Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2026 – 03:09 pm GMT

PDB ID	:	9TJP / pdb_00009tjp
Title	:	X-ray structure of CYP123 from Mycobacterium smegmatis with bound polyethylene glycol (PEG)
Authors	:	Dongxu, Y.; Remi, Z.; Yi, J.
Deposited on	:	2025-12-07
Resolution	:	2.19 Å(reported)

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

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

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

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

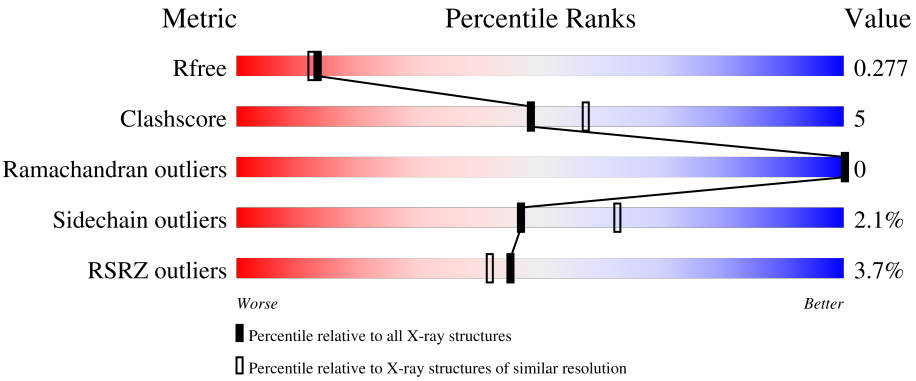
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	397	3% 85% 14%
1	B	397	4% 84% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6582 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.

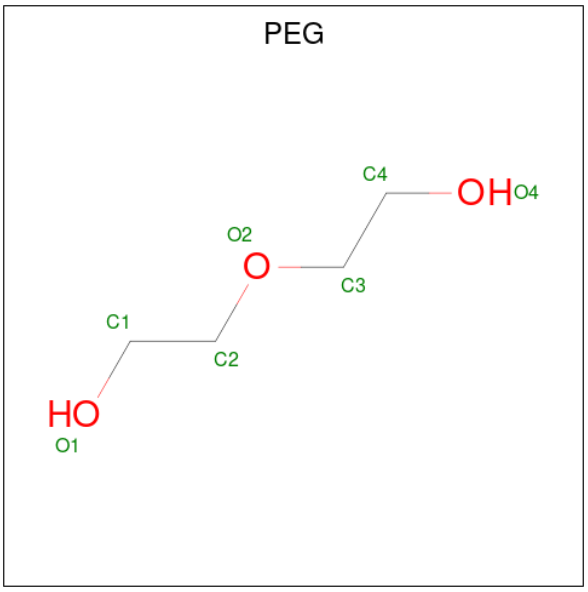
- Molecule 1 is a protein called Steroid C26-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3149	1980	556	604	9			
1	B	396	Total	C	N	O	S	0	0	0
			3140	1975	555	601	9			

There are 4 discrepancies between the modelled and reference sequences:

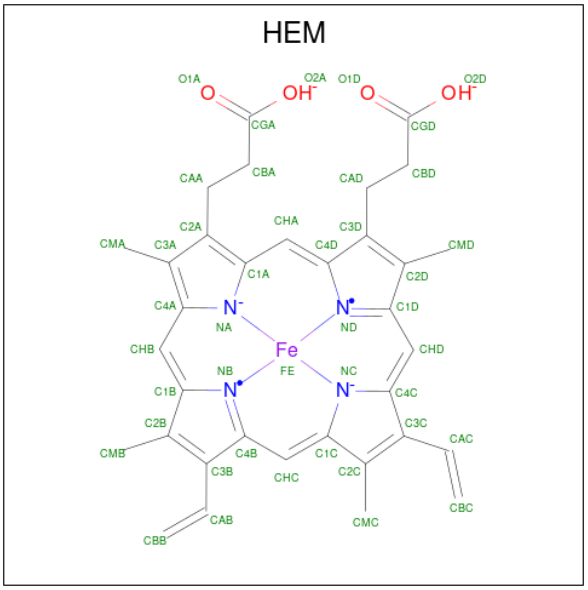
Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LEU	-	expression tag	UNP I7G922
A	402	GLU	-	expression tag	UNP I7G922
B	401	LEU	-	expression tag	UNP I7G922
B	402	GLU	-	expression tag	UNP I7G922

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



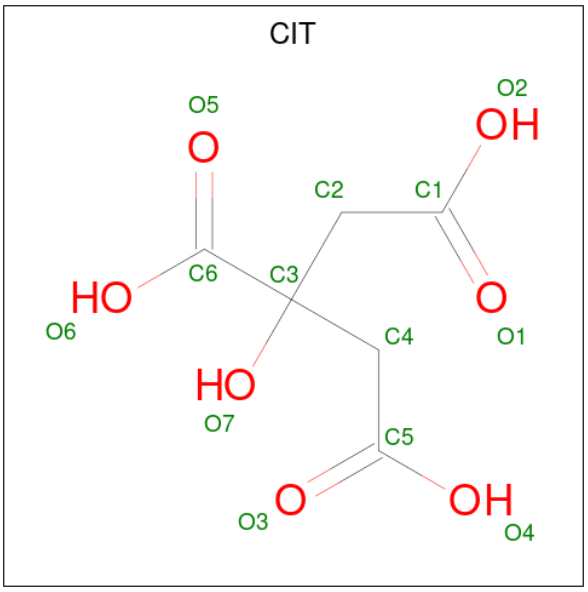
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

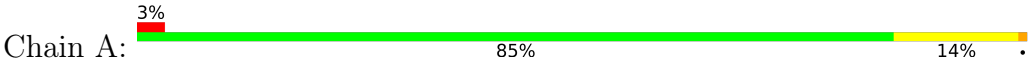
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	112	Total O 117 117	0	5
5	B	48	Total O 50 50	0	2

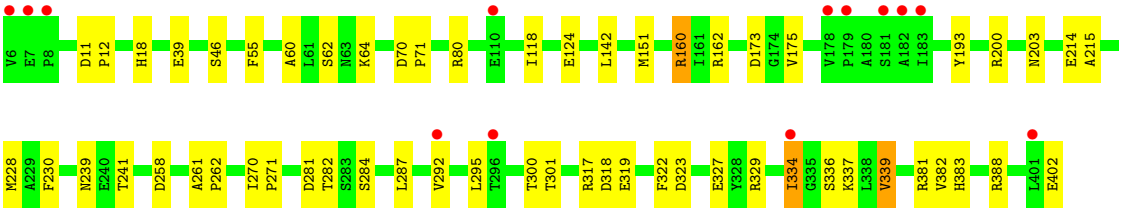
3 Residue-property plots (i)

