



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 06:03 PM EDT

PDB ID : 1ZRT
Title : Rhodobacter capsulatus cytochrome bc1 complex with stigmatellin bound
Authors : Berry, E.A.; Huang, L.S.; Saechao, L.K.; Pon, N.G.; Valkova-Valchanov, M.; Daldal, F.
Deposited on : 2005-05-22
Resolution : 3.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

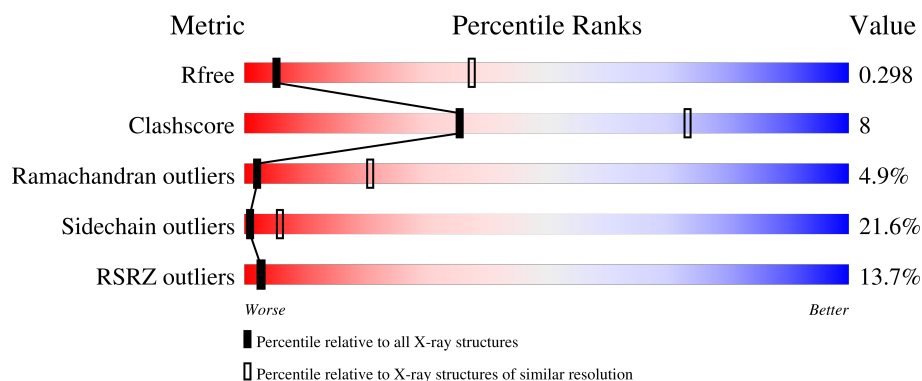
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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

Mol	Chain	Length	Quality of chain
1	C	437	<div> <div>3%</div> <div>68%</div> <div>24%</div> <div>7%</div> <div>.</div> </div>
1	P	437	<div> <div>5%</div> <div>67%</div> <div>24%</div> <div>6%</div> <div>..</div> </div>
2	D	258	<div> <div>33%</div> <div>59%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>
2	Q	258	<div> <div>24%</div> <div>59%</div> <div>31%</div> <div>6%</div> <div>.</div> </div>
3	E	191	<div> <div>12%</div> <div>58%</div> <div>32%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	R	191	

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
6	UNL	P	504	-	-	-	X
9	PG6	Q	502	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13919 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 Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	431	Total	C	N	O	S	0	1	0
			3472	2345	543	570	14			
1	P	431	Total	C	N	O	S	0	1	0
			3468	2342	542	570	14			

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	248	Total	C	N	O	S	0	0	0
			1908	1213	319	359	17			
2	Q	248	Total	C	N	O	S	0	0	0
			1904	1210	318	359	17			

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

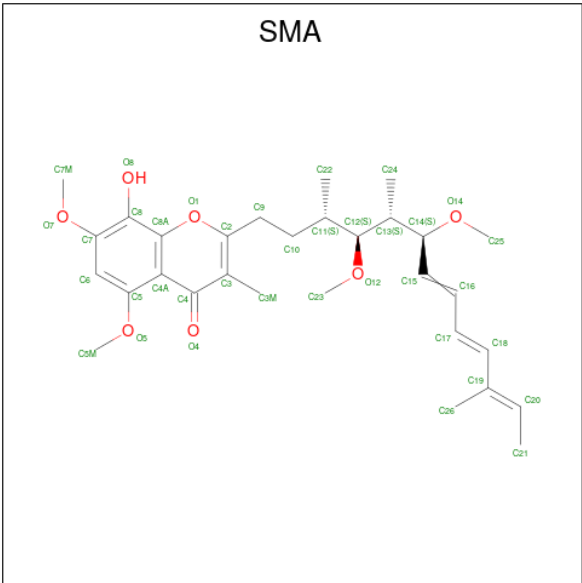
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	183	Total	C	N	O	S	0	0	0
			1372	859	248	257	8			
3	R	183	Total	C	N	O	S	0	0	0
			1376	861	248	259	8			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇) (labeled as "Ligand of Interest" by depositor).

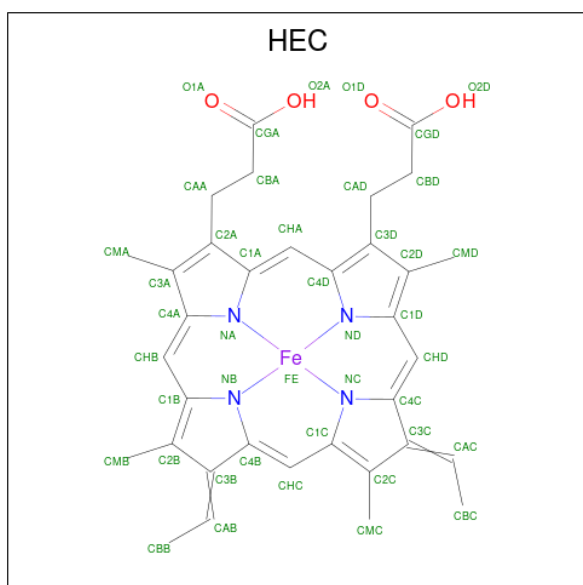


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			37	30	7		
5	P	1	Total	C	O	0	0
			37	30	7		

- Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	2	Total	C	O	0	0
			25	18	7		
6	P	2	Total	C	O	0	0
			36	27	9		

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



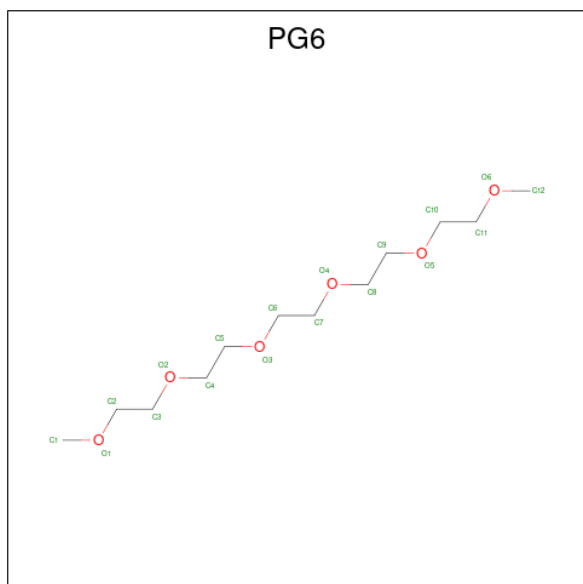
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).

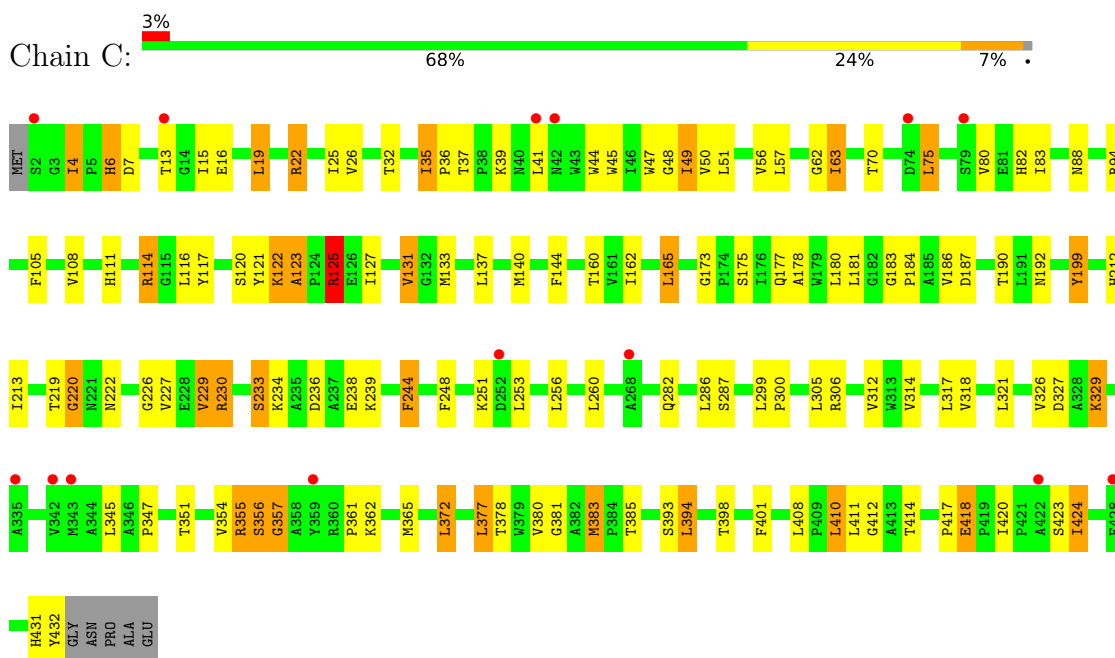


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Q	1	Total	C	O	0	0
			18	12	6		

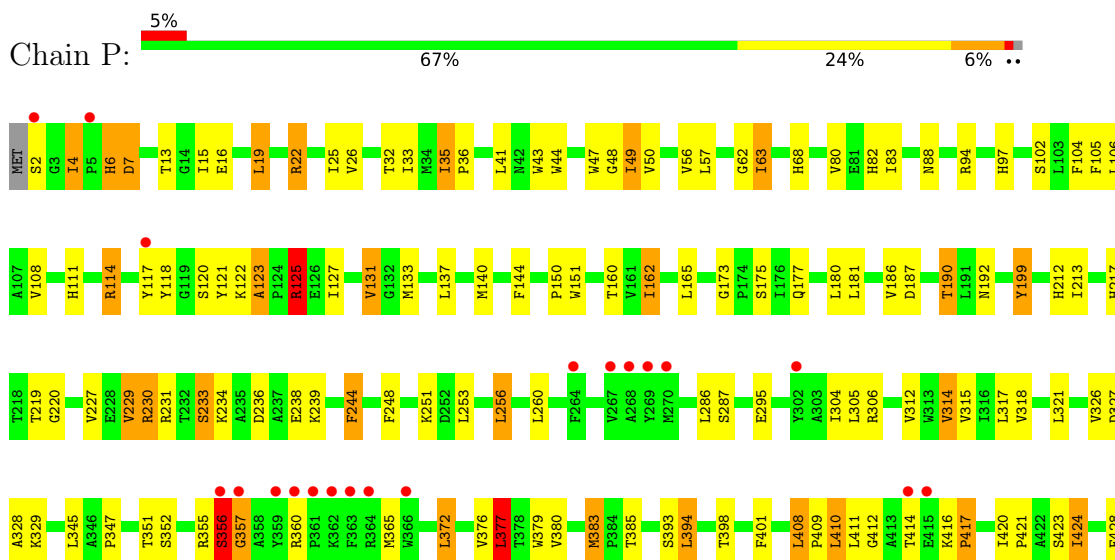
3 Residue-property plots [i](#)

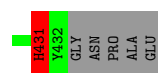
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

