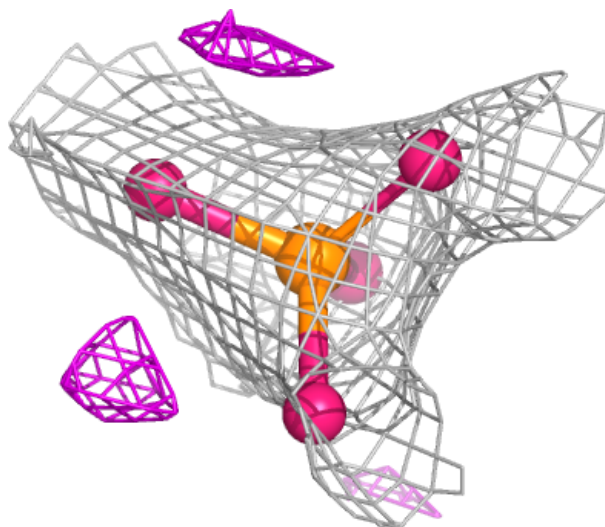
Electron density around UQ C 2002:

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



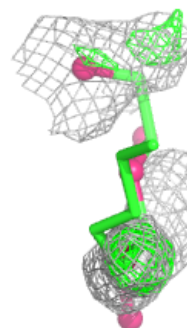
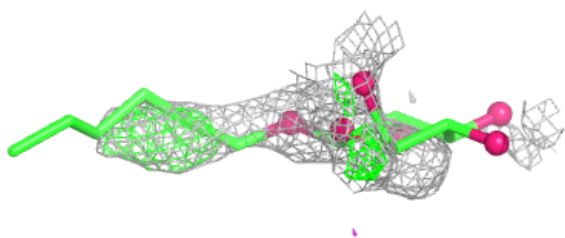
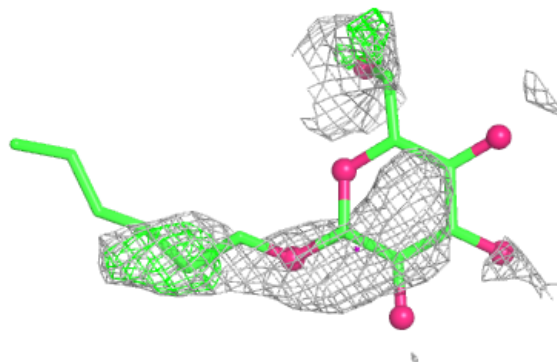
Electron density around PEE C 1012:

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

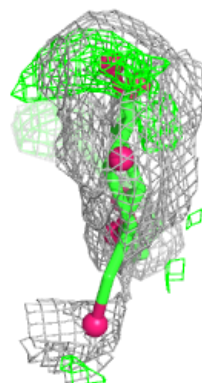
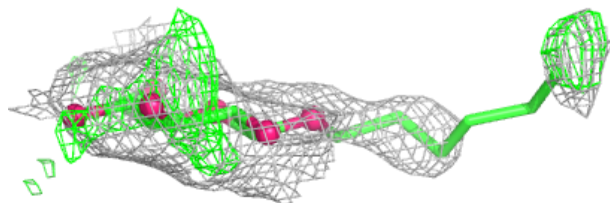
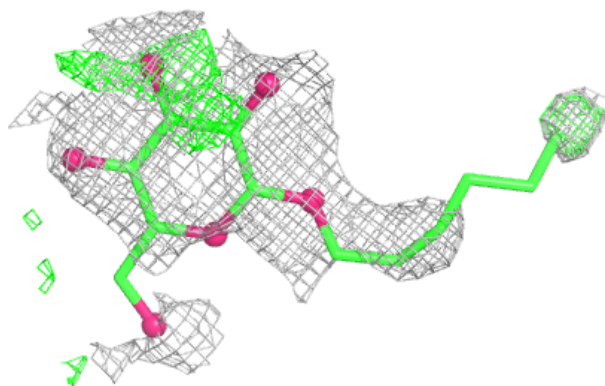


Electron density around JZR F 4001:

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

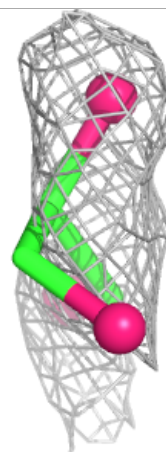
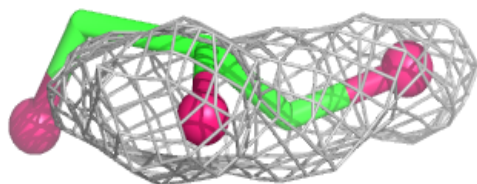
**Electron density around JZR C 2008:**

