



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:46 am BST

PDB ID : 6JBN
Title : Crystal structure of *Sphingomonas* sp. A1 peroxidase EfeB responsible for import of iron
Authors : Okumura, K.; Takase, R.; Mikami, B.; Murata, K.; Hashimoto, W.
Deposited on : 2019-01-26
Resolution : 2.30 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

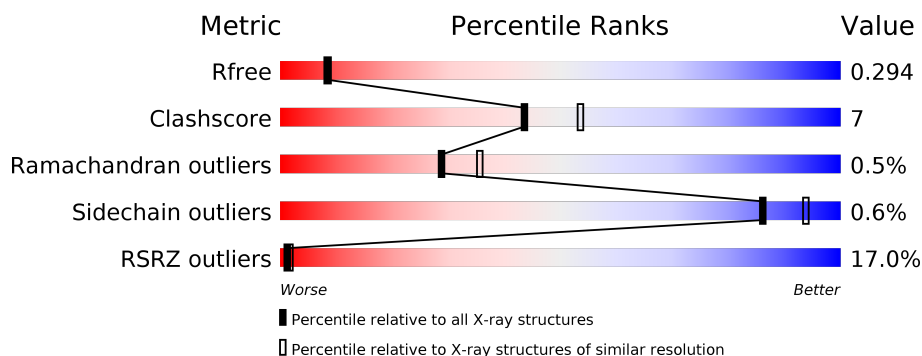
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	447	<div> <div>15%</div> <div>76%</div> <div>11%</div> <div>13%</div> </div>
1	B	447	<div> <div>14%</div> <div>74%</div> <div>13%</div> <div>13%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	505	-	-	-	X
5	EDO	A	506	-	-	-	X
5	EDO	A	507	-	-	X	-
5	EDO	B	509	-	-	X	X

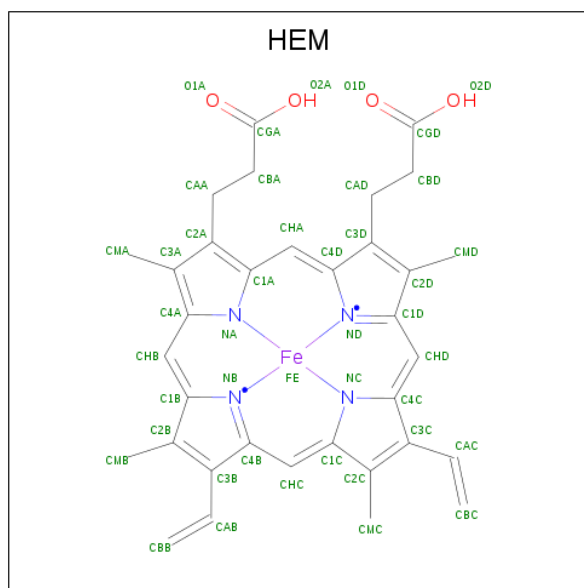
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In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peroxidase EfeB.

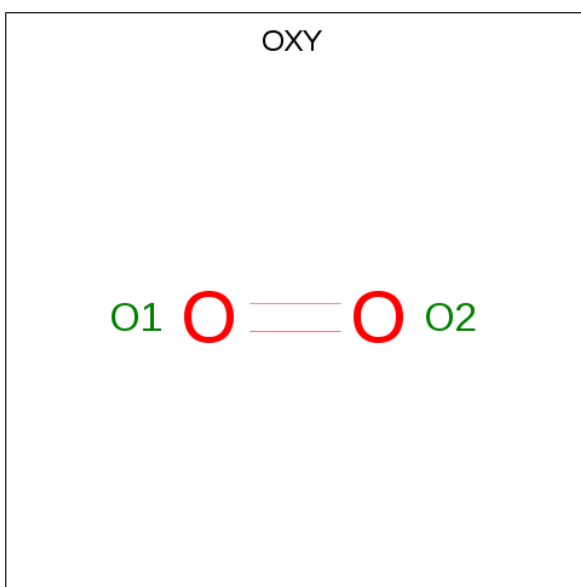
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total 3006	C 1884	N 544	O 572	S 6	0	0	0
1	B	390	Total 3009	C 1887	N 544	O 572	S 6	0	2	0

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



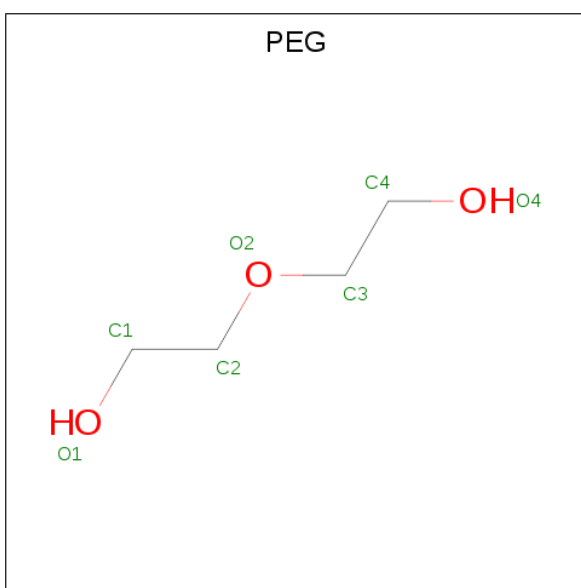
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



