



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:23 AM UTC

PDB ID : 2RFB / pdb_00002rfb
Title : Crystal Structure of a Cytochrome P450 from the Thermoacidophilic Archaeon
Picophilus Torridus
Authors : Ho, W.W.; Li, H.; Poulos, T.L.; Nishida, C.R.; Ortiz de Montellano, P.R.
Deposited on : 2007-09-28
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

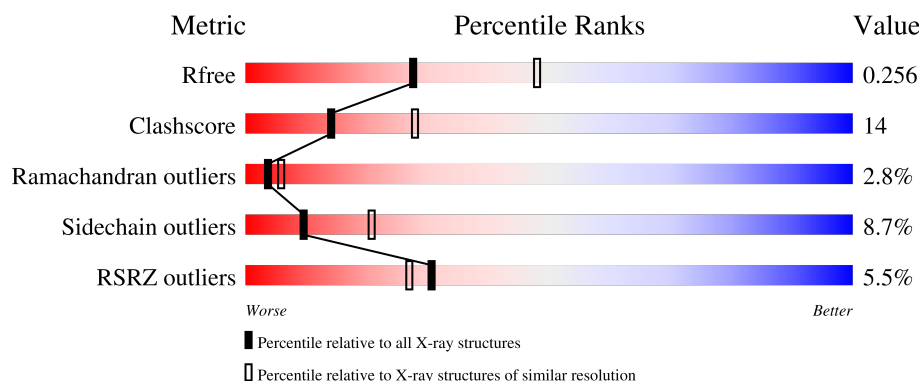
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	343	3% 68% 26% • •
1	B	343	8% 68% 24% 5% • •
1	C	343	5% 62% 30% 5% •

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
2	SO4	C	910	-	-	X	-

2 Entry composition [i](#)

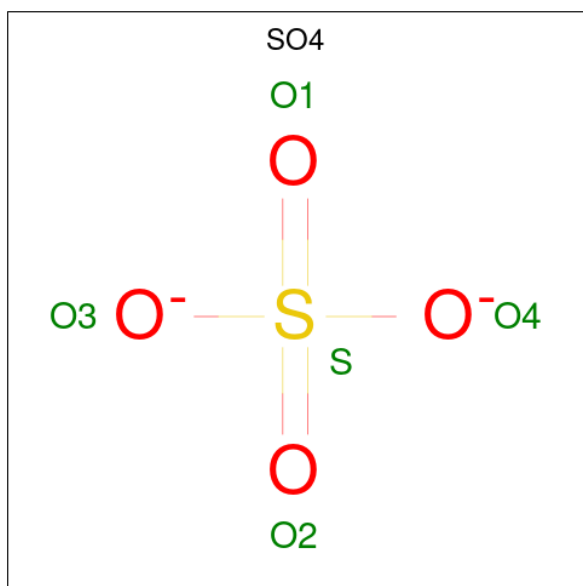
There are 4 unique types of molecules in this entry. The entry contains 8465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2752	1763	467	511	11			
1	B	335	Total	C	N	O	S	0	0	0
			2721	1744	460	505	12			
1	C	333	Total	C	N	O	S	0	0	0
			2708	1736	458	503	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



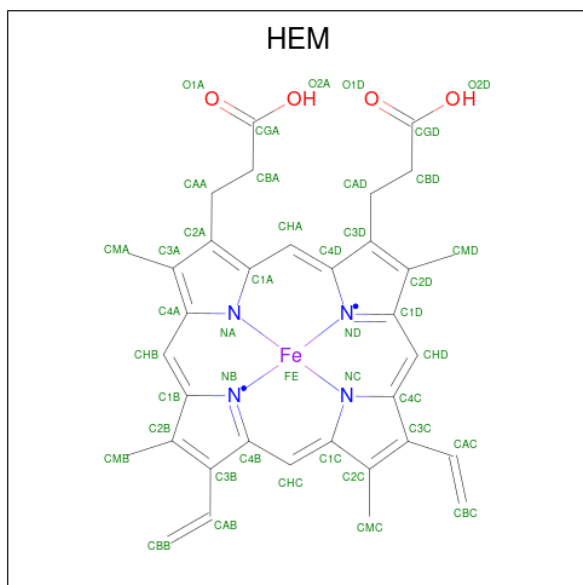
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

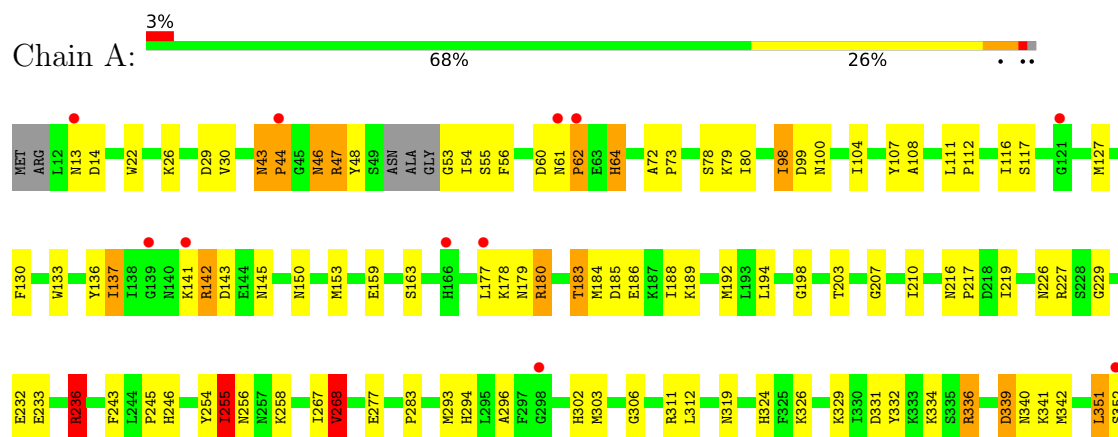
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	33	Total O 33 33	0	0
4	C	26	Total O 26 26	0	0

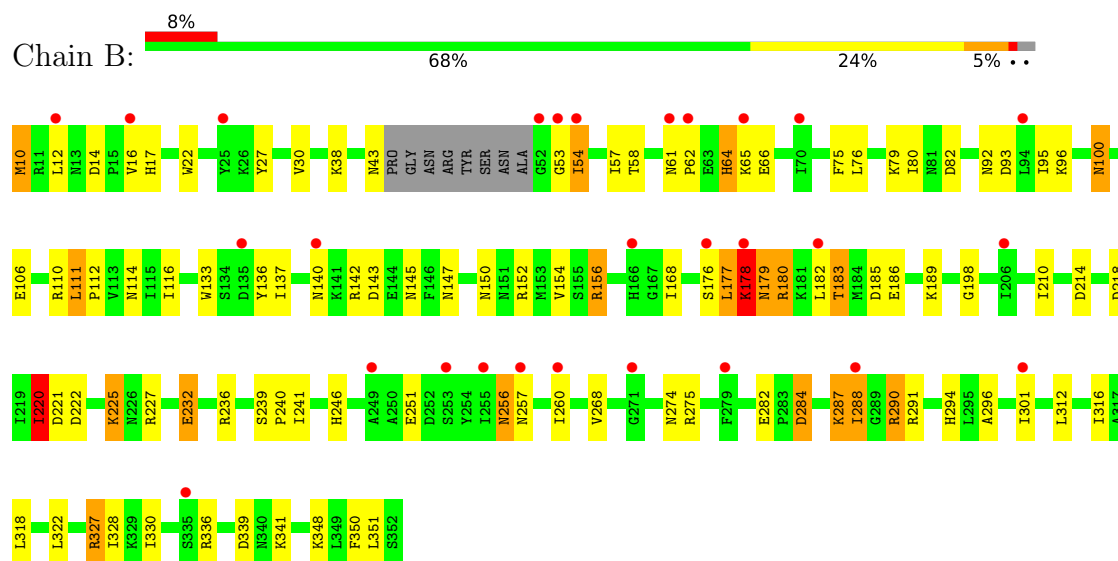
3 Residue-property plots [i](#)