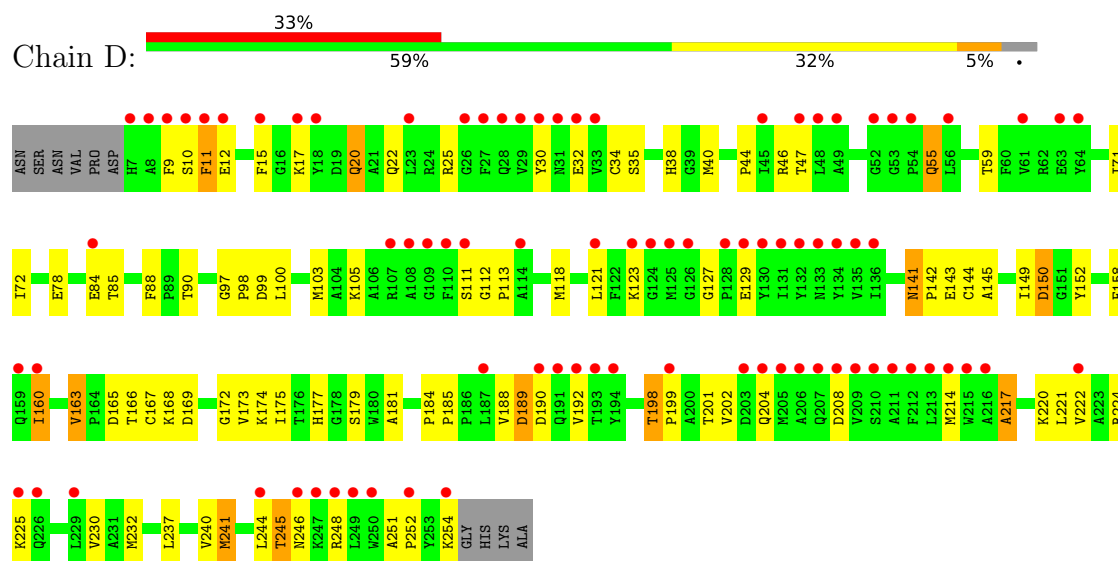


• Molecule 1: Cytochrome b

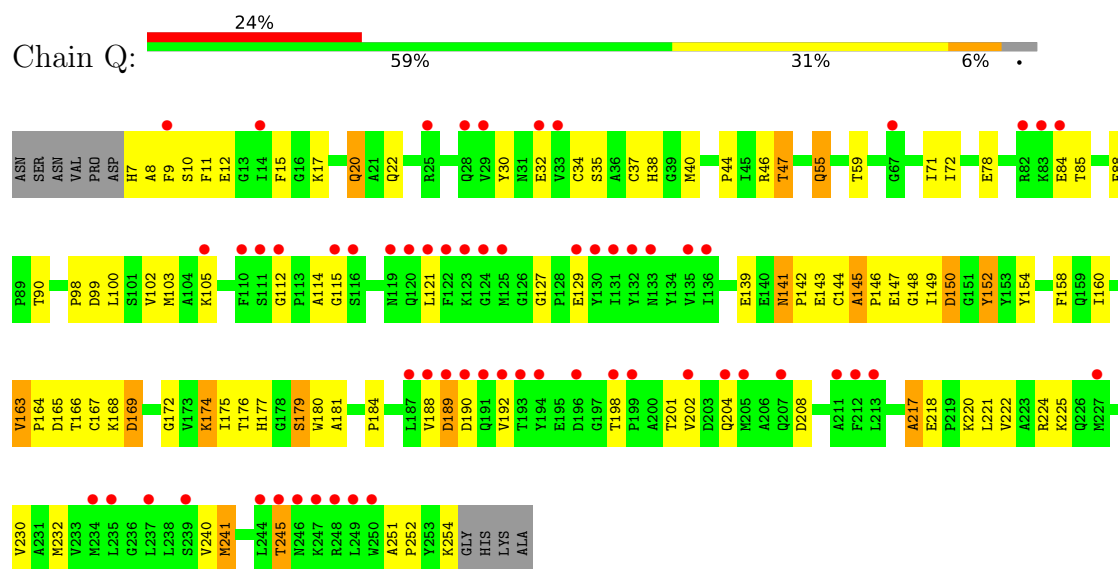




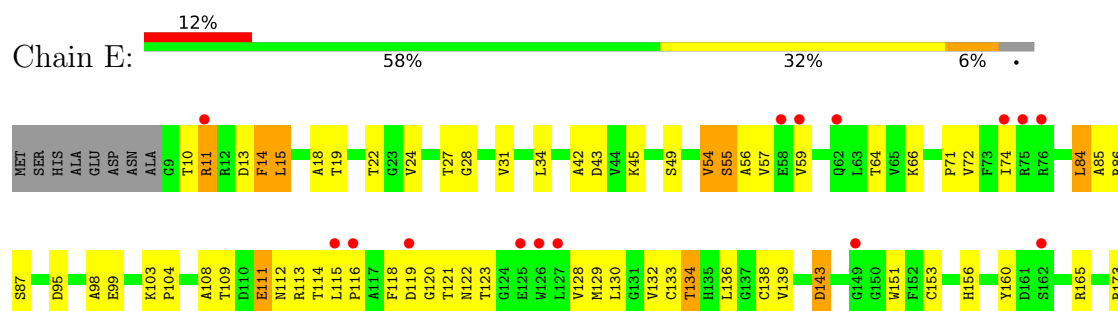
• Molecule 2: Cytochrome c1

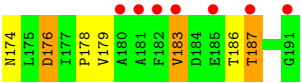


• Molecule 2: Cytochrome c1

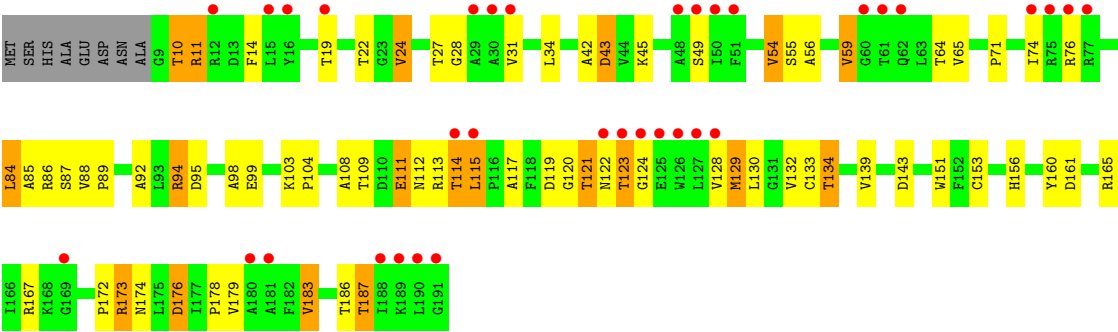


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





● Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.63Å 154.36Å 103.06Å 90.00° 113.57° 90.00°	Depositor
Resolution (Å)	59.77 – 3.51 59.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	96.5 (59.77-3.51) 96.6 (59.77-3.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 3.49Å)	Xtriage
Refinement program	PHENIX dev_3885, CNS 1.1	Depositor
R, R_{free}	0.221 , 0.289 0.226 , 0.298	Depositor DCC
R_{free} test set	1661 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13919	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, UNL, SMA, HEM, PG6, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	0.90	0/3608	1.08	10/4955 (0.2%)
1	P	0.96	1/3604 (0.0%)	1.09	7/4951 (0.1%)
2	D	0.72	0/1956	0.92	0/2647
2	Q	0.70	0/1952	0.91	0/2643
3	E	0.75	1/1402 (0.1%)	0.95	1/1905 (0.1%)
3	R	0.76	0/1406	0.95	4/1910 (0.2%)
All	All	0.84	2/13928 (0.0%)	1.01	22/19011 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
2	D	0	1
2	Q	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	138	CYS	CB-SG	-6.92	1.70	1.82
1	P	118	TYR	CB-CG	-5.40	1.43	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	84	LEU	CA-CB-CG	7.76	133.15	115.30
1	P	256	LEU	CB-CG-CD1	-7.04	99.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	84	LEU	CA-CB-CG	6.99	131.37	115.30
1	C	355	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	P	19	LEU	CA-CB-CG	6.84	131.03	115.30
1	C	19	LEU	CA-CB-CG	6.53	130.32	115.30
1	C	377	LEU	CB-CG-CD2	-6.52	99.91	111.00
1	C	165	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	P	377	LEU	CB-CG-CD2	-5.90	100.98	111.00
1	C	51	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	C	173	GLY	N-CA-C	5.65	127.23	113.10
1	P	372	LEU	CA-CB-CG	5.57	128.12	115.30
3	R	115	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	372	LEU	CA-CB-CG	5.52	128.00	115.30
3	R	129	MET	CG-SD-CE	5.43	108.90	100.20
1	C	220	GLY	N-CA-C	-5.40	99.60	113.10
1	P	260	LEU	CB-CG-CD1	-5.40	101.83	111.00
3	R	167	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	C	282	GLN	CA-CB-CG	5.37	125.21	113.40
1	P	162	ILE	CG1-CB-CG2	-5.19	99.98	111.40
1	P	173	GLY	N-CA-C	5.17	126.01	113.10
1	C	75	LEU	CB-CG-CD2	-5.10	102.32	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	167	CYS	Peptide
1	P	356	SER	Peptide
2	Q	148	GLY	Peptide
2	Q	167	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3472	0	3424	52	0
1	P	3468	0	3413	56	0
2	D	1908	0	1840	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1904	0	1829	32	0
3	E	1372	0	1346	28	0
3	R	1376	0	1350	28	0
4	C	86	0	60	2	0
4	P	86	0	60	3	0
5	C	37	0	42	3	0
5	P	37	0	42	3	0
6	C	25	0	0	0	0
6	P	36	0	0	1	0
7	D	43	0	30	5	0
7	Q	43	0	30	7	0
8	E	4	0	0	0	0
8	R	4	0	0	1	0
9	Q	18	0	26	0	0
All	All	13919	0	13492	222	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 8.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:TRP:HB3	1:C:114:ARG:HG3	1.72	0.71
1:P:4:ILE:HG13	1:P:231:ARG:HE	1.56	0.69
1:C:162:ILE:HA	1:C:165:LEU:HD12	1.76	0.68
1:P:44:TRP:HB3	1:P:114:ARG:HG3	1.75	0.67
1:C:123:ALA:O	1:C:355:ARG:NH1	2.28	0.67
3:E:74:ILE:HG23	3:E:128:VAL:HG22	1.77	0.67
1:P:123:ALA:O	1:P:355:ARG:NH1	2.27	0.66
1:P:356:SER:OG	1:P:357:GLY:N	2.29	0.66
2:Q:37:CYS:SG	7:Q:501:HEC:C3C	2.83	0.66
2:D:22:GLN:HE21	2:D:208:ASP:HA	1.61	0.64
1:P:6:HIS:HB3	1:P:36:PRO:HG3	1.80	0.62
2:D:165:ASP:HA	2:D:168:LYS:HB2	1.82	0.62
3:R:98:ALA:O	3:R:113:ARG:NH1	2.32	0.62
3:E:31:VAL:HA	3:E:34:LEU:HD12	1.82	0.61
1:C:356:SER:OG	1:C:357:GLY:N	2.32	0.61
2:Q:165:ASP:HA	2:Q:168:LYS:HB2	1.81	0.61
1:P:4:ILE:HB	1:P:36:PRO:HG2	1.82	0.61
3:R:108:ALA:O	3:R:165:ARG:NH1	2.31	0.61
1:C:180:LEU:HD22	5:C:503:SMA:H28	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:139:GLU:HB2	2:Q:154:TYR:HD2	1.66	0.60
1:P:144:PHE:HE2	5:P:503:SMA:H25	1.66	0.60
1:P:162:ILE:HA	1:P:165:LEU:HD12	1.82	0.60
1:C:4:ILE:HB	1:C:36:PRO:HG2	1.83	0.59
1:C:121:TYR:HB2	1:C:347:PRO:HG3	1.84	0.59
3:E:55:SER:OG	3:E:56:ALA:N	2.36	0.59
1:C:131:VAL:HG12	1:C:212:HIS:HD1	1.67	0.59
2:D:168:LYS:HA	2:D:174:LYS:HA	1.84	0.59
3:E:134:THR:HG21	3:E:173:ARG:HB2	1.85	0.58
1:C:47:TRP:O	1:C:111:HIS:ND1	2.36	0.58
3:R:74:ILE:HG23	3:R:128:VAL:HG22	1.84	0.58
1:P:131:VAL:HG12	1:P:212:HIS:HD1	1.68	0.58
1:C:361:PRO:HD3	1:C:418:GLU:HG3	1.86	0.58
1:C:70:THR:HG21	1:C:75:LEU:HD13	1.84	0.57
3:R:156:HIS:N	8:R:501:FES:S1	2.76	0.57
2:D:141:ASN:OD1	2:D:141:ASN:N	2.36	0.57
2:D:44:PRO:O	2:D:47:THR:OG1	2.20	0.57
1:P:306:ARG:NH2	1:P:383:MET:O	2.38	0.57
1:P:41:LEU:O	1:P:251:LYS:NZ	2.38	0.57
2:Q:22:GLN:HE21	2:Q:208:ASP:HA	1.70	0.57
1:C:286:LEU:HD23	3:R:71:PRO:HB3	1.85	0.57
3:R:31:VAL:HA	3:R:34:LEU:HD12	1.85	0.57
1:P:121:TYR:HB2	1:P:347:PRO:HG3	1.85	0.56
1:P:428:PHE:O	1:P:431:HIS:ND1	2.32	0.56
2:D:163:VAL:HG23	2:D:179:SER:HB2	1.86	0.56
3:E:108:ALA:O	3:E:165:ARG:NH1	2.38	0.56
3:R:134:THR:HG21	3:R:173:ARG:HB2	1.88	0.55
1:C:230:ARG:NH2	1:C:423:SER:OG	2.39	0.55
1:C:306:ARG:NH2	1:C:383:MET:O	2.39	0.55
1:P:233:SER:OG	1:P:234:LYS:N	2.40	0.55
1:P:180:LEU:HD13	5:P:503:SMA:H28	1.89	0.55
2:D:244:LEU:HB3	3:E:15:LEU:HD11	1.88	0.55
3:E:134:THR:HG22	3:E:173:ARG:HH21	1.71	0.54
2:Q:40:MET:HB2	2:Q:88:PHE:HB2	1.89	0.54
3:R:99:GLU:HB3	3:R:176:ASP:HA	1.88	0.54
3:R:42:ALA:HA	3:R:45:LYS:HB2	1.90	0.54
2:D:165:ASP:OD1	2:D:165:ASP:N	2.40	0.54
3:R:10:THR:HG22	3:R:14:PHE:HB2	1.90	0.54
3:E:99:GLU:HB3	3:E:176:ASP:HA	1.90	0.53
3:R:151:TRP:HB2	3:R:160:TYR:HB2	1.90	0.53
3:E:85:ALA:O	3:E:165:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:SER:OG	1:C:234:LYS:N	2.41	0.53
1:P:230:ARG:NH2	1:P:423:SER:OG	2.41	0.53
3:E:10:THR:HG22	3:E:11:ARG:HH21	1.74	0.53
2:D:144:CYS:SG	2:D:145:ALA:N	2.77	0.53
3:E:98:ALA:O	3:E:113:ARG:NH1	2.35	0.53
3:E:109:THR:OG1	3:E:112:ASN:ND2	2.42	0.53
1:P:102:SER:O	1:P:106:LEU:N	2.35	0.53
2:Q:184:PRO:HD2	7:Q:501:HEC:HBC2	1.91	0.53
2:D:40:MET:HB2	2:D:88:PHE:HB2	1.90	0.53
2:Q:112:GLY:HA2	2:Q:115:GLY:H	1.75	0.52
1:P:144:PHE:CE2	5:P:503:SMA:H25	2.45	0.52
3:E:151:TRP:HB2	3:E:160:TYR:HB2	1.92	0.52
2:Q:141:ASN:N	2:Q:141:ASN:OD1	2.43	0.52
1:C:312:VAL:HG13	1:C:394:LEU:HD11	1.91	0.52
3:E:43:ASP:OD1	3:E:43:ASP:N	2.40	0.52
1:P:80:VAL:HG21	1:P:150:PRO:HB3	1.93	0.51
3:E:71:PRO:HB3	1:P:286:LEU:HD23	1.92	0.51
3:R:85:ALA:O	3:R:165:ARG:NH2	2.43	0.51
3:R:103:LYS:NZ	3:R:111:GLU:O	2.39	0.51
1:C:6:HIS:HB3	1:C:36:PRO:HG3	1.91	0.51
3:E:14:PHE:O	3:E:18:ALA:N	2.41	0.51
1:P:379:TRP:HE1	2:Q:114:ALA:HB1	1.75	0.51
2:Q:44:PRO:O	2:Q:47:THR:OG1	2.26	0.51
2:Q:30:TYR:HD1	2:Q:34:CYS:HB2	1.76	0.51
3:R:54:VAL:O	3:R:56:ALA:N	2.45	0.50
3:E:66:LYS:HB2	1:P:286:LEU:HD21	1.91	0.50
1:C:410:LEU:O	1:C:412:GLY:N	2.45	0.50
1:C:178:ALA:HA	1:C:181:LEU:HB2	1.94	0.49
2:D:251:ALA:HA	2:D:254:LYS:HB3	1.94	0.49
1:C:219:THR:OG1	1:C:220:GLY:O	2.29	0.49
2:Q:251:ALA:HA	2:Q:254:LYS:HB3	1.94	0.49
3:R:109:THR:OG1	3:R:112:ASN:ND2	2.44	0.49
2:D:184:PRO:HD2	7:D:501:HEC:HBC2	1.94	0.49
1:C:41:LEU:O	1:C:251:LYS:NZ	2.45	0.49
3:E:143:ASP:O	2:Q:168:LYS:NZ	2.46	0.49
1:C:244:PHE:HA	1:C:248:PHE:HB2	1.94	0.49
2:Q:189:ASP:OD1	2:Q:202:VAL:N	2.45	0.49
7:D:501:HEC:HBA1	7:D:501:HEC:HBD2	1.94	0.49
1:P:236:ASP:HA	1:P:239:LYS:HE2	1.94	0.49
1:P:230:ARG:HD2	1:P:236:ASP:HB2	1.95	0.49
2:Q:102:VAL:HG23	2:Q:217:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:318:VAL:HG12	1:P:326:VAL:HB	1.95	0.48
2:Q:164:PRO:O	2:Q:168:LYS:N	2.46	0.48
2:D:30:TYR:HD1	2:D:34:CYS:HB2	1.77	0.48
1:C:122:LYS:NZ	1:C:354:VAL:O	2.42	0.48
2:Q:37:CYS:CB	7:Q:501:HEC:C3C	2.92	0.48
2:D:241:MET:O	2:D:245:THR:OG1	2.31	0.48
7:Q:501:HEC:HHA	7:Q:501:HEC:HBD2	1.95	0.48
3:R:183:VAL:HG23	3:R:187:THR:HB	1.96	0.48
1:C:120:SER:HA	1:C:125:ARG:HD3	1.97	0.47
2:D:38:HIS:HE1	2:D:98:PRO:HD2	1.79	0.47
1:C:39:LYS:HA	1:C:248:PHE:HZ	1.80	0.47
1:C:318:VAL:HG12	1:C:326:VAL:HB	1.97	0.47
1:P:7:ASP:OD1	1:P:7:ASP:N	2.43	0.47
7:Q:501:HEC:HBD2	7:Q:501:HEC:HBA1	1.97	0.47
1:P:229:VAL:HG13	1:P:424:ILE:HD12	1.97	0.47
2:D:9:PHE:HE2	2:D:129:GLU:HG3	1.80	0.47
1:P:219:THR:OG1	1:P:220:GLY:O	2.31	0.47
2:Q:241:MET:O	2:Q:245:THR:OG1	2.34	0.46
1:C:22:ARG:HH11	1:C:22:ARG:HB2	1.80	0.46
6:P:504:UNL:O4	2:Q:220:LYS:NZ	2.46	0.46
1:P:63:ILE:H	1:P:63:ILE:HG12	1.56	0.46
3:R:43:ASP:OD1	3:R:43:ASP:N	2.37	0.46
1:C:144:PHE:HE2	5:C:503:SMA:H25	1.81	0.46
2:Q:9:PHE:HE2	2:Q:129:GLU:HG3	1.80	0.46
2:D:105:LYS:HG3	2:D:217:ALA:HB1	1.97	0.46
2:Q:165:ASP:OD1	2:Q:165:ASP:N	2.40	0.46
2:Q:139:GLU:HB2	2:Q:154:TYR:CD2	2.48	0.46
2:D:189:ASP:OD1	2:D:202:VAL:N	2.44	0.46
1:P:410:LEU:O	1:P:412:GLY:N	2.49	0.46
3:E:42:ALA:HA	3:E:45:LYS:HB2	1.98	0.46
1:P:244:PHE:HA	1:P:248:PHE:HB2	1.97	0.46
1:P:47:TRP:O	1:P:111:HIS:ND1	2.49	0.45
1:P:304:ILE:HD11	1:P:377:LEU:HD21	1.98	0.45
2:D:20:GLN:HE22	2:D:55:GLN:HB2	1.81	0.45
2:D:141:ASN:HA	2:D:142:PRO:HD3	1.79	0.45
2:Q:17:LYS:HD2	2:Q:222:VAL:HG12	1.98	0.45
2:Q:152:TYR:HB3	2:Q:180:TRP:HB3	1.98	0.45
1:C:226:GLY:HA3	1:C:356:SER:HB2	1.99	0.45
1:C:49:ILE:HD13	1:C:49:ILE:HA	1.84	0.45
3:E:95:ASP:OD2	3:E:174:ASN:ND2	2.50	0.45
3:E:103:LYS:NZ	3:E:111:GLU:O	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASP:HA	1:C:239:LYS:HE2	1.99	0.45
1:P:22:ARG:HB2	1:P:22:ARG:HH11	1.82	0.45
3:E:183:VAL:HG23	3:E:187:THR:HB	1.98	0.45
2:Q:38:HIS:HE1	2:Q:98:PRO:HD2	1.82	0.45
3:E:54:VAL:O	3:E:57:VAL:N	2.50	0.44
2:Q:38:HIS:CD2	7:Q:501:HEC:NB	2.85	0.44
2:D:248:ARG:HH22	3:E:11:ARG:NH1	2.15	0.44
1:P:312:VAL:HG13	1:P:394:LEU:HD11	1.98	0.44
1:P:352:SER:HB2	1:P:412:GLY:HA2	2.00	0.44
2:Q:168:LYS:HB3	2:Q:169:ASP:H	1.57	0.44
7:Q:501:HEC:HHA	7:Q:501:HEC:HBA1	1.99	0.44
2:D:174:LYS:HB2	2:D:174:LYS:HE3	1.79	0.44
1:C:229:VAL:HG13	1:C:424:ILE:HD12	1.99	0.44
2:Q:163:VAL:HG13	2:Q:179:SER:HB2	2.00	0.44
1:C:230:ARG:HD2	1:C:236:ASP:HB2	1.99	0.44
1:C:35:ILE:HA	1:C:36:PRO:HD3	1.88	0.43
7:D:501:HEC:HBD2	7:D:501:HEC:HHA	2.00	0.43
1:P:315:VAL:HG11	1:P:328:ALA:HB2	2.01	0.43
3:E:54:VAL:O	3:E:56:ALA:N	2.51	0.43
1:P:181:LEU:HA	1:P:190:THR:HG23	2.01	0.43
1:C:22:ARG:HG2	1:P:219:THR:HG22	2.00	0.43
1:C:62:GLY:O	4:C:501:HEM:HBC2	2.18	0.43
1:P:97:HIS:HE1	4:P:501:HEM:NC	2.17	0.43
1:C:63:ILE:H	1:C:63:ILE:HG12	1.61	0.43
3:R:117:ALA:H	3:R:121:THR:HG23	1.83	0.43
1:C:127:ILE:HD12	1:C:127:ILE:HA	1.82	0.43
1:P:105:PHE:CZ	1:P:140:MET:HG2	2.53	0.42
1:C:180:LEU:HD13	5:C:503:SMA:H28	2.01	0.42
2:D:17:LYS:HD2	2:D:222:VAL:HG12	2.00	0.42
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.87	0.42
2:D:38:HIS:CE1	2:D:97:GLY:HA3	2.54	0.42
1:P:127:ILE:HD12	1:P:127:ILE:HA	1.80	0.42
1:P:416:LYS:HA	1:P:417:PRO:HD2	1.80	0.42
2:Q:174:LYS:HB2	2:Q:174:LYS:HE3	1.75	0.42
3:R:59:VAL:HG22	3:R:76:ARG:HH12	1.83	0.42
1:C:80:VAL:HA	1:C:83:ILE:HD12	2.00	0.42
3:E:136:LEU:HD12	3:E:156:HIS:CE1	2.54	0.42
1:C:114:ARG:HE	1:C:114:ARG:HB3	1.68	0.42
1:P:35:ILE:HG13	1:P:217:HIS:CD2	2.55	0.42
1:P:35:ILE:HG13	1:P:217:HIS:HD2	1.85	0.42
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:TYR:CE2	4:C:501:HEM:HBC1	2.54	0.42
1:C:105:PHE:CZ	1:C:140:MET:HG2	2.55	0.42
7:D:501:HEC:HBA1	7:D:501:HEC:HHA	2.01	0.42
1:P:408:LEU:HD13	1:P:408:LEU:HA	1.89	0.41
1:C:306:ARG:NH2	1:C:381:GLY:O	2.53	0.41
1:P:49:ILE:HD13	1:P:49:ILE:HA	1.80	0.41
3:R:114:THR:HG21	3:R:124:GLY:HA2	2.01	0.41
2:D:198:THR:HA	2:D:199:PRO:HD2	1.97	0.41
1:P:120:SER:HA	1:P:125:ARG:HD3	2.03	0.41
1:C:4:ILE:H	1:C:4:ILE:HG13	1.42	0.41
1:C:125:ARG:HE	1:C:222:ASN:HB2	1.85	0.41
1:P:62:GLY:O	4:P:501:HEM:HBC2	2.21	0.41
1:P:199:TYR:CE2	4:P:501:HEM:HBC1	2.55	0.41
3:R:88:VAL:HA	3:R:89:PRO:HD2	1.77	0.41
3:R:94:ARG:HB2	3:R:95:ASP:H	1.71	0.41
1:P:35:ILE:HA	1:P:36:PRO:HD3	1.87	0.41
1:P:312:VAL:HG12	1:P:314:VAL:HG13	2.01	0.41
1:C:219:THR:HG22	1:P:22:ARG:HG2	2.03	0.41
1:P:68:HIS:HB3	1:P:83:ILE:HG12	2.03	0.41
3:R:95:ASP:OD2	3:R:174:ASN:ND2	2.54	0.41
2:Q:20:GLN:HE22	2:Q:55:GLN:HB2	1.86	0.41
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.92	0.41
2:D:11:PHE:CE1	2:D:214:MET:HG2	2.56	0.41
1:P:114:ARG:HE	1:P:114:ARG:HB3	1.75	0.41
3:R:89:PRO:HG2	3:R:92:ALA:HB3	2.03	0.41
1:C:300:PRO:HD3	1:C:378:THR:HG22	2.03	0.41
2:Q:105:LYS:HD3	2:Q:218:GLU:HG2	2.03	0.41
2:Q:144:CYS:SG	2:Q:145:ALA:N	2.92	0.41
2:D:160:ILE:H	2:D:160:ILE:HG13	1.69	0.40
3:E:99:GLU:HB2	3:E:113:ARG:HH12	1.86	0.40
3:E:99:GLU:HG3	3:E:174:ASN:HB2	2.03	0.40
1:C:183:GLY:HA3	1:C:184:PRO:HD2	1.79	0.40
2:D:22:GLN:HG3	2:D:25:ARG:NH2	2.36	0.40
3:R:11:ARG:H	3:R:11:ARG:HE	1.69	0.40
3:R:172:PRO:HG2	3:R:173:ARG:HD3	2.03	0.40
2:D:38:HIS:CD2	7:D:501:HEC:NB	2.90	0.40
3:R:123:THR:O	3:R:123:THR:OG1	2.38	0.40
1:P:424:ILE:H	1:P:424:ILE:HG12	1.55	0.40
3:R:165:ARG:HA	3:R:174:ASN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	430/437 (98%)	363 (84%)	55 (13%)	12 (3%)	5	34
1	P	430/437 (98%)	359 (84%)	58 (14%)	13 (3%)	4	32
2	D	246/258 (95%)	195 (79%)	32 (13%)	19 (8%)	1	11
2	Q	246/258 (95%)	195 (79%)	32 (13%)	19 (8%)	1	11
3	E	181/191 (95%)	146 (81%)	24 (13%)	11 (6%)	1	16
3	R	181/191 (95%)	142 (78%)	29 (16%)	10 (6%)	2	19
All	All	1714/1772 (97%)	1400 (82%)	230 (13%)	84 (5%)	2	21