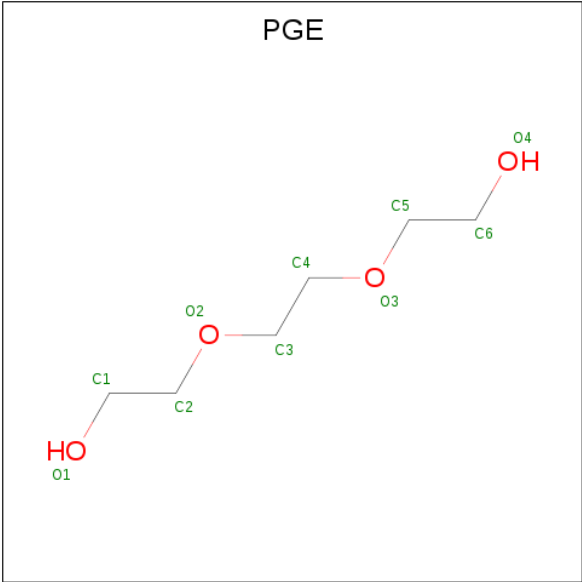
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	141	Total	O	0	0
			141	141		
7	B	116	Total	O	0	0
			116	116		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.02Å 104.99Å 83.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 – 2.30 44.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.49-2.30) 99.1 (44.49-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.54 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.234 , 0.297 0.235 , 0.294	Depositor DCC
R_{free} test set	1976 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	1.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6523	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7539e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PEG, HEM, PGE, OXY, EDO

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	0.44	0/3076	0.59	0/4189
1	B	0.42	0/3085	0.59	0/4202
All	All	0.43	0/6161	0.59	0/8391

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	3006	0	2951	36	0
1	B	3009	0	2959	44	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	21	0	30	4	0
4	B	14	0	20	2	0
5	A	56	0	84	7	0
5	B	40	0	60	8	0
6	B	30	0	42	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	141	0	0	3	0
7	B	116	0	0	3	0
All	All	6523	0	6206	84	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 7.