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: Steroid C26-monooxygenase

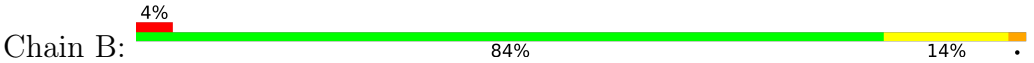
Chain A:

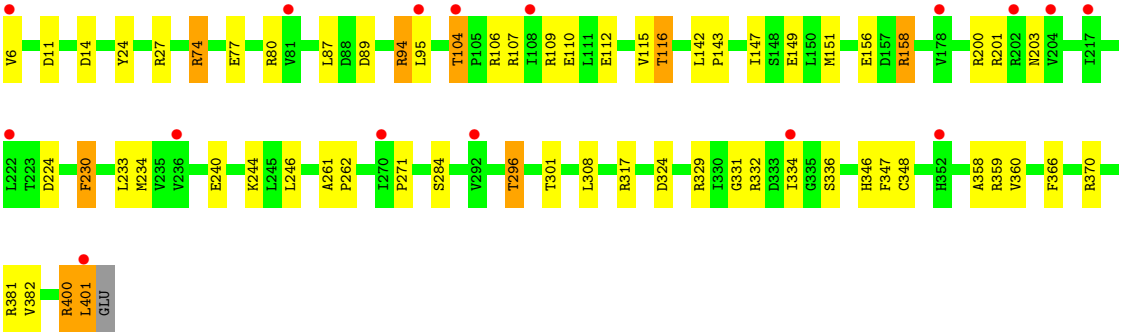




• Molecule 1: Steroid C26-monooxygenase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.90Å 132.90Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.54 – 2.19 66.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.54-2.19) 100.0 (66.54-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.210 , 0.272 0.216 , 0.277	Depositor DCC
R_{free} test set	3072 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k 0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6582	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: CIT, HEM, PEG

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	0.63	0/3214	1.16	10/4359 (0.2%)
1	B	0.59	0/3205	1.14	6/4347 (0.1%)
All	All	0.61	0/6419	1.15	16/8706 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	ARG	CG-CD-NE	-6.32	98.10	112.00
1	A	241	THR	CA-CB-OG1	-6.21	100.29	109.60
1	A	323	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	318	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	282	THR	OG1-CB-CG2	-5.78	97.74	109.30
1	A	300	THR	CA-CB-OG1	-5.76	100.96	109.60
1	A	151	MET	CG-SD-CE	5.65	113.34	100.90
1	A	339	VAL	N-CA-CB	-5.59	104.89	112.22
1	A	11	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	296	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	230	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	89	ASP	CB-CA-C	5.39	116.62	108.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	230	PHE	CA-CB-CG	-5.32	108.48	113.80
1	B	24	TYR	N-CA-CB	5.16	117.79	110.16
1	B	156	GLU	CB-CG-CD	5.12	121.30	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ARG	Sidechain
1	A	317	ARG	Sidechain
1	A	388	ARG	Sidechain
1	B	109	ARG	Sidechain
1	B	158	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	74	ARG	Sidechain
1	B	94	ARG	Sidechain

5.2 Too-close contacts (i)

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	3149	0	3070	26	0
1	B	3140	0	3064	36	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
3	A	43	0	30	3	0
3	B	43	0	30	5	0
4	A	13	0	5	0	0
4	B	13	0	5	1	0
5	A	117	0	0	2	0
5	B	50	0	0	1	0
All	All	6582	0	6224	69	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 5.