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



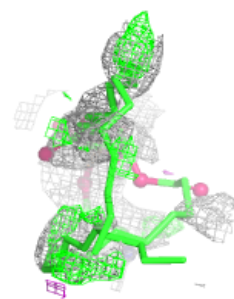
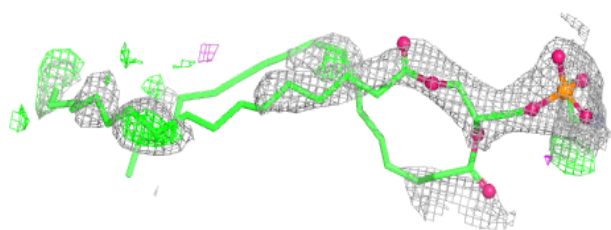
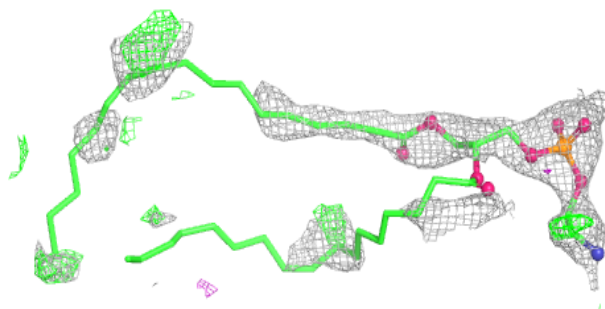
Electron density around PEE A 4003:

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

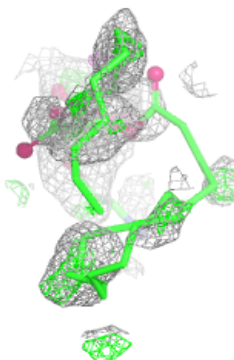
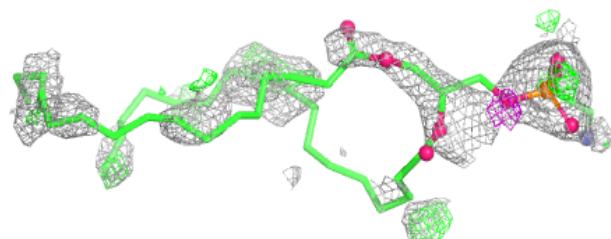
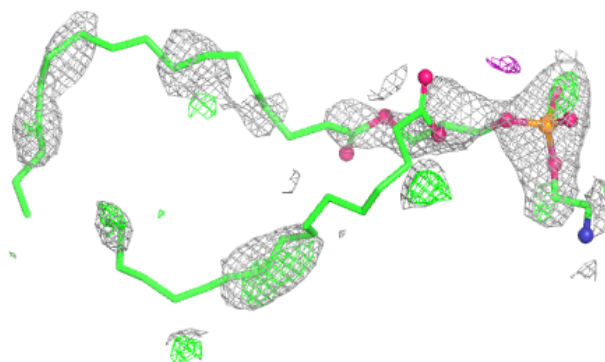


Electron density around PEE T 3005:

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

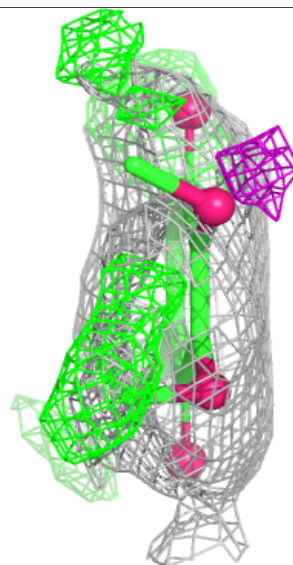
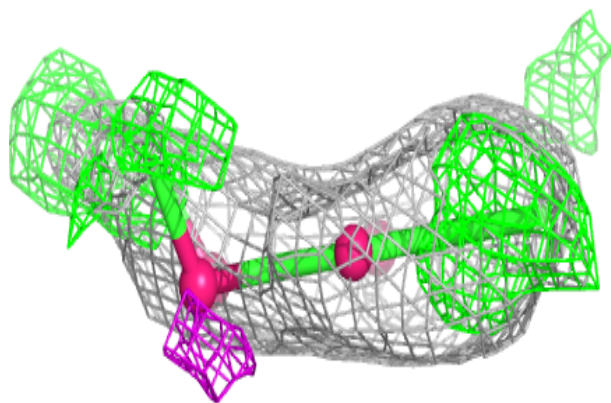
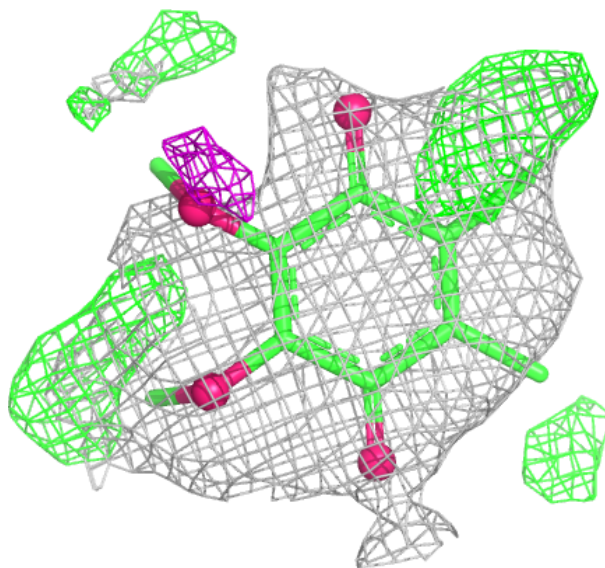
**Electron density around PEE G 2005:**

