Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2026 – 06:32 am BST

PDB ID	:	4UH9 / pdb_00004uh9
Title	:	Structure of bovine endothelial nitric oxide synthase heme domain in complex with N1-(3-(2-(6-Amino-4-methylpyridin-2-yl)ethyl)-5- fluorophenyl)-N1,N2-dimethylethane-1,2-diamine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2015-03-23
Resolution	:	2.14 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:

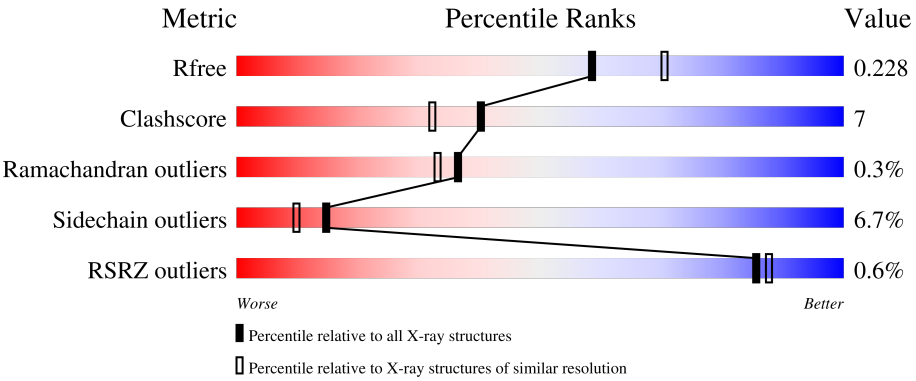
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	443	% 76% 13% • 9%
1	B	443	74% 14% • 9%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6885 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.

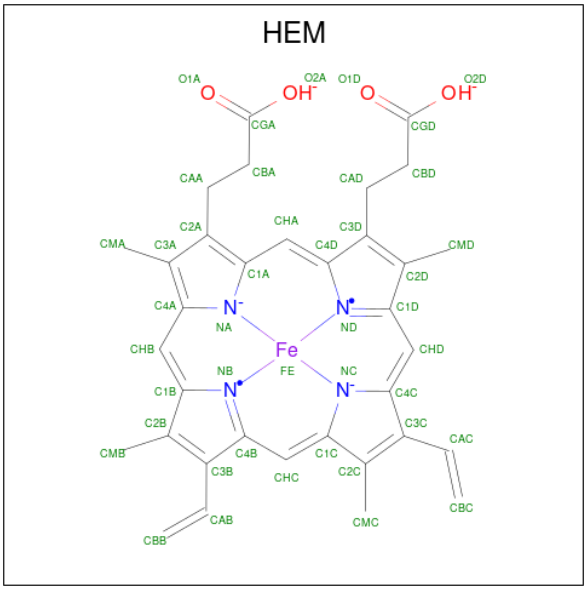
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	As	C	N	O	S	0	0	0
			3212	1	2043	564	588	16			
1	B	403	Total	As	C	N	O	S	0	0	0
			3212	1	2042	566	587	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	variant	UNP P29473
B	100	ARG	CYS	variant	UNP P29473