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	ALA
1	C	125	ARG
1	C	411	LEU
1	C	417	PRO
2	D	12	GLU
3	E	55	SER
3	E	119	ASP
1	P	125	ARG
1	P	411	LEU
1	P	417	PRO
1	P	431	HIS
2	Q	12	GLU
2	Q	145	ALA
2	Q	181	ALA
3	R	55	SER
1	C	356	SER
1	C	431	HIS
2	D	72	ILE
2	D	143	GLU
2	D	152	TYR

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Mol	Chain	Res	Type
2	D	172	GLY
2	D	177	HIS
2	D	181	ALA
3	E	13	ASP
3	E	118	PHE
1	P	230	ARG
1	P	356	SER
2	Q	72	ILE
2	Q	143	GLU
2	Q	146	PRO
2	Q	150	ASP
2	Q	152	TYR
2	Q	158	PHE
1	C	35	ILE
1	C	230	ARG
2	D	46	ARG
2	D	150	ASP
2	D	158	PHE
2	D	189	ASP
2	D	217	ALA
3	E	24	VAL
3	E	104	PRO
3	E	116	PRO
3	E	122	ASN
1	P	35	ILE
1	P	357	GLY
2	Q	8	ALA
2	Q	142	PRO
2	Q	147	GLU
2	Q	189	ASP
2	Q	217	ALA
3	R	24	VAL
3	R	104	PRO
3	R	119	ASP
3	R	122	ASN
1	C	48	GLY
1	C	329	LYS
2	D	55	GLN
2	D	198	THR
3	E	178	PRO
1	P	123	ALA
2	Q	198	THR

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Mol	Chain	Res	Type
3	R	94	ARG
1	C	187	ASP
1	C	357	GLY
2	D	111	SER
2	D	113	PRO
1	P	43	TRP
1	P	187	ASP
1	P	329	LYS
2	Q	46	ARG
2	Q	55	GLN
3	R	161	ASP
3	R	178	PRO
2	D	112	GLY
3	E	120	GLY
1	P	48	GLY
3	R	28	GLY
3	E	28	GLY
2	Q	127	GLY
2	Q	172	GLY
2	D	127	GLY
3	R	120	GLY
2	D	185	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	356/360 (99%)	285 (80%)	71 (20%)	1	7
1	P	355/360 (99%)	279 (79%)	76 (21%)	1	6
2	D	197/206 (96%)	153 (78%)	44 (22%)	1	5
2	Q	196/206 (95%)	152 (78%)	44 (22%)	1	5
3	E	142/149 (95%)	110 (78%)	32 (22%)	1	5
3	R	143/149 (96%)	109 (76%)	34 (24%)	0	4
All	All	1389/1430 (97%)	1088 (78%)	301 (22%)	1	6

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	ILE
1	C	6	HIS
1	C	7	ASP
1	C	13	THR
1	C	15	ILE
1	C	16	GLU
1	C	19	LEU
1	C	22	ARG
1	C	25	ILE
1	C	26	VAL
1	C	32	THR
1	C	37	THR
1	C	45	TRP
1	C	49	ILE
1	C	50	VAL
1	C	56	VAL
1	C	57	LEU
1	C	63	ILE
1	C	82	HIS
1	C	88	ASN
1	C	94	ARG
1	C	108	VAL
1	C	114	ARG
1	C	117	TYR
1	C	122	LYS
1	C	125	ARG
1	C	131	VAL
1	C	133	MET
1	C	137	LEU
1	C	160	THR
1	C	175	SER
1	C	177	GLN
1	C	186	VAL
1	C	190	THR
1	C	192	ASN
1	C	199	TYR
1	C	213	ILE
1	C	227	VAL
1	C	229	VAL
1	C	233	SER
1	C	238	GLU
1	C	244	PHE

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Mol	Chain	Res	Type
1	C	253	LEU
1	C	256	LEU
1	C	287	SER
1	C	305	LEU
1	C	314	VAL
1	C	317	LEU
1	C	321	LEU
1	C	327	ASP
1	C	329	LYS
1	C	345	LEU
1	C	351	THR
1	C	362	LYS
1	C	365	MET
1	C	372	LEU
1	C	377	LEU
1	C	380	VAL
1	C	383	MET
1	C	385	THR
1	C	393	SER
1	C	394	LEU
1	C	398	THR
1	C	401	PHE
1	C	408	LEU
1	C	410	LEU
1	C	414	THR
1	C	418	GLU
1	C	420	ILE
1	C	424	ILE
1	C	432	TYR
2	D	10	SER
2	D	11	PHE
2	D	15	PHE
2	D	20	GLN
2	D	32	GLU
2	D	35	SER
2	D	59	THR
2	D	71	ILE
2	D	78	GLU
2	D	84	GLU
2	D	85	THR
2	D	90	THR
2	D	99	ASP

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Mol	Chain	Res	Type
2	D	100	LEU
2	D	103	MET
2	D	118	MET
2	D	121	LEU
2	D	123	LYS
2	D	141	ASN
2	D	149	ILE
2	D	150	ASP
2	D	160	ILE
2	D	163	VAL
2	D	166	THR
2	D	169	ASP
2	D	173	VAL
2	D	175	ILE
2	D	188	VAL
2	D	190	ASP
2	D	192	VAL
2	D	201	THR
2	D	204	GLN
2	D	220	LYS
2	D	221	LEU
2	D	224	ARG
2	D	225	LYS
2	D	230	VAL
2	D	232	MET
2	D	237	LEU
2	D	240	VAL
2	D	241	MET
2	D	245	THR
2	D	246	ASN
2	D	252	PRO
3	E	11	ARG
3	E	14	PHE
3	E	15	LEU
3	E	19	THR
3	E	22	THR
3	E	27	THR
3	E	49	SER
3	E	54	VAL
3	E	59	VAL
3	E	64	THR
3	E	72	VAL

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Mol	Chain	Res	Type
3	E	84	LEU
3	E	86	ARG
3	E	87	SER
3	E	111	GLU
3	E	114	THR
3	E	115	LEU
3	E	121	THR
3	E	123	THR
3	E	129	MET
3	E	130	LEU
3	E	132	VAL
3	E	133	CYS
3	E	134	THR
3	E	139	VAL
3	E	143	ASP
3	E	153	CYS
3	E	176	ASP
3	E	179	VAL
3	E	183	VAL
3	E	186	THR
3	E	187	THR
1	P	2	SER
1	P	4	ILE
1	P	6	HIS
1	P	7	ASP
1	P	13	THR
1	P	15	ILE
1	P	16	GLU
1	P	19	LEU
1	P	22	ARG
1	P	25	ILE
1	P	26	VAL
1	P	32	THR
1	P	33	ILE
1	P	49	ILE
1	P	50	VAL
1	P	56	VAL
1	P	57	LEU
1	P	63	ILE
1	P	82	HIS
1	P	88	ASN
1	P	94	ARG

