Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 03:39 am BST

PDB ID	:	1OAF / pdb_00001oaf
Title	:	Ascobate peroxidase from soybean cytosol in complex with ascorbate
Authors	:	Sharp, K.H.; Raven, E.L.; Moody, P.C.E.
Deposited on	:	2003-01-13
Resolution	:	1.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

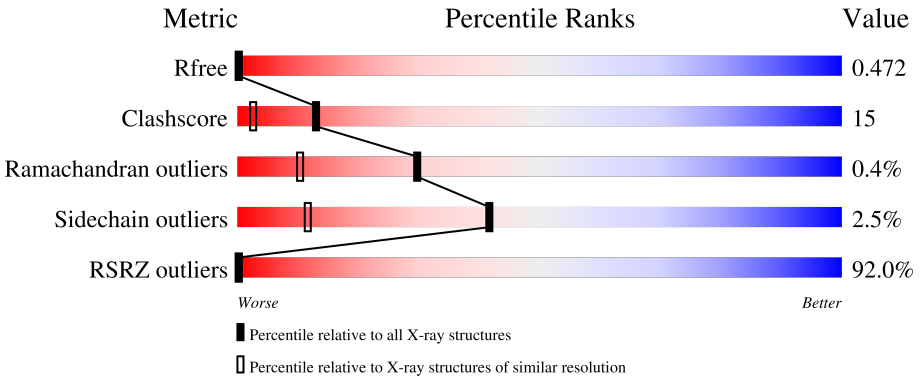
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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

Mol	Chain	Length	Quality of chain
1	A	261	88% 81% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2472 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.

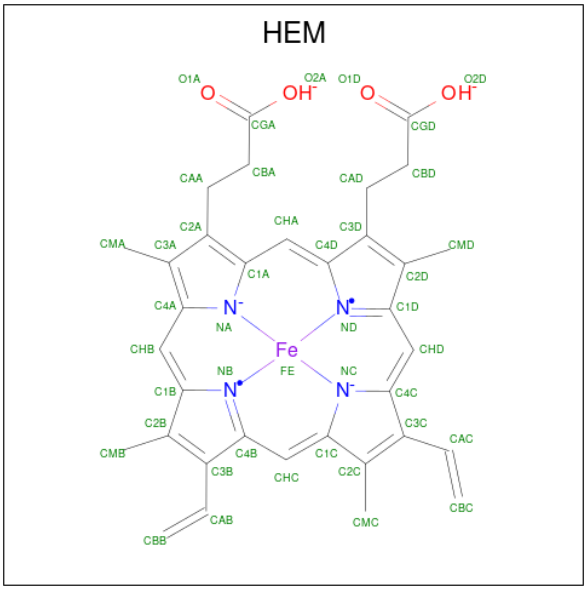
- Molecule 1 is a protein called ASCORBATE PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1911	1220	323	365	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	expression tag	UNP Q43758

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

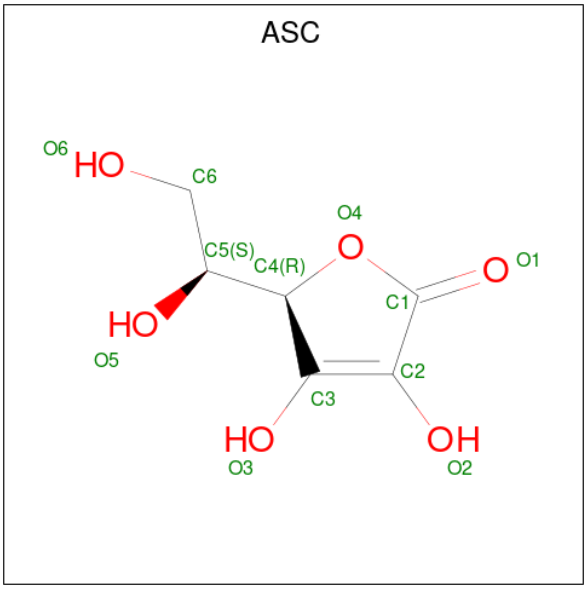


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is ASCORBIC ACID (CCD ID: ASC) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