All (84) 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:372:LYS:HA	6:B:516:PGE:H6	1.61	0.82
1:A:53:GLN:HG2	5:A:516:EDO:H12	1.67	0.76
1:A:99:GLU:HG2	5:A:507:EDO:H11	1.68	0.74
1:B:221:LYS:NZ	1:B:223:GLU:OE1	2.21	0.73
1:A:425:ARG:HB3	1:A:427:ASP:OD1	1.91	0.71
1:B:362[B]:ARG:HH21	1:B:362[B]:ARG:HB3	1.54	0.71
1:B:66:ARG:HD3	1:B:141:PRO:HG3	1.72	0.70
1:B:66:ARG:HD2	1:B:116:GLN:HA	1.73	0.69
1:A:305:ARG:HB3	1:A:339:PRO:HG2	1.75	0.68
1:B:124:ASP:HB3	1:B:127:LEU:HD23	1.76	0.68
1:B:275:ALA:H	5:B:511:EDO:H12	1.58	0.68
1:A:224:GLY:HA2	4:A:503:PEG:H12	1.77	0.67
1:B:357:ASN:OD1	1:B:399:ARG:NH2	2.31	0.63
1:B:362[B]:ARG:NH1	1:B:364:PHE:HE1	1.96	0.63
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.82	0.62
1:A:427:ASP:OD1	1:A:427:ASP:N	2.32	0.61
1:B:66:ARG:NH1	1:B:116:GLN:OE1	2.33	0.60
1:A:102:ARG:HE	5:A:507:EDO:H21	1.67	0.59
1:B:165:LYS:HD3	1:B:169:LEU:HB3	1.84	0.59
1:A:222:GLN:NE2	1:A:366:TYR:HB2	2.21	0.56
1:A:372:LYS:HA	1:A:372:LYS:HE3	1.87	0.56
1:A:436:ASP:OD1	5:A:519:EDO:O2	2.24	0.55
1:B:90:PHE:HE2	1:B:209:LEU:HD21	1.70	0.54
1:A:103:LEU:HD12	1:A:212:LEU:HD13	1.90	0.54
1:B:238:GLU:OE2	1:B:247:ARG:NH2	2.35	0.54
1:B:186:HIS:HB3	5:B:509:EDO:H22	1.90	0.54
1:B:362[B]:ARG:NH2	1:B:362[B]:ARG:HB3	2.23	0.54
5:B:509:EDO:H21	7:B:611:HOH:O	2.07	0.53
1:A:367:SER:H	4:A:503:PEG:H11	1.74	0.53
1:A:96:ASP:OD1	1:A:99:GLU:HG3	2.09	0.53
1:A:228:PRO:HG2	1:B:197:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:HB3	1:B:196:ASN:ND2	2.24	0.51
1:B:62:ASN:O	1:B:65[A]:GLN:HG2	2.11	0.50
5:A:507:EDO:H22	5:A:508:EDO:C2	2.42	0.50
1:A:142:ASP:OD1	1:A:196:ASN:HB2	2.11	0.50
1:A:66:ARG:NH1	1:A:116:GLN:OE1	2.46	0.49
1:A:321:ARG:HD3	1:A:322:THR:HG22	1.95	0.49
1:B:288:ILE:HG21	2:B:501:HEM:HBB1	1.94	0.49
1:A:301:GLY:O	1:A:305:ARG:HG3	2.14	0.48
1:B:149:SER:O	1:B:189:LEU:HD12	2.13	0.48
1:A:197:THR:HG21	1:B:228:PRO:HG2	1.96	0.48
1:A:305:ARG:HG2	5:A:509:EDO:H21	1.95	0.48
1:B:231:HIS:CD2	1:B:233:PRO:HD3	2.48	0.48
1:A:172:MET:HA	1:A:416:TYR:CE2	2.48	0.47
1:B:423:ILE:HD12	1:B:423:ILE:O	2.14	0.47
1:A:321:ARG:HH11	1:A:322:THR:HG22	1.78	0.47
1:A:335:GLY:HA3	1:A:340:LEU:HD22	1.96	0.47
6:B:516:PGE:H5	6:B:516:PGE:H32	1.67	0.47
1:B:109:GLU:HG3	5:B:513:EDO:H22	1.97	0.46
1:A:144:LEU:HA	1:A:194:CYS:O	2.15	0.46
1:B:269:ALA:HA	1:B:278:ALA:HB2	1.96	0.46
1:A:318:ASP:HB3	1:A:337:ARG:HB3	1.98	0.46
1:A:178:ASP:OD1	1:A:286:ARG:NH2	2.44	0.46
4:A:503:PEG:H31	7:A:703:HOH:O	2.15	0.46
1:B:317:LEU:O	1:B:337:ARG:HD2	2.16	0.46
1:B:110:ARG:NH1	6:B:515:PGE:H42	2.31	0.45
1:A:326:VAL:HG23	1:A:327:PRO:HD2	1.99	0.44
1:B:305:ARG:HG3	4:B:504:PEG:H12	1.99	0.44
1:B:429:TYR:CE1	1:B:432:ARG:HB2	2.52	0.44
1:B:151:GLY:HA3	5:B:509:EDO:H12	2.00	0.44
1:B:337:ARG:HA	1:B:337:ARG:HD3	1.55	0.44
1:A:372:LYS:HA	1:A:372:LYS:CE	2.47	0.43
1:B:50:ALA:C	1:B:52:THR:H	2.22	0.43
1:A:306:ILE:HG12	1:A:404:PRO:HB2	2.00	0.42
1:B:142:ASP:HB3	1:B:200:THR:HG21	2.01	0.42
4:A:504:PEG:H21	7:A:612:HOH:O	2.19	0.42
1:B:136:GLY:HA3	5:B:508:EDO:H12	2.00	0.42
1:B:142:ASP:HB2	7:B:619:HOH:O	2.19	0.42
1:B:142:ASP:OD1	1:B:196:ASN:HB2	2.20	0.42
1:B:144:LEU:HA	1:B:194:CYS:O	2.20	0.42
1:B:339:PRO:HG3	4:B:504:PEG:H42	2.02	0.42
1:A:102:ARG:HE	5:A:507:EDO:C2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CE2	1:A:165:LYS:HA	2.54	0.41
1:B:73:HIS:HB3	1:B:266:TRP:CH2	2.55	0.41
1:A:241:ARG:NH2	1:A:312:PRO:O	2.49	0.41
1:B:172:MET:HA	1:B:416:TYR:CE2	2.54	0.41
1:B:152:ASP:N	5:B:509:EDO:H12	2.35	0.41
1:A:334:LYS:HB2	7:A:647:HOH:O	2.20	0.41
1:B:173:THR:HG23	7:B:605:HOH:O	2.20	0.41
1:A:357:ASN:OD1	1:A:399:ARG:NH2	2.54	0.41
1:B:109:GLU:HG3	5:B:513:EDO:C2	2.51	0.41
1:A:239:SER:O	1:A:247:ARG:HG2	2.20	0.40
1:A:94:ALA:HB1	1:A:99:GLU:HB2	2.03	0.40
1:B:144:LEU:HD21	1:B:146:ILE:HD11	2.03	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	389/447 (87%)	373 (96%)	14 (4%)	2 (0%)	29	35
1	B	390/447 (87%)	375 (96%)	13 (3%)	2 (0%)	29	35
All	All	779/894 (87%)	748 (96%)	27 (4%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	269	ALA
1	B	269	ALA
1	B	320	GLY

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	316/353 (90%)	312 (99%)	4 (1%)	69	82
1	B	317/353 (90%)	317 (100%)	0	100	100
All	All	633/706 (90%)	629 (99%)	4 (1%)	86	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASP
1	A	167	ARG
1	A	321	ARG
1	A	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	231	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

