Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 06:43 am BST

PDB ID	:	4COO / pdb_00004coo
Title	:	Crystal structure of human cystathionine beta-synthase (delta516-525) at 2.0 angstrom resolution
Authors	:	McCorvie, T.J.; Kopec, J.; Vollamar, M.; Strain-Damerell, C.; Bushell, S.; Bradley, A.; Tallant, C.; Kiyani, W.; Froese, D.S.; Carpenter, E.S.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.; Edwards, A.; Bountra, C.; Yue, W.W.
Deposited on	:	2014-01-29
Resolution	:	2.00 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:

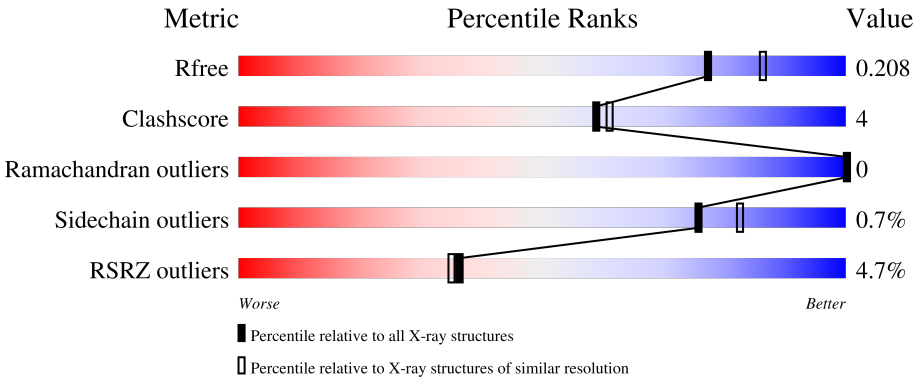
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	563	3% 81% 7% 12%
1	B	563	5% 81% 5% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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
3	ACT	A	1550	-	-	X	-
3	ACT	B	1540	-	-	X	-
3	ACT	B	1542	-	-	X	-
3	ACT	B	1546	-	-	X	-
5	EDO	A	1554	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8055 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 CYSTATHIONINE BETA-SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	5	0
			3822	2424	668	708	22			
1	B	487	Total	C	N	O	S	0	5	0
			3766	2392	657	695	22			

There are 64 discrepancies between the modelled and reference sequences:

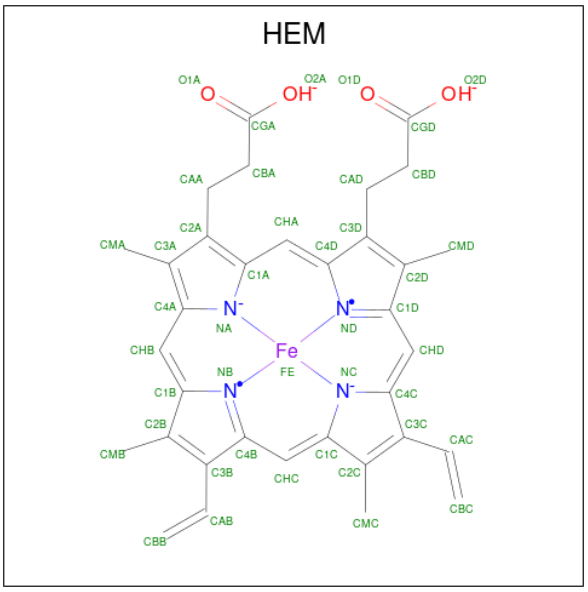
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P35520
A	-20	HIS	-	expression tag	UNP P35520
A	-19	HIS	-	expression tag	UNP P35520
A	-18	HIS	-	expression tag	UNP P35520
A	-17	HIS	-	expression tag	UNP P35520
A	-16	HIS	-	expression tag	UNP P35520
A	-15	HIS	-	expression tag	UNP P35520
A	-14	SER	-	expression tag	UNP P35520
A	-13	SER	-	expression tag	UNP P35520
A	-12	GLY	-	expression tag	UNP P35520
A	-11	VAL	-	expression tag	UNP P35520
A	-10	ASP	-	expression tag	UNP P35520
A	-9	LEU	-	expression tag	UNP P35520
A	-8	GLY	-	expression tag	UNP P35520
A	-7	THR	-	expression tag	UNP P35520
A	-6	GLU	-	expression tag	UNP P35520
A	-5	ASN	-	expression tag	UNP P35520
A	-4	LEU	-	expression tag	UNP P35520
A	-3	TYR	-	expression tag	UNP P35520
A	-2	PHE	-	expression tag	UNP P35520
A	-1	GLN	-	expression tag	UNP P35520
A	0	SER	-	expression tag	UNP P35520
A	?	-	ILE	deletion	UNP P35520
A	?	-	GLN	deletion	UNP P35520
A	?	-	TYR	deletion	UNP P35520

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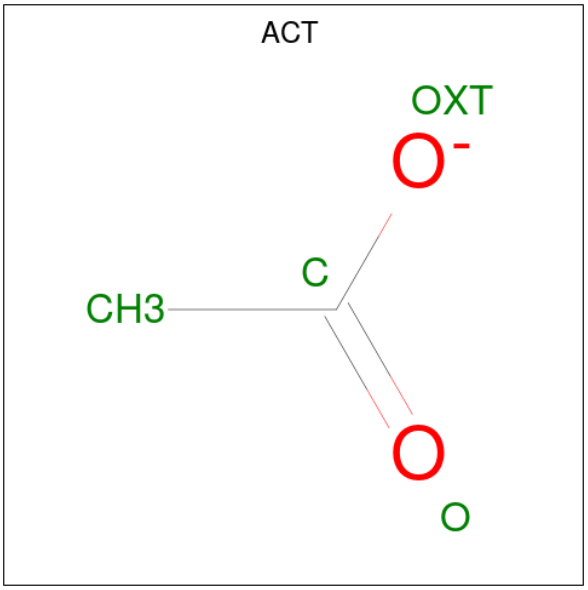
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	THR	deletion	UNP P35520
A	?	-	GLY	deletion	UNP P35520
A	?	-	LYS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
B	-21	MET	-	expression tag	UNP P35520
B	-20	HIS	-	expression tag	UNP P35520
B	-19	HIS	-	expression tag	UNP P35520
B	-18	HIS	-	expression tag	UNP P35520
B	-17	HIS	-	expression tag	UNP P35520
B	-16	HIS	-	expression tag	UNP P35520
B	-15	HIS	-	expression tag	UNP P35520
B	-14	SER	-	expression tag	UNP P35520
B	-13	SER	-	expression tag	UNP P35520
B	-12	GLY	-	expression tag	UNP P35520
B	-11	VAL	-	expression tag	UNP P35520
B	-10	ASP	-	expression tag	UNP P35520
B	-9	LEU	-	expression tag	UNP P35520
B	-8	GLY	-	expression tag	UNP P35520
B	-7	THR	-	expression tag	UNP P35520
B	-6	GLU	-	expression tag	UNP P35520
B	-5	ASN	-	expression tag	UNP P35520
B	-4	LEU	-	expression tag	UNP P35520
B	-3	TYR	-	expression tag	UNP P35520
B	-2	PHE	-	expression tag	UNP P35520
B	-1	GLN	-	expression tag	UNP P35520
B	0	SER	-	expression tag	UNP P35520
B	?	-	ILE	deletion	UNP P35520
B	?	-	GLN	deletion	UNP P35520
B	?	-	TYR	deletion	UNP P35520
B	?	-	HIS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	THR	deletion	UNP P35520
B	?	-	GLY	deletion	UNP P35520
B	?	-	LYS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520

