



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:41 am BST

PDB ID : 2W72
Title : DEOXYGENATED STRUCTURE OF A DISTAL SITE HEMOGLOBIN
MUTANT PLUS XE
Authors : Miele, A.E.; Draghi, F.; Sciara, G.; Johnson, K.A.; Renzi, F.; Vallone, B.;
Brunori, M.; Savino, C.
Deposited on : 2008-12-19
Resolution : 1.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

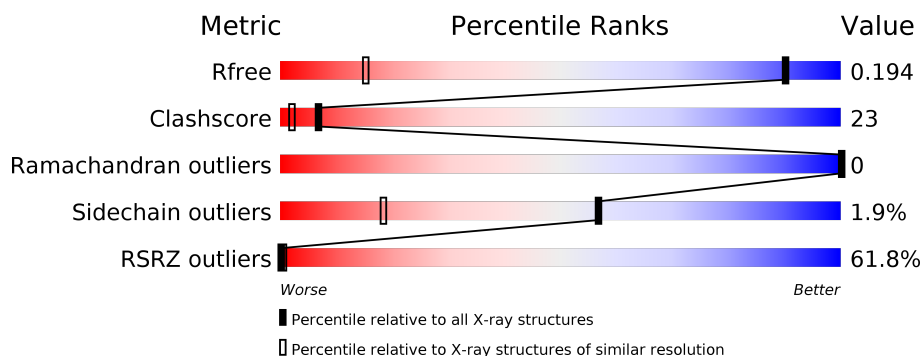
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.07 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	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>57%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>..</div> </div> </div>
2	B	146	<div> <div>65%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
2	D	146	<div> <div>64%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
3	C	141	<div> <div>62%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1144	-	-	X	-
5	SO4	C	1144	-	-	X	-
5	SO4	D	1148	-	-	X	-
6	XE	A	1146[A]	-	-	X	-
6	XE	A	1147[A]	-	-	X	-
6	XE	A	1147[B]	-	-	X	-
6	XE	A	1148	-	-	X	-
6	XE	A	1149	-	-	X	-
6	XE	A	1150	-	-	X	-
6	XE	B	1152	-	-	X	-
6	XE	C	1148[B]	-	-	X	-
6	XE	C	1149	-	-	X	-
6	XE	C	1150	-	-	X	-
6	XE	D	1149[B]	-	-	X	-
6	XE	D	1150	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6291 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 HUMAN HEMOGLOBIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	34	0
			1278	846	211	217	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	TYR	LEU	engineered mutation	UNP P69905
A	58	GLN	HIS	engineered mutation	UNP P69905

- Molecule 2 is a protein called HUMAN HEMOGLOBIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	43	0
			1365	904	225	230	6			
2	D	146	Total	C	N	O	S	0	34	0
			1322	867	221	229	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	VAL	conflict	UNP P69905
B	28	TYR	LEU	engineered mutation	UNP P68871
B	63	GLN	HIS	engineered mutation	UNP P68871
D	1	MET	VAL	conflict	UNP P69905
D	28	TYR	LEU	engineered mutation	UNP P68871
D	63	GLN	HIS	engineered mutation	UNP P68871

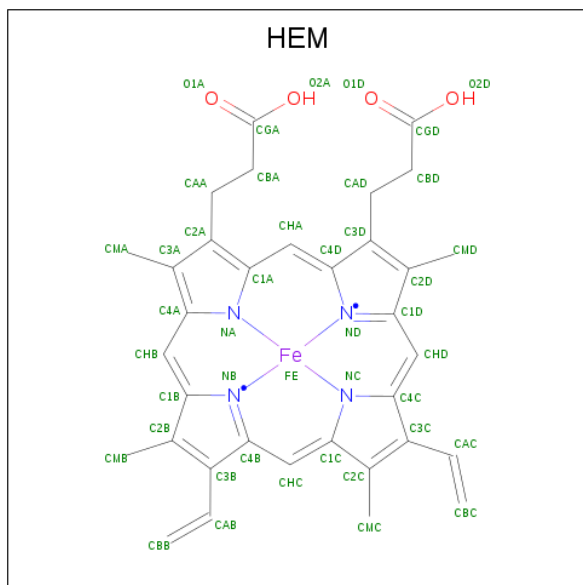
- Molecule 3 is a protein called HUMAN HEMOGLOBIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	141	Total	C	N	O	S	0	34	0
			1264	831	208	219	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	VAL	conflict	UNP P69905
C	29	TYR	LEU	engineered mutation	UNP P69905
C	58	GLN	HIS	engineered mutation	UNP P69905

- 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	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	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	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	1
			10	8	2		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

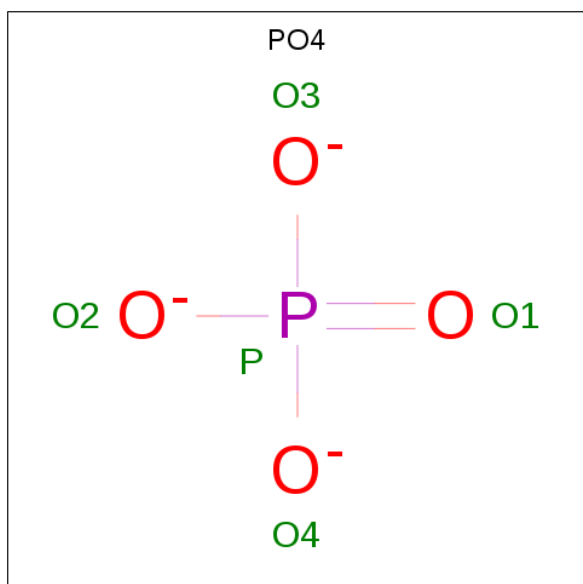
- Molecule 6 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Xe	0	1
			4	4		
6	A	6	Total	Xe	0	2
			8	8		
6	D	2	Total	Xe	0	1
			4	4		
6	C	5	Total	Xe	0	2
			7	7		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total K 1 1	0	0
7	A	1	Total K 1 1	0	0
7	C	1	Total K 1 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O P 5 4 1	0	0

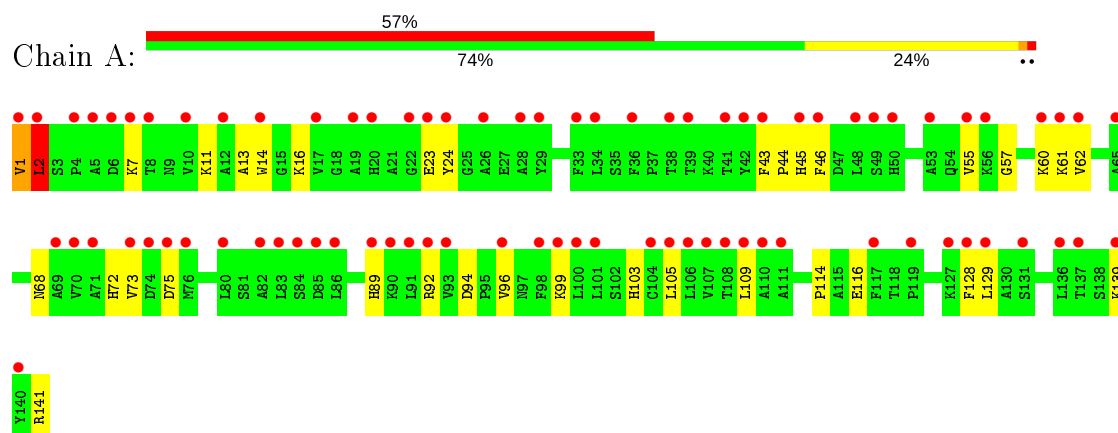
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	193	Total O 193 193	0	0
9	B	201	Total O 201 201	0	0
9	C	205	Total O 205 205	0	0
9	D	215	Total O 215 215	0	0

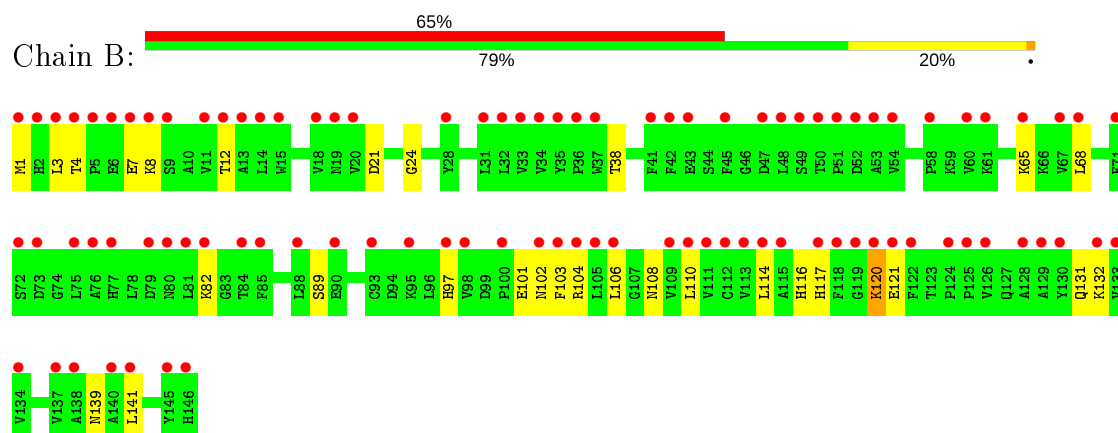
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

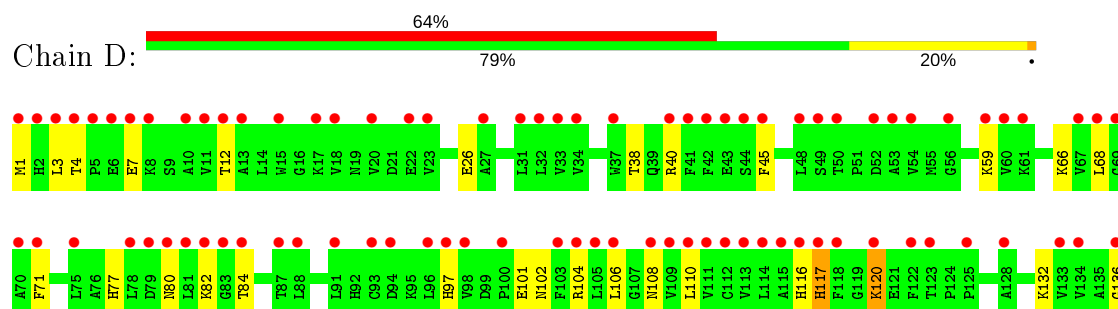
• Molecule 1: HUMAN HEMOGLOBIN A

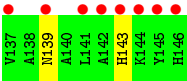


• Molecule 2: HUMAN HEMOGLOBIN A

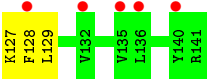
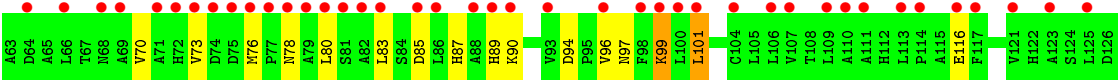
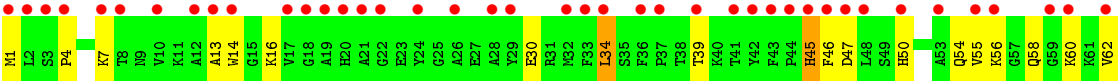