All (69) 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:296:THR:OG1	1:B:301:THR:HG22	1.86	0.75
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.59	0.68
3:B:501:HEM:HMC1	3:B:501:HEM:HBC2	1.75	0.67
1:A:334:ILE:HG23	1:A:336:SER:O	1.94	0.66
1:B:104:THR:HG23	1:B:107:ARG:H	1.61	0.65
1:A:193:TYR:HB2	1:A:228:MET:HE1	1.78	0.64
3:B:501:HEM:HBC2	3:B:501:HEM:CMC	2.27	0.64
1:B:201:ARG:NH2	1:B:224:ASP:OD1	2.33	0.61
1:B:346:HIS:O	1:B:347:PHE:C	2.44	0.59
1:B:366:PHE:O	1:B:400:ARG:NH1	2.37	0.58
1:A:258:ASP:HB2	5:A:680:HOH:O	2.02	0.58
1:B:233:LEU:HD21	3:B:501:HEM:HMA2	1.85	0.57
4:B:503:CIT:O3	4:B:503:CIT:O7	2.21	0.57
1:A:12:PRO:O	1:A:18:HIS:NE2	2.39	0.56
1:B:149:GLU:HB2	1:B:158:ARG:HH22	1.69	0.56
1:B:6:VAL:CG2	1:B:27:ARG:HH22	2.18	0.56
1:A:381:ARG:HG2	1:A:382:VAL:O	2.06	0.56
1:A:160:ARG:HG3	1:A:160:ARG:NH1	2.18	0.55
1:B:6:VAL:HG21	1:B:27:ARG:HH22	1.73	0.54
1:A:62:SER:OG	1:A:64:LYS:HG2	2.07	0.54
1:B:246:LEU:HD21	1:B:358:ALA:HA	1.89	0.54
1:A:118:ILE:HG22	1:A:142:LEU:HD12	1.92	0.52
3:A:502:HEM:HMC1	3:A:502:HEM:HBC2	1.92	0.52
1:A:295:LEU:O	1:A:301:THR:HA	2.11	0.51
1:B:115:VAL:HG12	1:B:360:VAL:HG11	1.92	0.51
1:B:106:ARG:HB3	1:B:106:ARG:CZ	2.42	0.49
3:B:501:HEM:HMC1	3:B:501:HEM:CBC	2.42	0.49
1:B:112:GLU:O	1:B:116:THR:OG1	2.29	0.48
1:A:39:GLU:OE2	1:A:39:GLU:N	2.44	0.48
1:B:149:GLU:HA	1:B:158:ARG:HH12	1.78	0.47
3:B:501:HEM:HHC	3:B:501:HEM:HBB2	1.96	0.47
1:B:147:ILE:HG22	1:B:151:MET:HE3	1.96	0.47
1:B:240:GLU:O	1:B:244:LYS:HG2	2.14	0.47
1:B:359:ARG:HB2	5:B:612:HOH:O	2.15	0.47
1:B:149:GLU:OE1	1:B:158:ARG:NH2	2.47	0.46
1:B:147:ILE:CG2	1:B:151:MET:HE3	2.45	0.46
1:B:308:LEU:C	1:B:308:LEU:HD23	2.39	0.46
1:A:200:ARG:HA	1:A:203:ASN:O	2.16	0.45
1:B:370:ARG:NH1	1:B:401:LEU:HD13	2.31	0.45
1:A:270:ILE:N	1:A:271:PRO:CD	2.79	0.45
1:A:193:TYR:CB	1:A:228:MET:HE1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:HA	1:A:322:PHE:O	2.17	0.45
1:B:271:PRO:HG3	1:B:359:ARG:HD3	1.98	0.45
1:B:347:PHE:O	1:B:348:CYS:C	2.59	0.45
1:B:331:GLY:O	1:B:332:ARG:C	2.59	0.44
1:B:106:ARG:NH2	1:B:110:GLU:OE2	2.50	0.44
1:B:324:ASP:OD2	1:B:329:ARG:NH2	2.49	0.44
1:A:327:GLU:OE1	1:A:329:ARG:NH2	2.51	0.44
1:B:400:ARG:O	1:B:401:LEU:C	2.61	0.44
1:A:402:GLU:N	1:A:402:GLU:OE1	2.52	0.43
1:A:70:ASP:HA	1:A:71:PRO:HD2	1.93	0.43
1:A:160:ARG:HH11	1:A:160:ARG:CG	2.31	0.42
1:A:287:LEU:CD2	3:A:502:HEM:HBA2	2.49	0.42
1:B:381:ARG:HG2	1:B:382:VAL:O	2.19	0.42
1:A:239:ASN:HB3	5:A:675:HOH:O	2.20	0.42
3:A:502:HEM:HHC	3:A:502:HEM:HBB2	2.00	0.42
1:B:230:PHE:CE2	1:B:234:MET:HE2	2.55	0.42
1:B:77:GLU:HG3	1:B:80:ARG:NH1	2.35	0.41
1:B:334:ILE:CG2	1:B:336:SER:O	2.67	0.41
1:A:261:ALA:HB3	1:A:262:PRO:HD3	2.03	0.41
1:B:261:ALA:HB3	1:B:262:PRO:HD3	2.03	0.41
1:B:200:ARG:O	1:B:203:ASN:O	2.39	0.41
1:A:173:ASP:OD2	1:A:383:HIS:ND1	2.54	0.41
1:A:214:GLU:O	1:A:215:ALA:C	2.64	0.41
1:B:142:LEU:N	1:B:143:PRO:CD	2.83	0.41
1:B:87:LEU:CD1	1:B:95:LEU:HD12	2.52	0.40
1:A:55:PHE:CE2	1:A:339:VAL:HG22	2.56	0.40
1:B:11:ASP:HB3	1:B:14:ASP:HB2	2.03	0.40
1:A:60:ALA:O	1:A:292:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

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	395/397 (100%)	385 (98%)	10 (2%)	0	100	100
1	B	394/397 (99%)	379 (96%)	15 (4%)	0	100	100
All	All	789/794 (99%)	764 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	336/336 (100%)	328 (98%)	8 (2%)	43	58
1	B	335/336 (100%)	329 (98%)	6 (2%)	51	68
All	All	671/672 (100%)	657 (98%)	14 (2%)	47	63

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	80	ARG
1	A	124	GLU
1	A	160	ARG
1	A	175	VAL
1	A	284	SER
1	A	334	ILE
1	A	337	LYS
1	B	94	ARG
1	B	104	THR
1	B	116	THR
1	B	284	SER
1	B	400	ARG
1	B	401	LEU

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

Mol	Chain	Res	Type
1	A	269	GLN
1	A	352	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	CIT	A	503	-	12,12,12	1.27	2 (16%)	17,17,17	1.50	2 (11%)
4	CIT	B	503	-	12,12,12	1.24	1 (8%)	17,17,17	1.52	3 (17%)
3	HEM	B	501	1	50,50,50	1.63	11 (22%)	66,82,82	1.18	9 (13%)
3	HEM	A	502	5,1	50,50,50	1.57	11 (22%)	66,82,82	1.23	6 (9%)
2	PEG	A	501	-	6,6,6	0.36	0	5,5,5	0.23	0
2	PEG	B	502	-	6,6,6	0.42	0	5,5,5	0.37	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
4	CIT	A	503	-	-	3/16/16/16	-
4	CIT	B	503	-	-	9/16/16/16	-
3	HEM	B	501	1	-	1/14/54/54	-
3	HEM	A	502	5,1	-	3/14/54/54	-
2	PEG	A	501	-	-	0/4/4/4	-
2	PEG	B	502	-	-	2/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	HEM	FE-NB	4.09	2.07	1.94
3	B	501	HEM	C1D-C2D	-4.08	1.36	1.44
3	B	501	HEM	C3C-C4C	-4.04	1.38	1.46
3	A	502	HEM	FE-NB	3.85	2.06	1.94
3	B	501	HEM	C4D-C3D	-3.53	1.39	1.45
3	A	502	HEM	C4D-C3D	-3.46	1.39	1.45
3	A	502	HEM	C3C-C4C	-3.40	1.40	1.46
3	A	502	HEM	C1D-C2D	-3.11	1.38	1.44
3	B	501	HEM	FE-NA	3.08	2.05	1.95
3	A	502	HEM	FE-NC	3.06	2.05	1.95
3	B	501	HEM	C1A-C2A	-2.84	1.39	1.44
3	B	501	HEM	C3B-C4B	-2.75	1.39	1.44
3	A	502	HEM	C1A-C2A	-2.69	1.39	1.44
3	A	502	HEM	C4A-C3A	-2.65	1.37	1.43
3	B	501	HEM	C1B-C2B	-2.58	1.39	1.44
3	A	502	HEM	C3B-C4B	-2.57	1.39	1.44
3	B	501	HEM	C4A-C3A	-2.55	1.37	1.43
3	A	502	HEM	FE-NA	2.47	2.03	1.95
4	A	503	CIT	C3-C6	2.47	1.56	1.53
3	B	501	HEM	C1C-C2C	-2.36	1.40	1.45
3	A	502	HEM	FE-ND	2.29	2.01	1.94
3	B	501	HEM	C1A-NA	-2.20	1.35	1.39
4	A	503	CIT	O4-C5	-2.19	1.23	1.30
4	B	503	CIT	C3-C6	2.09	1.55	1.53
3	A	502	HEM	CHD-C4C	2.01	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	CIT	O5-C6-C3	-3.97	116.63	122.25
4	B	503	CIT	O5-C6-C3	-3.54	117.24	122.25
3	A	502	HEM	CAB-C3B-C2B	-3.42	117.34	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	HEM	CMB-C2B-C1B	3.37	130.17	125.04
4	A	503	CIT	O6-C6-C3	2.92	118.12	113.05
3	B	501	HEM	CMB-C2B-C1B	2.91	129.47	125.04
3	B	501	HEM	CAB-C3B-C2B	-2.90	119.04	128.60
3	B	501	HEM	O1A-CGA-CBA	-2.57	114.82	123.08
3	A	502	HEM	CHC-C4B-NB	-2.48	121.72	124.42
4	B	503	CIT	O6-C6-C3	2.38	117.18	113.05
3	B	501	HEM	CMC-C2C-C1C	2.37	128.88	124.71
3	B	501	HEM	O2A-CGA-CBA	2.30	121.42	114.03
3	A	502	HEM	CAB-C3B-C4B	2.15	134.49	124.47
3	B	501	HEM	O1D-CGD-CBD	-2.12	116.28	123.08
4	B	503	CIT	O3-C5-C4	-2.08	116.86	122.94
3	A	502	HEM	C3C-C2C-C1C	-2.08	105.09	107.08
3	B	501	HEM	CAD-C3D-C4D	2.07	128.27	124.66
3	B	501	HEM	O2D-CGD-CBD	2.05	120.62	114.03
3	A	502	HEM	CHB-C1B-NB	-2.04	121.86	124.37
3	B	501	HEM	CHC-C1C-NC	-2.00	122.27	124.44