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



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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



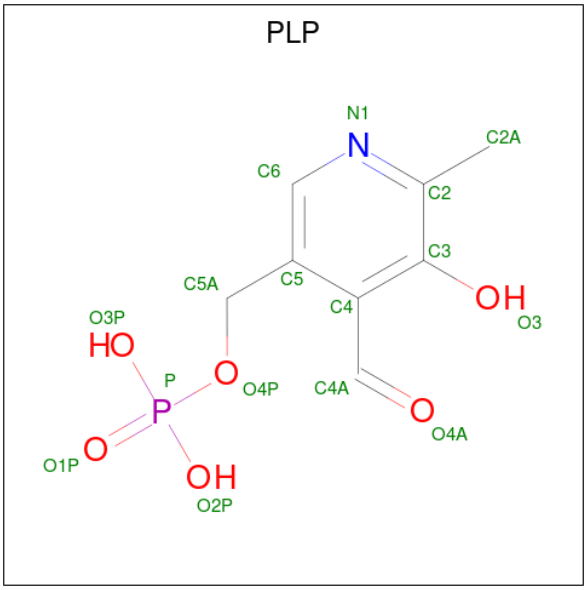
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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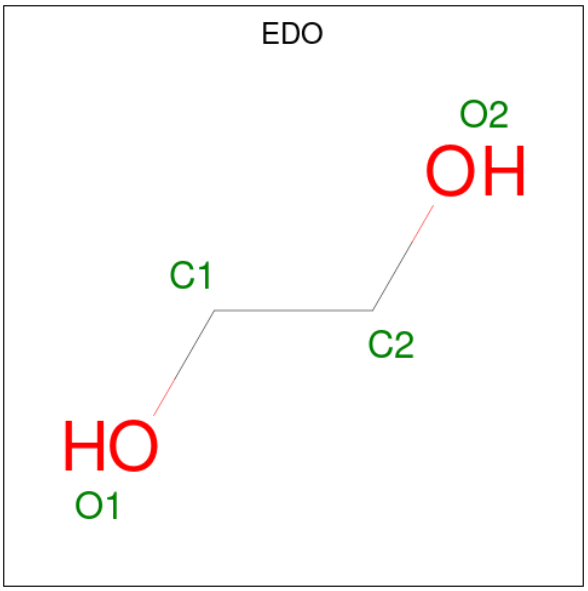
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



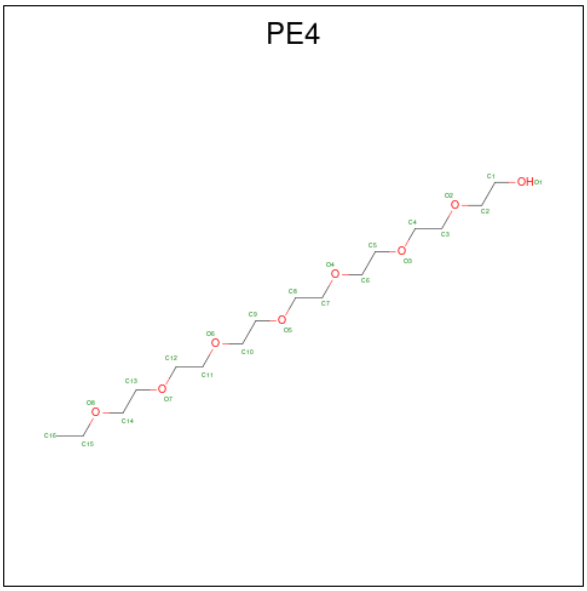
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 15 8 1 5 1	0	0
4	B	1	Total C N O P 15 8 1 5 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 5 2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	191	Total O 191 191	0	0
8	B	103	Total O 103 103	0	0

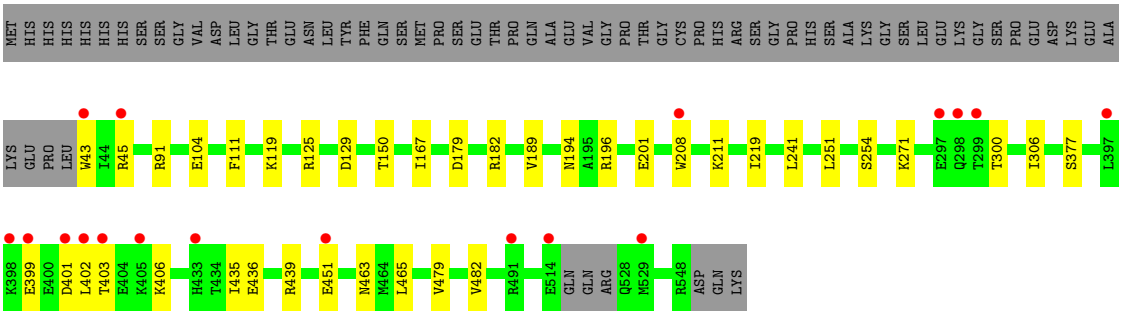
3 Residue-property plots (i)

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: CYSTATHIONINE BETA-SYNTHASE

Chain A:

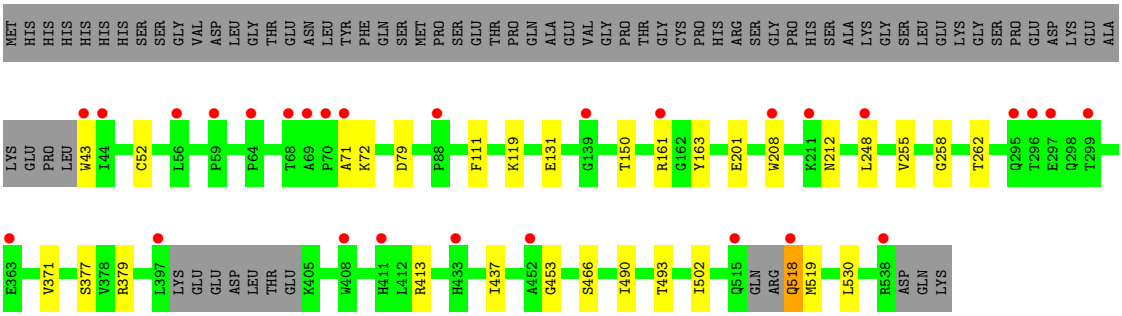




• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.26Å 116.19Å 167.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.56 – 2.00 95.56 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.56-2.00) 99.6 (95.56-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.201 0.184 , 0.208	Depositor DCC
R_{free} test set	4662 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: PLP, PE4, EDO, ACT, NA, HEM

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	0.73	0/3905	0.84	0/5295
1	B	0.64	0/3846	0.80	0/5216
All	All	0.69	0/7751	0.82	0/10511

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	3822	0	3856	31	0
1	B	3766	0	3778	25	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	4	0	3	4	0
3	B	16	0	12	13	0
4	A	15	0	6	0	0
4	B	15	0	6	3	0
5	A	24	0	36	5	0
5	B	4	0	6	1	0
6	A	7	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	191	0	0	8	0
8	B	103	0	0	4	0
All	All	8055	0	7769	68	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 4.

