Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 06:26 PM EDT

PDB ID	:	1PPJ / pdb_00001ppj
Title	:	Bovine cytochrome bc1 complex with stigmatellin and antimycin
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 (i) 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 (i)) were used in the production of this report:

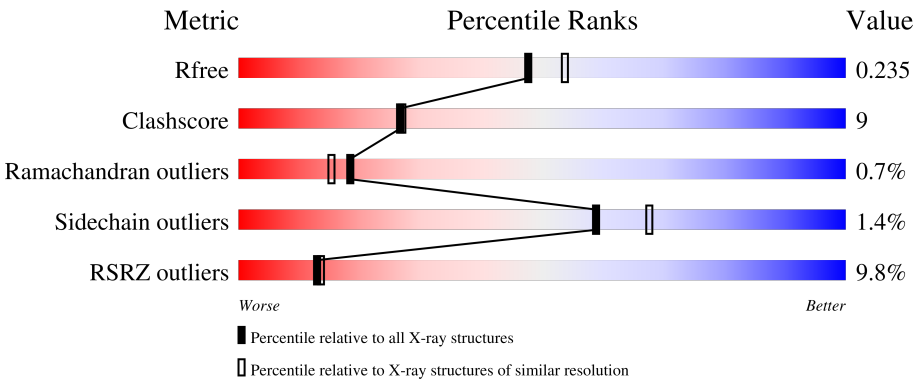
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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 <=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	5%, 78%, 19%, • •
1	N	446	9%, 78%, 19%, • •
2	B	439	4%, 78%, 18%, • •
2	O	439	10%, 80%, 16%, •
3	C	379	2%, 78%, 16%, • •

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Mol	Chain	Length	Quality of chain
3	P	379	3% 77% 18%
4	D	241	2% 85% 15%
4	Q	241	4% 84% 16%
5	E	196	26% 78% 19%
5	R	196	9% 74% 23%
6	F	110	5% 78% 9% 10%
6	S	110	9% 74% 14% 10%
7	G	81	17% 64% 25% 7%
7	T	81	16% 68% 22% 6%
8	H	78	9% 71% 14% 15%
8	U	78	15% 69% 14% 15%
9	I	78	40% 24% 28% 45%
9	V	78	40% 28% 26% 45%
10	J	62	11% 40% 11% 47%
10	W	62	44% 53% 44%

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
13	AZI	A	4011	-	X	-	X
13	AZI	C	2005	-	X	-	-
13	AZI	G	4009	-	X	-	-
13	AZI	O	4010	-	X	-	-
13	AZI	P	3005	-	X	-	-
18	ANY	P	3002	X	-	-	-
19	HEC	D	501	X	-	-	-
19	HEC	Q	501	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 33549 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
			Total	C	N	O	S			
1	A	442	3396	2117	601	658	20	0	0	1
1	N	442	3396	2117	601	658	20	10	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	3178	1997	562	612	7	0	0	1
2	O	424	3156	1984	558	607	7	0	0	1

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	365	2892	1940	450	485	17	0	0	0
3	P	365	2891	1940	449	485	17	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1510	954	263	285	8	0	0	0
5	R	196	1517	956	263	290	8	0	0	0

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

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

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

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

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

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

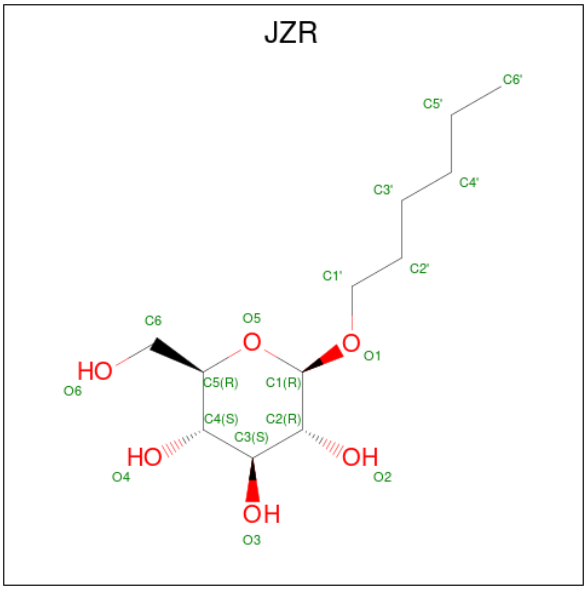
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	43	285	175	53	56	1	0	0	0
9	V	43	285	175	53	56	1	0	0	0

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

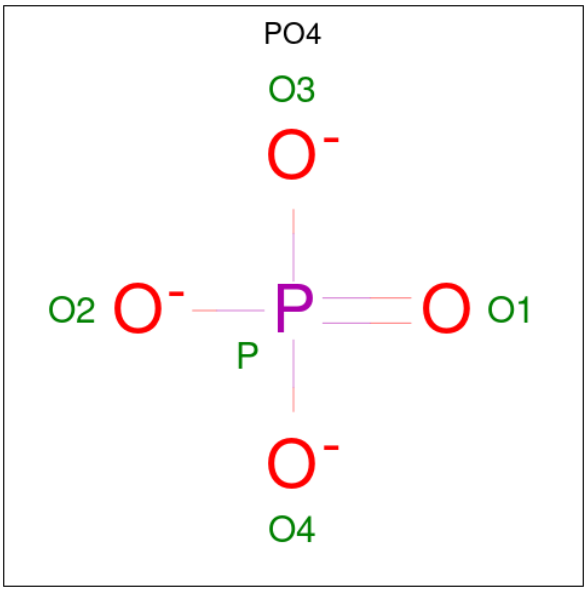
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	33	284	185	50	49	0	0	1
			Total	C	N	O			
10	W	62	506	332	88	86	0	0	1

- Molecule 11 is hexyl beta-D-glucopyranoside (CCD ID: JZR) (formula: $C_{12}H_{24}O_6$).



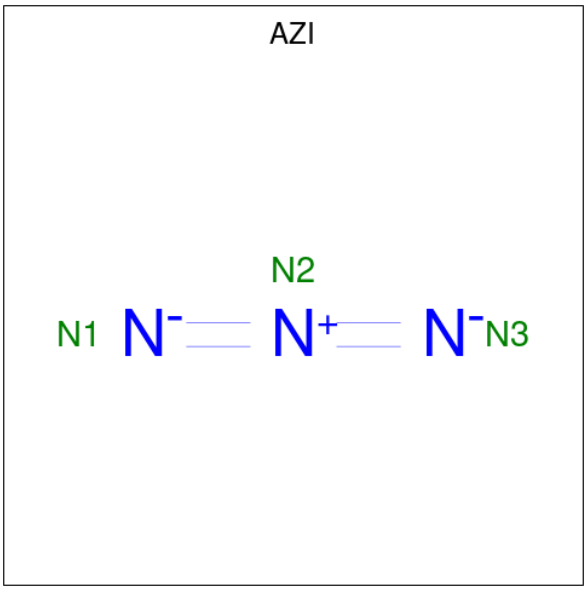
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
11	A	1	18	12	6		0	0
			Total	C	O			
11	C	1	18	12	6		0	0
			Total	C	O			
11	C	1	18	12	6		0	0
			Total	C	O			
11	D	1	18	12	6		0	0
			Total	C	O			
11	F	1	18	12	6		0	0
			Total	C	O			
11	F	1	18	12	6		0	0
			Total	C	O			
11	P	1	18	12	6		0	0
			Total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

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



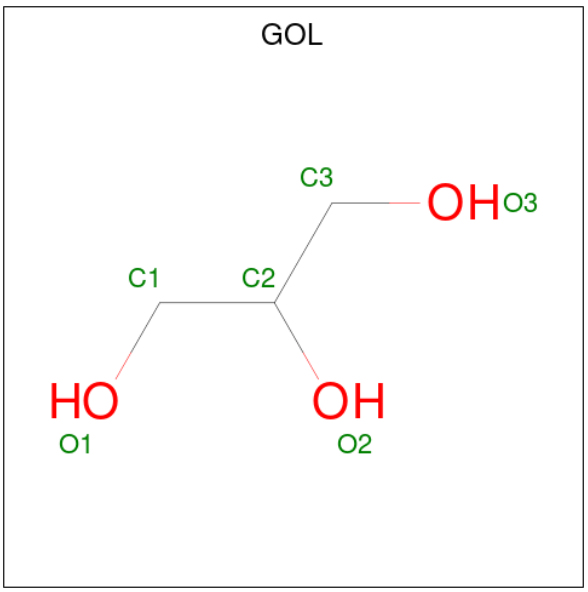
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O P 5 4 1	0	0
12	C	1	Total O P 5 4 1	0	0
12	F	1	Total O P 5 4 1	0	0
12	P	1	Total O P 5 4 1	0	0
12	S	1	Total O P 5 4 1	0	0

- Molecule 13 is AZIDE ION (CCD ID: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 3 3	0	0
13	C	1	Total N 3 3	0	0
13	G	1	Total N 3 3	0	0
13	O	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

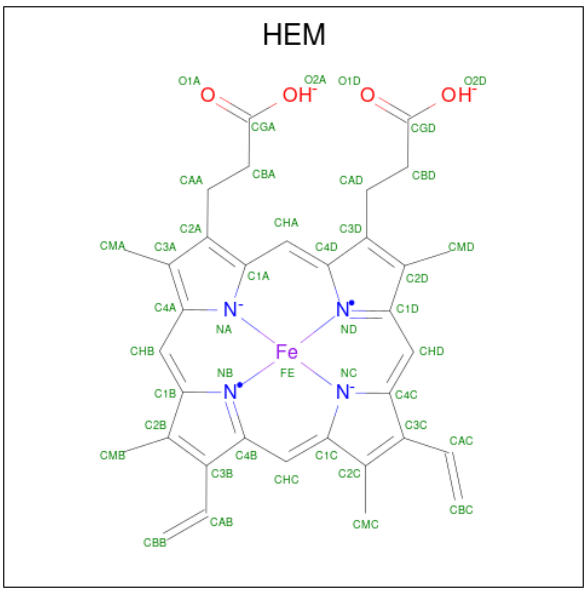
- Molecule 14 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

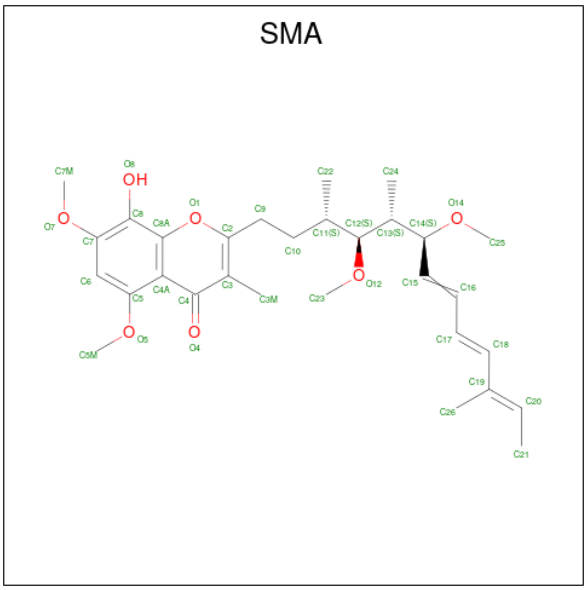
- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

$C_{34}H_{32}FeN_4O_4$).



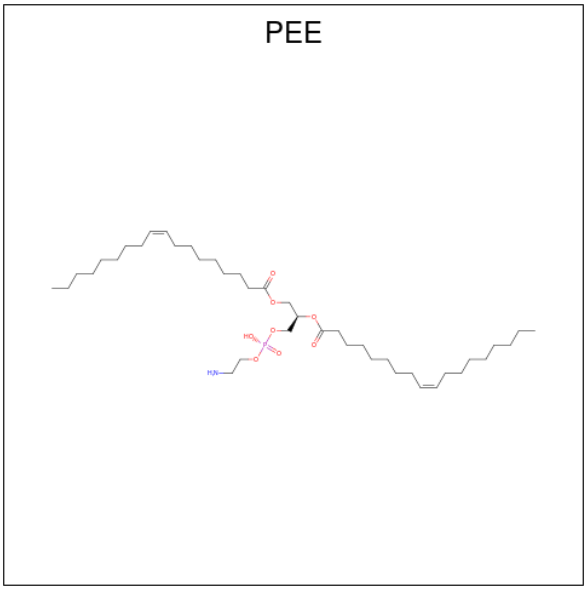
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
15	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
15	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
15	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
15	P	1	43	34	1	4	4	0	0

- Molecule 16 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



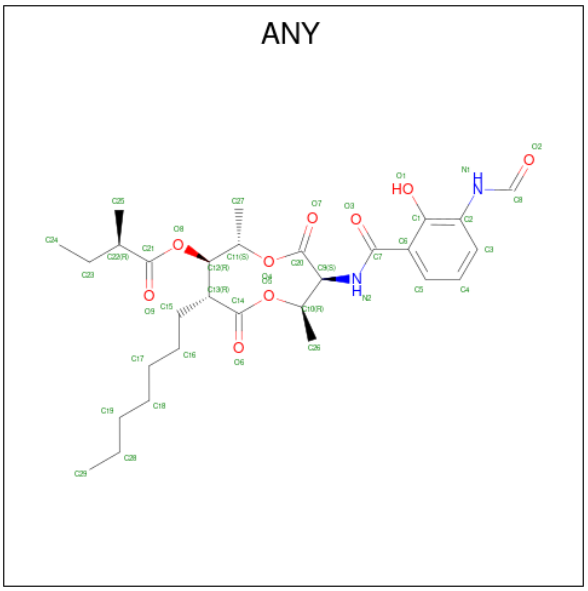
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	C	1	37	30	7	0	0
			Total	C	O		
16	P	1	37	30	7	0	0

- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



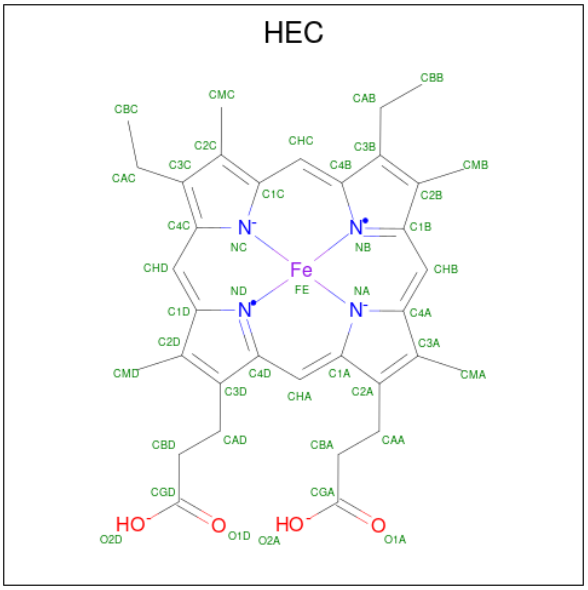
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
17	C	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
17	D	1	26	16	1	8	1	0	0
			Total	C	N	O	P		
17	P	1	49	39	1	8	1	0	0
			Total	C	N	O	P		
17	Q	1	51	41	1	8	1	0	0

- Molecule 18 is 2-METHYL-BUTYRIC ACID 3-(3-FORMYLAMINO-2-HYDROXY-BENZOYLAMINO)-8-HEPTYL-2,6-DIMETHYL-4,9-DIOXO-[1,5]DIOXONAN-7-YL ESTER (CCD ID: ANY) (formula: $C_{29}H_{42}N_2O_9$).



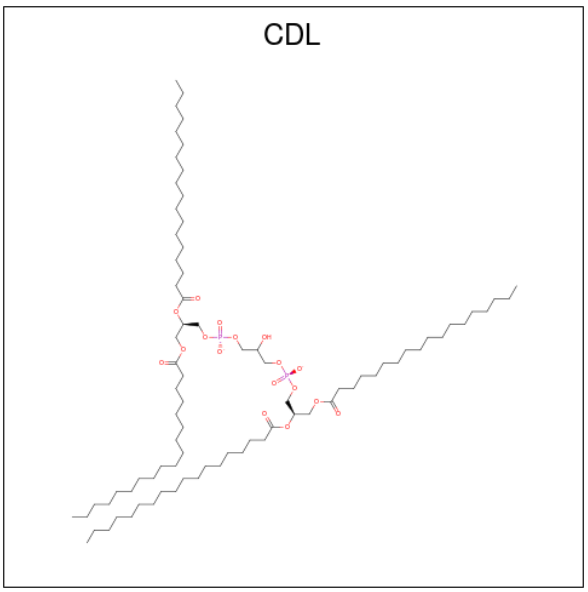
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
18	C	1	37	26	2	9	0	0
			Total	C	N	O		
18	P	1	37	26	2	9	0	0

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



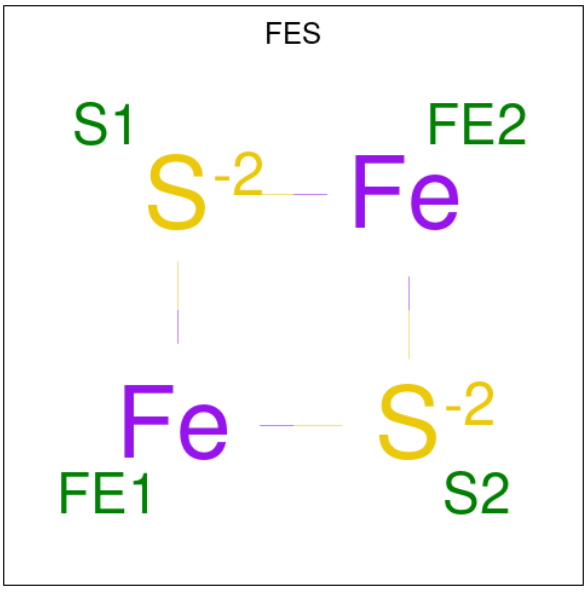
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
19	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
19	Q	1	43	34	1	4	4	0	0

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	D	1	39	24	13	2	0	0
			Total	C	O	P		
20	G	1	44	25	17	2	0	0
			Total	C	O	P		
20	P	1	39	24	13	2	0	0
			Total	C	O	P		
20	T	1	49	30	17	2	0	0

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
22	A	219	219	219	0	0
			Total	O		
22	B	167	167	167	0	0
			Total	O		
22	C	123	123	123	0	0
			Total	O		
22	D	96	96	96	0	0
			Total	O		
22	E	50	50	50	0	0
			Total	O		
22	F	63	63	63	0	0
			Total	O		
22	G	17	17	17	0	0
			Total	O		
22	H	17	17	17	0	0
			Total	O		
22	I	16	16	16	0	0
			Total	O		
22	J	4	4	4	0	0
			Total	O		
22	N	98	98	98	0	0
			Total	O		
22	O	127	127	127	0	0
			Total	O		
22	P	115	115	115	0	0
			Total	O		
22	Q	89	89	89	0	0
			Total	O		
22	R	63	63	63	0	0
			Total	O		
22	S	63	63	63	0	0
			Total	O		
22	T	20	20	20	0	0
			Total	O		
22	U	6	6	6	0	0

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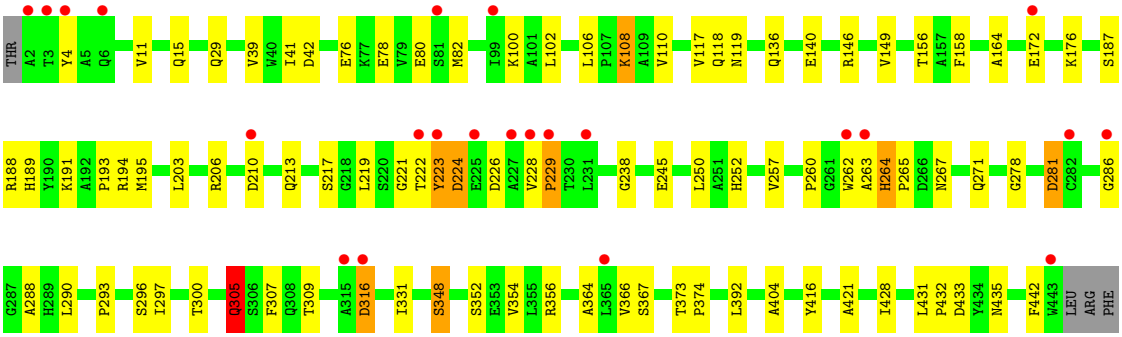
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
22	V	8	8	8	0	0
			Total	O		
22	W	9	9	9	0	0

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.

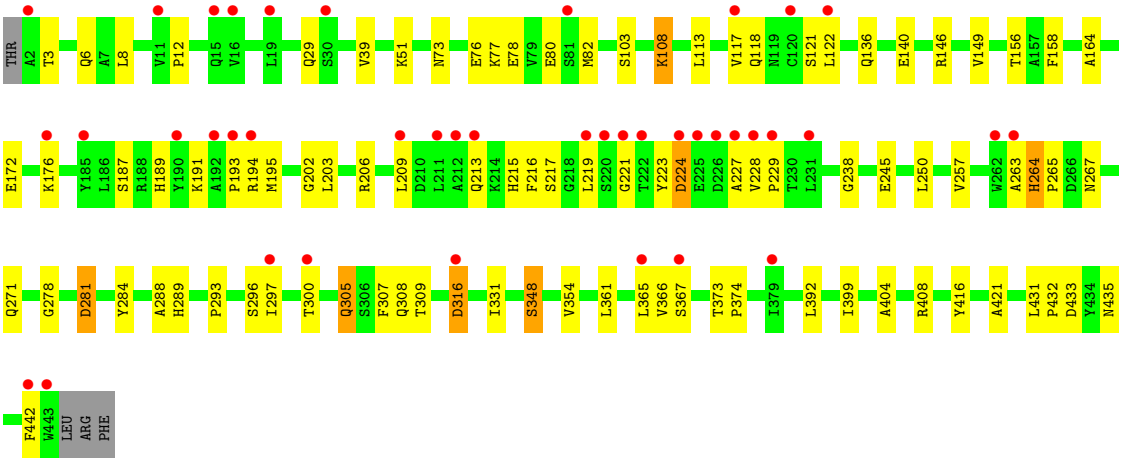
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A:



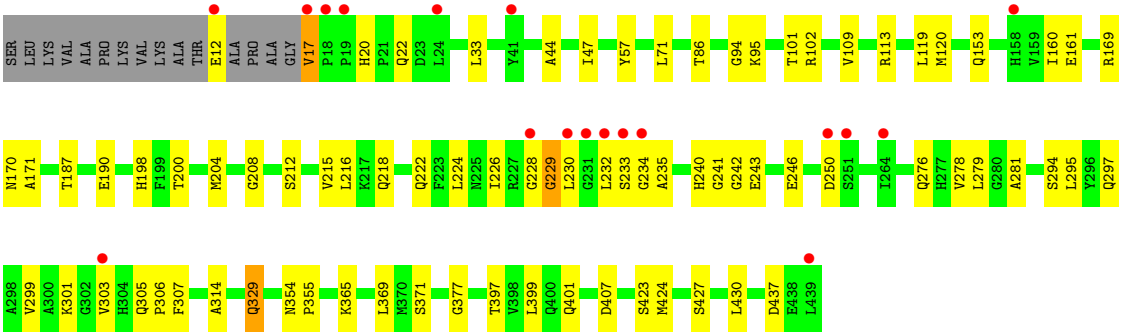
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain N:



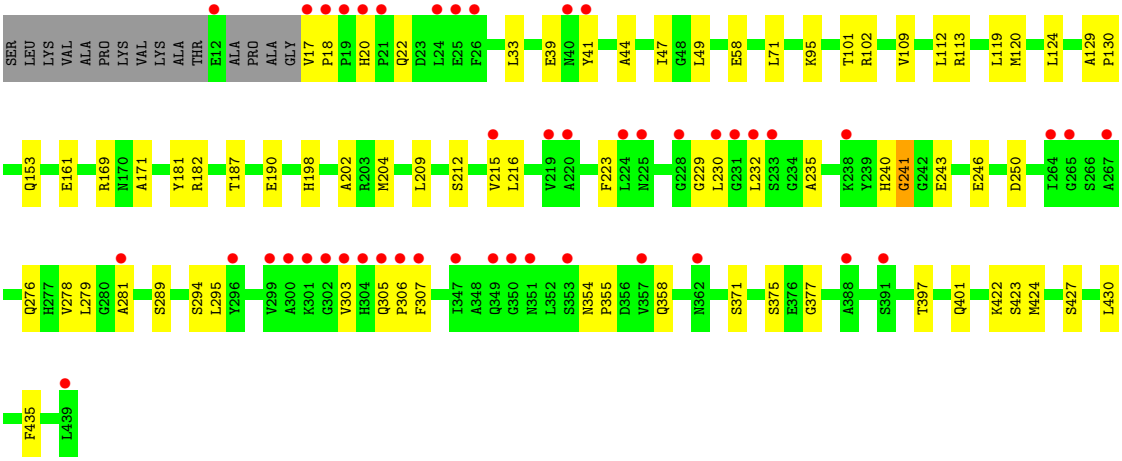
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain B:



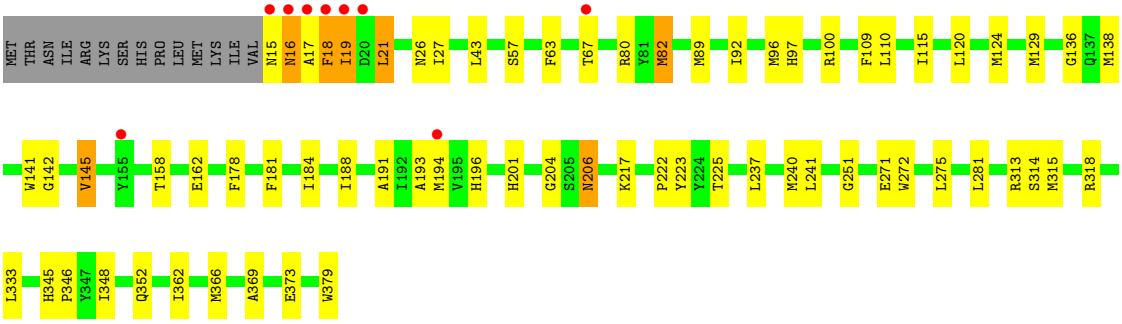
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain O:



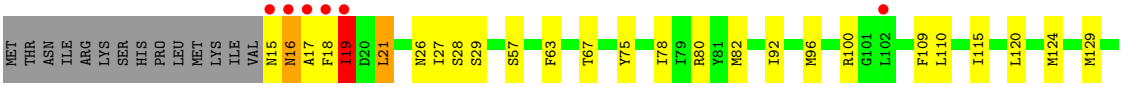
- Molecule 3: Cytochrome b

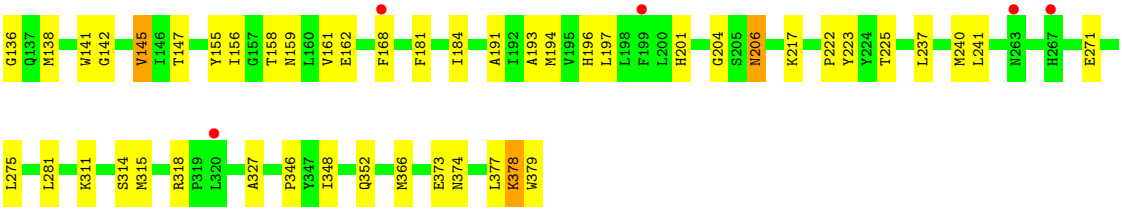
Chain C:



- Molecule 3: Cytochrome b

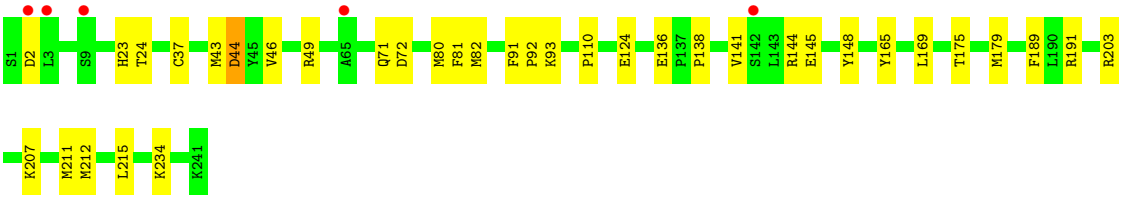
Chain P:





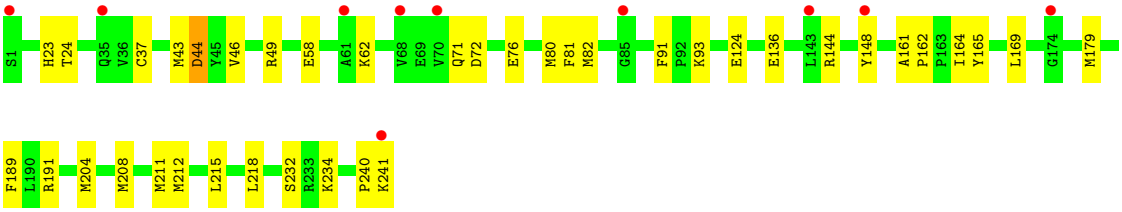
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



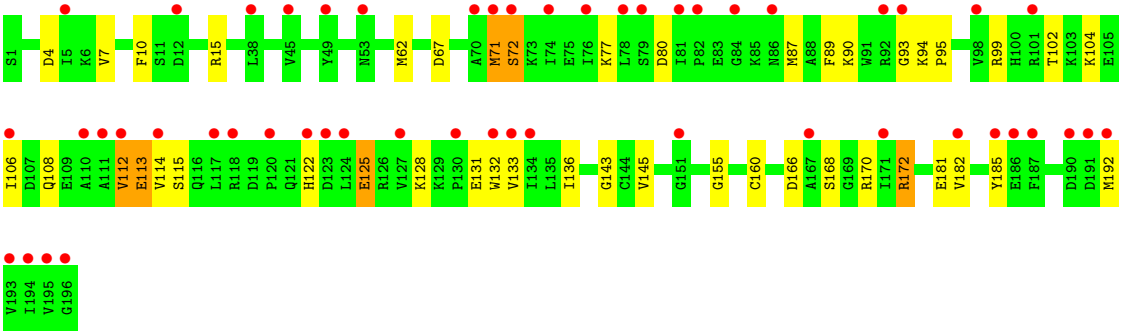
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



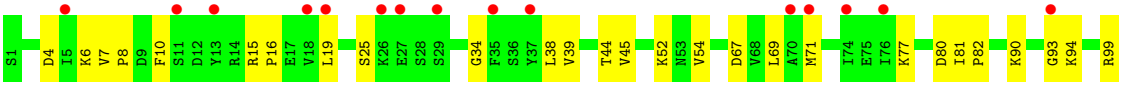
• Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

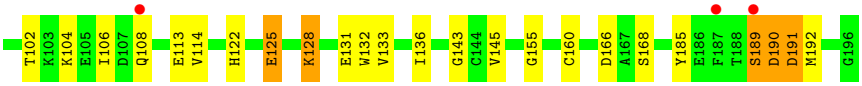
Chain E:



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

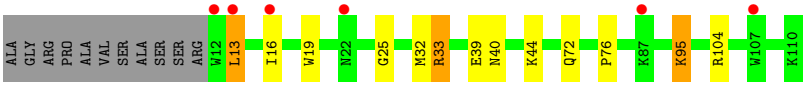
Chain R:





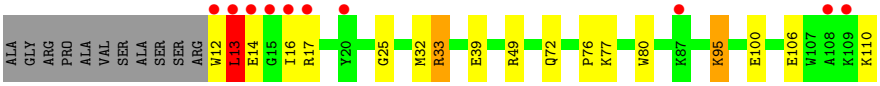
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



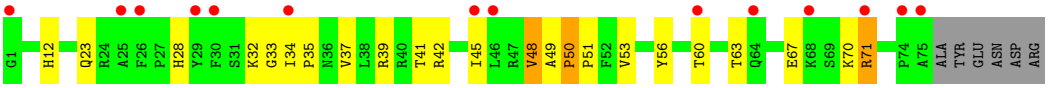
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain S:



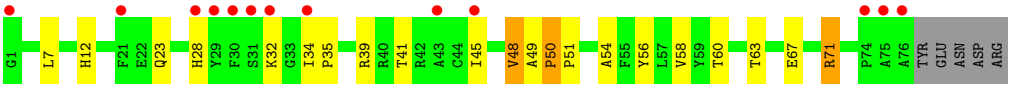
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



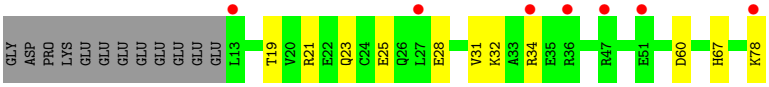
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain T:



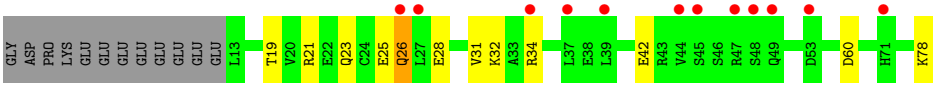
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



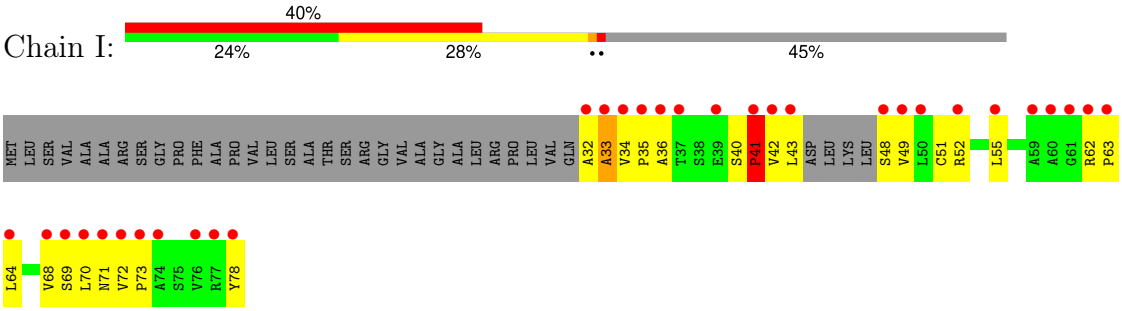
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain U:



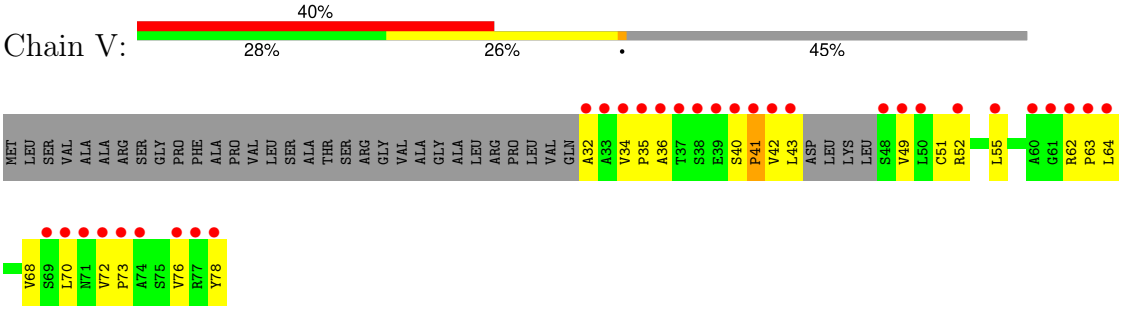
• Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain I:



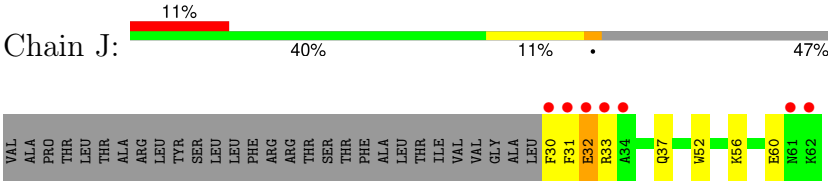
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain V:



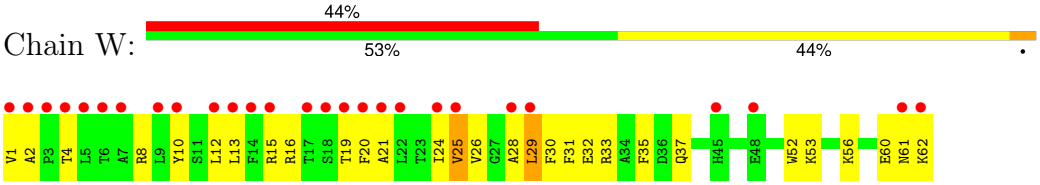
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.53Å 168.75Å 231.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.53 – 2.10 93.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (93.53-2.10) 97.8 (93.53-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.260 0.220 , 0.235	Depositor DCC
R_{free} test set	14181 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33549	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SMA, PO4, AZI, PEE, ANY, FES, JZR, CDL, HEM, GOL, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/3465	0.97	17/4704 (0.4%)
1	N	0.37	0/3465	0.95	13/4704 (0.3%)
2	B	0.41	0/3236	0.93	10/4388 (0.2%)
2	O	0.39	0/3213	0.94	11/4354 (0.3%)
3	C	0.42	0/2986	1.00	23/4089 (0.6%)
3	P	0.42	0/2985	1.01	20/4087 (0.5%)
4	D	0.39	0/1978	0.96	7/2684 (0.3%)
4	Q	0.39	0/1978	0.93	7/2684 (0.3%)
5	E	0.37	0/1544	0.99	6/2087 (0.3%)
5	R	0.38	0/1551	1.01	11/2097 (0.5%)
6	F	0.40	0/878	0.96	5/1175 (0.4%)
6	S	0.37	0/878	0.91	4/1175 (0.3%)
7	G	0.37	0/642	0.97	6/869 (0.7%)
7	T	0.35	0/647	0.96	5/876 (0.6%)
8	H	0.35	0/544	0.93	1/729 (0.1%)
8	U	0.35	0/544	0.92	1/729 (0.1%)
9	I	0.49	0/286	1.35	4/387 (1.0%)
9	V	0.48	0/286	1.30	4/387 (1.0%)
10	J	0.34	0/292	0.74	0/386
10	W	0.35	0/518	0.83	0/696
All	All	0.40	0/31916	0.97	155/43287 (0.4%)

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	143	GLY	N-CA-C	8.72	127.35	115.32
5	E	143	GLY	N-CA-C	8.51	127.06	115.32
3	P	26	ASN	N-CA-C	8.38	122.81	112.59
3	C	26	ASN	N-CA-C	8.16	122.55	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	153	GLN	N-CA-C	-7.67	103.90	113.18
9	I	35	PRO	N-CA-CB	7.50	110.31	103.33
7	T	48	VAL	N-CA-C	7.32	117.92	110.82
5	R	114	VAL	N-CA-C	7.30	118.95	110.62
3	P	184	ILE	N-CA-C	7.28	118.94	111.00
3	C	206	ASN	N-CA-C	-7.19	100.16	110.59
2	O	278	VAL	N-CA-C	-6.92	104.11	110.82
3	P	204	GLY	N-CA-C	-6.92	102.58	112.81
7	G	48	VAL	N-CA-C	6.90	117.87	111.45
3	P	223	TYR	N-CA-C	6.87	119.40	111.02
2	B	153	GLN	N-CA-C	-6.87	104.37	112.89
9	I	40	SER	CA-C-N	6.85	128.40	119.84
9	I	40	SER	C-N-CA	6.85	128.40	119.84
3	P	206	ASN	N-CA-C	-6.85	100.90	110.35
9	V	40	SER	CA-C-N	6.84	128.39	119.84
9	V	40	SER	C-N-CA	6.84	128.39	119.84
3	C	223	TYR	N-CA-C	6.81	119.33	111.02
3	C	109	PHE	N-CA-C	-6.77	96.79	108.56
3	C	184	ILE	N-CA-C	6.71	118.31	111.00
3	P	241	LEU	N-CA-C	-6.69	104.07	111.36
1	A	305	GLN	N-CA-C	-6.65	104.19	112.90
3	C	204	GLY	N-CA-C	-6.64	102.99	112.81
4	D	215	LEU	N-CA-C	6.63	118.50	111.28
3	C	115	ILE	N-CA-C	-6.62	104.03	110.72
3	P	136	GLY	N-CA-C	-6.57	103.57	112.57
3	P	109	PHE	N-CA-C	-6.54	97.17	108.56
3	C	57	SER	N-CA-C	6.54	120.25	112.93
2	O	430	LEU	N-CA-C	6.54	120.25	112.93
2	B	278	VAL	N-CA-C	-6.47	104.54	110.82
2	B	113	ARG	N-CA-C	6.41	119.08	111.71
4	Q	215	LEU	N-CA-C	6.40	118.25	111.28
7	T	49	ALA	N-CA-C	6.39	121.44	112.75
1	A	331	ILE	N-CA-C	6.37	116.53	110.42
3	C	145	VAL	N-CA-C	6.37	116.53	110.42
1	N	278	GLY	N-CA-C	6.37	123.30	112.22
2	O	113	ARG	N-CA-C	6.36	119.03	111.71
4	Q	44	ASP	N-CA-C	6.36	119.89	111.75
7	G	49	ALA	N-CA-C	6.33	121.35	112.75
3	P	145	VAL	N-CA-C	6.31	116.47	110.42
4	D	24	THR	N-CA-C	-6.30	104.50	111.36
6	S	25	GLY	N-CA-C	6.29	124.04	115.30
5	E	15	ARG	N-CA-C	-6.19	101.54	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	241	LEU	N-CA-C	-6.14	104.66	111.36
1	N	331	ILE	N-CA-C	6.12	116.30	110.42
1	A	238	GLY	N-CA-C	-6.12	101.43	110.97
1	A	348	SER	N-CA-C	6.12	119.91	111.71
3	C	136	GLY	N-CA-C	-6.09	104.23	112.57
3	C	110	LEU	N-CA-C	6.08	118.41	111.11
1	N	264	HIS	N-CA-C	6.08	118.44	109.50
3	P	82	MET	N-CA-C	-6.08	104.74	111.36
9	I	33	ALA	N-CA-C	6.07	117.57	111.07
5	R	136	ILE	N-CA-C	-6.07	98.94	108.23
3	C	271	GLU	N-CA-C	-6.05	102.12	110.35
9	V	35	PRO	N-CA-CB	6.05	109.73	103.38
5	E	136	ILE	N-CA-C	-6.03	99.00	108.23
2	O	235	ALA	N-CA-C	-6.03	102.41	110.55
6	F	25	GLY	N-CA-C	6.00	123.64	115.30
3	C	82	MET	N-CA-C	-5.94	104.93	111.82
3	P	110	LEU	N-CA-C	5.93	118.23	111.11
6	F	13	LEU	N-CA-C	-5.92	104.90	111.71
5	E	168	SER	N-CA-C	-5.92	106.02	113.72
7	G	53	VAL	N-CA-C	-5.91	104.75	110.72
1	N	238	GLY	N-CA-C	-5.90	101.76	110.97
4	D	44	ASP	N-CA-C	5.86	119.25	111.75
3	P	271	GLU	N-CA-C	-5.86	102.39	110.35
1	N	263	ALA	N-CA-C	5.84	119.50	112.38
5	R	128	LYS	N-CA-C	-5.83	105.83	113.12
1	N	348	SER	N-CA-C	5.81	119.50	111.71
7	T	50	PRO	N-CA-C	5.81	117.79	110.70
1	N	309	THR	N-CA-C	-5.78	101.97	110.52
1	A	262	TRP	N-CA-C	5.77	120.83	111.37
7	G	23	GLN	N-CA-C	5.76	118.16	109.41
1	A	278	GLY	N-CA-C	5.70	122.63	112.02
1	N	257	VAL	N-CA-C	-5.70	101.20	109.29
3	C	19	ILE	N-CA-C	5.69	121.18	109.34
3	P	115	ILE	N-CA-C	-5.69	104.82	110.62
5	R	168	SER	N-CA-C	-5.67	106.34	113.72
7	T	12	HIS	N-CA-C	5.67	119.50	112.58
7	G	12	HIS	N-CA-C	5.67	119.49	112.58
3	C	188	ILE	N-CA-C	-5.66	105.01	110.72
7	T	23	GLN	N-CA-C	5.63	117.97	109.41
6	F	32	MET	N-CA-C	-5.62	101.43	110.14
3	P	225	THR	N-CA-C	-5.61	105.25	111.36
7	G	50	PRO	N-CA-C	5.60	117.53	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	421	ALA	N-CA-C	-5.59	100.06	109.07
3	P	275	LEU	N-CA-C	5.58	117.37	111.28
1	N	416	TYR	N-CA-C	5.57	118.26	109.96
1	A	264	HIS	N-CA-C	5.57	117.69	109.50
5	E	4	ASP	N-CA-C	-5.55	106.28	113.16
3	P	57	SER	N-CA-C	5.54	119.67	113.02
1	A	263	ALA	N-CA-C	5.53	119.13	112.38
1	A	119	ASN	N-CA-C	5.53	119.56	112.26
3	C	333	LEU	N-CA-C	-5.51	105.35	111.36
2	O	101	THR	N-CA-C	-5.50	99.08	110.80
3	P	378	LYS	N-CA-C	5.50	119.16	111.74
2	B	430	LEU	N-CA-C	5.47	119.05	112.93
3	P	19	ILE	N-CA-C	5.47	120.71	109.34
3	C	275	LEU	N-CA-C	5.45	117.22	111.28
6	S	32	MET	N-CA-C	-5.45	101.69	110.14
1	A	100	LYS	N-CA-C	-5.42	100.33	109.07
5	R	38	LEU	N-CA-C	-5.41	105.04	111.69
5	R	4	ASP	N-CA-C	-5.40	106.47	113.16
1	A	260	PRO	N-CA-C	5.39	120.63	113.57
2	B	329	GLN	N-CA-C	-5.38	102.92	110.50
5	R	15	ARG	N-CA-C	-5.38	102.66	110.08
8	U	26	GLN	N-CA-C	-5.38	106.56	113.23
5	R	125	GLU	N-CA-C	-5.37	106.78	113.38
1	A	416	TYR	N-CA-C	5.36	117.94	109.96
1	N	305	GLN	N-CA-C	-5.35	105.11	111.69
2	B	198	HIS	N-CA-C	5.30	120.61	114.04
1	A	421	ALA	N-CA-C	-5.30	100.54	109.07
2	B	17	VAL	CA-C-N	5.29	125.83	120.38
2	B	17	VAL	C-N-CA	5.29	125.83	120.38
3	C	313	ARG	N-CA-C	5.27	116.83	111.14
1	N	215	HIS	N-CA-C	5.27	119.98	113.50
1	A	309	THR	N-CA-C	-5.26	102.74	110.52
4	Q	37	CYS	N-CA-C	5.25	117.08	111.36
4	Q	24	THR	N-CA-C	-5.23	105.66	111.36
8	H	67	HIS	N-CA-C	-5.23	105.58	111.28
2	B	226	ILE	N-CA-C	5.22	115.63	108.12
2	O	198	HIS	N-CA-C	5.22	120.51	114.04
4	D	37	CYS	N-CA-C	5.22	117.71	111.71
2	O	422	LYS	N-CA-C	5.21	118.23	110.52
2	B	101	THR	N-CA-C	-5.20	99.72	110.80
3	C	142	GLY	N-CA-C	-5.20	106.11	112.77
3	C	225	THR	N-CA-C	-5.20	105.69	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	136	GLU	CA-C-N	5.17	123.43	119.66
4	Q	136	GLU	C-N-CA	5.17	123.43	119.66
5	R	81	ILE	CA-C-N	5.14	125.42	119.92
5	R	81	ILE	C-N-CA	5.14	125.42	119.92
5	E	125	GLU	N-CA-C	-5.12	107.08	113.38
2	O	241	GLY	N-CA-C	-5.12	106.28	112.48
6	S	39	GLU	N-CA-C	5.11	116.60	108.67
3	P	142	GLY	N-CA-C	-5.09	106.25	112.77
2	O	58	GLU	N-CA-C	-5.07	103.70	110.55
6	S	76	PRO	N-CA-C	-5.07	103.15	111.21
9	V	70	LEU	N-CA-C	-5.07	105.45	111.69
2	O	112	LEU	N-CA-C	-5.06	103.36	110.50
1	A	41	ILE	N-CA-C	5.04	115.98	108.46
4	D	136	GLU	CA-C-N	5.04	123.34	119.66
4	D	136	GLU	C-N-CA	5.04	123.34	119.66
3	C	362	ILE	N-CA-C	5.04	115.81	110.72
6	F	39	GLU	N-CA-C	5.03	116.47	108.67
1	A	428	ILE	N-CA-C	5.03	119.80	109.34
4	D	23	HIS	N-CA-C	5.03	118.68	112.54
6	F	76	PRO	N-CA-C	-5.03	103.21	111.21
1	N	51	LYS	N-CA-C	5.03	117.66	111.82
3	C	272	TRP	N-CA-C	5.02	117.41	111.33
4	Q	23	HIS	N-CA-C	5.02	118.66	112.54
3	P	155	TYR	N-CA-C	5.01	121.47	110.80
1	A	257	VAL	N-CA-C	-5.00	102.19	109.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3396	0	3292	68	0
1	N	3396	0	3292	60	0
2	B	3178	0	3153	74	0
2	O	3156	0	3123	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2892	0	2938	41	0
3	P	2891	0	2937	49	0
4	D	1919	0	1868	33	0
4	Q	1919	0	1868	37	0
5	E	1510	0	1495	33	0
5	R	1517	0	1499	35	0
6	F	861	0	854	12	0
6	S	861	0	854	19	0
7	G	621	0	626	15	0
7	T	626	0	631	15	0
8	H	539	0	524	11	0
8	U	539	0	524	10	0
9	I	285	0	280	50	0
9	V	285	0	280	24	0
10	J	284	0	264	5	0
10	W	506	0	512	35	0
11	A	18	0	24	0	0
11	C	36	0	48	2	0
11	D	18	0	24	3	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	R	18	0	24	1	0
11	S	18	0	24	3	0
12	A	5	0	0	0	0
12	C	5	0	0	0	0
12	F	5	0	0	0	0
12	P	5	0	0	0	0
12	S	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	G	3	0	0	0	0
13	O	3	0	0	0	0
13	P	3	0	0	0	0
14	B	6	0	8	0	0
14	C	12	0	16	1	0
14	O	6	0	8	0	0
14	P	6	0	8	0	0
14	R	6	0	8	2	0
15	C	86	0	60	3	0
15	P	86	0	60	2	0
16	C	37	0	42	2	0
16	P	37	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	49	0	72	0	0
17	D	26	0	26	3	0
17	P	49	0	72	1	0
17	Q	51	0	82	4	0
18	C	37	0	28	1	0
18	P	37	0	29	2	0
19	D	43	0	30	2	0
19	Q	43	0	30	0	0
20	D	39	0	39	1	0
20	G	44	0	32	0	0
20	P	39	0	39	2	0
20	T	49	0	42	2	0
21	E	4	0	0	0	0
21	R	4	0	0	0	0
22	A	219	0	0	7	0
22	B	167	0	0	5	0
22	C	123	0	0	1	0
22	D	96	0	0	1	0
22	E	50	0	0	0	0
22	F	63	0	0	0	0
22	G	17	0	0	0	0
22	H	17	0	0	0	0
22	I	16	0	0	2	0
22	J	4	0	0	0	0
22	N	98	0	0	1	0
22	O	127	0	0	2	0
22	P	115	0	0	5	0
22	Q	89	0	0	0	0
22	R	63	0	0	5	0
22	S	63	0	0	1	0
22	T	20	0	0	0	0
22	U	6	0	0	0	0
22	V	8	0	0	1	0
22	W	9	0	0	0	0
All	All	33549	0	31803	595	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 9.