• Molecule 2: HUMAN HEMOGLOBIN A





● Molecule 3: HUMAN HEMOGLOBIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.96Å 82.45Å 53.53Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	17.32 – 1.07 17.60 – 1.07	Depositor EDS
% Data completeness (in resolution range)	94.2 (17.32-1.07) 94.2 (17.60-1.07)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 1.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.129 , 0.153 0.175 , 0.194	Depositor DCC
R_{free} test set	11886 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	8.2	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.1	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	6291	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, HEM, K, SO4, XE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	0/1411	0.90	5/1909 (0.3%)
2	B	0.74	0/1528	0.84	0/2061
2	D	0.82	0/1463	0.83	0/1975
3	C	0.66	0/1400	0.84	0/1894
All	All	0.74	0/5802	0.85	5/7839 (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
3	C	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	92	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	2[A]	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	2[B]	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	139[A]	LYS	CD-CE-NZ	-5.05	100.09	111.70
1	A	139[B]	LYS	CD-CE-NZ	-5.05	100.09	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	45[A]	HIS	Mainchain

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Mol	Chain	Res	Type	Group
3	C	45[B]	HIS	Mainchain

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	1278	0	1379	69	1
2	B	1365	0	1485	59	0
2	D	1322	0	1391	57	0
3	C	1264	0	1345	75	1
4	A	43	0	30	3	0
4	B	43	0	30	2	0
4	C	43	0	30	3	1
4	D	43	0	30	4	0
5	A	15	0	0	2	0
5	B	15	0	0	1	0
5	C	10	0	0	9	0
5	D	5	0	0	2	0
6	A	8	0	0	34	0
6	B	4	0	0	4	0
6	C	7	0	0	12	0
6	D	4	0	0	7	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	C	5	0	0	0	0
9	A	193	0	0	16	2
9	B	201	0	0	27	0
9	C	205	0	0	16	1
9	D	215	0	0	29	4
All	All	6291	0	5720	260	5

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 23.