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: Cytochrome P450

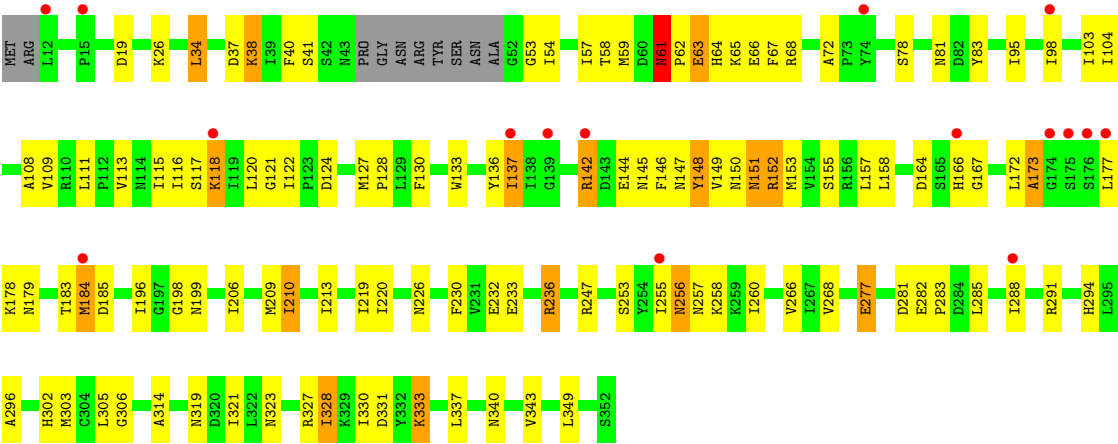


• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.79Å 168.46Å 88.23Å 90.00° 96.25° 90.00°	Depositor
Resolution (Å)	48.51 – 2.50 48.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.51-2.50) 98.4 (48.51-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.268 0.205 , 0.256	Depositor DCC
R_{free} test set	2414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8465	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: HEM, SO4

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	1.01	2/2809 (0.1%)	1.11	11/3785 (0.3%)
1	B	0.98	11/2776 (0.4%)	1.03	6/3739 (0.2%)
1	C	0.67	0/2763	1.00	4/3722 (0.1%)
All	All	0.90	13/8348 (0.2%)	1.05	21/11246 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	LYS	CD-CE	16.19	2.01	1.52
1	B	221	ASP	CG-OD1	15.80	1.55	1.25
1	B	221	ASP	CG-OD2	10.69	1.45	1.25
1	B	287	LYS	CE-NZ	9.26	1.77	1.49
1	B	222	ASP	CG-OD1	9.15	1.42	1.25
1	B	225	LYS	CD-CE	9.04	1.79	1.52
1	B	290	ARG	NE-CZ	8.29	1.42	1.33
1	B	218	ASP	CG-OD2	6.63	1.38	1.25
1	B	220	ILE	CB-CG1	6.20	1.65	1.53
1	B	218	ASP	CG-OD1	6.07	1.36	1.25
1	A	255	ILE	CA-CB	-5.93	1.46	1.54
1	A	61	ASN	CA-C	-5.31	1.47	1.52
1	B	287	LYS	CG-CD	5.09	1.67	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	ASN	CA-C-N	-10.04	107.28	119.84
1	C	61	ASN	C-N-CA	-10.04	107.28	119.84
1	B	287	LYS	CG-CD-CE	-7.78	93.40	111.30
1	B	282	GLU	CA-C-N	7.19	126.81	119.19
1	B	282	GLU	C-N-CA	7.19	126.81	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ASN	O-C-N	6.59	126.64	120.51
1	A	217	PRO	CA-C-N	-6.19	112.75	122.65
1	A	217	PRO	C-N-CA	-6.19	112.75	122.65
1	A	210	ILE	N-CA-C	-5.98	104.68	110.72
1	C	61	ASN	N-CA-C	5.96	122.97	109.81
1	A	268	VAL	N-CA-CB	-5.60	103.68	111.41
1	A	203	THR	N-CA-C	-5.52	105.34	111.36
1	A	236	ARG	CG-CD-NE	-5.50	99.91	112.00
1	A	22	TRP	N-CA-C	-5.43	100.84	109.96
1	A	98	ILE	N-CA-C	-5.37	107.14	113.42
1	B	27	TYR	N-CA-C	5.21	117.36	111.11
1	B	76	LEU	CA-C-N	5.18	124.62	119.24
1	B	76	LEU	C-N-CA	5.18	124.62	119.24
1	A	43	ASN	CA-C-N	5.09	126.21	119.84
1	A	43	ASN	C-N-CA	5.09	126.21	119.84
1	C	226	ASN	N-CA-C	5.01	116.06	107.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	2756	83	0
1	B	2721	0	2727	72	0
1	C	2708	0	2716	79	0
2	A	15	0	0	1	0
2	C	5	0	0	4	0
3	A	43	0	30	5	0
3	B	43	0	30	3	0
3	C	43	0	30	6	0
4	A	76	0	0	7	0
4	B	33	0	0	3	0
4	C	26	0	0	1	0
All	All	8465	0	8289	237	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 14.