All (68) 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:119:LYS:NZ	4:B:1543:PLP:C4A	1.67	1.51
1:B:379:ARG:NH2	8:B:2011:HOH:O	1.81	1.09
1:B:119:LYS:HZ3	4:B:1543:PLP:C4A	1.81	0.90
1:B:150:THR:H	3:B:1540:ACT:H1	1.40	0.87
1:A:150:THR:H	3:A:1550:ACT:H1	1.41	0.85
5:A:1554:EDO:O2	3:B:1542:ACT:H2	1.83	0.79
8:A:2190:HOH:O	3:B:1542:ACT:H1	1.83	0.77
1:B:530:LEU:HA	3:B:1542:ACT:H3	1.66	0.74
1:A:194[B]:ASN:ND2	8:A:2082:HOH:O	2.19	0.74
1:B:201:GLU:OE1	8:B:2041:HOH:O	2.06	0.72
1:A:201:GLU:OE1	8:A:2086:HOH:O	2.07	0.72
1:A:194[B]:ASN:CG	8:A:2082:HOH:O	2.32	0.72
2:A:1549:HEM:HMC2	2:A:1549:HEM:HBC2	1.74	0.69
1:A:91:ARG:NH1	1:A:104:GLU:OE2	2.26	0.69
2:B:1539:HEM:HMC1	2:B:1539:HEM:HBC2	1.77	0.66
5:A:1554:EDO:H11	3:B:1546:ACT:CH3	2.28	0.64
1:A:208[A]:TRP:CZ3	1:A:211:LYS:HE2	2.33	0.63
3:A:1550:ACT:H3	8:A:2047:HOH:O	2.00	0.60
1:A:43:TRP:CZ3	1:A:45[A]:ARG:HG2	2.38	0.59
1:B:530:LEU:CA	3:B:1542:ACT:H3	2.32	0.58
1:A:211:LYS:HD3	1:A:219:ILE:HG13	1.85	0.58
1:A:194[A]:ASN:OD1	1:A:300:THR:CG2	2.52	0.57
1:B:119:LYS:NZ	3:B:1540:ACT:H2	2.21	0.56
1:A:403:THR:HA	1:A:406:LYS:HG2	1.88	0.56
1:A:125:ARG:HD2	1:A:129:ASP:OD2	2.07	0.55
1:A:150:THR:H	3:A:1550:ACT:CH3	2.15	0.55
3:B:1540:ACT:H3	8:B:2019:HOH:O	2.07	0.55
1:B:111:PHE:HB2	1:B:377:SER:HB3	1.89	0.54
1:A:196:ARG:HD3	1:B:466:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:NH2	8:A:2084:HOH:O	2.29	0.53
1:A:439:ARG:HH21	6:A:1557:PE4:C6	2.22	0.53
2:B:1539:HEM:HMB1	2:B:1539:HEM:HBB2	1.89	0.52
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.92	0.51
1:B:119:LYS:CE	4:B:1543:PLP:C4A	2.81	0.51
2:A:1549:HEM:HBC2	2:A:1549:HEM:CMC	2.40	0.51
1:A:479:VAL:HG22	8:A:2162:HOH:O	2.12	0.49
1:A:119:LYS:HG3	3:A:1550:ACT:H2	1.94	0.49
1:B:453:GLY:HA3	1:B:518:GLN:OE1	2.13	0.48
1:B:262:THR:HG21	5:B:1544:EDO:H22	1.95	0.48
5:A:1554:EDO:C1	3:B:1546:ACT:CH3	2.91	0.48
1:A:194[A]:ASN:OD1	1:A:300:THR:HG22	2.12	0.48
1:A:403:THR:HA	1:A:406:LYS:CG	2.43	0.48
1:A:189:VAL:HG22	3:B:1546:ACT:H2	1.95	0.47
2:B:1539:HEM:HBC2	2:B:1539:HEM:CMC	2.44	0.47
1:A:451:GLU:H	1:A:451:GLU:CD	2.22	0.47
1:B:208[B]:TRP:NE1	1:B:212:ASN:HD21	2.13	0.47
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.98	0.46
2:A:1549:HEM:HBB2	2:A:1549:HEM:HHC	1.97	0.46
1:A:435:ILE:HD12	1:A:465:LEU:HG	1.97	0.45
1:A:179:ASP:OD2	8:A:2074:HOH:O	2.21	0.45
1:B:131:GLU:OE2	1:B:163:TYR:OH	2.33	0.45
1:B:71:ALA:O	1:B:72:LYS:C	2.61	0.44
1:B:79:ASP:OD2	1:B:161[B]:ARG:NH1	2.43	0.44
1:A:463:ASN:HB2	1:B:201:GLU:OE2	2.17	0.43
1:B:52:CYS:HA	2:B:1539:HEM:C1A	2.53	0.43
1:B:413:ARG:HD2	1:B:493:THR:O	2.19	0.43
1:A:399:GLU:HA	1:A:402:LEU:HB3	2.01	0.43
1:B:490:ILE:HD12	1:B:502:ILE:HD12	2.00	0.43
1:A:182:ARG:HD3	8:B:2096:HOH:O	2.19	0.42
5:A:1554:EDO:O2	3:B:1542:ACT:CH3	2.59	0.42
1:A:436:GLU:HG2	6:A:1557:PE4:H31	2.00	0.42
1:B:43:TRP:N	1:B:208[B]:TRP:CZ2	2.88	0.42
1:B:150:THR:H	3:B:1540:ACT:CH3	2.22	0.42
1:A:482:VAL:O	1:A:482:VAL:HG12	2.20	0.42
1:A:241:LEU:HD13	1:A:271:LYS:HE3	2.02	0.42
1:A:254:SER:HB2	1:A:306:ILE:HG21	2.02	0.41
1:B:248:LEU:HD13	1:B:371:VAL:HG23	2.01	0.41
5:A:1554:EDO:H11	3:B:1546:ACT:H1	2.01	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	494/563 (88%)	484 (98%)	10 (2%)	0	100	100
1	B	486/563 (86%)	475 (98%)	11 (2%)	0	100	100
All	All	980/1126 (87%)	959 (98%)	21 (2%)	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	412/476 (87%)	409 (99%)	3 (1%)	76	82
1	B	402/476 (84%)	399 (99%)	3 (1%)	76	82
All	All	814/952 (86%)	808 (99%)	6 (1%)	76	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ILE
1	A	251	LEU
1	A	401	ASP
1	B	437	ILE
1	B	518	GLN
1	B	519	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	B	67	HIS
1	B	222	GLN
1	B	501	HIS
1	B	515	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	EDO	A	1552	-	3,3,3	0.51	0	2,2,2	0.28	0
2	HEM	B	1539	1	50,50,50	1.61	7 (14%)	66,82,82	1.69	14 (21%)
3	ACT	B	1541	-	3,3,3	0.76	0	3,3,3	0.77	0
3	ACT	A	1550	-	3,3,3	1.56	0	3,3,3	0.76	0
5	EDO	A	1555	-	3,3,3	0.35	0	2,2,2	0.39	0
3	ACT	B	1546	-	3,3,3	0.84	0	3,3,3	1.11	0
5	EDO	A	1554	-	3,3,3	0.36	0	2,2,2	0.35	0
5	EDO	A	1553	-	3,3,3	0.37	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACT	B	1542	-	3,3,3	0.71	0	3,3,3	1.15	0
5	EDO	A	1559	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1556	-	3,3,3	0.43	0	2,2,2	0.26	0
2	HEM	A	1549	1	50,50,50	1.53	7 (14%)	66,82,82	1.81	18 (27%)
3	ACT	B	1540	-	3,3,3	1.17	0	3,3,3	0.59	0