All (260) 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:A:105[B]:LEU:HD21	6:A:1149:XE:XE	1.50	1.89
1:A:46[A]:PHE:CD1	6:A:1148:XE:XE	2.39	1.52
1:A:105[B]:LEU:CD2	6:A:1149:XE:XE	2.44	1.41
1:A:46[A]:PHE:CE1	6:A:1148:XE:XE	2.57	1.34
3:C:1[B]:MET:CE	5:C:1144:SO4:O3	1.83	1.25
2:D:26[A]:GLU:OE1	2:D:117[A]:HIS:CE1	1.91	1.24
4:A:1142:HEM:HBB1	6:A:1150:XE:XE	2.19	1.20
1:A:109[B]:LEU:CD1	6:A:1147[B]:XE:XE	2.69	1.19
3:C:34[A]:LEU:HD21	9:D:2005:HOH:O	1.38	1.18
4:A:1142:HEM:CBB	6:A:1150:XE:XE	2.70	1.17
3:C:1[B]:MET:HE3	5:C:1144:SO4:O3	1.00	1.17
4:C:1142:HEM:HBB1	6:C:1150:XE:XE	2.24	1.15
4:C:1142:HEM:CBB	6:C:1150:XE:XE	2.72	1.15
3:C:7[B]:LYS:HE2	3:C:73[B]:VAL:HG12	1.22	1.14
1:A:46[A]:PHE:HD1	6:A:1148:XE:XE	1.93	1.14
3:C:7[B]:LYS:CG	3:C:73[B]:VAL:HG11	1.76	1.13
3:C:14:TRP:HH2	9:C:2043:HOH:O	1.25	1.13
3:C:34[A]:LEU:CD2	9:D:2005:HOH:O	1.88	1.11
3:C:1[B]:MET:HG3	5:C:1144:SO4:O4	1.52	1.09
2:D:143[B]:HIS:HD2	9:D:2137:HOH:O	1.36	1.06
3:C:7[B]:LYS:HG2	3:C:73[B]:VAL:HG11	1.07	1.06
2:D:26[A]:GLU:OE1	2:D:117[A]:HIS:HE1	1.29	1.06
1:A:109[B]:LEU:HD11	6:A:1147[B]:XE:XE	2.36	1.04
1:A:99[A]:LYS:HG3	9:A:2147:HOH:O	1.57	1.02
2:B:12[A]:THR:HG22	9:B:2024:HOH:O	1.60	1.00
3:C:1[B]:MET:HG3	5:C:1144:SO4:S	2.00	1.00
1:A:128:PHE:CE2	6:A:1146[A]:XE:XE	2.94	0.99
3:C:7[B]:LYS:CE	3:C:73[B]:VAL:HG12	1.92	0.98
2:B:101[B]:GLU:HG3	3:C:96[B]:VAL:HG11	1.45	0.98
1:A:109[B]:LEU:HD13	6:A:1147[B]:XE:XE	2.40	0.97
1:A:128:PHE:HE2	6:A:1146[A]:XE:XE	2.25	0.96
3:C:85[B]:ASP:OD1	3:C:89[B]:HIS:CD2	2.19	0.95
3:C:1[B]:MET:CE	9:C:2198:HOH:O	2.14	0.94
3:C:1[B]:MET:HE1	9:C:2198:HOH:O	1.66	0.94
2:D:40[B]:ARG:NH1	9:D:2081:HOH:O	1.97	0.94
2:B:97[B]:HIS:HD2	9:B:2138:HOH:O	1.50	0.93
3:C:1[A]:MET:O	3:C:127[A]:LYS:NZ	2.03	0.92
3:C:7[B]:LYS:HG2	3:C:73[B]:VAL:CG1	1.99	0.92
2:B:121[A]:GLU:CD	9:B:2166:HOH:O	2.08	0.91
2:D:40[B]:ARG:NH2	9:D:2081:HOH:O	2.03	0.91
1:A:96[B]:VAL:HG11	2:D:101[B]:GLU:HG3	1.51	0.90
2:B:101[B]:GLU:HG3	3:C:96[B]:VAL:CG1	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105[B]:LEU:HD11	6:A:1149:XE:XE	2.50	0.89
1:A:7[A]:LYS:HE3	1:A:11:LYS:HE3	1.55	0.89
2:D:40[B]:ARG:CZ	9:D:2081:HOH:O	2.16	0.89
3:C:7[B]:LYS:HE2	3:C:73[B]:VAL:CG1	2.02	0.88
2:D:97[B]:HIS:HD2	9:D:2153:HOH:O	1.54	0.88
2:B:89:SER:HA	2:B:141[B]:LEU:HD23	1.55	0.87
3:C:96[B]:VAL:HG22	9:C:2152:HOH:O	1.73	0.87
4:D:1147:HEM:HBB1	6:D:1149[B]:XE:XE	2.53	0.86
2:D:12[B]:THR:HG22	9:D:2031:HOH:O	1.74	0.86
1:A:96[B]:VAL:CG2	9:A:2148:HOH:O	2.23	0.86
3:C:85[B]:ASP:OD1	3:C:89[B]:HIS:HD2	1.57	0.86
2:D:108[B]:ASN:OD1	9:D:2175:HOH:O	1.96	0.83
3:C:7[B]:LYS:CD	3:C:73[B]:VAL:CG1	2.57	0.83
2:B:121[A]:GLU:OE1	9:B:2166:HOH:O	1.97	0.83
3:C:56[A]:LYS:HG2	9:C:2098:HOH:O	1.79	0.82
1:A:45[A]:HIS:CD2	9:A:2071:HOH:O	2.34	0.81
3:C:1[B]:MET:CE	5:C:1144:SO4:S	2.69	0.80
2:D:104[B]:ARG:NH2	2:D:139[B]:ASN:OD1	2.14	0.80
3:C:1[B]:MET:HE3	5:C:1144:SO4:S	2.22	0.80
1:A:96[B]:VAL:HG23	9:A:2148:HOH:O	1.82	0.80
2:D:108[B]:ASN:ND2	9:D:2175:HOH:O	2.15	0.79
3:C:47[B]:ASP:HB3	3:C:54[B]:GLN:HE21	1.48	0.79
3:C:34[A]:LEU:HD23	9:C:2060:HOH:O	1.83	0.79
3:C:7[B]:LYS:CD	3:C:73[B]:VAL:HG11	2.14	0.78
2:D:3[B]:LEU:HA	2:D:7[B]:GLU:OE2	1.82	0.78
1:A:96[B]:VAL:CG1	2:D:101[B]:GLU:HG3	2.13	0.77
1:A:105[A]:LEU:HD11	6:A:1147[A]:XE:XE	2.63	0.77
1:A:105[B]:LEU:CG	6:A:1149:XE:XE	3.10	0.77
2:B:24:GLY:HA2	2:B:68[B]:LEU:HD22	1.66	0.77
2:D:80:ASN:O	2:D:84[B]:THR:HG23	1.83	0.77
2:D:77[B]:HIS:HB2	2:D:84[B]:THR:HG21	1.68	0.76
4:D:1147:HEM:CBB	6:D:1149[B]:XE:XE	3.12	0.76
2:B:104[B]:ARG:NH2	9:B:2156:HOH:O	2.17	0.76
3:C:47[B]:ASP:HB3	3:C:54[B]:GLN:NE2	2.01	0.76
2:D:1[B]:MET:HG2	9:D:2194:HOH:O	1.86	0.75
3:C:101[A]:LEU:HD13	6:C:1150:XE:XE	2.65	0.75
4:D:1147:HEM:HBB1	6:D:1149[C]:XE:XE	2.65	0.74
1:A:46[A]:PHE:HE1	6:A:1148:XE:XE	2.27	0.73
2:B:3:LEU:HB2	2:B:8[B]:LYS:HG3	1.68	0.73
2:B:110:LEU:O	2:B:114[B]:LEU:HD13	1.88	0.73
2:B:101[B]:GLU:CG	3:C:96[B]:VAL:HG11	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1147:HEM:HBB1	6:B:1151[A]:XE:XE	2.67	0.73
3:C:1[B]:MET:HE2	5:C:1144:SO4:O2	1.90	0.72
2:D:1[B]:MET:CE	9:D:2194:HOH:O	2.37	0.72
1:A:24:TYR:HB3	6:A:1147[B]:XE:XE	2.69	0.71
3:C:96[B]:VAL:CG2	9:C:2152:HOH:O	2.33	0.71
6:C:1149:XE:XE	6:C:1150:XE:XE	3.64	0.71
2:B:110:LEU:HD22	6:B:1151[B]:XE:XE	2.69	0.71
3:C:7[B]:LYS:CE	3:C:73[B]:VAL:CG1	2.67	0.70
1:A:23[A]:GLU:HG2	9:A:2043:HOH:O	1.90	0.70
2:B:103:PHE:CE1	2:B:141[B]:LEU:HD13	2.27	0.70
3:C:1[B]:MET:HG2	9:C:2197:HOH:O	1.92	0.69
3:C:45[A]:HIS:CD2	3:C:45[A]:HIS:H	2.09	0.69
3:C:7[B]:LYS:CD	3:C:73[B]:VAL:HG12	2.22	0.69
2:D:117[A]:HIS:CE1	9:D:2180:HOH:O	2.45	0.69
1:A:13:ALA:HB1	6:A:1151:XE:XE	2.71	0.69
2:D:26[A]:GLU:HG3	5:D:1148:SO4:O2	1.92	0.68
1:A:105[B]:LEU:CD1	6:A:1149:XE:XE	3.18	0.68
3:C:1[B]:MET:CG	5:C:1144:SO4:O4	2.36	0.67
2:D:116[A]:HIS:HD2	2:D:117[A]:HIS:ND1	1.93	0.67
2:D:77[B]:HIS:CB	2:D:84[B]:THR:HG21	2.24	0.67
2:B:24:GLY:CA	2:B:68[B]:LEU:HD22	2.25	0.66
1:A:116[B]:GLU:OE2	5:A:1144:SO4:O2	2.14	0.65
2:D:45:PHE:HA	2:D:59[A]:LYS:HD3	1.76	0.65
2:D:77[B]:HIS:HE1	9:D:2125:HOH:O	1.79	0.65
3:C:127[A]:LYS:NZ	9:C:2173:HOH:O	2.28	0.65
2:B:4:THR:OG1	2:B:7[B]:GLU:HG2	1.96	0.64
2:B:121[A]:GLU:OE1	9:B:2167:HOH:O	2.15	0.64
1:A:141:ARG:O	3:C:1[B]:MET:HB3	1.98	0.64
2:D:110:LEU:HD22	6:D:1149[B]:XE:XE	2.76	0.64
2:D:12[B]:THR:HG21	9:D:2030:HOH:O	1.98	0.64
1:A:96[B]:VAL:HG11	2:D:101[B]:GLU:CG	2.25	0.64
2:B:117[B]:HIS:HD2	5:B:1149[B]:SO4:O3	1.82	0.63
3:C:47[B]:ASP:H	3:C:54[B]:GLN:NE2	1.96	0.63
3:C:30:GLU:OE2	3:C:50[A]:HIS:HD2	1.81	0.63
2:B:65[A]:LYS:HG3	9:B:2039:HOH:O	1.99	0.63
3:C:76[B]:MET:HG2	3:C:80:LEU:HD12	1.79	0.63
1:A:96[B]:VAL:HG22	9:A:2148:HOH:O	1.92	0.62
2:B:82[B]:LYS:HE3	2:B:139[B]:ASN:ND2	2.15	0.62
1:A:1[A]:VAL:HG13	9:C:2185:HOH:O	2.00	0.62
1:A:60[A]:LYS:HD3	9:A:2100:HOH:O	1.99	0.62
2:B:104[A]:ARG:NH2	9:B:2152:HOH:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97[B]:HIS:CD2	9:D:2153:HOH:O	2.37	0.62
3:C:60[B]:LYS:NZ	9:C:2107:HOH:O	2.25	0.62
1:A:57:GLY:O	1:A:61[B]:LYS:HE2	2.00	0.61
2:B:132[B]:LYS:NZ	9:B:2170:HOH:O	2.04	0.61
2:B:116:HIS:HD2	9:B:2055:HOH:O	1.84	0.61
3:C:7[B]:LYS:HD3	3:C:73[B]:VAL:CG1	2.30	0.61
1:A:16[B]:LYS:NZ	1:A:116[B]:GLU:OE2	2.30	0.61
2:D:77[B]:HIS:CE1	9:D:2125:HOH:O	2.51	0.61
3:C:46[A]:PHE:HA	3:C:54[A]:GLN:OE1	2.02	0.60
3:C:47[B]:ASP:H	3:C:54[B]:GLN:HE22	1.48	0.60
1:A:129:LEU:HD21	6:A:1146[B]:XE:XE	2.80	0.60
2:B:131[B]:GLN:HG3	9:B:2169:HOH:O	2.01	0.60
3:C:34[A]:LEU:HD22	9:D:2005:HOH:O	1.70	0.60
1:A:89[A]:HIS:NE2	9:A:2130:HOH:O	2.32	0.60
2:B:21:ASP:OD1	2:B:65[B]:LYS:HG3	2.02	0.59
1:A:60[A]:LYS:HE2	9:A:2106:HOH:O	2.01	0.59
1:A:89[B]:HIS:HD2	9:A:2137:HOH:O	1.86	0.58
1:A:105[B]:LEU:CD2	6:A:1147[B]:XE:XE	3.30	0.58
1:A:105[B]:LEU:HD22	6:A:1147[B]:XE:XE	2.82	0.57
1:A:7[A]:LYS:CE	1:A:11:LYS:HE3	2.32	0.57
2:B:82[B]:LYS:CE	2:B:139[B]:ASN:ND2	2.68	0.57
2:D:3[B]:LEU:HG	2:D:7[B]:GLU:HG3	1.85	0.57
2:D:38:THR:HG22	2:D:102:ASN:HD22	1.68	0.56
3:C:34[A]:LEU:CD2	9:C:2060:HOH:O	2.48	0.56
2:B:121[A]:GLU:OE2	9:B:2166:HOH:O	2.14	0.56
2:B:103:PHE:CZ	2:B:141[B]:LEU:HD13	2.41	0.56
3:C:47[B]:ASP:CB	3:C:54[B]:GLN:NE2	2.69	0.55
1:A:62:VAL:HG11	6:A:1149:XE:XE	2.85	0.55
1:A:105[A]:LEU:CD1	6:A:1147[A]:XE:XE	3.33	0.55
3:C:45[A]:HIS:H	3:C:45[A]:HIS:HD2	1.51	0.55
3:C:1[B]:MET:HE2	5:C:1144:SO4:S	2.46	0.54
3:C:55:VAL:HG22	6:C:1148[B]:XE:XE	2.86	0.54
1:A:2[B]:LEU:O	1:A:7[B]:LYS:HE2	2.08	0.53
2:D:117[B]:HIS:HE1	9:D:2037:HOH:O	1.90	0.53
3:C:7[B]:LYS:CG	3:C:73[B]:VAL:CG1	2.63	0.53
2:B:82[B]:LYS:CE	2:B:139[B]:ASN:HD21	2.21	0.53
2:D:108[B]:ASN:CG	9:D:2175:HOH:O	2.33	0.53
3:C:128:PHE:CE2	6:C:1147[A]:XE:XE	3.40	0.53
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.23	0.53
1:A:45[A]:HIS:CE1	9:A:2074:HOH:O	2.62	0.52
3:C:39:THR:HG22	3:C:97:ASN:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLN:HG2	6:C:1148[B]:XE:XE	2.88	0.52
1:A:128:PHE:CD2	6:A:1146[A]:XE:XE	3.40	0.52
2:D:117[A]:HIS:NE2	9:D:2182:HOH:O	1.86	0.52
3:C:83:LEU:O	3:C:87[A]:HIS:HD2	1.93	0.52
3:C:45[A]:HIS:HE1	4:C:1142:HEM:O2D	1.93	0.51
1:A:1[A]:VAL:CG1	9:C:2185:HOH:O	2.55	0.51
1:A:55:VAL:HG22	6:A:1148:XE:XE	2.88	0.51
1:A:99[B]:LYS:HG3	9:A:2147:HOH:O	2.11	0.51
3:C:55:VAL:HG22	6:C:1148[A]:XE:XE	2.89	0.51
1:A:105[B]:LEU:HD23	6:A:1147[B]:XE:XE	2.88	0.51
1:A:43:PHE:CD2	6:A:1148:XE:XE	3.42	0.51
3:C:62:VAL:HG11	6:C:1149:XE:XE	2.89	0.50
2:B:101[B]:GLU:HG3	3:C:96[B]:VAL:HG12	1.90	0.50
2:B:120[A]:LYS:NZ	9:B:2162:HOH:O	2.44	0.50
1:A:44:PRO:HA	9:A:2069:HOH:O	2.11	0.50
3:C:16:LYS:HG2	3:C:116[A]:GLU:HG2	1.92	0.50
2:D:106:LEU:HD11	6:D:1150:XE:XE	2.90	0.49
2:B:97[B]:HIS:CD2	9:B:2138:HOH:O	2.38	0.49
1:A:75[A]:ASP:OD2	9:A:2114:HOH:O	2.20	0.49
2:B:108[B]:ASN:CG	9:B:2157:HOH:O	2.51	0.49
2:D:1[B]:MET:HG3	2:D:136:GLY:HA3	1.94	0.49
3:C:70:VAL:O	3:C:73[B]:VAL:HG23	2.13	0.49
1:A:94:ASP:OD1	1:A:96[A]:VAL:HG22	2.13	0.48
1:A:62:VAL:CG1	6:A:1149:XE:XE	3.39	0.48
3:C:129:LEU:HD22	6:C:1150:XE:XE	2.91	0.48
2:B:3:LEU:CB	2:B:8[B]:LYS:HG3	2.38	0.48
3:C:4[B]:PRO:HG2	9:C:2009:HOH:O	2.14	0.48
2:B:7[A]:GLU:OE2	2:B:132[A]:LYS:NZ	2.39	0.48
2:B:121[A]:GLU:CG	9:B:2165:HOH:O	2.61	0.48
3:C:127[B]:LYS:NZ	9:C:2174:HOH:O	2.30	0.47
1:A:129:LEU:HD22	6:A:1150:XE:XE	2.93	0.47
2:D:117[A]:HIS:ND1	9:D:2180:HOH:O	2.35	0.47
2:D:82[A]:LYS:NZ	2:D:139[A]:ASN:HD21	2.12	0.47
2:D:71:PHE:CD1	6:D:1149[B]:XE:XE	3.45	0.47
2:D:104[B]:ARG:NH2	2:D:139[B]:ASN:CG	2.68	0.47
2:D:4:THR:N	2:D:7[B]:GLU:HG2	2.30	0.47
2:D:97[A]:HIS:HD2	9:D:2153:HOH:O	1.96	0.47
2:D:82[A]:LYS:HZ2	2:D:143[A]:HIS:CD2	2.33	0.47
1:A:14[A]:TRP:CE3	6:A:1146[A]:XE:XE	3.46	0.46
2:D:1[B]:MET:HE2	9:D:2194:HOH:O	2.08	0.46
2:B:120[A]:LYS:HG3	9:B:2161:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1[B]:MET:HG3	2:D:136:GLY:CA	2.45	0.46
2:B:65[A]:LYS:HE3	9:B:2039:HOH:O	2.15	0.46
2:B:1[A]:MET:HE1	9:B:2172:HOH:O	2.15	0.45
2:D:116[A]:HIS:CE1	9:D:2178:HOH:O	2.69	0.45
2:B:24:GLY:N	2:B:68[B]:LEU:HD22	2.32	0.45
1:A:55:VAL:HA	6:A:1148:XE:XE	2.95	0.45
2:B:121[A]:GLU:HG3	9:B:2165:HOH:O	2.16	0.45
3:C:1[B]:MET:HE3	9:C:2198:HOH:O	1.98	0.45
2:D:116[A]:HIS:CD2	9:D:2180:HOH:O	2.69	0.45
2:D:26[B]:GLU:OE1	5:D:1148:SO4:O3	2.35	0.45
2:B:38:THR:HG22	2:B:102:ASN:ND2	2.31	0.45
2:B:103:PHE:CD1	4:B:1147:HEM:HBB2	2.52	0.45
2:B:106:LEU:HD11	6:B:1152:XE:XE	2.95	0.45
2:B:89:SER:HA	2:B:141[B]:LEU:CD2	2.38	0.45
2:B:24:GLY:HA2	2:B:68[B]:LEU:CD2	2.44	0.44
1:A:45[A]:HIS:HD2	9:A:2071:HOH:O	1.87	0.44
2:D:120[A]:LYS:HE3	2:D:120[A]:LYS:HA	2.00	0.44
3:C:129:LEU:HD21	6:C:1147[B]:XE:XE	2.95	0.44
1:A:141:ARG:O	3:C:1[B]:MET:CB	2.64	0.44
1:A:45[A]:HIS:CD2	9:A:2074:HOH:O	2.71	0.43
3:C:94:ASP:OD2	3:C:96[A]:VAL:HG22	2.18	0.43
2:B:65[A]:LYS:CE	9:B:2039:HOH:O	2.65	0.43
2:B:97[B]:HIS:HE1	9:B:2147:HOH:O	2.02	0.43
1:A:114[A]:PRO:HD2	5:A:1144:SO4:O3	2.19	0.43
2:D:66:LYS:HD3	4:D:1147:HEM:HAA1	2.01	0.43
1:A:103:HIS:CE1	2:B:108[B]:ASN:HB2	2.53	0.42
2:B:108[B]:ASN:ND2	9:B:2157:HOH:O	2.51	0.42
2:D:82[A]:LYS:HZ1	2:D:139[A]:ASN:HD21	1.66	0.42
1:A:68[B]:ASN:ND2	1:A:72[B]:HIS:ND1	2.67	0.42
2:B:121[A]:GLU:HG2	9:B:2165:HOH:O	2.20	0.42
2:B:82[B]:LYS:HE3	2:B:139[B]:ASN:HD21	1.81	0.42
2:D:77[A]:HIS:HD2	9:D:2134:HOH:O	2.03	0.42
1:A:109[B]:LEU:HD12	6:A:1147[B]:XE:XE	2.89	0.42
1:A:7[A]:LYS:HG3	1:A:73:VAL:HG11	2.00	0.42
2:B:68[A]:LEU:HD13	6:B:1152:XE:XE	2.97	0.42
2:B:38:THR:HG22	2:B:102:ASN:HD22	1.85	0.42
2:D:7[B]:GLU:OE2	2:D:132:LYS:NZ	2.44	0.42
3:C:1[A]:MET:HG3	3:C:1[A]:MET:O	2.20	0.42
2:D:68:LEU:HD13	6:D:1150:XE:XE	2.98	0.42
2:D:77[A]:HIS:HE1	9:D:2129:HOH:O	2.03	0.42
2:B:7[B]:GLU:HA	2:B:7[B]:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61[B]:LYS:HD3	4:A:1142:HEM:CAA	2.51	0.41
1:A:24:TYR:CB	6:A:1147[B]:XE:XE	3.46	0.41
2:D:84[B]:THR:HG22	9:D:2144:HOH:O	2.20	0.41
2:B:104[A]:ARG:CZ	9:B:2152:HOH:O	2.69	0.41
3:C:13:ALA:HB1	6:C:1151:XE:XE	2.99	0.41
2:B:139[A]:ASN:ND2	9:B:2175:HOH:O	2.54	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2052:HOH:O	9:D:2024:HOH:O[2_656]	1.70	0.50
1:A:45[A]:HIS:CE1	4:C:1142:HEM:O2D[1_556]	1.95	0.25
9:A:2136:HOH:O	9:D:2125:HOH:O[2_656]	2.09	0.11
3:C:1[A]:MET:SD	9:D:2123:HOH:O[2_656]	2.15	0.05
9:C:2116:HOH:O	9:D:2012:HOH:O[2_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	174/141 (123%)	170 (98%)	4 (2%)	0	100	100
2	B	186/146 (127%)	184 (99%)	2 (1%)	0	100	100
2	D	177/146 (121%)	176 (99%)	1 (1%)	0	100	100
3	C	173/141 (123%)	165 (95%)	8 (5%)	0	100	100
All	All	710/574 (124%)	695 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	149/113 (132%)	145 (97%)	4 (3%)	44 9
2	B	161/118 (136%)	159 (99%)	2 (1%)	71 35
2	D	152/118 (129%)	148 (97%)	4 (3%)	46 9
3	C	148/113 (131%)	140 (95%)	8 (5%)	22 2
All	All	610/462 (132%)	592 (97%)	18 (3%)	57 7