All (595) 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:B:204:MET:HE1	2:B:224:LEU:HD22	1.41	1.03
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.23	1.01
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.21	1.01
2:B:95:LYS:HE2	9:I:32:ALA:HB3	1.47	0.94
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.48	0.94
2:O:95:LYS:HE2	9:V:32:ALA:N	1.82	0.94
1:A:136:GLN:HE21	9:I:51:CYS:HB3	1.30	0.93
1:A:146:ARG:HA	22:A:4191:HOH:O	1.69	0.92
9:I:32:ALA:HA	9:I:71:ASN:CB	1.99	0.91
6:S:13:LEU:H	6:S:13:LEU:HD23	1.32	0.91
2:B:200:THR:HG21	2:B:228:GLY:HA3	1.51	0.90
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.07	0.90
1:N:136:GLN:HE21	9:V:51:CYS:HB3	1.38	0.88
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.08	0.88
8:H:25:GLU:HB2	8:H:34:ARG:HH22	1.38	0.88
2:B:95:LYS:HE2	9:I:32:ALA:CB	2.03	0.88
8:U:25:GLU:HB2	8:U:34:ARG:HH22	1.37	0.87
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.10	0.86
1:A:39:VAL:HG11	1:A:195:MET:HE3	1.57	0.86
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.39	0.85
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.42	0.84
1:N:136:GLN:NE2	9:V:51:CYS:HB3	1.93	0.83
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.14	0.83
1:N:39:VAL:HG11	1:N:195:MET:HE3	1.61	0.82
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.61	0.81
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.63	0.81
9:V:49:VAL:HG11	9:V:55:LEU:HD13	1.62	0.81
6:F:13:LEU:O	6:F:16:ILE:HG12	1.80	0.80
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.62	0.80
1:A:136:GLN:NE2	9:I:51:CYS:HB3	1.96	0.80
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.63	0.80
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.65	0.78
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.65	0.77
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.68	0.74
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.02	0.74
5:R:34:GLY:CA	10:W:10:TYR:HB2	2.17	0.74
10:W:21:ALA:O	10:W:25:VAL:HG23	1.88	0.74
5:R:34:GLY:HA2	10:W:10:TYR:HB2	1.70	0.74
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.70	0.74
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.04	0.72
7:T:63:THR:O	7:T:67:GLU:HG2	1.90	0.72
8:U:28:GLU:O	8:U:31:VAL:HG22	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.05	0.71
8:H:28:GLU:O	8:H:31:VAL:HG22	1.91	0.71
3:P:17:ALA:HA	3:P:201:HIS:HE1	1.55	0.70
7:G:63:THR:O	7:G:67:GLU:HG2	1.91	0.70
5:R:189:SER:O	5:R:190:ASP:C	2.33	0.70
3:C:17:ALA:HA	3:C:201:HIS:HE1	1.57	0.69
9:I:62:ARG:HB3	9:I:63:PRO:HD2	1.74	0.69
9:I:72:VAL:HG13	9:I:73:PRO:HD2	1.74	0.69
1:N:209:LEU:O	1:N:213:GLN:HG3	1.93	0.69
5:R:104:LYS:O	5:R:108:GLN:HG3	1.91	0.69
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.27	0.69
9:V:62:ARG:HB3	9:V:63:PRO:HD2	1.74	0.69
5:E:104:LYS:O	5:E:108:GLN:HG3	1.92	0.68
1:A:293:PRO:O	1:A:297:ILE:HG12	1.93	0.68
2:B:200:THR:CG2	2:B:228:GLY:HA3	2.23	0.68
1:N:293:PRO:O	1:N:297:ILE:HG12	1.94	0.68
9:I:32:ALA:HA	9:I:71:ASN:HB3	1.76	0.68
2:B:20:HIS:HB2	2:B:22:GLN:HG2	1.74	0.67
8:U:25:GLU:CB	8:U:34:ARG:HH22	2.08	0.67
22:A:4203:HOH:O	9:I:73:PRO:HG3	1.94	0.67
8:U:28:GLU:O	8:U:32:LYS:HG2	1.95	0.67
8:H:25:GLU:CB	8:H:34:ARG:HH22	2.07	0.67
4:D:81:PHE:C	4:D:82:MET:HE2	2.20	0.67
2:B:95:LYS:HE2	9:I:32:ALA:N	2.10	0.67
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.77	0.66
8:H:28:GLU:O	8:H:32:LYS:HG2	1.95	0.66
2:O:358:GLN:HB2	22:O:4120:HOH:O	1.95	0.66
1:A:39:VAL:CG1	1:A:195:MET:HE3	2.25	0.66
8:H:21:ARG:O	8:H:25:GLU:HG2	1.96	0.66
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.29	0.66
6:F:95:LYS:HB2	6:F:95:LYS:HZ2	1.61	0.66
1:A:316:ASP:OD1	1:A:316:ASP:N	2.26	0.66
1:N:82:MET:HE1	1:N:108:LYS:HG2	1.77	0.65
3:P:129:MET:CE	3:P:181:PHE:HD2	2.05	0.65
10:W:33:ARG:O	10:W:37:GLN:HG3	1.96	0.65
3:C:16:ASN:N	3:C:16:ASN:HD22	1.93	0.65
1:A:136:GLN:O	1:A:140:GLU:HG3	1.97	0.65
4:Q:81:PHE:C	4:Q:82:MET:HE2	2.21	0.65
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.79	0.65
9:I:32:ALA:N	9:I:72:VAL:HG23	2.13	0.64
4:Q:144:ARG:HH11	4:Q:144:ARG:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.32	0.64
1:N:113:LEU:O	1:N:117:VAL:HG12	1.97	0.64
2:O:306:PRO:HA	9:V:52:ARG:HG3	1.80	0.64
10:W:16:ARG:HH11	10:W:19:THR:HG21	1.63	0.64
1:N:39:VAL:CG1	1:N:195:MET:HE3	2.27	0.64
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.79	0.64
9:V:72:VAL:HG13	9:V:73:PRO:HD2	1.78	0.64
1:A:172:GLU:OE2	1:A:176:LYS:HE3	1.98	0.64
5:E:112:VAL:HG21	5:E:170:ARG:HH22	1.61	0.64
4:D:144:ARG:HG2	4:D:144:ARG:HH11	1.64	0.63
2:B:204:MET:CE	2:B:224:LEU:HD22	2.23	0.63
1:A:305:GLN:HE21	1:A:305:GLN:HA	1.62	0.63
3:C:129:MET:CE	3:C:181:PHE:HD2	2.05	0.63
2:B:94:GLY:O	9:I:32:ALA:HB2	1.99	0.63
3:C:89:MET:HE1	20:D:2003:CDL:H812	1.81	0.63
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.34	0.62
8:U:21:ARG:O	8:U:25:GLU:HG2	1.98	0.62
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.80	0.62
9:I:32:ALA:CA	9:I:71:ASN:CB	2.74	0.62
2:B:299:VAL:HG12	2:B:303:VAL:CG1	2.30	0.62
1:N:136:GLN:O	1:N:140:GLU:HG3	2.00	0.62
1:A:352:SER:HB3	6:S:110:LYS:OXT	1.99	0.62
2:B:95:LYS:CE	9:I:32:ALA:HB3	2.25	0.61
1:N:316:ASP:OD1	1:N:316:ASP:N	2.33	0.61
15:P:501:HEM:HMC1	15:P:501:HEM:HBC2	1.83	0.61
5:R:71:MET:HE1	14:R:4005:GOL:H31	1.82	0.61
4:D:165:TYR:HA	4:D:179:MET:HE2	1.82	0.61
1:N:224:ASP:OD1	1:N:227:ALA:HB3	1.99	0.61
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.30	0.61
2:O:202:ALA:HB3	2:O:229:GLY:O	2.00	0.61
7:T:71:ARG:HH22	8:U:60:ASP:CG	2.08	0.61
9:I:32:ALA:N	9:I:71:ASN:HB2	2.16	0.61
4:Q:218:LEU:HD13	22:R:4057:HOH:O	1.99	0.61
9:I:32:ALA:HA	9:I:71:ASN:CG	2.25	0.61
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.00	0.61
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.26	0.61
2:O:250:ASP:HB3	22:O:4111:HOH:O	1.99	0.60
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.84	0.60
22:A:4157:HOH:O	9:I:41:PRO:HB3	2.00	0.60
15:C:501:HEM:HMC1	15:C:501:HEM:HBC2	1.82	0.60
6:F:13:LEU:HD12	6:F:16:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:16:ASN:N	3:P:16:ASN:HD22	1.99	0.60
4:Q:71:GLN:HG3	4:Q:82:MET:HE1	1.82	0.60
5:E:71:MET:O	5:E:72:SER:HB3	2.01	0.60
6:S:95:LYS:HB2	6:S:95:LYS:HZ2	1.66	0.60
5:E:94:LYS:HE3	3:P:168:PHE:O	2.01	0.59
1:N:193:PRO:HD3	1:N:221:GLY:HA2	1.84	0.59
2:O:33:LEU:HD12	2:O:204:MET:HE2	1.85	0.59
9:I:32:ALA:HA	9:I:71:ASN:HB2	1.84	0.59
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.32	0.59
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.85	0.59
3:P:100:ARG:HD2	3:P:100:ARG:C	2.27	0.59
6:S:13:LEU:HD23	6:S:13:LEU:N	2.12	0.59
10:W:15:ARG:HH11	10:W:15:ARG:HG3	1.67	0.59
5:R:39:VAL:HG13	22:R:4057:HOH:O	2.02	0.58
4:Q:218:LEU:HD22	22:R:4057:HOH:O	2.01	0.58
1:N:117:VAL:HG13	1:N:118:GLN:HG3	1.85	0.58
1:A:305:GLN:HB3	9:I:41:PRO:HA	1.85	0.58
1:A:252:HIS:ND1	22:A:4191:HOH:O	2.32	0.58
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.38	0.58
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.85	0.58
3:P:15:ASN:OD1	3:P:19:ILE:HB	2.03	0.58
4:Q:211:MET:HE1	10:W:31:PHE:HZ	1.67	0.58
4:D:43:MET:HE3	4:D:46:VAL:HG21	1.86	0.57
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.39	0.57
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.86	0.57
9:I:42:VAL:HG12	9:I:43:LEU:CG	2.35	0.57
2:B:12:GLU:HG2	2:B:17:VAL:N	2.19	0.57
4:D:145:GLU:HA	11:D:4003:JZR:H2	1.87	0.57
4:Q:43:MET:HE2	4:Q:91:PHE:CD2	2.40	0.56
3:C:251:GLY:HA2	14:C:2008:GOL:H11	1.87	0.56
10:W:13:LEU:O	10:W:19:THR:HG23	2.05	0.56
1:A:118:GLN:HG2	1:A:219:LEU:HD13	1.88	0.56
2:B:299:VAL:O	2:B:303:VAL:HG12	2.05	0.56
2:B:354:ASN:HB2	2:B:355:PRO:HD3	1.85	0.56
4:D:71:GLN:HG3	4:D:82:MET:HE1	1.87	0.56
1:A:188:ARG:NH1	1:A:229:PRO:HD3	2.20	0.56
2:B:299:VAL:HG12	2:B:303:VAL:HG12	1.87	0.56
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.05	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.88	0.56
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:VAL:O	1:N:228:VAL:HG13	2.06	0.56
1:A:191:LYS:HE2	1:A:223:TYR:CB	2.36	0.56
17:Q:3006:PEE:H18	5:R:54:VAL:HG22	1.88	0.56
5:R:128:LYS:HE3	5:R:185:TYR:O	2.05	0.56
11:F:3011:JZR:H1	1:N:289:HIS:NE2	2.21	0.55
3:P:80:ARG:HD3	3:P:80:ARG:C	2.31	0.55
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.06	0.55
10:J:32:GLU:HG3	10:J:33:ARG:N	2.20	0.55
2:O:202:ALA:HB3	2:O:229:GLY:C	2.30	0.55
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.89	0.55
4:Q:211:MET:HE1	10:W:31:PHE:CZ	2.41	0.55
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.55
1:N:361:LEU:O	1:N:365:LEU:HG	2.07	0.55
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.89	0.55
2:B:212:SER:O	2:B:215:VAL:HG22	2.07	0.55
1:N:117:VAL:HG21	1:N:195:MET:HE1	1.89	0.55
1:N:281:ASP:OD2	9:V:73:PRO:HG3	2.07	0.55
2:O:202:ALA:HB1	2:O:230:LEU:HD23	1.89	0.55
1:A:193:PRO:HD3	1:A:221:GLY:HA2	1.88	0.54
1:A:267:ASN:O	1:A:271:GLN:HG2	2.07	0.54
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.07	0.54
1:A:228:VAL:O	1:A:228:VAL:HG13	2.06	0.54
7:G:71:ARG:HH22	8:H:60:ASP:CG	2.15	0.54
5:R:44:THR:CG2	10:W:24:ILE:HD13	2.37	0.54
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.43	0.54
9:V:42:VAL:HG12	9:V:43:LEU:CG	2.38	0.54
1:A:136:GLN:NE2	9:I:51:CYS:CB	2.70	0.54
3:C:80:ARG:C	3:C:80:ARG:HD3	2.33	0.54
3:P:18:PHE:O	3:P:21:LEU:HB2	2.07	0.54
3:P:314:SER:O	3:P:318:ARG:HD3	2.08	0.54
10:W:10:TYR:OH	10:W:15:ARG:NH1	2.41	0.54
1:A:296:SER:O	1:A:300:THR:HG23	2.08	0.54
3:C:15:ASN:C	3:C:17:ALA:H	2.15	0.54
7:G:32:LYS:C	7:G:35:PRO:HD2	2.32	0.54
1:N:78:GLU:OE2	1:N:108:LYS:HD3	2.08	0.54
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.90	0.54
10:W:15:ARG:HG3	10:W:15:ARG:NH1	2.23	0.54
1:A:78:GLU:OE2	1:A:108:LYS:HD3	2.08	0.53
3:C:17:ALA:HA	3:C:201:HIS:CE1	2.42	0.53
4:D:144:ARG:HG2	4:D:144:ARG:NH1	2.23	0.53
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:32:ALA:CA	9:I:71:ASN:HB3	2.38	0.53
1:N:373:THR:HB	1:N:374:PRO:HD3	1.90	0.53
6:S:106:GLU:HG2	22:S:3048:HOH:O	2.06	0.53
10:J:33:ARG:O	10:J:37:GLN:HG3	2.09	0.53
7:T:71:ARG:NH2	8:U:60:ASP:OD1	2.42	0.53
3:C:18:PHE:O	3:C:21:LEU:HB2	2.08	0.53
3:C:158:THR:O	3:C:162:GLU:HG3	2.09	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.90	0.53
4:Q:164:ILE:O	4:Q:179:MET:HE2	2.09	0.53
4:Q:208:MET:HA	17:Q:3006:PEE:H49	1.88	0.53
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.53
4:Q:43:MET:HE2	4:Q:91:PHE:HE2	1.72	0.53
4:Q:144:ARG:HG2	4:Q:144:ARG:NH1	2.21	0.53
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.39	0.53
3:P:138:MET:HA	3:P:138:MET:HE2	1.90	0.53
9:I:70:LEU:HB3	22:I:1016:HOH:O	2.09	0.53
4:Q:165:TYR:HA	4:Q:179:MET:HE2	1.90	0.53
1:N:195:MET:SD	1:N:219:LEU:HD21	2.49	0.53
2:O:305:GLN:N	2:O:306:PRO:HD3	2.23	0.53
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.89	0.52
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.06	0.52
1:A:82:MET:HE1	1:A:108:LYS:HG2	1.91	0.52
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.91	0.52
10:W:4:THR:O	10:W:8:ARG:HG2	2.09	0.52
1:N:267:ASN:O	1:N:271:GLN:HG2	2.09	0.52
1:N:365:LEU:HD11	1:N:399:ILE:HD11	1.91	0.52
2:O:212:SER:O	2:O:215:VAL:HG22	2.08	0.52
9:I:32:ALA:CA	9:I:71:ASN:HB2	2.40	0.52
7:T:41:THR:O	7:T:45:ILE:HG12	2.09	0.52
1:A:4:TYR:HB2	22:B:2124:HOH:O	2.10	0.52
3:C:138:MET:HE2	3:C:138:MET:HA	1.90	0.52
7:G:41:THR:O	7:G:45:ILE:HG12	2.09	0.52
4:D:148:TYR:OH	11:D:4003:JZR:H6	2.08	0.52
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.90	0.52
2:B:86:THR:HG23	9:I:70:LEU:HD11	1.92	0.52
1:N:158:PHE:O	1:N:164:ALA:HB2	2.10	0.52
10:W:52:TRP:O	10:W:56:LYS:HB2	2.09	0.52
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.10	0.52
3:P:206:ASN:HB3	15:P:502:HEM:O2D	2.10	0.52
5:R:94:LYS:HE3	14:R:4005:GOL:O3	2.09	0.52
8:U:19:THR:O	8:U:23:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:62:LYS:C	10:W:62:LYS:HD2	2.35	0.52
1:A:364:ALA:HB2	9:I:33:ALA:HB1	1.92	0.52
6:F:19:TRP:CD1	11:F:4001:JZR:H1	2.46	0.51
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.51
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.92	0.51
2:B:33:LEU:HD12	2:B:204:MET:HE2	1.91	0.51
3:P:158:THR:O	3:P:162:GLU:HG3	2.11	0.51
3:P:315:MET:HE1	3:P:366:MET:HE2	1.93	0.51
2:O:305:GLN:N	2:O:305:GLN:C	2.68	0.51
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.51
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.91	0.51
4:D:110:PRO:HG3	19:D:501:HEC:HMD3	1.93	0.51
1:N:296:SER:O	1:N:300:THR:HG23	2.10	0.51
3:P:17:ALA:HA	3:P:201:HIS:CE1	2.42	0.51
3:C:191:ALA:HA	3:C:194:MET:HE2	1.92	0.51
5:E:114:VAL:O	5:E:114:VAL:HG12	2.10	0.51
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.51
2:B:397:THR:O	2:B:401:GLN:HG3	2.11	0.51
3:C:16:ASN:N	3:C:16:ASN:ND2	2.59	0.51
3:C:206:ASN:HB3	15:C:502:HEM:O2D	2.11	0.51
4:D:2:ASP:OD1	7:G:70:LYS:HE3	2.11	0.51
1:N:213:GLN:O	1:N:217:SER:OG	2.29	0.51
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.41	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.50
2:B:94:GLY:O	9:I:32:ALA:CB	2.59	0.50
2:O:49:LEU:HD11	2:O:204:MET:HE3	1.92	0.50
6:S:12:TRP:N	6:S:13:LEU:HD23	2.27	0.50
6:S:95:LYS:NZ	6:S:95:LYS:CB	2.72	0.50
2:B:95:LYS:NZ	9:I:34:VAL:HG22	2.27	0.50
7:T:48:VAL:O	7:T:51:PRO:HD2	2.12	0.50
10:J:52:TRP:O	10:J:56:LYS:HB2	2.12	0.50
1:N:366:VAL:HG21	2:O:44:ALA:HB2	1.94	0.50
6:F:13:LEU:O	6:F:16:ILE:CG1	2.56	0.50
9:I:32:ALA:HA	9:I:71:ASN:ND2	2.26	0.50
3:P:281:LEU:C	3:P:281:LEU:HD23	2.37	0.50
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.93	0.49
8:H:19:THR:O	8:H:23:GLN:HG3	2.11	0.49
2:O:102:ARG:HH22	2:O:161:GLU:CD	2.20	0.49
2:O:95:LYS:NZ	9:V:34:VAL:HG22	2.26	0.49
5:R:25:SER:HA	22:R:4016:HOH:O	2.12	0.49
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
1:A:213:GLN:O	1:A:217:SER:OG	2.25	0.49
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.38	0.49
5:R:90:LYS:HE3	5:R:93:GLY:O	2.12	0.49
1:A:140:GLU:HB3	9:I:48:SER:O	2.12	0.49
3:C:281:LEU:C	3:C:281:LEU:HD23	2.37	0.49
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.12	0.49
5:E:71:MET:O	5:E:72:SER:CB	2.60	0.49
3:P:378:LYS:HE3	6:S:17:ARG:HD3	1.95	0.49
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.49
7:G:56:TYR:O	7:G:60:THR:HG23	2.12	0.49
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.48	0.49
10:W:16:ARG:NH1	10:W:19:THR:HG21	2.25	0.49
20:P:3003:CDL:H511	20:P:3003:CDL:H721	1.95	0.49
5:E:102:THR:O	5:E:106:ILE:HG13	2.12	0.48
2:B:47:ILE:HD13	2:B:120:MET:HE3	1.96	0.48
1:N:408:ARG:HD2	22:N:522:HOH:O	2.12	0.48
2:O:39:GLU:OE2	2:O:41:TYR:N	2.44	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
3:C:100:ARG:HD2	3:C:100:ARG:C	2.37	0.48
3:P:29:SER:HB3	20:P:3003:CDL:H722	1.94	0.48
1:A:281:ASP:OD2	9:I:73:PRO:HG3	2.13	0.48
4:Q:124:GLU:OE2	4:Q:191:ARG:CD	2.62	0.48
4:Q:165:TYR:HA	4:Q:179:MET:CE	2.44	0.48
9:V:32:ALA:HB1	22:V:1505:HOH:O	2.13	0.48
2:B:297:GLN:O	2:B:301:LYS:HG3	2.14	0.48
3:C:129:MET:HE2	3:C:178:PHE:CD1	2.49	0.48
6:F:72:GLN:OE1	6:F:72:GLN:HA	2.14	0.48
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.14	0.48
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.13	0.48
4:D:81:PHE:O	4:D:82:MET:HE2	2.14	0.48
3:C:191:ALA:HA	3:C:194:MET:CE	2.43	0.47
3:C:217:LYS:HE3	22:C:4101:HOH:O	2.14	0.47
4:D:124:GLU:OE2	4:D:191:ARG:HD3	2.13	0.47
1:N:366:VAL:HG23	1:N:367:SER:N	2.28	0.47
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.44	0.47
6:S:100:GLU:HB3	11:S:2011:JZR:H6A	1.94	0.47
3:C:27:ILE:HD12	18:C:2002:ANY:H3	1.96	0.47
3:C:63:PHE:O	3:C:67:THR:HG23	2.14	0.47
3:P:191:ALA:HA	3:P:194:MET:HE2	1.95	0.47
2:B:95:LYS:HE2	9:I:32:ALA:CA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:LEU:O	3:C:124:MET:HG3	2.13	0.47
2:O:187:THR:OG1	2:O:190:GLU:HG3	2.14	0.47
3:C:43:LEU:HD11	3:C:82:MET:HE2	1.95	0.47
5:E:62:MET:HG2	22:P:3114:HOH:O	2.14	0.47
2:O:279:LEU:HA	2:O:294:SER:HB3	1.97	0.47
7:T:39:ARG:HG2	7:T:39:ARG:HH11	1.79	0.47
7:G:39:ARG:HG2	7:G:39:ARG:HH11	1.78	0.47
2:O:33:LEU:CD1	2:O:204:MET:HE2	2.44	0.47
2:O:95:LYS:NZ	9:V:34:VAL:CG2	2.78	0.47
5:R:77:LYS:HA	5:R:192:MET:HG2	1.96	0.47
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.45	0.47
4:Q:81:PHE:O	4:Q:82:MET:HE2	2.14	0.47
1:A:223:TYR:O	1:A:224:ASP:HB3	2.14	0.47
3:C:315:MET:HE1	3:C:366:MET:HE2	1.95	0.47
9:I:72:VAL:HG13	9:I:73:PRO:CD	2.43	0.47
9:I:72:VAL:CG1	9:I:73:PRO:HD2	2.44	0.47
7:T:56:TYR:O	7:T:60:THR:HG23	2.14	0.47
2:B:250:ASP:HB3	22:B:2139:HOH:O	2.14	0.47
3:C:314:SER:O	3:C:318:ARG:HD3	2.14	0.47
2:O:209:LEU:HD23	2:O:375:SER:HB2	1.96	0.47
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.80	0.47
1:A:11:VAL:HG21	1:A:392:LEU:HD12	1.97	0.47
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.14	0.47
1:N:250:LEU:HD13	1:N:305:GLN:HG3	1.98	0.47
2:O:215:VAL:HG23	2:O:216:LEU:N	2.28	0.47
2:O:241:GLY:HA2	2:O:423:SER:OG	2.14	0.47
5:E:112:VAL:CG2	5:E:170:ARG:HH22	2.28	0.46
3:P:78:ILE:HD12	4:Q:204:MET:HE1	1.97	0.46
5:R:44:THR:HG21	10:W:24:ILE:HG21	1.97	0.46
5:R:77:LYS:HB2	5:R:192:MET:HE3	1.97	0.46
6:S:72:GLN:OE1	6:S:72:GLN:HA	2.15	0.46
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.51	0.46
3:P:237:LEU:HD13	4:Q:212:MET:HG3	1.98	0.46
2:B:95:LYS:CE	9:I:32:ALA:N	2.76	0.46
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.96	0.46
5:E:160:CYS:HB3	16:P:3001:SMA:H4	1.95	0.46
1:N:29:GLN:O	2:O:18:PRO:HG3	2.15	0.46
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.64	0.46
1:N:206:ARG:HG3	1:N:206:ARG:HH11	1.80	0.46
2:B:187:THR:HB	22:B:2093:HOH:O	2.14	0.46
4:D:165:TYR:HA	4:D:179:MET:CE	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:124:GLU:OE2	4:Q:191:ARG:HD3	2.15	0.46
6:S:16:ILE:HG13	6:S:17:ARG:N	2.30	0.46
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.97	0.46
4:D:82:MET:HE3	22:D:4089:HOH:O	2.14	0.46
4:D:138:PRO:HG2	4:D:141:VAL:CG2	2.46	0.46
9:I:69:SER:HB2	22:I:1441:HOH:O	2.14	0.46
3:P:191:ALA:HA	3:P:194:MET:CE	2.46	0.46
1:N:224:ASP:OD2	1:N:227:ALA:N	2.49	0.46
2:B:229:GLY:C	2:B:230:LEU:HD12	2.41	0.46
16:C:2001:SMA:H4	5:R:160:CYS:HB3	1.97	0.46
3:P:120:LEU:O	3:P:124:MET:HG3	2.16	0.46
3:P:348:ILE:O	3:P:352:GLN:HG3	2.16	0.46
7:T:28:HIS:CG	7:T:32:LYS:HE2	2.51	0.46
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.63	0.45
1:A:373:THR:HB	1:A:374:PRO:HD3	1.96	0.45
3:C:379:TRP:CE3	6:F:33:ARG:HD3	2.50	0.45
4:Q:72:ASP:O	4:Q:80:MET:HE3	2.16	0.45
1:A:366:VAL:HG23	1:A:367:SER:N	2.31	0.45
3:C:97:HIS:CD2	15:C:502:HEM:NC	2.83	0.45
2:O:71:LEU:CD2	9:V:68:VAL:HG21	2.44	0.45
10:W:8:ARG:O	10:W:12:LEU:HB2	2.16	0.45
3:C:345:HIS:NE2	11:C:4002:JZR:H3	2.32	0.45
3:P:158:THR:HB	22:P:3127:HOH:O	2.17	0.45
4:Q:240:PRO:O	4:Q:241:LYS:HB2	2.16	0.45
1:A:29:GLN:HB3	2:B:12:GLU:O	2.17	0.45
1:A:102:LEU:HD21	2:B:369:LEU:HD12	1.98	0.45
7:G:28:HIS:CG	7:G:32:LYS:HE2	2.51	0.45
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.80	0.45
4:D:43:MET:HE2	4:D:91:PHE:HE2	1.81	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.45
5:R:52:LYS:HE3	10:W:32:GLU:OE2	2.17	0.45
6:S:49:ARG:HH22	11:S:2011:JZR:H4	1.81	0.45
9:V:72:VAL:HG13	9:V:73:PRO:CD	2.46	0.45
2:B:307:PHE:CD1	2:B:307:PHE:C	2.94	0.45
6:S:13:LEU:H	6:S:13:LEU:CD2	2.07	0.45
9:V:64:LEU:HB3	9:V:78:TYR:OXT	2.17	0.45
2:B:240:HIS:CE1	2:O:435:PHE:CD1	3.05	0.45
9:I:32:ALA:N	9:I:71:ASN:CB	2.79	0.45
2:O:109:VAL:HB	2:O:119:LEU:HD12	1.98	0.45
5:R:102:THR:O	5:R:106:ILE:HG13	2.17	0.45
3:C:145:VAL:HG21	16:C:2001:SMA:H6	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LYS:HE3	1:A:108:LYS:HA	1.99	0.44
1:A:206:ARG:HG3	1:A:206:ARG:NH1	2.31	0.44
2:B:241:GLY:HA2	2:B:423:SER:OG	2.17	0.44
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.52	0.44
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.26	0.44
3:C:240:MET:HE2	17:D:2006:PEE:H50	1.99	0.44
1:N:206:ARG:HG3	1:N:206:ARG:NH1	2.32	0.44
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.98	0.44
1:A:213:GLN:HG2	22:A:4063:HOH:O	2.16	0.44
2:B:160:ILE:HG22	22:B:2146:HOH:O	2.16	0.44
2:O:246:GLU:O	2:O:427:SER:HA	2.17	0.44
2:O:354:ASN:HB3	2:O:355:PRO:HD3	2.00	0.44
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.53	0.44
10:W:25:VAL:O	10:W:28:ALA:HB3	2.17	0.44
3:C:237:LEU:HD13	4:D:212:MET:HG3	1.99	0.44
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.65	0.44
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.52	0.44
3:P:197:LEU:CD1	18:P:3002:ANY:H12	2.48	0.44
1:N:431:LEU:HD12	1:N:432:PRO:HD2	1.99	0.44
4:Q:43:MET:CE	4:Q:91:PHE:HE2	2.31	0.44
5:E:113:GLU:C	5:E:115:SER:H	2.26	0.44
7:G:71:ARG:NH2	8:H:60:ASP:OD1	2.50	0.44
1:N:103:SER:HB3	1:N:202:GLY:O	2.18	0.44
2:O:397:THR:O	2:O:401:GLN:HG3	2.18	0.44
3:P:145:VAL:HG21	16:P:3001:SMA:H6	1.99	0.44
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.33	0.43
2:B:218:GLN:O	2:B:222:GLN:HG3	2.18	0.43
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.71	0.43
5:E:77:LYS:HA	5:E:192:MET:HG2	1.99	0.43
4:Q:148:TYR:CD1	4:Q:148:TYR:N	2.86	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	0.43
1:A:223:TYR:O	1:A:224:ASP:CB	2.66	0.43
2:B:120:MET:HE2	2:B:120:MET:HA	1.99	0.43
6:F:104:ARG:HH21	11:F:3011:JZR:H6'B	1.83	0.43
3:P:78:ILE:CD1	4:Q:204:MET:HE1	2.49	0.43
2:B:279:LEU:HA	2:B:294:SER:HB3	2.00	0.43
1:A:222:THR:O	1:A:223:TYR:CB	2.66	0.43
1:A:307:PHE:CD1	1:A:307:PHE:C	2.96	0.43
1:A:356:ARG:NH1	22:A:4058:HOH:O	2.51	0.43
5:E:77:LYS:HB2	5:E:192:MET:HE3	1.99	0.43
4:Q:161:ALA:O	4:Q:162:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:ARG:NH2	5:E:67:ASP:HB3	2.33	0.43
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.43
3:P:21:LEU:HD13	22:P:3100:HOH:O	2.18	0.43
5:R:69:LEU:O	5:R:71:MET:HG3	2.18	0.43
5:R:155:GLY:HA3	5:R:166:ASP:C	2.44	0.43
10:W:60:GLU:HB3	10:W:61:ASN:C	2.43	0.43
2:B:299:VAL:HG12	2:B:303:VAL:HG11	1.98	0.43
5:E:90:LYS:HE2	5:E:93:GLY:HA2	2.00	0.43
3:P:240:MET:HE2	17:Q:3006:PEE:H16	1.99	0.43
2:B:12:GLU:CG	2:B:17:VAL:N	2.82	0.43
2:O:305:GLN:N	2:O:306:PRO:CD	2.82	0.43
5:R:16:PRO:HA	5:R:19:LEU:HD12	2.00	0.43
22:B:2146:HOH:O	9:I:64:LEU:CG	2.66	0.43
9:I:64:LEU:HB3	9:I:78:TYR:OXT	2.18	0.43
1:N:288:ALA:CB	1:N:300:THR:HG22	2.48	0.43
1:A:149:VAL:CG1	22:A:4191:HOH:O	2.66	0.42
1:A:281:ASP:HA	1:A:305:GLN:O	2.18	0.42
3:C:92:ILE:O	3:C:96:MET:HG2	2.19	0.42
4:D:145:GLU:HG2	11:D:4003:JZR:O3	2.19	0.42
6:S:95:LYS:HB2	6:S:95:LYS:HZ3	1.82	0.42
9:V:34:VAL:HG23	9:V:34:VAL:O	2.19	0.42
1:A:187:SER:O	1:A:191:LYS:HD3	2.18	0.42
2:B:232:LEU:HB3	2:B:235:ALA:CB	2.49	0.42
1:A:288:ALA:CB	1:A:300:THR:HG22	2.48	0.42
3:C:315:MET:HE1	3:C:366:MET:CE	2.50	0.42
5:E:122:HIS:HB3	5:E:125:GLU:HG3	2.02	0.42
6:F:40:ASN:O	6:F:44:LYS:HG3	2.19	0.42
10:W:1:VAL:O	10:W:2:ALA:HB2	2.19	0.42
1:A:286:GLY:HA3	1:A:290:LEU:HD21	2.01	0.42
2:B:305:GLN:NE2	2:B:305:GLN:HA	2.35	0.42
4:D:175:THR:HG23	8:H:78:LYS:HE3	2.01	0.42
4:D:211:MET:HE1	10:J:31:PHE:CZ	2.54	0.42
7:G:39:ARG:HG2	7:G:39:ARG:NH1	2.34	0.42
8:H:31:VAL:HG23	8:H:32:LYS:N	2.33	0.42
2:O:120:MET:HA	2:O:120:MET:HE2	2.01	0.42
3:P:217:LYS:HG3	7:T:7:LEU:HD13	2.01	0.42
3:P:315:MET:HE1	3:P:366:MET:CE	2.49	0.42
1:A:156:THR:HA	5:E:7:VAL:HG21	2.00	0.42
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.42
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.81	0.42
3:P:92:ILE:O	3:P:96:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:PRO:HG3	19:D:501:HEC:CMD	2.49	0.42
9:V:42:VAL:HG12	9:V:43:LEU:N	2.34	0.42
1:A:42:ASP:O	1:A:194:ARG:CZ	2.68	0.42
4:D:203:ARG:HD2	17:D:2006:PEE:N	2.34	0.42
7:G:33:GLY:O	7:G:37:VAL:HG23	2.20	0.42
2:O:202:ALA:HB3	2:O:230:LEU:HA	2.01	0.42
2:O:371:SER:O	2:O:377:GLY:HA3	2.20	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
8:U:31:VAL:HG23	8:U:32:LYS:N	2.34	0.42
2:B:57:TYR:HD1	2:B:233:SER:HA	1.85	0.42
2:B:303:VAL:O	2:B:303:VAL:HG13	2.20	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
4:D:207:LYS:NZ	17:D:2006:PEE:H11	2.35	0.42
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.42
3:P:147:THR:HG22	3:P:161:VAL:HG13	2.00	0.42
1:A:223:TYR:C	1:A:224:ASP:OD1	2.63	0.42
2:B:230:LEU:HD12	2:B:230:LEU:N	2.35	0.42
3:C:345:HIS:CD2	11:C:4002:JZR:H3	2.55	0.42
10:W:8:ARG:HG2	10:W:8:ARG:HH11	1.84	0.42
5:E:77:LYS:HD3	5:E:80:ASP:OD1	2.20	0.42
2:O:17:VAL:HA	2:O:18:PRO:HD3	1.78	0.42
2:O:307:PHE:CD1	2:O:307:PHE:C	2.97	0.42
2:B:243:GLU:HA	2:B:424:MET:O	2.20	0.41
3:C:369:ALA:O	3:C:373:GLU:HG3	2.20	0.41
1:N:117:VAL:HG11	1:N:216:PHE:HE2	1.85	0.41
2:O:47:ILE:HD13	2:O:120:MET:HE3	2.01	0.41
2:O:243:GLU:HA	2:O:424:MET:O	2.21	0.41
8:U:26:GLN:OE1	8:U:26:GLN:HA	2.19	0.41
9:V:72:VAL:CG1	9:V:73:PRO:HD2	2.48	0.41
8:H:25:GLU:HB2	8:H:34:ARG:NH2	2.20	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.83	0.41
2:B:200:THR:O	2:B:204:MET:HG3	2.20	0.41
2:B:371:SER:O	2:B:377:GLY:HA3	2.20	0.41
5:E:172:ARG:HB3	5:E:172:ARG:HH11	1.85	0.41
3:P:63:PHE:O	3:P:67:THR:HG23	2.21	0.41
4:Q:204:MET:HE3	17:Q:3006:PEE:C10	2.50	0.41
4:Q:218:LEU:HB3	22:R:4057:HOH:O	2.19	0.41
6:S:49:ARG:NH2	11:S:2011:JZR:H4	2.35	0.41
5:E:87:MET:CG	5:E:89:PHE:CZ	3.03	0.41
1:N:117:VAL:HG11	1:N:216:PHE:CE2	2.56	0.41
1:N:187:SER:O	1:N:191:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:34:GLY:HA3	10:W:10:TYR:HB2	1.97	0.41
5:R:122:HIS:HB3	5:R:125:GLU:HG3	2.01	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.56	0.41
9:I:62:ARG:CB	9:I:63:PRO:HD2	2.49	0.41
2:O:95:LYS:O	2:O:109:VAL:HA	2.20	0.41
3:P:28:SER:HB2	20:T:3004:CDL:HA21	2.01	0.41
5:E:113:GLU:C	5:E:115:SER:N	2.79	0.41
1:N:12:PRO:HG3	2:O:18:PRO:HA	2.02	0.41
3:P:377:LEU:HD11	22:P:3086:HOH:O	2.21	0.41
4:Q:58:GLU:O	4:Q:62:LYS:HG3	2.21	0.41
5:E:87:MET:HG2	5:E:89:PHE:CZ	2.56	0.41
1:A:117:VAL:HG11	1:A:195:MET:CE	2.50	0.41
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.51	0.41
2:O:124:LEU:HD13	2:O:223:PHE:CB	2.50	0.41
4:Q:211:MET:HE2	10:W:35:PHE:CZ	2.56	0.41
1:A:250:LEU:HD13	1:A:305:GLN:HG3	2.03	0.41
2:B:354:ASN:ND2	2:B:407:ASP:OD2	2.54	0.41
5:E:155:GLY:HA3	5:E:166:ASP:C	2.45	0.41
1:N:73:ASN:O	1:N:77:LYS:HG3	2.20	0.41
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.85	0.41
2:O:129:ALA:N	2:O:130:PRO:CD	2.84	0.41
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.55	0.41
5:R:80:ASP:O	5:R:82:PRO:HD3	2.20	0.41
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.41
3:C:348:ILE:O	3:C:352:GLN:HG3	2.20	0.41
1:N:76:GLU:CD	2:O:289:SER:H	2.28	0.41
1:N:82:MET:CE	1:N:108:LYS:HG2	2.48	0.41
1:N:264:HIS:ND1	1:N:265:PRO:HD2	2.36	0.41
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.46	0.41
4:Q:232:SER:O	5:R:10:PHE:HE1	2.04	0.41
10:W:56:LYS:HG2	10:W:60:GLU:CD	2.46	0.41
4:D:72:ASP:O	4:D:80:MET:HE3	2.21	0.40
5:E:128:LYS:HE3	5:E:185:TYR:O	2.21	0.40
7:T:39:ARG:HG2	7:T:39:ARG:NH1	2.35	0.40
10:W:26:VAL:O	10:W:30:PHE:HD1	2.04	0.40
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.86	0.40
2:B:170:ASN:HD22	2:B:232:LEU:HD23	1.86	0.40
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.97	0.40
3:P:159:ASN:ND2	22:P:3127:HOH:O	2.54	0.40
17:P:3007:PEE:H2	20:T:3004:CDL:OB3	2.21	0.40
1:A:106:LEU:O	1:A:110:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:HB	2:B:119:LEU:HD12	2.03	0.40
2:B:242:GLY:O	2:B:423:SER:HA	2.21	0.40
2:B:365:LYS:HB3	2:B:399:LEU:HD22	2.03	0.40
1:N:121:SER:O	1:N:122:LEU:HB2	2.22	0.40
4:Q:49:ARG:NH2	5:R:67:ASP:HB3	2.36	0.40
2:B:95:LYS:HB2	9:I:32:ALA:HB2	2.02	0.40
2:B:232:LEU:HB3	2:B:235:ALA:HB3	2.04	0.40
5:E:112:VAL:O	5:E:114:VAL:N	2.54	0.40
3:P:318:ARG:HB3	3:P:373:GLU:OE2	2.21	0.40
9:V:76:VAL:O	9:V:76:VAL:HG13	2.21	0.40
1:A:224:ASP:OD2	1:A:226:ASP:OD1	2.40	0.40
2:B:95:LYS:O	2:B:109:VAL:HA	2.21	0.40
5:E:181:GLU:HG2	5:E:182:VAL:N	2.36	0.40
1:N:146:ARG:O	1:N:149:VAL:HG12	2.21	0.40
3:P:27:ILE:HD12	18:P:3002:ANY:H3	2.03	0.40
3:P:75:TYR:CE2	11:R:4007:JZR:H6	2.56	0.40
4:Q:234:LYS:HD2	5:R:8:PRO:HB2	2.04	0.40
7:T:54:ALA:O	7:T:58:VAL:HG23	2.22	0.40
10:W:29:LEU:HD12	10:W:29:LEU:HA	1.86	0.40
10:W:53:LYS:HE3	10:W:53:LYS:HB2	1.90	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	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	14	10
1	N	440/446 (99%)	425 (97%)	11 (2%)	4 (1%)	14	10
2	B	418/439 (95%)	405 (97%)	10 (2%)	3 (1%)	18	15
2	O	419/439 (95%)	404 (96%)	13 (3%)	2 (0%)	24	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	363/379 (96%)	352 (97%)	9 (2%)	2 (1%)	21	18
3	P	363/379 (96%)	352 (97%)	10 (3%)	1 (0%)	36	36
4	D	239/241 (99%)	233 (98%)	6 (2%)	0	100	100
4	Q	239/241 (99%)	232 (97%)	7 (3%)	0	100	100
5	E	194/196 (99%)	181 (93%)	10 (5%)	3 (2%)	8	4
5	R	194/196 (99%)	183 (94%)	8 (4%)	3 (2%)	8	4
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	94 (97%)	1 (1%)	2 (2%)	5	2
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	69 (93%)	5 (7%)	0	100	100
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	64 (100%)	0	0	100	100
9	I	39/78 (50%)	37 (95%)	1 (3%)	1 (3%)	4	1
9	V	39/78 (50%)	36 (92%)	2 (5%)	1 (3%)	4	1
10	J	30/62 (48%)	28 (93%)	2 (7%)	0	100	100
10	W	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	3
All	All	3945/4220 (94%)	3803 (96%)	115 (3%)	27 (1%)	18	15

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	19	ILE
5	E	71	MET
5	E	72	SER
9	I	41	PRO
1	N	224	ASP
2	O	171	ALA
2	O	303	VAL
3	P	19	ILE
5	R	191	ASP
9	V	41	PRO
2	B	171	ALA
2	B	229	GLY
5	E	113	GLU
5	R	189	SER

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Mol	Chain	Res	Type
5	R	190	ASP
6	S	13	LEU
1	A	223	TYR
3	C	18	PHE
1	N	223	TYR
1	A	229	PRO
1	A	442	PHE
1	N	229	PRO
1	N	442	PHE
6	S	14	GLU
10	W	25	VAL
2	B	234	GLY

5.3.2 Protein sidechains (i)

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	363/370 (98%)	355 (98%)	8 (2%)	45	53
1	N	363/370 (98%)	357 (98%)	6 (2%)	53	62
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	328/343 (96%)	327 (100%)	1 (0%)	86	91
3	C	312/327 (95%)	308 (99%)	4 (1%)	61	69
3	P	311/327 (95%)	307 (99%)	4 (1%)	61	69
4	D	206/206 (100%)	205 (100%)	1 (0%)	81	88
4	Q	206/206 (100%)	204 (99%)	2 (1%)	68	76
5	E	165/168 (98%)	163 (99%)	2 (1%)	63	72
5	R	167/168 (99%)	164 (98%)	3 (2%)	51	60
6	F	90/98 (92%)	88 (98%)	2 (2%)	45	53
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%)	65 (98%)	1 (2%)	57	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	63/74 (85%)	63 (100%)	0	100	100
8	U	63/74 (85%)	61 (97%)	2 (3%)	34	38
9	I	27/60 (45%)	26 (96%)	1 (4%)	30	33
9	V	27/60 (45%)	26 (96%)	1 (4%)	30	33
10	J	27/52 (52%)	25 (93%)	2 (7%)	13	10
10	W	51/52 (98%)	50 (98%)	1 (2%)	48	56
All	All	3323/3538 (94%)	3278 (99%)	45 (1%)	59	67

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	203	LEU
1	A	210	ASP
1	A	245	GLU
1	A	281	ASP
1	A	305	GLN
1	A	316	ASP
1	A	348	SER
3	C	16	ASN
3	C	21	LEU
3	C	222	PRO
3	C	346	PRO
4	D	169	LEU
5	E	112	VAL
5	E	172	ARG
6	F	33	ARG
6	F	95	LYS
7	G	71	ARG
9	I	41	PRO
10	J	30	PHE
10	J	32	GLU
1	N	108	LYS
1	N	203	LEU
1	N	245	GLU
1	N	281	ASP
1	N	316	ASP
1	N	348	SER
2	O	232	LEU
3	P	16	ASN

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Mol	Chain	Res	Type
3	P	21	LEU
3	P	222	PRO
3	P	346	PRO
4	Q	76	GLU
4	Q	169	LEU
5	R	6	LYS
5	R	113	GLU
5	R	191	ASP
6	S	13	LEU
6	S	33	ARG
6	S	95	LYS
7	T	71	ARG
8	U	42	GLU
8	U	78	LYS
9	V	41	PRO
10	W	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	53	ASN
1	A	136	GLN
1	A	159	GLN
1	A	165	GLN
1	A	213	GLN
1	A	267	ASN
1	A	271	GLN
1	A	289	HIS
1	A	305	GLN
1	A	311	ASN
2	B	240	HIS
2	B	305	GLN
2	B	343	GLN
2	B	354	ASN
2	B	412	ASN
3	C	16	ASN
3	C	159	ASN
3	C	201	HIS
3	C	312	GLN
5	E	57	GLN
5	E	108	GLN

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Mol	Chain	Res	Type
7	G	6	HIS
8	H	71	HIS
9	I	58	GLN
1	N	18	GLN
1	N	61	HIS
1	N	136	GLN
1	N	159	GLN
1	N	165	GLN
1	N	213	GLN
1	N	215	HIS
1	N	267	ASN
1	N	271	GLN
1	N	311	ASN
2	O	218	GLN
2	O	240	HIS
2	O	343	GLN
2	O	412	ASN
3	P	16	ASN
3	P	159	ASN
3	P	201	HIS
4	Q	225	HIS
5	R	57	GLN
5	R	108	GLN
6	S	38	HIS
6	S	79	GLN
8	U	71	HIS
8	U	75	ASN
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)