All (237) 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:B:225:LYS:CE	1:B:225:LYS:CD	1.79	1.55
1:B:287:LYS:NZ	1:B:287:LYS:CE	1.77	1.47
1:B:287:LYS:CE	1:B:287:LYS:CD	2.01	1.37
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.21	1.04
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.23	1.01
1:A:133:TRP:HE1	1:A:150:ASN:HD22	1.18	0.90
1:A:294:HIS:HD2	1:A:296:ALA:H	1.19	0.88
1:C:61:ASN:HD21	1:C:65:LYS:HG2	1.40	0.87
1:C:133:TRP:HE1	1:C:150:ASN:HD22	1.24	0.85
1:A:133:TRP:HE1	1:A:150:ASN:ND2	1.75	0.84
1:C:232:GLU:OE1	1:C:294:HIS:HE1	1.59	0.83
3:C:410:HEM:HBC2	3:C:410:HEM:HHD	1.62	0.82
1:B:143:ASP:HB3	1:B:145:ASN:H	1.45	0.81
1:B:288:ILE:HD12	1:B:288:ILE:H	1.46	0.80
1:C:166:HIS:CD2	1:C:167:GLY:H	1.98	0.79
1:C:166:HIS:HD2	1:C:167:GLY:H	1.32	0.77
1:B:177:LEU:O	1:B:179:ASN:N	2.17	0.76
1:C:61:ASN:ND2	1:C:65:LYS:HG2	2.01	0.75
1:A:26:LYS:HE3	1:A:29:ASP:OD2	1.88	0.74
1:A:142:ARG:HH11	1:A:142:ARG:CG	2.00	0.73
1:B:287:LYS:CE	1:B:287:LYS:CG	2.69	0.71
1:C:209:MET:HE1	1:C:314:ALA:HB1	1.72	0.70
1:A:142:ARG:HG3	1:A:142:ARG:NH1	2.01	0.70
1:A:183:THR:HG22	1:A:186:GLU:H	1.55	0.70
1:B:30:VAL:HG13	1:B:268:VAL:CG1	2.23	0.69
1:B:225:LYS:CE	1:B:225:LYS:CG	2.70	0.69
1:A:48:TYR:CE2	1:A:246:HIS:HE1	2.11	0.68
1:C:232:GLU:OE1	1:C:294:HIS:CE1	2.46	0.68
1:B:53:GLY:HA2	1:B:189:LYS:HD3	1.74	0.68
1:B:136:TYR:HE2	1:B:143:ASP:HB2	1.57	0.68
1:B:178:LYS:O	1:B:179:ASN:HB2	1.94	0.68
1:B:246:HIS:NE2	4:B:419:HOH:O	2.22	0.68
1:A:339:ASP:OD1	1:A:339:ASP:N	2.25	0.67
1:B:294:HIS:HD2	1:B:296:ALA:H	1.42	0.67
1:B:54:ILE:O	1:B:57:ILE:HG22	1.94	0.67
1:A:226:ASN:ND2	1:A:229:GLY:H	1.93	0.67
1:B:328:ILE:HG23	1:B:351:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:OD2	1:A:334:LYS:NZ	2.18	0.67
1:A:133:TRP:NE1	1:A:150:ASN:HD22	1.93	0.66
1:C:198:GLY:HA2	3:C:410:HEM:C2C	2.30	0.66
1:B:180:ARG:NH2	1:B:186:GLU:OE1	2.29	0.66
1:A:277:GLU:CG	1:A:283:PRO:HG3	2.26	0.66
1:C:210:ILE:HD11	1:C:321:ILE:HD13	1.78	0.66
1:C:236:ARG:NH2	1:C:283:PRO:O	2.27	0.66
1:A:294:HIS:HD2	1:A:296:ALA:N	1.91	0.65
1:C:83:TYR:HD2	1:C:118:LYS:HZ1	1.45	0.65
1:A:137:ILE:HD12	1:A:192:MET:HE3	1.78	0.64
1:B:92:ASN:O	1:B:95:ILE:HG22	1.97	0.64
1:A:277:GLU:HG2	1:A:283:PRO:HG3	1.79	0.64
1:B:176:SER:O	1:B:177:LEU:HB2	1.97	0.64
1:C:220:ILE:HD11	1:C:328:ILE:HD11	1.81	0.62
1:B:64:HIS:CD2	1:B:65:LYS:HG2	2.35	0.62
1:C:103:ILE:HD12	1:C:349:LEU:HD22	1.80	0.62
1:A:340:ASN:HD22	1:A:341:LYS:N	1.98	0.62
1:C:282:GLU:HB3	1:C:285:LEU:HG	1.82	0.62
1:B:133:TRP:HE1	1:B:150:ASN:HD22	1.48	0.61
1:A:48:TYR:HE2	1:A:246:HIS:HE1	1.48	0.61
1:B:30:VAL:HG13	1:B:268:VAL:HG13	1.82	0.61
1:C:117:SER:HA	1:C:120:LEU:HD12	1.82	0.60
1:C:294:HIS:HD2	1:C:296:ALA:H	1.50	0.60
1:B:183:THR:HG22	1:B:186:GLU:H	1.67	0.60
1:B:232:GLU:OE2	1:B:294:HIS:HE1	1.85	0.60
1:A:47:ARG:HH11	1:A:47:ARG:HA	1.67	0.59
1:C:104:ILE:HA	1:C:108:ALA:HB3	1.83	0.59
1:A:30:VAL:HG13	1:A:268:VAL:HG13	1.84	0.59
1:C:184:MET:SD	1:C:184:MET:N	2.64	0.59
1:C:233:GLU:OE2	1:C:236:ARG:NH1	2.35	0.58
1:A:55:SER:OG	1:A:56:PHE:N	2.36	0.58
1:A:232:GLU:OE2	1:A:294:HIS:HE1	1.87	0.58
1:C:340:ASN:HB3	1:C:343:VAL:HG22	1.86	0.58
1:C:281:ASP:CB	2:C:910:SO4:O1	2.52	0.58
1:A:64:HIS:HE1	3:A:410:HEM:O2D	1.87	0.58
1:B:275:ARG:HH11	1:B:284:ASP:HB3	1.70	0.57
1:B:53:GLY:HA2	1:B:189:LYS:CD	2.35	0.57
1:A:53:GLY:HA2	4:A:980:HOH:O	2.04	0.57
1:A:78:SER:HA	4:A:955:HOH:O	2.03	0.57
1:A:142:ARG:CG	1:A:142:ARG:NH1	2.63	0.57
1:B:198:GLY:HA2	3:B:410:HEM:C2C	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:HB2	1:A:46:ASN:H	1.69	0.56
1:A:294:HIS:CD2	1:A:296:ALA:H	2.11	0.56
1:C:83:TYR:HD2	1:C:118:LYS:NZ	2.01	0.56
1:C:206:ILE:O	1:C:210:ILE:HD12	2.05	0.56
1:C:288:ILE:HD12	1:C:288:ILE:H	1.69	0.56
1:C:277:GLU:HG3	1:C:283:PRO:HG3	1.87	0.56
1:A:255:ILE:O	1:A:256:ASN:C	2.48	0.56
1:B:256:ASN:O	1:B:257:ASN:HB2	2.05	0.56
1:B:136:TYR:CE2	1:B:143:ASP:HB2	2.41	0.55
1:B:348:LYS:HD2	1:B:350:PHE:HE1	1.71	0.55
1:C:61:ASN:ND2	1:C:64:HIS:HD2	2.04	0.55
1:C:37:ASP:OD2	1:C:38:LYS:HD3	2.07	0.55
1:A:48:TYR:HE2	1:A:246:HIS:CE1	2.24	0.55
1:C:302:HIS:O	1:C:303:MET:C	2.50	0.55
1:A:185:ASP:O	1:A:189:LYS:HG2	2.06	0.54
1:C:111:LEU:O	1:C:115:ILE:HD12	2.08	0.54
1:C:281:ASP:HB3	2:C:910:SO4:O1	2.07	0.54
1:C:209:MET:CE	1:C:314:ALA:HB1	2.38	0.54
1:B:348:LYS:HD2	1:B:350:PHE:CE1	2.43	0.54
1:C:155:SER:HA	1:C:158:LEU:HD12	1.89	0.54
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.02	0.53
3:C:410:HEM:HHD	3:C:410:HEM:CBC	2.35	0.53
1:A:98:ILE:CD1	1:A:107:TYR:HB2	2.39	0.52
1:C:117:SER:HB3	1:C:130:PHE:CE2	2.43	0.52
1:B:43:ASN:C	1:B:43:ASN:OD1	2.52	0.52
1:A:184:MET:O	1:A:188:ILE:HG12	2.10	0.52
1:A:329:LYS:O	1:A:352:SER:N	2.30	0.52
1:B:220:ILE:HG12	1:B:322:LEU:HD22	1.92	0.52
1:A:311:ARG:HD2	4:A:938:HOH:O	2.08	0.52
1:A:332:TYR:O	1:A:336:ARG:NH2	2.43	0.52
1:C:78:SER:O	1:C:81:ASN:HB3	2.10	0.52
1:B:177:LEU:HG	1:B:178:LYS:H	1.75	0.52
1:C:109:VAL:O	1:C:113:VAL:HG23	2.10	0.52
1:A:99:ASP:O	1:A:100:ASN:HB2	2.09	0.51
1:B:246:HIS:O	1:B:246:HIS:CG	2.63	0.51
1:C:40:PHE:CZ	1:C:255:ILE:HD11	2.46	0.51
1:A:14:ASP:OD1	1:A:26:LYS:NZ	2.42	0.51
1:A:311:ARG:NH1	4:A:938:HOH:O	2.41	0.51
1:C:151:ASN:O	1:C:152:ARG:C	2.54	0.51
1:A:277:GLU:HG3	1:A:283:PRO:HG3	1.93	0.51
1:A:306:GLY:HA3	3:A:410:HEM:C3C	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG13	1:B:268:VAL:HG11	1.92	0.51
1:B:64:HIS:HE1	3:B:410:HEM:O2D	1.94	0.51
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.09	0.51
1:C:72:ALA:HA	1:C:305:LEU:HD11	1.93	0.50