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	VAL
1	A	1[B]	VAL
1	A	2[A]	LEU
1	A	2[B]	LEU
2	B	120[A]	LYS
2	B	120[B]	LYS
3	C	34[A]	LEU
3	C	34[B]	LEU
3	C	78[A]	ASN
3	C	78[B]	ASN
3	C	99[A]	LYS
3	C	99[B]	LYS
3	C	101[A]	LEU
3	C	101[B]	LEU
2	D	117[A]	HIS
2	D	117[B]	HIS
2	D	120[A]	LYS
2	D	120[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	116	HIS
3	C	97	ASN
2	D	102	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 26 are monoatomic - leaving 14 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	$\# Z > 2$
5	SO4	A	1144	1	4,4,4	0.42	0	6,6,6	0.59	0
5	SO4	B	1149[B]	-	4,4,4	0.80	0	6,6,6	1.17	0
4	HEM	B	1147	2	27,50,50	1.60	2 (7%)	17,82,82	1.73	5 (29%)
5	SO4	D	1148	2	4,4,4	0.18	0	6,6,6	0.67	0
4	HEM	C	1142	3	27,50,50	1.41	4 (14%)	17,82,82	1.52	5 (29%)
5	SO4	C	1143	-	4,4,4	0.14	0	6,6,6	0.62	0
5	SO4	C	1144	-	4,4,4	0.11	0	6,6,6	0.44	0
5	SO4	A	1143	-	4,4,4	0.20	0	6,6,6	0.30	0
4	HEM	A	1142	1	27,50,50	1.42	3 (11%)	17,82,82	1.43	3 (17%)
4	HEM	D	1147	2	27,50,50	1.44	4 (14%)	17,82,82	1.54	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	1148	-	4,4,4	0.28	0	6,6,6	0.76	0
5	SO4	A	1145	-	4,4,4	0.30	0	6,6,6	1.28	1 (16%)
5	SO4	B	1149[A]	-	4,4,4	0.15	0	6,6,6	1.17	1 (16%)
8	PO4	C	1145	-	4,4,4	1.48	1 (25%)	6,6,6	1.66	1 (16%)