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



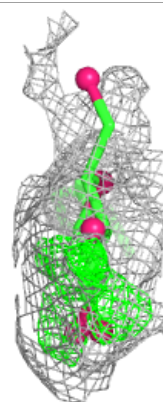
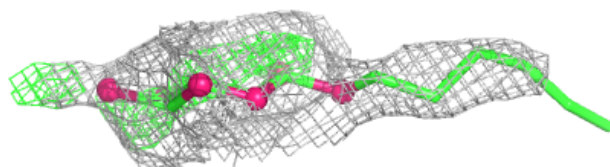
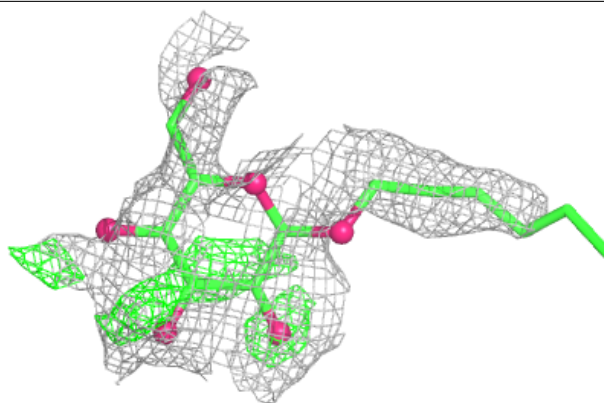
Electron density around UQ P 3002:

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

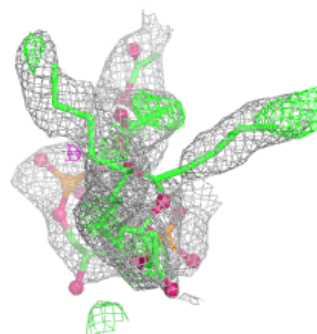
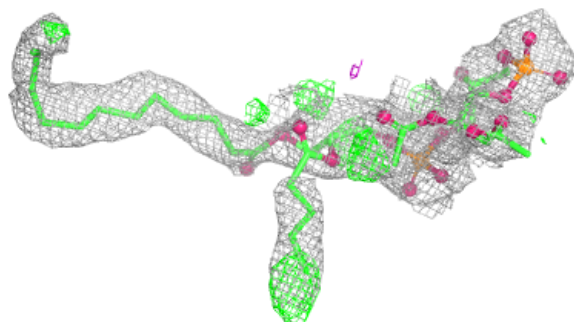
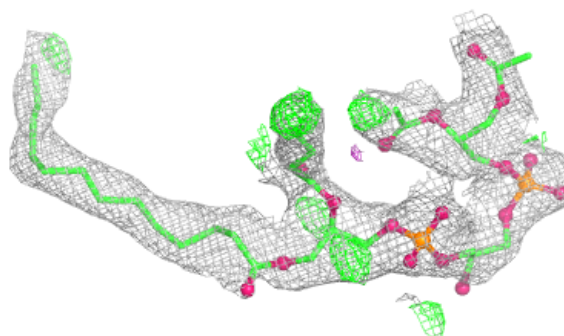


Electron density around JZR P 3008:

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

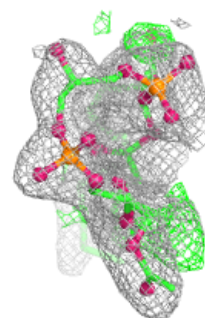
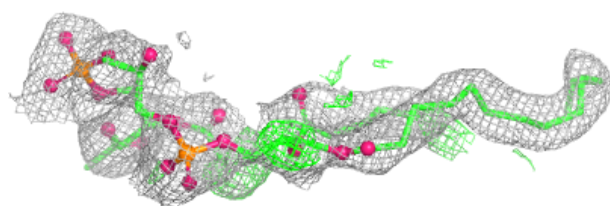
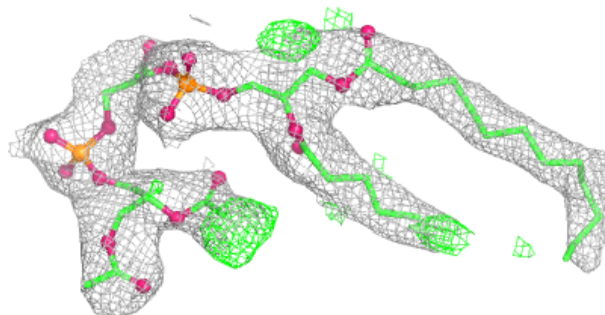
**Electron density around CDL G 2003:**