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Mol	Chain	Res	Type
1	P	104	PHE
1	P	108	VAL
1	P	114	ARG
1	P	117	TYR
1	P	122	LYS
1	P	125	ARG
1	P	131	VAL
1	P	133	MET
1	P	137	LEU
1	P	151	TRP
1	P	160	THR
1	P	175	SER
1	P	177	GLN
1	P	186	VAL
1	P	190	THR
1	P	192	ASN
1	P	199	TYR
1	P	213	ILE
1	P	227	VAL
1	P	229	VAL
1	P	233	SER
1	P	238	GLU
1	P	244	PHE
1	P	253	LEU
1	P	256	LEU
1	P	287	SER
1	P	295[A]	GLU
1	P	295[B]	GLU
1	P	305	LEU
1	P	314	VAL
1	P	317	LEU
1	P	321	LEU
1	P	327	ASP
1	P	345	LEU
1	P	351	THR
1	P	360	ARG
1	P	365	MET
1	P	372	LEU
1	P	376	VAL
1	P	377	LEU
1	P	380	VAL
1	P	383	MET

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Mol	Chain	Res	Type
1	P	385	THR
1	P	393	SER
1	P	394	LEU
1	P	398	THR
1	P	401	PHE
1	P	408	LEU
1	P	409	PRO
1	P	410	LEU
1	P	414	THR
1	P	420	ILE
1	P	421	PRO
1	P	424	ILE
1	P	431	HIS
2	Q	7	HIS
2	Q	10	SER
2	Q	11	PHE
2	Q	15	PHE
2	Q	20	GLN
2	Q	32	GLU
2	Q	35	SER
2	Q	47	THR
2	Q	59	THR
2	Q	71	ILE
2	Q	78	GLU
2	Q	84	GLU
2	Q	85	THR
2	Q	90	THR
2	Q	99	ASP
2	Q	100	LEU
2	Q	103	MET
2	Q	121	LEU
2	Q	141	ASN
2	Q	149	ILE
2	Q	150	ASP
2	Q	160	ILE
2	Q	163	VAL
2	Q	166	THR
2	Q	169	ASP
2	Q	174	LYS
2	Q	175	ILE
2	Q	176	THR
2	Q	177	HIS

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Mol	Chain	Res	Type
2	Q	179	SER
2	Q	188	VAL
2	Q	190	ASP
2	Q	192	VAL
2	Q	201	THR
2	Q	204	GLN
2	Q	221	LEU
2	Q	224	ARG
2	Q	225	LYS
2	Q	230	VAL
2	Q	232	MET
2	Q	240	VAL
2	Q	241	MET
2	Q	245	THR
2	Q	252	PRO
3	R	10	THR
3	R	11	ARG
3	R	19	THR
3	R	22	THR
3	R	24	VAL
3	R	27	THR
3	R	43	ASP
3	R	49	SER
3	R	54	VAL
3	R	59	VAL
3	R	64	THR
3	R	65	VAL
3	R	84	LEU
3	R	86	ARG
3	R	87	SER
3	R	111	GLU
3	R	114	THR
3	R	115	LEU
3	R	121	THR
3	R	123	THR
3	R	129	MET
3	R	130	LEU
3	R	132	VAL
3	R	133	CYS
3	R	134	THR
3	R	139	VAL
3	R	143	ASP

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Mol	Chain	Res	Type
3	R	153	CYS
3	R	173	ARG
3	R	176	ASP
3	R	179	VAL
3	R	183	VAL
3	R	186	THR
3	R	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	C	177	GLN
2	D	20	GLN
2	D	22	GLN
2	D	133	ASN
2	D	204	GLN
3	E	36	ASN
3	E	39	ASN
3	E	112	ASN
3	E	159	HIS
1	P	88	ASN
1	P	177	GLN
2	Q	20	GLN
2	Q	22	GLN
2	Q	204	GLN
3	R	36	ASN
3	R	39	ASN
3	R	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are unknown - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	HEM	C	501	1	41,50,50	1.91	8 (19%)	45,82,82	1.92	12 (26%)
7	HEC	Q	501	2	32,50,50	2.30	7 (21%)	24,82,82	2.71	7 (29%)
4	HEM	C	502	1	41,50,50	1.59	7 (17%)	45,82,82	2.28	16 (35%)
8	FES	E	501	3	0,4,4	-	-	-	-	-
4	HEM	P	501	1	41,50,50	1.63	6 (14%)	45,82,82	1.90	14 (31%)
9	PG6	Q	502	-	17,17,17	0.71	0	16,16,16	0.56	0
4	HEM	P	502	1	41,50,50	1.58	7 (17%)	45,82,82	2.02	13 (28%)
7	HEC	D	501	2	32,50,50	2.09	8 (25%)	24,82,82	2.88	8 (33%)
8	FES	R	501	3	0,4,4	-	-	-	-	-
5	SMA	P	503	-	38,38,38	2.24	6 (15%)	48,52,52	2.14	17 (35%)
5	SMA	C	503	-	38,38,38	2.32	6 (15%)	48,52,52	2.55	18 (37%)

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
4	HEM	C	501	1	-	3/12/54/54	-
7	HEC	Q	501	2	-	7/10/54/54	-
4	HEM	C	502	1	-	3/12/54/54	-
8	FES	E	501	3	-	-	0/1/1/1
4	HEM	P	501	1	-	3/12/54/54	-
9	PG6	Q	502	-	-	5/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	P	502	1	-	5/12/54/54	-
7	HEC	D	501	2	-	6/10/54/54	-
8	FES	R	501	3	-	-	0/1/1/1
5	SMA	P	503	-	-	15/34/34/34	0/2/2/2
5	SMA	C	503	-	-	14/34/34/34	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	503	SMA	C3-C2	8.54	1.51	1.34
5	C	503	SMA	C8-C8A	8.19	1.52	1.39
5	P	503	SMA	C7-C8	7.28	1.50	1.40
5	C	503	SMA	C3-C2	6.76	1.48	1.34
4	C	501	HEM	FE-NB	6.51	2.29	1.96
7	Q	501	HEC	C2B-C3B	-6.32	1.34	1.40
4	P	501	HEM	C3C-C2C	-5.94	1.32	1.40
7	D	501	HEC	C2B-C3B	-5.83	1.34	1.40
4	C	502	HEM	C3C-CAC	5.72	1.59	1.47
7	Q	501	HEC	C3D-C2D	5.32	1.53	1.37
5	C	503	SMA	C4A-C5	5.19	1.49	1.40
4	C	501	HEM	C3C-C2C	-5.13	1.33	1.40
5	C	503	SMA	C7-C8	5.12	1.47	1.40
7	D	501	HEC	CAD-C3D	5.12	1.59	1.52
4	P	502	HEM	C3C-C2C	-4.85	1.33	1.40
7	D	501	HEC	C3D-C2D	4.75	1.51	1.37
5	P	503	SMA	C4A-C5	4.62	1.48	1.40
7	Q	501	HEC	C3C-C2C	-4.60	1.36	1.40
4	P	502	HEM	C3C-CAC	4.34	1.56	1.47
7	Q	501	HEC	CAD-C3D	4.34	1.58	1.52
5	C	503	SMA	C4A-C8A	4.32	1.50	1.40
5	P	503	SMA	C8-C8A	4.04	1.46	1.39
4	C	502	HEM	C3C-C2C	-3.68	1.35	1.40
7	D	501	HEC	C3C-C2C	-3.33	1.37	1.40
4	C	501	HEM	C3C-CAC	3.29	1.54	1.47
4	P	501	HEM	FE-NB	3.28	2.13	1.96
5	P	503	SMA	C4A-C8A	3.27	1.48	1.40
7	Q	501	HEC	C3C-C4C	3.00	1.48	1.43
4	C	501	HEM	CMB-C2B	2.97	1.57	1.50
4	P	501	HEM	C3C-CAC	2.94	1.53	1.47
4	P	501	HEM	CMB-C2B	2.81	1.56	1.50
7	Q	501	HEC	CAA-C2A	2.79	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	502	HEM	CAA-C2A	2.73	1.56	1.52
7	Q	501	HEC	C4D-CHA	-2.72	1.33	1.41
4	C	502	HEM	C3B-C2B	-2.66	1.31	1.37
4	P	501	HEM	CMD-C2D	2.61	1.56	1.50
4	P	502	HEM	FE-NB	2.60	2.09	1.96
4	P	501	HEM	C1A-NA	2.59	1.41	1.36
4	C	502	HEM	CAB-C3B	2.54	1.54	1.47
5	C	503	SMA	C4A-C4	2.39	1.52	1.46
4	C	501	HEM	CAB-C3B	2.38	1.53	1.47
7	D	501	HEC	C3C-C4C	2.37	1.47	1.43
4	C	501	HEM	FE-ND	-2.31	1.85	1.96
4	P	502	HEM	C3B-C2B	-2.30	1.32	1.37
4	P	502	HEM	CAB-C3B	2.25	1.53	1.47
4	C	501	HEM	CMC-C2C	2.18	1.56	1.51
7	D	501	HEC	CAA-C2A	2.17	1.56	1.52
4	C	502	HEM	CAA-C2A	2.17	1.55	1.52
4	C	502	HEM	CAD-C3D	2.16	1.56	1.51
4	C	502	HEM	O1D-CGD	2.11	1.29	1.22
4	C	501	HEM	CMD-C2D	2.10	1.55	1.50
7	D	501	HEC	C4D-CHA	-2.08	1.35	1.41
5	P	503	SMA	O1-C8A	-2.08	1.35	1.38
4	P	502	HEM	CAD-C3D	2.06	1.56	1.51
7	D	501	HEC	C2A-C1A	2.03	1.47	1.42

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	SMA	C14-C15-C16	-8.55	108.86	125.61
7	D	501	HEC	CMC-C2C-C1C	-7.69	116.64	128.46
7	Q	501	HEC	CBD-CAD-C3D	7.68	125.73	112.62
7	D	501	HEC	CBD-CAD-C3D	7.55	125.50	112.62
7	Q	501	HEC	CMC-C2C-C1C	-6.58	118.35	128.46
4	C	502	HEM	C4B-CHC-C1C	6.37	130.97	122.56
4	C	501	HEM	C2C-C3C-C4C	6.22	111.25	106.90
5	P	503	SMA	O7-C7-C8	6.10	120.70	114.54
5	C	503	SMA	C9-C2-C3	-6.02	118.26	127.07
4	C	502	HEM	C3B-C2B-C1B	5.33	110.44	106.49
4	P	502	HEM	C4B-CHC-C1C	5.11	129.30	122.56
7	D	501	HEC	CBA-CAA-C2A	4.96	120.96	112.60
5	P	503	SMA	C14-C15-C16	-4.88	116.06	125.61
5	C	503	SMA	C17-C18-C19	-4.70	113.20	126.42
5	C	503	SMA	O1-C8A-C8	4.69	123.85	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	HEM	CMD-C2D-C1D	-4.51	118.17	125.04
4	C	502	HEM	C1D-C2D-C3D	4.50	111.69	106.96
7	Q	501	HEC	CBA-CAA-C2A	4.44	120.09	112.60
4	P	502	HEM	CMC-C2C-C3C	4.35	132.82	124.68
4	P	501	HEM	C2C-C3C-C4C	4.28	109.89	106.90
4	P	501	HEM	CBA-CAA-C2A	-4.24	105.39	112.62
5	C	503	SMA	O1-C2-C9	4.19	119.46	110.58
4	C	501	HEM	CBA-CAA-C2A	-4.10	105.62	112.62
4	P	502	HEM	CMB-C2B-C1B	3.96	131.06	125.04
5	C	503	SMA	C7M-O7-C7	3.87	123.38	117.53
5	P	503	SMA	C16-C17-C18	-3.84	115.09	124.67
5	P	503	SMA	C22-C11-C12	3.82	117.40	111.15
5	P	503	SMA	C9-C10-C11	-3.79	107.60	114.52
5	C	503	SMA	O5-C5-C6	-3.77	117.62	124.12
5	C	503	SMA	C22-C11-C10	3.76	116.25	110.36
4	P	501	HEM	C4C-CHD-C1D	3.63	127.35	122.56
4	P	501	HEM	C4A-C3A-C2A	3.59	109.49	107.00
4	C	502	HEM	CMB-C2B-C3B	-3.57	119.56	128.30
5	P	503	SMA	C7M-O7-C7	3.45	122.73	117.53
4	P	502	HEM	CMB-C2B-C3B	-3.41	119.95	128.30
5	P	503	SMA	O5-C5-C4A	3.40	120.59	115.85
5	C	503	SMA	O4-C4-C3	-3.40	115.84	120.25
4	P	502	HEM	C3B-C2B-C1B	3.37	108.98	106.49
4	C	501	HEM	C4C-CHD-C1D	3.35	126.98	122.56
4	P	501	HEM	C4B-C3B-C2B	3.33	109.76	107.11
5	P	503	SMA	O8-C8-C7	3.30	126.40	119.24
4	C	502	HEM	CMB-C2B-C1B	3.26	130.00	125.04
7	Q	501	HEC	CMC-C2C-C3C	3.20	129.58	125.82
4	P	502	HEM	C1D-C2D-C3D	3.10	110.22	106.96
4	C	501	HEM	C4B-C3B-C2B	3.07	109.56	107.11
4	C	502	HEM	CMC-C2C-C3C	3.07	130.43	124.68
7	D	501	HEC	CMC-C2C-C3C	3.04	129.39	125.82
4	P	502	HEM	CMD-C2D-C1D	-3.02	120.44	125.04
5	C	503	SMA	O8-C8-C7	-2.97	112.81	119.24
7	D	501	HEC	O1A-CGA-CBA	-2.95	113.60	123.08
4	P	502	HEM	C1B-NB-C4B	2.92	108.09	105.07
5	C	503	SMA	C4A-C8A-C8	-2.86	117.14	121.27
5	C	503	SMA	O8-C8-C8A	2.84	126.10	119.85
4	C	501	HEM	CAA-CBA-CGA	-2.83	105.82	113.76
4	P	501	HEM	CMB-C2B-C1B	-2.82	120.74	125.04
4	C	501	HEM	C4A-C3A-C2A	2.81	108.95	107.00
7	D	501	HEC	CMB-C2B-C1B	-2.78	124.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	HEM	C2B-C1B-NB	-2.76	106.56	109.84
4	C	502	HEM	C2D-C1D-ND	-2.76	106.58	109.88
4	P	502	HEM	C2B-C1B-NB	-2.75	106.58	109.84
5	P	503	SMA	O5-C5-C6	-2.74	119.40	124.12
4	C	501	HEM	CBD-CAD-C3D	-2.72	105.08	112.63
5	P	503	SMA	C7-C6-C5	2.69	124.29	118.97
4	C	502	HEM	C4D-ND-C1D	2.66	107.82	105.07
4	C	501	HEM	CHC-C4B-NB	2.66	127.32	124.43
7	Q	501	HEC	CMB-C2B-C1B	-2.62	124.43	128.46
4	P	501	HEM	C1B-NB-C4B	2.61	107.77	105.07
4	C	502	HEM	C1B-NB-C4B	2.60	107.76	105.07
5	C	503	SMA	O12-C12-C13	2.57	111.77	107.97
4	P	501	HEM	CBD-CAD-C3D	-2.55	105.55	112.63
7	Q	501	HEC	O1A-CGA-CBA	-2.53	114.94	123.08
4	P	502	HEM	O1D-CGD-CBD	-2.52	114.97	123.08
5	C	503	SMA	C8A-O1-C2	2.50	123.20	119.35
4	P	501	HEM	C4D-ND-C1D	2.47	107.63	105.07
5	C	503	SMA	C16-C17-C18	-2.47	118.51	124.67
4	P	501	HEM	CAD-CBD-CGD	-2.44	108.34	113.60
4	P	501	HEM	C3C-C4C-NC	-2.43	106.36	110.94
5	P	503	SMA	C22-C11-C10	2.41	114.14	110.36
5	C	503	SMA	O4-C4-C4A	2.40	126.53	121.99
4	C	501	HEM	C4D-ND-C1D	2.35	107.50	105.07
4	P	501	HEM	CHD-C1D-C2D	2.34	128.63	124.98
4	C	501	HEM	C3C-C4C-NC	-2.32	106.57	110.94
4	C	501	HEM	CAD-CBD-CGD	-2.31	108.62	113.60
4	P	502	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
4	P	501	HEM	CAA-CBA-CGA	-2.29	107.34	113.76
4	C	502	HEM	C4C-CHD-C1D	-2.28	119.54	122.56
7	D	501	HEC	C3C-C4C-NC	-2.24	106.72	110.94
5	P	503	SMA	O8-C8-C8A	-2.19	115.03	119.85
5	P	503	SMA	C13-C14-C15	2.19	116.91	112.13
4	C	502	HEM	CAB-C3B-C2B	-2.17	121.47	128.60
4	P	502	HEM	CAB-C3B-C2B	-2.15	121.52	128.60
5	P	503	SMA	O7-C7-C6	-2.13	120.45	124.12
4	P	502	HEM	C4D-ND-C1D	2.11	107.25	105.07
4	C	501	HEM	C1B-NB-C4B	2.10	107.25	105.07
5	P	503	SMA	C11-C12-C13	-2.07	108.77	114.29
7	Q	501	HEC	C3C-C4C-NC	-2.06	107.05	110.94
5	C	503	SMA	C25-O14-C14	2.06	117.96	113.01
4	C	502	HEM	O2D-CGD-O1D	2.05	128.41	123.30
7	D	501	HEC	CAA-C2A-C3A	-2.04	121.37	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	503	SMA	O4-C4-C3	-2.04	117.60	120.25
4	P	501	HEM	CMB-C2B-C3B	2.03	133.27	128.30
4	C	502	HEM	CAD-C3D-C2D	2.03	131.65	127.88
5	P	503	SMA	C17-C18-C19	-2.02	120.73	126.42
4	C	502	HEM	O1D-CGD-CBD	-2.02	116.60	123.08
5	C	503	SMA	C3M-C3-C4	2.01	119.60	116.27