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	1142	3	-	0/6/54/54	-
4	HEM	A	1142	1	-	0/6/54/54	-
4	HEM	B	1147	2	-	0/6/54/54	-
4	HEM	D	1147	2	-	0/6/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1147	HEM	C3B-C2B	-4.98	1.33	1.40
4	D	1147	HEM	C3B-C2B	-4.19	1.34	1.40
4	B	1147	HEM	C3C-C2C	-3.87	1.35	1.40
4	A	1142	HEM	C3B-C2B	-3.79	1.35	1.40
4	A	1142	HEM	C3C-C2C	-3.70	1.35	1.40
4	C	1142	HEM	C3C-C2C	-3.03	1.36	1.40
4	C	1142	HEM	C3B-C2B	-3.03	1.36	1.40
4	C	1142	HEM	CMA-C3A	2.35	1.56	1.51
4	D	1147	HEM	C3C-C2C	-2.32	1.37	1.40
8	C	1145	PO4	P-O3	-2.27	1.47	1.54
4	D	1147	HEM	C1B-C2B	2.23	1.47	1.42
4	C	1142	HEM	CAA-C2A	2.11	1.55	1.52
4	A	1142	HEM	C3D-C2D	2.08	1.43	1.37
4	D	1147	HEM	CAD-C3D	-2.03	1.48	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1147	HEM	CBD-CAD-C3D	-4.04	105.04	112.48
4	A	1142	HEM	CMA-C3A-C4A	-3.69	122.79	128.46
8	C	1145	PO4	O4-P-O1	-3.14	99.39	110.89
4	C	1142	HEM	C4A-C3A-C2A	3.09	109.14	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1147	HEM	CMC-C2C-C3C	2.91	130.12	124.68
4	D	1147	HEM	CMC-C2C-C3C	2.90	130.10	124.68
4	D	1147	HEM	CBA-CAA-C2A	-2.85	107.23	112.49
5	A	1145	SO4	O4-S-O3	-2.76	97.26	109.06
4	B	1147	HEM	CMA-C3A-C4A	-2.71	124.30	128.46
4	A	1142	HEM	CMA-C3A-C2A	2.60	129.84	124.94
4	C	1142	HEM	CMA-C3A-C4A	-2.58	124.51	128.46
4	A	1142	HEM	CMC-C2C-C3C	2.54	129.42	124.68
4	C	1142	HEM	CMC-C2C-C3C	2.51	129.37	124.68
4	D	1147	HEM	CMB-C2B-C3B	2.45	129.26	124.68
4	B	1147	HEM	CBA-CAA-C2A	-2.41	108.05	112.49
4	C	1142	HEM	CMB-C2B-C3B	2.36	129.09	124.68
4	D	1147	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
4	B	1147	HEM	C4C-C3C-C2C	2.10	108.36	106.90
4	C	1142	HEM	CBD-CAD-C3D	-2.02	108.76	112.48
5	B	1149[A]	SO4	O3-S-O1	2.02	119.83	109.31

There are no chirality outliers.

There are no torsion outliers.

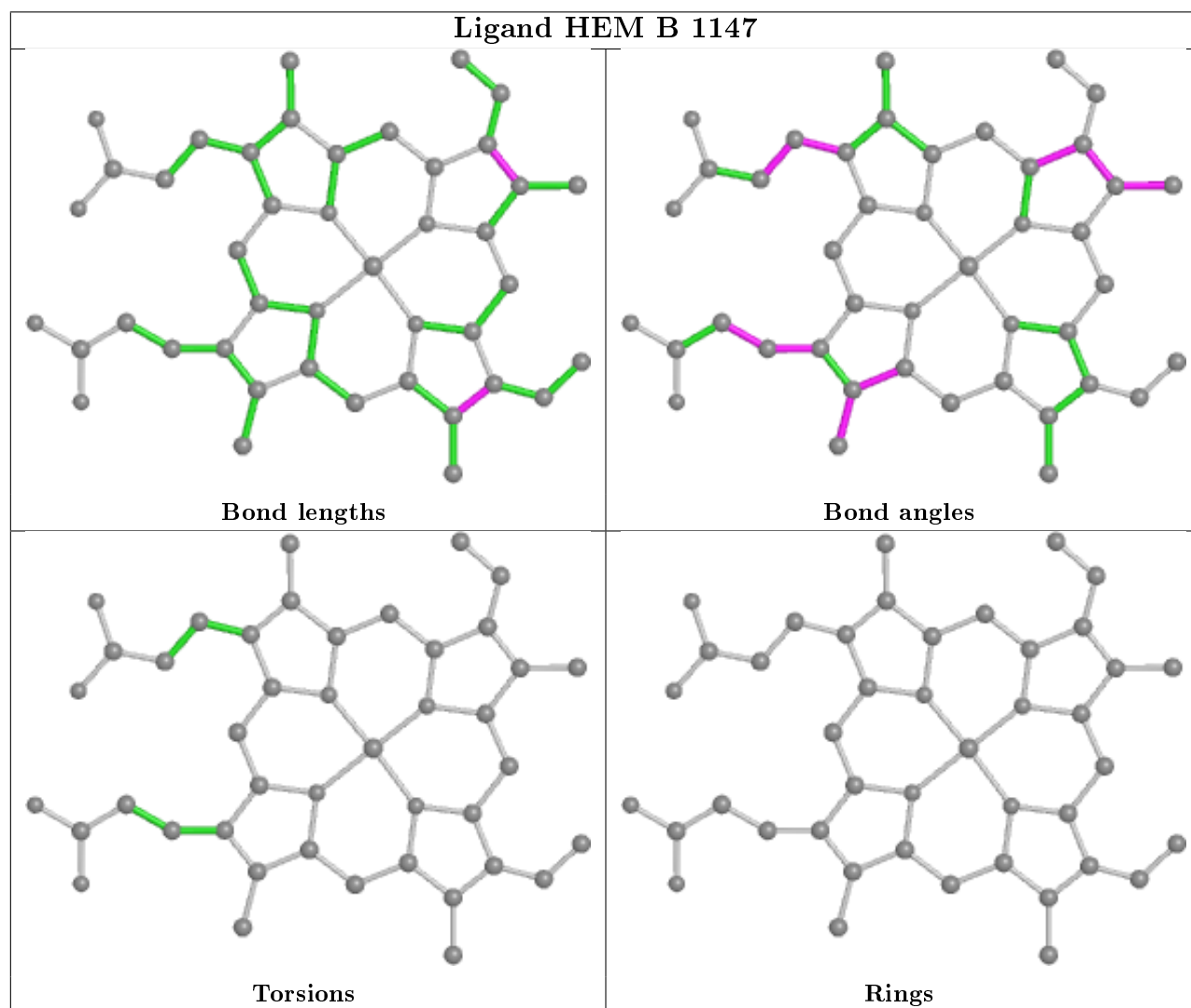
There are no ring outliers.

8 monomers are involved in 27 short contacts:

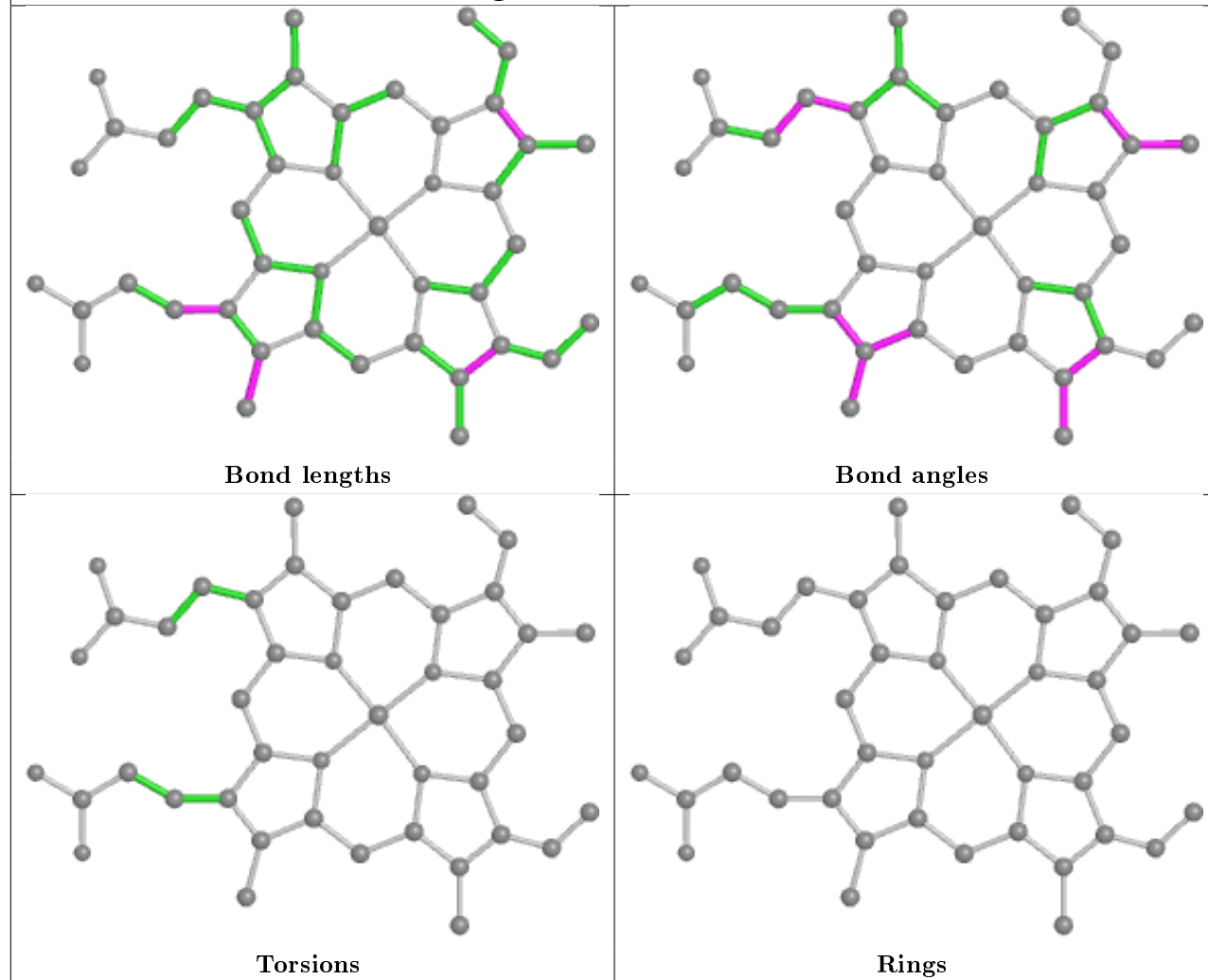
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1144	SO4	2	0
5	B	1149[B]	SO4	1	0
4	B	1147	HEM	2	0
5	D	1148	SO4	2	0
4	C	1142	HEM	3	1
5	C	1144	SO4	9	0
4	A	1142	HEM	3	0
4	D	1147	HEM	4	0

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.