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

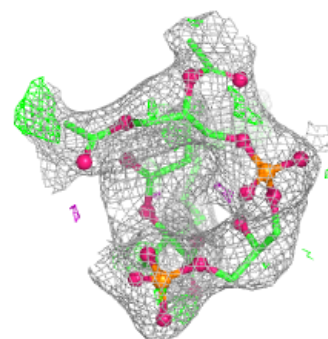
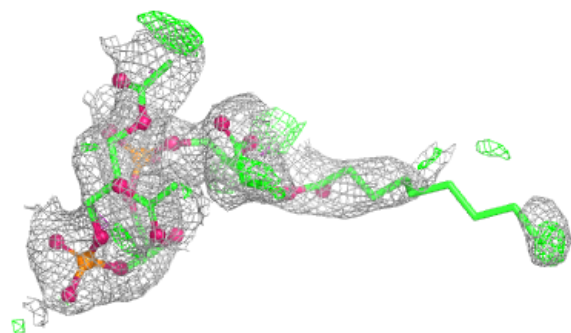
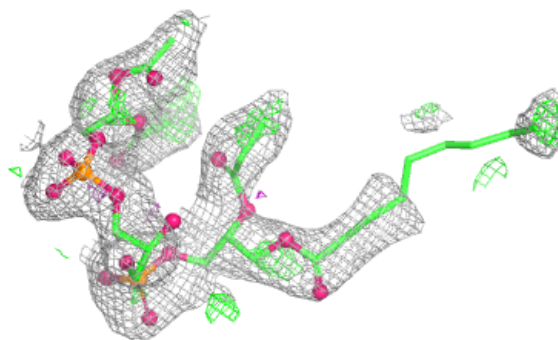


Electron density around CDL Q 3003:

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

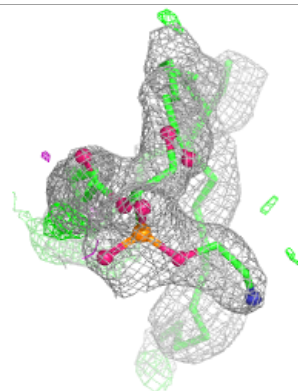
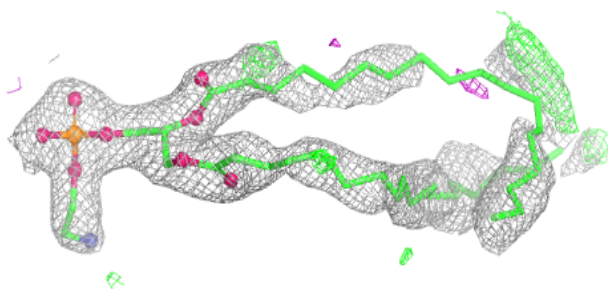
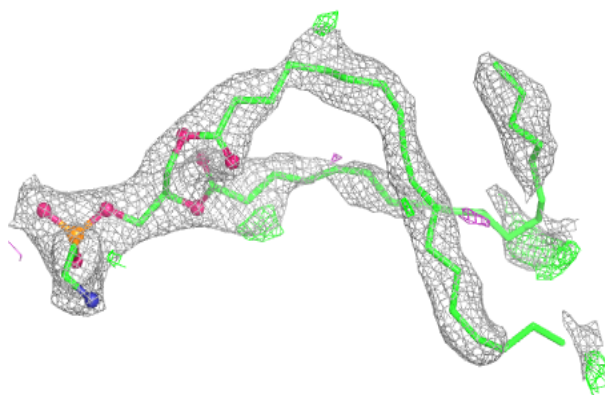
**Electron density around CDL G 2004:**

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

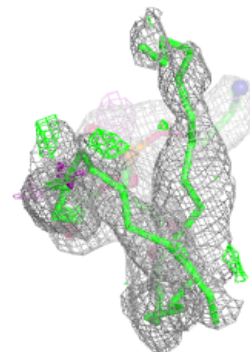
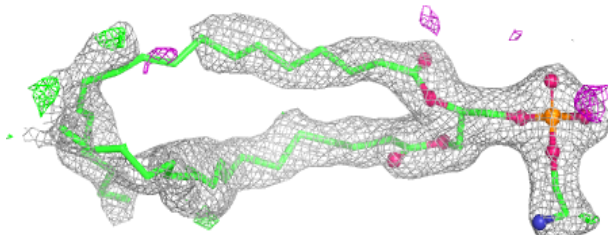
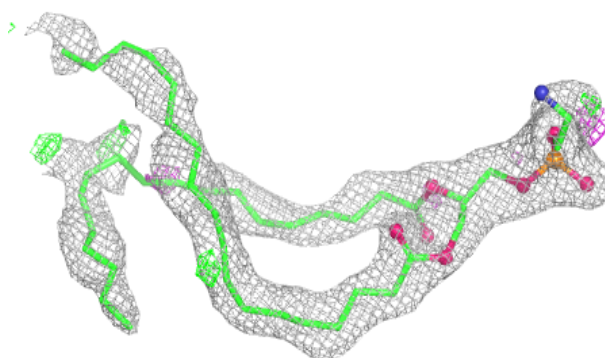