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	502	HEM	C2A-CAA-CBA-CGA
4	P	502	HEM	C2A-CAA-CBA-CGA
5	C	503	SMA	C13-C14-O14-C25
5	C	503	SMA	C17-C18-C19-C20
5	C	503	SMA	C17-C18-C19-C26
5	P	503	SMA	C3-C2-C9-C10
5	P	503	SMA	O1-C2-C9-C10
5	P	503	SMA	C17-C18-C19-C20
5	P	503	SMA	C17-C18-C19-C26
7	D	501	HEC	C1A-C2A-CAA-CBA
7	D	501	HEC	C3A-C2A-CAA-CBA
7	D	501	HEC	C2D-C3D-CAD-CBD
7	D	501	HEC	C4D-C3D-CAD-CBD
7	Q	501	HEC	C1A-C2A-CAA-CBA
7	Q	501	HEC	C3A-C2A-CAA-CBA
7	Q	501	HEC	C2D-C3D-CAD-CBD
7	Q	501	HEC	C4D-C3D-CAD-CBD
5	C	503	SMA	C9-C10-C11-C22
4	C	501	HEM	C3D-CAD-CBD-CGD
4	P	501	HEM	C3D-CAD-CBD-CGD
5	C	503	SMA	C6-C5-O5-C5M
5	P	503	SMA	C6-C5-O5-C5M
5	P	503	SMA	C4A-C5-O5-C5M
5	C	503	SMA	C4A-C5-O5-C5M
5	C	503	SMA	C15-C14-O14-C25
9	Q	502	PG6	O3-C6-C7-O4
5	P	503	SMA	C15-C16-C17-C18
5	P	503	SMA	C24-C13-C14-O14
5	P	503	SMA	C12-C13-C14-O14
5	C	503	SMA	C8-C7-O7-C7M
5	C	503	SMA	C11-C10-C9-C2

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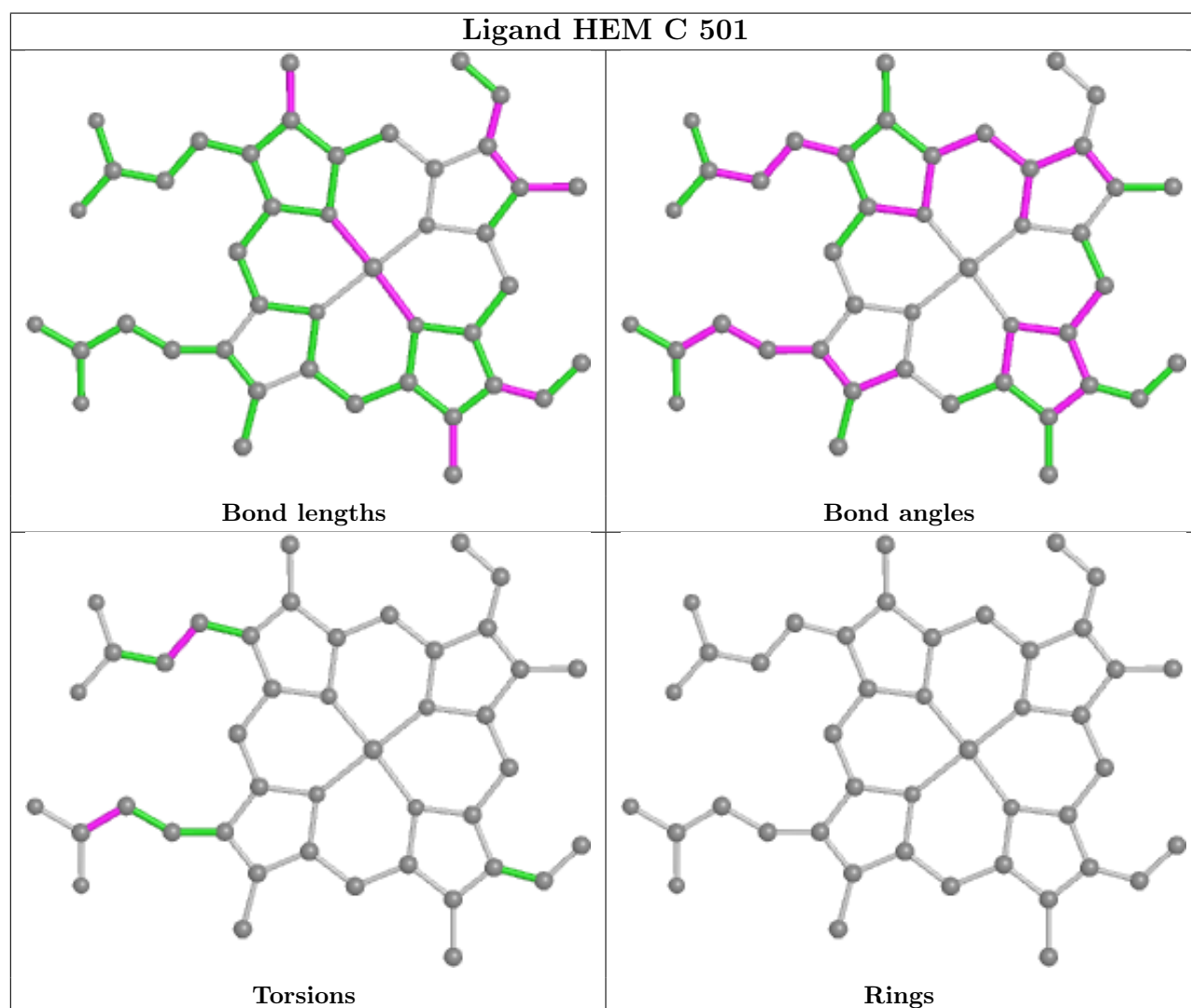
Mol	Chain	Res	Type	Atoms
5	P	503	SMA	C15-C14-O14-C25
5	C	503	SMA	C6-C7-O7-C7M
5	C	503	SMA	C24-C13-C14-C15
5	P	503	SMA	C24-C13-C14-C15
5	P	503	SMA	C12-C13-C14-C15
5	P	503	SMA	C13-C14-O14-C25
7	Q	501	HEC	C3D-CAD-CBD-CGD
7	D	501	HEC	CAD-CBD-CGD-O2D
7	Q	501	HEC	CAD-CBD-CGD-O2D
5	C	503	SMA	C12-C13-C14-C15
4	C	501	HEM	CAA-CBA-CGA-O1A
4	P	501	HEM	CAA-CBA-CGA-O1A
5	P	503	SMA	O14-C14-C15-C16
9	Q	502	PG6	O4-C8-C9-O5
7	Q	501	HEC	CAD-CBD-CGD-O1D
7	D	501	HEC	CAD-CBD-CGD-O1D
4	P	502	HEM	C3D-CAD-CBD-CGD
4	C	502	HEM	CAA-CBA-CGA-O2A
4	P	502	HEM	CAA-CBA-CGA-O2A
4	P	502	HEM	CAA-CBA-CGA-O1A
4	C	501	HEM	CAA-CBA-CGA-O2A
4	C	502	HEM	CAA-CBA-CGA-O1A
4	P	501	HEM	CAA-CBA-CGA-O2A
5	C	503	SMA	C24-C13-C14-O14
5	C	503	SMA	C12-C13-C14-O14
9	Q	502	PG6	O2-C4-C5-O3
5	P	503	SMA	C9-C10-C11-C22
9	Q	502	PG6	O5-C10-C11-O6
9	Q	502	PG6	O1-C2-C3-O2
4	P	502	HEM	CAD-CBD-CGD-O2D

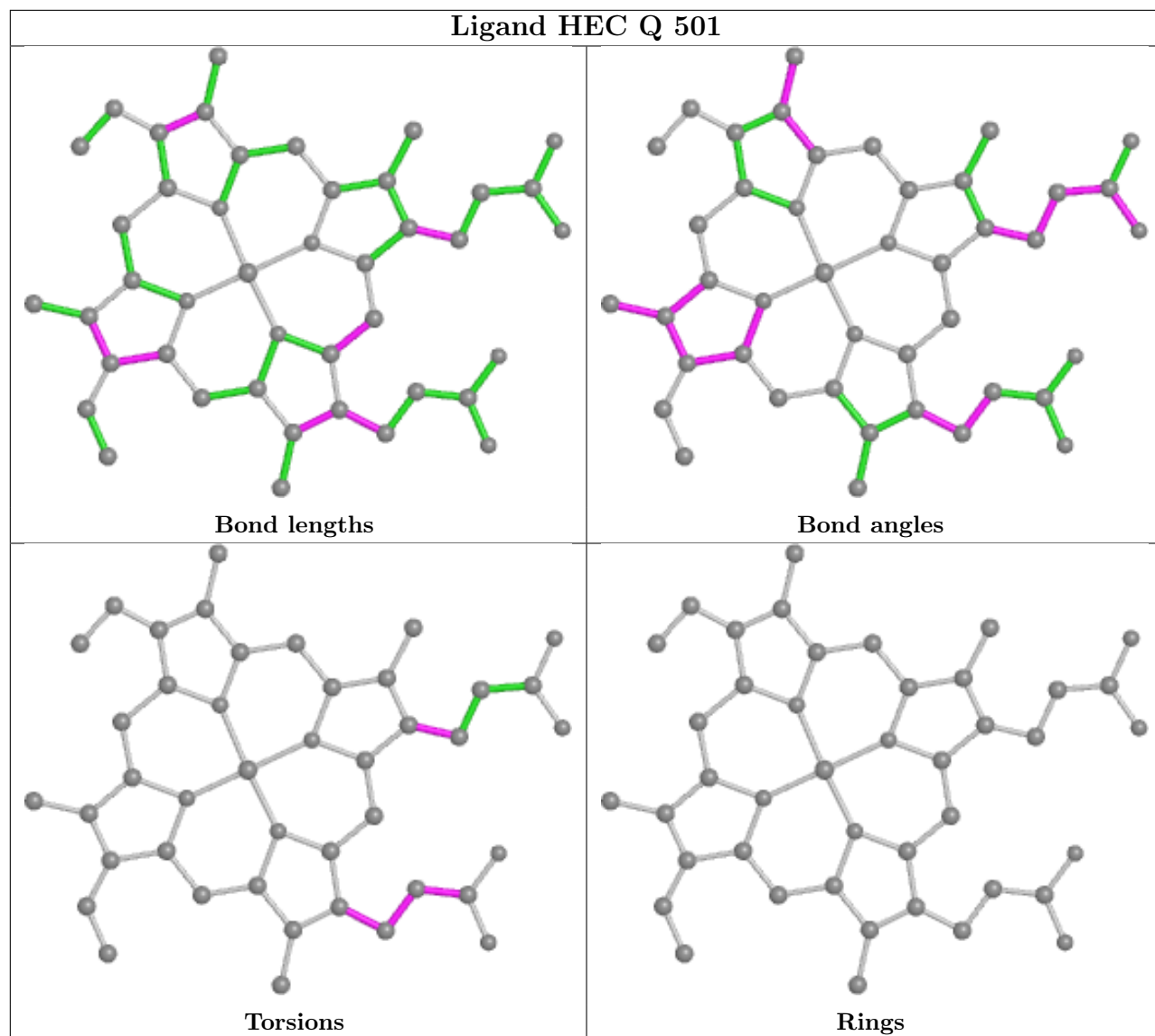
There are no ring outliers.