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	CIT	C2-C3-C6-O5
4	B	503	CIT	C2-C3-C6-O6
4	B	503	CIT	O7-C3-C6-O5
4	B	503	CIT	O7-C3-C6-O6
4	B	503	CIT	C1-C2-C3-O7
4	B	503	CIT	C1-C2-C3-C4
2	B	502	PEG	O2-C3-C4-O4
4	B	503	CIT	C1-C2-C3-C6
3	A	502	HEM	C4B-C3B-CAB-CBB
3	B	501	HEM	C4B-C3B-CAB-CBB
2	B	502	PEG	C4-C3-O2-C2
4	B	503	CIT	O2-C1-C2-C3
4	B	503	CIT	O1-C1-C2-C3
4	A	503	CIT	C2-C3-C4-C5
4	A	503	CIT	O1-C1-C2-C3
4	A	503	CIT	O2-C1-C2-C3
3	A	502	HEM	CAD-CBD-CGD-O2D
3	A	502	HEM	CAD-CBD-CGD-O1D

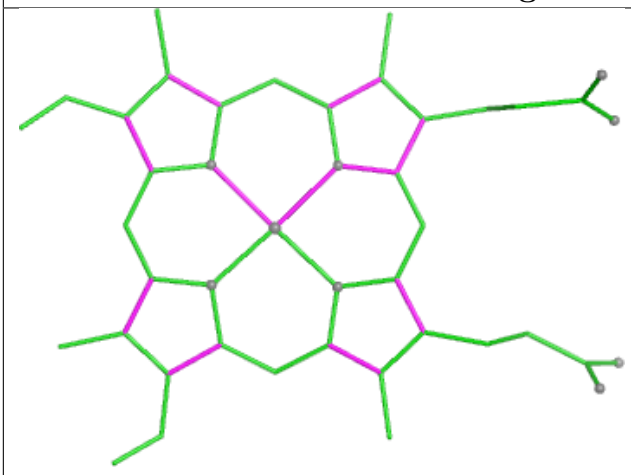
There are no ring outliers.

3 monomers are involved in 9 short contacts:

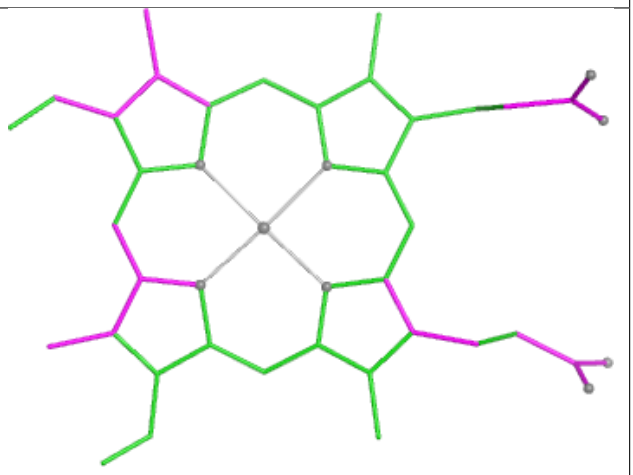
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	CIT	1	0
3	B	501	HEM	5	0
3	A	502	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