4	PLP	B	1543	-	15,15,16	2.37	4 (26%)	20,22,23	2.47	11 (55%)
4	PLP	A	1551	-	15,15,16	2.20	4 (26%)	20,22,23	2.42	10 (50%)
6	PE4	A	1557	-	6,6,23	0.80	0	5,5,22	0.65	0
5	EDO	B	1544	-	3,3,3	0.47	0	2,2,2	0.19	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	A	1552	-	-	0/1/1/1	-
2	HEM	B	1539	1	-	0/14/54/54	-
5	EDO	A	1555	-	-	0/1/1/1	-
5	EDO	A	1554	-	-	1/1/1/1	-
5	EDO	A	1553	-	-	1/1/1/1	-
5	EDO	A	1559	-	-	1/1/1/1	-
5	EDO	A	1556	-	-	0/1/1/1	-
2	HEM	A	1549	1	-	3/14/54/54	-
4	PLP	B	1543	-	-	1/6/6/8	0/1/1/1
4	PLP	A	1551	-	-	0/6/6/8	0/1/1/1
6	PE4	A	1557	-	-	3/4/4/21	-
5	EDO	B	1544	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1543	PLP	C5-C4	5.67	1.46	1.40
2	B	1539	HEM	FE-NB	5.52	2.12	1.94
4	A	1551	PLP	C3-C2	4.71	1.45	1.40
2	A	1549	HEM	FE-NB	4.65	2.09	1.94
2	A	1549	HEM	C1B-NB	-4.26	1.33	1.40
2	B	1539	HEM	FE-NC	4.25	2.09	1.95
4	B	1543	PLP	C3-C2	4.11	1.45	1.40
4	A	1551	PLP	C4A-C4	-4.00	1.43	1.51
4	B	1543	PLP	C4A-C4	-3.89	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1551	PLP	C3-C4	3.73	1.47	1.40
4	A	1551	PLP	C5-C4	3.65	1.44	1.40
2	B	1539	HEM	C1B-NB	-3.47	1.34	1.40
4	B	1543	PLP	C3-C4	3.23	1.46	1.40
2	A	1549	HEM	FE-NC	3.13	2.05	1.95
2	B	1539	HEM	C4D-ND	-2.99	1.35	1.40
2	A	1549	HEM	C3B-C4B	2.75	1.50	1.44
2	A	1549	HEM	C4D-ND	-2.58	1.35	1.40
2	B	1539	HEM	C3B-C4B	2.55	1.50	1.44
2	A	1549	HEM	C1C-C2C	-2.44	1.40	1.45
2	A	1549	HEM	C1D-ND	-2.38	1.33	1.38
2	B	1539	HEM	C1C-C2C	-2.30	1.40	1.45
2	B	1539	HEM	C4B-NB	-2.11	1.34	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1549	HEM	C1B-NB-C4B	5.76	111.02	105.07
2	B	1539	HEM	C1B-NB-C4B	5.26	110.51	105.07
2	B	1539	HEM	C4C-NC-C1C	4.61	109.86	105.35
4	A	1551	PLP	C4A-C4-C5	-4.61	116.19	120.94
2	A	1549	HEM	C4C-NC-C1C	4.41	109.67	105.35
4	B	1543	PLP	C6-C5-C4	-4.15	114.89	118.16
4	B	1543	PLP	O4P-C5A-C5	4.10	117.17	109.35
4	B	1543	PLP	C3-C4-C5	4.02	123.08	118.74
4	A	1551	PLP	C6-N1-C2	4.02	126.61	119.17
2	B	1539	HEM	CHA-C4D-ND	3.97	129.27	124.37
4	A	1551	PLP	C6-C5-C4	-3.94	115.06	118.16
2	B	1539	HEM	CHC-C4B-NB	3.68	128.42	124.42
2	A	1549	HEM	CHB-C1B-NB	3.62	128.84	124.37
4	B	1543	PLP	C6-N1-C2	3.52	125.69	119.17
2	A	1549	HEM	C1A-CHA-C4D	-3.49	118.06	126.34
2	B	1539	HEM	CAA-CBA-CGA	-3.45	106.17	113.60
4	B	1543	PLP	C4-C3-C2	-3.40	115.04	120.07
4	A	1551	PLP	C3-C4-C5	3.30	122.31	118.74
4	A	1551	PLP	C5A-C5-C6	3.16	124.57	119.37
2	B	1539	HEM	CBD-CAD-C3D	-3.08	104.07	112.63
2	B	1539	HEM	CHD-C1D-ND	3.05	127.73	124.42
2	A	1549	HEM	CBD-CAD-C3D	-3.04	104.18	112.63
2	A	1549	HEM	CAB-C3B-C2B	-3.02	118.64	128.60
2	B	1539	HEM	CHA-C4D-C3D	-2.93	119.82	125.33
4	B	1543	PLP	C4A-C4-C5	-2.90	117.95	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1551	PLP	C3-C2-N1	-2.90	117.03	120.77
2	A	1549	HEM	CHC-C4B-NB	2.80	127.46	124.42
4	A	1551	PLP	O3-C3-C2	2.76	123.50	117.49
4	B	1543	PLP	O3-C3-C2	2.70	123.39	117.49
4	A	1551	PLP	O4P-C5A-C5	2.68	114.46	109.35
2	A	1549	HEM	CHD-C1D-ND	2.67	127.31	124.42
2	A	1549	HEM	O2D-CGD-CBD	2.63	122.49	114.03
2	A	1549	HEM	CHA-C4D-C3D	-2.55	120.54	125.33
4	A	1551	PLP	C4-C3-C2	-2.55	116.31	120.07
2	A	1549	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
2	A	1549	HEM	C1C-CHC-C4B	-2.46	120.75	126.06
2	B	1539	HEM	C1A-CHA-C4D	-2.44	120.55	126.34
2	A	1549	HEM	CHA-C4D-ND	2.44	127.38	124.37
4	B	1543	PLP	O2P-P-O4P	-2.38	100.40	106.73
2	A	1549	HEM	CMB-C2B-C1B	2.34	128.60	125.04
2	A	1549	HEM	CAB-C3B-C4B	2.33	135.32	124.47
2	B	1539	HEM	CMD-C2D-C1D	2.32	128.58	125.04
2	A	1549	HEM	C4C-C3C-C2C	2.27	108.62	106.75
4	B	1543	PLP	O3P-P-O2P	2.26	116.26	107.64
4	B	1543	PLP	O2P-P-O1P	2.22	119.38	110.68
2	B	1539	HEM	C4A-NA-C1A	2.21	107.51	105.35
2	A	1549	HEM	CHD-C4C-NC	2.18	126.80	124.44
2	B	1539	HEM	O2A-CGA-O1A	-2.14	117.97	123.30
2	A	1549	HEM	O2A-CGA-CBA	2.09	120.75	114.03
2	B	1539	HEM	CHD-C1D-C2D	-2.07	121.74	124.98
4	A	1551	PLP	C2A-C2-N1	2.05	121.68	117.67
2	B	1539	HEM	C4B-C3B-C2B	-2.05	105.49	107.11
4	B	1543	PLP	C5A-C5-C6	2.04	122.72	119.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1543	PLP	C6-C5-C5A-O4P
2	A	1549	HEM	C4B-C3B-CAB-CBB
6	A	1557	PE4	C6-C5-O3-C4
6	A	1557	PE4	C4-C3-O2-C2
5	A	1553	EDO	O1-C1-C2-O2
6	A	1557	PE4	C3-C4-O3-C5
5	A	1554	EDO	O1-C1-C2-O2
2	A	1549	HEM	CAA-CBA-CGA-O2A
5	B	1544	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	1549	HEM	CAA-CBA-CGA-O1A
5	A	1559	EDO	O1-C1-C2-O2