1:B:110:ARG:O	1:B:114:ASN:ND2	2.41	0.50
1:C:281:ASP:HB2	2:C:910:SO4:O1	2.11	0.50
1:A:48:TYR:CE2	1:A:246:HIS:CE1	2.95	0.50
1:A:183:THR:HB	1:A:186:GLU:OE1	2.12	0.50
1:C:137:ILE:HG23	1:C:196:ILE:HD11	1.93	0.50
1:A:340:ASN:ND2	1:A:342:MET:H	2.10	0.50
1:B:75:PHE:HA	1:B:80:ILE:CD1	2.42	0.50
1:A:326:LYS:N	2:A:900:SO4:O3	2.44	0.49
1:A:294:HIS:CD2	1:A:296:ALA:HB3	2.47	0.49
1:A:73:PRO:O	1:A:79:LYS:HG3	2.13	0.49
1:B:178:LYS:O	1:B:179:ASN:CB	2.61	0.49
1:C:255:ILE:O	1:C:256:ASN:C	2.56	0.49
1:A:216:ASN:O	1:A:219:ILE:HG22	2.13	0.48
1:A:351:LEU:O	1:A:352:SER:HB3	2.13	0.48
1:C:306:GLY:HA3	3:C:410:HEM:C3C	2.48	0.48
1:A:183:THR:HG22	1:A:186:GLU:N	2.25	0.48
1:C:127:MET:N	1:C:128:PRO:HD2	2.29	0.48
1:A:47:ARG:HA	1:A:47:ARG:NH1	2.27	0.48
1:A:233:GLU:OE1	1:A:236:ARG:HD3	2.13	0.48
1:A:254:TYR:HA	1:A:258:LYS:O	2.14	0.48
1:A:98:ILE:HD12	1:A:107:TYR:HB2	1.96	0.48
1:C:209:MET:HB3	1:C:230:PHE:HE2	1.78	0.48
1:C:147:ASN:O	1:C:148:TYR:C	2.56	0.47
1:A:183:THR:HG23	1:A:185:ASP:H	1.79	0.47
1:A:13:ASN:ND2	4:A:977:HOH:O	2.47	0.47
1:A:277:GLU:HG2	1:A:283:PRO:CG	2.44	0.47
1:A:245:PRO:HA	1:A:267:ILE:HG23	1.96	0.47
1:C:34:LEU:HD21	1:C:268:VAL:HG21	1.97	0.47
1:C:327:ARG:HB3	4:C:924:HOH:O	2.13	0.47
1:A:60:ASP:C	1:A:62:PRO:HD2	2.40	0.47
1:C:136:TYR:HB3	1:C:146:PHE:CD1	2.50	0.47
1:B:111:LEU:N	1:B:112:PRO:HD2	2.29	0.46
1:B:142:ARG:O	1:B:142:ARG:HG2	2.16	0.46
1:B:156:ARG:NH1	1:B:156:ARG:CG	2.75	0.46
1:C:142:ARG:HD2	1:C:142:ARG:O	2.15	0.46
1:A:198:GLY:HA2	3:A:410:HEM:C2C	2.50	0.46
1:B:100:ASN:C	1:B:100:ASN:HD22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:O	1:B:154:VAL:HG23	2.15	0.46
1:A:293:MET:HG2	1:A:294:HIS:O	2.16	0.46
1:A:194:LEU:O	3:A:410:HEM:HBC2	2.15	0.45
1:C:63:GLU:HG2	1:C:64:HIS:N	2.31	0.45
1:A:99:ASP:OD2	1:A:324:HIS:HE1	1.97	0.45
1:A:136:TYR:HE2	1:A:143:ASP:HB2	1.80	0.45
1:B:227:ARG:HG2	1:B:318:LEU:HD23	1.99	0.45
1:C:116:ILE:HG22	1:C:120:LEU:HD11	1.98	0.45
1:C:281:ASP:HB2	2:C:910:SO4:S	2.57	0.45
1:B:17:HIS:HB2	1:B:22:TRP:CZ3	2.52	0.44
1:A:302:HIS:O	1:A:303:MET:C	2.60	0.44
1:C:172:LEU:O	1:C:173:ALA:C	2.61	0.44
1:A:179:ASN:O	1:A:180:ARG:HB2	2.17	0.44
1:A:340:ASN:HD22	1:A:340:ASN:C	2.22	0.44
1:B:177:LEU:C	1:B:179:ASN:H	2.20	0.44
1:B:185:ASP:OD2	1:B:189:LYS:HD2	2.18	0.44
1:C:68:ARG:NH1	3:C:410:HEM:O2D	2.45	0.44
1:A:98:ILE:O	1:A:99:ASP:C	2.59	0.44
1:B:54:ILE:HG13	1:B:58:THR:OG1	2.17	0.44
1:B:316:ILE:HG23	4:B:421:HOH:O	2.17	0.44
1:C:136:TYR:OH	1:C:145:ASN:HB2	2.18	0.44
1:C:210:ILE:HG22	1:C:330:ILE:HD11	2.00	0.44
1:A:207:GLY:HA3	4:A:936:HOH:O	2.17	0.43
1:C:149:VAL:O	1:C:152:ARG:HB3	2.17	0.43
1:B:10:MET:HE2	1:C:26:LYS:NZ	2.33	0.43
1:C:59:MET:HE1	1:C:67:PHE:CZ	2.54	0.43
1:A:111:LEU:N	1:A:112:PRO:HD2	2.34	0.43
1:A:133:TRP:CD2	1:A:153:MET:HG2	2.54	0.43
1:B:328:ILE:HA	1:B:351:LEU:HD21	1.99	0.43
1:C:57:ILE:HG23	1:C:58:THR:HG23	2.00	0.43
1:C:121:GLY:O	1:C:122:ILE:C	2.62	0.43
1:B:54:ILE:H	1:B:54:ILE:HG12	1.19	0.43
1:B:93:ASP:HA	1:B:96:LYS:HE3	2.01	0.43
1:B:176:SER:HB3	1:B:177:LEU:H	1.61	0.42
1:B:14:ASP:OD1	1:B:256:ASN:O	2.36	0.42
1:B:236:ARG:NH1	1:B:274:ASN:O	2.52	0.42
1:A:72:ALA:HB3	1:A:73:PRO:HD3	2.02	0.42
1:A:43:ASN:OD1	1:A:43:ASN:N	2.52	0.42
3:A:410:HEM:HAB	3:A:410:HEM:HHC	1.66	0.42
1:B:246:HIS:CD2	4:B:419:HOH:O	2.67	0.42
1:B:287:LYS:NZ	1:B:287:LYS:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:TYR:O	1:C:149:VAL:C	2.63	0.42
1:C:331:ASP:OD1	1:C:333:LYS:HB2	2.19	0.42
1:C:83:TYR:CD2	1:C:118:LYS:NZ	2.82	0.41
1:A:232:GLU:OE1	1:A:311:ARG:NE	2.39	0.41
1:C:117:SER:CB	1:C:130:PHE:CE2	3.03	0.41
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.94	0.41
3:B:410:HEM:HBC2	3:B:410:HEM:CMC	2.50	0.41
1:C:66:GLU:HG2	1:C:177:LEU:HD23	2.01	0.41
1:C:258:LYS:O	1:C:260:ILE:HD12	2.21	0.41
1:C:277:GLU:H	1:C:277:GLU:CD	2.28	0.41
1:A:104:ILE:HA	1:A:108:ALA:HB3	2.03	0.41
1:C:66:GLU:HA	1:C:177:LEU:HD23	2.02	0.41
1:B:177:LEU:HD12	1:B:177:LEU:HA	1.95	0.41
1:B:210:ILE:HG22	1:B:330:ILE:HD11	2.02	0.41
1:C:152:ARG:HB3	1:C:153:MET:H	1.72	0.41
1:A:340:ASN:ND2	1:A:340:ASN:C	2.79	0.41
1:B:64:HIS:CD2	1:B:301:ILE:HD12	2.56	0.41
1:C:61:ASN:ND2	1:C:64:HIS:CD2	2.86	0.41
1:C:61:ASN:HA	1:C:64:HIS:HB3	2.02	0.41
1:A:227:ARG:CD	1:A:319:ASN:HB2	2.50	0.41
1:A:341:LYS:NZ	4:A:997:HOH:O	2.44	0.41
1:A:14:ASP:HA	1:A:26:LYS:HE2	2.02	0.41
1:B:232:GLU:OE2	1:B:294:HIS:CE1	2.68	0.41
1:B:239:SER:HA	1:B:240:PRO:HD3	1.95	0.41
1:C:256:ASN:O	1:C:257:ASN:HB2	2.20	0.41
1:A:243:PHE:CE2	1:A:342:MET:HA	2.55	0.41
1:B:294:HIS:CD2	1:B:294:HIS:C	2.99	0.41
1:B:79:LYS:O	1:B:82:ASP:HB2	2.21	0.40
1:A:331:ASP:OD1	1:A:331:ASP:C	2.65	0.40
1:B:179:ASN:O	1:B:180:ARG:HB2	2.21	0.40
1:C:153:MET:HE3	1:C:157:LEU:HG	2.03	0.40
1:C:198:GLY:HA2	3:C:410:HEM:CMC	2.51	0.40
1:A:117:SER:HB3	1:A:130:PHE:CE2	2.57	0.40
1:C:319:ASN:O	1:C:323:ASN:HB2	2.20	0.40
1:C:41:SER:O	1:C:247:ARG:HA	2.21	0.40
1:B:287:LYS:HB2	1:B:290:ARG:NE	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/343 (97%)	308 (92%)	20 (6%)	6 (2%)	6	12
1	B	331/343 (96%)	286 (86%)	35 (11%)	10 (3%)	3	5
1	C	329/343 (96%)	289 (88%)	28 (8%)	12 (4%)	2	3
All	All	994/1029 (97%)	883 (89%)	83 (8%)	28 (3%)	4	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	B	12	LEU
1	B	177	LEU
1	B	178	LYS
1	B	179	ASN
1	C	19	ASP
1	B	66	GLU
1	C	53	GLY
1	C	62	PRO
1	C	152	ARG
1	C	256	ASN
1	A	46	ASN
1	A	62	PRO
1	B	62	PRO
1	B	256	ASN
1	C	173	ALA
1	A	163	SER
1	A	178	LYS
1	A	180	ARG
1	C	61	ASN
1	C	151	ASN
1	C	178	LYS
1	C	179	ASN
1	C	199	ASN