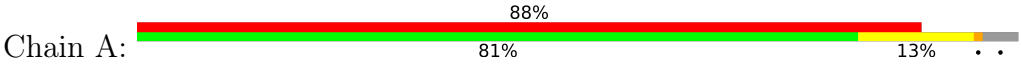
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	505	Total O 505 505	0	0

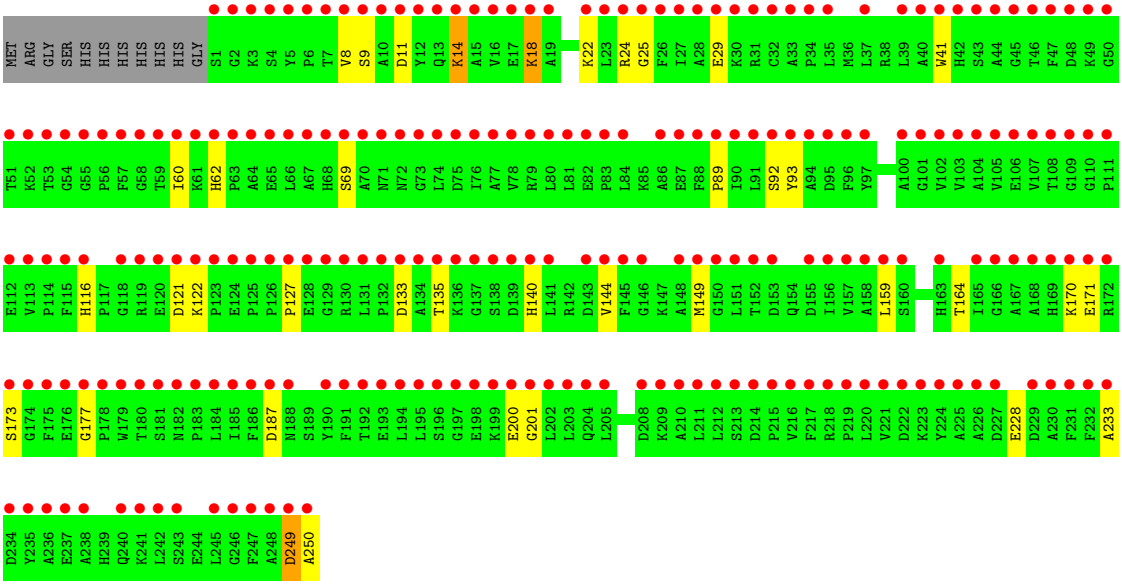
3 Residue-property plots (i)

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: ASCORBATE PEROXIDASE

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	81.33Å 81.33Å 74.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.74 – 1.40 57.51 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (57.74-1.40) 96.3 (57.51-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.38Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.196 0.471 , 0.472	Depositor DCC
R_{free} test set	2518 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	2472	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, HEM, NA

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	0.61	0/1962	0.78	0/2658

There are no bond length outliers.

There are no bond angle outliers.

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	1911	0	1871	58	3
2	A	43	0	30	1	0
3	A	1	0	0	0	0
4	A	12	0	6	0	0
5	A	505	0	0	48	6
All	All	2472	0	1907	58	9

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 15.