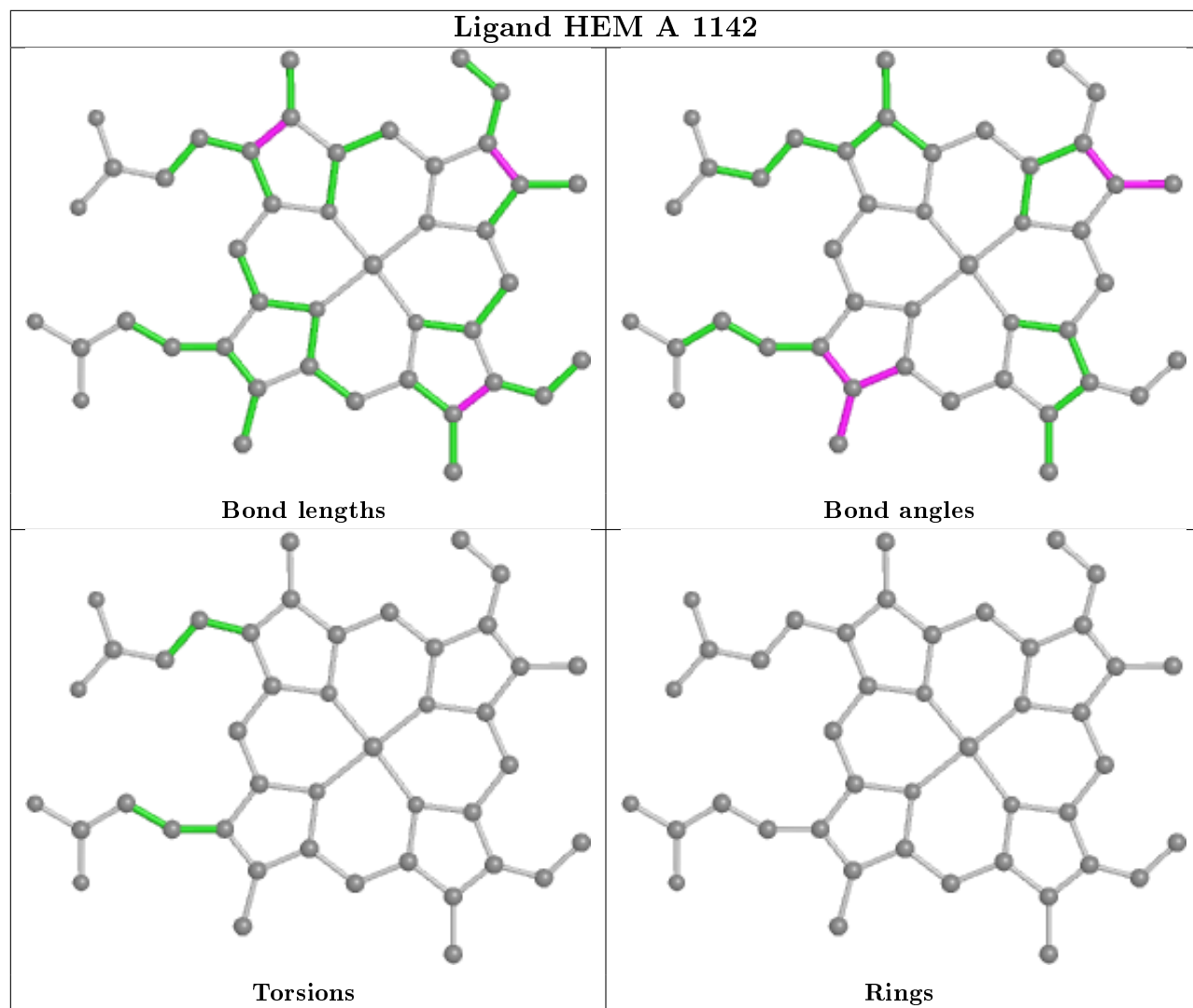
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

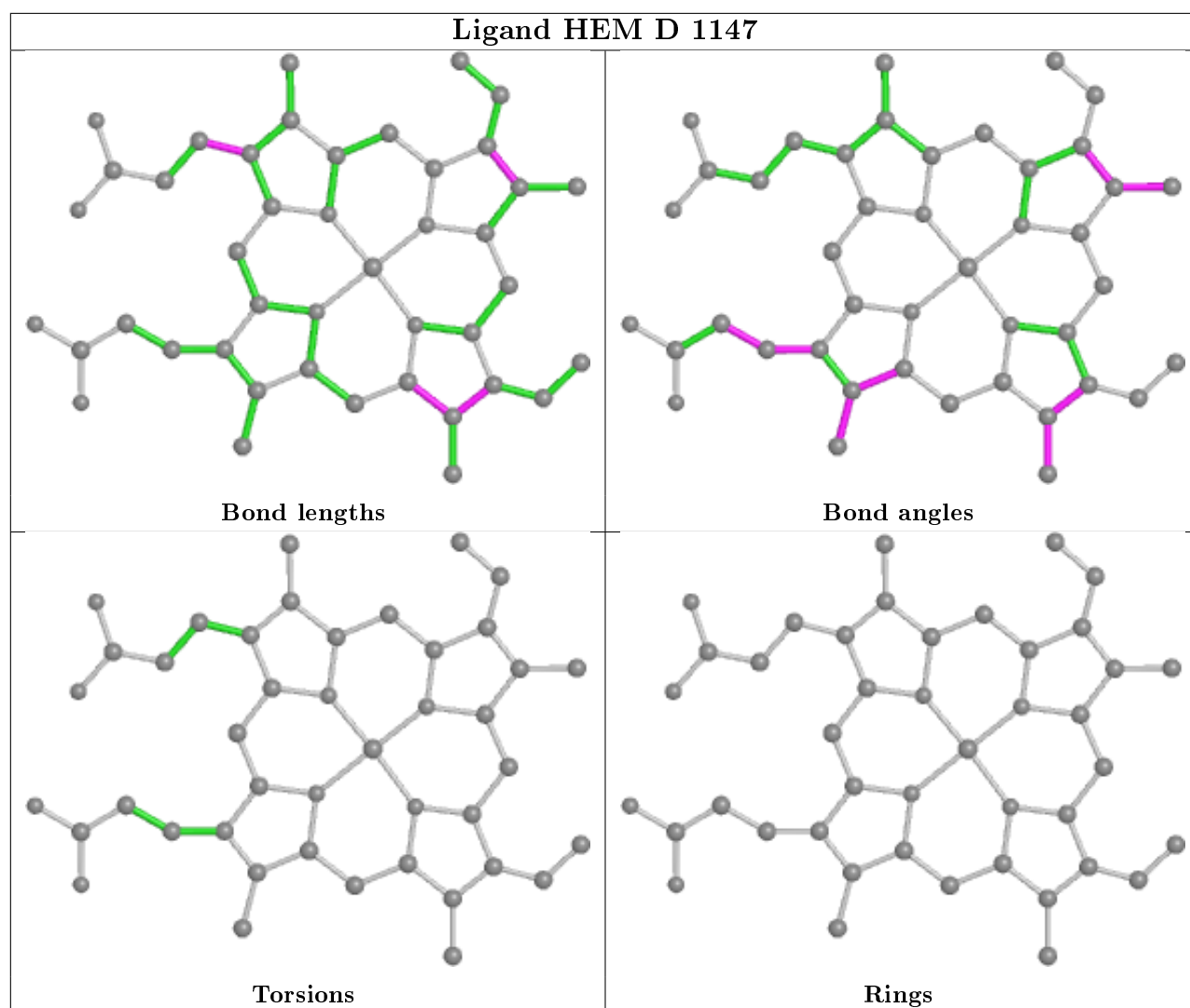


Ligand HEM C 1142



Ligand HEM A 1142





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	141/141 (100%)	2.38	80 (56%) 0 1	8, 11, 18, 25	1 (0%)
2	B	146/146 (100%)	2.58	95 (65%) 0 0	8, 11, 22, 32	4 (2%)
2	D	146/146 (100%)	2.38	93 (63%) 0 0	8, 11, 17, 27	0
3	C	141/141 (100%)	2.55	87 (61%) 0 0	8, 11, 20, 24	0
All	All	574/574 (100%)	2.47	355 (61%) 0 0	8, 11, 20, 32	5 (0%)