45 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	HEM	C	501	3	50,50,50	1.44	4 (8%)	67,82,82	1.03	3 (4%)
20	CDL	G	2004	-	43,43,99	1.12	3 (6%)	49,55,111	1.24	6 (12%)
13	AZI	O	4010	-	2,2,2	3.49	2 (100%)	0,1,1	-	-
20	CDL	P	3003	-	38,38,99	1.04	1 (2%)	42,47,111	1.04	4 (9%)
11	JZR	P	3010	-	18,18,18	1.82	5 (27%)	23,23,23	0.70	0
11	JZR	S	2011	-	18,18,18	1.79	3 (16%)	23,23,23	0.73	0
19	HEC	D	501	4	50,50,50	0.95	1 (2%)	68,82,82	1.19	3 (4%)
18	ANY	C	2002	-	38,38,41	1.88	11 (28%)	32,52,55	1.73	7 (21%)
14	GOL	P	3008	-	5,5,5	1.28	0	5,5,5	0.56	0
16	SMA	P	3001	-	38,38,38	1.62	8 (21%)	47,52,52	0.88	2 (4%)
13	AZI	A	4011	-	2,2,2	4.67	2 (100%)	0,1,1	-	-
20	CDL	D	2003	-	38,38,99	1.07	1 (2%)	42,47,111	1.04	3 (7%)
15	HEM	P	502	3	50,50,50	1.53	4 (8%)	67,82,82	1.02	2 (2%)
12	PO4	A	2013	-	4,4,4	1.42	1 (25%)	6,6,6	0.90	0
21	FES	E	501	5	0,4,4	-	-	-		
11	JZR	F	4001	-	18,18,18	1.84	5 (27%)	23,23,23	0.71	0
20	CDL	T	3004	-	48,48,99	1.15	3 (6%)	54,60,111	1.19	3 (5%)
14	GOL	R	4005	-	5,5,5	1.30	0	5,5,5	0.56	0
11	JZR	C	2010	-	18,18,18	1.81	4 (22%)	23,23,23	0.70	0
16	SMA	C	2001	-	38,38,38	1.64	9 (23%)	47,52,52	0.89	2 (4%)
14	GOL	B	2009	-	5,5,5	1.21	0	5,5,5	0.56	0
14	GOL	C	4006	-	5,5,5	1.32	0	5,5,5	0.61	0
11	JZR	F	3011	-	18,18,18	1.80	5 (27%)	23,23,23	0.67	0
17	PEE	D	2006	-	25,25,50	1.50	6 (24%)	28,30,55	0.77	1 (3%)
14	GOL	O	3009	-	5,5,5	1.15	0	5,5,5	0.50	0
11	JZR	R	4007	-	18,18,18	1.85	4 (22%)	23,23,23	0.71	0
13	AZI	C	2005	-	2,2,2	4.06	2 (100%)	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	JZR	A	4004	-	18,18,18	1.58	3 (16%)	23,23,23	0.62	0
12	PO4	P	3013	-	4,4,4	1.41	1 (25%)	6,6,6	0.87	0
11	JZR	C	4002	-	18,18,18	1.87	4 (22%)	23,23,23	0.76	1 (4%)
13	AZI	P	3005	-	2,2,2	3.88	2 (100%)	0,1,1	-	-
12	PO4	C	4008	-	4,4,4	1.46	1 (25%)	6,6,6	0.89	0
17	PEE	C	2007	-	48,48,50	1.29	5 (10%)	51,53,55	0.75	2 (3%)
14	GOL	C	2008	-	5,5,5	1.45	0	5,5,5	0.75	0
12	PO4	S	3012	-	4,4,4	1.40	1 (25%)	6,6,6	0.89	0
15	HEM	C	502	3	50,50,50	1.46	5 (10%)	67,82,82	1.04	2 (2%)
15	HEM	P	501	3	50,50,50	1.49	5 (10%)	67,82,82	0.99	2 (2%)
11	JZR	D	4003	-	18,18,18	1.84	4 (22%)	23,23,23	0.72	0
12	PO4	F	2012	-	4,4,4	1.34	1 (25%)	6,6,6	0.89	0
21	FES	R	501	5	0,4,4	-	-	-		
19	HEC	Q	501	4	50,50,50	0.93	1 (2%)	68,82,82	1.28	5 (7%)
18	ANY	P	3002	-	38,38,41	1.88	12 (31%)	32,52,55	1.59	6 (18%)
17	PEE	Q	3006	-	50,50,50	1.33	5 (10%)	53,55,55	0.75	2 (3%)
13	AZI	G	4009	-	2,2,2	3.80	2 (100%)	0,1,1	-	-
17	PEE	P	3007	-	48,48,50	1.30	5 (10%)	51,53,55	0.75	2 (3%)

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	HEM	C	501	3	-	5/14/54/54	-
20	CDL	G	2004	-	-	34/52/52/110	-
20	CDL	P	3003	-	-	23/43/43/110	-
11	JZR	P	3010	-	-	5/9/29/29	0/1/1/1
11	JZR	S	2011	-	-	5/9/29/29	0/1/1/1
19	HEC	D	501	4	1/1/3/7	8/14/54/54	-
18	ANY	C	2002	-	-	2/37/52/56	0/1/2/2
14	GOL	P	3008	-	-	2/4/4/4	-
16	SMA	P	3001	-	-	0/34/34/34	0/2/2/2
20	CDL	D	2003	-	-	19/43/43/110	-
15	HEM	P	502	3	-	4/14/54/54	-
21	FES	E	501	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	JZR	F	4001	-	-	2/9/29/29	0/1/1/1
20	CDL	T	3004	-	-	27/57/57/110	-
14	GOL	R	4005	-	-	2/4/4/4	-
11	JZR	C	2010	-	-	4/9/29/29	0/1/1/1
16	SMA	C	2001	-	-	2/34/34/34	0/2/2/2
14	GOL	B	2009	-	-	2/4/4/4	-
14	GOL	C	4006	-	-	3/4/4/4	-
11	JZR	F	3011	-	-	3/9/29/29	0/1/1/1
17	PEE	D	2006	-	-	18/29/29/54	-
14	GOL	O	3009	-	-	4/4/4/4	-
11	JZR	R	4007	-	-	2/9/29/29	0/1/1/1
11	JZR	A	4004	-	-	0/9/29/29	0/1/1/1
11	JZR	C	4002	-	-	3/9/29/29	0/1/1/1
17	PEE	C	2007	-	-	19/52/52/54	-
14	GOL	C	2008	-	-	4/4/4/4	-
15	HEM	C	502	3	-	4/14/54/54	-
15	HEM	P	501	3	-	5/14/54/54	-
11	JZR	D	4003	-	-	4/9/29/29	0/1/1/1
21	FES	R	501	5	-	-	0/1/1/1
19	HEC	Q	501	4	1/1/3/7	7/14/54/54	-
18	ANY	P	3002	-	1/1/10/13	3/37/52/56	0/1/2/2
17	PEE	Q	3006	-	-	24/54/54/54	-
17	PEE	P	3007	-	-	19/52/52/54	-

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	502	HEM	CBB-CAB	5.48	1.56	1.30
15	P	501	HEM	CBB-CAB	5.42	1.56	1.30
15	C	501	HEM	CBC-CAC	5.33	1.56	1.30
15	P	501	HEM	CBC-CAC	5.00	1.54	1.30
15	C	502	HEM	CBC-CAC	5.00	1.54	1.30
15	P	502	HEM	CBC-CAC	4.95	1.54	1.30
18	P	3002	ANY	C8-N1	4.95	1.40	1.34
11	C	4002	JZR	O1-C1	4.93	1.48	1.40
11	S	2011	JZR	O1-C1	4.92	1.48	1.40
13	A	4011	AZI	N1-N2	-4.91	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	4003	JZR	O1-C1	4.87	1.48	1.40
11	F	4001	JZR	O1-C1	4.82	1.48	1.40
11	C	2010	JZR	O1-C1	4.78	1.48	1.40
11	R	4007	JZR	O1-C1	4.78	1.48	1.40
18	C	2002	ANY	C2-C1	4.71	1.47	1.40
15	C	502	HEM	CBB-CAB	4.69	1.52	1.30
11	P	3010	JZR	O1-C1	4.64	1.47	1.40
11	F	3011	JZR	O1-C1	4.61	1.47	1.40
15	C	501	HEM	CBB-CAB	4.54	1.52	1.30
13	A	4011	AZI	N3-N2	-4.42	1.14	1.23
18	P	3002	ANY	C2-C1	4.40	1.46	1.40
13	C	2005	AZI	N1-N2	-4.31	1.14	1.23
18	C	2002	ANY	C8-N1	4.27	1.40	1.34
13	P	3005	AZI	N1-N2	-4.26	1.14	1.23
17	P	3007	PEE	C39-C38	4.13	1.55	1.31
17	C	2007	PEE	C39-C38	4.09	1.54	1.31
17	Q	3006	PEE	C39-C38	4.08	1.54	1.31
13	G	4009	AZI	N1-N2	-3.96	1.15	1.23
13	O	4010	AZI	N1-N2	-3.83	1.15	1.23
13	C	2005	AZI	N3-N2	-3.79	1.15	1.23
16	P	3001	SMA	O1-C2	3.75	1.41	1.36
18	C	2002	ANY	C3-C2	3.69	1.45	1.39
16	C	2001	SMA	O1-C2	3.67	1.40	1.36
13	G	4009	AZI	N3-N2	-3.63	1.15	1.23
18	P	3002	ANY	C3-C2	3.62	1.45	1.39
18	P	3002	ANY	C12-C11	3.57	1.60	1.52
18	C	2002	ANY	C12-C11	3.56	1.60	1.52
13	P	3005	AZI	N3-N2	-3.46	1.16	1.23
15	P	502	HEM	CAB-C3B	-3.45	1.38	1.47
17	Q	3006	PEE	C21-C22	-3.41	1.34	1.51
17	C	2007	PEE	C21-C22	-3.39	1.34	1.51
11	A	4004	JZR	O1-C1	3.38	1.45	1.40
11	S	2011	JZR	O5-C1	3.38	1.50	1.41
11	F	3011	JZR	O5-C1	3.37	1.50	1.41
17	P	3007	PEE	C21-C22	-3.37	1.35	1.51
11	R	4007	JZR	O5-C1	3.30	1.50	1.41
16	P	3001	SMA	C6-C5	3.30	1.44	1.38
11	D	4003	JZR	O5-C1	3.29	1.50	1.41
16	P	3001	SMA	C6-C7	3.24	1.44	1.38
16	C	2001	SMA	C6-C7	3.23	1.44	1.38
11	C	4002	JZR	O5-C1	3.23	1.50	1.41
11	F	4001	JZR	O5-C1	3.23	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	3002	ANY	C13-C12	3.21	1.59	1.53
11	C	2010	JZR	O5-C1	3.19	1.50	1.41
17	C	2007	PEE	O3-C30	3.17	1.42	1.33
16	C	2001	SMA	C7-C8	3.17	1.44	1.40
16	C	2001	SMA	C4A-C5	3.15	1.46	1.40
18	C	2002	ANY	C10-C9	3.13	1.60	1.53
13	O	4010	AZI	N3-N2	-3.10	1.16	1.23
16	C	2001	SMA	C20-C19	3.09	1.35	1.33
16	P	3001	SMA	C7-C8	3.08	1.44	1.40
17	D	2006	PEE	P-O1P	3.06	1.61	1.50
11	A	4004	JZR	O5-C1	3.06	1.49	1.41
11	P	3010	JZR	O5-C1	3.06	1.49	1.41
15	P	502	HEM	CAC-C3C	-3.06	1.39	1.47
17	Q	3006	PEE	P-O1P	3.04	1.61	1.50
17	Q	3006	PEE	O3-C30	3.03	1.42	1.33
17	P	3007	PEE	P-O1P	3.03	1.61	1.50
17	P	3007	PEE	O3-C30	2.98	1.42	1.33
15	P	501	HEM	CAB-C3B	-2.97	1.39	1.47
17	P	3007	PEE	O2-C10	2.92	1.42	1.34
15	C	501	HEM	CAB-C3B	-2.91	1.39	1.47
17	D	2006	PEE	O2-C10	2.90	1.42	1.34
16	C	2001	SMA	C6-C5	2.87	1.43	1.38
18	C	2002	ANY	C13-C12	2.86	1.58	1.53
15	C	501	HEM	CAC-C3C	-2.85	1.39	1.47
15	P	501	HEM	CAC-C3C	-2.84	1.39	1.47
16	P	3001	SMA	C4A-C5	2.83	1.45	1.40
17	Q	3006	PEE	O2-C10	2.83	1.42	1.34
16	P	3001	SMA	C20-C19	2.77	1.35	1.33
17	C	2007	PEE	O2-C10	2.72	1.42	1.34
11	A	4004	JZR	C4-C5	2.71	1.58	1.53
18	C	2002	ANY	O8-C21	2.67	1.40	1.34
17	D	2006	PEE	O3-C30	2.67	1.41	1.33
18	C	2002	ANY	O5-C14	2.66	1.40	1.34
16	P	3001	SMA	C8-C8A	2.63	1.43	1.39
15	C	502	HEM	CAB-C3B	-2.63	1.40	1.47
11	C	4002	JZR	C4-C5	2.61	1.58	1.53
11	P	3010	JZR	C4-C5	2.58	1.58	1.53
12	C	4008	PO4	P-O1	2.56	1.56	1.50
17	C	2007	PEE	P-O1P	2.56	1.59	1.50
18	P	3002	ANY	C7-N2	2.55	1.40	1.34
11	R	4007	JZR	C4-C5	2.54	1.58	1.53
16	C	2001	SMA	C3-C2	2.49	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	ANY	C5-C6	2.47	1.43	1.39
15	C	502	HEM	CAC-C3C	-2.47	1.40	1.47
20	T	3004	CDL	O1-C1	2.45	1.50	1.43
11	F	4001	JZR	C4-C5	2.45	1.58	1.53
12	A	2013	PO4	P-O1	2.45	1.56	1.50
16	C	2001	SMA	C4A-C8A	2.43	1.46	1.40
12	S	3012	PO4	P-O1	2.42	1.56	1.50
20	G	2004	CDL	O1-C1	2.42	1.50	1.43
12	P	3013	PO4	P-O1	2.42	1.56	1.50
18	P	3002	ANY	C10-C9	2.41	1.58	1.53
20	T	3004	CDL	OB8-CB6	-2.41	1.39	1.45
18	P	3002	ANY	C5-C6	2.40	1.43	1.39
19	D	501	HEC	C4C-C3C	2.40	1.49	1.44
18	P	3002	ANY	O5-C14	2.38	1.39	1.34
11	F	3011	JZR	C4-C5	2.38	1.58	1.53
18	P	3002	ANY	O8-C21	2.38	1.39	1.34
11	D	4003	JZR	C4-C5	2.37	1.58	1.53
12	F	2012	PO4	P-O1	2.33	1.56	1.50
20	D	2003	CDL	O1-C1	2.31	1.50	1.43
11	C	4002	JZR	O5-C5	2.30	1.50	1.44
11	S	2011	JZR	O5-C5	2.29	1.50	1.44
11	R	4007	JZR	O5-C5	2.28	1.49	1.44
11	D	4003	JZR	O5-C5	2.25	1.49	1.44
17	D	2006	PEE	C3-C2	2.24	1.57	1.50
20	T	3004	CDL	OA8-CA6	-2.24	1.40	1.45
20	P	3003	CDL	O1-C1	2.20	1.49	1.43
15	P	501	HEM	FE-NB	2.20	2.01	1.94
16	C	2001	SMA	C8-C8A	2.20	1.43	1.39
11	F	4001	JZR	O5-C5	2.18	1.49	1.44
18	P	3002	ANY	C6-C1	2.16	1.45	1.41
11	C	2010	JZR	C4-C5	2.16	1.57	1.53
20	G	2004	CDL	OA8-CA6	-2.14	1.40	1.45
20	G	2004	CDL	OB8-CB6	-2.12	1.40	1.45
11	F	3011	JZR	O5-C5	2.12	1.49	1.44
18	C	2002	ANY	C7-N2	2.11	1.39	1.34
11	C	2010	JZR	O5-C5	2.11	1.49	1.44
18	P	3002	ANY	C4-C3	2.10	1.42	1.38
16	P	3001	SMA	C3-C2	2.09	1.38	1.34
17	D	2006	PEE	C31-C30	2.08	1.56	1.50
11	P	3010	JZR	O5-C5	2.07	1.49	1.44
11	P	3010	JZR	C1-C2	2.07	1.58	1.52
15	C	502	HEM	C3B-C4B	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	ANY	C6-C1	2.05	1.44	1.41
11	F	3011	JZR	C1-C2	2.02	1.58	1.52
17	D	2006	PEE	C1-C2	2.02	1.57	1.50
19	Q	501	HEC	C4C-C3C	2.01	1.48	1.44
11	F	4001	JZR	C1-C2	2.00	1.58	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	2002	ANY	C25-C22-C23	5.41	133.03	111.60
19	Q	501	HEC	CAC-C3C-C4C	-4.79	118.33	124.91
20	T	3004	CDL	CB4-OB6-CB5	-4.54	109.82	117.85
19	Q	501	HEC	CAC-C3C-C2C	4.31	133.70	126.89
20	G	2004	CDL	CB4-OB6-CB5	-4.01	110.77	117.85
18	P	3002	ANY	C23-C22-C21	4.00	123.05	110.94
19	D	501	HEC	CAC-C3C-C2C	3.86	133.00	126.89
18	C	2002	ANY	O5-C14-O6	-3.65	119.58	124.10
15	C	502	HEM	C3B-C4B-NB	3.65	112.09	109.47
15	P	502	HEM	C3B-C4B-NB	3.63	112.08	109.47
18	P	3002	ANY	O5-C14-O6	-3.56	119.69	124.10
15	P	501	HEM	C3B-C4B-NB	3.47	111.96	109.47
19	D	501	HEC	CAC-C3C-C4C	-3.36	120.29	124.91
16	P	3001	SMA	C9-C10-C11	-3.11	108.65	114.46
20	T	3004	CDL	CA4-OA6-CA5	-3.08	110.42	117.80
15	C	501	HEM	C3B-C4B-NB	2.98	111.61	109.47
19	D	501	HEC	CMB-C2B-C1B	2.96	129.66	125.03
18	P	3002	ANY	C25-C22-C23	2.89	123.05	111.60
18	C	2002	ANY	O2-C8-N1	-2.84	121.82	125.72
20	G	2004	CDL	CA4-OA6-CA5	-2.82	111.06	117.80
17	Q	3006	PEE	C22-C21-C20	2.80	127.32	113.86
16	C	2001	SMA	C9-C10-C11	-2.80	109.23	114.46
18	C	2002	ANY	C25-C22-C21	2.79	119.39	110.94
18	P	3002	ANY	O2-C8-N1	-2.72	121.99	125.72
16	C	2001	SMA	C4A-C4-C3	-2.71	114.79	118.78
20	G	2004	CDL	CA6-CA4-CA3	-2.70	105.50	111.78
20	D	2003	CDL	CB4-OB6-CB5	-2.66	111.44	117.80
17	C	2007	PEE	C21-C22-C23	2.65	127.74	114.37
17	P	3007	PEE	C21-C22-C23	2.63	127.67	114.37
20	P	3003	CDL	CB6-CB4-CB3	-2.62	105.68	111.78
17	P	3007	PEE	C22-C21-C20	2.62	126.44	113.86
15	C	501	HEM	C2D-C1D-ND	2.60	112.90	109.90
17	C	2007	PEE	C22-C21-C20	2.59	126.32	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	2003	CDL	CB6-CB4-CB3	-2.53	105.89	111.78
20	P	3003	CDL	CB4-OB6-CB5	-2.46	111.90	117.80
18	P	3002	ANY	O4-C20-O7	-2.43	121.09	124.10
15	C	502	HEM	C4B-C3B-C2B	-2.41	105.06	107.28
16	P	3001	SMA	C4A-C4-C3	-2.40	115.25	118.78
18	C	2002	ANY	O8-C21-O9	-2.37	119.67	123.95
20	D	2003	CDL	OA4-PA1-OA2	2.36	112.81	106.67
18	P	3002	ANY	O8-C21-O9	-2.34	119.72	123.95
11	C	4002	JZR	C1'-O1-C1	2.29	117.58	113.68
20	G	2004	CDL	CB6-CB4-CB3	-2.28	106.47	111.78
19	Q	501	HEC	CAD-C3D-C4D	2.25	128.62	124.70
17	Q	3006	PEE	C21-C22-C23	2.25	125.74	114.37
20	T	3004	CDL	CB6-OB8-CB7	-2.24	111.57	117.08
15	P	501	HEM	CMD-C2D-C1D	2.23	128.52	125.03
15	P	502	HEM	C4B-C3B-C2B	-2.16	105.29	107.28
20	P	3003	CDL	OA4-PA1-OA2	2.16	112.30	106.67
20	G	2004	CDL	CB6-OB8-CB7	-2.16	111.76	117.08
18	C	2002	ANY	C23-C22-C21	-2.15	104.43	110.94
15	C	501	HEM	CMD-C2D-C1D	2.07	128.27	125.03
19	Q	501	HEC	C4A-C3A-C2A	-2.06	103.92	106.97
18	C	2002	ANY	O4-C20-O7	-2.04	121.56	124.10
17	D	2006	PEE	O3-C3-C2	2.02	114.22	108.40
20	G	2004	CDL	OB6-CB5-OB7	2.01	126.88	122.99
19	Q	501	HEC	CMA-C3A-C4A	2.01	128.27	124.73
20	P	3003	CDL	OA2-PA1-OA3	2.00	111.85	106.44

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	P	3002	ANY	C22
19	D	501	HEC	NA
19	Q	501	HEC	NA

All (268) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	2008	GOL	C1-C2-C3-O3
14	O	3009	GOL	O1-C1-C2-C3
14	O	3009	GOL	C1-C2-C3-O3
14	P	3008	GOL	O1-C1-C2-C3
14	R	4005	GOL	O1-C1-C2-C3
17	C	2007	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
17	D	2006	PEE	C2-C1-O3P-P
17	D	2006	PEE	C4-O4P-P-O3P
17	D	2006	PEE	C4-O4P-P-O2P
17	D	2006	PEE	C4-O4P-P-O1P
17	P	3007	PEE	C4-O4P-P-O1P
17	Q	3006	PEE	C4-O4P-P-O3P
17	Q	3006	PEE	C4-O4P-P-O2P
17	Q	3006	PEE	C4-O4P-P-O1P
17	Q	3006	PEE	O4P-C4-C5-N
20	D	2003	CDL	CA2-OA2-PA1-OA4
20	D	2003	CDL	CA2-OA2-PA1-OA5
20	D	2003	CDL	CB2-OB2-PB2-OB3
20	D	2003	CDL	CB2-OB2-PB2-OB4
20	D	2003	CDL	CB2-OB2-PB2-OB5
20	D	2003	CDL	OB5-CB3-CB4-OB6
20	G	2004	CDL	O1-C1-CB2-OB2
20	G	2004	CDL	CA2-C1-CB2-OB2
20	G	2004	CDL	CA2-OA2-PA1-OA3
20	G	2004	CDL	CA2-OA2-PA1-OA4
20	G	2004	CDL	CA2-OA2-PA1-OA5
20	G	2004	CDL	C11-CA5-OA6-CA4
20	G	2004	CDL	CB2-OB2-PB2-OB5
20	P	3003	CDL	CA2-C1-CB2-OB2
20	P	3003	CDL	CA2-OA2-PA1-OA3
20	P	3003	CDL	CA2-OA2-PA1-OA5
20	P	3003	CDL	OB6-CB4-CB6-OB8
20	T	3004	CDL	O1-C1-CA2-OA2
20	T	3004	CDL	O1-C1-CB2-OB2
20	T	3004	CDL	CB2-OB2-PB2-OB3
20	T	3004	CDL	C51-CB5-OB6-CB4
20	G	2004	CDL	C51-CB5-OB6-CB4
20	T	3004	CDL	OB7-CB5-OB6-CB4
20	G	2004	CDL	C71-CB7-OB8-CB6
20	G	2004	CDL	OA7-CA5-OA6-CA4
20	T	3004	CDL	OA9-CA7-OA8-CA6
20	G	2004	CDL	OB9-CB7-OB8-CB6
20	G	2004	CDL	OB7-CB5-OB6-CB4
17	C	2007	PEE	C37-C38-C39-C40
17	P	3007	PEE	C37-C38-C39-C40
17	D	2006	PEE	O5-C30-O3-C3
20	P	3003	CDL	O1-C1-CB2-OB2
17	D	2006	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
20	T	3004	CDL	C31-CA7-OA8-CA6
20	T	3004	CDL	C71-CB7-OB8-CB6
20	G	2004	CDL	C31-CA7-OA8-CA6
17	Q	3006	PEE	C17-C18-C19-C20
19	D	501	HEC	C4C-C3C-CAC-CBC
11	S	2011	JZR	C4-C5-C6-O6
20	G	2004	CDL	CA7-C31-C32-C33
20	T	3004	CDL	C11-CA5-OA6-CA4
14	O	3009	GOL	O1-C1-C2-O2
14	O	3009	GOL	O2-C2-C3-O3
19	D	501	HEC	C2B-C3B-CAB-CBB
11	F	3011	JZR	O1-C1'-C2'-C3'
11	P	3010	JZR	O1-C1'-C2'-C3'
17	C	2007	PEE	C21-C22-C23-C24
17	P	3007	PEE	C21-C22-C23-C24
20	T	3004	CDL	OB9-CB7-OB8-CB6
17	C	2007	PEE	C10-C11-C12-C13
17	P	3007	PEE	C10-C11-C12-C13
11	D	4003	JZR	O5-C5-C6-O6
17	Q	3006	PEE	C10-C11-C12-C13
17	Q	3006	PEE	C30-C31-C32-C33
20	T	3004	CDL	CA5-C11-C12-C13
20	G	2004	CDL	OA9-CA7-OA8-CA6
17	Q	3006	PEE	C37-C38-C39-C40
11	S	2011	JZR	O5-C5-C6-O6
11	D	4003	JZR	O1-C1'-C2'-C3'
20	T	3004	CDL	OA7-CA5-OA6-CA4
20	T	3004	CDL	CB2-C1-CA2-OA2
20	T	3004	CDL	CA2-C1-CB2-OB2
14	B	2009	GOL	C1-C2-C3-O3
14	C	2008	GOL	O1-C1-C2-C3
14	C	4006	GOL	C1-C2-C3-O3
11	P	3010	JZR	O5-C5-C6-O6
20	D	2003	CDL	C51-CB5-OB6-CB4
20	T	3004	CDL	C11-C12-C13-C14
17	C	2007	PEE	C12-C13-C14-C15
17	P	3007	PEE	C12-C13-C14-C15
14	B	2009	GOL	O2-C2-C3-O3
14	C	2008	GOL	O1-C1-C2-O2
14	C	2008	GOL	O2-C2-C3-O3
14	C	4006	GOL	O2-C2-C3-O3
14	R	4005	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
11	D	4003	JZR	C2'-C3'-C4'-C5'
20	T	3004	CDL	C13-C14-C15-C16
20	D	2003	CDL	C78-C79-C80-C81
19	D	501	HEC	C2C-C3C-CAC-CBC
17	C	2007	PEE	C20-C21-C22-C23
20	D	2003	CDL	CB3-CB4-CB6-OB8
17	C	2007	PEE	C41-C42-C43-C44
17	P	3007	PEE	C20-C21-C22-C23
17	P	3007	PEE	C41-C42-C43-C44
20	P	3003	CDL	C77-C78-C79-C80
17	Q	3006	PEE	C13-C14-C15-C16
20	T	3004	CDL	C32-C33-C34-C35
20	T	3004	CDL	C31-C32-C33-C34
17	Q	3006	PEE	C43-C44-C45-C46
20	D	2003	CDL	OB7-CB5-OB6-CB4
17	C	2007	PEE	C33-C34-C35-C36
20	D	2003	CDL	C73-C74-C75-C76
20	P	3003	CDL	C73-C74-C75-C76
11	C	2010	JZR	C1'-C2'-C3'-C4'
11	D	4003	JZR	C1'-C2'-C3'-C4'
11	C	4002	JZR	C2'-C3'-C4'-C5'
17	Q	3006	PEE	C40-C41-C42-C43
17	Q	3006	PEE	C42-C43-C44-C45
11	R	4007	JZR	C1'-C2'-C3'-C4'
17	D	2006	PEE	C11-C10-O2-C2
20	P	3003	CDL	C72-C73-C74-C75
17	C	2007	PEE	C19-C20-C21-C22
17	P	3007	PEE	C19-C20-C21-C22
17	P	3007	PEE	C33-C34-C35-C36
17	Q	3006	PEE	C34-C35-C36-C37
20	P	3003	CDL	CB5-C51-C52-C53
20	P	3003	CDL	CB7-C71-C72-C73
17	D	2006	PEE	O4-C10-O2-C2
20	P	3003	CDL	C78-C79-C80-C81
17	Q	3006	PEE	C23-C24-C25-C26
11	C	4002	JZR	O5-C5-C6-O6
11	P	3010	JZR	C1'-C2'-C3'-C4'
20	D	2003	CDL	CB7-C71-C72-C73
17	Q	3006	PEE	C35-C36-C37-C38
11	F	4001	JZR	C1'-C2'-C3'-C4'
17	Q	3006	PEE	C22-C23-C24-C25
11	S	2011	JZR	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
14	P	3008	GOL	O1-C1-C2-O2
20	T	3004	CDL	C34-C35-C36-C37
20	G	2004	CDL	OA5-CA3-CA4-CA6
20	G	2004	CDL	OB5-CB3-CB4-CB6
20	P	3003	CDL	OB5-CB3-CB4-CB6
17	P	3007	PEE	C22-C23-C24-C25
17	C	2007	PEE	C22-C23-C24-C25
19	Q	501	HEC	C2B-C3B-CAB-CBB
17	Q	3006	PEE	C20-C21-C22-C23
20	P	3003	CDL	CB3-CB4-CB6-OB8
19	Q	501	HEC	C4C-C3C-CAC-CBC
17	C	2007	PEE	C35-C36-C37-C38
17	P	3007	PEE	C13-C14-C15-C16
17	C	2007	PEE	C13-C14-C15-C16
20	D	2003	CDL	CA2-OA2-PA1-OA3
14	C	4006	GOL	O1-C1-C2-C3
17	P	3007	PEE	C35-C36-C37-C38
17	Q	3006	PEE	C15-C16-C17-C18
20	P	3003	CDL	C51-C52-C53-C54
20	D	2003	CDL	C72-C73-C74-C75
17	Q	3006	PEE	C39-C40-C41-C42
11	C	4002	JZR	C3'-C4'-C5'-C6'
19	D	501	HEC	C4B-C3B-CAB-CBB
17	D	2006	PEE	C33-C34-C35-C36
11	P	3010	JZR	C2'-C3'-C4'-C5'
20	D	2003	CDL	OB5-CB3-CB4-CB6
17	P	3007	PEE	C23-C24-C25-C26
17	C	2007	PEE	C23-C24-C25-C26
20	T	3004	CDL	CA3-CA4-CA6-OA8
20	G	2004	CDL	C35-C36-C37-C38
11	C	2010	JZR	C4-C5-C6-O6
20	P	3003	CDL	OB5-CB3-CB4-OB6
20	T	3004	CDL	OB5-CB3-CB4-OB6
20	G	2004	CDL	C34-C35-C36-C37
20	G	2004	CDL	OA6-CA4-CA6-OA8
18	P	3002	ANY	C16-C17-C18-C19
17	D	2006	PEE	C32-C33-C34-C35
20	D	2003	CDL	C76-C77-C78-C79
18	P	3002	ANY	C15-C16-C17-C18
17	D	2006	PEE	C10-C11-C12-C13
19	Q	501	HEC	C4B-C3B-CAB-CBB
17	Q	3006	PEE	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
17	Q	3006	PEE	O3P-C1-C2-O2
20	G	2004	CDL	OA5-CA3-CA4-OA6
20	G	2004	CDL	OB5-CB3-CB4-OB6
11	F	3011	JZR	C1'-C2'-C3'-C4'
17	D	2006	PEE	O3P-C1-C2-C3
20	T	3004	CDL	OB5-CB3-CB4-CB6
20	P	3003	CDL	C51-CB5-OB6-CB4
20	P	3003	CDL	OB7-CB5-OB6-CB4
17	D	2006	PEE	O3P-C1-C2-O2
20	G	2004	CDL	C33-C34-C35-C36
20	D	2003	CDL	OB6-CB4-CB6-OB8
20	T	3004	CDL	OA6-CA4-CA6-OA8
20	G	2004	CDL	CA3-CA4-CA6-OA8
17	P	3007	PEE	C38-C39-C40-C41
17	D	2006	PEE	C1-O3P-P-O2P
17	D	2006	PEE	C1-O3P-P-O1P
17	D	2006	PEE	C1-O3P-P-O4P
20	G	2004	CDL	CA3-OA5-PA1-OA2
20	G	2004	CDL	CA3-OA5-PA1-OA3
20	G	2004	CDL	CB2-OB2-PB2-OB3
20	G	2004	CDL	CB3-OB5-PB2-OB3
20	P	3003	CDL	CB2-OB2-PB2-OB3
20	P	3003	CDL	CB3-OB5-PB2-OB3
20	T	3004	CDL	CA2-OA2-PA1-OA3
20	T	3004	CDL	CB2-OB2-PB2-OB5
20	G	2004	CDL	C12-C11-CA5-OA6
20	G	2004	CDL	CA4-CA3-OA5-PA1
11	S	2011	JZR	O1-C1'-C2'-C3'
17	C	2007	PEE	C38-C39-C40-C41
17	D	2006	PEE	C3-C2-O2-C10
20	P	3003	CDL	C75-C76-C77-C78
11	F	3011	JZR	C3'-C4'-C5'-C6'
17	Q	3006	PEE	O3P-C1-C2-C3
17	Q	3006	PEE	C36-C37-C38-C39
20	G	2004	CDL	C12-C11-CA5-OA7
11	C	2010	JZR	O5-C5-C6-O6
15	C	502	HEM	CAA-CBA-CGA-O1A
20	D	2003	CDL	CB5-C51-C52-C53
17	C	2007	PEE	C16-C17-C18-C19
20	D	2003	CDL	C71-C72-C73-C74
15	P	502	HEM	CAA-CBA-CGA-O1A
15	C	502	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	P	502	HEM	CAA-CBA-CGA-O2A
17	P	3007	PEE	C16-C17-C18-C19
17	C	2007	PEE	C42-C43-C44-C45
15	C	501	HEM	CAD-CBD-CGD-O1D
17	P	3007	PEE	C42-C43-C44-C45
15	P	501	HEM	CAD-CBD-CGD-O1D
11	F	4001	JZR	C2'-C3'-C4'-C5'
15	C	502	HEM	CAD-CBD-CGD-O2D
16	C	2001	SMA	C9-C10-C11-C22
15	P	501	HEM	CAD-CBD-CGD-O2D
20	G	2004	CDL	O1-C1-CA2-OA2
15	P	502	HEM	CAD-CBD-CGD-O2D
19	D	501	HEC	CAA-CBA-CGA-O2A
19	Q	501	HEC	CAD-CBD-CGD-O1D
15	C	501	HEM	CAD-CBD-CGD-O2D
19	Q	501	HEC	CAA-CBA-CGA-O2A
11	C	2010	JZR	C2'-C3'-C4'-C5'
11	S	2011	JZR	C2'-C3'-C4'-C5'
20	P	3003	CDL	CA2-OA2-PA1-OA4
17	D	2006	PEE	C30-C31-C32-C33
15	C	501	HEM	CAA-CBA-CGA-O1A
15	C	501	HEM	CAA-CBA-CGA-O2A
19	D	501	HEC	CAA-CBA-CGA-O1A
19	D	501	HEC	CAD-CBD-CGD-O1D
11	R	4007	JZR	C3'-C4'-C5'-C6'
15	C	502	HEM	CAD-CBD-CGD-O1D
19	Q	501	HEC	CAA-CBA-CGA-O1A
18	C	2002	ANY	C9-C10-O5-C14
18	P	3002	ANY	C9-C10-O5-C14
15	P	502	HEM	CAD-CBD-CGD-O1D
15	P	501	HEM	CAA-CBA-CGA-O2A
17	P	3007	PEE	C36-C37-C38-C39
19	Q	501	HEC	CAD-CBD-CGD-O2D
15	P	501	HEM	CAA-CBA-CGA-O1A
16	C	2001	SMA	C13-C14-C15-C16
18	C	2002	ANY	C16-C17-C18-C19
20	G	2004	CDL	C32-C31-CA7-OA8
19	D	501	HEC	CAD-CBD-CGD-O2D
17	C	2007	PEE	O3-C30-C31-C32
20	T	3004	CDL	C12-C13-C14-C15
20	P	3003	CDL	C71-C72-C73-C74
20	P	3003	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
17	P	3007	PEE	O3-C30-C31-C32
20	T	3004	CDL	C32-C31-CA7-OA8
17	Q	3006	PEE	C31-C32-C33-C34
20	G	2004	CDL	C32-C31-CA7-OA9
15	C	501	HEM	C3D-CAD-CBD-CGD
15	P	501	HEM	C3D-CAD-CBD-CGD
17	C	2007	PEE	C36-C37-C38-C39
17	C	2007	PEE	O5-C30-C31-C32
11	P	3010	JZR	C4-C5-C6-O6
17	P	3007	PEE	O5-C30-C31-C32

There are no ring outliers.