- 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		

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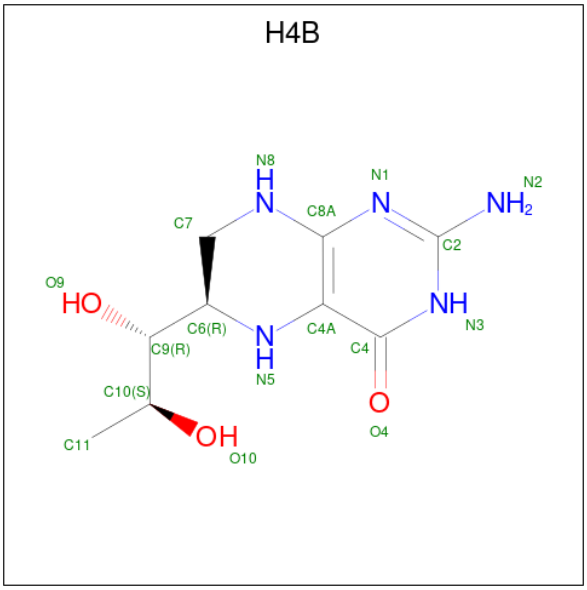
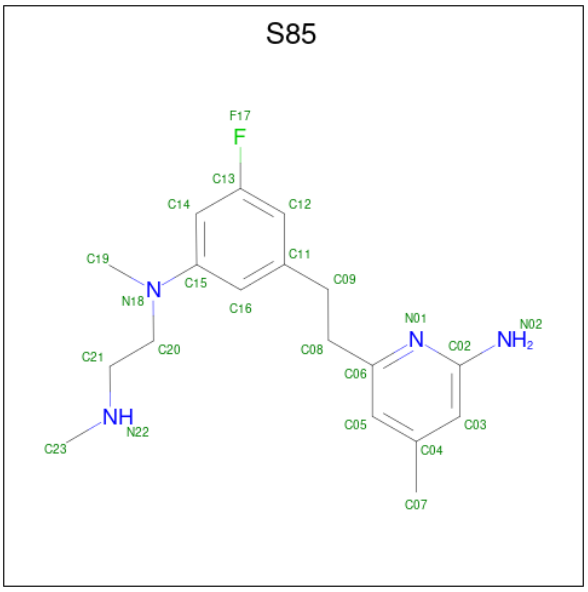
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



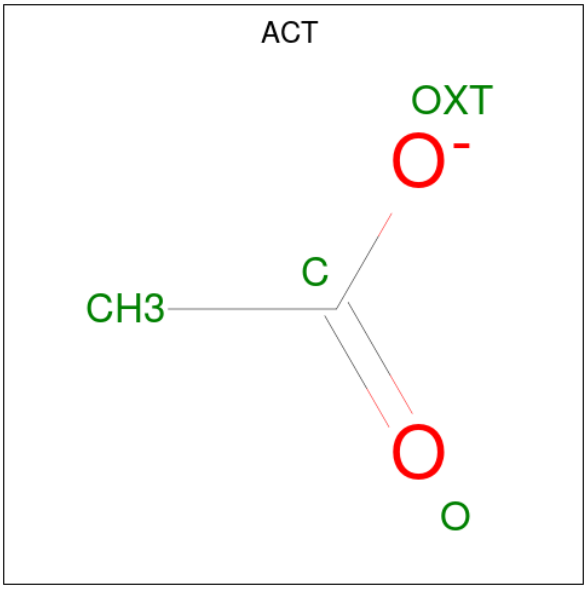
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			17	9	5	3			
3	B	1	Total	C	N	O		0	0
			17	9	5	3			

- Molecule 4 is N1-(3-(2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL)-5-FLUOROPHEN YL)-N1,N2-DIMETHYLETHANE-1,2-DIAMINE (CCD ID: S85) (formula: $C_{18}H_{25}FN_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	18	1	4		
4	A	1	Total	C	F	N	0	0
			23	18	1	4		
4	B	1	Total	C	F	N	0	0
			23	18	1	4		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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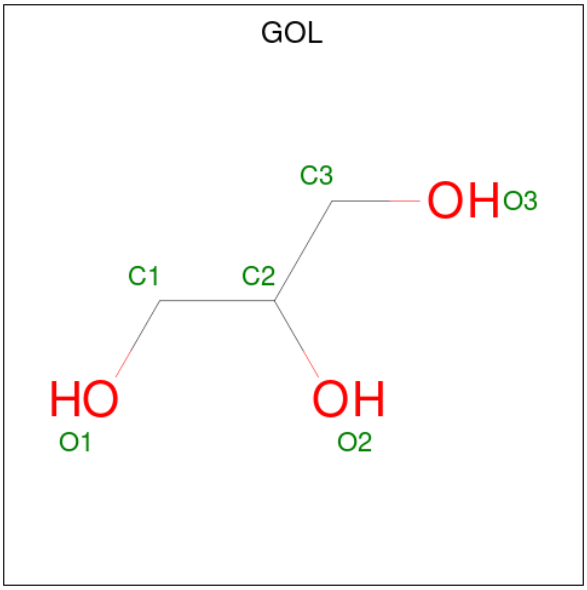
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	134	Total O 134 134	0	0