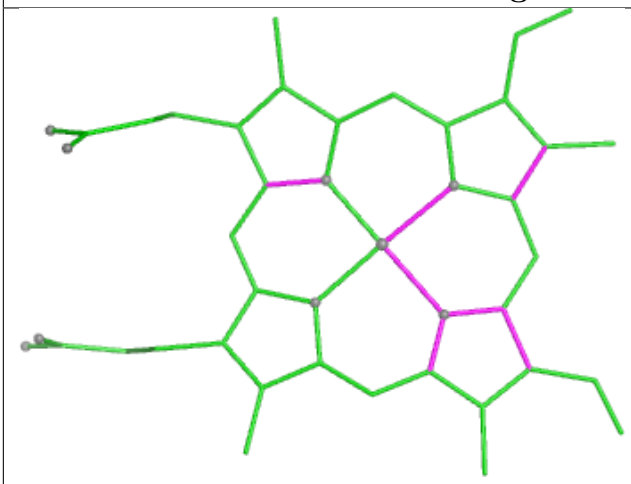
There are no ring outliers.

10 monomers are involved in 30 short contacts:

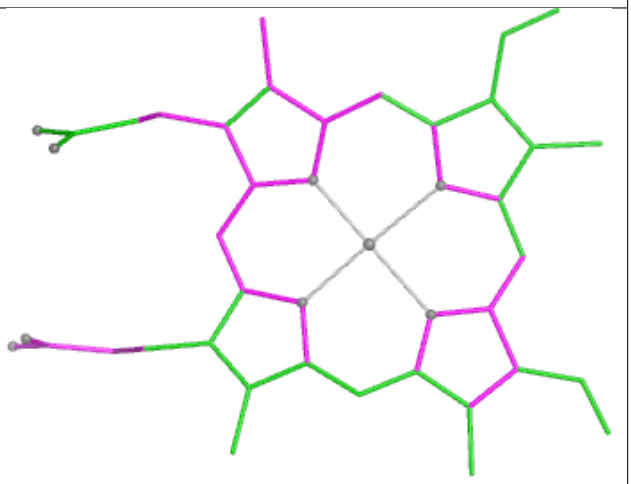
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1539	HEM	4	0
3	A	1550	ACT	4	0
3	B	1546	ACT	4	0
5	A	1554	EDO	5	0
3	B	1542	ACT	5	0
2	A	1549	HEM	3	0
3	B	1540	ACT	4	0
4	B	1543	PLP	3	0
6	A	1557	PE4	2	0
5	B	1544	EDO	1	0

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.