All (58) 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:135:THR:HG21	5:A:2363:HOH:O	1.40	1.18
1:A:200:GLU:OE1	5:A:2437:HOH:O	1.58	1.17
1:A:121:ASP:CG	5:A:2325:HOH:O	1.89	1.15
1:A:121:ASP:CB	5:A:2325:HOH:O	1.94	1.12
1:A:11:ASP:OD2	5:A:2071:HOH:O	1.66	1.10
1:A:69:SER:HB2	5:A:2229:HOH:O	1.51	1.09
1:A:121:ASP:OD2	5:A:2325:HOH:O	1.66	1.08
1:A:201:GLY:CA	5:A:2438:HOH:O	2.03	1.06
1:A:171:GLU:OE1	5:A:2397:HOH:O	1.82	0.98
1:A:93:TYR:CE1	5:A:2290:HOH:O	2.14	0.97
1:A:25:GLY:HA3	5:A:2115:HOH:O	1.65	0.97
1:A:249:ASP:OD1	5:A:2494:HOH:O	1.83	0.97
1:A:201:GLY:N	5:A:2438:HOH:O	1.96	0.96
1:A:201:GLY:HA2	5:A:2438:HOH:O	1.61	0.93
1:A:89:PRO:HB3	5:A:2145:HOH:O	1.71	0.91
1:A:69:SER:CB	5:A:2229:HOH:O	2.12	0.89
1:A:250:ALA:HB1	5:A:2496:HOH:O	1.71	0.88
1:A:133:ASP:H	1:A:140:HIS:HE1	1.20	0.87
1:A:200:GLU:CD	5:A:2437:HOH:O	2.15	0.81
1:A:116:HIS:NE2	5:A:2313:HOH:O	2.01	0.80
1:A:93:TYR:CZ	5:A:2290:HOH:O	2.34	0.78
1:A:93:TYR:OH	5:A:2290:HOH:O	2.03	0.77
1:A:171:GLU:HG3	5:A:2394:HOH:O	1.86	0.75
1:A:135:THR:HG23	5:A:2353:HOH:O	1.87	0.74
1:A:133:ASP:H	1:A:140:HIS:CE1	2.04	0.73
1:A:93:TYR:HE1	5:A:2290:HOH:O	1.60	0.71
1:A:62:HIS:CD2	5:A:2210:HOH:O	2.47	0.68
1:A:177:GLY:HA2	5:A:2407:HOH:O	1.94	0.68
1:A:11:ASP:HB2	5:A:2070:HOH:O	1.92	0.68
1:A:29:GLU:HG3	5:A:2123:HOH:O	1.93	0.67
1:A:62:HIS:HD2	5:A:2210:HOH:O	1.78	0.66
1:A:171:GLU:CG	5:A:2394:HOH:O	2.45	0.62
1:A:62:HIS:CD2	5:A:2211:HOH:O	2.53	0.62
1:A:121:ASP:HB2	5:A:2322:HOH:O	2.00	0.61
1:A:127:PRO:HA	5:A:2332:HOH:O	2.00	0.61
1:A:18:LYS:NZ	1:A:22:LYS:HG2	2.15	0.60
1:A:127:PRO:HB3	5:A:2332:HOH:O	2.01	0.60
1:A:233:ALA:HA	5:A:2475:HOH:O	2.05	0.57
1:A:24:ARG:CD	5:A:2108:HOH:O	2.53	0.56
1:A:11:ASP:CG	5:A:2071:HOH:O	2.29	0.56
1:A:133:ASP:N	1:A:140:HIS:HE1	1.97	0.56
1:A:170:LYS:HG2	5:A:2397:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:CB	5:A:2324:HOH:O	2.59	0.51
1:A:24:ARG:HD3	5:A:2108:HOH:O	2.09	0.51
1:A:116:HIS:CE1	5:A:2313:HOH:O	2.54	0.51
1:A:187:ASP:HB2	1:A:228:GLU:OE2	2.13	0.49
1:A:69:SER:HB3	5:A:2229:HOH:O	1.97	0.48
1:A:127:PRO:CA	5:A:2332:HOH:O	2.61	0.47
1:A:18:LYS:HZ2	1:A:22:LYS:NZ	2.12	0.47
1:A:121:ASP:HB3	5:A:2325:HOH:O	1.87	0.46
1:A:159:LEU:HB3	2:A:1251:HEM:HMC3	1.97	0.45
1:A:177:GLY:CA	5:A:2407:HOH:O	2.60	0.45
1:A:18:LYS:HZ2	1:A:22:LYS:HG2	1.81	0.43
1:A:14:LYS:O	1:A:14:LYS:HD3	2.19	0.42
1:A:127:PRO:CB	5:A:2332:HOH:O	2.65	0.42
1:A:121:ASP:HB2	5:A:2325:HOH:O	1.89	0.42
1:A:144:VAL:HG12	1:A:149:MET:HE3	2.03	0.41
1:A:92:SER:HB2	5:A:2324:HOH:O	2.21	0.40