36 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
5	EDO	B	511	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	A	511	-	3,3,3	0.51	0	2,2,2	0.33	0
5	EDO	B	509	-	3,3,3	0.39	0	2,2,2	0.34	0
2	HEM	B	501	1,3	27,50,50	0.78	1 (3%)	17,82,82	1.21	2 (11%)
4	PEG	A	505	-	6,6,6	0.66	0	5,5,5	0.71	0
2	HEM	A	501	1,3	27,50,50	0.95	2 (7%)	17,82,82	1.23	3 (17%)
4	PEG	B	504	-	6,6,6	0.52	0	5,5,5	0.32	0
5	EDO	B	505	-	3,3,3	0.38	0	2,2,2	0.46	0
5	EDO	B	508	-	3,3,3	0.45	0	2,2,2	0.87	0
5	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	515	-	3,3,3	0.46	0	2,2,2	0.35	0
4	PEG	A	504	-	6,6,6	0.39	0	5,5,5	0.41	0
5	EDO	A	510	-	3,3,3	0.49	0	2,2,2	0.34	0
5	EDO	A	519	-	3,3,3	0.54	0	2,2,2	0.25	0
5	EDO	A	514	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	B	506	-	3,3,3	0.50	0	2,2,2	0.39	0
5	EDO	A	506	-	3,3,3	0.53	0	2,2,2	0.16	0
5	EDO	B	514	-	3,3,3	0.51	0	2,2,2	0.21	0
5	EDO	A	512	-	3,3,3	0.53	0	2,2,2	0.31	0
3	OXY	B	502	2	1,1,1	0.04	0	-		
5	EDO	A	513	-	3,3,3	0.50	0	2,2,2	0.43	0
5	EDO	A	516	-	3,3,3	0.57	0	2,2,2	0.12	0
4	PEG	B	503	-	6,6,6	0.58	0	5,5,5	0.46	0
5	EDO	A	518	-	3,3,3	0.52	0	2,2,2	0.34	0
5	EDO	A	517	-	3,3,3	0.50	0	2,2,2	0.33	0
6	PGE	B	515	-	9,9,9	0.34	0	8,8,8	0.47	0
4	PEG	A	503	-	6,6,6	0.56	0	5,5,5	0.36	0
5	EDO	B	512	-	3,3,3	0.45	0	2,2,2	0.36	0
3	OXY	A	502	2	1,1,1	0.01	0	-		
5	EDO	B	510	-	3,3,3	0.49	0	2,2,2	0.61	0
5	EDO	A	509	-	3,3,3	0.50	0	2,2,2	0.25	0
5	EDO	A	508	-	3,3,3	0.35	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGE	B	517	-	9,9,9	0.37	0	8,8,8	0.73	0
5	EDO	B	513	-	3,3,3	0.55	0	2,2,2	0.10	0
6	PGE	B	516	-	9,9,9	0.35	0	8,8,8	0.34	0
5	EDO	A	507	-	3,3,3	0.58	0	2,2,2	0.17	0

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
5	EDO	B	511	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	B	509	-	-	0/1/1/1	-
2	HEM	B	501	1,3	-	0/6/54/54	-
4	PEG	A	505	-	-	2/4/4/4	-
2	HEM	A	501	1,3	-	0/6/54/54	-
4	PEG	B	504	-	-	2/4/4/4	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	B	508	-	-	1/1/1/1	-
5	EDO	B	507	-	-	0/1/1/1	-
5	EDO	A	515	-	-	0/1/1/1	-
4	PEG	A	504	-	-	0/4/4/4	-
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	519	-	-	0/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	514	-	-	0/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	A	513	-	-	1/1/1/1	-
5	EDO	A	516	-	-	1/1/1/1	-
4	PEG	B	503	-	-	1/4/4/4	-
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	A	517	-	-	1/1/1/1	-
6	PGE	B	515	-	-	4/7/7/7	-
4	PEG	A	503	-	-	2/4/4/4	-
5	EDO	B	512	-	-	0/1/1/1	-
5	EDO	B	510	-	-	0/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-
6	PGE	B	517	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	513	-	-	0/1/1/1	-
6	PGE	B	516	-	-	4/7/7/7	-
5	EDO	A	507	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C4D-C3D	2.31	1.47	1.42
2	A	501	HEM	C3C-C2C	-2.16	1.37	1.40
2	B	501	HEM	C4D-C3D	2.16	1.47	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4A-C3A-C2A	2.41	108.67	107.00
2	B	501	HEM	C1D-C2D-C3D	-2.33	105.37	107.00
2	A	501	HEM	CBA-CAA-C2A	2.28	116.70	112.49
2	A	501	HEM	CMB-C2B-C3B	2.07	128.56	124.68
2	B	501	HEM	CMB-C2B-C3B	2.00	128.43	124.68