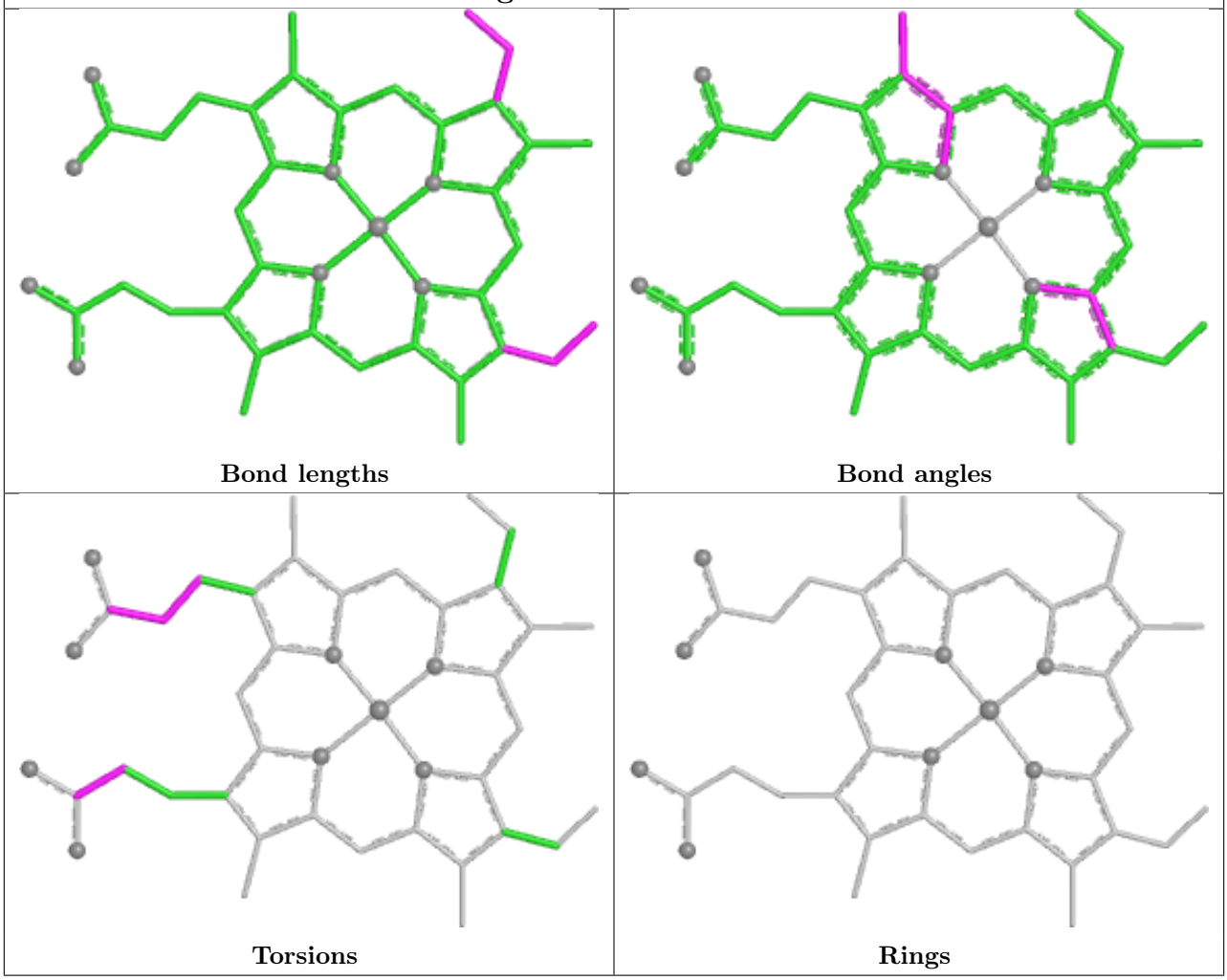
23 monomers are involved in 41 short contacts:

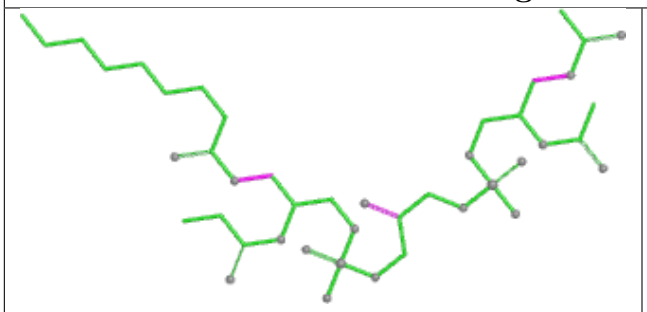
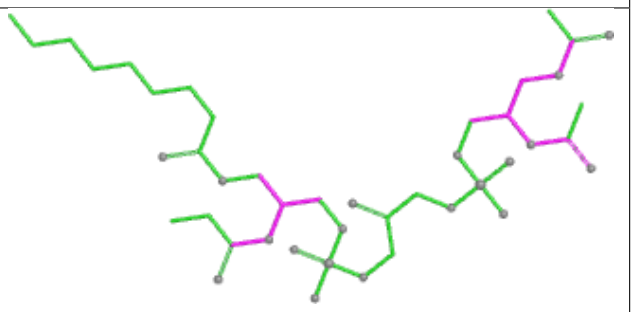
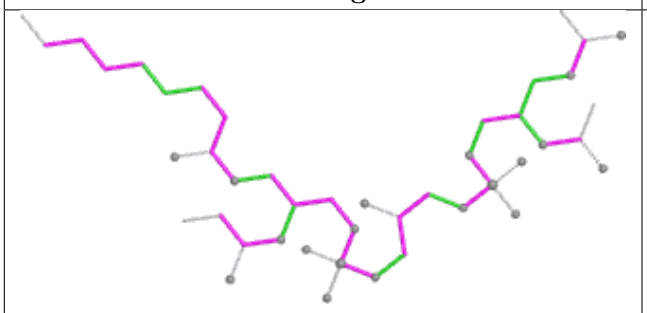
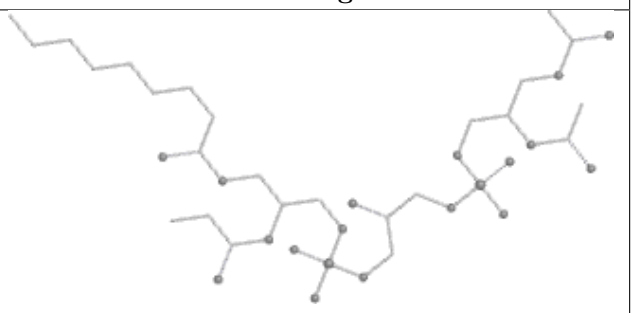
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	501	HEM	1	0
20	P	3003	CDL	2	0
11	S	2011	JZR	3	0
19	D	501	HEC	2	0
18	C	2002	ANY	1	0
16	P	3001	SMA	2	0
20	D	2003	CDL	1	0
15	P	502	HEM	1	0
11	F	4001	JZR	1	0
20	T	3004	CDL	2	0
14	R	4005	GOL	2	0
16	C	2001	SMA	2	0
11	F	3011	JZR	2	0
17	D	2006	PEE	3	0
11	R	4007	JZR	1	0
11	C	4002	JZR	2	0
14	C	2008	GOL	1	0
15	C	502	HEM	2	0
15	P	501	HEM	1	0
11	D	4003	JZR	3	0
18	P	3002	ANY	2	0
17	Q	3006	PEE	4	0
17	P	3007	PEE	1	0

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

also be included. For torsion angles, if less then 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 HEM C 501



Ligand CDL G 2004	
 Bond lengths	 Bond angles
 Torsions	 Rings

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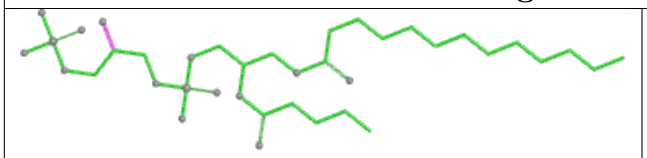
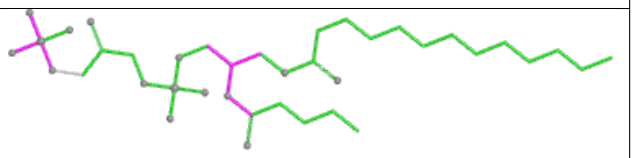
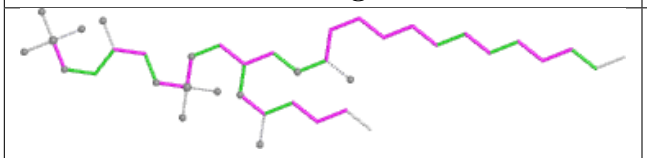
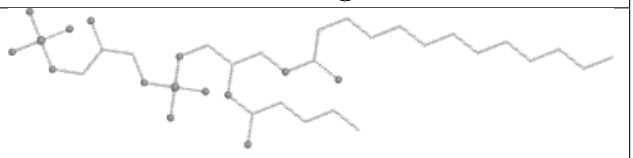
 Bond lengths	 Bond angles
 Torsions	 Rings

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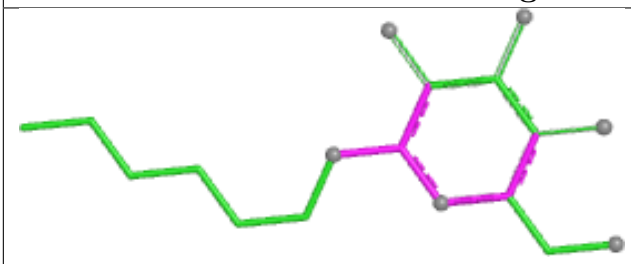

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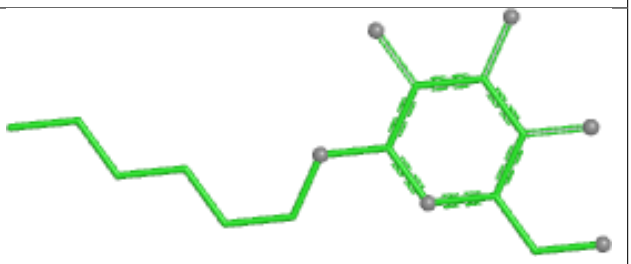

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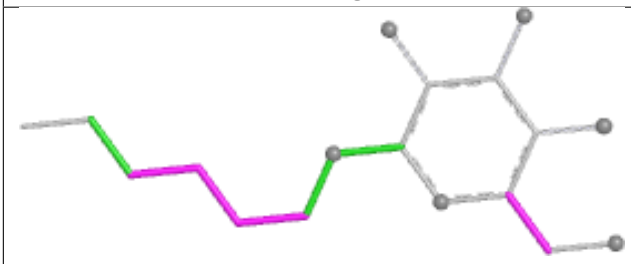

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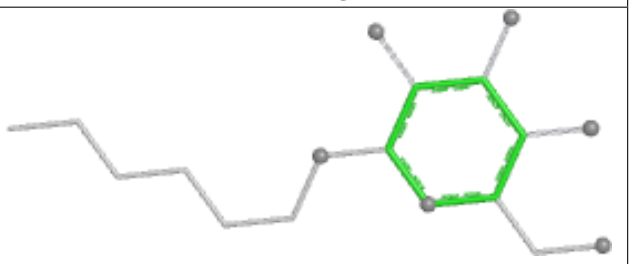

Rings

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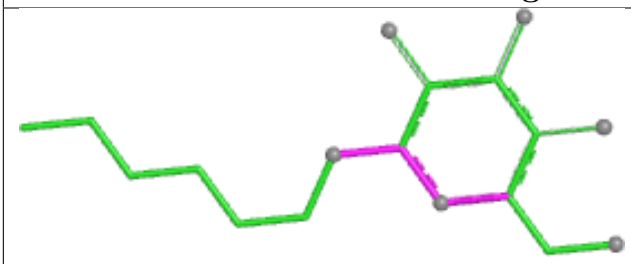

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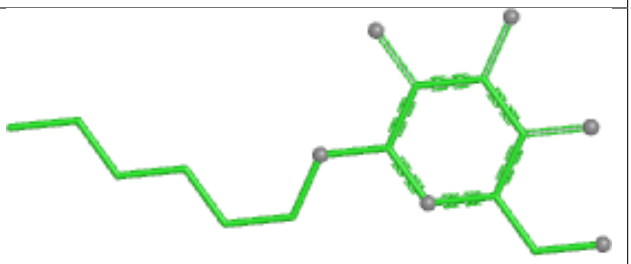

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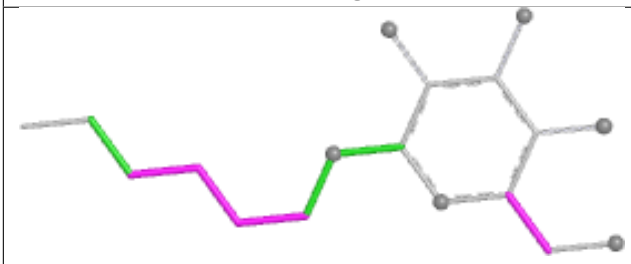

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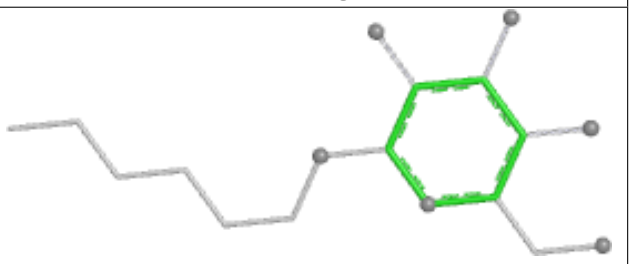

Rings

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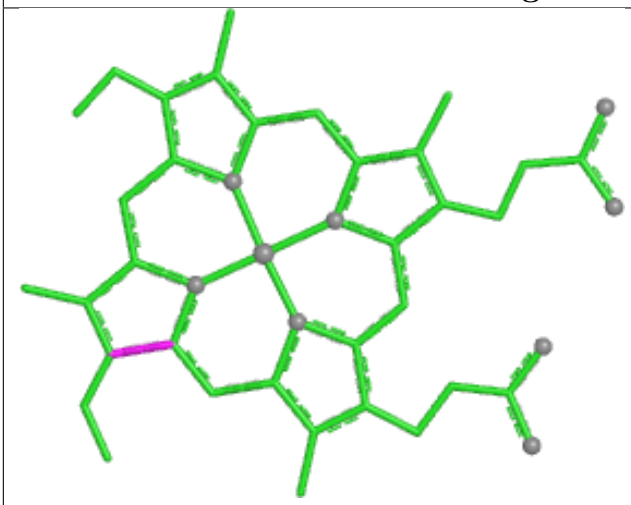

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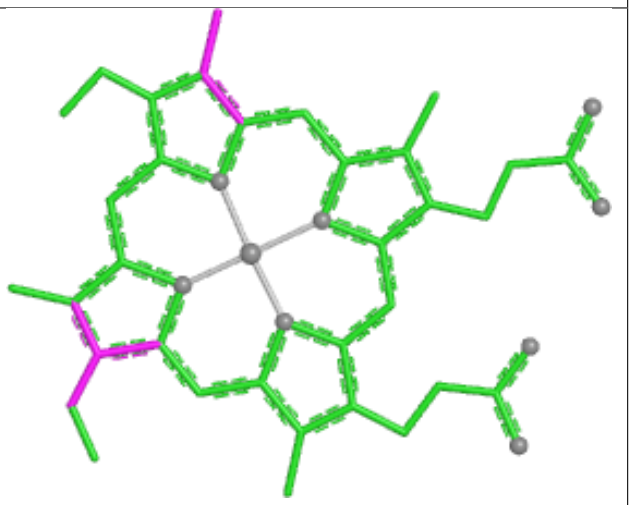

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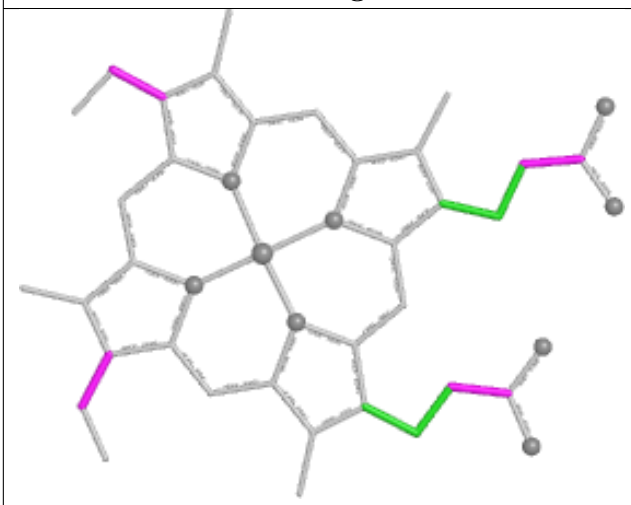

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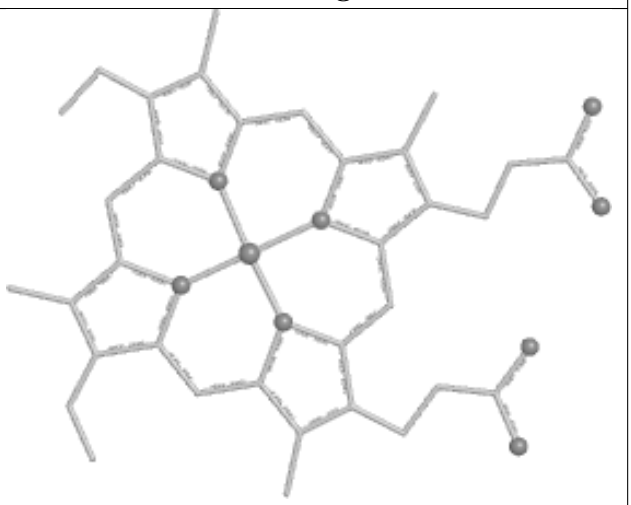

Rings

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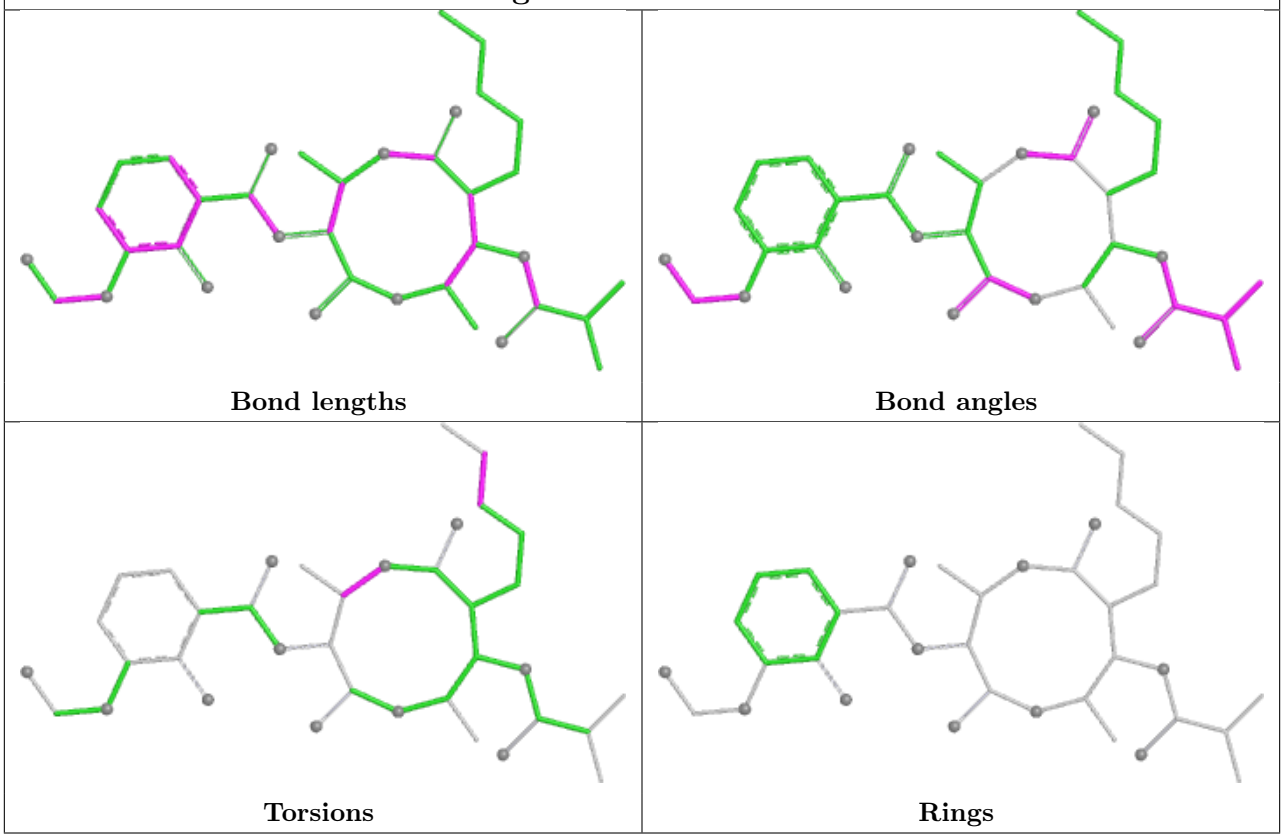

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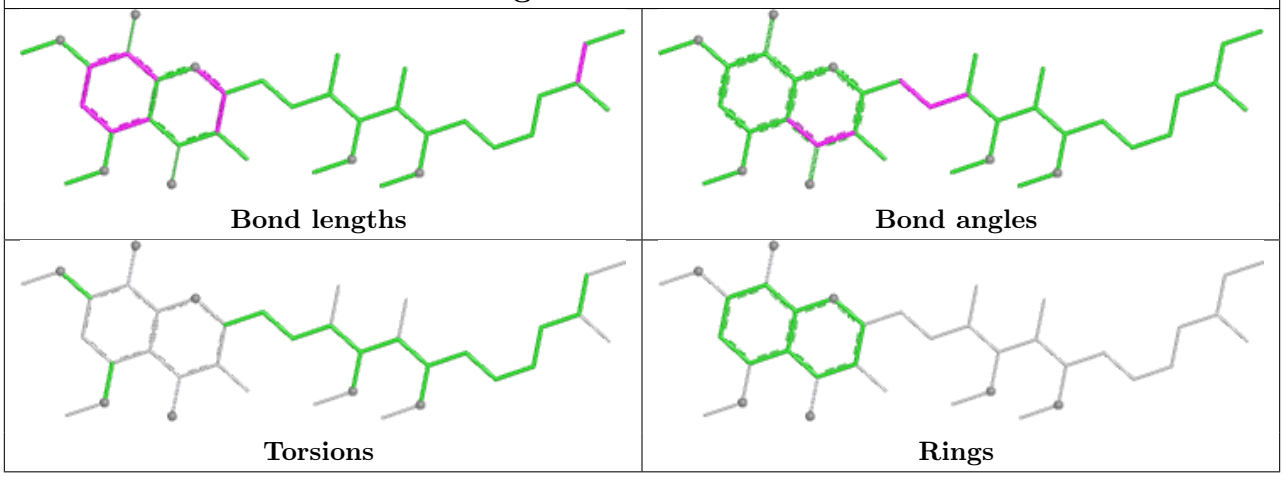

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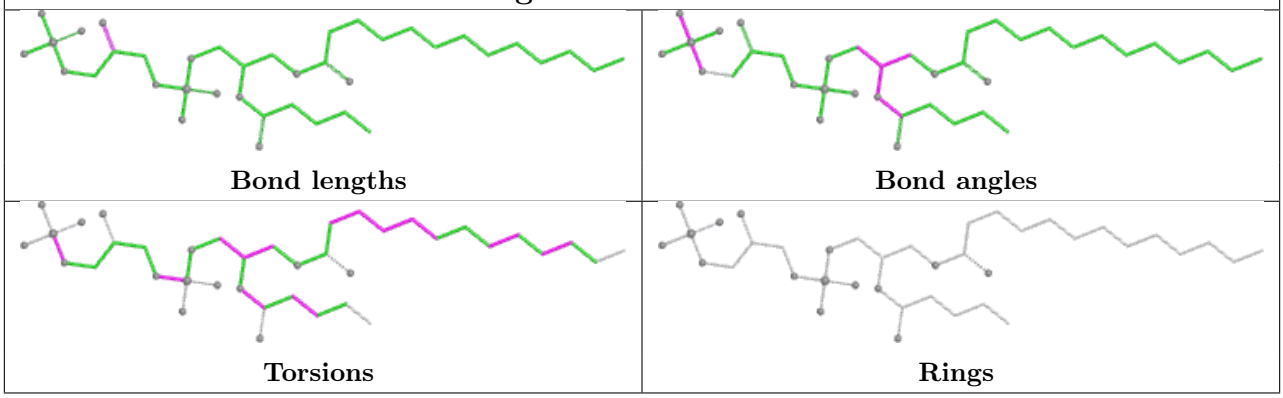

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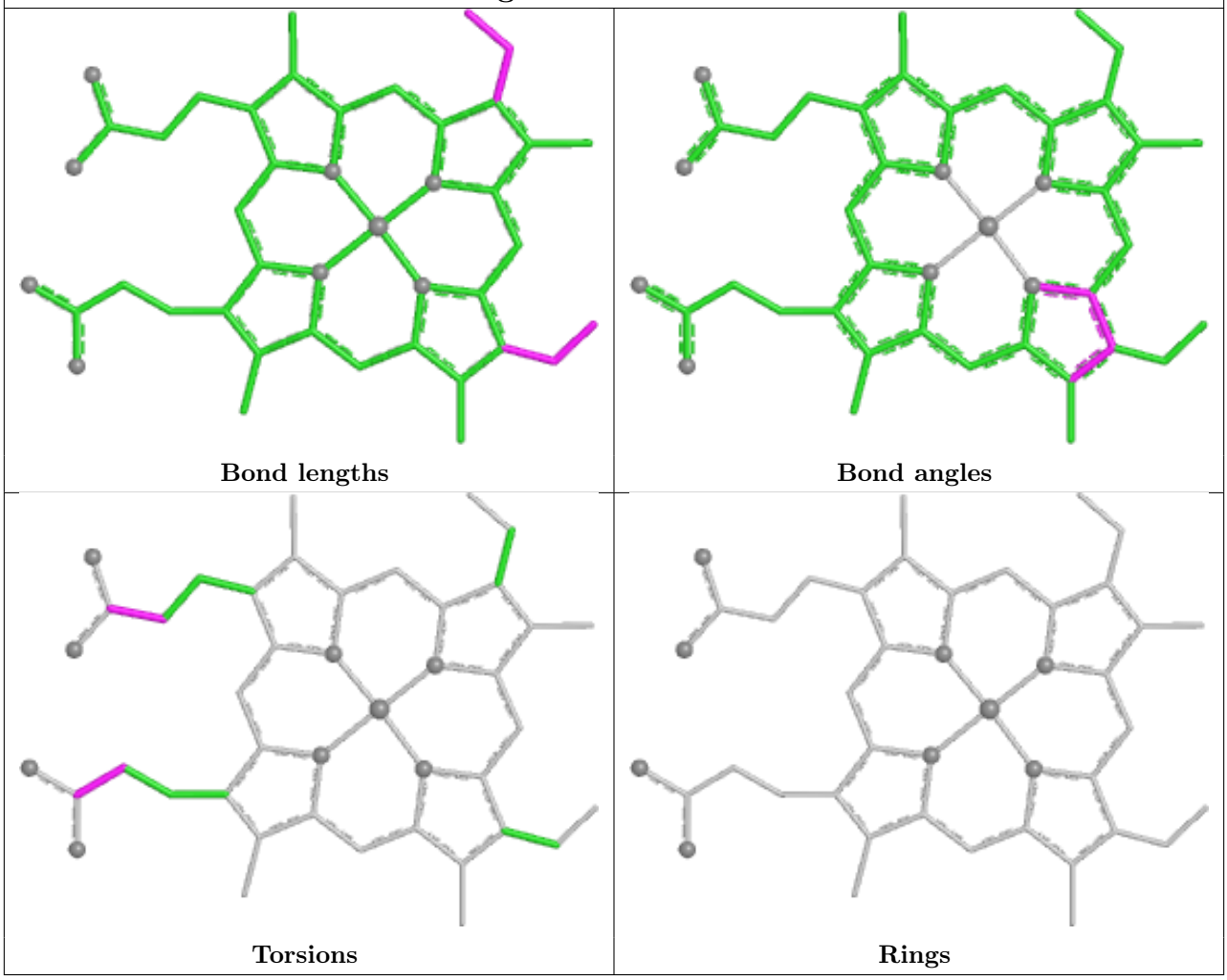

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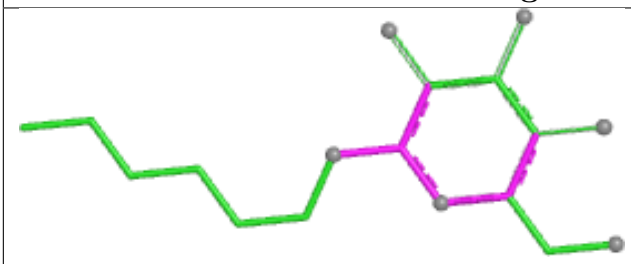

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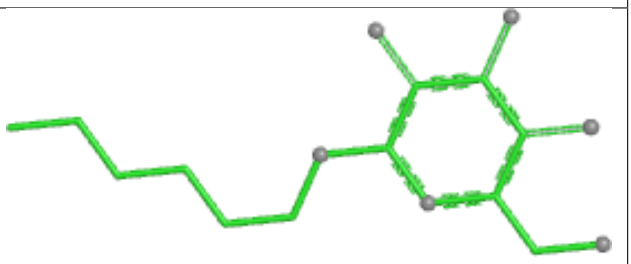
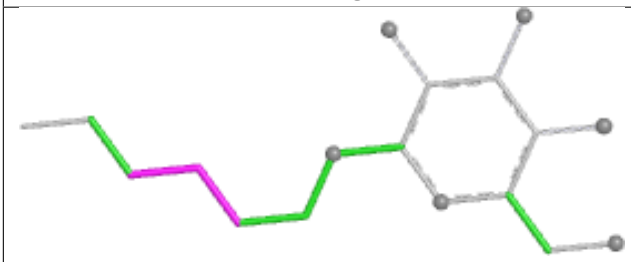
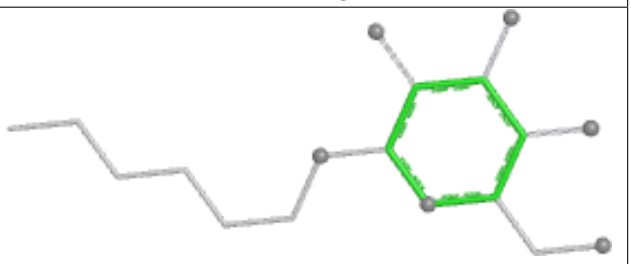


Bond angles

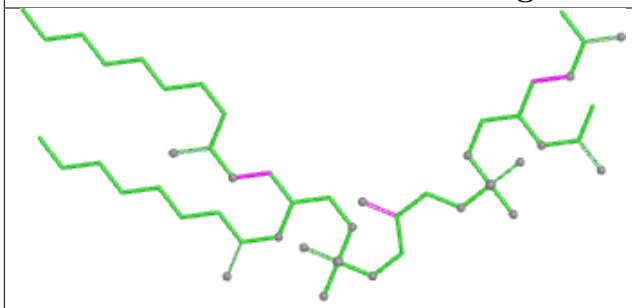


Torsions



Rings

Ligand CDL T 3004



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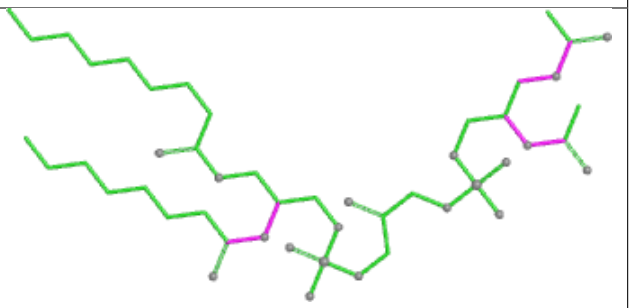