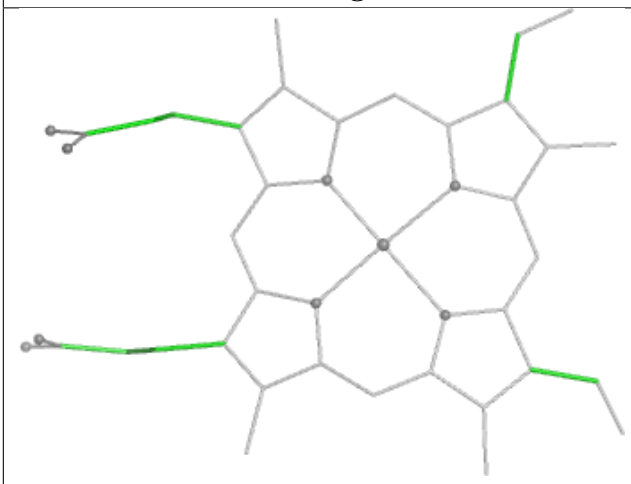
Ligand HEM B 1539



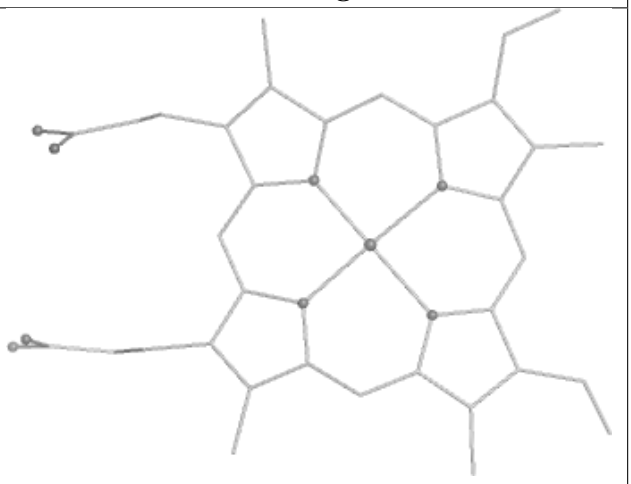
Bond lengths



Bond angles

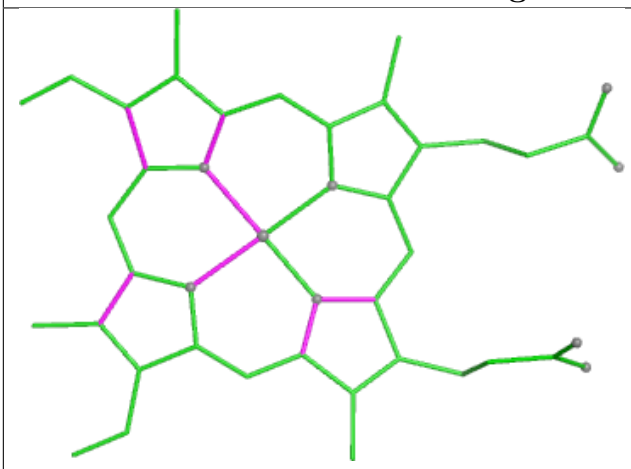


Torsions

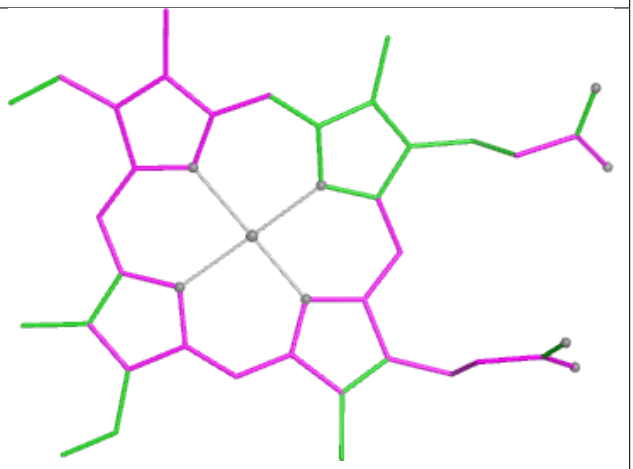


Rings

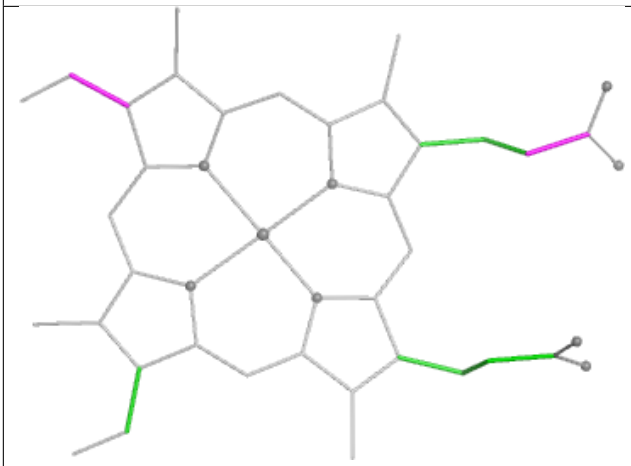
Ligand HEM A 1549



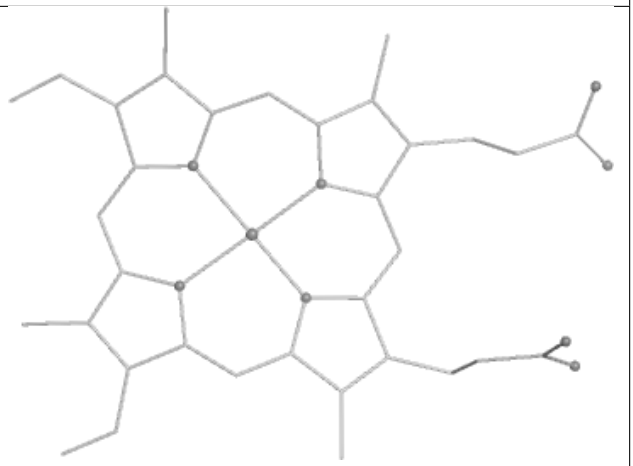
Bond lengths



Bond angles

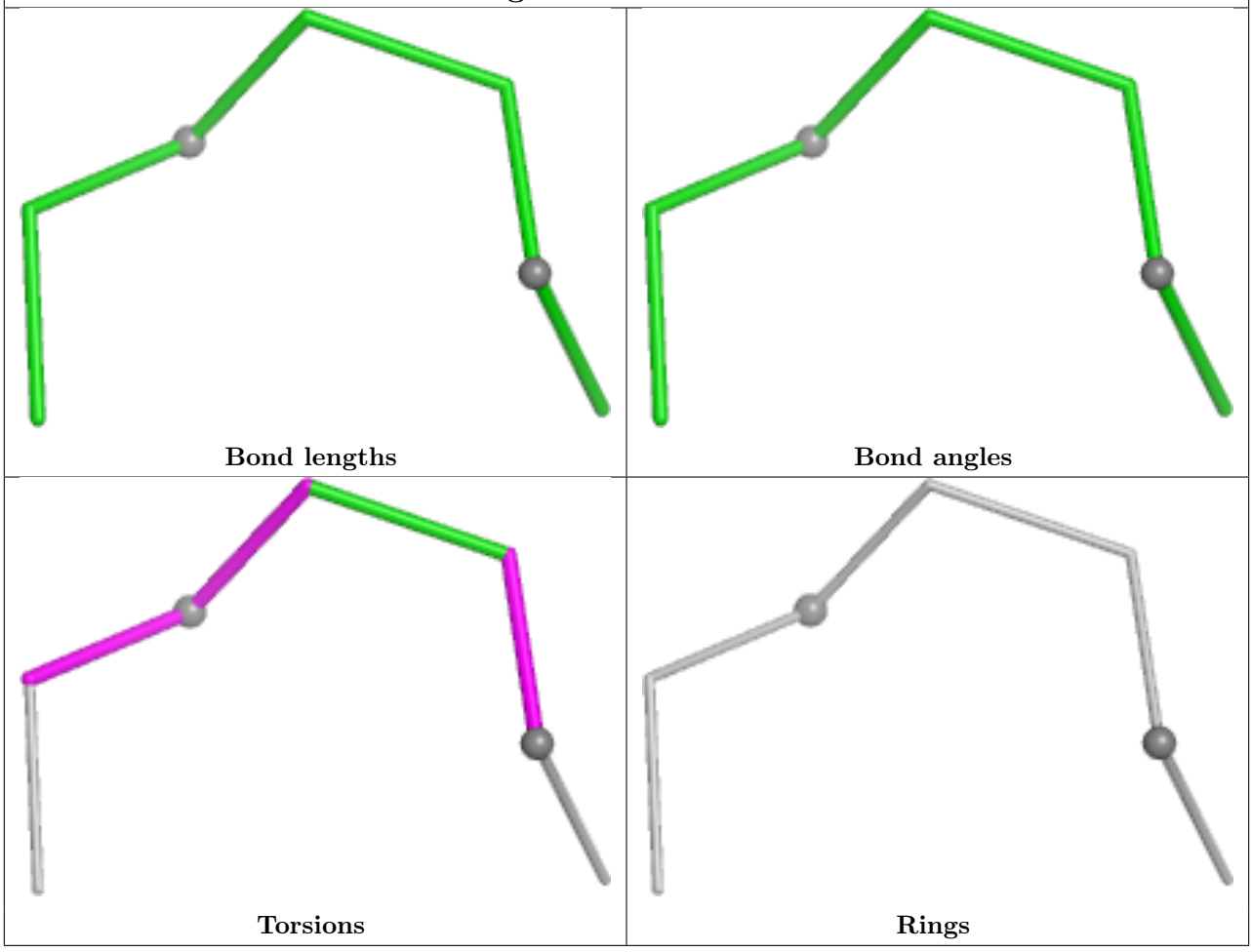


Torsions



Rings

Ligand PE4 A 1557



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	493/563 (87%)	-0.04	18 (3%)	45	44	15, 36, 64, 107	5 (1%)
1	B	487/563 (86%)	0.19	28 (5%)	29	28	21, 44, 76, 126	5 (1%)
All	All	980/1126 (87%)	0.07	46 (4%)	36	35	15, 40, 74, 126	10 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208[A]	TRP	4.3
1	A	297	GLU	4.2
1	B	43	TRP	4.1
1	A	298	GLN	4.1
1	B	68	THR	4.1
1	B	538	ARG	4.0
1	B	44	ILE	3.8
1	B	69	ALA	3.6
1	B	71	ALA	3.6
1	A	514	GLU	3.5
1	B	433[A]	HIS	3.5
1	B	70	PRO	3.4
1	A	403	THR	3.4
1	A	399	GLU	3.4
1	A	43	TRP	3.3
1	B	208[A]	TRP	3.3
1	B	515	GLN	3.3
1	A	402	LEU	3.3
1	B	299	THR	3.2
1	B	397	LEU	3.2
1	B	518	GLN	3.1
1	A	398	LYS	3.1
1	B	56	LEU	2.9
1	A	433[A]	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	45[A]	ARG	2.8
1	A	405	LYS	2.8
1	A	451	GLU	2.7
1	A	529	MET	2.5
1	B	295	GLN	2.4
1	A	397	LEU	2.4
1	B	452	ALA	2.3