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	515	PGE	O2-C3-C4-O3
6	B	516	PGE	O2-C3-C4-O3
6	B	515	PGE	O1-C1-C2-O2
4	A	505	PEG	O1-C1-C2-O2
6	B	517	PGE	C6-C5-O3-C4
6	B	516	PGE	C3-C4-O3-C5
5	A	513	EDO	O1-C1-C2-O2
5	A	509	EDO	O1-C1-C2-O2
4	B	504	PEG	O1-C1-C2-O2
4	B	504	PEG	O2-C3-C4-O4
4	B	503	PEG	O2-C3-C4-O4
6	B	517	PGE	O1-C1-C2-O2
4	A	503	PEG	O2-C3-C4-O4
6	B	516	PGE	C1-C2-O2-C3
5	B	511	EDO	O1-C1-C2-O2
6	B	516	PGE	C4-C3-O2-C2
4	A	503	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	505	PEG	O2-C3-C4-O4
6	B	515	PGE	C4-C3-O2-C2
6	B	517	PGE	C3-C4-O3-C5
6	B	517	PGE	C1-C2-O2-C3
6	B	515	PGE	C1-C2-O2-C3
5	B	508	EDO	O1-C1-C2-O2
5	A	514	EDO	O1-C1-C2-O2
5	A	516	EDO	O1-C1-C2-O2
5	A	517	EDO	O1-C1-C2-O2
5	A	507	EDO	O1-C1-C2-O2
6	B	517	PGE	O3-C5-C6-O4

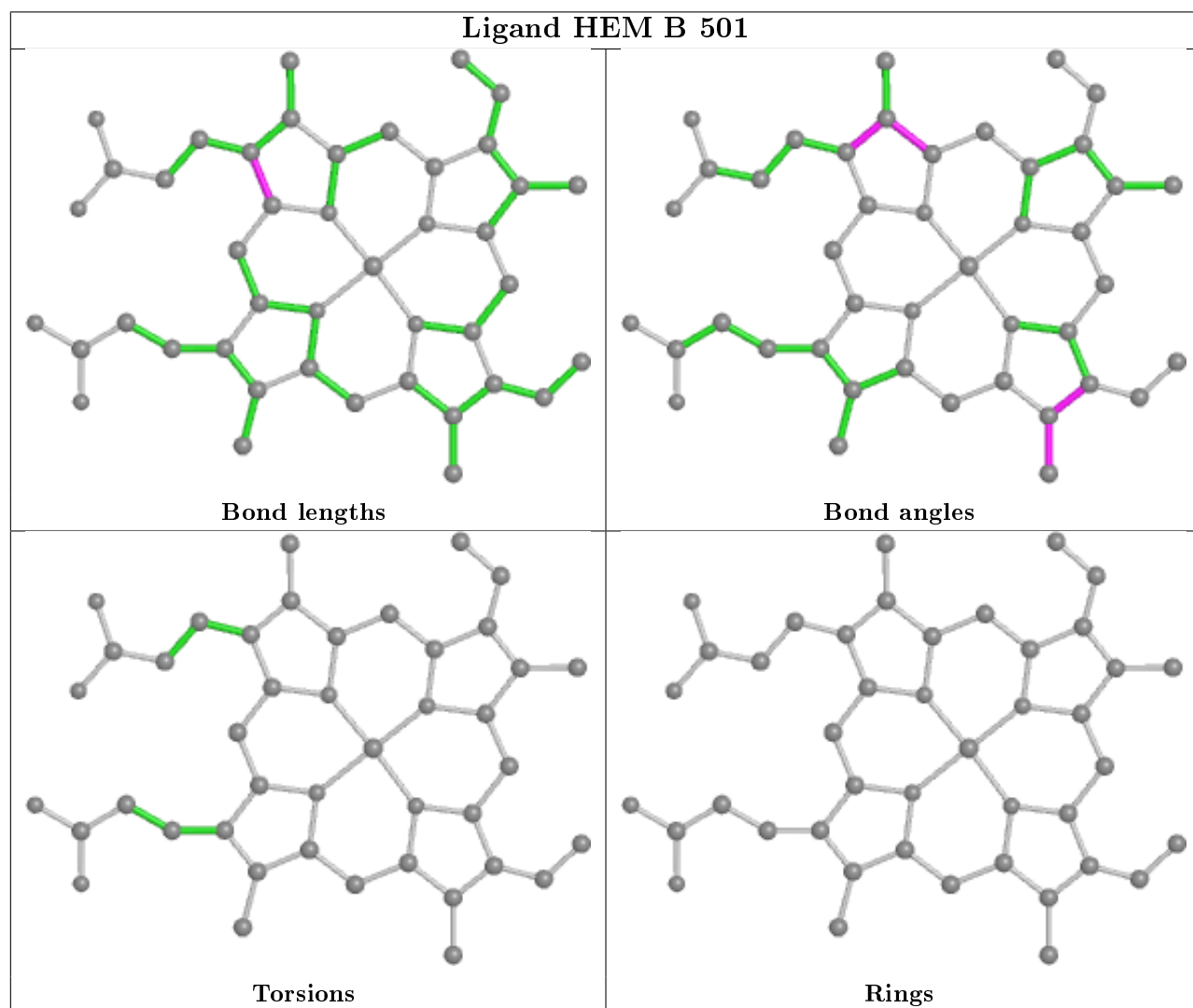
There are no ring outliers.