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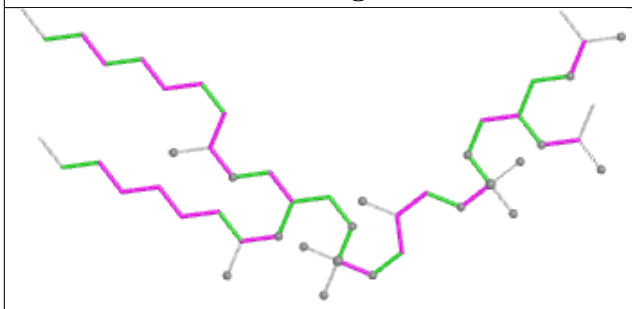

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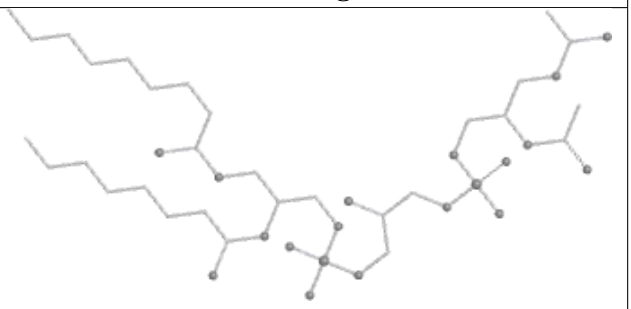
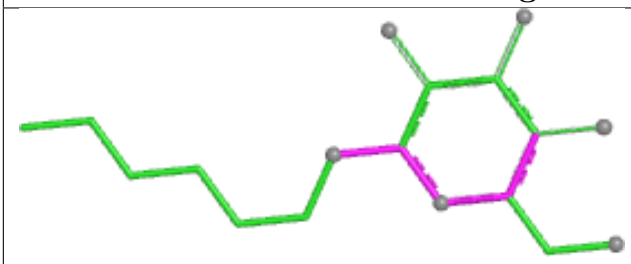


Rings

Ligand JZR C 2010



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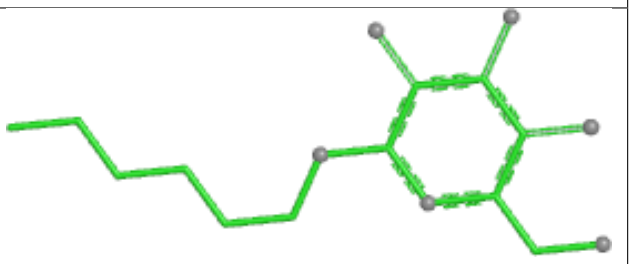

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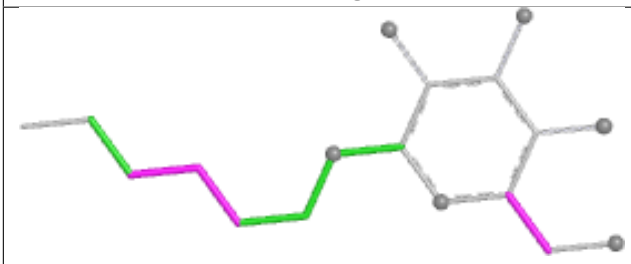

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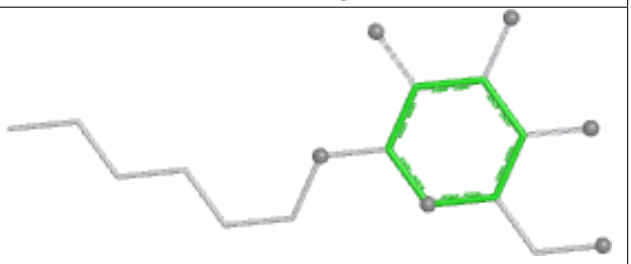
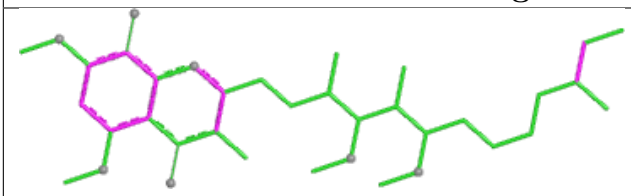


Rings

Ligand SMA C 2001



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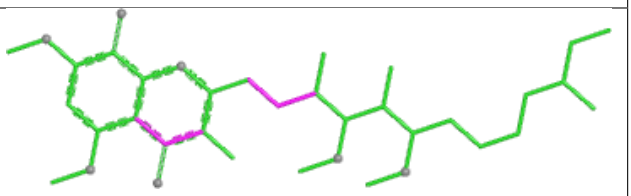

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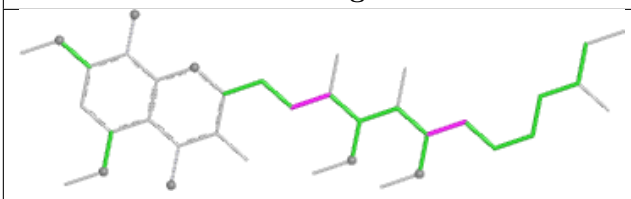

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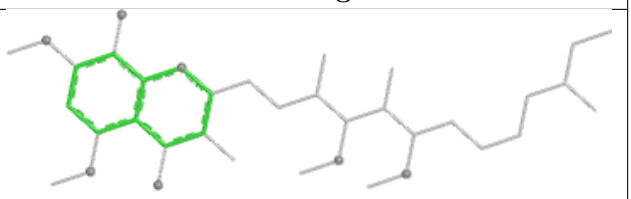
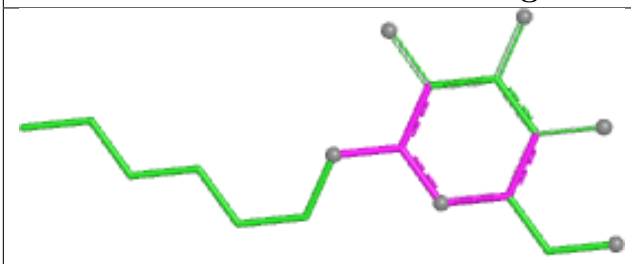


Rings

Ligand JZR F 3011



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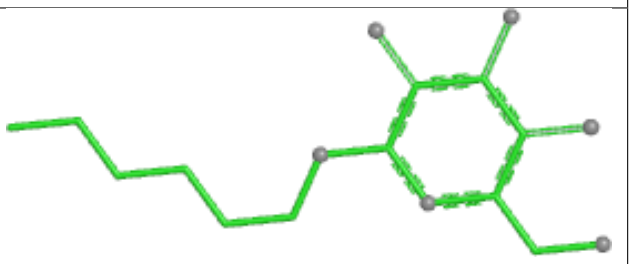
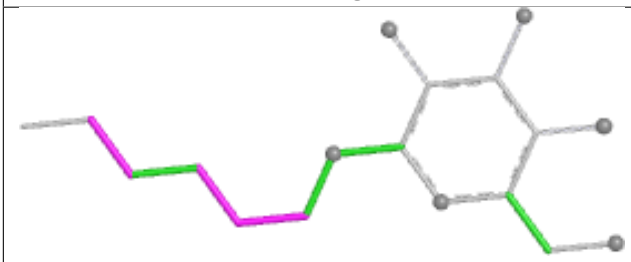


Bond angles



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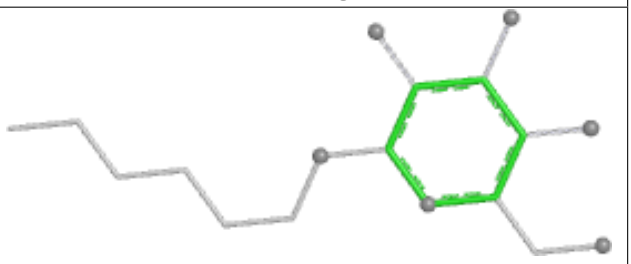
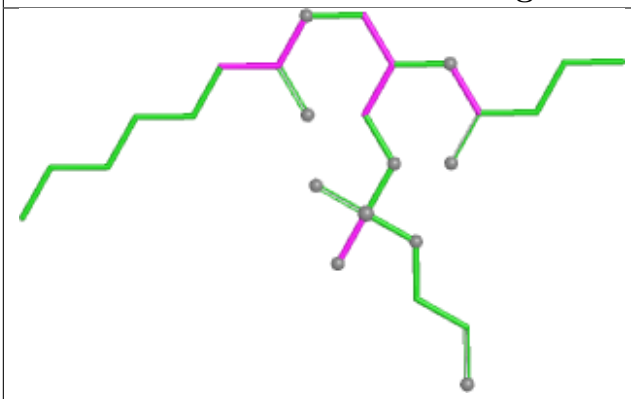


Rings

Ligand PEE D 2006



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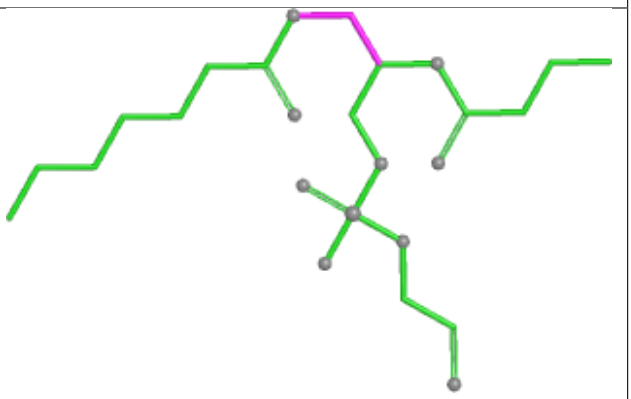
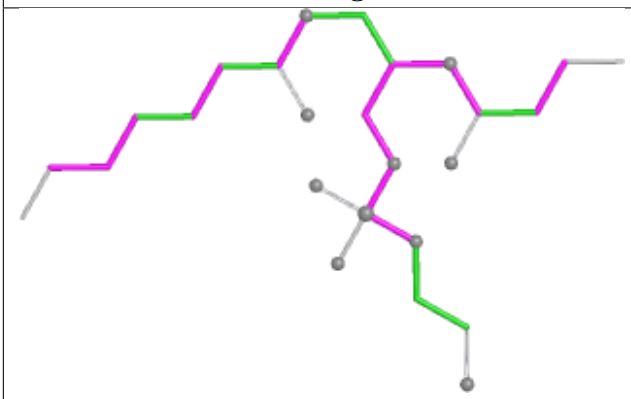


Bond angles



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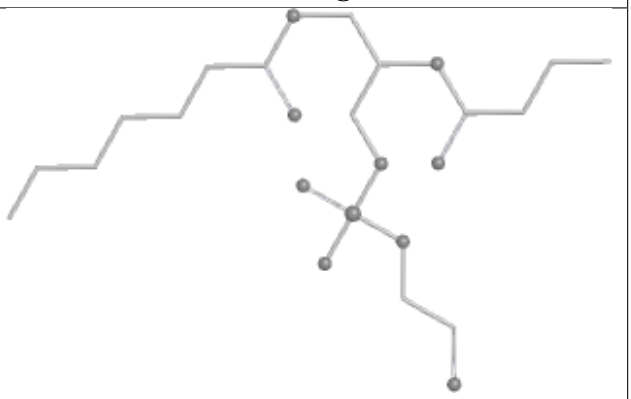
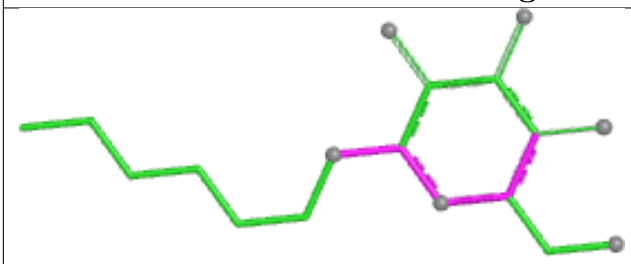


Rings

Ligand JZR R 4007



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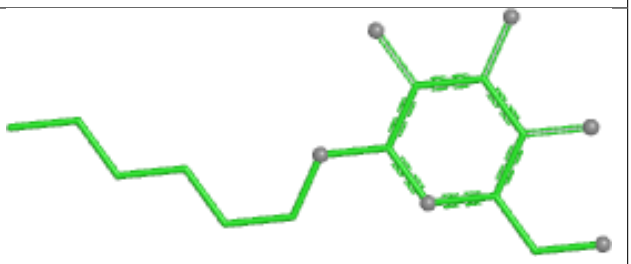
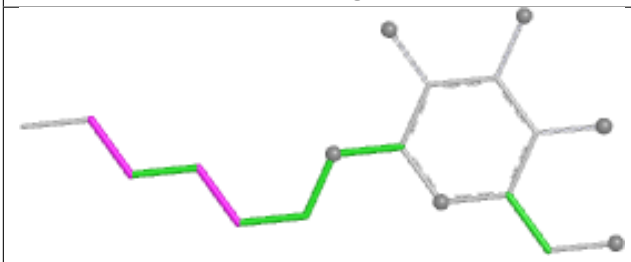


Bond angles



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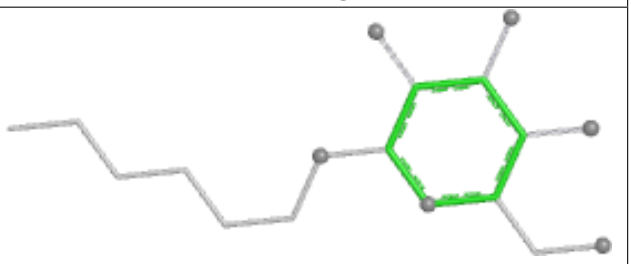
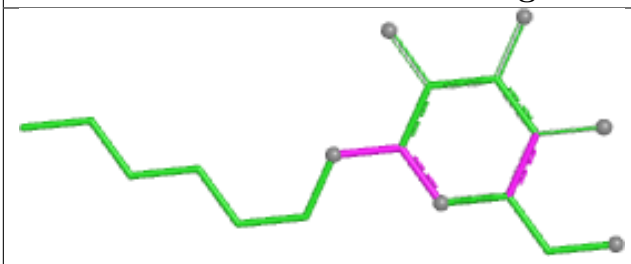


Rings

Ligand JZR A 4004



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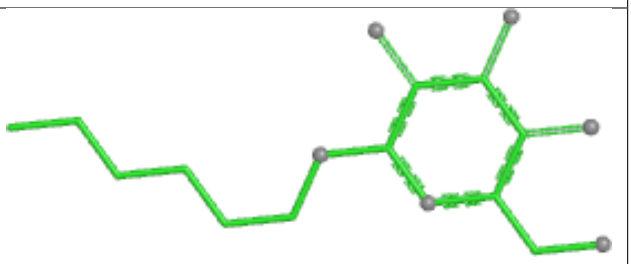
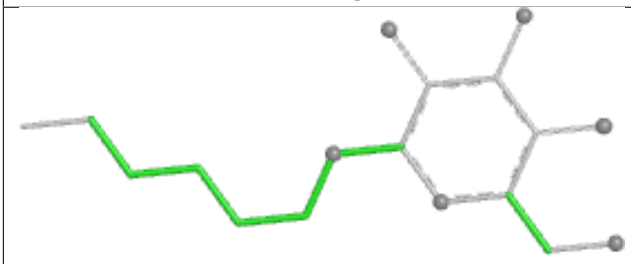
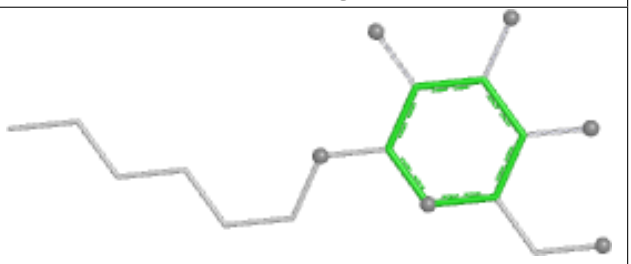