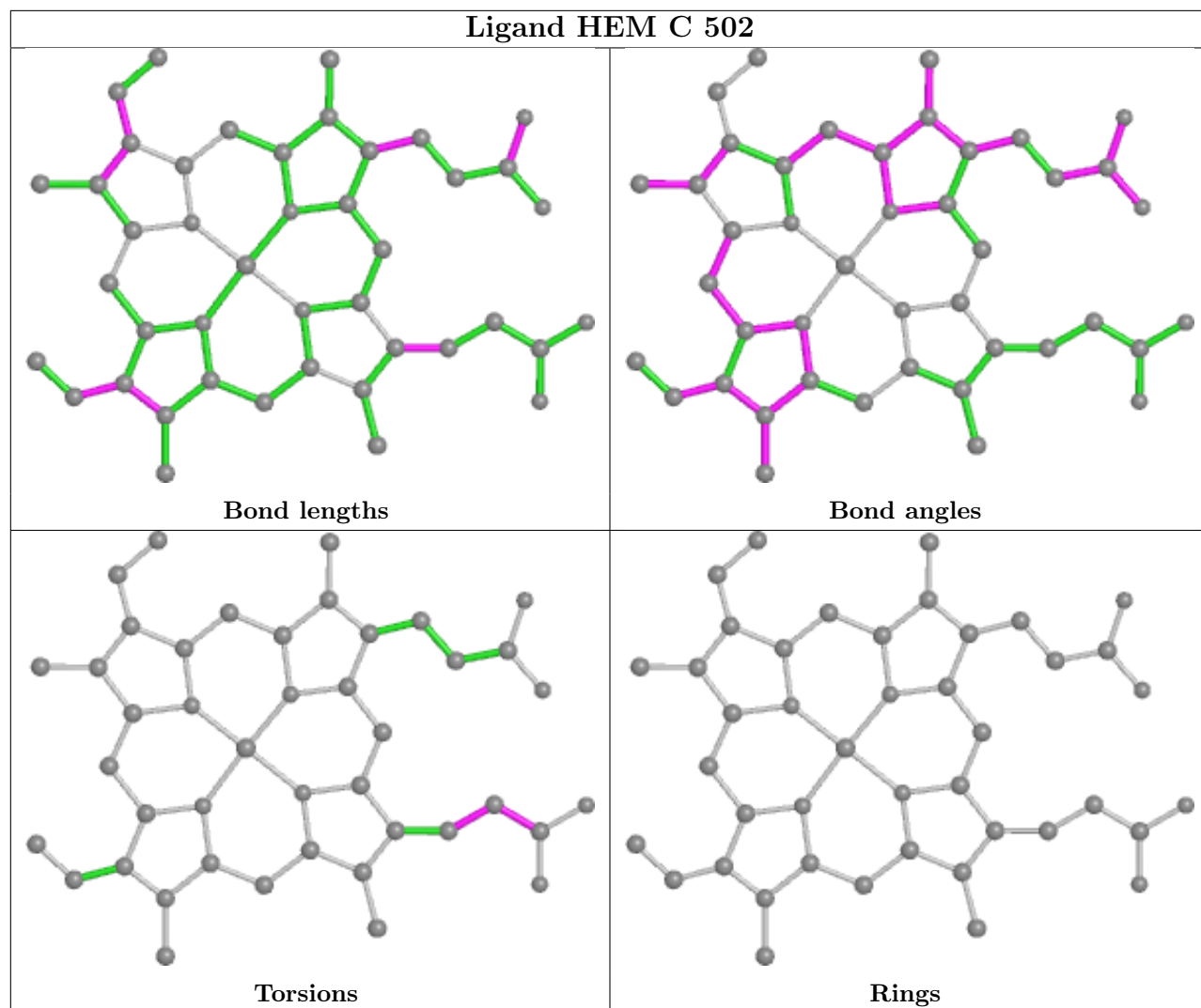
7 monomers are involved in 24 short contacts:

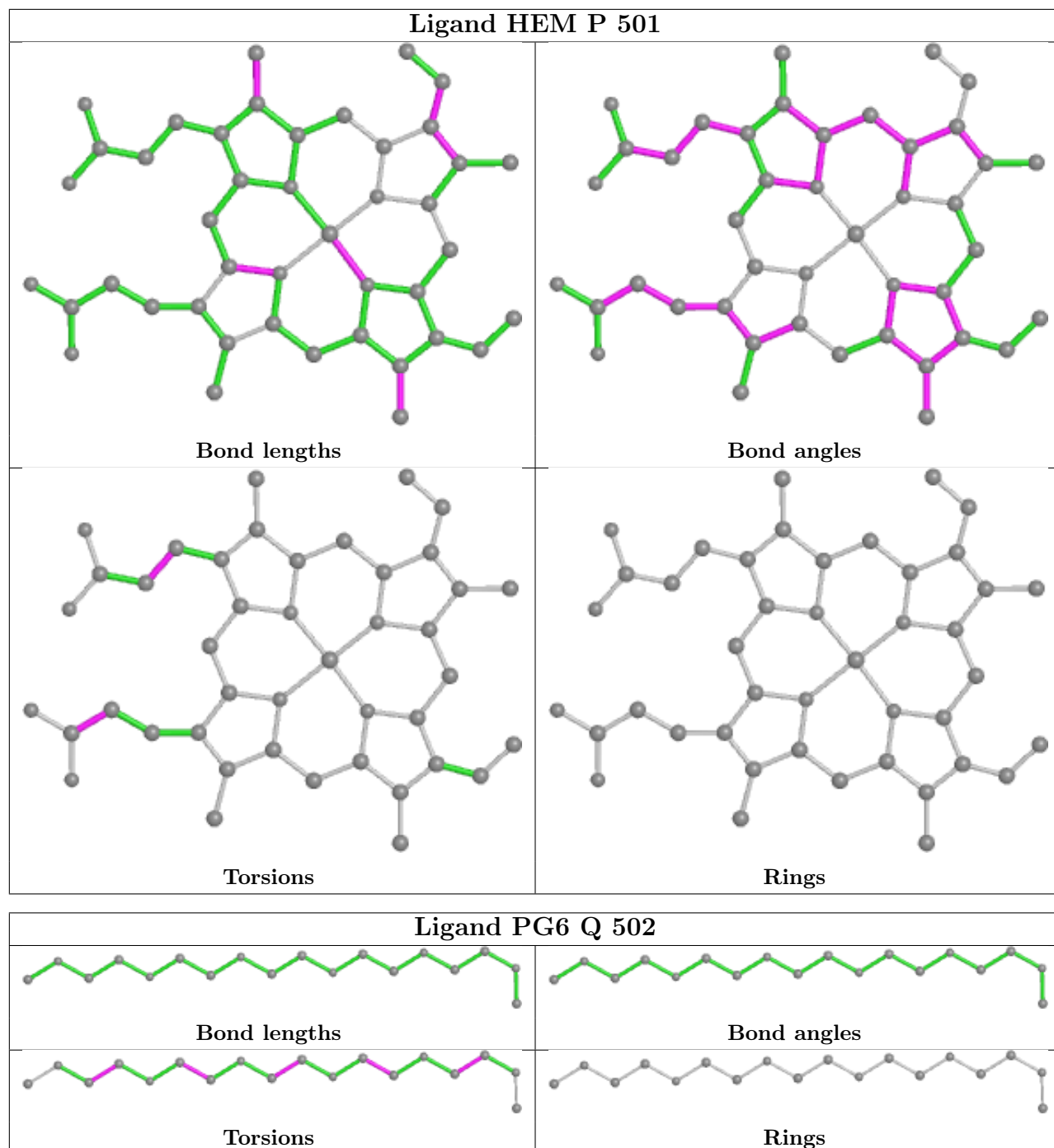
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	HEM	2	0
7	Q	501	HEC	7	0
4	P	501	HEM	3	0
7	D	501	HEC	5	0
8	R	501	FES	1	0
5	P	503	SMA	3	0
5	C	503	SMA	3	0

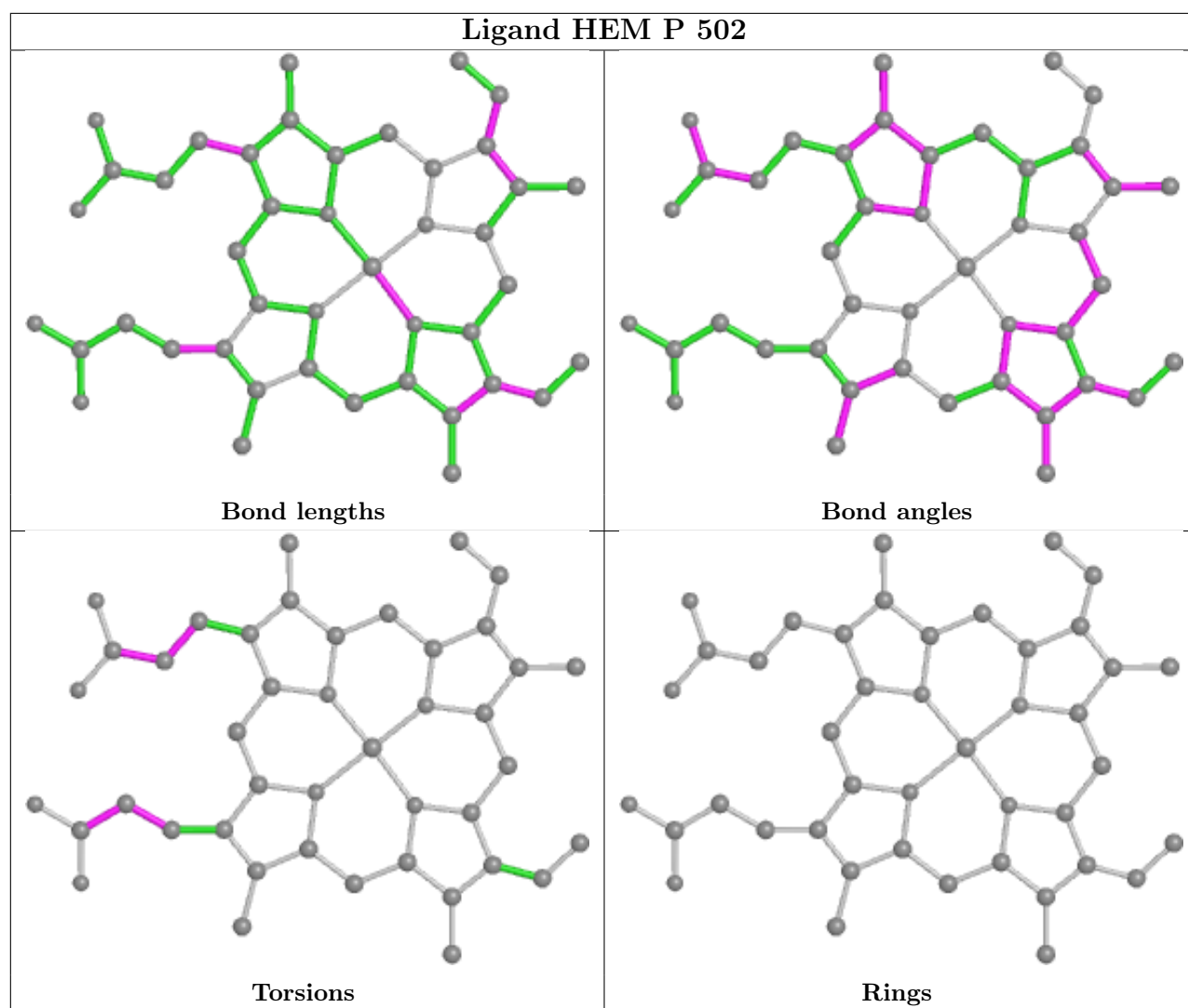
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