1	B	411	HIS	2.3
1	B	408	TRP	2.3
1	B	59	PRO	2.3
1	B	64	PRO	2.3
1	A	491	ARG	2.2
1	A	401	ASP	2.2
1	B	363	GLU	2.1
1	B	161[A]	ARG	2.1
1	B	248	LEU	2.1
1	B	211	LYS	2.1
1	B	297	GLU	2.1
1	A	299	THR	2.1
1	B	139	GLY	2.1
1	B	88	PRO	2.0
1	B	296	THR	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
5	EDO	A	1559	4/4	0.69	0.30	20,20,20,20	0

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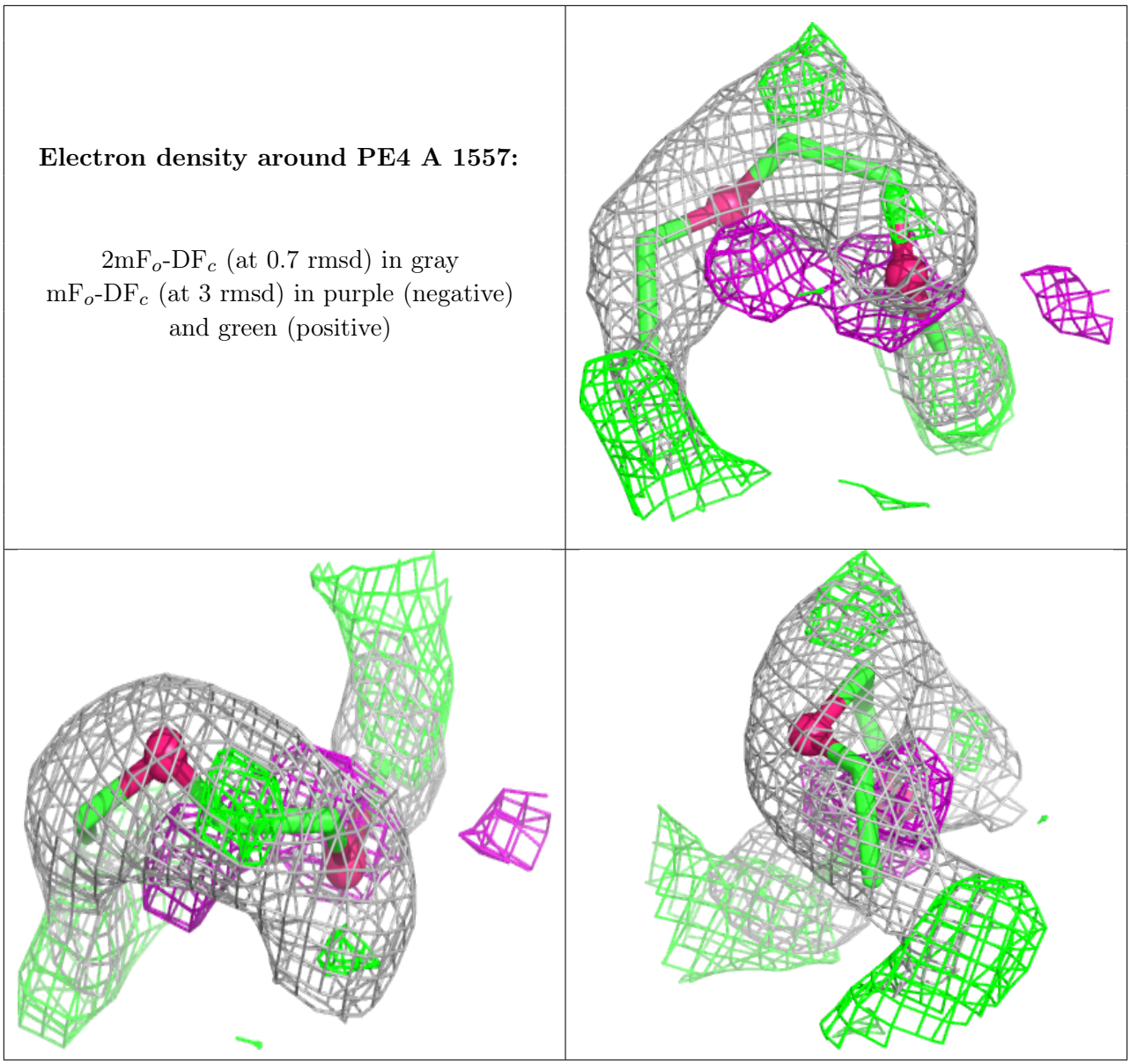
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PE4	A	1557	7/24	0.75	0.25	50,56,63,66	0
3	ACT	B	1546	4/4	0.79	0.24	42,64,65,67	0
5	EDO	A	1555	4/4	0.87	0.15	54,54,55,58	0
3	ACT	B	1541	4/4	0.88	0.17	52,53,55,56	0
3	ACT	B	1542	4/4	0.88	0.14	57,62,62,64	0
3	ACT	A	1550	4/4	0.88	0.14	24,28,29,42	0
5	EDO	A	1556	4/4	0.91	0.12	41,45,47,47	0
5	EDO	A	1554	4/4	0.91	0.15	44,45,47,47	0
3	ACT	B	1540	4/4	0.91	0.12	29,34,39,47	0
5	EDO	A	1553	4/4	0.92	0.16	34,46,47,49	0
5	EDO	B	1544	4/4	0.92	0.15	51,53,53,57	0
5	EDO	A	1552	4/4	0.92	0.14	43,43,45,45	0
2	HEM	B	1539	43/43	0.93	0.14	48,60,71,74	0
2	HEM	A	1549	43/43	0.97	0.08	26,33,46,60	0
4	PLP	A	1551	15/16	0.98	0.05	23,26,28,31	0
4	PLP	B	1543	15/16	0.98	0.05	29,32,34,35	0
7	NA	A	1558	1/1	0.98	0.10	28,28,28,28	0
7	NA	B	1545	1/1	0.99	0.07	34,34,34,34	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.