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	180	ARG
1	C	148	TYR
1	B	327	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/310 (99%)	287 (94%)	20 (6%)	15	32
1	B	303/310 (98%)	271 (89%)	32 (11%)	6	14
1	C	302/310 (97%)	275 (91%)	27 (9%)	9	20
All	All	912/930 (98%)	833 (91%)	79 (9%)	9	21

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	54	ILE
1	A	64	HIS
1	A	80	ILE
1	A	116	ILE
1	A	127	MET
1	A	137	ILE
1	A	141	LYS
1	A	142	ARG
1	A	145	ASN
1	A	159	GLU
1	A	177	LEU
1	A	183	THR
1	A	236	ARG
1	A	255	ILE
1	A	268	VAL
1	A	312	LEU
1	A	336	ARG

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Mol	Chain	Res	Type
1	A	339	ASP
1	A	351	LEU
1	B	10	MET
1	B	16	VAL
1	B	38	LYS
1	B	54	ILE
1	B	64	HIS
1	B	100	ASN
1	B	106	GLU
1	B	111	LEU
1	B	116	ILE
1	B	137	ILE
1	B	140	ASN
1	B	147	ASN
1	B	152	ARG
1	B	156	ARG
1	B	168	ILE
1	B	178	LYS
1	B	182	LEU
1	B	183	THR
1	B	214	ASP
1	B	220	ILE
1	B	232	GLU
1	B	241	ILE
1	B	251	GLU
1	B	260	ILE
1	B	284	ASP
1	B	288	ILE
1	B	291	ARG
1	B	312	LEU
1	B	327	ARG
1	B	336	ARG
1	B	339	ASP
1	B	341	LYS
1	C	34	LEU
1	C	38	LYS
1	C	54	ILE
1	C	61	ASN
1	C	63	GLU
1	C	95	ILE
1	C	98	ILE
1	C	118	LYS

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Mol	Chain	Res	Type
1	C	124	ASP
1	C	137	ILE
1	C	142	ARG
1	C	144	GLU
1	C	164	ASP
1	C	183	THR
1	C	184	MET
1	C	185	ASP
1	C	210	ILE
1	C	213	ILE
1	C	219	ILE
1	C	236	ARG
1	C	253	SER
1	C	266	VAL
1	C	277	GLU
1	C	291	ARG
1	C	328	ILE
1	C	333	LYS
1	C	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	64	HIS
1	A	81	ASN
1	A	150	ASN
1	A	151	ASN
1	A	170	ASN
1	A	199	ASN
1	A	226	ASN
1	A	246	HIS
1	A	256	ASN
1	A	294	HIS
1	A	319	ASN
1	A	324	HIS
1	A	340	ASN
1	B	17	HIS
1	B	32	HIS
1	B	64	HIS
1	B	92	ASN
1	B	100	ASN

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Mol	Chain	Res	Type
1	B	150	ASN
1	B	166	HIS
1	B	199	ASN
1	B	208	ASN
1	B	226	ASN
1	B	256	ASN
1	B	294	HIS
1	C	32	HIS
1	C	61	ASN
1	C	64	HIS
1	C	100	ASN
1	C	150	ASN
1	C	166	HIS
1	C	226	ASN
1	C	246	HIS
1	C	294	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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
2	SO4	A	900	-	4,4,4	0.29	0	6,6,6	0.45	0
3	HEM	B	410	1	50,50,50	1.97	11 (22%)	67,82,82	1.46	13 (19%)
2	SO4	A	920	-	4,4,4	0.27	0	6,6,6	0.32	0
3	HEM	C	410	1	50,50,50	1.76	8 (16%)	67,82,82	1.11	5 (7%)
2	SO4	A	910	-	4,4,4	0.22	0	6,6,6	0.88	0
2	SO4	C	910	-	4,4,4	0.87	0	6,6,6	0.36	0
3	HEM	A	410	1	50,50,50	2.69	19 (38%)	67,82,82	2.07	21 (31%)

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
3	HEM	C	410	1	-	0/14/54/54	-
3	HEM	B	410	1	-	1/14/54/54	-
3	HEM	A	410	1	-	2/14/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	HEM	C3D-C2D	8.19	1.54	1.36
3	B	410	HEM	C3D-C2D	7.97	1.54	1.36
3	C	410	HEM	C3D-C2D	7.63	1.53	1.36
3	A	410	HEM	FE-NC	6.02	2.15	1.95
3	A	410	HEM	CMA-C3A	5.34	1.61	1.50
3	A	410	HEM	CAB-C3B	5.19	1.61	1.47
3	A	410	HEM	FE-NA	5.12	2.12	1.95
3	A	410	HEM	FE-NB	5.08	2.10	1.94
3	A	410	HEM	CMC-C2C	4.53	1.60	1.50
3	A	410	HEM	CMB-C2B	4.40	1.59	1.50
3	A	410	HEM	CAC-C3C	4.17	1.58	1.47
3	B	410	HEM	FE-NC	4.14	2.08	1.95
3	B	410	HEM	FE-NB	3.92	2.07	1.94
3	B	410	HEM	FE-ND	3.91	2.06	1.94
3	C	410	HEM	FE-NB	3.60	2.06	1.94
3	B	410	HEM	FE-NA	3.55	2.06	1.95
3	C	410	HEM	CAB-C3B	3.30	1.56	1.47
3	A	410	HEM	CHC-C1C	3.09	1.44	1.38
3	A	410	HEM	CMD-C2D	2.88	1.56	1.50
3	B	410	HEM	CMC-C2C	2.87	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	HEM	C3C-C4C	-2.69	1.41	1.46
3	A	410	HEM	CBB-CAB	2.64	1.43	1.30
3	C	410	HEM	FE-NA	2.64	2.03	1.95
3	B	410	HEM	CMD-C2D	2.61	1.56	1.50
3	B	410	HEM	CMB-C2B	2.60	1.56	1.50
3	B	410	HEM	CAB-C3B	2.60	1.54	1.47
3	B	410	HEM	CAC-C3C	2.59	1.54	1.47
3	C	410	HEM	CMC-C2C	2.34	1.55	1.50
3	A	410	HEM	CAA-C2A	2.31	1.57	1.51
3	A	410	HEM	C4D-C3D	-2.27	1.41	1.45
3	C	410	HEM	CAC-C3C	2.24	1.53	1.47
3	A	410	HEM	CAD-C3D	2.24	1.57	1.51
3	C	410	HEM	CMB-C2B	2.19	1.55	1.50
3	B	410	HEM	CMA-C3A	2.19	1.55	1.50
3	C	410	HEM	C3C-C2C	-2.13	1.32	1.37
3	A	410	HEM	CHC-C4B	2.12	1.44	1.39
3	A	410	HEM	O1A-CGA	2.11	1.29	1.22
3	A	410	HEM	CHD-C1D	2.04	1.43	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	HEM	CHC-C4B-NB	5.93	130.80	124.42
3	B	410	HEM	C4D-ND-C1D	5.56	111.79	105.21
3	A	410	HEM	CHA-C4D-ND	4.82	130.32	124.37
3	C	410	HEM	C4D-ND-C1D	4.42	110.44	105.21
3	A	410	HEM	C4D-ND-C1D	4.03	109.98	105.21
3	A	410	HEM	CMC-C2C-C1C	4.01	131.80	124.73
3	A	410	HEM	CHC-C1C-C2C	3.89	133.59	125.49
3	B	410	HEM	CHC-C4B-NB	3.72	128.43	124.42
3	A	410	HEM	CHC-C1C-NC	-3.54	120.60	124.45
3	A	410	HEM	CAA-CBA-CGA	-3.44	104.55	113.67
3	A	410	HEM	CHA-C4D-C3D	-3.42	118.93	125.23
3	A	410	HEM	CMA-C3A-C4A	-3.40	120.24	125.42
3	A	410	HEM	CMA-C3A-C2A	3.39	132.81	125.62
3	A	410	HEM	CMC-C2C-C3C	-3.18	120.73	128.43
3	A	410	HEM	CHC-C4B-C3B	-3.11	118.87	125.07
3	A	410	HEM	CAB-C3B-C2B	3.00	138.18	128.43
3	A	410	HEM	CAB-C3B-C4B	-2.75	112.23	124.39
3	C	410	HEM	CHA-C4D-ND	2.71	127.72	124.37
3	B	410	HEM	C1B-NB-C4B	2.67	108.37	105.21
3	B	410	HEM	C4C-C3C-C2C	2.53	109.00	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	HEM	CAD-C3D-C2D	2.52	132.58	127.87
3	A	410	HEM	C4B-C3B-C2B	2.50	109.58	107.28
3	C	410	HEM	CBD-CAD-C3D	-2.49	105.64	112.53
3	B	410	HEM	CMD-C2D-C1D	2.49	128.93	125.03
3	A	410	HEM	CMD-C2D-C1D	2.41	128.80	125.03
3	A	410	HEM	C4A-CHB-C1B	-2.37	120.68	126.25
3	A	410	HEM	CHB-C4A-NA	2.34	128.11	123.86
3	A	410	HEM	CHB-C4A-C3A	-2.34	120.65	127.43
3	B	410	HEM	C3A-C4A-NA	-2.24	106.55	110.14
3	B	410	HEM	CAD-C3D-C4D	2.19	128.51	124.70
3	C	410	HEM	CHC-C4B-NB	2.18	126.77	124.42
3	B	410	HEM	C4A-NA-C1A	2.15	109.32	105.82
3	A	410	HEM	C2C-C1C-NC	-2.11	105.74	109.64
3	B	410	HEM	CBD-CAD-C3D	-2.09	106.75	112.53
3	B	410	HEM	C2A-C1A-NA	-2.08	107.84	110.15
3	B	410	HEM	C3B-C4B-NB	-2.07	107.98	109.47
3	B	410	HEM	CHD-C4C-NC	2.05	126.69	124.45
3	C	410	HEM	CMD-C2D-C1D	2.03	128.20	125.03
3	B	410	HEM	CBC-CAC-C3C	-2.01	117.46	127.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	HEM	C2C-C3C-CAC-CBC
3	A	410	HEM	C4C-C3C-CAC-CBC
3	B	410	HEM	C2B-C3B-CAB-CBB