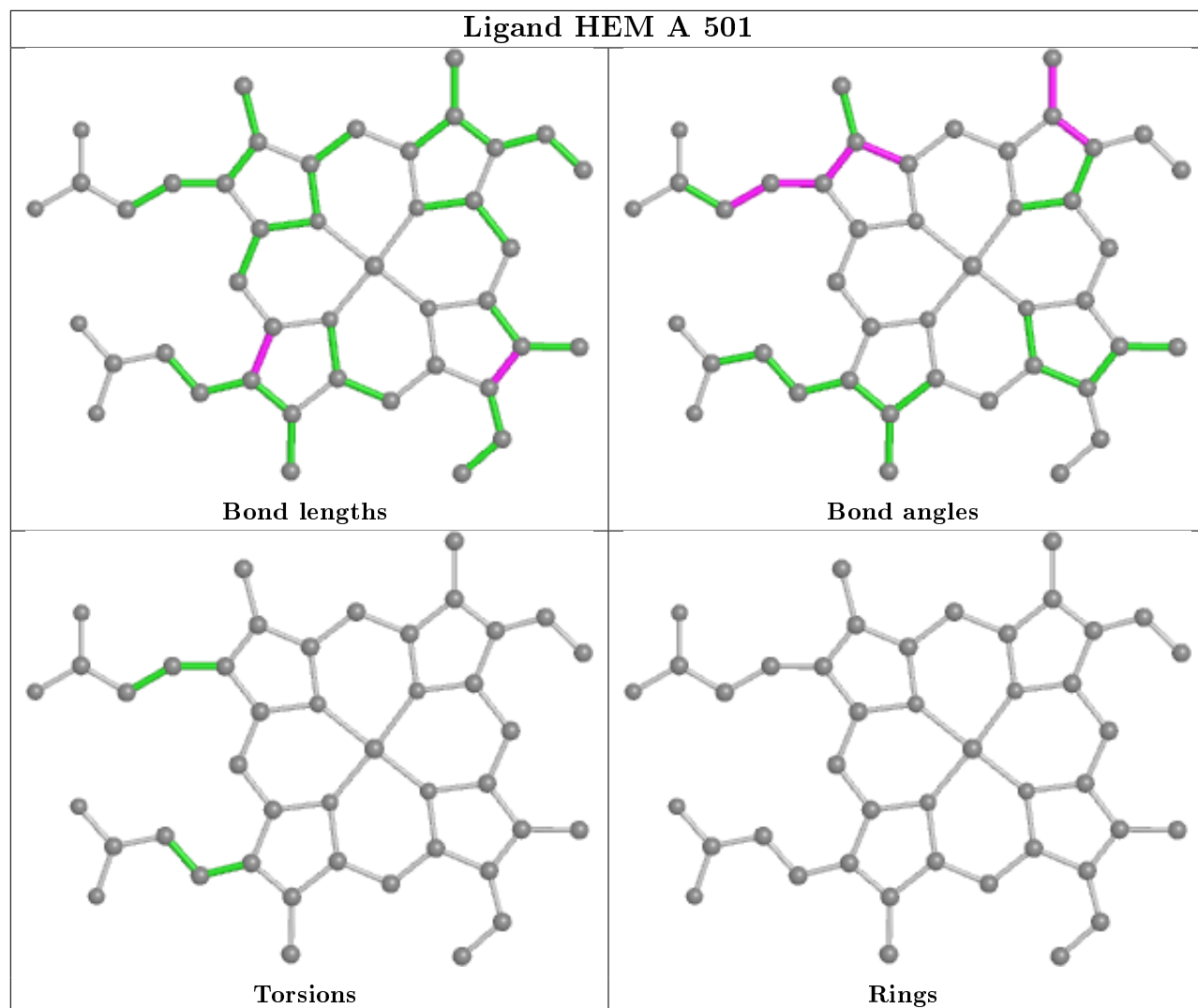
15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	511	EDO	1	0
5	B	509	EDO	4	0
2	B	501	HEM	2	0
4	B	504	PEG	2	0
5	B	508	EDO	1	0
4	A	504	PEG	1	0
5	A	519	EDO	1	0
5	A	516	EDO	1	0
6	B	515	PGE	1	0
4	A	503	PEG	3	0
5	A	509	EDO	1	0
5	A	508	EDO	1	0
5	B	513	EDO	2	0
6	B	516	PGE	2	0
5	A	507	EDO	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.