All (9) 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)
1:A:9:SER:OG	1:A:173:SER:O[6_565]	1.57	0.63
5:A:2101:HOH:O	5:A:2225:HOH:O[8_666]	1.62	0.58
5:A:2287:HOH:O	5:A:2406:HOH:O[6_565]	1.69	0.51
5:A:2144:HOH:O	5:A:2452:HOH:O[5_555]	1.71	0.49
1:A:122:LYS:O	1:A:200:GLU:CG[6_565]	2.14	0.06
1:A:8:VAL:CA	1:A:170:LYS:O[6_565]	2.15	0.05
5:A:2184:HOH:O	5:A:2288:HOH:O[6_465]	2.16	0.04
5:A:2061:HOH:O	5:A:2225:HOH:O[8_666]	2.17	0.03
5:A:2337:HOH:O	5:A:2337:HOH:O[8_665]	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	248/261 (95%)	243 (98%)	4 (2%)	1 (0%)	30 10

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/206 (96%)	192 (98%)	5 (2%)	42 11

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	18	LYS
1	A	41	TRP
1	A	60	ILE
1	A	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	140	HIS
1	A	204	GLN

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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ASC	A	1253	-	12,12,12	1.19	1 (8%)	17,17,17	1.00	0
2	HEM	A	1251	5,1	50,50,50	1.57	7 (14%)	66,82,82	1.38	11 (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	ASC	A	1253	-	-	0/6/22/22	0/1/1/1
2	HEM	A	1251	5,1	-	2/14/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1251	HEM	C3D-C2D	5.14	1.47	1.36
2	A	1251	HEM	FE-NB	3.94	2.07	1.94
4	A	1253	ASC	O4-C1	3.87	1.41	1.36
2	A	1251	HEM	FE-ND	3.56	2.05	1.94
2	A	1251	HEM	FE-NA	3.01	2.05	1.95
2	A	1251	HEM	FE-NC	2.65	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1251	HEM	CAB-C3B	2.31	1.53	1.47
2	A	1251	HEM	CAC-C3C	2.10	1.53	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1251	HEM	C4A-NA-C1A	3.57	108.85	105.35
2	A	1251	HEM	C4D-ND-C1D	3.47	108.65	105.07
2	A	1251	HEM	C1B-NB-C4B	2.93	108.10	105.07
2	A	1251	HEM	CAA-CBA-CGA	-2.72	107.75	113.60
2	A	1251	HEM	C4C-NC-C1C	2.64	107.93	105.35
2	A	1251	HEM	CMD-C2D-C1D	2.44	128.75	125.04
2	A	1251	HEM	C4C-C3C-C2C	2.33	108.67	106.75
2	A	1251	HEM	C2A-C1A-NA	-2.26	107.62	110.15
2	A	1251	HEM	O2D-CGD-CBD	2.17	121.00	114.03
2	A	1251	HEM	C3B-C2B-C1B	2.12	108.06	106.49
2	A	1251	HEM	CHA-C1A-NA	2.07	127.66	123.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1251	HEM	CAA-CBA-CGA-O2A
2	A	1251	HEM	CAA-CBA-CGA-O1A