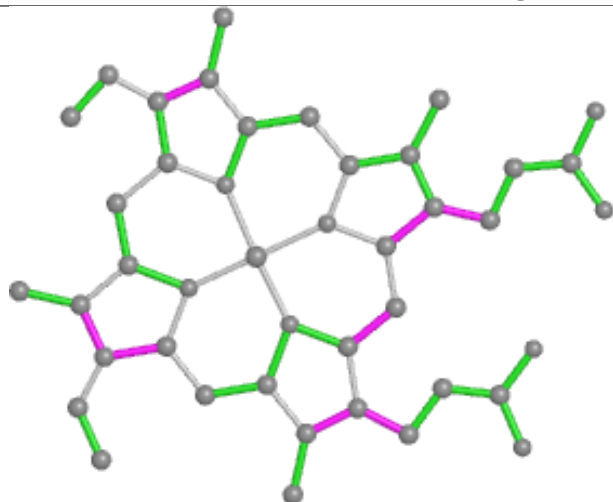




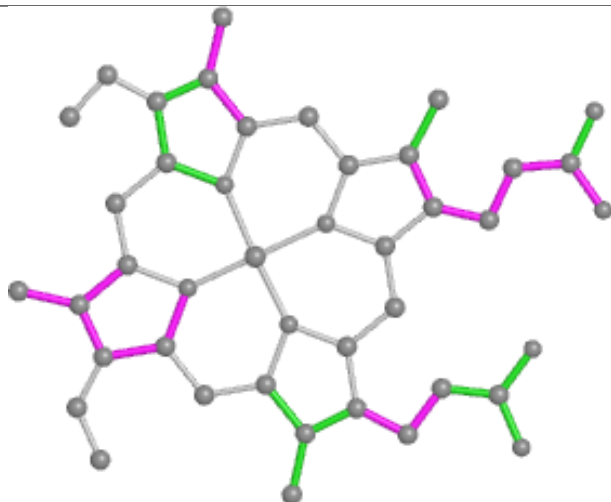




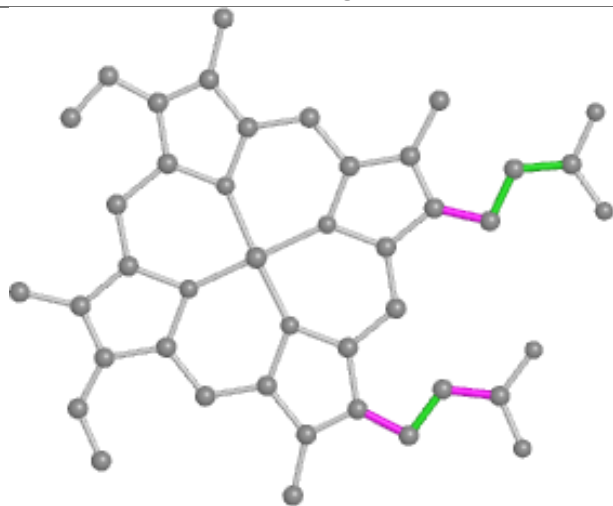
Ligand HEC D 501



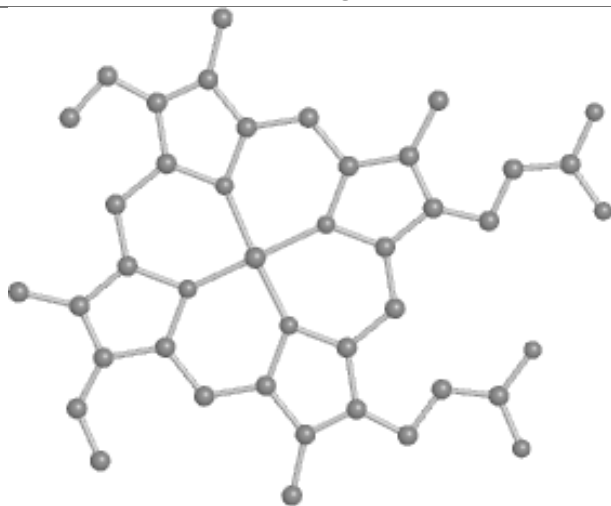
Bond lengths



Bond angles

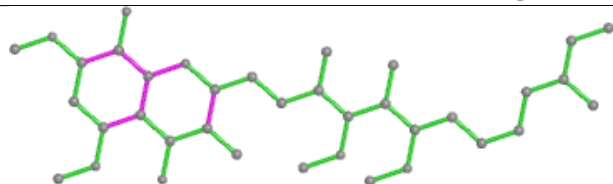


Torsions

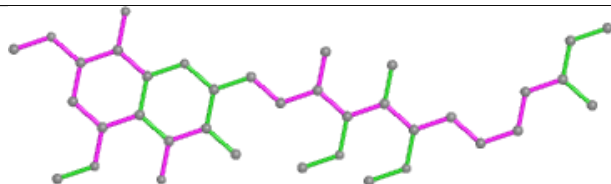


Rings

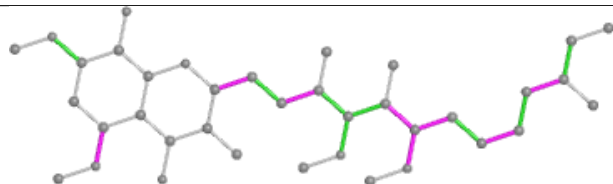
Ligand SMA P 503



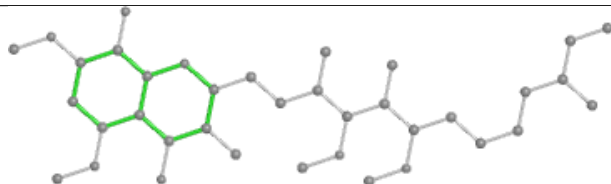
Bond lengths



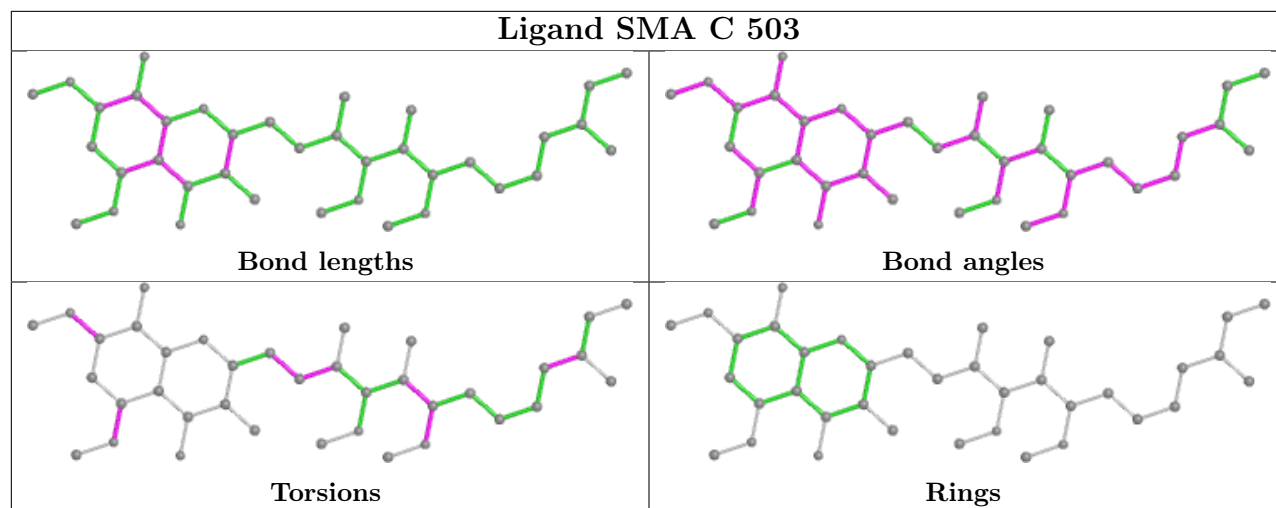
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	C	431/437 (98%)	0.05	14 (3%)	47	36	69, 101, 141, 197	0
1	P	431/437 (98%)	0.17	20 (4%)	32	24	66, 101, 141, 170	0
2	D	248/258 (96%)	1.52	85 (34%)	0	0	97, 140, 179, 228	0
2	Q	248/258 (96%)	1.12	61 (24%)	0	0	95, 139, 181, 230	0
3	E	183/191 (95%)	0.32	22 (12%)	4	4	84, 126, 167, 185	0
3	R	183/191 (95%)	0.62	34 (18%)	1	1	88, 129, 170, 190	0
All	All	1724/1772 (97%)	0.53	236 (13%)	3	3	66, 118, 167, 230	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	121	LEU	11.3
2	D	212	PHE	9.5
2	D	110	PHE	9.3
2	Q	124	GLY	8.7
2	D	226	GLN	8.6
2	Q	119	ASN	8.1
2	D	111	SER	8.0
2	D	109	GLY	8.0
2	D	124	GLY	7.9
2	D	9	PHE	7.9
2	D	207	GLN	7.2
3	R	181	ALA	7.1
2	Q	125	MET	7.1
2	Q	120	GLN	6.6
2	Q	247	LYS	6.5
2	D	213	LEU	6.5
2	Q	111	SER	6.4
2	D	210	SER	6.4
2	D	247	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	7	HIS	6.1
3	R	189	LYS	6.0
2	D	209	VAL	5.8
2	D	54	PRO	5.8
2	Q	205	MET	5.8
3	R	180	ALA	5.8
3	R	124	GLY	5.7
2	D	211	ALA	5.7
2	Q	123	LYS	5.6
3	R	191	GLY	5.4
3	R	49	SER	5.3
2	D	206	ALA	5.3
1	C	2	SER	5.3
1	P	363	PHE	5.3
2	D	125	MET	5.3
2	D	28	GLN	5.2
2	D	135	VAL	5.1
2	Q	187	LEU	5.0
2	D	48	LEU	4.9
2	D	12	GLU	4.9
2	D	49	ALA	4.8
1	P	362	LYS	4.8
2	D	108	ALA	4.8
2	D	32	GLU	4.7
2	Q	193	THR	4.7
2	D	131	ILE	4.7
2	D	27	PHE	4.7
2	Q	67	GLY	4.7
2	D	23	LEU	4.6
3	E	149	GLY	4.6
2	D	134	TYR	4.5
2	D	208	ASP	4.5
2	D	84	GLU	4.5
3	R	62	GLN	4.4
3	R	76	ARG	4.4
2	Q	248	ARG	4.3
2	Q	246	ASN	4.3
3	R	125	GLU	4.3
2	D	126	GLY	4.2
1	P	361	PRO	4.1
2	D	205	MET	4.1
3	R	15	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	R	16	TYR	4.1
2	Q	188	VAL	4.1
2	D	214	MET	4.1
2	Q	194	TYR	4.1
2	Q	32	GLU	4.0
1	P	2	SER	4.0
2	Q	245	THR	4.0
2	Q	198	THR	3.9
2	D	128	PRO	3.9
2	D	132	TYR	3.9
2	Q	191	GLN	3.9
3	E	58	GLU	3.9
2	Q	204	GLN	3.8
3	R	126	TRP	3.8
2	D	123	LYS	3.8
3	R	61	THR	3.8
1	P	359	TYR	3.8
1	P	415	GLU	3.8
2	D	56	LEU	3.8
2	Q	129	GLU	3.8
2	Q	133	ASN	3.7
3	R	60	GLY	3.7
1	C	42	ASN	3.7
2	D	8	ALA	3.7
2	D	129	GLU	3.7
3	R	190	LEU	3.7
2	D	246	ASN	3.7
2	D	53	GLY	3.7
2	D	250	TRP	3.6
1	P	264	PHE	3.6
2	D	30	TYR	3.5
2	D	26	GLY	3.5
2	D	10	SER	3.5
2	D	192	VAL	3.5
2	D	11	PHE	3.5
2	D	29	VAL	3.5
2	D	136	ILE	3.5
2	D	249	LEU	3.4
2	D	18	TYR	3.4
2	Q	234	MET	3.4
2	Q	211	ALA	3.4
2	Q	82	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	Q	212	PHE	3.4
2	Q	110	PHE	3.3
2	Q	122	PHE	3.3
1	C	252	ASP	3.3
3	E	126	TRP	3.3
2	Q	135	VAL	3.3
2	Q	213	LEU	3.3
2	Q	235	LEU	3.3
2	D	248	ARG	3.3
3	E	181	ALA	3.3
2	D	225	LYS	3.3
2	D	222	VAL	3.3
3	R	77	ARG	3.2
2	D	130	TYR	3.2
3	E	180	ALA	3.2
3	R	188	ILE	3.2
2	Q	29	VAL	3.2
3	E	62	GLN	3.2
3	R	50	ILE	3.2
1	P	117	TYR	3.1
3	R	75	ARG	3.1
2	Q	250	TRP	3.1
2	Q	136	ILE	3.0
2	Q	28	GLN	3.0
1	P	364	ARG	3.0
3	R	114	THR	3.0
2	Q	112	GLY	3.0
2	D	215	TRP	3.0
2	D	45	ILE	3.0
3	E	119	ASP	2.9
1	C	343	MET	2.9
3	R	12	ARG	2.9
2	D	15	PHE	2.9
2	D	203	ASP	2.9
3	R	123	THR	2.9
3	E	125	GLU	2.9
2	D	33	VAL	2.9
3	R	127	LEU	2.9
1	P	414	THR	2.8
2	Q	192	VAL	2.8
2	D	63	GLU	2.8
3	E	11	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
3	R	128	VAL	2.8
2	D	133	ASN	2.8
1	P	268	ALA	2.8
2	Q	199	PRO	2.8
2	Q	207	GLN	2.8
1	C	41	LEU	2.7
1	C	268	ALA	2.7
3	R	30	ALA	2.7
1	C	13	THR	2.7
1	C	359	TYR	2.7
3	R	122	ASN	2.7
3	R	51	PHE	2.7
2	Q	84	GLU	2.6
3	E	59	VAL	2.6
2	D	107	ARG	2.6
2	Q	115	GLY	2.6
1	P	302	TYR	2.6
2	Q	83	LYS	2.6
3	E	162	SER	2.6
1	P	269	TYR	2.6
2	D	52	GLY	2.6
1	P	270	MET	2.5
2	Q	14	ILE	2.5
2	Q	244	LEU	2.5
2	Q	189	ASP	2.5
2	D	17	LYS	2.5
1	P	5	PRO	2.5
3	E	76	ARG	2.5
1	C	74	ASP	2.5
2	D	121	LEU	2.5
3	R	48	ALA	2.5
1	P	360	ARG	2.5
2	Q	249	LEU	2.5
1	P	267	VAL	2.5
2	D	254	LYS	2.5
2	D	244	LEU	2.5
2	Q	9	PHE	2.4
2	D	187	LEU	2.4
2	Q	130	TYR	2.4
3	E	116	PRO	2.4
2	D	31	ASN	2.4
2	Q	131	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	74	ILE	2.3
3	R	31	VAL	2.3
2	D	229	LEU	2.3
1	P	357	GLY	2.3
2	Q	132	TYR	2.3
2	Q	202	VAL	2.3
2	D	190	ASP	2.3
2	D	204	GLN	2.3
2	Q	239	SER	2.3
2	D	47	THR	2.3
3	R	29	ALA	2.3
1	C	335	ALA	2.3
3	E	127	LEU	2.3
2	D	61	VAL	2.3
2	D	193	THR	2.3
2	D	252	PRO	2.2
3	E	183	VAL	2.2
2	D	216	ALA	2.2
2	D	194	TYR	2.2
1	C	342	VAL	2.2
3	R	74	ILE	2.2
3	E	115	LEU	2.2
1	C	422	ALA	2.2
3	E	182	PHE	2.2
3	E	191	GLY	2.2
2	Q	25	ARG	2.2
2	Q	105	LYS	2.2
2	Q	237	LEU	2.2
3	R	19	THR	2.2
2	D	114	ALA	2.2
3	E	75	ARG	2.2
3	R	169	GLY	2.2
2	Q	33	VAL	2.2
3	R	115	LEU	2.1
2	D	64	TYR	2.1
3	E	185	GLU	2.1
1	C	428	PHE	2.1
2	D	199	PRO	2.1
3	E	187	THR	2.1
2	D	160	ILE	2.1
1	P	356	SER	2.1
2	Q	196	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	Q	227	MET	2.1
2	D	159	GLN	2.1
1	P	366	TRP	2.0
2	D	191	GLN	2.0
2	Q	190	ASP	2.0
1	C	79	SER	2.0
2	Q	116	SER	2.0

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

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

6.3 Carbohydrates [i](#)

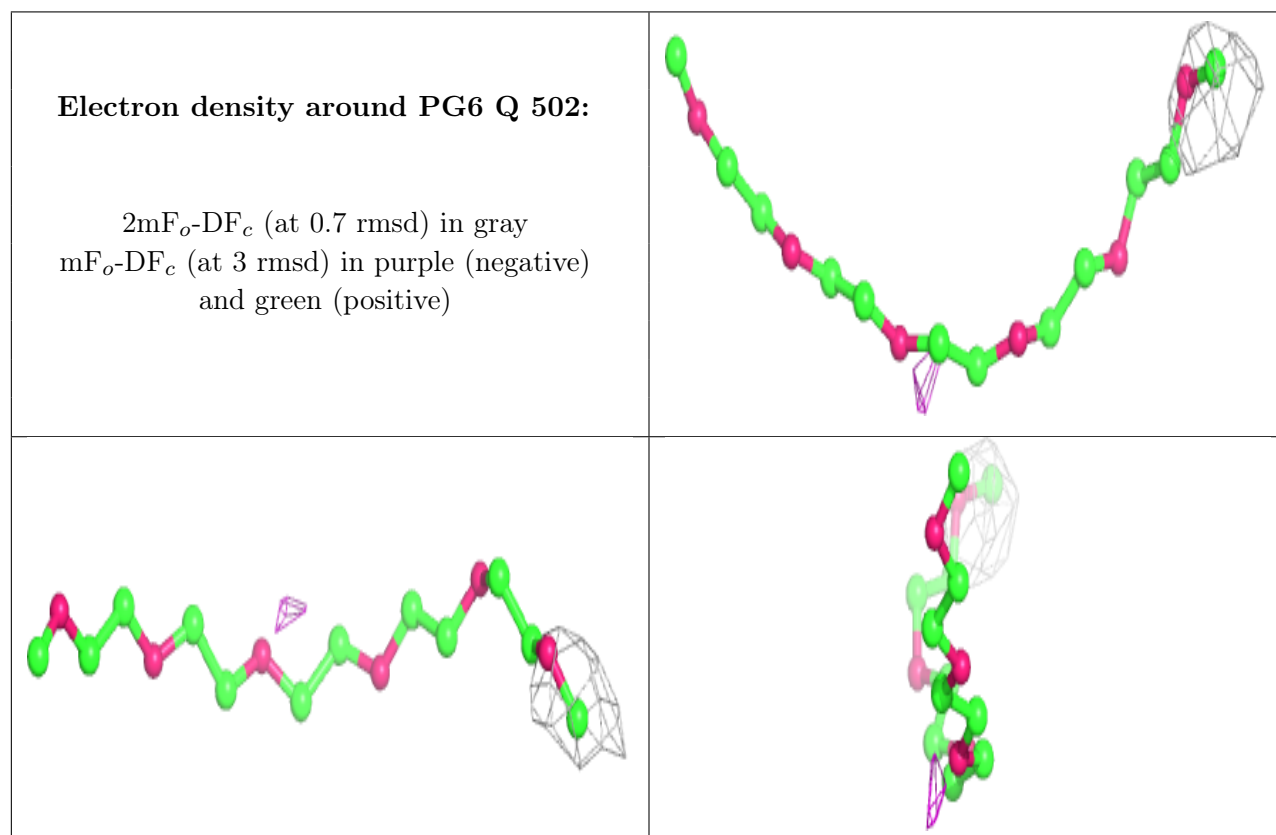
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

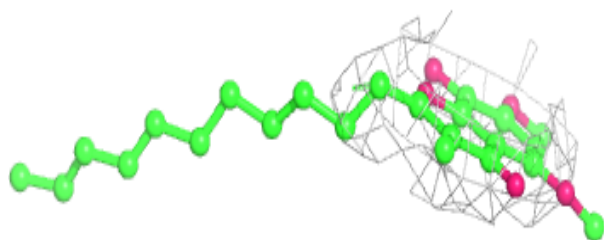
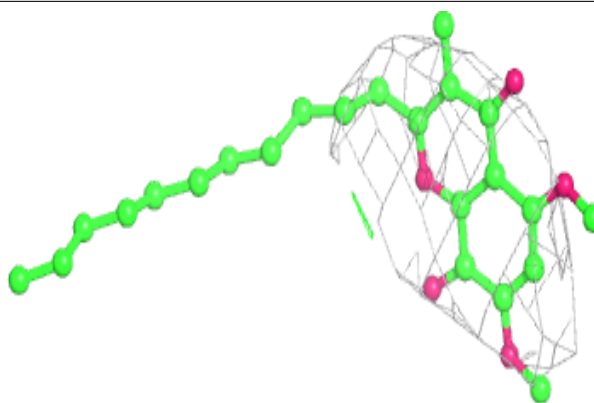
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PG6	Q	502	18/18	0.42	1.53	71,114,137,139	0
6	UNL	P	504	28/-	0.75	0.56	72,136,156,165	0
6	UNL	C	505	8/-	0.81	0.21	99,113,116,122	0
6	UNL	P	505	8/-	0.83	0.25	82,94,101,110	0
6	UNL	C	504	17/-	0.85	0.28	97,127,136,148	17
7	HEC	D	501	43/43	0.90	0.47	100,114,130,135	0
5	SMA	C	503	37/37	0.90	0.54	78,98,110,112	0
5	SMA	P	503	37/37	0.91	0.43	85,102,111,117	0
7	HEC	Q	501	43/43	0.94	0.26	100,113,129,136	0
4	HEM	C	502	43/43	0.96	0.35	80,107,117,126	0
4	HEM	C	501	43/43	0.97	0.30	80,92,112,124	0
4	HEM	P	501	43/43	0.97	0.37	73,91,105,129	0
8	FES	E	501	4/4	0.97	0.22	88,99,112,114	0
4	HEM	P	502	43/43	0.97	0.31	79,106,117,128	0
8	FES	R	501	4/4	0.99	0.20	102,103,110,120	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.