Electron density around PEE D 2006:

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

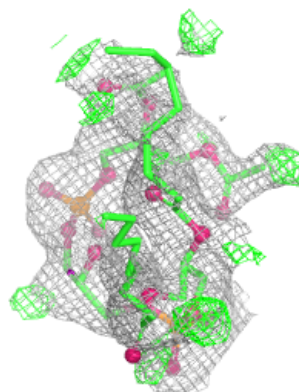
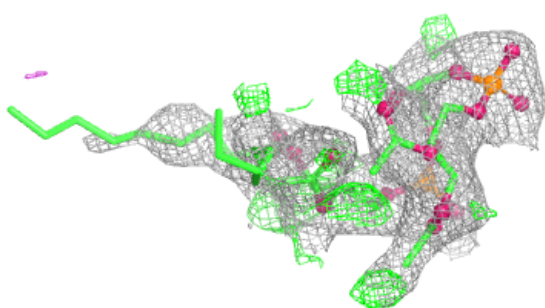
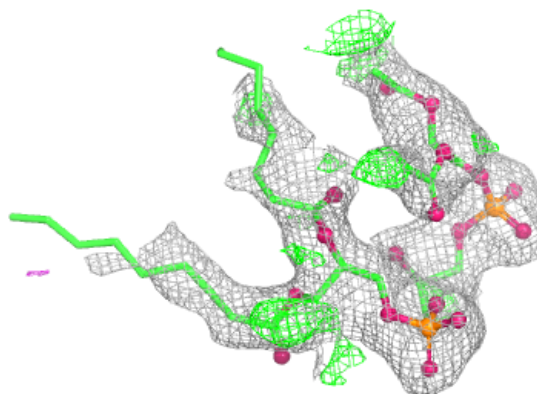
**Electron density around PEE Q 3006:**

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

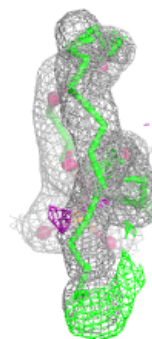
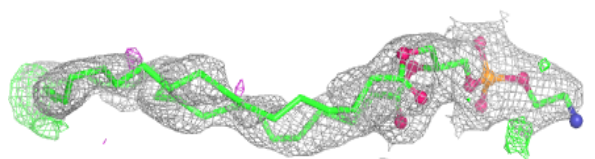
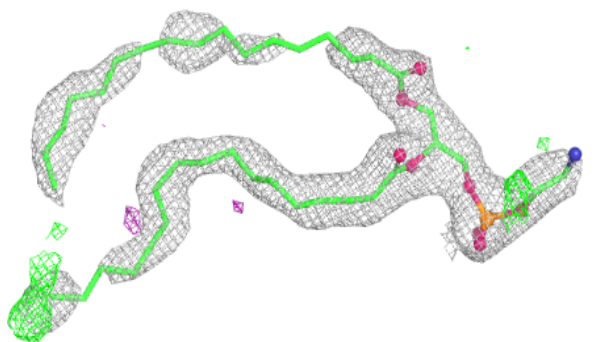


Electron density around CDL T 3004:

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

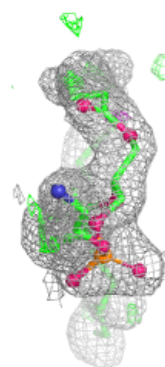
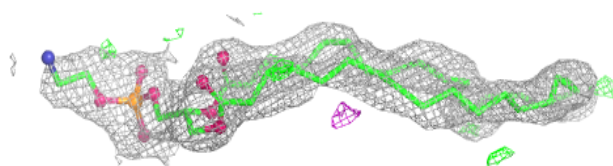
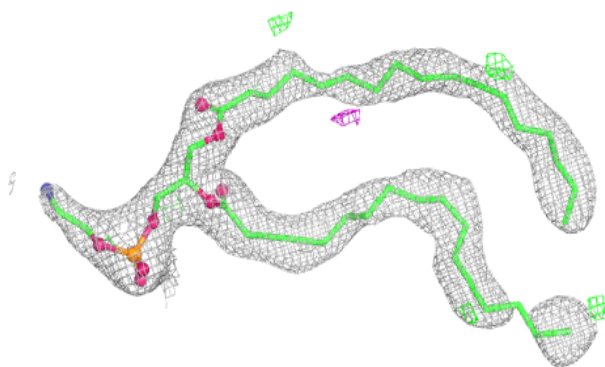
**Electron density around PEE C 2007:**