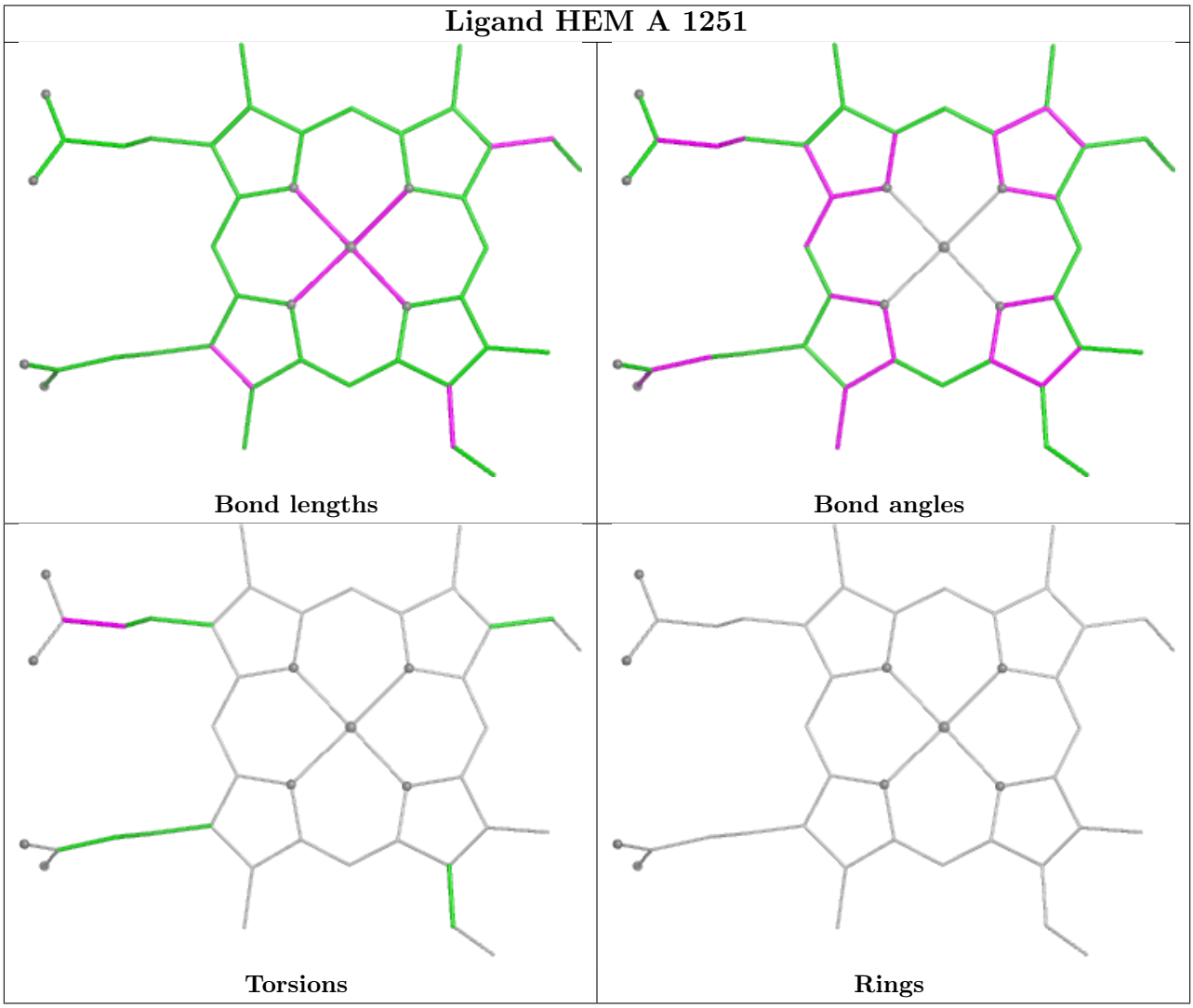
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1251	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