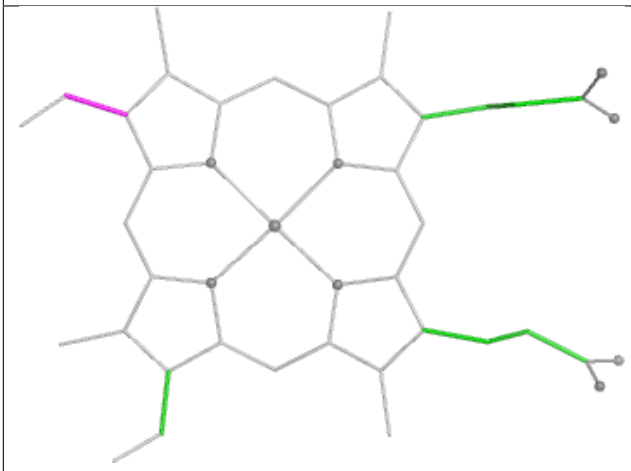
Ligand HEM B 501



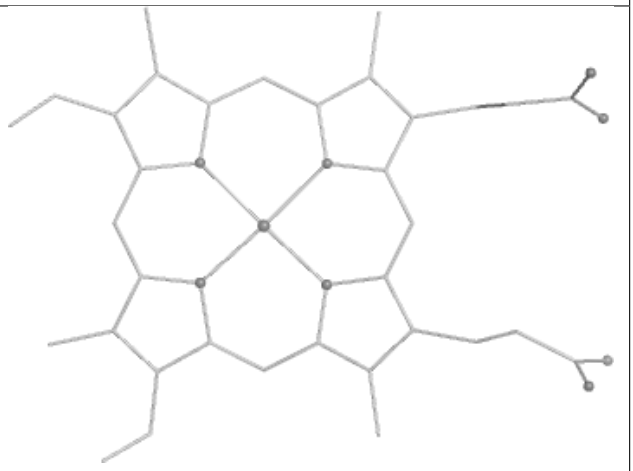
Bond lengths



Bond angles

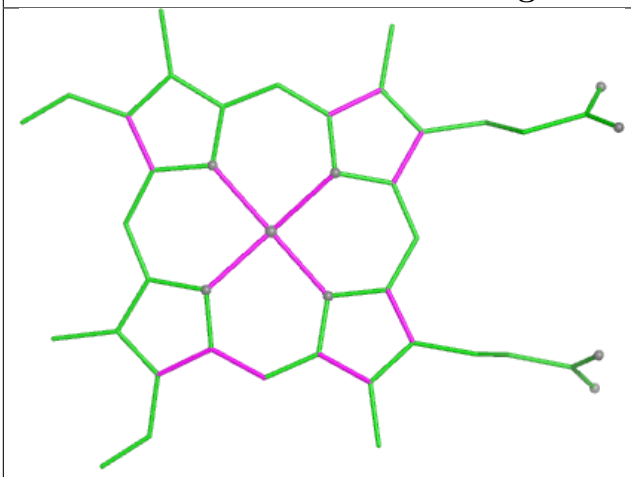


Torsions

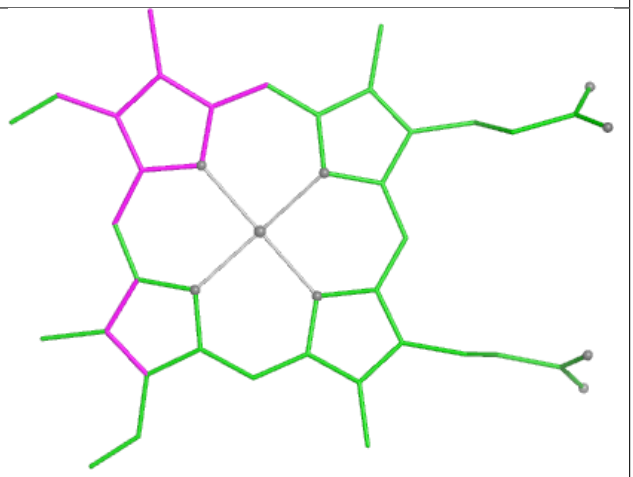


Rings

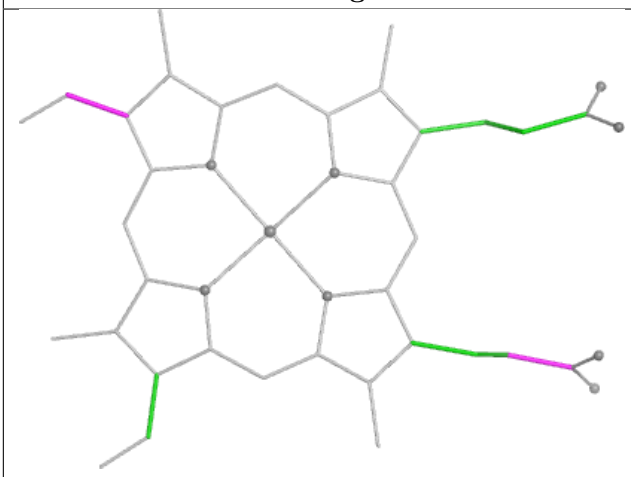
Ligand HEM A 502



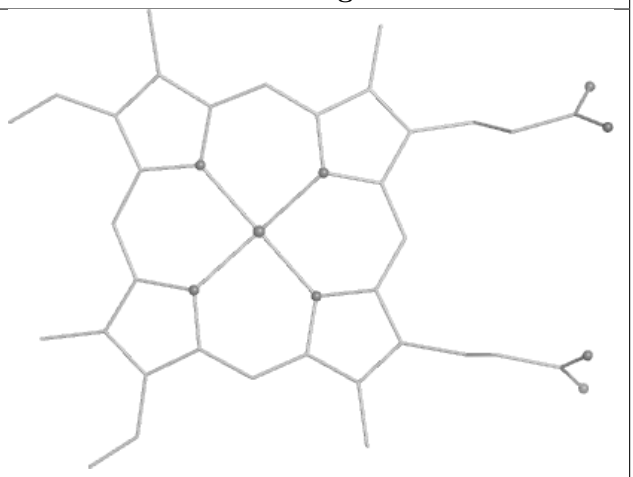
Bond lengths



Bond angles

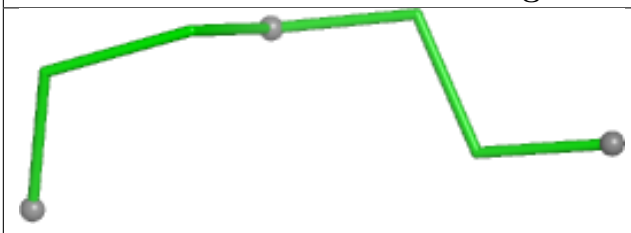


Torsions

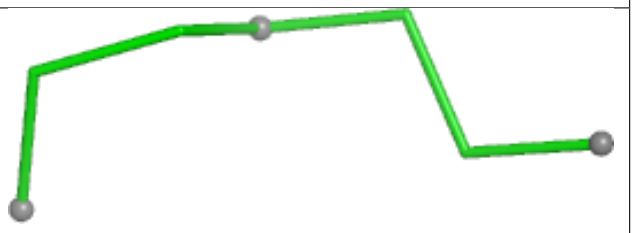


Rings

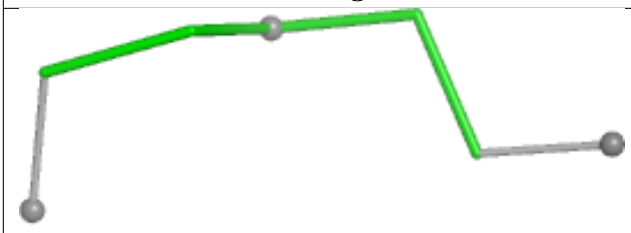
Ligand PEG A 501



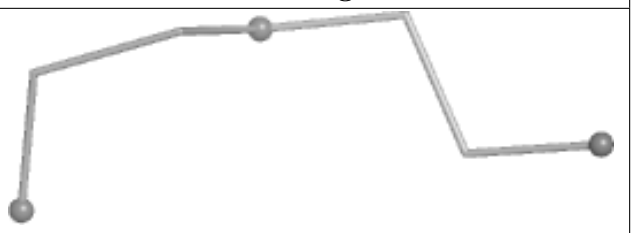
Bond lengths



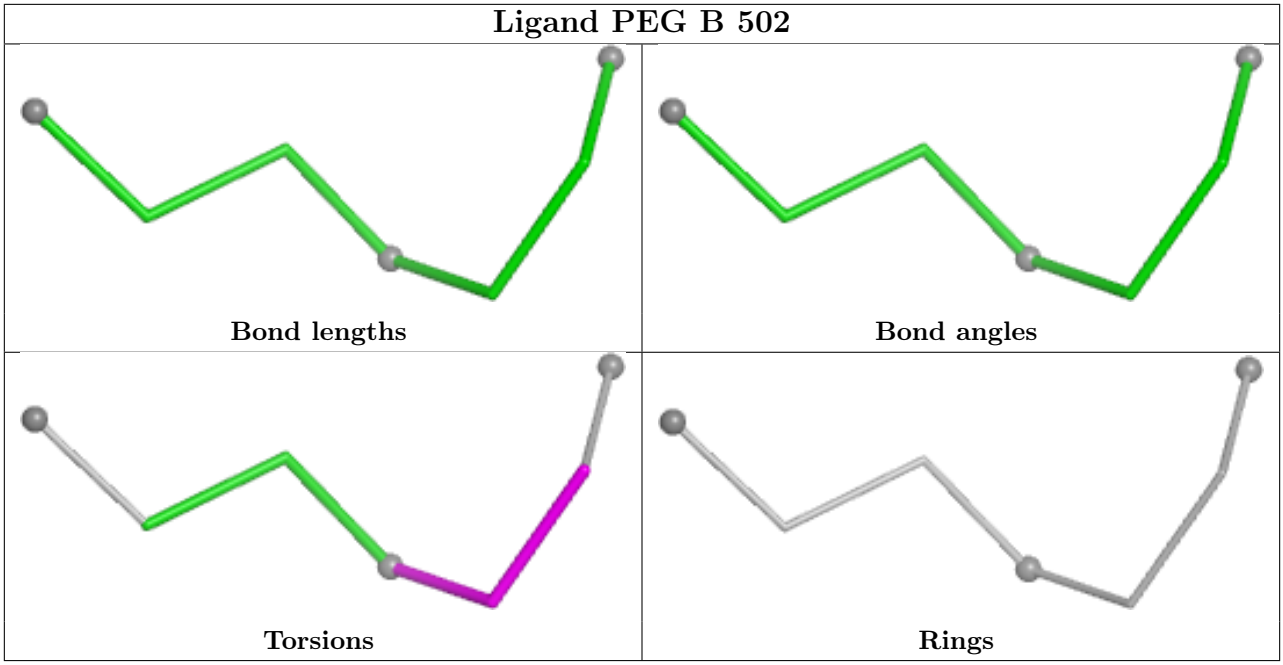
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	397/397 (100%)	0.19	13 (3%)	49	46	35, 49, 71, 105	3 (0%)
1	B	396/397 (99%)	0.50	16 (4%)	42	39	37, 58, 89, 106	1 (0%)
All	All	793/794 (99%)	0.34	29 (3%)	45	42	35, 52, 84, 106	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	ARG	8.5