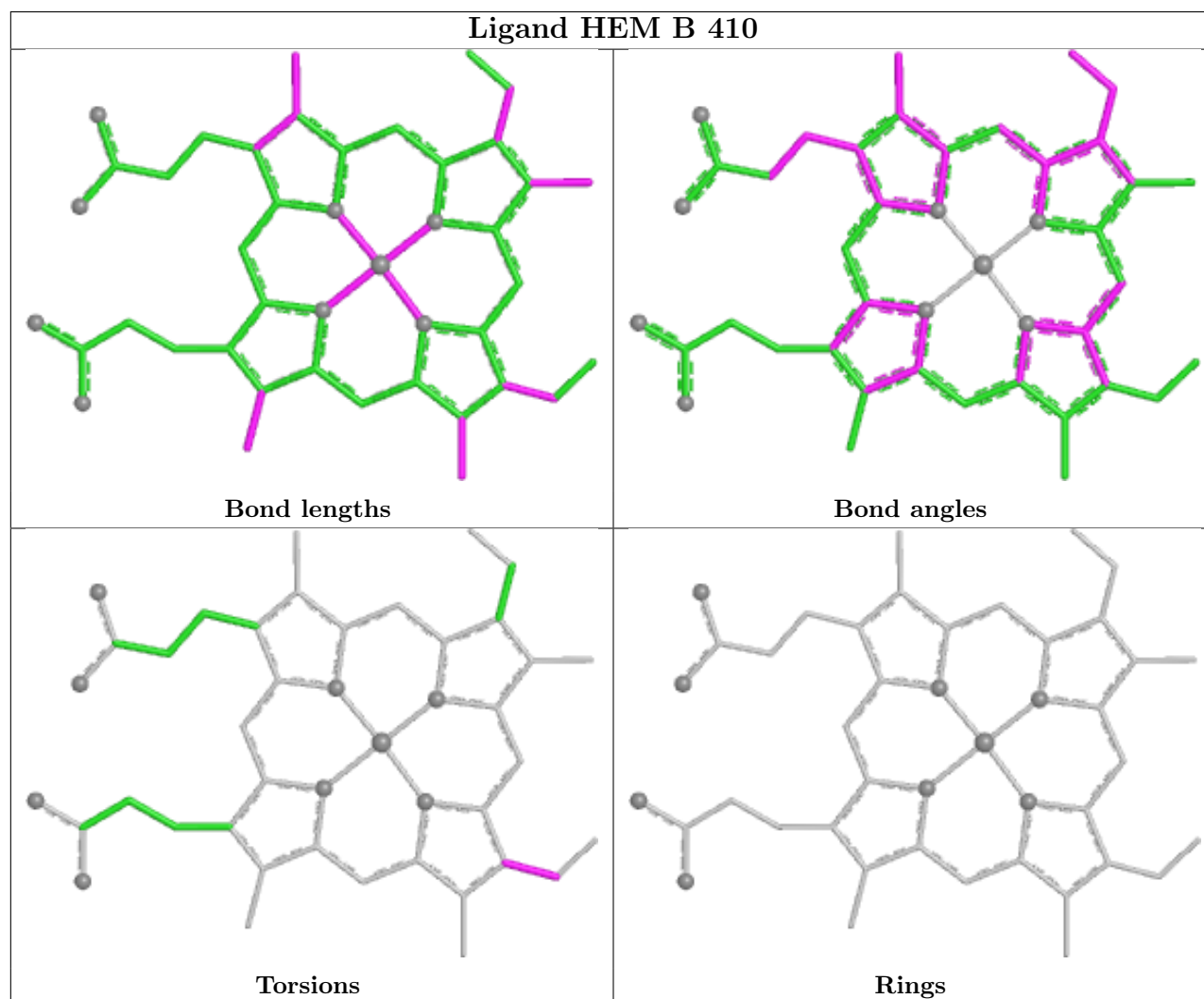
There are no ring outliers.

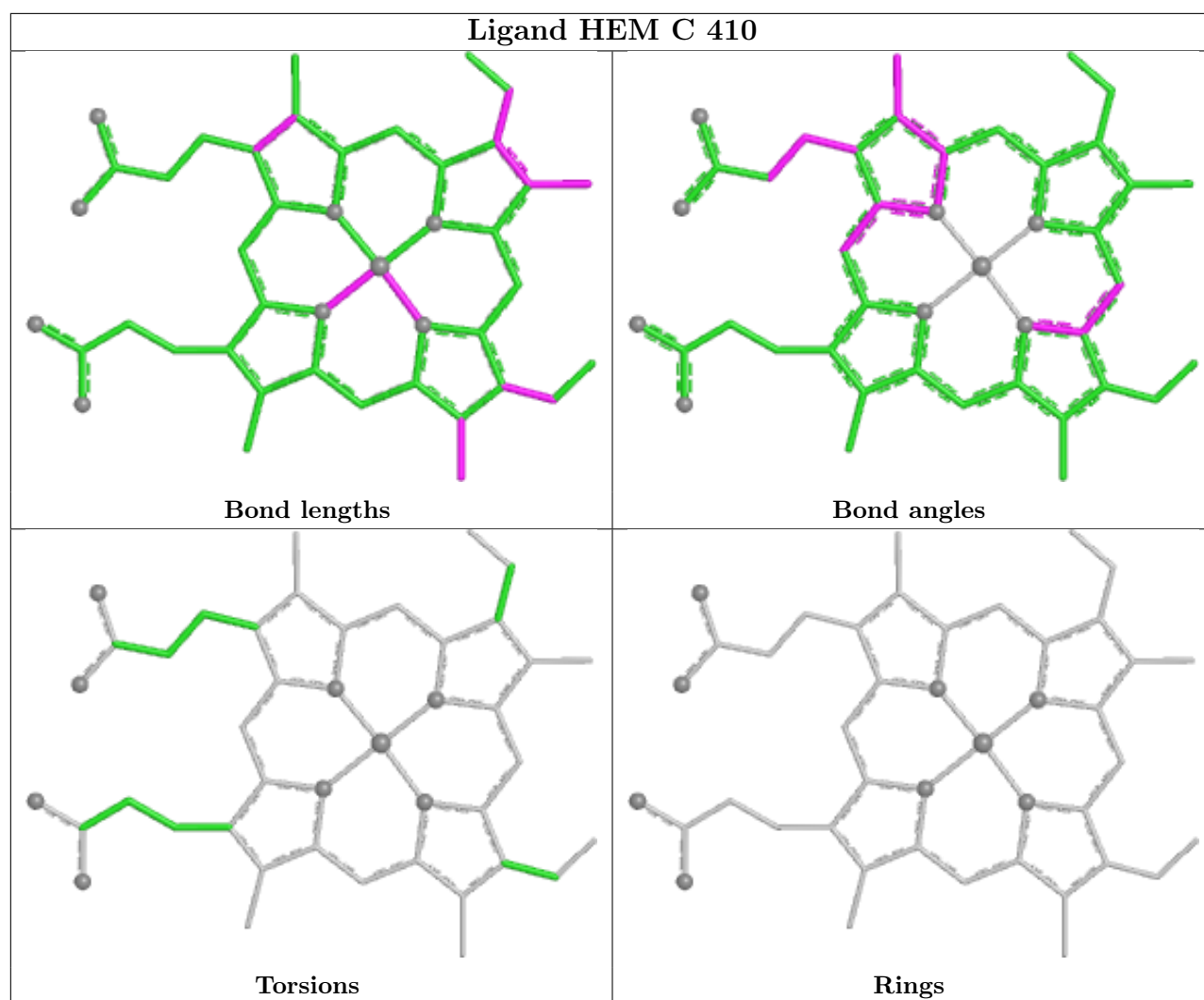
5 monomers are involved in 19 short contacts:

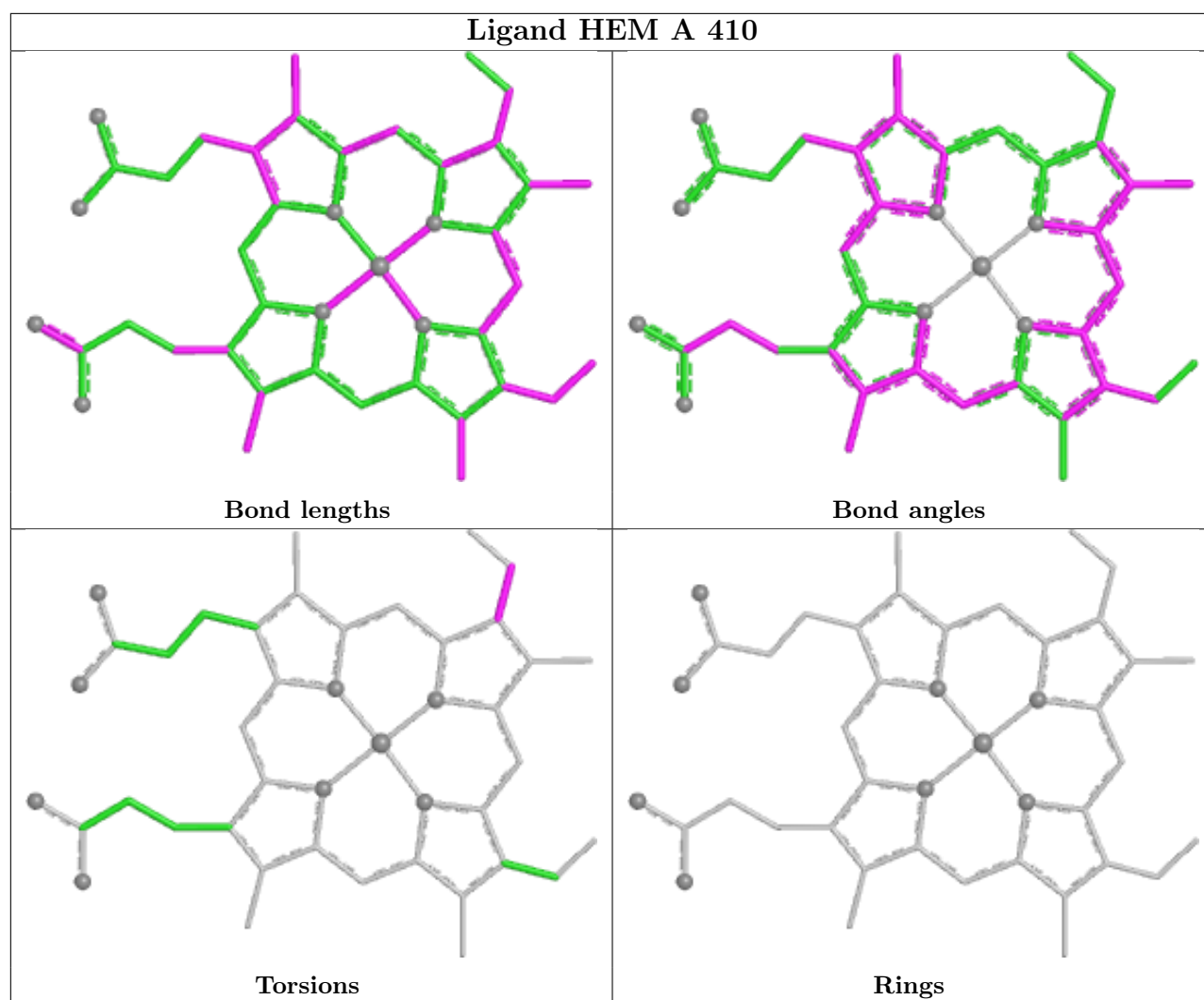
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	SO4	1	0
3	B	410	HEM	3	0
3	C	410	HEM	6	0
2	C	910	SO4	4	0
3	A	410	HEM	5	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	338/343 (98%)	0.55	11 (3%)	49 45	59, 68, 85, 114	0
1	B	335/343 (97%)	0.88	28 (8%)	17 15	58, 69, 82, 86	0
1	C	333/343 (97%)	0.59	16 (4%)	35 31	57, 70, 80, 88	0
All	All	1006/1029 (97%)	0.67	55 (5%)	30 27	57, 69, 82, 114	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	ASN	4.2
1	B	178	LYS	4.2
1	B	260	ILE	4.1
1	B	52	GLY	3.7
1	C	74	TYR	3.7
1	B	53	GLY	3.7
1	A	177	LEU	3.5
1	B	65	LYS	3.5
1	B	62	PRO	3.5
1	B	140	ASN	3.4
1	B	70	ILE	3.3
1	C	137	ILE	3.1
1	C	177	LEU	3.1
1	B	61	ASN	3.0
1	A	139	GLY	3.0
1	B	288	ILE	3.0
1	B	271	GLY	3.0
1	C	12	LEU	2.9
1	C	15	PRO	2.8
1	B	206	ILE	2.8
1	A	13	ASN	2.7
1	C	166	HIS	2.7
1	A	166	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	2.6
1	A	121	GLY	2.5
1	B	255	ILE	2.5
1	B	335	SER	2.4
1	A	62	PRO	2.4
1	B	257	ASN	2.4
1	B	253	SER	2.4
1	B	279	PHE	2.4
1	B	16	VAL	2.4
1	C	175	SER	2.3
1	B	54	ILE	2.3
1	C	288	ILE	2.3
1	A	44	PRO	2.3
1	A	298	GLY	2.3
1	A	352	SER	2.3
1	B	25	TYR	2.3
1	A	141	LYS	2.2
1	B	182	LEU	2.2
1	B	301	ILE	2.2
1	B	135	ASP	2.2
1	C	98	ILE	2.1
1	C	184	MET	2.1
1	C	139	GLY	2.1
1	B	12	LEU	2.1
1	C	142	ARG	2.1
1	C	176	SER	2.1
1	B	166	HIS	2.1
1	B	249	ALA	2.0
1	C	255	ILE	2.0
1	C	118	LYS	2.0
1	C	174	GLY	2.0
1	B	176	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](#)