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2[A]	HIS	11.8
1	A	2[A]	LEU	9.6
1	A	1[A]	VAL	9.4
2	D	2[A]	HIS	8.6
2	B	1[A]	MET	7.6
1	A	74[A]	ASP	7.5
3	C	1[A]	MET	7.5
2	B	3	LEU	7.1
1	A	45[A]	HIS	6.9
3	C	78[A]	ASN	6.8
3	C	74[A]	ASP	6.5
3	C	2	LEU	6.2
3	C	48	LEU	6.2
2	B	8[A]	LYS	5.8
1	A	14[A]	TRP	5.7
2	B	5[A]	PRO	5.7
2	B	141[A]	LEU	5.7
3	C	19	ALA	5.6
1	A	75[A]	ASP	5.5
3	C	73[A]	VAL	5.3
1	A	105[A]	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	1[A]	MET	5.1
2	B	48	LEU	5.0
2	D	3[A]	LEU	4.8
2	B	76	ALA	4.7
2	B	15	TRP	4.7
2	B	50	THR	4.7
3	C	71	ALA	4.7
2	B	77[A]	HIS	4.5
3	C	8	THR	4.5
1	A	109[A]	LEU	4.4
3	C	89[A]	HIS	4.4
3	C	75[A]	ASP	4.4
3	C	34[A]	LEU	4.3
3	C	60[A]	LYS	4.3
3	C	20[A]	HIS	4.3
2	D	8[A]	LYS	4.3
2	B	4	THR	4.2
2	D	48	LEU	4.1
2	B	68[A]	LEU	4.1
3	C	4[A]	PRO	4.1
2	B	6[A]	GLU	4.0
3	C	80	LEU	4.0
3	C	46[A]	PHE	4.0
2	B	82[A]	LYS	4.0
3	C	99[A]	LYS	3.9
2	D	34	VAL	3.9
2	B	112	CYS	3.9
2	B	45	PHE	3.9
2	B	104[A]	ARG	3.9
1	A	33	PHE	3.8
3	C	33	PHE	3.8
2	B	9[A]	SER	3.8
1	A	56[A]	LYS	3.8
2	B	12[A]	THR	3.8
3	C	37[A]	PRO	3.8
3	C	90[A]	LYS	3.8
3	C	45[A]	HIS	3.8
2	D	41	PHE	3.8
1	A	60[A]	LYS	3.8
2	D	33	VAL	3.7
1	A	117	PHE	3.7
3	C	50[A]	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	82	ALA	3.7
3	C	101[A]	LEU	3.7
2	B	118	PHE	3.7
2	D	96	LEU	3.6
1	A	71	ALA	3.6
2	B	18	VAL	3.6
2	B	49[A]	SER	3.6
2	B	7[A]	GLU	3.6
2	D	49	SER	3.6
1	A	23[A]	GLU	3.6
2	B	93[A]	CYS	3.5
2	D	137	VAL	3.5
2	D	122	PHE	3.5
2	B	37	TRP	3.5
3	C	136	LEU	3.5
2	D	43[A]	GLU	3.5
2	D	134	VAL	3.5
1	A	50[A]	HIS	3.5
3	C	93	VAL	3.4
3	C	18	GLY	3.4
2	B	42	PHE	3.4
2	B	65[A]	LYS	3.4
3	C	77	PRO	3.4
3	C	3	SER	3.4
1	A	73	VAL	3.4
2	B	34	VAL	3.4
3	C	81[A]	SER	3.3
3	C	98	PHE	3.3
2	B	138	ALA	3.3
2	D	82[A]	LYS	3.3
2	D	110	LEU	3.3
1	A	89[A]	HIS	3.3
3	C	140	TYR	3.3
2	D	79[A]	ASP	3.3
3	C	47[A]	ASP	3.3
2	D	68	LEU	3.2
2	B	28	TYR	3.2
2	D	61[A]	LYS	3.2
2	B	80[A]	ASN	3.2
2	D	120[A]	LYS	3.2
2	D	15	TRP	3.2
3	C	24	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	64[A]	ASP	3.2
2	B	33	VAL	3.2
3	C	86	LEU	3.2
2	B	109[A]	VAL	3.2
2	D	22[A]	GLU	3.1
2	D	143[A]	HIS	3.1
2	D	146	HIS	3.1
2	B	88	LEU	3.1
3	C	79	ALA	3.1
2	D	104[A]	ARG	3.1
1	A	10[A]	VAL	3.1
2	D	98	VAL	3.1
3	C	106	LEU	3.1
2	D	37	TRP	3.1
1	A	19	ALA	3.1
3	C	53	ALA	3.1
1	A	62	VAL	3.1
2	B	11	VAL	3.1
1	A	101	LEU	3.1
2	D	109	VAL	3.1
2	D	133	VAL	3.1
2	B	60	VAL	3.0
2	B	52[A]	ASP	3.0
2	D	144[A]	LYS	3.0
2	D	42	PHE	3.0
2	D	54	VAL	3.0
1	A	48	LEU	3.0
2	B	61[A]	LYS	2.9
2	B	95[A]	LYS	2.9
2	B	98	VAL	2.9
3	C	85[A]	ASP	2.9
2	B	75[A]	LEU	2.9
2	D	5	PRO	2.9
3	C	66	LEU	2.9
2	B	146	HIS	2.9
1	A	46[A]	PHE	2.9
2	B	125[A]	PRO	2.9
1	A	136	LEU	2.9
2	D	75	LEU	2.9
1	A	49[A]	SER	2.9
2	D	6[A]	GLU	2.9
2	D	45	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	2.9
1	A	107	VAL	2.9
2	D	60	VAL	2.9
3	C	10	VAL	2.9
3	C	113	LEU	2.9
2	B	72[A]	SER	2.9
2	D	128	ALA	2.9
1	A	98	PHE	2.9
2	B	41	PHE	2.9
2	D	108[A]	ASN	2.9
1	A	55	VAL	2.8
1	A	70	VAL	2.8
1	A	34	LEU	2.8
3	C	114	PRO	2.8
3	C	14	TRP	2.8
2	D	97[A]	HIS	2.8
2	D	103	PHE	2.8
1	A	96[A]	VAL	2.8
3	C	22	GLY	2.8
2	B	31	LEU	2.8
2	B	32	LEU	2.8
1	A	108	THR	2.8
3	C	76[A]	MET	2.8
2	D	67	VAL	2.8
2	D	105	LEU	2.8
2	D	114	LEU	2.8
1	A	5	ALA	2.8
3	C	135	VAL	2.7
2	B	58	PRO	2.7
2	B	97[A]	HIS	2.7
2	D	7[A]	GLU	2.7
1	A	140	TYR	2.7
2	B	111	VAL	2.7
2	B	113	VAL	2.7
2	D	11	VAL	2.7
2	D	80	ASN	2.7
2	D	116[A]	HIS	2.7
3	C	44	PRO	2.7
1	A	24	TYR	2.7
1	A	29	TYR	2.7
2	B	35	TYR	2.7
3	C	88	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	106	LEU	2.7
3	C	104	CYS	2.7
2	B	84[A]	THR	2.7
2	D	145	TYR	2.7
1	A	36	PHE	2.7
1	A	110	ALA	2.7
2	D	53	ALA	2.7
2	D	20	VAL	2.6
2	D	136	GLY	2.6
3	C	83	LEU	2.6
3	C	42	TYR	2.6
2	B	51	PRO	2.6
2	B	124	PRO	2.6
1	A	17	VAL	2.6
2	B	126	VAL	2.6
3	C	107	VAL	2.6
2	D	94	ASP	2.6
3	C	72[A]	HIS	2.6
2	B	114[A]	LEU	2.6
2	D	32	LEU	2.6
3	C	100	LEU	2.6
3	C	125	LEU	2.6
3	C	13	ALA	2.6
3	C	29	TYR	2.6
2	B	54	VAL	2.6
1	A	80	LEU	2.6
1	A	91	LEU	2.6
2	D	31	LEU	2.6
2	D	88	LEU	2.6
2	D	115	ALA	2.6
2	D	117[A]	HIS	2.6
2	B	145	TYR	2.6
3	C	128	PHE	2.6
1	A	41	THR	2.5
2	B	67	VAL	2.5
3	C	62	VAL	2.5
3	C	96[A]	VAL	2.5
1	A	104	CYS	2.5
2	B	130	TYR	2.5
2	D	112	CYS	2.5
1	A	43	PHE	2.5
1	A	128	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	122	PHE	2.5
2	D	87[A]	THR	2.5
2	D	123	THR	2.5
2	B	13	ALA	2.5
2	B	115	ALA	2.5
1	A	100	LEU	2.5
1	A	39	THR	2.5
2	B	119	GLY	2.5
3	C	21	ALA	2.5
2	B	20	VAL	2.5
2	B	137	VAL	2.5
2	B	81	LEU	2.5
3	C	7[A]	LYS	2.5
2	D	93	CYS	2.5
1	A	93	VAL	2.4
1	A	7[A]	LYS	2.4
1	A	76[A]	MET	2.4
1	A	6	ASP	2.4
1	A	20[A]	HIS	2.4
1	A	90[A]	LYS	2.4
1	A	119	PRO	2.4
3	C	55	VAL	2.4
2	B	106	LEU	2.4
3	C	32	MET	2.4
1	A	28	ALA	2.4
2	D	13	ALA	2.4
3	C	12	ALA	2.4
3	C	59	GLY	2.4
2	D	50	THR	2.4
1	A	106	LEU	2.4
1	A	53	ALA	2.4
2	D	27	ALA	2.4
3	C	110	ALA	2.4
1	A	42	TYR	2.4
2	B	43[A]	GLU	2.3
3	C	41	THR	2.3
1	A	99[A]	LYS	2.3
2	B	129	ALA	2.3
2	B	140	ALA	2.3
2	D	10	ALA	2.3
2	D	142	ALA	2.3
2	D	78	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	91	LEU	2.3
3	C	109	LEU	2.3
2	B	19[A]	ASN	2.3
1	A	4	PRO	2.3
2	B	36	PRO	2.3
2	B	133	VAL	2.3
2	D	113	VAL	2.3
3	C	17	VAL	2.3
3	C	132	VAL	2.3
1	A	83	LEU	2.3
2	D	81	LEU	2.3
1	A	22	GLY	2.3
2	D	56	GLY	2.3
2	D	125	PRO	2.3
3	C	117	PHE	2.3
1	A	61[A]	LYS	2.3
2	B	90[A]	GLU	2.3
3	C	123	ALA	2.3
2	B	71	PHE	2.3
2	D	118	PHE	2.3
1	A	85[A]	ASP	2.2
2	D	111	VAL	2.2
3	C	121	VAL	2.2
2	D	141	LEU	2.2
3	C	116[A]	GLU	2.2
2	B	103	PHE	2.2
3	C	36	PHE	2.2
3	C	43	PHE	2.2
2	B	128	ALA	2.2
2	D	69	GLY	2.2
3	C	68	ASN	2.2
1	A	131[A]	SER	2.2
2	D	44	SER	2.2
2	B	73	ASP	2.2
1	A	65	ALA	2.2
2	B	53	ALA	2.2
3	C	28	ALA	2.2
2	B	102	ASN	2.2
2	D	100	PRO	2.2
3	C	56[A]	LYS	2.2
1	A	8	THR	2.2
2	B	134	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	127[A]	LYS	2.2
2	D	40[A]	ARG	2.2
1	A	82	ALA	2.2
2	D	70	ALA	2.1
3	C	26	ALA	2.1
2	B	117[A]	HIS	2.1
2	B	132[A]	LYS	2.1
2	B	85	PHE	2.1
1	A	139[A]	LYS	2.1
2	D	17[A]	LYS	2.1
2	B	121[A]	GLU	2.1
2	D	18	VAL	2.1
1	A	26	ALA	2.1
3	C	69	ALA	2.1
1	A	38	THR	2.1
1	A	137	THR	2.1
2	D	4	THR	2.1
1	A	86	LEU	2.1
1	A	129	LEU	2.1
2	B	105	LEU	2.1
2	D	59[A]	LYS	2.1
2	B	100	PRO	2.1
1	A	69	ALA	2.1
1	A	111	ALA	2.1
3	C	39	THR	2.1
2	B	120[A]	LYS	2.1
2	B	14	LEU	2.1
2	B	110	LEU	2.1
2	D	71	PHE	2.1
2	D	52[A]	ASP	2.0
1	A	92	ARG	2.0
2	B	47	ASP	2.0
1	A	84[A]	SER	2.0
2	D	83	GLY	2.0
2	D	12[A]	THR	2.0
2	D	84[A]	THR	2.0
3	C	111	ALA	2.0
2	B	79	ASP	2.0
2	D	23	VAL	2.0
2	D	139[A]	ASN	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 carbohydrates 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
7	K	A	1153	1/1	0.47	0.15	59,59,59,59	0
5	SO4	C	1144	5/5	0.75	0.23	13,14,17,17	5
5	SO4	C	1143	5/5	0.76	0.27	10,22,23,25	5
5	SO4	D	1148	5/5	0.81	0.26	11,15,18,21	5
5	SO4	A	1143	5/5	0.82	0.17	24,26,28,28	5
5	SO4	A	1144	5/5	0.83	0.19	16,23,25,27	5
5	SO4	B	1148	5/5	0.83	0.20	17,18,22,23	5
6	XE	C	1151	1/1	0.83	0.47	56,56,56,56	0
8	PO4	C	1145	5/5	0.90	0.15	15,16,17,20	5
5	SO4	A	1145	5/5	0.90	0.25	11,15,16,17	5
5	SO4	B	1149[A]	5/5	0.91	0.21	12,16,18,19	5
5	SO4	B	1149[B]	5/5	0.91	0.21	10,12,14,14	5
7	K	B	1150	1/1	0.93	0.31	32,32,32,32	1
6	XE	B	1152	1/1	0.95	0.19	17,17,17,17	1
6	XE	D	1150	1/1	0.95	0.41	21,21,21,21	1
7	K	C	1146	1/1	0.96	0.09	21,21,21,21	1
4	HEM	C	1142	43/43	0.96	0.15	7,9,20,23	0
4	HEM	B	1147	43/43	0.97	0.18	7,9,21,23	0
4	HEM	A	1142	43/43	0.97	0.15	7,8,22,27	0
4	HEM	D	1147	43/43	0.97	0.16	7,7,14,24	0
6	XE	A	1148	1/1	0.98	0.21	19,19,19,19	1
6	XE	A	1146[B]	1/1	0.99	0.11	22,22,22,22	1
6	XE	A	1150	1/1	0.99	0.13	12,12,12,12	1
6	XE	A	1151	1/1	0.99	0.11	15,15,15,15	1
6	XE	A	1146[A]	1/1	0.99	0.11	16,16,16,16	1
6	XE	A	1147[B]	1/1	0.99	0.10	19,19,19,19	1
6	XE	D	1149[C]	1/1	0.99	0.12	14,14,14,14	1