1	B	401	LEU	4.2
1	A	6	VAL	3.7
1	A	178	VAL	3.7
1	B	334	ILE	3.6
1	B	6	VAL	3.6
1	A	179	PRO	3.4
1	B	178	VAL	3.3
1	A	292	VAL	3.1
1	B	217	ILE	3.0
1	A	7	GLU	2.7
1	A	110	GLU	2.7
1	B	292	VAL	2.7
1	A	182	ALA	2.6
1	B	236	VAL	2.6
1	B	81	VAL	2.4
1	B	108	ILE	2.4
1	B	204	VAL	2.4
1	A	401	LEU	2.3
1	B	95	LEU	2.3
1	B	352	HIS	2.3
1	A	183	ILE	2.2
1	B	222	LEU	2.2
1	A	334	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	270	ILE	2.1
1	A	8	PRO	2.1
1	A	296	THR	2.0
1	B	104	THR	2.0
1	A	181	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

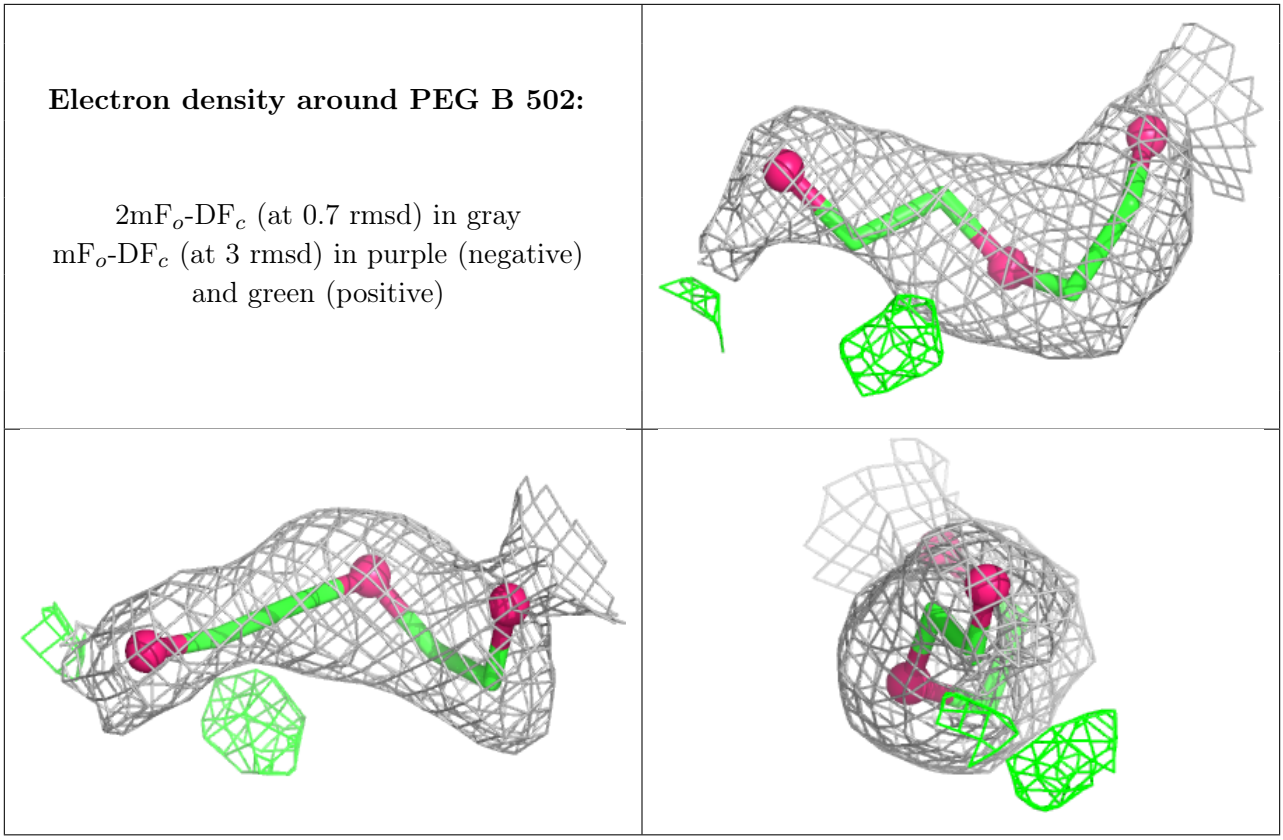
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	CIT	B	503	13/13	0.83	0.14	57,61,75,83	13
4	CIT	A	503	13/13	0.88	0.09	60,65,74,75	0
2	PEG	B	502	7/7	0.89	0.17	69,72,75,82	0
2	PEG	A	501	7/7	0.93	0.13	42,47,60,64	0
3	HEM	A	502	43/43	0.98	0.07	27,40,48,59	0
3	HEM	B	501	43/43	0.98	0.07	35,50,57,63	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.