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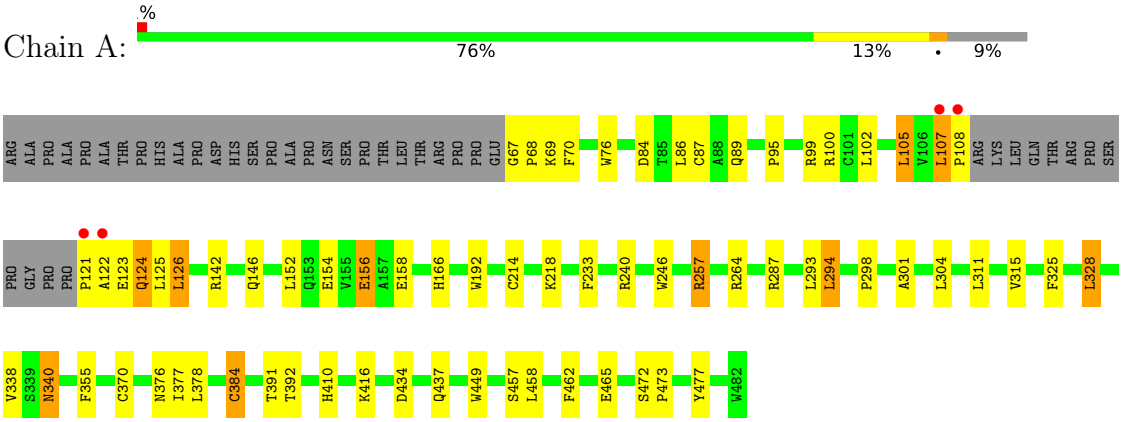
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	109	Total	O	0	0
			109	109		

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.

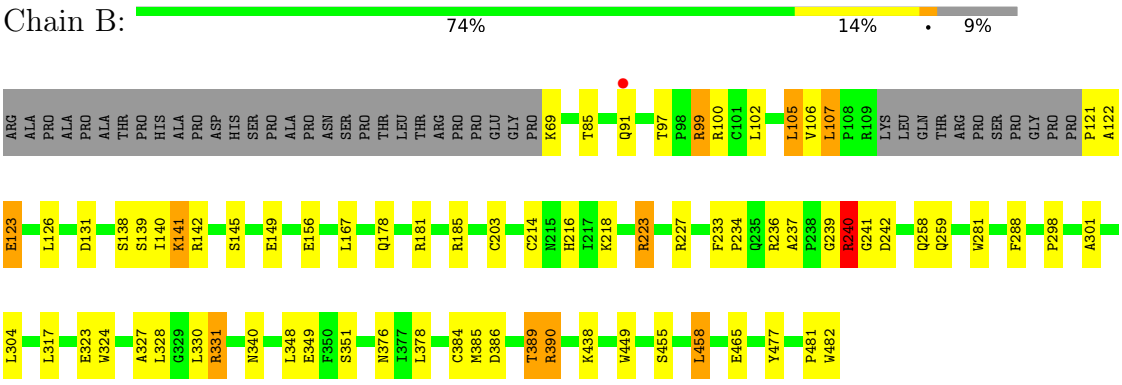
• Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

Chain A:



• Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

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	58.22Å 106.78Å 157.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.46 – 2.14 88.46 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.2 (88.46-2.14) 98.5 (88.46-2.14)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.227 0.174 , 0.228	Depositor DCC
R_{free} test set	2701 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.0	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	0.97	EDS
Total number of atoms	6885	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: ACT, CAS, GOL, ZN, S85, H4B, 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	1.14	4/3292 (0.1%)	1.19	12/4483 (0.3%)
1	B	1.05	2/3291 (0.1%)	1.15	11/4480 (0.2%)
All	All	1.10	6/6583 (0.1%)	1.17	23/8963 (0.3%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	VAL	CA-C	8.55	1.59	1.52
1	A	315	VAL	CA-CB	6.34	1.59	1.54
1	B	97	THR	CA-C	5.37	1.57	1.52
1	A	434	ASP	CA-C	5.19	1.59	1.52
1	A	377	ILE	N-CA	5.18	1.53	1.46
1	B	227	ARG	CA-C	-5.05	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	GLY	CA-C-N	10.16	131.49	120.11
1	A	67	GLY	C-N-CA	10.16	131.49	120.11
1	A	301	ALA	CA-C-N	-10.09	110.53	120.21
1	A	301	ALA	C-N-CA	-10.09	110.53	120.21
1	B	237	ALA	CA-C-N	7.21	128.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	237	ALA	C-N-CA	7.21	128.85	119.84
1	B	301	ALA	CA-C-N	-6.80	113.29	120.03
1	B	301	ALA	C-N-CA	-6.80	113.29	120.03
1	A	315	VAL	CA-C-N	6.45	126.21	119.76
1	A	315	VAL	C-N-CA	6.45	126.21	119.76
1	B	240	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	B	240	ARG	NE-CZ-NH1	5.91	127.41	121.50
1	A	437	GLN	N-CA-C	-5.89	104.77	111.07
1	B	85	THR	N-CA-C	-5.82	106.53	113.97
1	B	376	ASN	N-CA-C	5.60	119.11	111.39
1	A	68	PRO	N-CA-C	5.55	119.27	111.33
1	B	218	LYS	N-CA-C	-5.54	105.32	111.36
1	B	323	GLU	N-CA-C	5.53	118.23	111.82
1	A	233	PHE	CA-C-N	-5.52	114.07	119.76
1	A	233	PHE	C-N-CA	-5.52	114.07	119.76
1	B	389	THR	N-CA-C	5.26	119.33	113.01
1	A	392	THR	N-CA-C	-5.10	105.90	111.82
1	A	192	TRP	N-CA-C	5.00	118.15	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

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	3212	0	3114	50	0
1	B	3212	0	3117	37	1
2	A	43	0	30	5	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	46	0	50	3	0
4	B	23	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	134	0	0	5	1
8	B	109	0	0	3	0
All	All	6885	0	6424	86	1