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	391/447 (87%)	1.24	69 (17%)  	17, 26, 46, 71	0
1	B	390/447 (87%)	1.23	64 (16%)  	17, 27, 49, 71	0
All	All	781/894 (87%)	1.23	133 (17%)  	17, 27, 47, 71	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ASP	8.0
1	B	50	ALA	7.7
1	A	269	ALA	7.6
1	B	269	ALA	6.8
1	A	50	ALA	6.8
1	B	123	PRO	6.2
1	B	270	ASP	5.7
1	B	235	THR	5.4
1	B	319	GLY	5.3
1	A	124	ASP	5.2
1	B	321	ARG	5.0
1	A	321	ARG	4.7
1	B	271	SER	4.5
1	B	233	PRO	4.5
1	B	124	ASP	4.4
1	B	125	PRO	4.1
1	A	427	ASP	4.1
1	B	425	ARG	4.0
1	B	427	ASP	4.0
1	B	51	GLY	3.9
1	A	231	HIS	3.9
1	A	123	PRO	3.8
1	B	337	ARG	3.8
1	B	381	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	259	ARG	3.6
1	B	231	HIS	3.5
1	A	330	ALA	3.5
1	A	331	VAL	3.3
1	B	259	ARG	3.3
1	A	351	THR	3.3
1	B	426	ALA	3.3
1	B	126	ARG	3.2
1	A	299	PRO	3.2
1	A	83	ALA	3.1
1	A	271	SER	3.1
1	A	354	SER	3.0
1	B	100	LEU	3.0
1	B	111	ILE	3.0
1	A	167	ARG	3.0
1	A	297	ARG	3.0
1	B	272	ALA	2.9
1	B	432	ARG	2.9
1	A	329	TYR	2.9
1	A	426	ALA	2.9
1	A	412	ILE	2.9
1	B	200	THR	2.9
1	B	287	ILE	2.9
1	B	320	GLY	2.9
1	A	127	LEU	2.9
1	A	227	PRO	2.8
1	B	62	ASN	2.8
1	B	65[A]	GLN	2.8
1	B	275	ALA	2.8
1	B	297	ARG	2.8
1	A	126	ARG	2.8
1	A	372	LYS	2.8
1	B	368	ASN	2.7
1	A	368	ASN	2.7
1	B	362[A]	ARG	2.7
1	B	202	ILE	2.7
1	B	84	ALA	2.7
1	A	320	GLY	2.6
1	A	125	PRO	2.6
1	A	425	ARG	2.6
1	B	194	CYS	2.6
1	A	364	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	86	LEU	2.6
1	A	232	LYS	2.6
1	A	337	ARG	2.6
1	B	57	ALA	2.6
1	B	119	PRO	2.5
1	B	225	THR	2.5
1	B	383	ILE	2.5
1	A	230	ALA	2.5
1	B	274	PRO	2.5
1	B	209	LEU	2.5
1	A	318	ASP	2.5
1	A	179	ALA	2.5
1	A	324	HIS	2.5
1	A	169	LEU	2.5
1	B	83	ALA	2.4
1	B	157	ASP	2.4
1	A	237	SER	2.4
1	B	364	PHE	2.4
1	A	370	VAL	2.4
1	B	334	LYS	2.4
1	B	61	ASP	2.4
1	A	298	THR	2.3
1	A	371	THR	2.3
1	B	232	LYS	2.3
1	B	139	VAL	2.3
1	A	51	GLY	2.3
1	A	314	GLY	2.3
1	A	260	GLU	2.3
1	A	369	GLY	2.3
1	A	84	ALA	2.3
1	A	87	LEU	2.3
1	A	391	ALA	2.3
1	A	328	ASP	2.2
1	B	92	VAL	2.2
1	A	342	SER	2.2
1	A	373	SER	2.2
1	A	240	ALA	2.2
1	B	130	THR	2.2
1	B	336	THR	2.2
1	A	346	LEU	2.2
1	A	305	ARG	2.2
1	A	200	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	268	GLN	2.2
1	A	166	PRO	2.2
1	B	163	SER	2.2
1	B	391	ALA	2.2
1	B	305	ARG	2.2
1	A	229	VAL	2.1
1	B	179	ALA	2.1
1	A	316	PRO	2.1
1	A	121	VAL	2.1
1	A	440	ARG	2.1
1	B	263	ARG	2.1
1	A	235	THR	2.1
1	B	312	PRO	2.1
1	A	376	LEU	2.1
1	B	298	THR	2.1
1	A	94	ALA	2.1
1	A	436	ASP	2.0
1	B	207	ASP	2.0
1	A	348	ASN	2.0
1	A	143	ALA	2.0
1	A	65	GLN	2.0
1	B	64	GLN	2.0
1	B	276	TRP	2.0
1	A	294	ARG	2.0
1	B	282	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