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



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	250/261 (95%)	3.65	230 (92%)	0	0	10, 16, 27, 39	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	GLY	9.5
1	A	250	ALA	9.2
1	A	195	LEU	7.1
1	A	247	PHE	6.9
1	A	202	LEU	6.9
1	A	194	LEU	6.5
1	A	248	ALA	6.3
1	A	86	ALA	6.3
1	A	196	SER	6.2
1	A	1	SER	6.1
1	A	57	PHE	6.1
1	A	127	PRO	6.0
1	A	63	PRO	6.0
1	A	125	PRO	5.9
1	A	90	ILE	5.8
1	A	62	HIS	5.7
1	A	2	GLY	5.7
1	A	145	PHE	5.7
1	A	73	GLY	5.6
1	A	71	ASN	5.6
1	A	84	LEU	5.5
1	A	16	VAL	5.5
1	A	32	CYS	5.5
1	A	229	ASP	5.5
1	A	47	PHE	5.5
1	A	232	PHE	5.4
1	A	67	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	5.3
1	A	66	LEU	5.3
1	A	212	LEU	5.3
1	A	83	PRO	5.2
1	A	96	PHE	5.2
1	A	91	LEU	5.1
1	A	80	LEU	5.1
1	A	8	VAL	5.1
1	A	167	ALA	5.0
1	A	203	LEU	5.0
1	A	6	PRO	5.0
1	A	75	ASP	4.9
1	A	105	VAL	4.9
1	A	60	ILE	4.9
1	A	144	VAL	4.9
1	A	230	ALA	4.9
1	A	131	LEU	4.9
1	A	151	LEU	4.9
1	A	7	THR	4.9
1	A	107	VAL	4.9
1	A	41	TRP	4.8
1	A	93	TYR	4.8
1	A	97	TYR	4.8
1	A	65	GLU	4.8
1	A	54	GLY	4.8
1	A	15	ALA	4.7
1	A	137	GLY	4.7
1	A	4	SER	4.7
1	A	124	GLU	4.7
1	A	216	VAL	4.6
1	A	77	ALA	4.6
1	A	210	ALA	4.5
1	A	205	LEU	4.5
1	A	76	ILE	4.5
1	A	17	GLU	4.5
1	A	233	ALA	4.5
1	A	201	GLY	4.4
1	A	19	ALA	4.4
1	A	152	THR	4.4
1	A	44	ALA	4.4
1	A	53	THR	4.4
1	A	213	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	133	ASP	4.3
1	A	25	GLY	4.3
1	A	249	ASP	4.3
1	A	157	VAL	4.3
1	A	58	GLY	4.3
1	A	74	LEU	4.2
1	A	26	PHE	4.2
1	A	175	PHE	4.2
1	A	148	ALA	4.2
1	A	238	ALA	4.2
1	A	156	ILE	4.1
1	A	199	LYS	4.1
1	A	28	ALA	4.1
1	A	179	TRP	4.1
1	A	88	PHE	4.0
1	A	89	PRO	4.0
1	A	141	LEU	4.0
1	A	135	THR	4.0
1	A	245	LEU	4.0
1	A	226	ALA	4.0
1	A	174	GLY	3.9
1	A	43	SER	3.9
1	A	123	PRO	3.9
1	A	51	THR	3.9
1	A	40	ALA	3.9
1	A	100	ALA	3.9
1	A	139	ASP	3.9
1	A	198	GLU	3.8
1	A	217	PHE	3.8
1	A	246	GLY	3.8
1	A	59	THR	3.8
1	A	209	LYS	3.8
1	A	70	ALA	3.8
1	A	79	ARG	3.8
1	A	234	ASP	3.7
1	A	186	PHE	3.7
1	A	165	ILE	3.7
1	A	12	TYR	3.7
1	A	94	ALA	3.7
1	A	50	GLY	3.7
1	A	116	HIS	3.7