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 (86) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:CAS:SG	1:A:384:CAS:AS	2.52	1.27
1:A:107:LEU:HD12	1:A:108:PRO:HD2	1.35	1.04
1:A:158:GLU:OE2	1:A:166:HIS:HD2	1.49	0.94
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.33	0.93
1:A:121:PRO:HB3	1:A:124:GLN:HG2	1.59	0.84
1:B:214:CYS:SG	8:B:2045:HOH:O	2.41	0.77
1:B:99:ARG:NH1	1:B:100:ARG:HD2	1.99	0.77
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.66	0.77
1:B:223:ARG:HB2	1:B:223:ARG:NH1	1.99	0.76
1:B:99:ARG:HH11	1:B:100:ARG:HD2	1.49	0.75
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.69	0.74
1:A:158:GLU:OE2	1:A:166:HIS:CD2	2.39	0.73
1:A:294:LEU:HD13	1:A:304:LEU:HD13	1.73	0.70
1:B:106:VAL:HG12	1:B:107:LEU:HD13	1.72	0.70
1:A:107:LEU:HD12	1:A:108:PRO:CD	2.17	0.70
1:A:105:LEU:HD13	1:B:465:GLU:OE1	1.93	0.69
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.03	0.69
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.75	0.68
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.75	0.68
1:B:236:ARG:HD2	1:B:242:ASP:OD1	1.95	0.66
1:A:384:CAS:SG	1:A:384:CAS:CE2	2.85	0.64
4:B:800:S85:H231	8:B:2107:HOH:O	1.96	0.63
1:A:214:CYS:SG	8:A:2043:HOH:O	2.56	0.61
1:B:481:PRO:HD2	1:B:482:TRP:CE3	2.37	0.60
1:A:121:PRO:HB3	1:A:124:GLN:CG	2.29	0.60
1:B:223:ARG:HB2	1:B:223:ARG:HH11	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:TRP:O	1:B:327:ALA:HB3	2.07	0.55
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.89	0.54
1:A:87:CYS:SG	1:B:99:ARG:NH1	2.81	0.53
1:A:465:GLU:HB3	1:B:105:LEU:HD22	1.91	0.53
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.91	0.52
2:A:500:HEM:HHC	2:A:500:HEM:CBB	2.38	0.52
1:A:264:ARG:HD3	8:A:2064:HOH:O	2.10	0.51
1:A:340:ASN:H	1:A:340:ASN:HD22	1.58	0.51
1:A:376:ASN:ND2	8:A:2092:HOH:O	2.41	0.50
1:B:140:ILE:C	1:B:141:LYS:HG2	2.35	0.50
1:A:154:GLU:CG	4:A:801:S85:H092	2.42	0.49
1:A:76:TRP:HH2	1:B:107:LEU:HD22	1.78	0.49
1:A:384:CAS:AS	1:A:384:CAS:CB	3.21	0.48
1:B:317:LEU:HG	1:B:331:ARG:HA	1.95	0.48
1:A:214:CYS:O	1:A:218:LYS:HG3	2.14	0.47
1:A:152:LEU:O	1:A:156:GLU:HG2	2.14	0.47
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.96	0.47
1:B:223:ARG:HB2	1:B:223:ARG:CZ	2.42	0.47
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.61	0.47
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.96	0.47
1:B:390:ARG:HE	1:B:390:ARG:HB2	1.23	0.46
1:B:385:MET:O	1:B:386:ASP:HB3	2.15	0.46
1:A:472:SER:HA	1:A:473:PRO:C	2.40	0.46
1:A:257:ARG:NH1	1:A:257:ARG:CG	2.74	0.46
1:A:105:LEU:N	1:A:105:LEU:CD2	2.79	0.45
1:A:100:ARG:HD2	8:B:2008:HOH:O	2.16	0.45
1:A:338:VAL:HG21	4:A:800:S85:C13	2.46	0.45
1:A:287:ARG:NH1	8:A:2070:HOH:O	2.30	0.45
1:B:449:TRP:HA	3:B:600:H4B:N1	2.31	0.44
1:A:70:PHE:HB3	1:A:84:ASP:O	2.17	0.44
1:A:449:TRP:HA	3:A:600:H4B:N1	2.32	0.44
1:A:457:SER:HA	1:A:462:PHE:CG	2.53	0.44
1:A:477:TYR:OH	2:A:500:HEM:O2D	2.26	0.44
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.74	0.44
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.53	0.44
1:B:288:PHE:CB	1:B:331:ARG:HD3	2.48	0.44
1:A:142:ARG:HA	1:A:142:ARG:HD3	1.79	0.43
1:A:294:LEU:HD13	1:A:304:LEU:CD1	2.47	0.43
1:A:338:VAL:HG23	4:A:800:S85:H05	1.99	0.43
1:A:86:LEU:O	1:A:89:GLN:HB2	2.18	0.43
2:B:500:HEM:CBA	4:B:800:S85:H092	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:HIS:ND1	8:A:2104:HOH:O	2.35	0.43
1:A:449:TRP:HZ3	2:A:500:HEM:O2A	2.00	0.43
1:B:216:HIS:CD2	1:B:216:HIS:C	2.97	0.43
1:B:481:PRO:HD2	1:B:482:TRP:CZ3	2.54	0.43
1:B:121:PRO:HD2	1:B:123:GLU:OE1	2.19	0.43
1:A:457:SER:HA	1:A:462:PHE:CB	2.50	0.42
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.42
1:B:477:TYR:OH	2:B:500:HEM:O1D	2.25	0.42
1:A:340:ASN:HD22	1:A:340:ASN:N	2.17	0.42
1:A:355:PHE:CD1	2:A:500:HEM:CAC	3.02	0.42
1:B:142:ARG:O	1:B:145:SER:OG	2.29	0.42
1:B:122:ALA:O	1:B:126:LEU:HB2	2.20	0.41
1:B:241:GLY:O	1:B:298:PRO:HB3	2.20	0.41
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.60	0.41
1:A:76:TRP:CH2	1:B:107:LEU:HD22	2.56	0.41
1:B:236:ARG:HG3	1:B:349:GLU:HB2	2.03	0.41
1:A:325:PHE:O	1:A:328:LEU:HB2	2.21	0.41
1:A:87:CYS:SG	1:B:99:ARG:CZ	3.10	0.40
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ARG:NH2	8:A:2039:HOH:O[2_555]	2.19	0.01