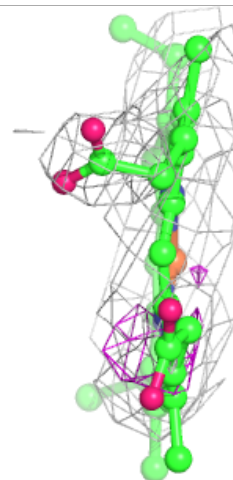
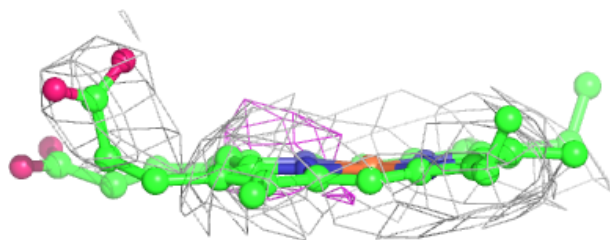
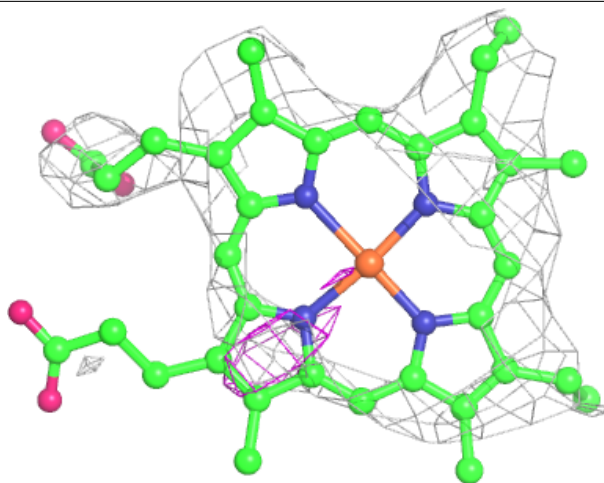
Electron density around UNL P 504:

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



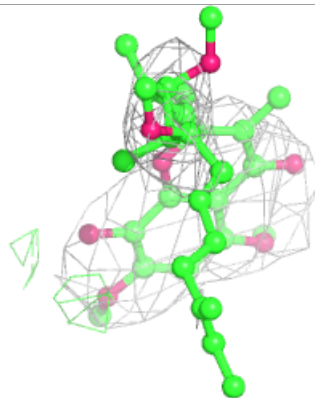
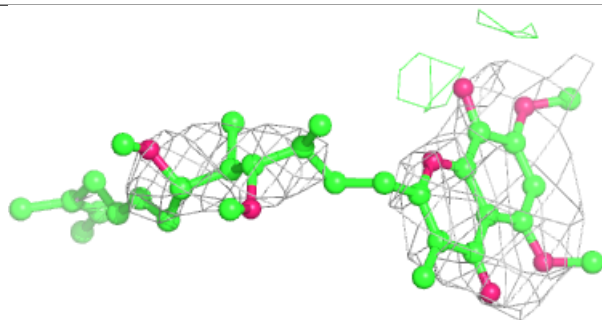
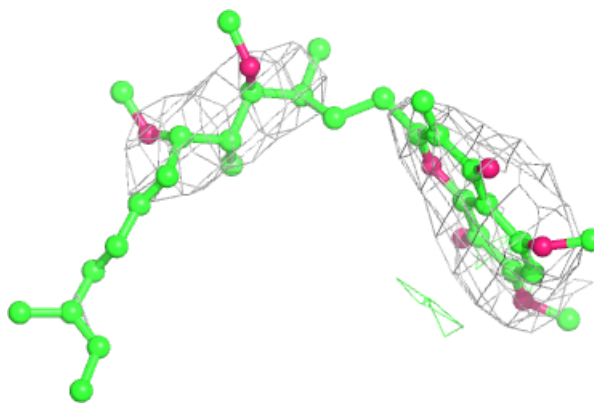
Electron density around HEC D 501:

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

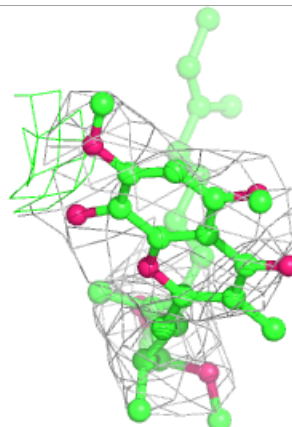
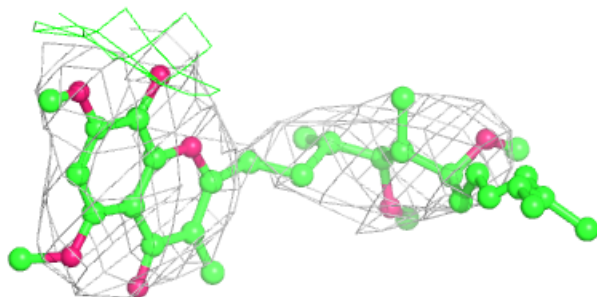
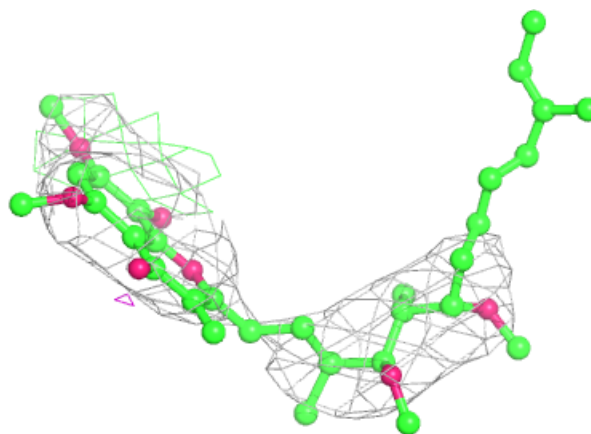


Electron density around SMA C 503:

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

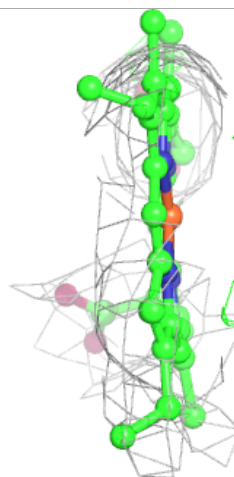
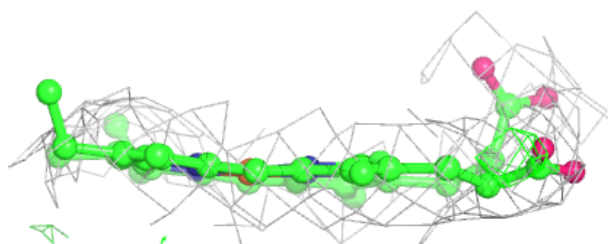
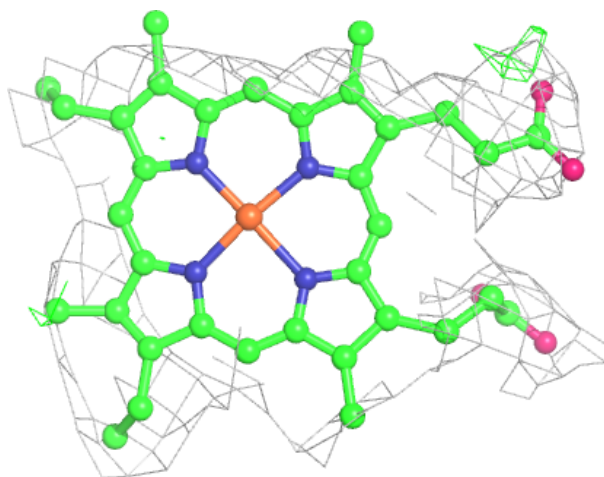
**Electron density around SMA P 503:**

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



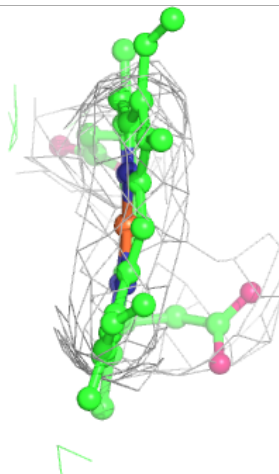
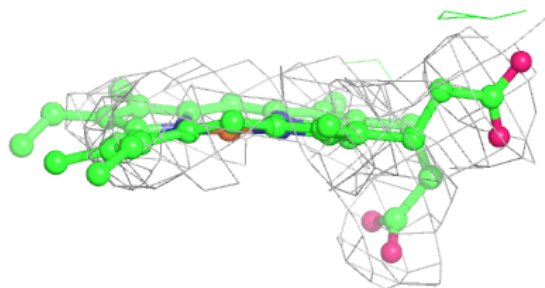
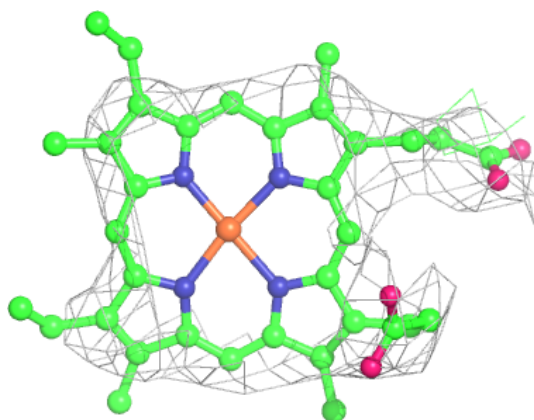
Electron density around HEC Q 501:

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



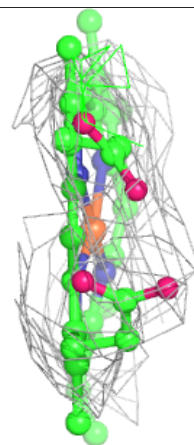
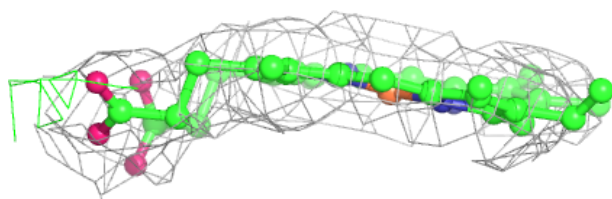
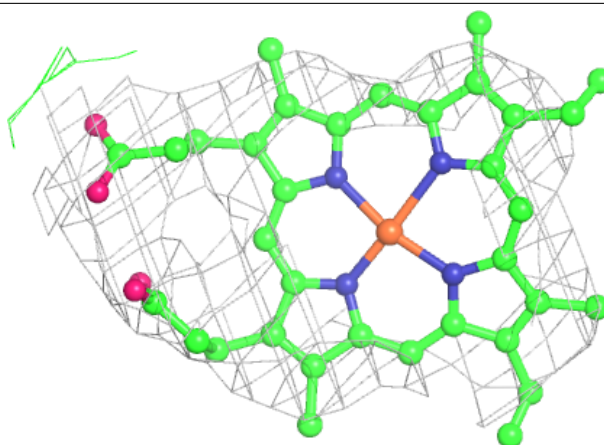
Electron density around HEM C 502:

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



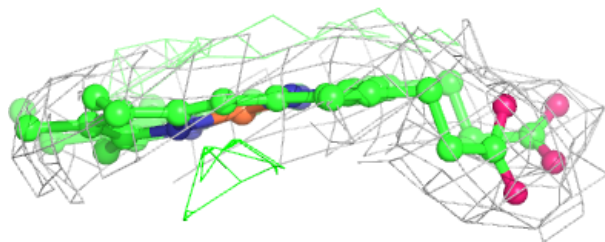
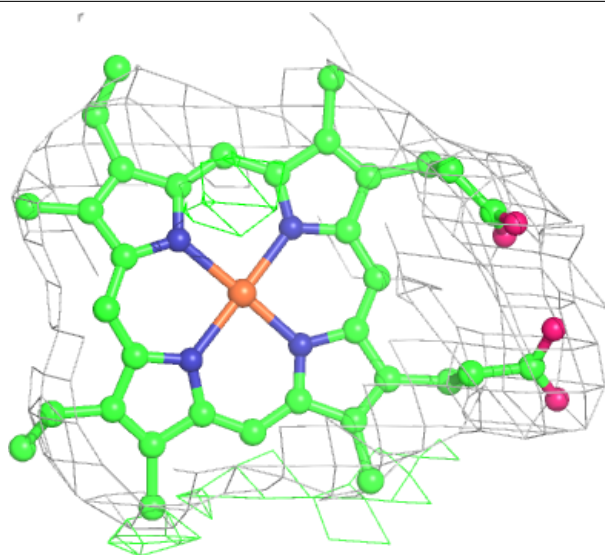
Electron density around HEM C 501:

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



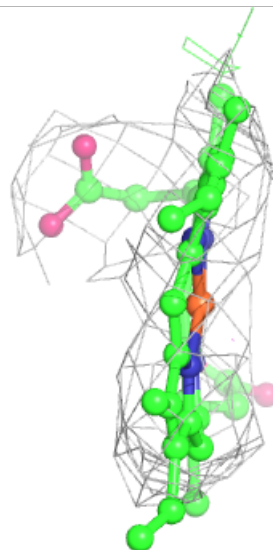
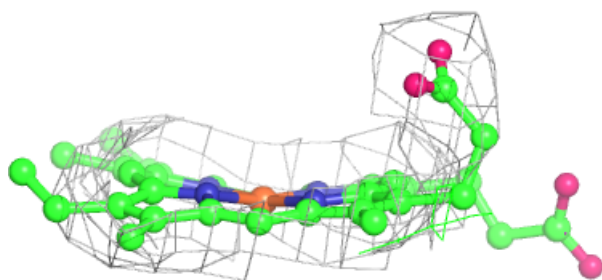
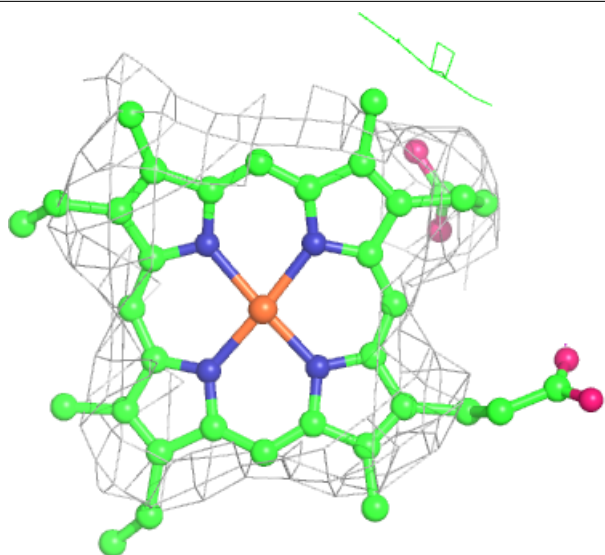
Electron density around HEM P 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.