Bond angles

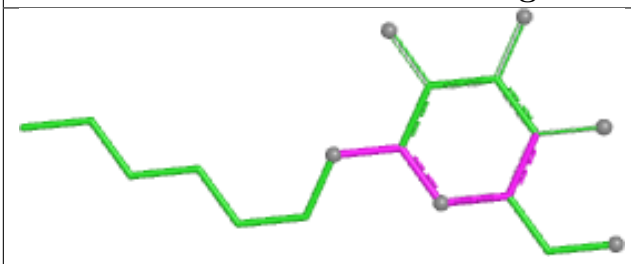


Torsions

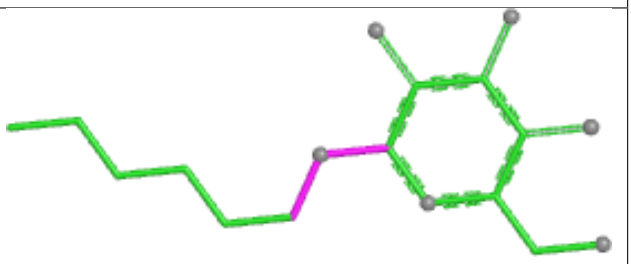


Rings

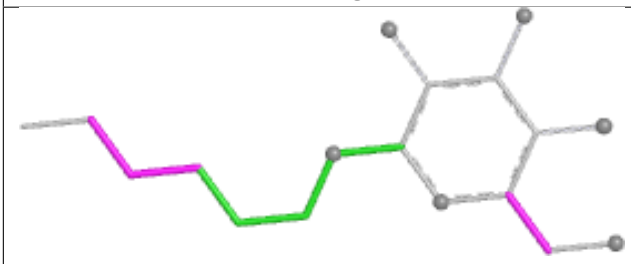
Ligand JZR C 4002



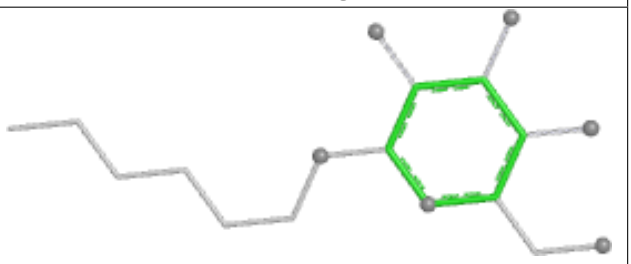
Bond lengths



Bond angles

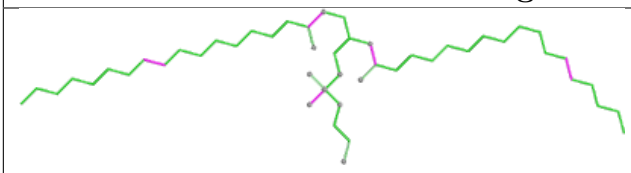


Torsions

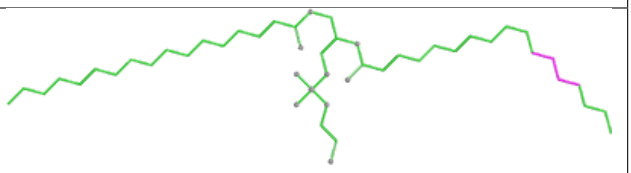


Rings

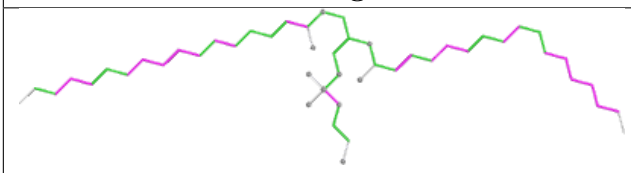
Ligand PEE C 2007



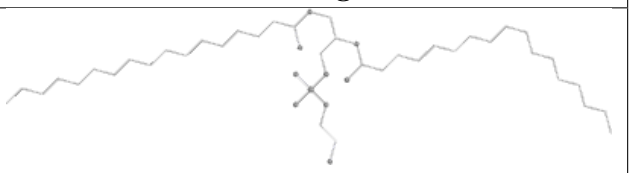
Bond lengths



Bond angles

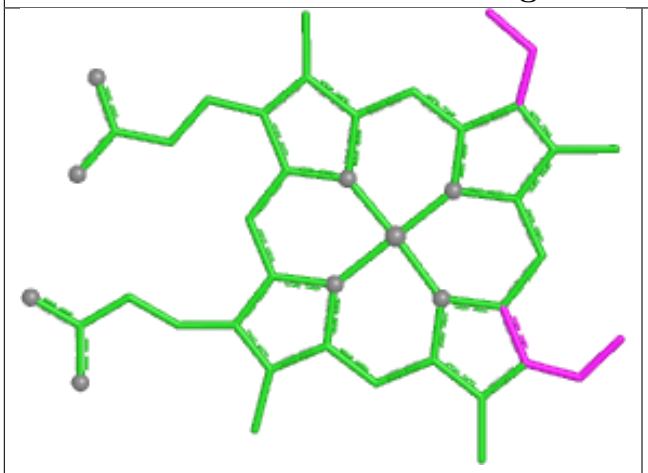


Torsions

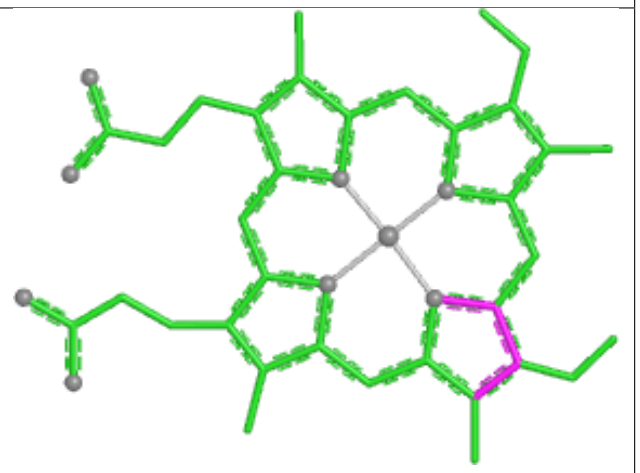


Rings

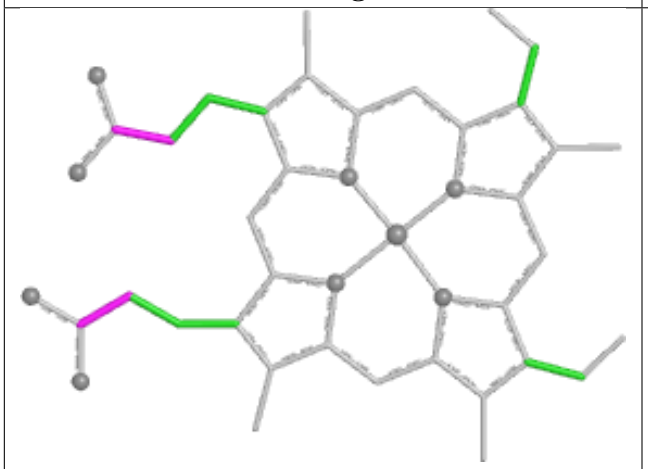
Ligand HEM C 502



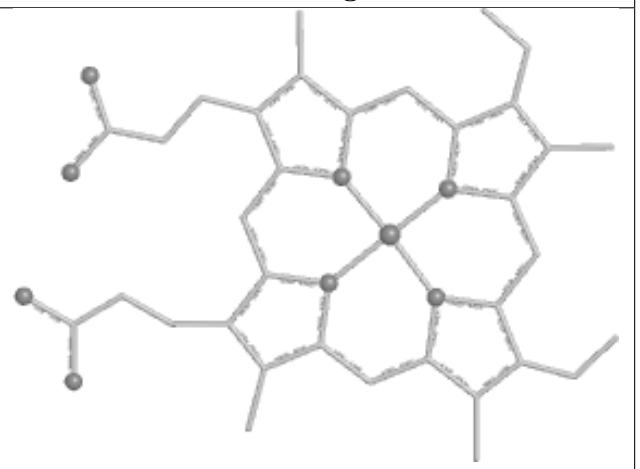
Bond lengths



Bond angles

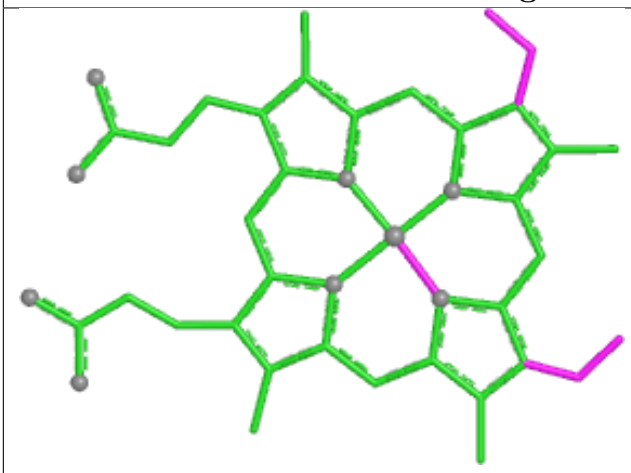


Torsions

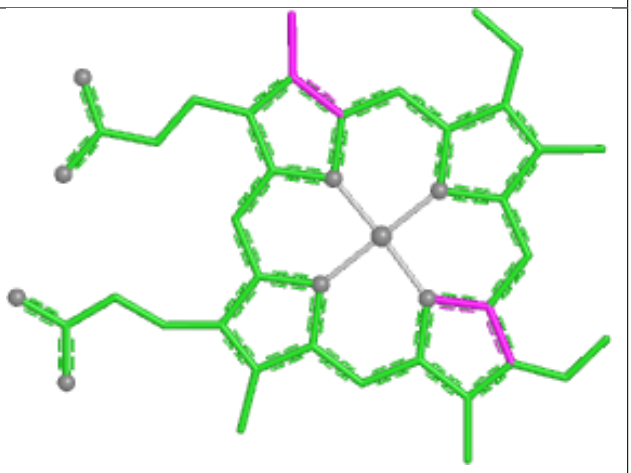


Rings

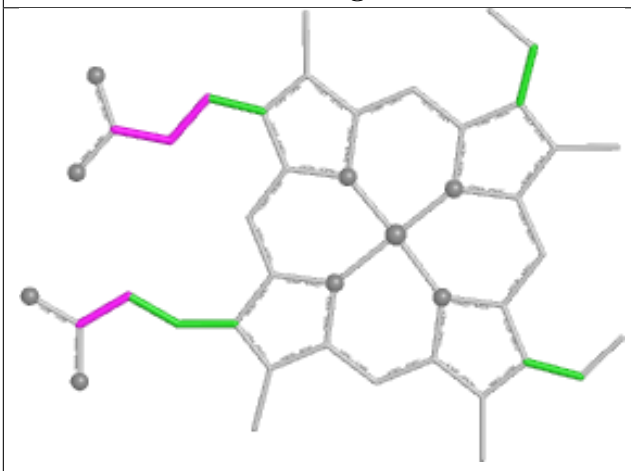
Ligand HEM P 501



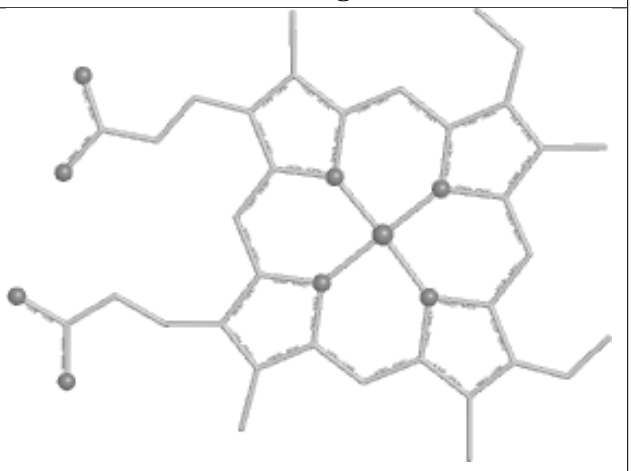
Bond lengths



Bond angles

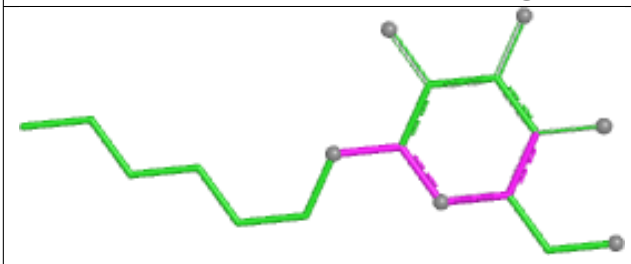


Torsions

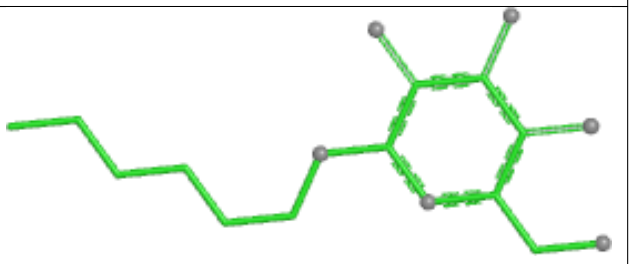


Rings

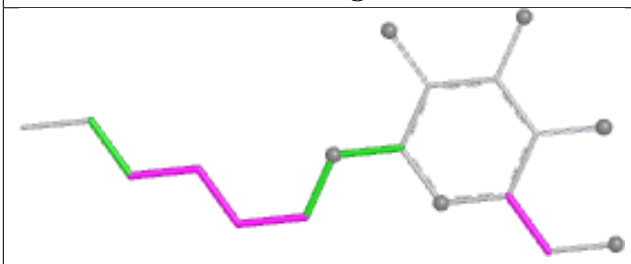
Ligand JZR D 4003



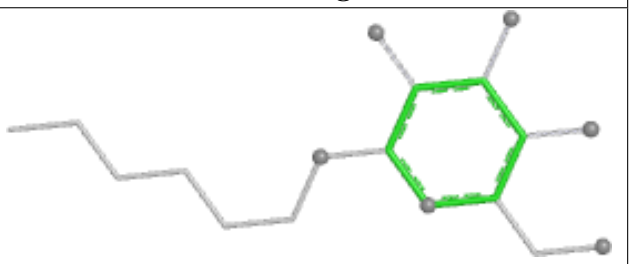
Bond lengths



Bond angles

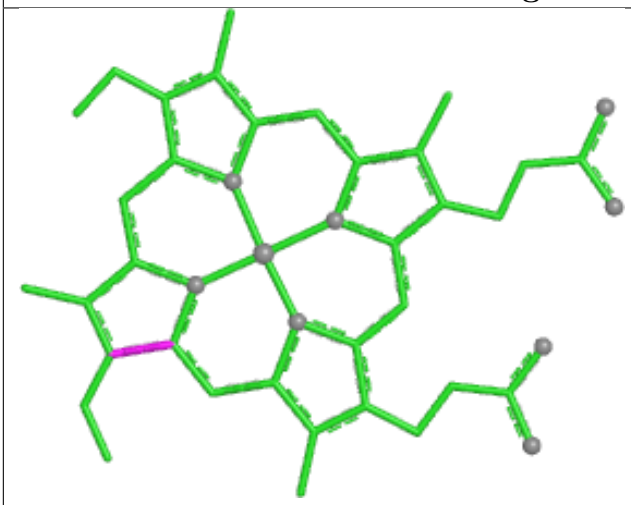


Torsions

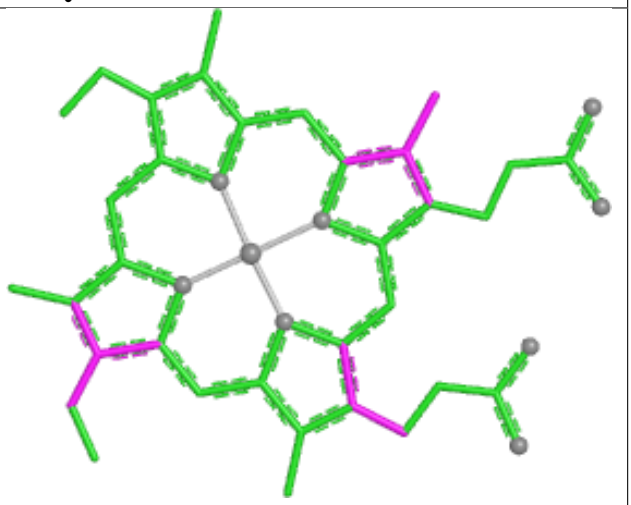


Rings

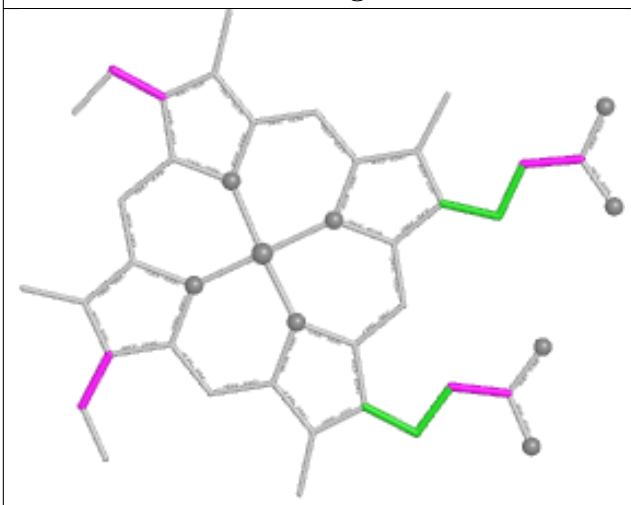
Ligand HEC Q 501



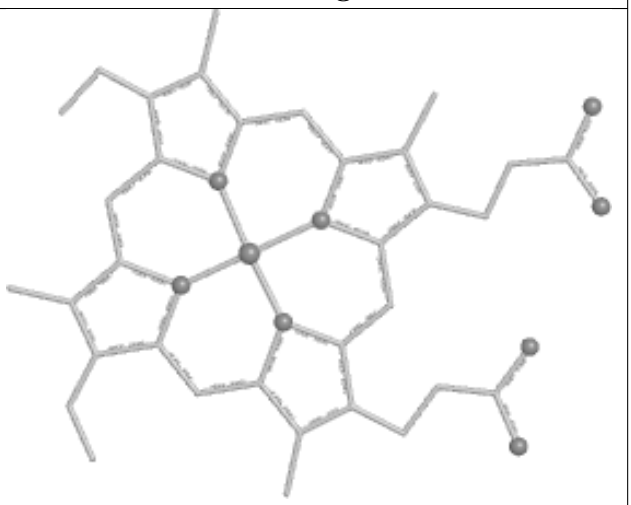
Bond lengths



Bond angles

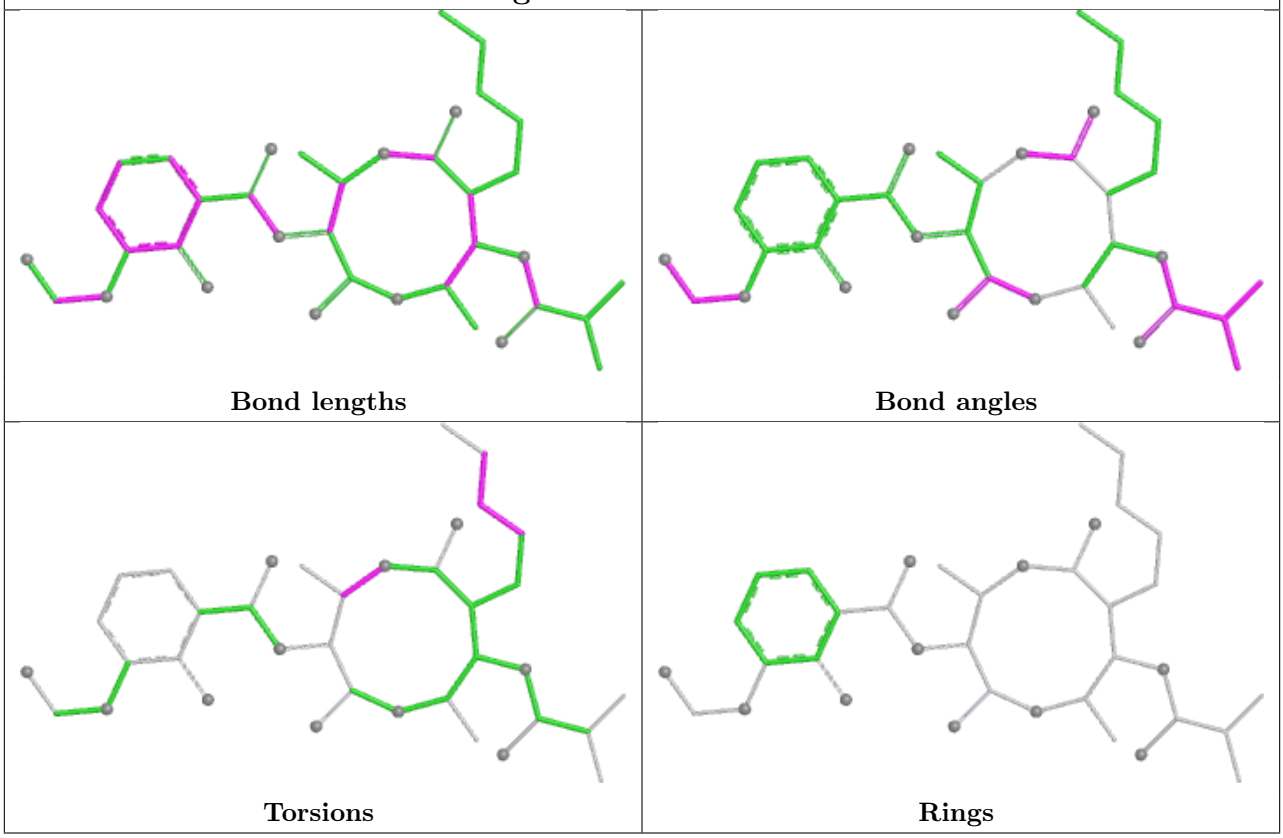


Torsions

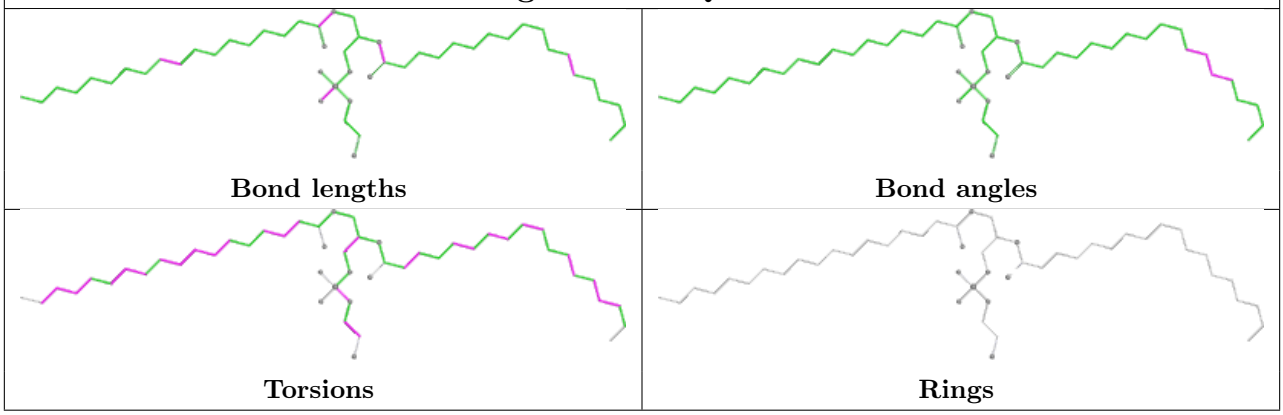


Rings

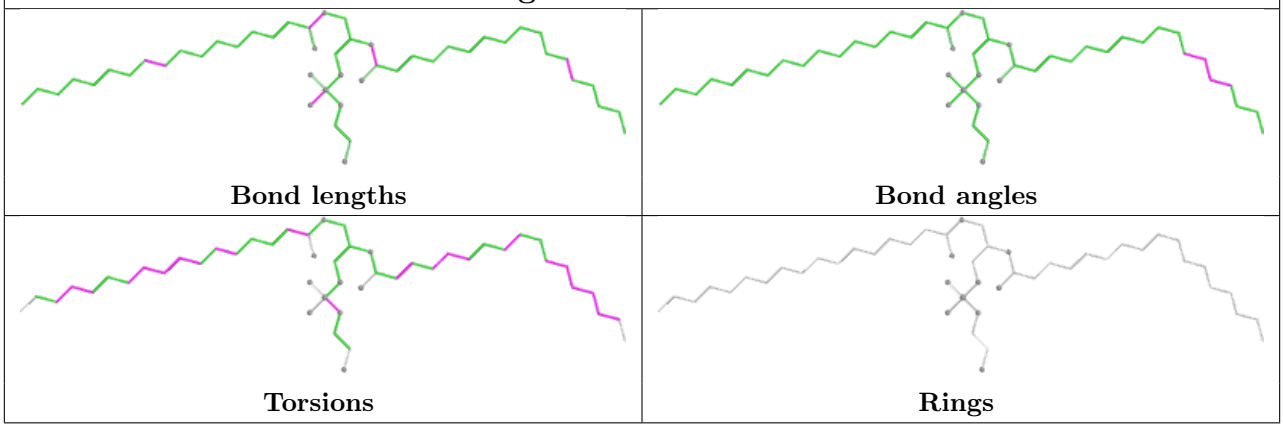
Ligand ANY P 3002



Ligand PEE Q 3006



Ligand PEE P 3007



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.42	23 (5%)	33	35	25, 39, 60, 115	0
1	N	441/446 (98%)	0.91	41 (9%)	14	15	30, 52, 76, 139	1 (0%)
2	B	424/439 (96%)	0.52	18 (4%)	40	42	29, 42, 66, 94	0
2	O	424/439 (96%)	0.83	46 (10%)	11	11	30, 47, 70, 124	0
3	C	365/379 (96%)	0.30	9 (2%)	58	61	23, 36, 53, 108	0
3	P	365/379 (96%)	0.38	11 (3%)	52	55	29, 39, 53, 106	0
4	D	241/241 (100%)	0.52	5 (2%)	63	66	31, 44, 64, 82	0
4	Q	241/241 (100%)	0.73	10 (4%)	41	43	35, 48, 67, 89	0
5	E	196/196 (100%)	1.46	51 (26%)	1	1	35, 62, 106, 111	0
5	R	196/196 (100%)	0.91	18 (9%)	14	15	34, 51, 77, 95	0
6	F	99/110 (90%)	0.47	6 (6%)	27	29	27, 40, 69, 78	0
6	S	99/110 (90%)	0.77	10 (10%)	12	13	33, 42, 80, 102	0
7	G	75/81 (92%)	1.20	14 (18%)	3	3	29, 53, 76, 89	0
7	T	76/81 (93%)	1.32	13 (17%)	4	4	37, 63, 93, 95	0
8	H	66/78 (84%)	0.98	7 (10%)	11	12	43, 59, 77, 81	0
8	U	66/78 (84%)	1.30	12 (18%)	3	3	50, 66, 89, 104	0
9	I	43/78 (55%)	2.87	31 (72%)	0	0	34, 65, 84, 89	0
9	V	43/78 (55%)	2.79	31 (72%)	0	0	38, 72, 86, 90	0
10	J	33/62 (53%)	1.24	7 (21%)	2	2	37, 54, 115, 130	0
10	W	62/62 (100%)	1.76	27 (43%)	0	1	44, 74, 129, 144	0
All	All	3997/4220 (94%)	0.76	390 (9%)	13	13	23, 45, 81, 144	1 (0%)

All (390) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	1	GLY	8.5
1	N	222	THR	8.0
6	S	13	LEU	7.2
2	B	231	GLY	7.0
9	I	78	TYR	6.9
6	S	12	TRP	6.8
9	V	78	TYR	6.8
2	B	232	LEU	6.6
7	T	1	GLY	6.5
2	B	233	SER	6.2
1	N	227	ALA	6.2
1	A	2	ALA	6.2
9	V	43	LEU	6.1
9	I	70	LEU	5.8
6	S	16	ILE	5.7
5	E	191	ASP	5.6
1	A	228	VAL	5.6
3	P	17	ALA	5.6
2	B	12	GLU	5.5
2	O	303	VAL	5.2
10	J	61	ASN	5.2
6	F	12	TRP	5.2
9	V	48	SER	5.1
3	C	17	ALA	5.1
2	B	230	LEU	5.1
9	V	41	PRO	5.0
5	E	76	ILE	4.9
7	G	75	ALA	4.8
2	O	26	PHE	4.8
1	N	221	GLY	4.7
9	V	33	ALA	4.7
9	I	48	SER	4.6
5	E	187	PHE	4.5
2	O	304	HIS	4.4
2	O	17	VAL	4.4
9	V	35	PRO	4.3
1	A	262	TRP	4.3
9	V	32	ALA	4.3
9	V	42	VAL	4.3
5	E	106	ILE	4.3
5	E	194	ILE	4.3
5	R	27	GLU	4.3
5	R	70	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
9	I	49	VAL	4.2
9	V	63	PRO	4.1
9	V	70	LEU	4.1
5	E	195	VAL	4.1
9	I	59	ALA	4.1
10	J	31	PHE	4.1
9	I	77	ARG	4.1
9	I	50	LEU	4.1
1	A	223	TYR	4.1
9	V	76	VAL	4.1
9	I	71	ASN	4.0
5	E	111	ALA	4.0
2	O	230	LEU	4.0
7	G	45	ILE	4.0
8	U	39	LEU	4.0
9	V	50	LEU	4.0
9	I	76	VAL	4.0
2	O	21	PRO	4.0
1	A	227	ALA	3.9
10	W	5	LEU	3.9
2	B	41	TYR	3.9
1	N	81	SER	3.9
10	J	30	PHE	3.9
9	I	61	GLY	3.9
3	P	18	PHE	3.8
5	E	49	TYR	3.8
9	I	35	PRO	3.8
2	O	302	GLY	3.8
9	I	62	ARG	3.8
7	G	29	TYR	3.7
1	N	443	TRP	3.6
10	W	1	VAL	3.6
9	I	60	ALA	3.6
10	W	6	THR	3.6
9	I	73	PRO	3.6
4	Q	85	GLY	3.6
9	I	52	ARG	3.5
5	E	190	ASP	3.5
2	O	224	LEU	3.5
6	F	13	LEU	3.5
3	P	15	ASN	3.5
1	A	222	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	3.4
9	I	63	PRO	3.4
9	V	61	GLY	3.4
10	W	61	ASN	3.4
8	U	47	ARG	3.4
5	E	193	VAL	3.4
9	I	32	ALA	3.4
1	A	229	PRO	3.4
2	O	306	PRO	3.4
5	E	130	PRO	3.4
5	E	84	GLY	3.4
2	O	232	LEU	3.4
9	I	55	LEU	3.4
5	E	132	TRP	3.3
5	E	78	LEU	3.3
3	P	168	PHE	3.3
6	S	14	GLU	3.3
1	N	229	PRO	3.3
6	S	15	GLY	3.3
10	W	3	PRO	3.3
1	A	4	TYR	3.3
1	N	365	LEU	3.3
9	V	71	ASN	3.3
10	W	22	LEU	3.3
7	G	30	PHE	3.3
5	E	112	VAL	3.2
10	J	34	ALA	3.2
10	W	24	ILE	3.2
2	O	301	LYS	3.2
2	B	17	VAL	3.2
4	Q	241	LYS	3.2
10	W	15	ARG	3.2
8	U	44	VAL	3.2
9	I	72	VAL	3.2
9	V	36	ALA	3.2
3	P	320	LEU	3.2
10	W	20	PHE	3.2
2	O	225	ASN	3.2
2	O	351	ASN	3.1
5	E	110	ALA	3.1
7	T	75	ALA	3.1
5	E	124	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
10	W	9	LEU	3.1
1	A	286	GLY	3.1
2	O	281	ALA	3.1
1	N	2	ALA	3.1
9	V	34	VAL	3.1
1	N	19	LEU	3.1
3	P	19	ILE	3.1
1	N	193	PRO	3.0
9	V	62	ARG	3.0
1	A	225	GLU	3.0
1	N	122	LEU	3.0
10	W	25	VAL	3.0
9	V	77	ARG	3.0
10	J	32	GLU	3.0
1	N	442	PHE	3.0
3	C	19	ILE	3.0
5	E	81	ILE	3.0
2	O	265	GLY	3.0
2	O	350	GLY	3.0
1	A	315	ALA	3.0
1	N	220	SER	3.0
9	I	34	VAL	3.0
10	W	12	LEU	3.0
5	E	5	ILE	3.0
2	O	41	TYR	3.0
2	O	305	GLN	2.9
3	C	18	PHE	3.0
10	W	14	PHE	3.0
9	I	42	VAL	2.9
9	V	72	VAL	2.9
2	O	233	SER	2.9
9	I	74	ALA	2.9
7	G	46	LEU	2.9
2	O	264	ILE	2.9
1	N	262	TRP	2.9
8	H	78	LYS	2.9
6	S	108	ALA	2.9
2	B	234	GLY	2.9
7	G	64	GLN	2.9
5	R	187	PHE	2.9
9	I	36	ALA	2.9
10	W	45	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	133	VAL	2.8
10	W	4	THR	2.8
2	O	18	PRO	2.8
2	O	362	ASN	2.8
7	T	30	PHE	2.8
5	R	37	TYR	2.8
2	O	388	ALA	2.8
3	C	20	ASP	2.8
7	T	76	ALA	2.8
2	O	12	GLU	2.8
3	C	155	TYR	2.8
1	N	117	VAL	2.8
5	R	76	ILE	2.8
9	V	39	GLU	2.8
9	I	41	PRO	2.8
1	N	194	ARG	2.7
3	C	16	ASN	2.7
5	E	192	MET	2.7
8	H	27	LEU	2.7
2	O	215	VAL	2.7
5	R	18	VAL	2.7
1	N	120	CYS	2.7
7	T	34	ILE	2.7
4	Q	1	SER	2.7
5	E	72	SER	2.7
1	N	316	ASP	2.7
1	A	6	GLN	2.7
2	B	303	VAL	2.7
5	E	167	ALA	2.7
5	E	38	LEU	2.7
10	W	17	THR	2.7
5	E	186	GLU	2.7
7	G	74	PRO	2.7
5	E	45	VAL	2.7
5	E	114	VAL	2.7
10	W	2	ALA	2.6
2	O	391	SER	2.6
4	Q	174	GLY	2.6
5	R	71	MET	2.6
2	O	267	ALA	2.6
1	N	231	LEU	2.6
2	O	19	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	82	PRO	2.6
7	T	29	TYR	2.6
1	N	297	ILE	2.6
5	E	74	ILE	2.6
5	E	182	VAL	2.6
7	T	43	ALA	2.6
9	I	33	ALA	2.6
9	I	37	THR	2.6
8	U	37	LEU	2.6
5	R	11	SER	2.6
8	H	51	GLU	2.6
1	N	263	ALA	2.6
8	H	34	ARG	2.6
10	W	7	ALA	2.6
9	I	43	LEU	2.6
5	E	93	GLY	2.5
6	S	109	LYS	2.5
1	A	263	ALA	2.5
4	Q	143	LEU	2.5
10	W	13	LEU	2.5
5	E	196	GLY	2.5
9	V	49	VAL	2.5
7	T	28	HIS	2.5
10	J	33	ARG	2.5
9	V	40	SER	2.5
2	O	24	LEU	2.5
4	D	3	LEU	2.5
5	E	117	LEU	2.5
8	U	27	LEU	2.5
7	G	26	PHE	2.5
2	O	20	HIS	2.5
5	E	134	ILE	2.5
7	G	34	ILE	2.5
9	I	68	VAL	2.5
1	N	185	TYR	2.5
10	W	48	GLU	2.5
5	R	189	SER	2.5
10	W	21	ALA	2.5
5	R	35	PHE	2.5
2	O	231	GLY	2.5
5	E	53	ASN	2.5
6	F	22	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	11	VAL	2.4
7	T	45	ILE	2.5
8	U	26	GLN	2.4
9	V	60	ALA	2.4
5	R	19	LEU	2.4
5	R	26	LYS	2.4
10	J	62	LYS	2.4
2	O	347	ILE	2.4
5	E	127	VAL	2.4
7	T	31	SER	2.4
9	V	37	THR	2.4
1	N	212	ALA	2.4
3	C	15	ASN	2.4
1	N	379	ILE	2.4
4	D	142	SER	2.4
9	V	73	PRO	2.4
8	U	71	HIS	2.4
5	E	70	ALA	2.4
2	B	439	LEU	2.4
1	N	225	GLU	2.4
8	U	49	GLN	2.4
5	E	12	ASP	2.4
5	E	123	ASP	2.4
10	W	18	SER	2.4
1	A	443	TRP	2.4
4	Q	148	TYR	2.3
1	N	192	ALA	2.3
4	Q	61	ALA	2.3
9	V	74	ALA	2.3
7	T	32	LYS	2.3
9	V	69	SER	2.3
10	W	28	ALA	2.3
3	P	16	ASN	2.3
1	N	211	LEU	2.3
2	O	238	LYS	2.3
2	O	307	PHE	2.3
4	D	9	SER	2.3
1	N	228	VAL	2.3
5	E	120	PRO	2.3
1	A	365	LEU	2.3
2	B	250	ASP	2.3
9	V	55	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	71	MET	2.3
2	O	353	SER	2.3
5	E	79	SER	2.3
2	O	349	GLN	2.3
4	Q	70	VAL	2.3
7	T	74	PRO	2.3
2	B	228	GLY	2.3
5	R	93	GLY	2.3
10	W	10	TYR	2.3
1	N	213	GLN	2.2
9	V	38	SER	2.2
7	T	21	PHE	2.2
5	R	5	ILE	2.2
2	O	219	VAL	2.2
1	N	224	ASP	2.2
2	O	228	GLY	2.2
2	O	300	ALA	2.2
3	P	199	PHE	2.2
5	E	86	ASN	2.2
6	F	16	ILE	2.2
1	N	16	VAL	2.2
5	E	98	VAL	2.2
6	F	87	LYS	2.2
4	D	65	ALA	2.2
2	O	439	LEU	2.2
1	N	15	GLN	2.2
5	E	122	HIS	2.2
5	R	29	SER	2.2
2	B	19	PRO	2.2
1	A	316	ASP	2.2
2	O	220	ALA	2.2
9	V	64	LEU	2.2
1	N	30	SER	2.2
5	E	92	ARG	2.2
5	E	118	ARG	2.2
6	S	20	TYR	2.2
6	S	87	LYS	2.2
2	O	40	ASN	2.2
1	A	210	ASP	2.2
1	N	226	ASP	2.2
3	C	67	THR	2.2
8	U	53	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
9	I	39	GLU	2.1
2	O	299	VAL	2.1
1	A	231	LEU	2.1
9	I	64	LEU	2.1
9	V	52	ARG	2.1
8	U	45	SER	2.1
8	U	48	SER	2.1
5	R	13	TYR	2.1
1	N	300	THR	2.1
3	P	267	HIS	2.1
2	B	24	LEU	2.1
3	P	102	LEU	2.1
1	A	172	GLU	2.1
3	P	263	ASN	2.1
1	N	190	TYR	2.1
1	A	3	THR	2.1
10	W	19	THR	2.1
2	B	158	HIS	2.1
1	A	99	ILE	2.1
5	E	101	ARG	2.1
5	E	151	GLY	2.1
6	F	107	TRP	2.1
2	O	357	VAL	2.1
4	Q	68	VAL	2.1
10	W	62	LYS	2.1
2	B	251	SER	2.1
8	H	13	LEU	2.1
9	I	69	SER	2.1
10	W	29	LEU	2.1
4	D	2	ASP	2.1
4	Q	35	GLN	2.1
7	G	60	THR	2.1
7	G	71	ARG	2.1
8	H	36	ARG	2.1
8	H	47	ARG	2.1
2	B	264	ILE	2.1
1	A	81	SER	2.1
7	G	25	ALA	2.1
1	N	209	LEU	2.0
1	N	219	LEU	2.0
6	S	17	ARG	2.0
8	U	34	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	176	LYS	2.0
2	O	296	TYR	2.0
7	G	68	LYS	2.0
5	E	171	ILE	2.0
5	R	74	ILE	2.0
2	O	25	GLU	2.0
1	N	367	SER	2.0
3	C	194	MET	2.0
5	R	108	GLN	2.0
1	A	282	CYS	2.0
5	E	185	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	JZR	F	4001	18/18	0.19	0.28	146,154,157,158	0
14	GOL	C	4006	6/6	0.54	0.16	96,98,99,100	0
11	JZR	S	2011	18/18	0.62	0.28	61,89,94,98	0
13	AZI	C	2005	3/3	0.64	0.32	54,54,56,58	0
11	JZR	F	3011	18/18	0.64	0.29	108,113,116,116	0
13	AZI	A	4011	3/3	0.66	0.44	61,61,66,69	0
12	PO4	A	2013	5/5	0.68	0.13	119,120,121,122	0
14	GOL	R	4005	6/6	0.68	0.17	81,83,84,85	0
13	AZI	P	3005	3/3	0.69	0.26	51,51,54,56	0
14	GOL	B	2009	6/6	0.69	0.25	84,85,86,86	0
11	JZR	R	4007	18/18	0.70	0.19	85,95,98,99	0
12	PO4	C	4008	5/5	0.71	0.19	153,153,153,153	0

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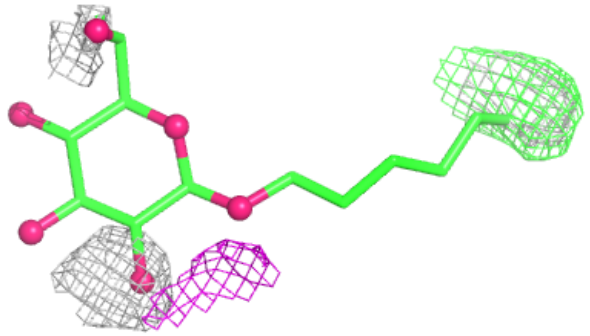
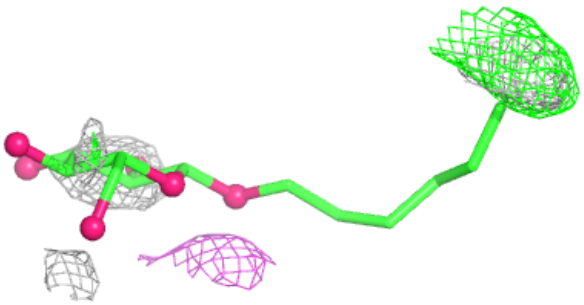
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	JZR	C	2010	18/18	0.72	0.23	94,103,108,108	0
11	JZR	D	4003	18/18	0.73	0.31	160,169,171,171	0
12	PO4	S	3012	5/5	0.73	0.15	97,97,99,100	0
14	GOL	O	3009	6/6	0.77	0.19	82,84,85,85	0
13	AZI	O	4010	3/3	0.78	0.14	102,102,104,104	0
14	GOL	P	3008	6/6	0.78	0.27	67,69,71,71	0
11	JZR	P	3010	18/18	0.78	0.24	103,107,112,112	0
17	PEE	D	2006	26/51	0.78	0.27	85,98,108,109	0
12	PO4	P	3013	5/5	0.80	0.11	104,105,106,106	0
20	CDL	D	2003	39/100	0.80	0.18	53,78,93,94	0
11	JZR	C	4002	18/18	0.81	0.24	114,122,125,125	0
20	CDL	G	2004	44/100	0.83	0.20	73,87,99,102	0
20	CDL	P	3003	39/100	0.83	0.18	61,89,111,111	0
20	CDL	T	3004	49/100	0.83	0.21	74,89,107,107	0
12	PO4	F	2012	5/5	0.84	0.11	81,82,83,84	0
17	PEE	Q	3006	51/51	0.86	0.20	65,75,98,100	0
14	GOL	C	2008	6/6	0.88	0.23	61,65,68,75	0
13	AZI	G	4009	3/3	0.90	0.25	66,66,67,68	0
17	PEE	P	3007	49/51	0.91	0.17	41,57,81,81	0
17	PEE	C	2007	49/51	0.92	0.15	35,55,81,83	0
11	JZR	A	4004	18/18	0.93	0.09	28,34,40,42	0
18	ANY	C	2002	37/40	0.94	0.10	31,39,65,70	0
18	ANY	P	3002	37/40	0.94	0.11	33,39,67,71	0
16	SMA	C	2001	37/37	0.95	0.08	31,39,44,48	0
16	SMA	P	3001	37/37	0.95	0.09	27,40,44,46	0
19	HEC	Q	501	43/43	0.96	0.09	38,45,48,51	0
19	HEC	D	501	43/43	0.97	0.08	35,41,44,45	0
15	HEM	C	501	43/43	0.97	0.08	20,31,38,47	0
15	HEM	P	502	43/43	0.97	0.08	27,31,36,40	0
21	FES	E	501	4/4	0.97	0.06	41,41,43,43	0
15	HEM	C	502	43/43	0.98	0.07	22,28,34,37	0
15	HEM	P	501	43/43	0.98	0.07	30,34,42,46	0
21	FES	R	501	4/4	0.98	0.04	35,35,37,37	0

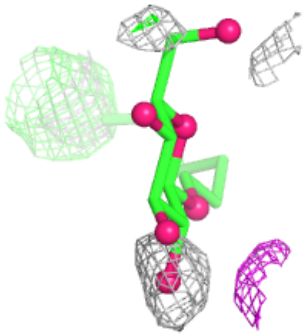
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZR 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)

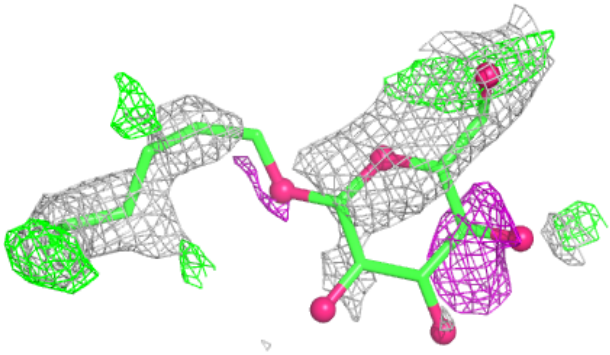


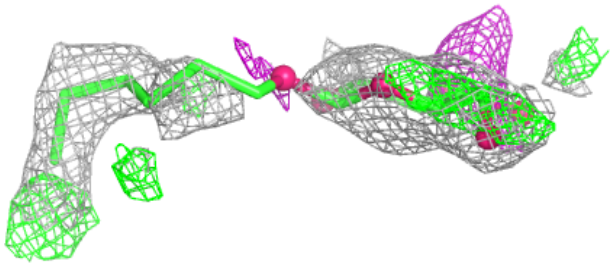


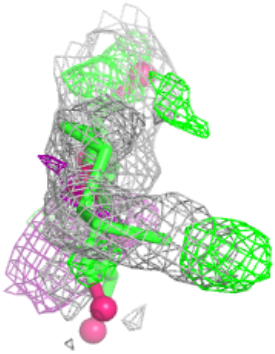


Electron density around JZR S 2011:

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

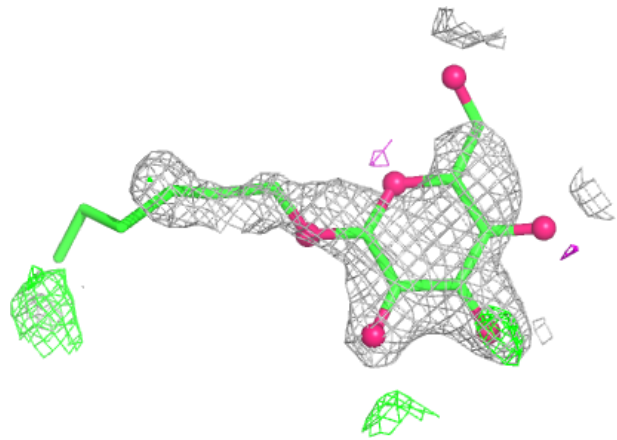


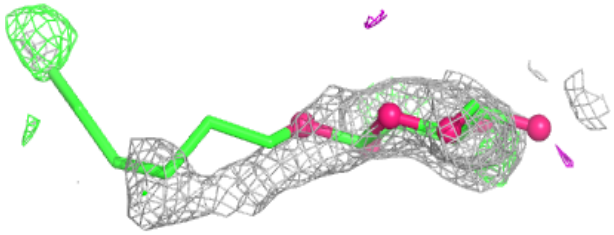


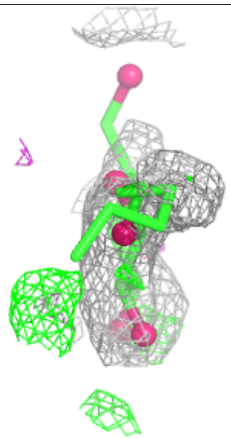


Electron density around JZR F 3011:

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

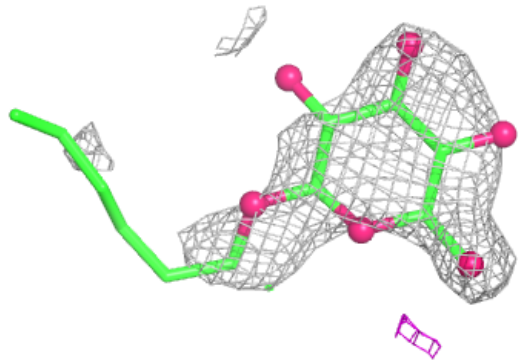


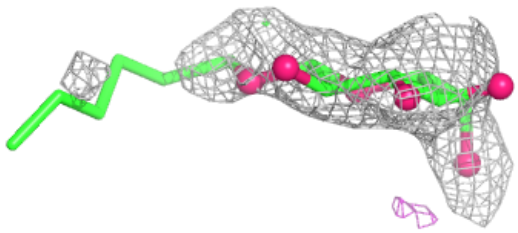


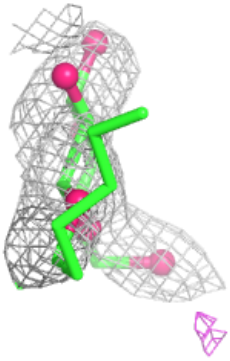


Electron density around JZR R 4007:

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

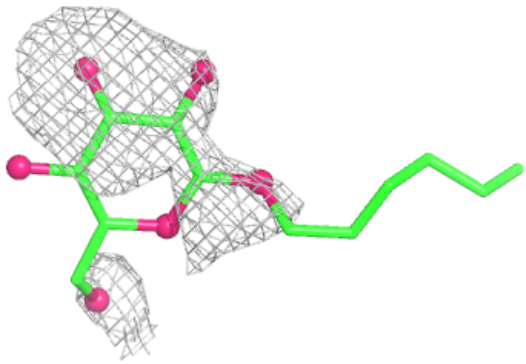


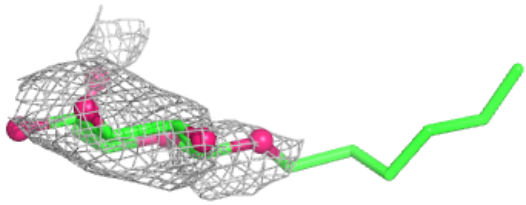


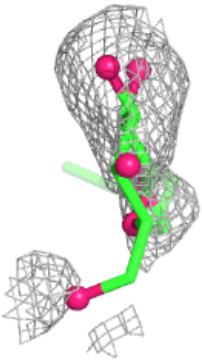


Electron density around JZR C 2010:

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

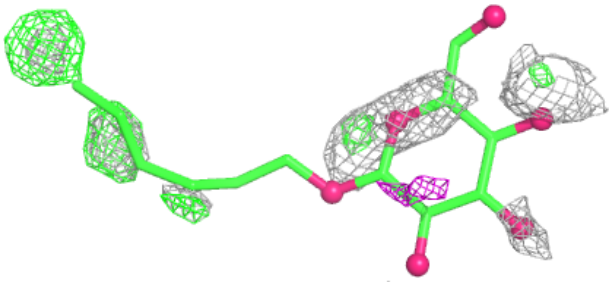


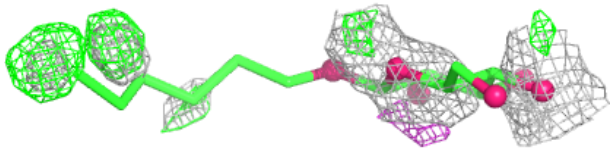


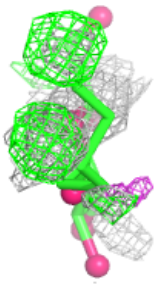


Electron density around JZR D 4003:

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

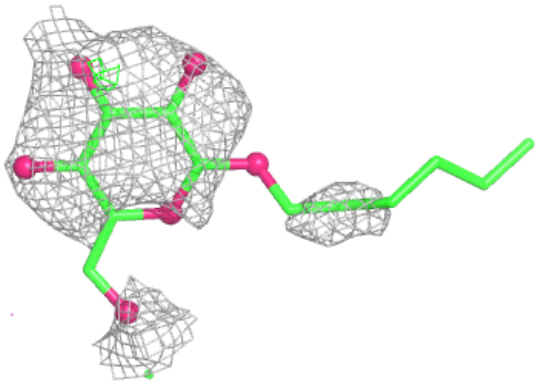


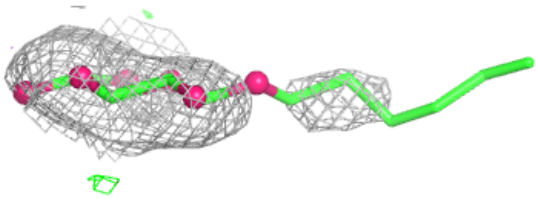


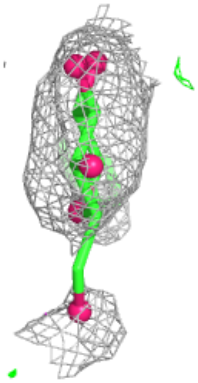


Electron density around JZR P 3010:

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

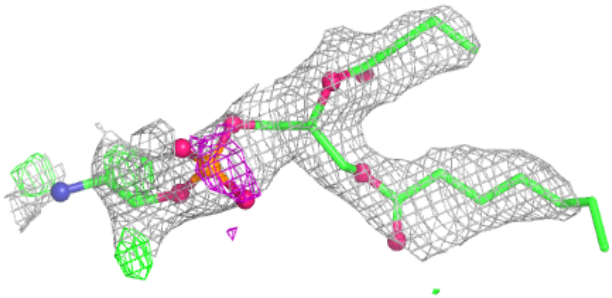


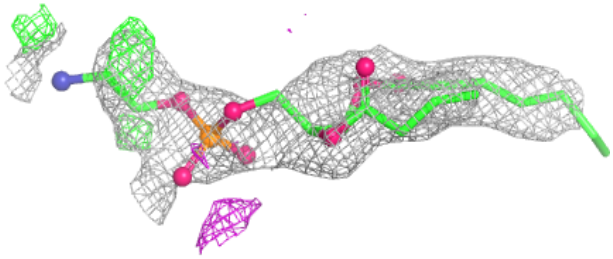


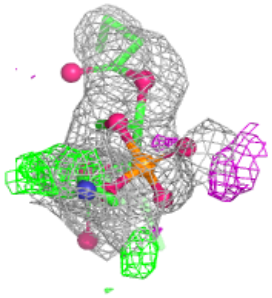


Electron density around PEE D 2006:

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

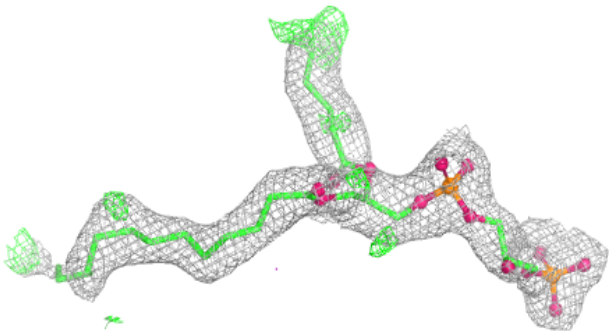


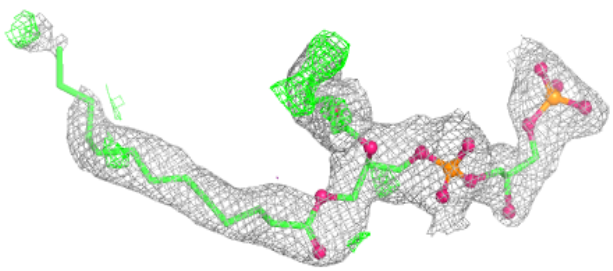




Electron density around CDL D 2003:

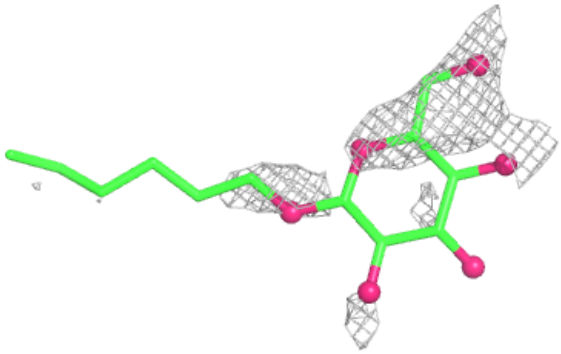
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

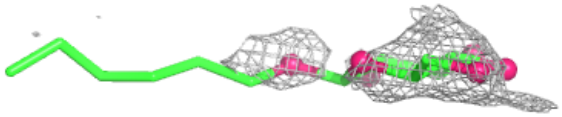


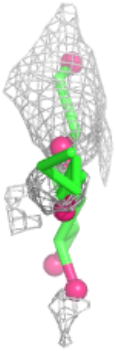


Electron density around JZR C 4002:

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

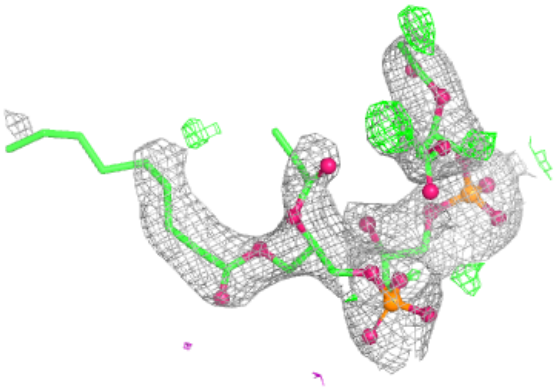


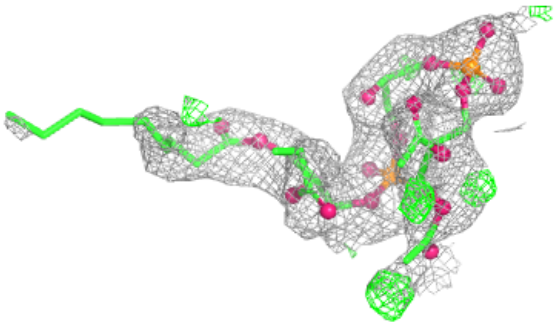


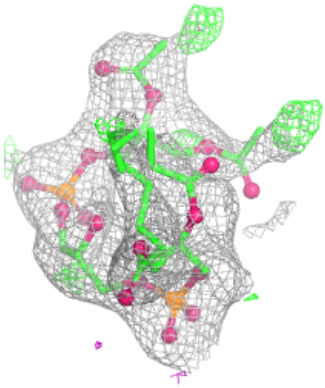


Electron density around CDL G 2004:

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

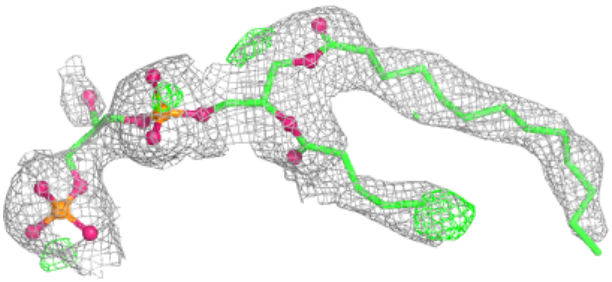


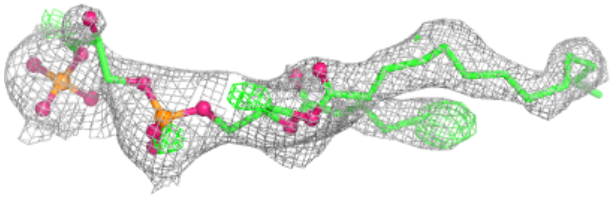


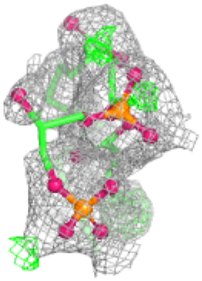


Electron density around CDL P 3003:

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

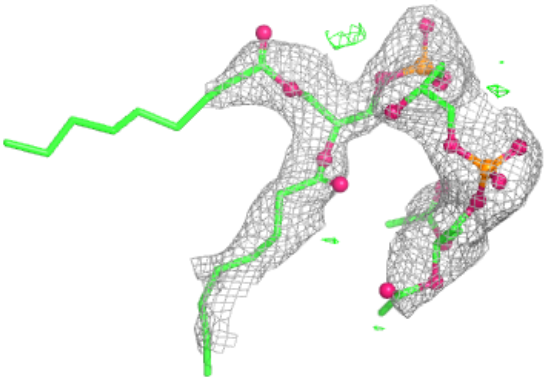


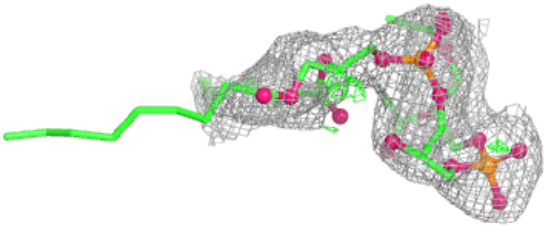


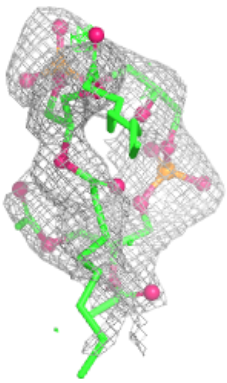


Electron density around CDL T 3004:

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

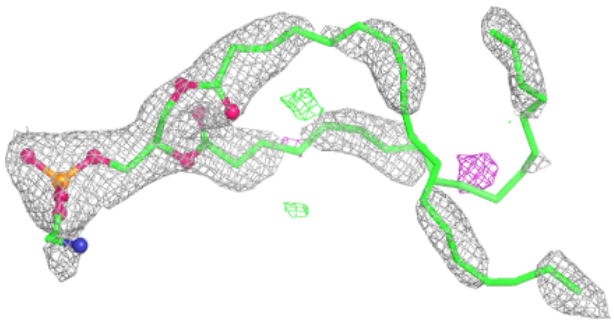


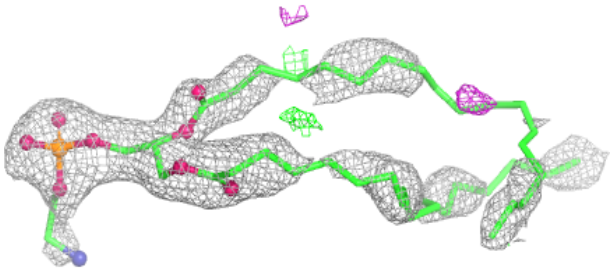




Electron density around PEE Q 3006:

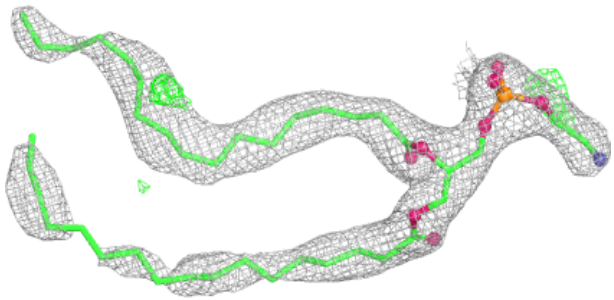
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

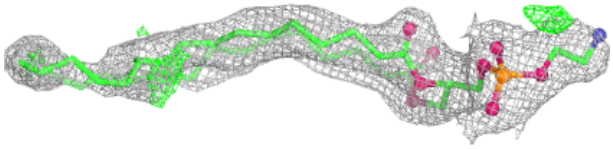


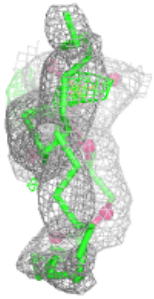


Electron density around PEE P 3007:

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

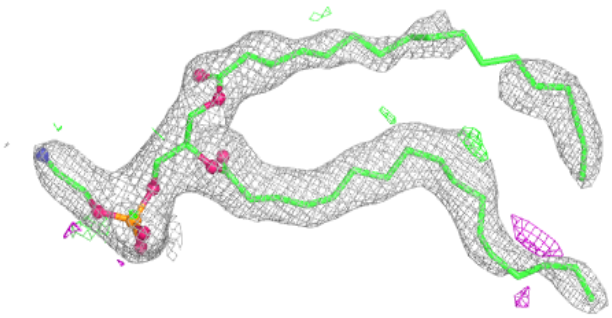


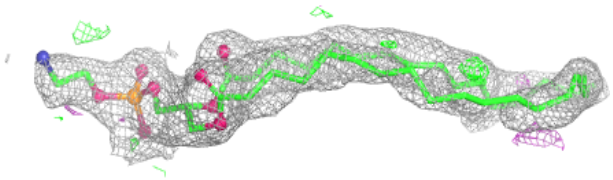


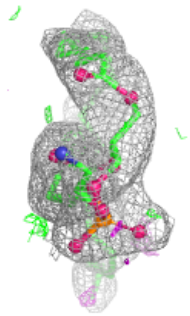


Electron density around PEE C 2007:

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

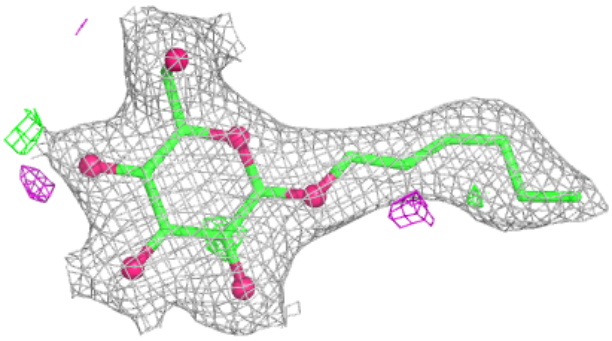


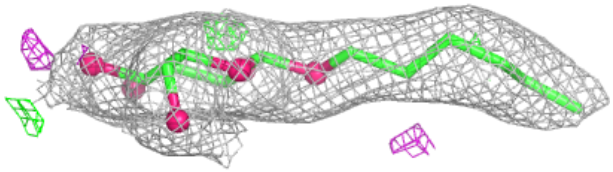


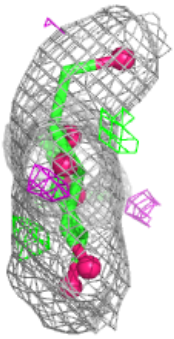


Electron density around JZR A 4004:

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

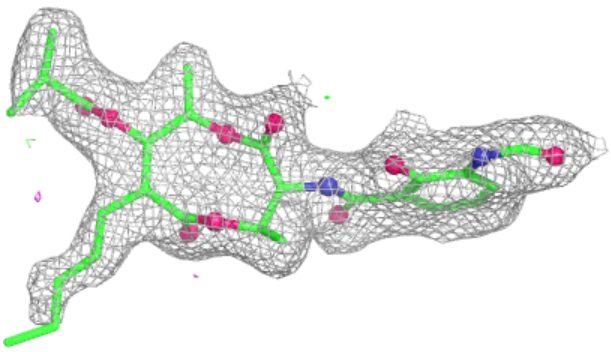


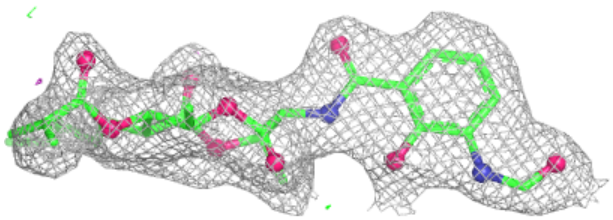


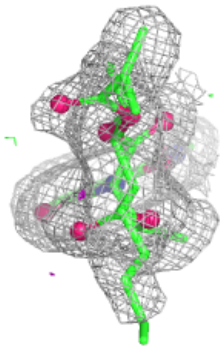


Electron density around ANY C 2002:

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

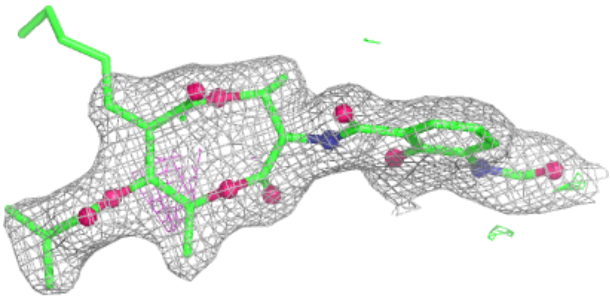


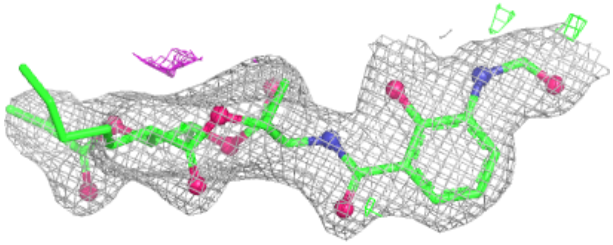


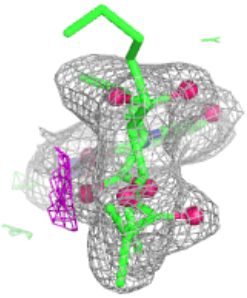


Electron density around ANY P 3002:

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

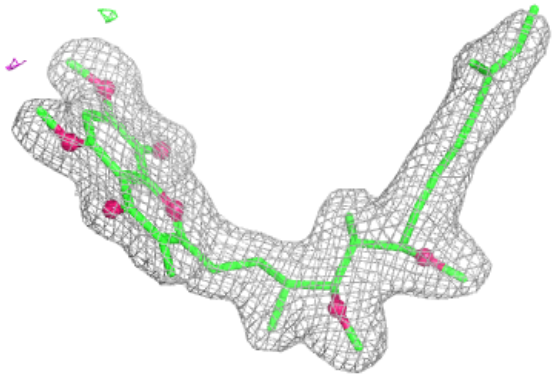


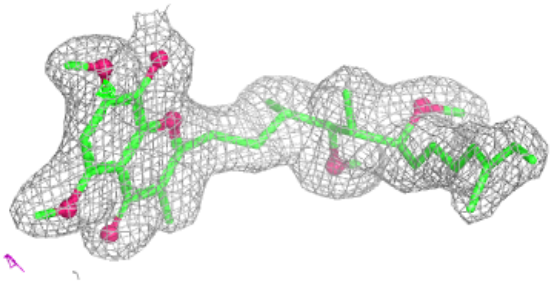




Electron density around SMA C 2001:

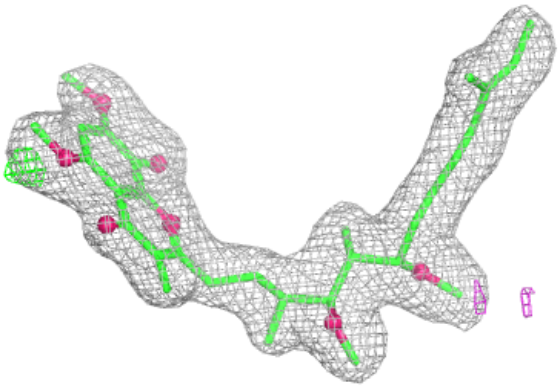
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

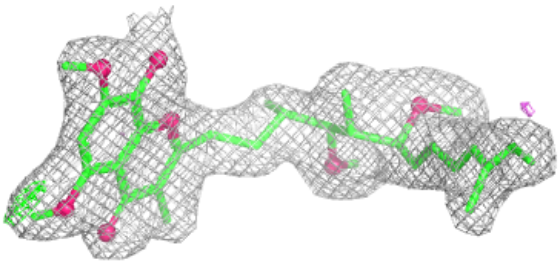


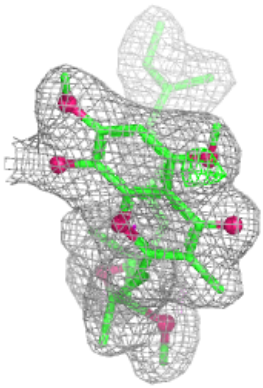


Electron density around SMA P 3001:

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

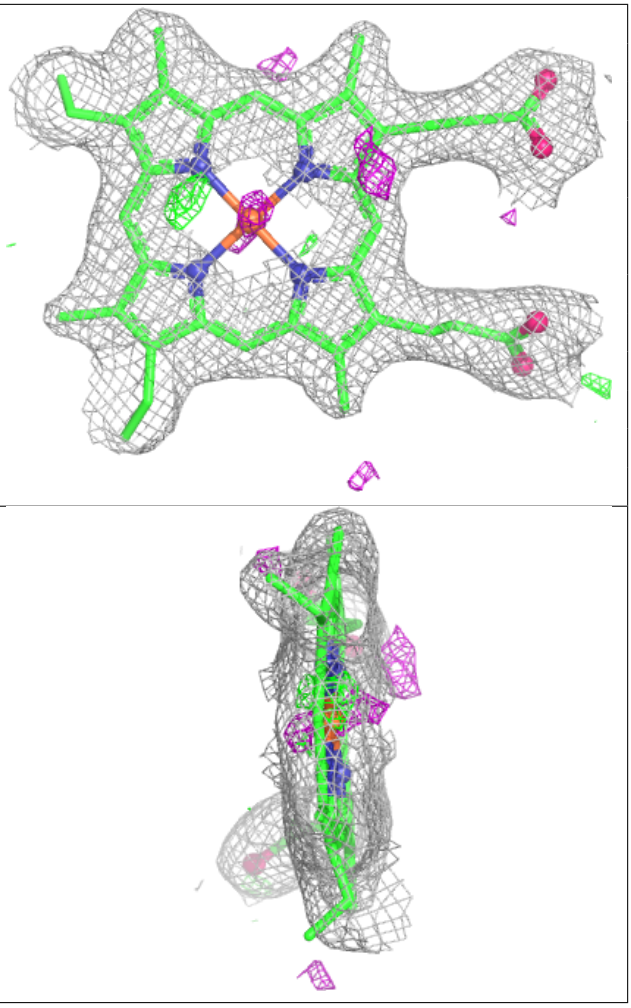






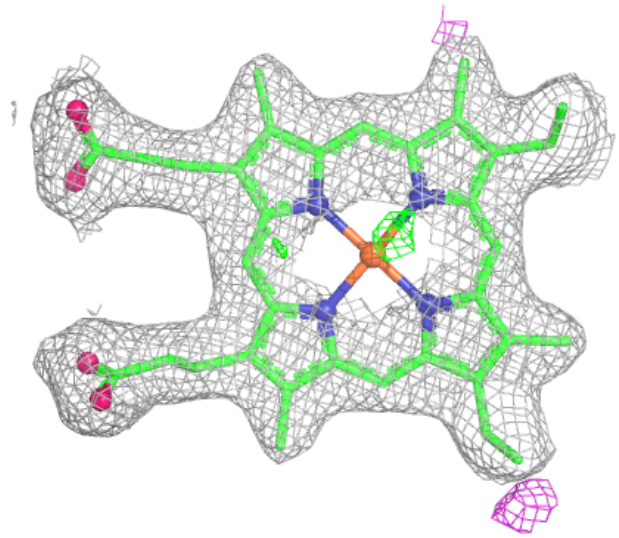
Electron density around HEC Q 501:

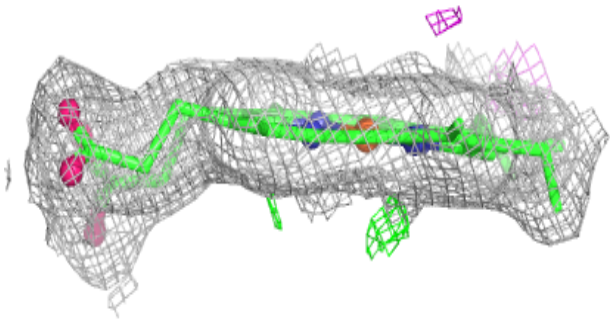
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

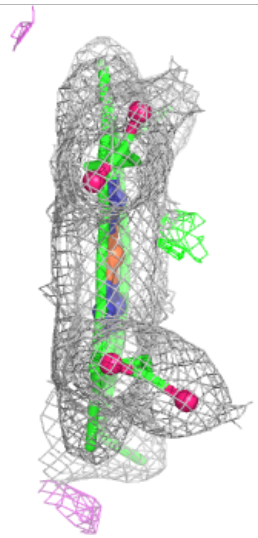


Electron density around HEC D 501:

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

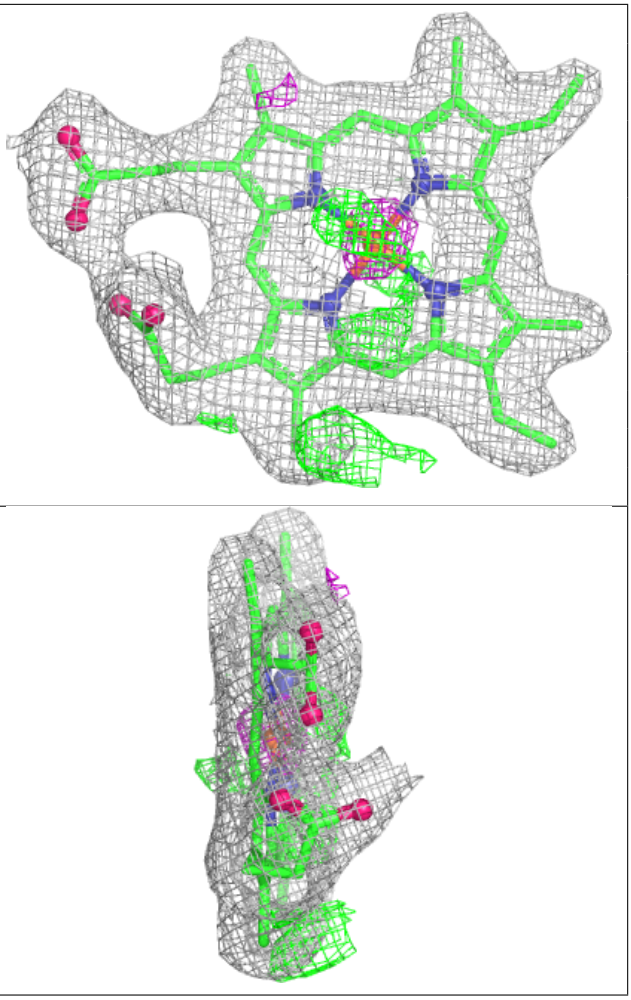






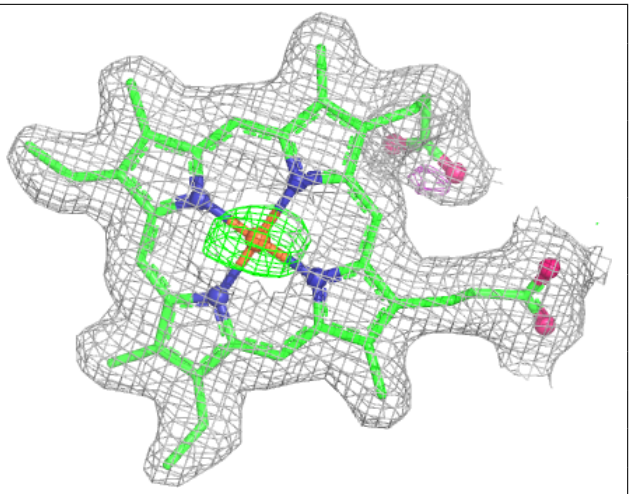
Electron density around HEM C 501:

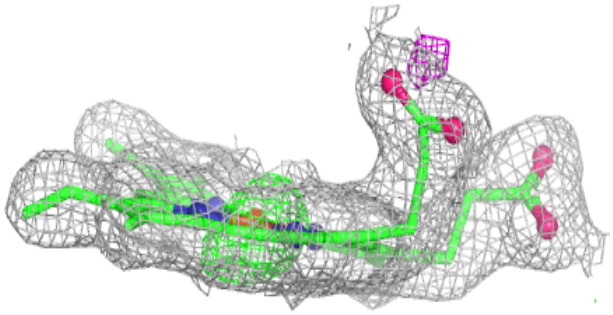
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

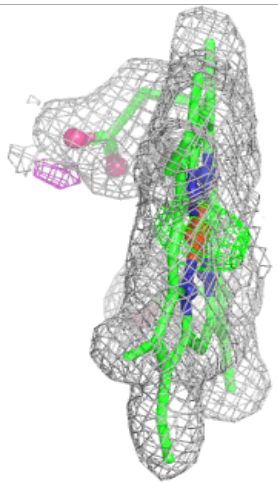


Electron density around HEM P 502:

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

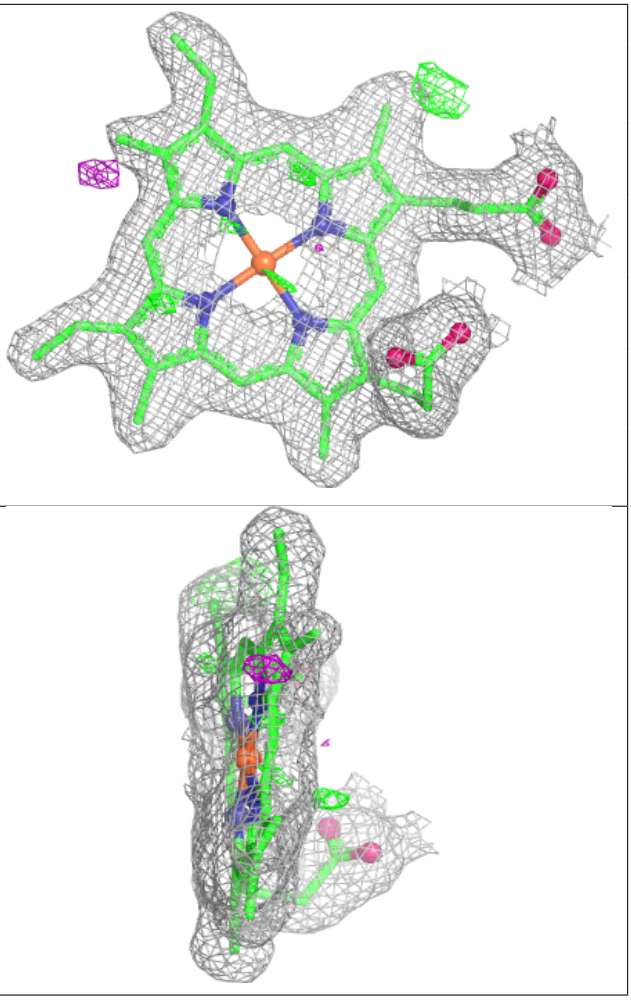






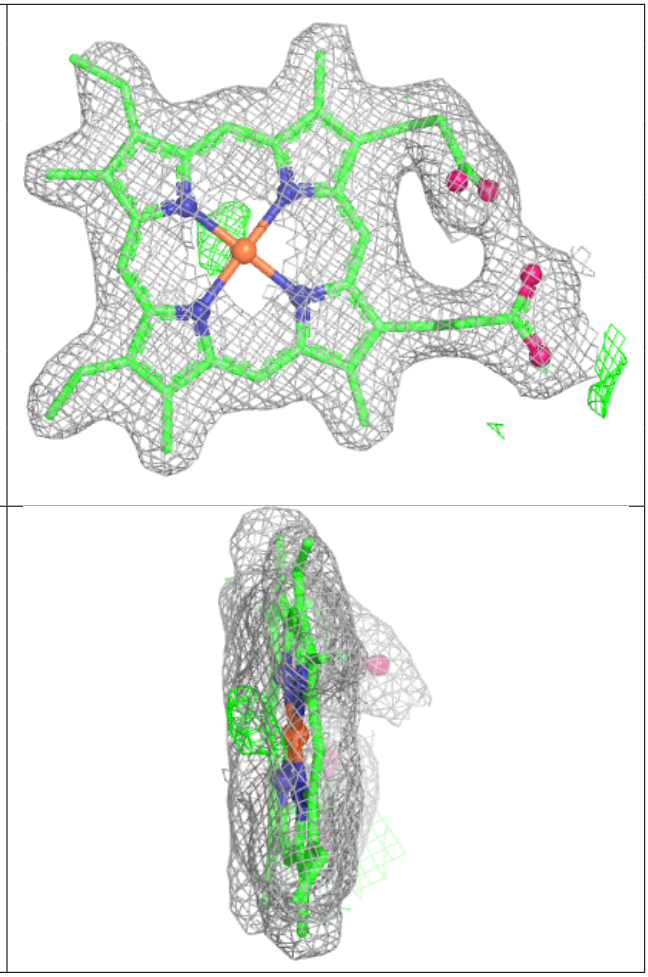
Electron density around HEM C 502:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.