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	399/443 (90%)	387 (97%)	11 (3%)	1 (0%)	36 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	398/443 (90%)	382 (96%)	15 (4%)	1 (0%)	36 33
All	All	797/886 (90%)	769 (96%)	26 (3%)	2 (0%)	36 33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	328	LEU
1	A	122	ALA

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	342/375 (91%)	322 (94%)	20 (6%)	18 13
1	B	342/375 (91%)	316 (92%)	26 (8%)	12 7
All	All	684/750 (91%)	638 (93%)	46 (7%)	15 10

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	102	LEU
1	A	105	LEU
1	A	107	LEU
1	A	123	GLU
1	A	124	GLN
1	A	125	LEU
1	A	126	LEU
1	A	146	GLN
1	A	156	GLU
1	A	257	ARG
1	A	293	LEU
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	311	LEU
1	A	328	LEU
1	A	340	ASN
1	A	391	THR
1	A	416	LYS
1	A	458	LEU
1	B	69	LYS
1	B	91	GLN
1	B	99	ARG
1	B	102	LEU
1	B	105	LEU
1	B	107	LEU
1	B	123	GLU
1	B	131	ASP
1	B	138	SER
1	B	139	SER
1	B	141	LYS
1	B	149	GLU
1	B	156	GLU
1	B	203	CYS
1	B	223	ARG
1	B	240	ARG
1	B	258	GLN
1	B	259	GLN
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	390	ARG
1	B	438	LYS
1	B	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	128	GLN
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	413	GLN
1	A	435	ASN
1	A	468	ASN
1	B	91	GLN
1	B	128	GLN
1	B	178	GLN
1	B	191	GLN
1	B	207	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
1	B	279	HIS
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CAS	A	384	1	5,8,9	1.79	1 (20%)	1,9,11	0.66	0
1	CAS	B	384	1	5,8,9	1.35	2 (40%)	1,9,11	0.85	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
1	CAS	A	384	1	-	0/0/7/9	-
1	CAS	B	384	1	-	0/0/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	CAS	AS-CE1	3.60	2.05	1.96
1	B	384	CAS	AS-CE2	2.23	2.01	1.96
1	B	384	CAS	AS-CE1	2.00	2.01	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\#\|Z\| > 2$
6	GOL	B	880	-	5,5,5	0.29	0	5,5,5	0.85	0
3	H4B	A	600	-	15,18,18	1.25	4 (26%)	11,26,26	2.23	5 (45%)
6	GOL	A	880	-	5,5,5	0.71	0	5,5,5	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	S85	B	800	-	24,24,24	0.95	1 (4%)	32,32,32	1.96	10 (31%)
3	H4B	B	600	-	15,18,18	1.18	2 (13%)	11,26,26	2.02	4 (36%)
5	ACT	B	861	-	3,3,3	1.02	0	3,3,3	0.52	0
4	S85	A	800	-	24,24,24	1.33	2 (8%)	32,32,32	2.21	10 (31%)
5	ACT	A	860	-	3,3,3	0.84	0	3,3,3	0.50	0
2	HEM	B	500	1	50,50,50	1.78	5 (10%)	66,82,82	1.64	14 (21%)
2	HEM	A	500	1	50,50,50	1.57	8 (16%)	66,82,82	2.26	21 (31%)
5	ACT	A	861	-	3,3,3	1.13	0	3,3,3	0.34	0
5	ACT	B	860	-	3,3,3	0.61	0	3,3,3	1.35	0
4	S85	A	801	-	24,24,24	1.21	1 (4%)	32,32,32	1.77	5 (15%)