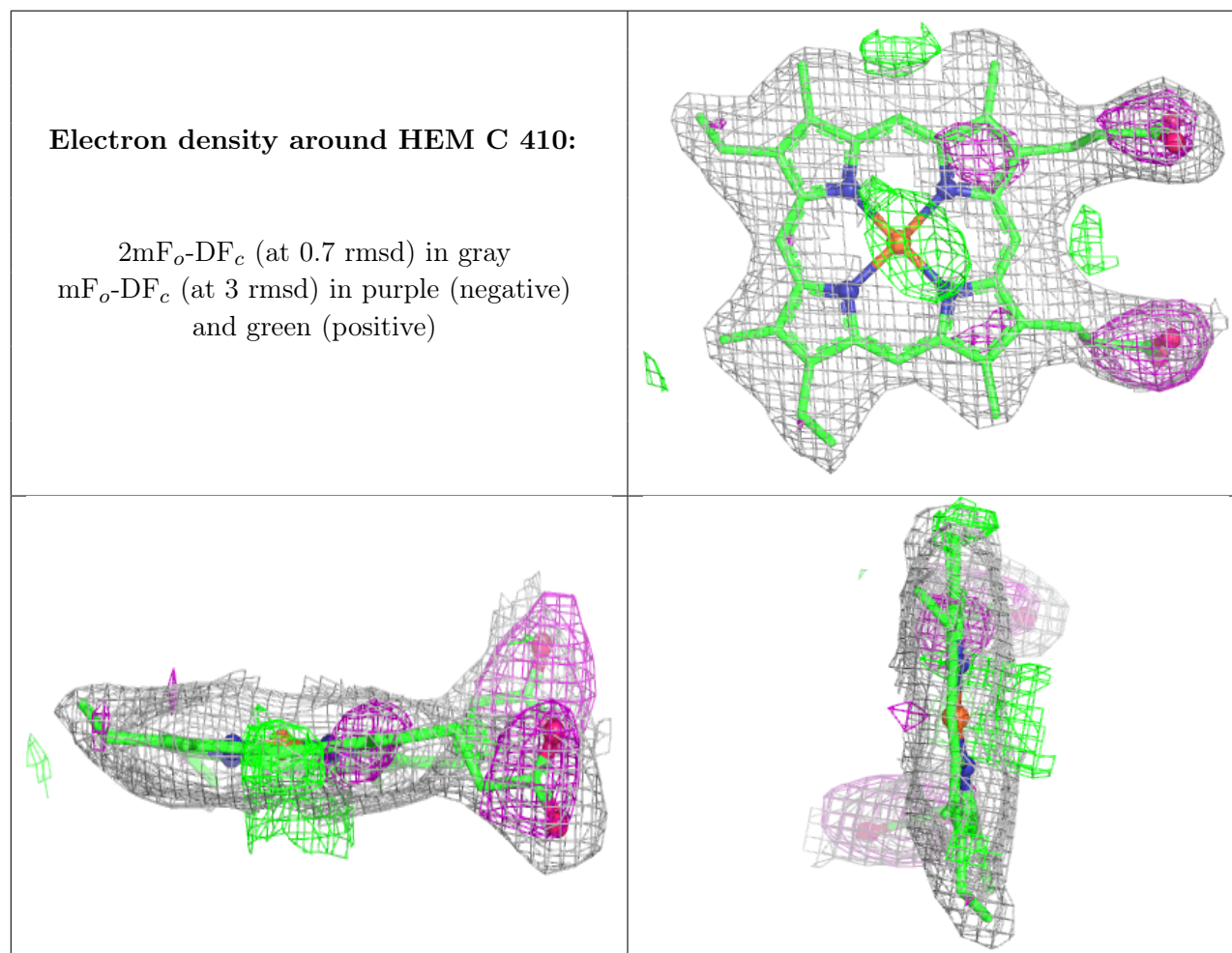
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

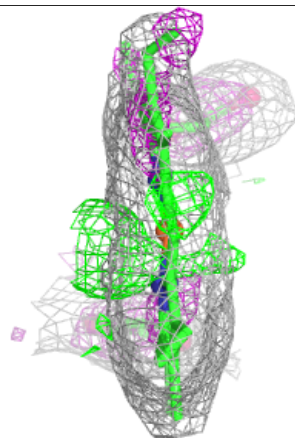
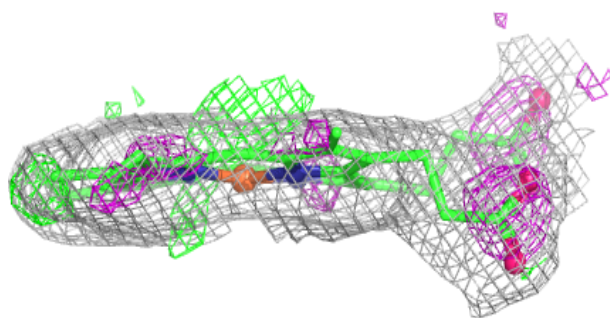
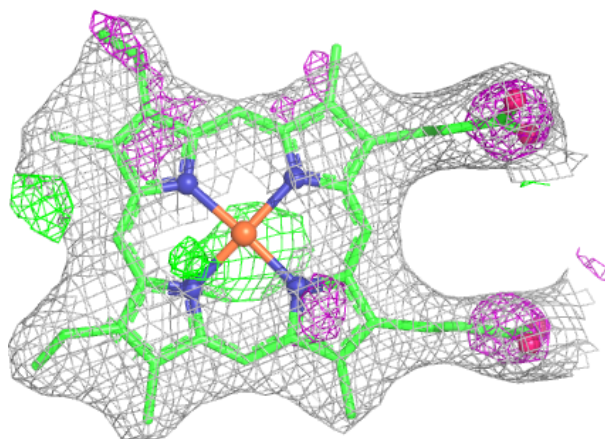
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	910	5/5	0.37	0.22	89,89,91,92	0
2	SO4	A	900	5/5	0.70	0.19	86,87,88,89	0
2	SO4	A	920	5/5	0.71	0.17	90,90,91,92	0
2	SO4	A	910	5/5	0.91	0.18	76,78,78,79	0
3	HEM	C	410	43/43	0.92	0.13	62,64,67,70	0
3	HEM	B	410	43/43	0.93	0.12	61,65,67,67	0
3	HEM	A	410	43/43	0.95	0.11	60,67,71,75	0

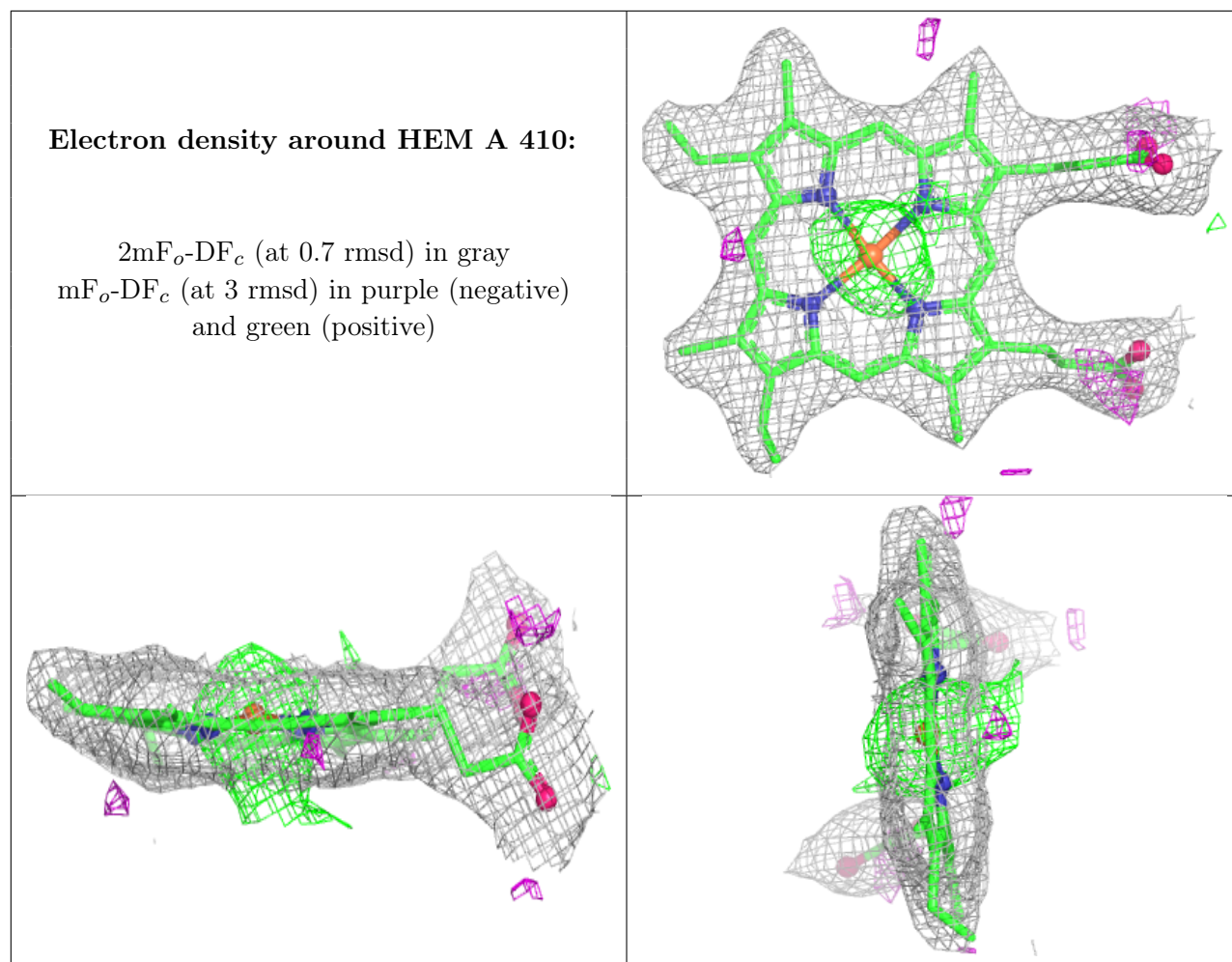
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around HEM B 410:

$2mF_o-DF_c$ (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.