1	A	78	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	138	SER	3.7
1	A	129	GLY	3.7
1	A	52	LYS	3.6
1	A	45	GLY	3.6
1	A	150	GLY	3.6
1	A	68	HIS	3.6
1	A	236	ALA	3.6
1	A	5	TYR	3.6
1	A	166	GLY	3.6
1	A	37	LEU	3.5
1	A	61	LYS	3.5
1	A	223	LYS	3.5
1	A	39	LEU	3.5
1	A	220	LEU	3.5
1	A	102	VAL	3.5
1	A	191	PHE	3.5
1	A	114	PRO	3.5
1	A	221	VAL	3.5
1	A	111	PRO	3.4
1	A	132	PRO	3.4
1	A	231	PHE	3.3
1	A	177	GLY	3.3
1	A	122	LYS	3.3
1	A	69	SER	3.3
1	A	146	GLY	3.3
1	A	46	THR	3.3
1	A	11	ASP	3.3
1	A	155	ASP	3.3
1	A	182	ASN	3.3
1	A	112	GLU	3.3
1	A	115	PHE	3.3
1	A	95	ASP	3.2
1	A	240	GLN	3.2
1	A	14	LYS	3.2
1	A	55	GLY	3.2
1	A	192	THR	3.2
1	A	178	PRO	3.2
1	A	219	PRO	3.2
1	A	218	ARG	3.2
1	A	30	LYS	3.2
1	A	113	VAL	3.2
1	A	184	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLN	3.1
1	A	126	PRO	3.1
1	A	10	ALA	3.1
1	A	92	SER	3.1
1	A	118	GLY	3.1
1	A	168	ALA	3.1
1	A	103	VAL	3.1
1	A	108	THR	3.1
1	A	81	LEU	3.1
1	A	27	ILE	3.1
1	A	35	LEU	3.0
1	A	170	LYS	3.0
1	A	211	LEU	3.0
1	A	9	SER	3.0
1	A	243	SER	3.0
1	A	22	LYS	3.0
1	A	193	GLU	3.0
1	A	29	GLU	2.9
1	A	31	ARG	2.9
1	A	34	PRO	2.9
1	A	64	ALA	2.9
1	A	18	LYS	2.9
1	A	136	LYS	2.9
1	A	188	ASN	2.9
1	A	120	GLU	2.9
1	A	200	GLU	2.9
1	A	187	ASP	2.8
1	A	224	TYR	2.8
1	A	183	PRO	2.8
1	A	128	GLU	2.7
1	A	23	LEU	2.7
1	A	176	GLU	2.7
1	A	208	ASP	2.7
1	A	48	ASP	2.7
1	A	153	ASP	2.7
1	A	180	THR	2.6
1	A	3	LYS	2.6
1	A	82	GLU	2.6
1	A	159	LEU	2.5
1	A	190	TYR	2.5
1	A	235	TYR	2.5
1	A	24	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	42	HIS	2.5
1	A	149	MET	2.5
1	A	225	ALA	2.5
1	A	227	ASP	2.5
1	A	110	GLY	2.5
1	A	181	SER	2.4
1	A	241	LYS	2.4
1	A	185	ILE	2.4
1	A	119	ARG	2.4
1	A	121	ASP	2.4
1	A	222	ASP	2.4
1	A	106	GLU	2.4
1	A	109	GLY	2.4
1	A	158	ALA	2.3
1	A	163	HIS	2.3
1	A	172	ARG	2.3
1	A	169	HIS	2.3
1	A	33	ALA	2.3
1	A	237	GLU	2.3
1	A	104	ALA	2.2
1	A	72	ASN	2.2
1	A	215	PRO	2.2
1	A	160	SER	2.2
1	A	204	GLN	2.2
1	A	49	LYS	2.2
1	A	214	ASP	2.2
1	A	130	ARG	2.1
1	A	101	GLY	2.1
1	A	242	LEU	2.1
1	A	87	GLU	2.1
1	A	173	SER	2.1
1	A	171	GLU	2.1
1	A	56	PRO	2.1
1	A	140	HIS	2.1
1	A	143	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