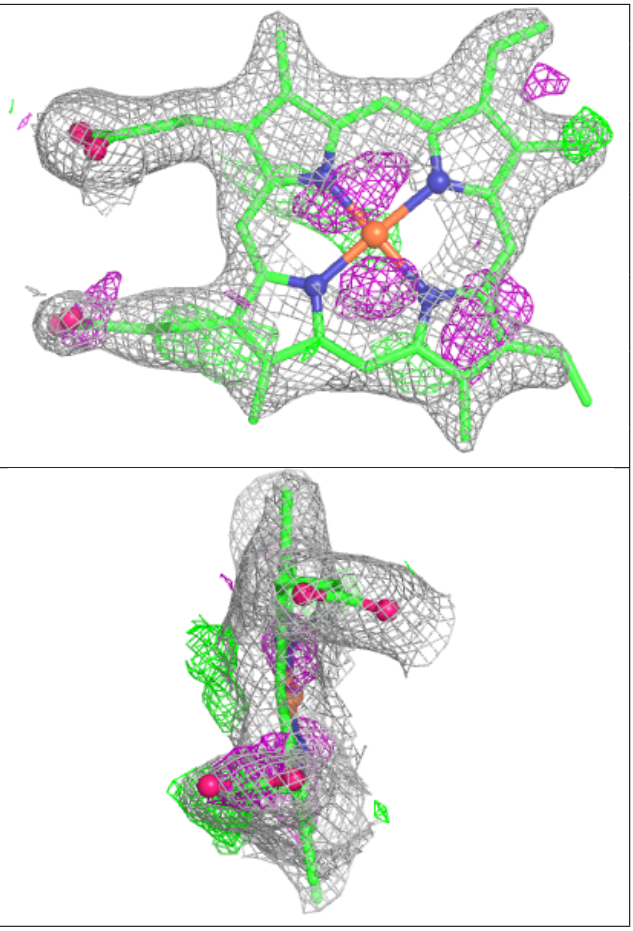
Electron density around PE4 A 1557:

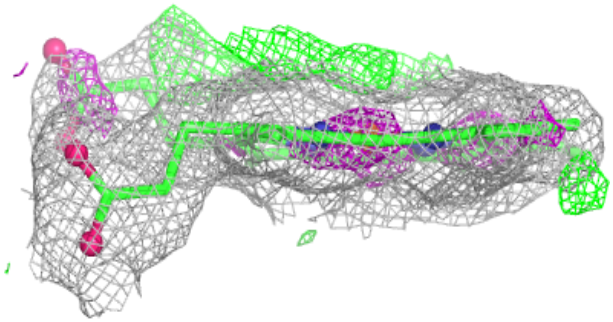
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEM B 1539:

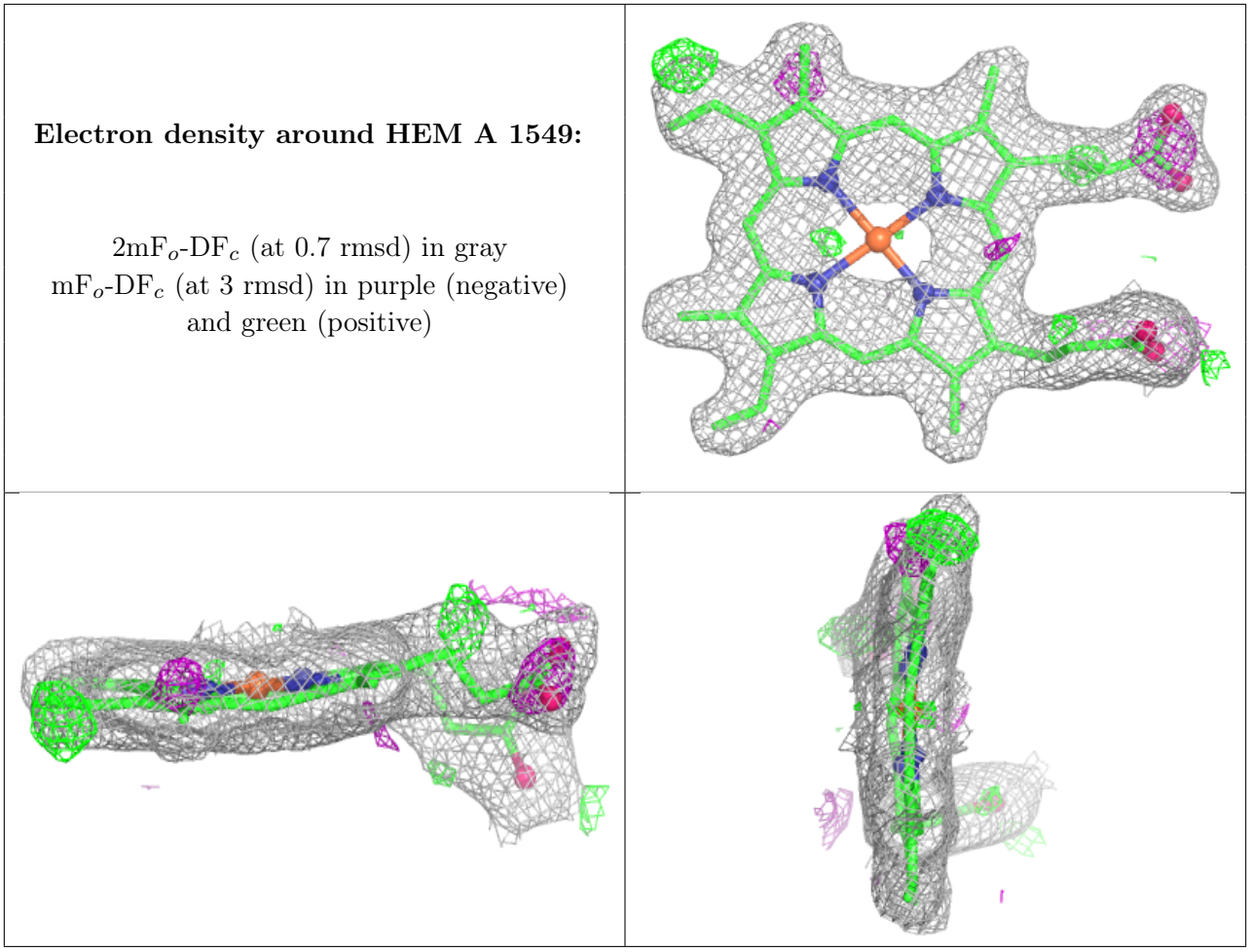
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEM A 1549:

$2mF_o$-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.