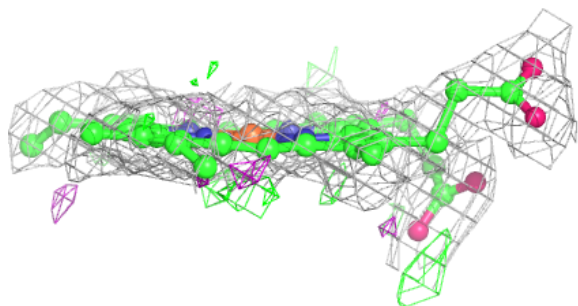
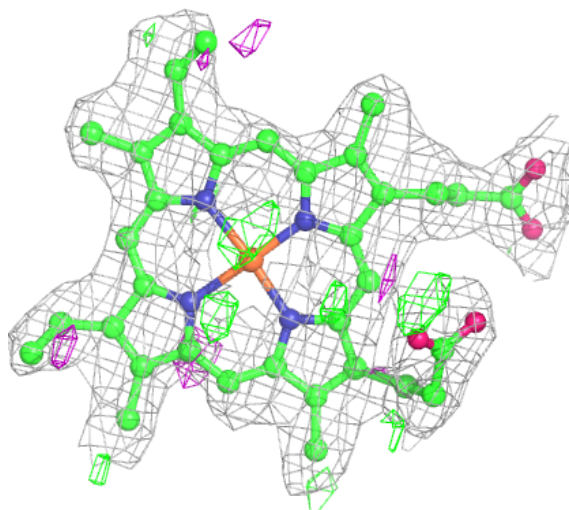
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	507	4/4	0.22	0.25	60,61,61,63	0
5	EDO	A	516	4/4	0.32	0.36	41,42,45,47	0
5	EDO	A	510	4/4	0.53	0.40	47,49,52,58	0
5	EDO	B	513	4/4	0.55	0.28	52,53,55,56	0
5	EDO	B	510	4/4	0.60	0.32	36,41,45,47	0
5	EDO	B	509	4/4	0.61	0.48	24,29,32,40	0
4	PEG	A	503	7/7	0.62	0.33	28,29,38,38	0
5	EDO	A	514	4/4	0.63	0.21	53,54,56,64	0
6	PGE	B	515	10/10	0.64	0.25	28,38,41,43	0
5	EDO	A	513	4/4	0.65	0.24	38,43,48,51	0
5	EDO	A	511	4/4	0.66	0.35	42,43,44,47	0
5	EDO	B	514	4/4	0.67	0.26	40,41,46,46	0
5	EDO	A	507	4/4	0.67	0.27	34,36,37,41	0
5	EDO	B	512	4/4	0.68	0.36	40,44,47,48	0
5	EDO	B	505	4/4	0.68	0.14	35,37,38,39	0
5	EDO	B	508	4/4	0.69	0.22	40,40,42,42	0
5	EDO	A	509	4/4	0.69	0.25	34,36,38,41	0
5	EDO	A	519	4/4	0.69	0.17	33,37,38,41	0
6	PGE	B	516	10/10	0.69	0.33	24,43,56,59	0
4	PEG	A	505	7/7	0.69	0.45	10,26,31,40	0
5	EDO	B	506	4/4	0.70	0.25	41,43,43,45	0
4	PEG	B	503	7/7	0.70	0.38	28,33,46,50	0
5	EDO	A	518	4/4	0.75	0.33	48,49,49,49	0
5	EDO	A	512	4/4	0.75	0.18	35,36,39,52	0
5	EDO	A	506	4/4	0.75	0.40	31,37,42,43	0
5	EDO	B	511	4/4	0.76	0.40	35,35,37,38	0
5	EDO	A	517	4/4	0.77	0.23	35,42,45,48	0
4	PEG	B	504	7/7	0.78	0.30	35,39,45,48	0
4	PEG	A	504	7/7	0.78	0.18	42,43,55,60	0
5	EDO	A	508	4/4	0.79	0.24	24,33,35,37	0
3	OXY	A	502	2/2	0.79	0.24	26,26,26,27	0
6	PGE	B	517	10/10	0.80	0.35	14,29,39,43	0
5	EDO	A	515	4/4	0.84	0.36	35,37,45,47	0
2	HEM	A	501	43/43	0.86	0.20	15,21,24,26	0
2	HEM	B	501	43/43	0.90	0.18	13,22,27,28	0
3	OXY	B	502	2/2	0.91	0.26	20,20,20,25	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.

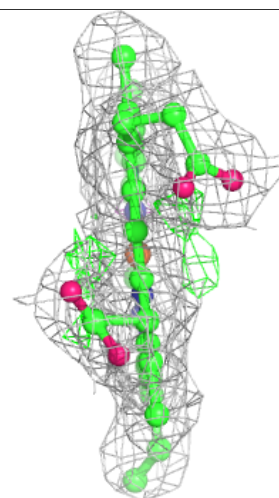
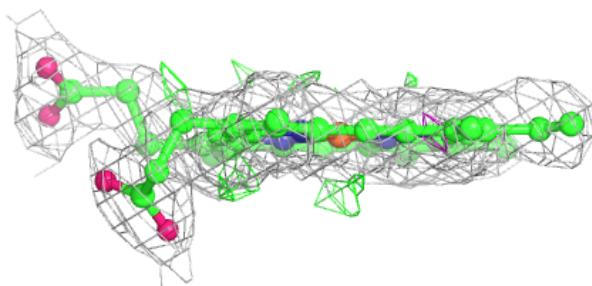
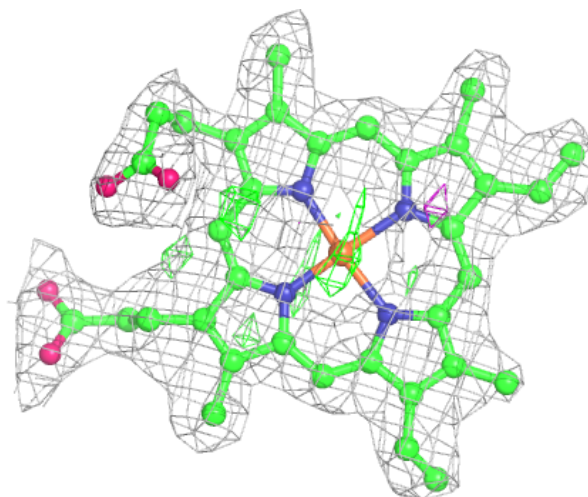
Electron density around HEM A 501:

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



Electron density around HEM B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.