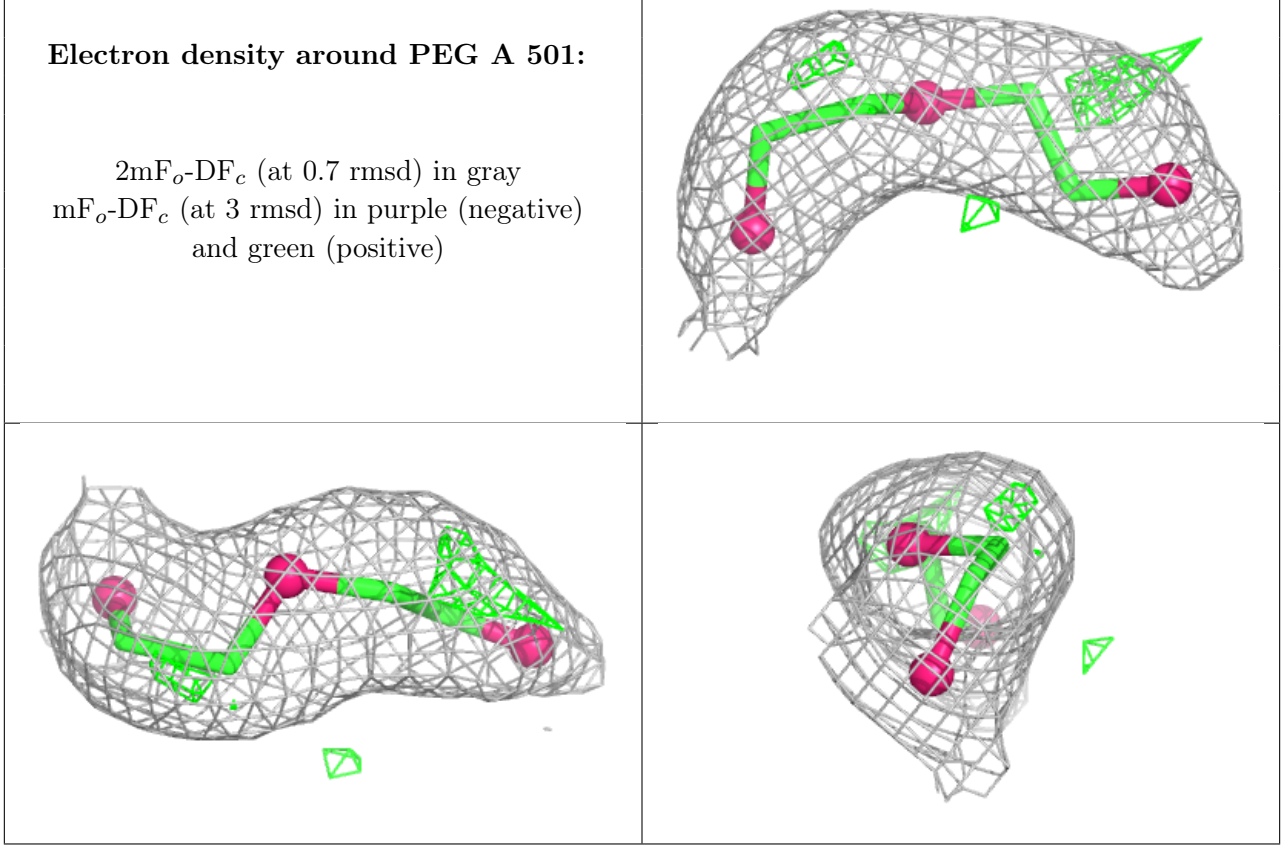
Electron density around PEG B 502:

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



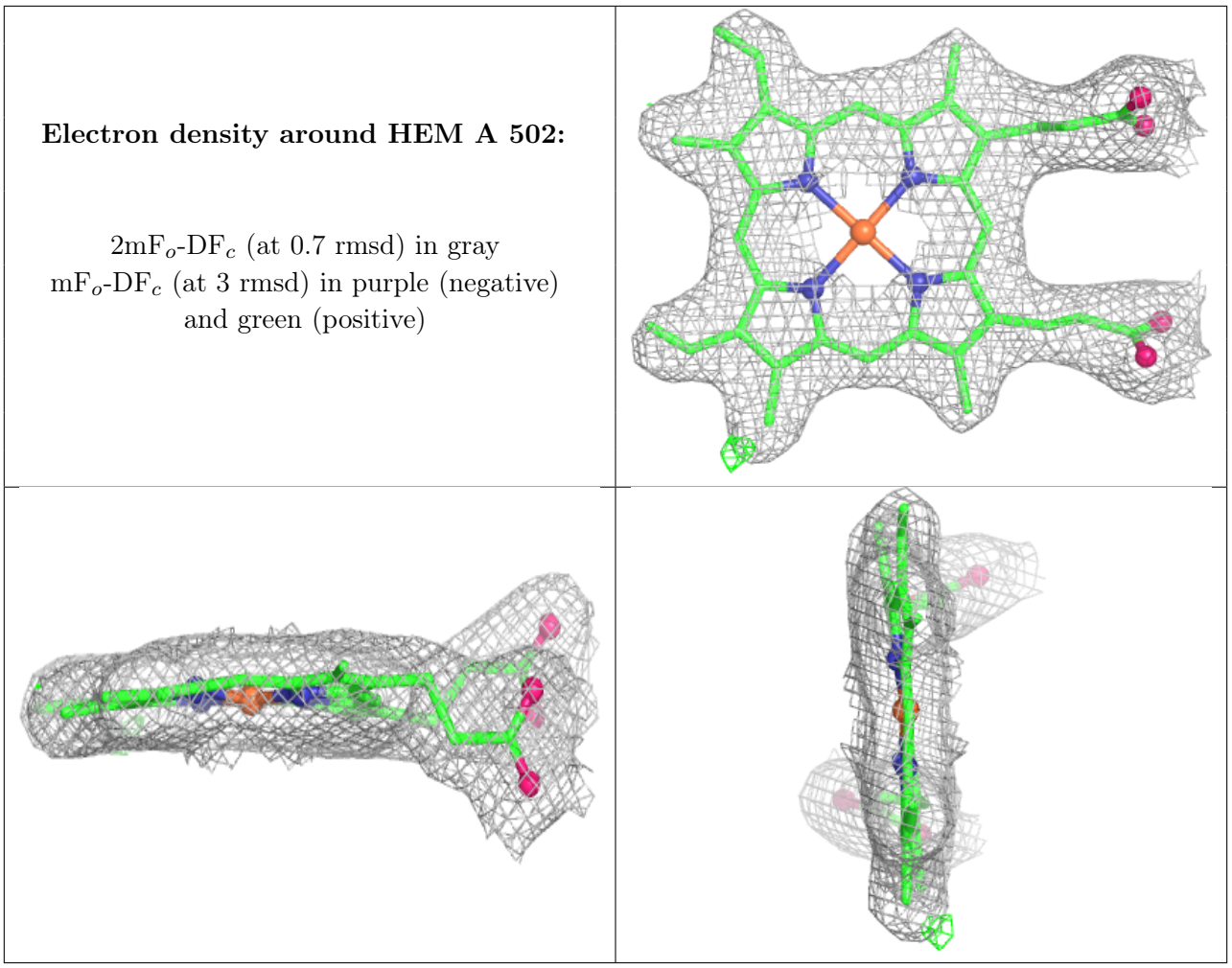
Electron density around PEG A 501:

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



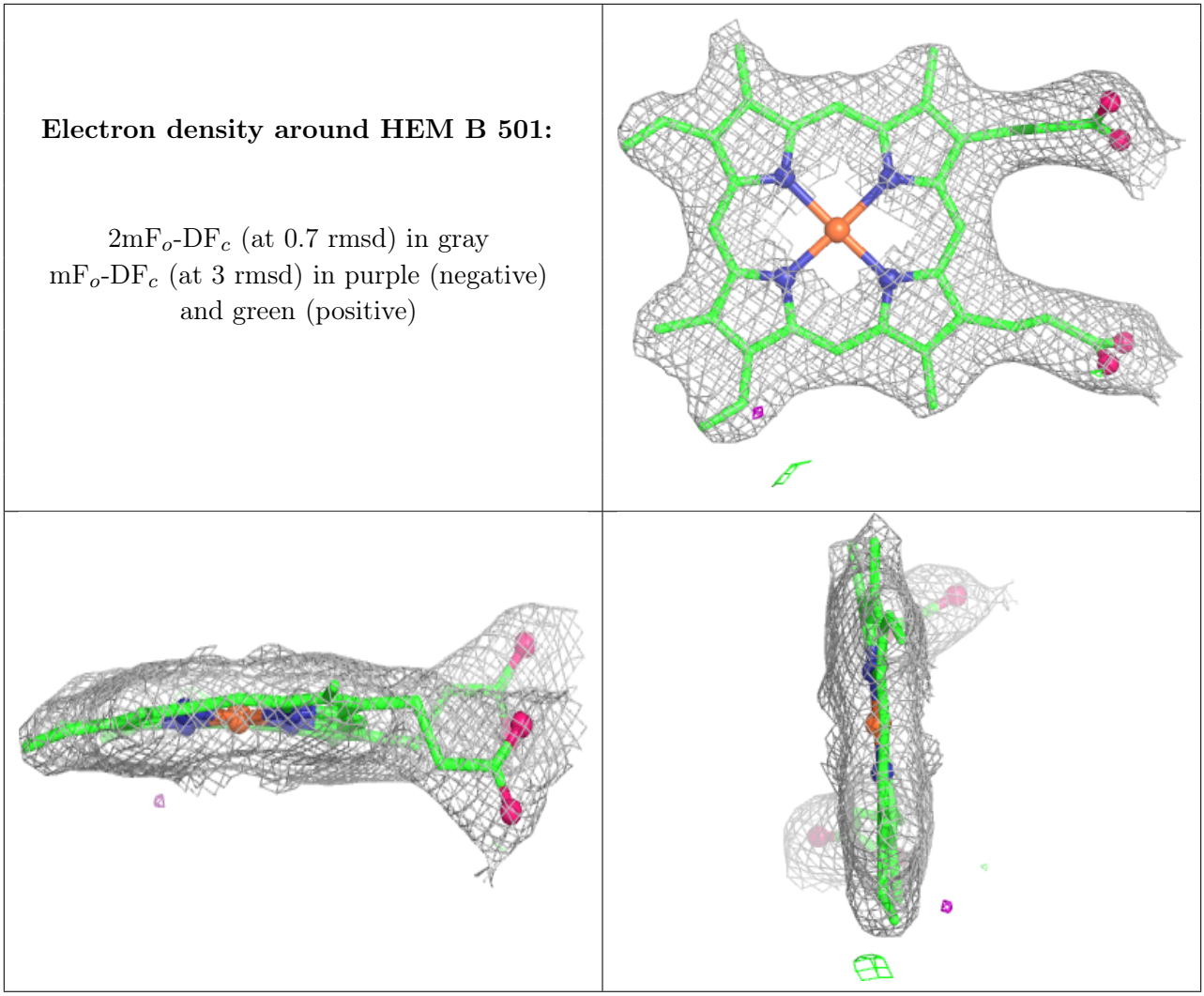
Electron density around HEM A 502:

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



Electron density around HEM 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

There are no such residues in this entry.