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

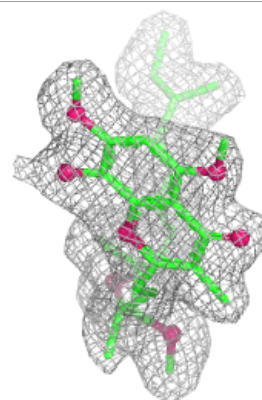
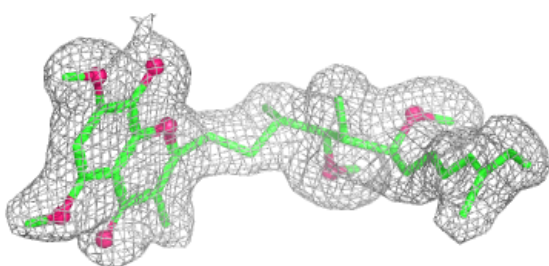
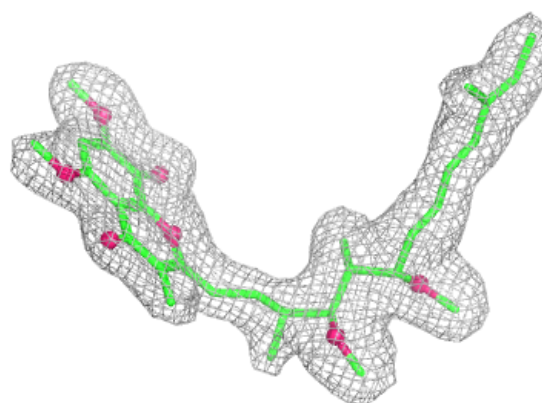


Electron density around PEE P 3007:

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

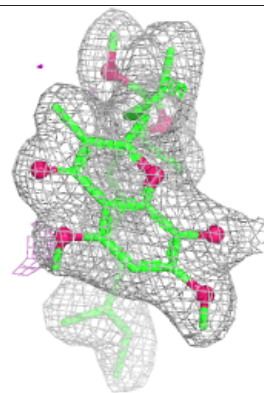
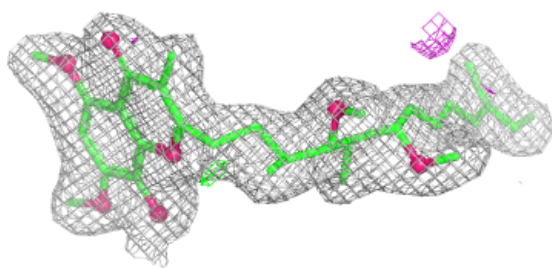
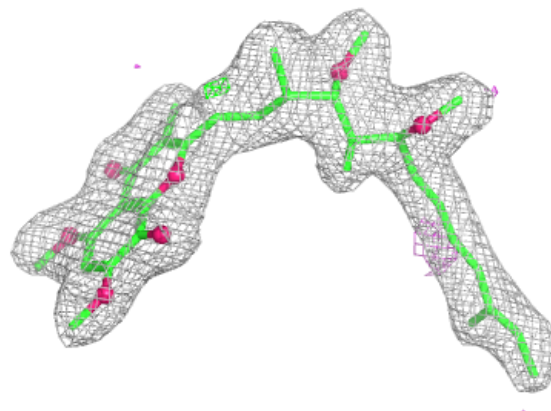
**Electron density around SMA C 2001:**

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



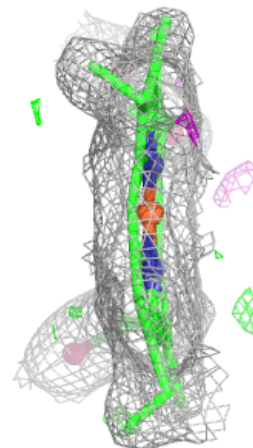
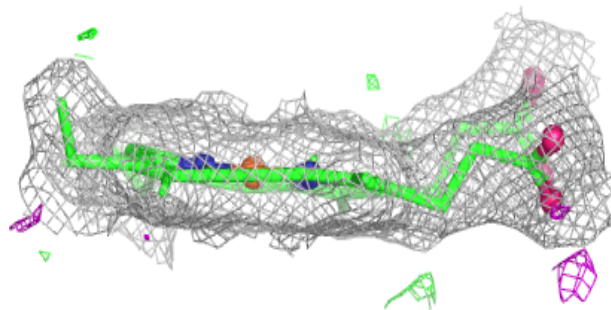
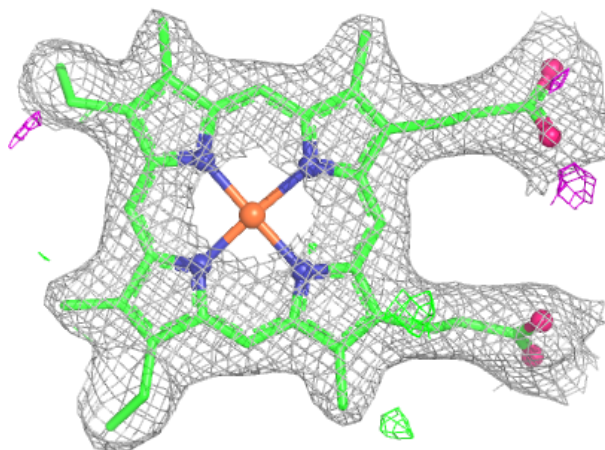
Electron density around SMA P 3001:

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



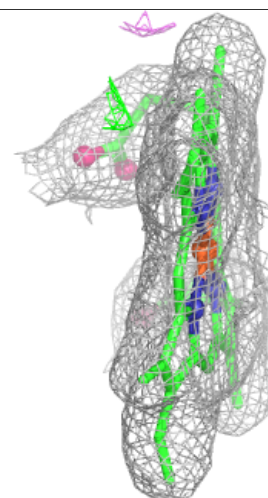
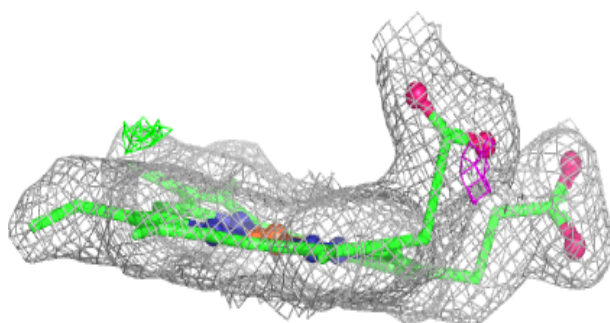
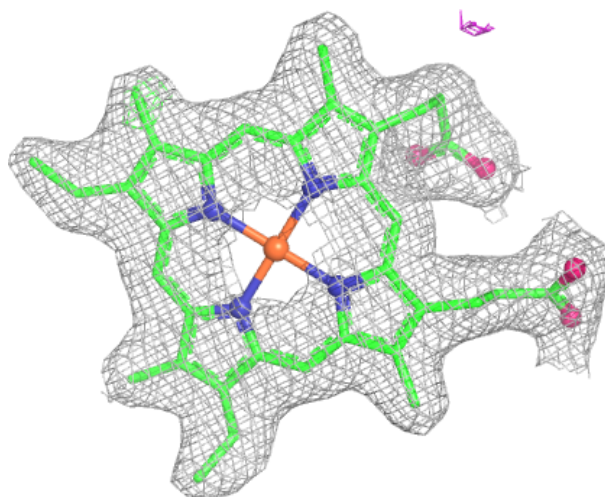
Electron density around HEC Q 501:

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



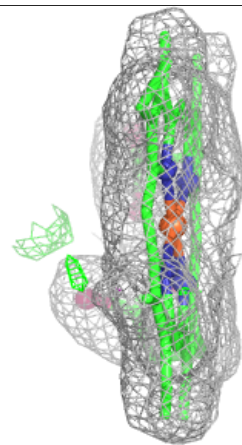
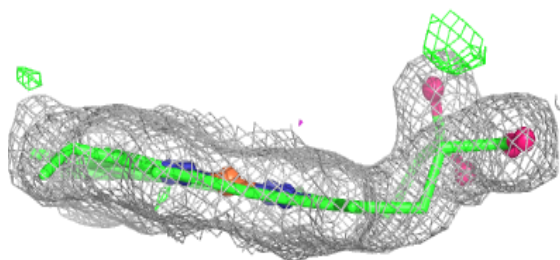
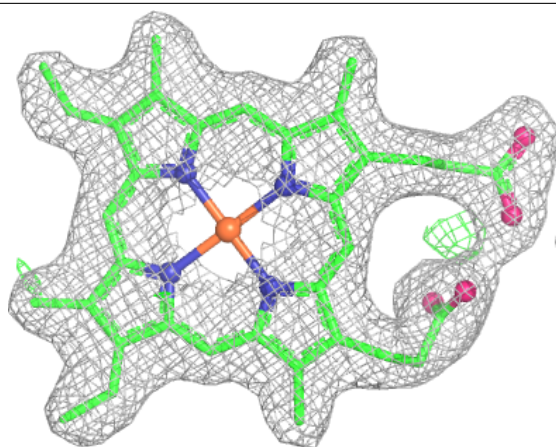
Electron density around HEM C 502:

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



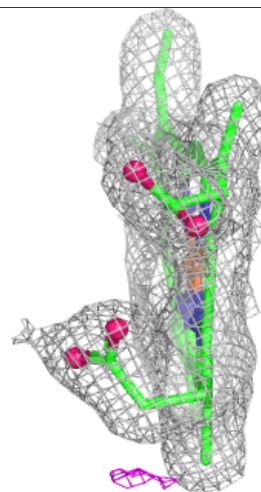
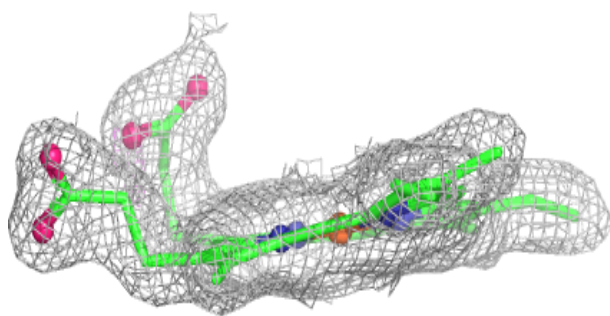
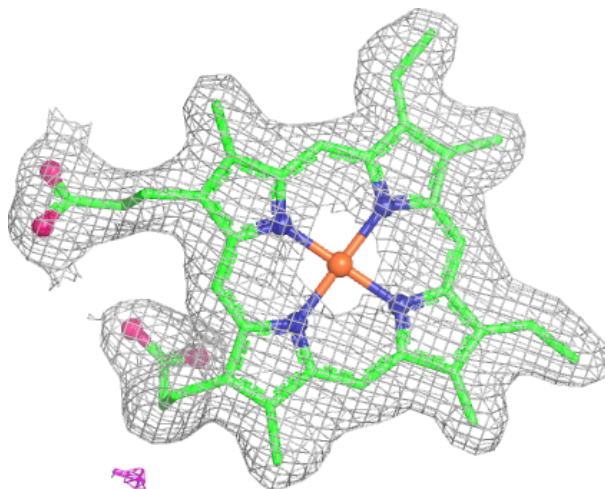
Electron density around HEM P 501:

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



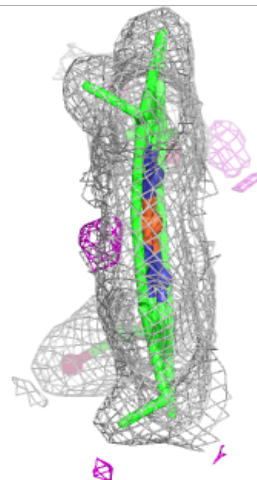
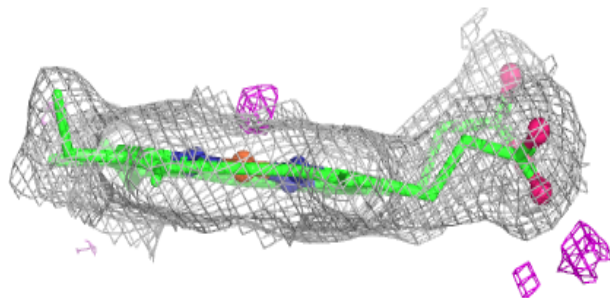
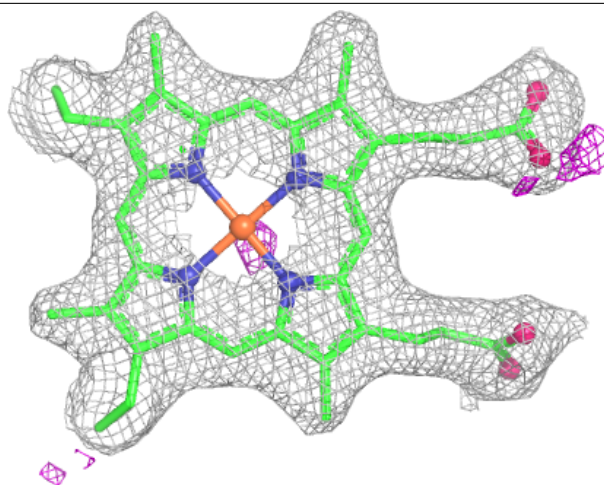
Electron density around HEM P 502:

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



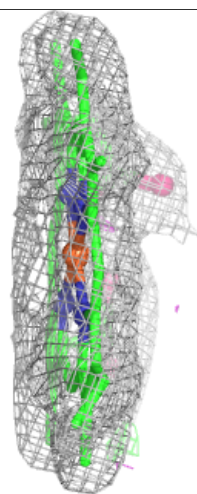
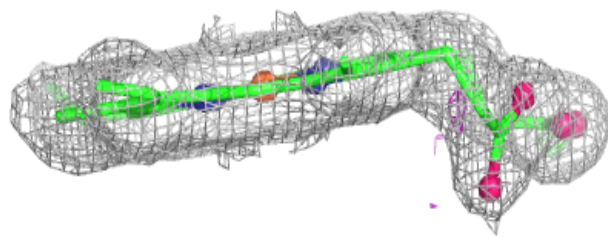
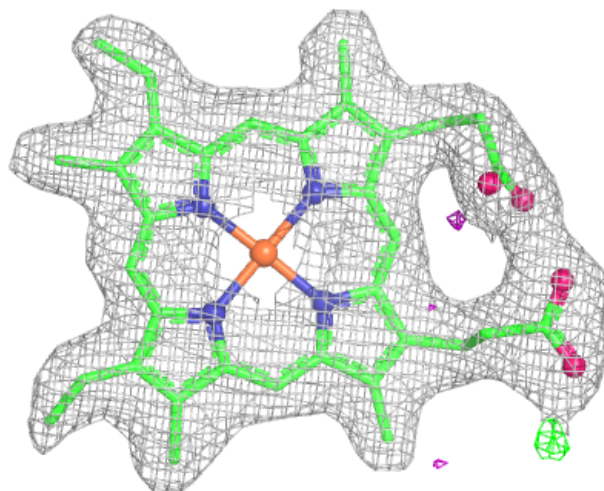
Electron density around HEC D 501:

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



Electron density around HEM C 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.