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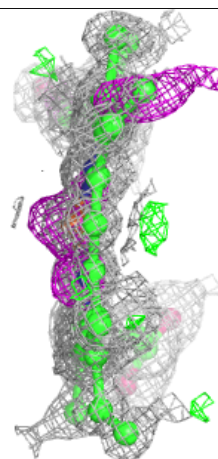
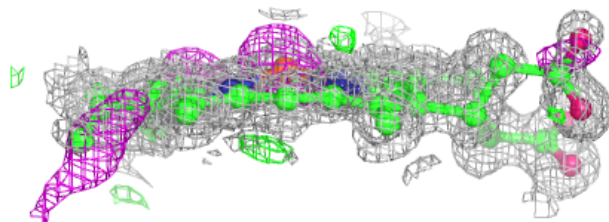
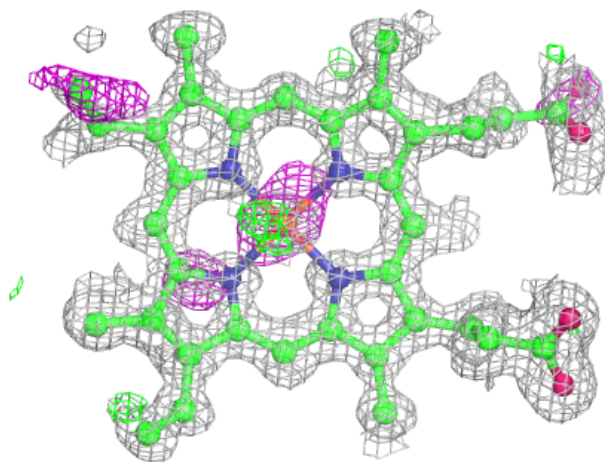
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	XE	C	1148[B]	1/1	0.99	0.11	15,15,15,15	1
6	XE	D	1149[B]	1/1	0.99	0.12	28,28,28,28	1
6	XE	C	1148[A]	1/1	0.99	0.11	14,14,14,14	1
6	XE	A	1147[A]	1/1	0.99	0.10	17,17,17,17	1
6	XE	B	1151[A]	1/1	0.99	0.11	12,12,12,12	1
6	XE	D	1149[A]	1/1	0.99	0.12	10,10,10,10	1
6	XE	B	1151[B]	1/1	0.99	0.11	20,20,20,20	1
6	XE	C	1150	1/1	0.99	0.15	14,14,14,14	1
6	XE	B	1151[C]	1/1	0.99	0.11	18,18,18,18	1
6	XE	A	1149	1/1	1.00	0.11	10,10,10,10	1
6	XE	C	1147[A]	1/1	1.00	0.10	14,14,14,14	1
6	XE	C	1149	1/1	1.00	0.11	12,12,12,12	1
6	XE	C	1147[B]	1/1	1.00	0.10	21,21,21,21	1

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.

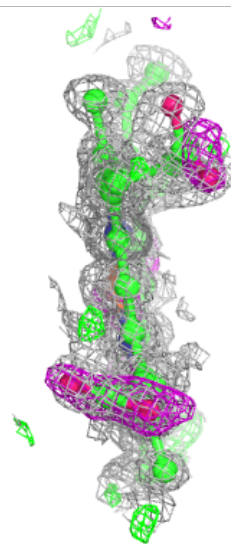
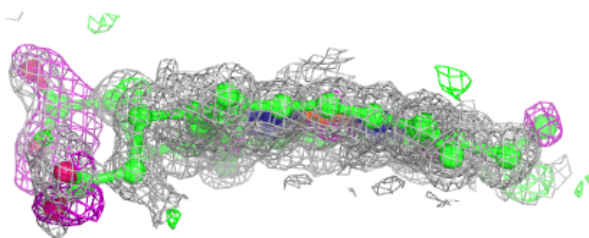
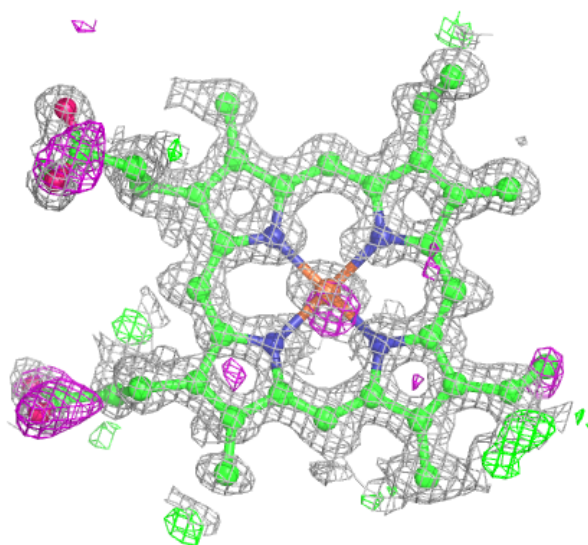
Electron density around HEM C 1142:

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



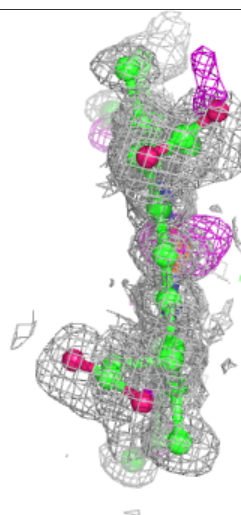
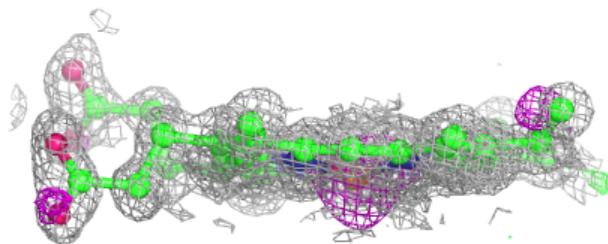
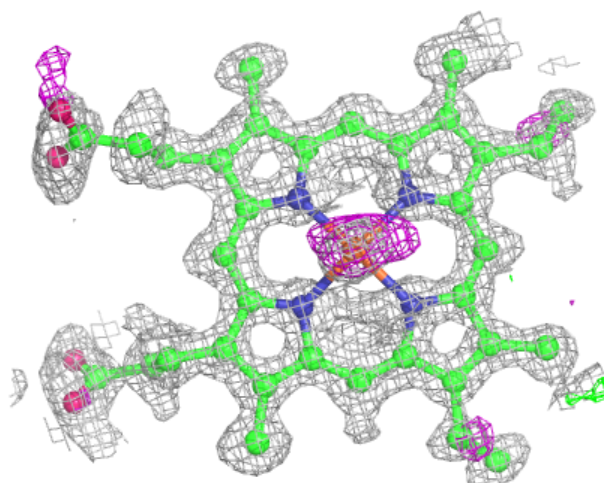
Electron density around HEM B 1147:

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



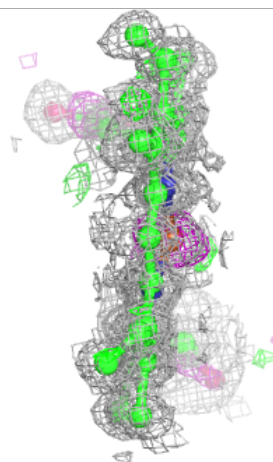
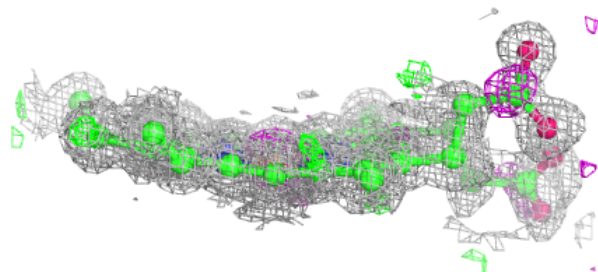
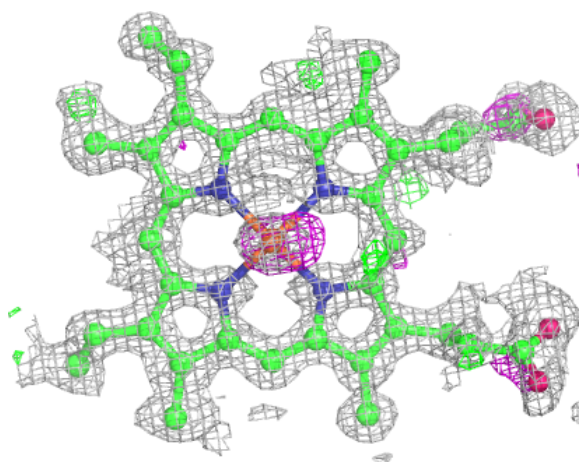
Electron density around HEM A 1142:

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



Electron density around HEM D 1147:

$2mF_o-DF_c$ (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.