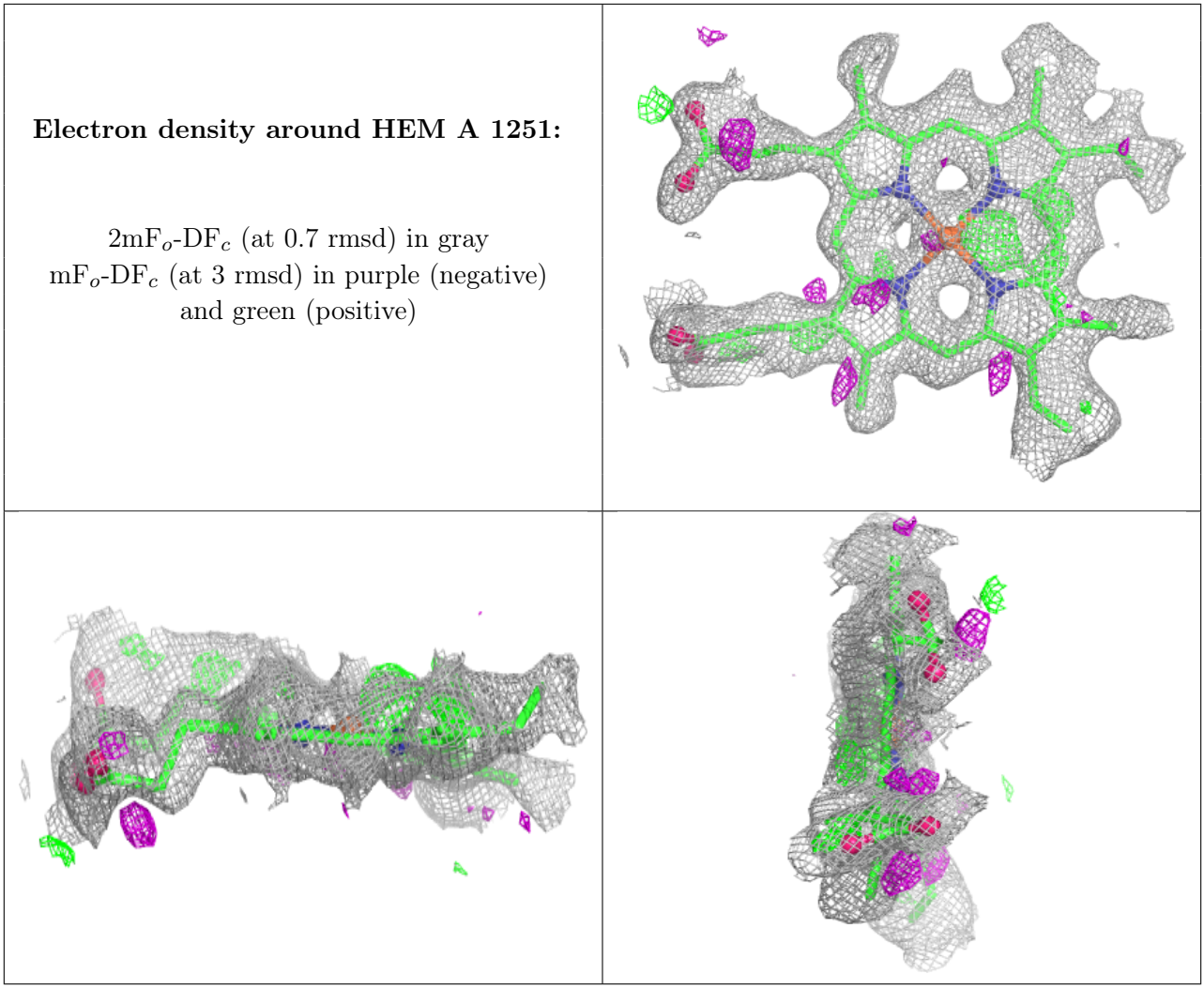
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ASC	A	1253	12/12	0.67	0.17	14,17,24,27	0
3	NA	A	1252	1/1	0.76	0.31	14,14,14,14	0
2	HEM	A	1251	43/43	0.82	0.17	9,11,14,15	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 A 1251:

$2mF_o$-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.