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
6	GOL	B	880	-	-	0/4/4/4	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
6	GOL	A	880	-	-	0/4/4/4	-
4	S85	B	800	-	-	3/13/13/13	0/2/2/2
3	H4B	B	600	-	-	3/8/17/17	0/2/2/2
4	S85	A	800	-	-	3/13/13/13	0/2/2/2
2	HEM	B	500	1	-	1/14/54/54	-
2	HEM	A	500	1	-	6/14/54/54	-
4	S85	A	801	-	-	3/13/13/13	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-NC	5.56	2.14	1.95
2	B	500	HEM	FE-NB	5.39	2.11	1.94
2	B	500	HEM	C1B-NB	-4.70	1.32	1.40
2	A	500	HEM	FE-ND	-4.53	1.80	1.94
2	A	500	HEM	C1B-NB	-4.17	1.33	1.40
2	A	500	HEM	FE-NC	3.81	2.08	1.95
2	B	500	HEM	C3B-C4B	2.87	1.50	1.44
2	A	500	HEM	C4D-ND	-2.83	1.35	1.40
2	B	500	HEM	C1D-C2D	2.67	1.49	1.44
4	B	800	S85	C14-C13	2.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	H4B	C7-C6	2.61	1.54	1.52
4	A	800	S85	C14-C13	2.51	1.41	1.37
4	A	801	S85	C05-C04	2.43	1.43	1.39
2	A	500	HEM	C1C-NC	-2.41	1.35	1.39
4	A	800	S85	C03-C02	2.24	1.43	1.39
3	A	600	H4B	O4-C4	2.20	1.27	1.23
3	A	600	H4B	C2-N2	2.19	1.39	1.34
2	A	500	HEM	C3C-C4C	-2.17	1.42	1.46
3	A	600	H4B	C4-N3	-2.08	1.35	1.38
2	A	500	HEM	C3B-C4B	2.07	1.49	1.44
3	B	600	H4B	C4A-C8A	2.06	1.42	1.38
3	A	600	H4B	C7-C6	2.03	1.54	1.52
2	A	500	HEM	C1D-ND	-2.02	1.34	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800	S85	C02-N01-C06	5.84	122.52	118.10
2	A	500	HEM	CHA-C4D-ND	5.69	131.40	124.37
2	A	500	HEM	CHA-C4D-C3D	-5.18	115.60	125.33
4	A	801	S85	C02-N01-C06	5.15	122.01	118.10
4	B	800	S85	C02-N01-C06	5.12	121.98	118.10
2	A	500	HEM	CHD-C1D-C2D	-5.02	117.14	124.98
3	A	600	H4B	C2-N1-C8A	4.89	122.25	113.43
4	A	800	S85	C09-C11-C12	-4.80	112.66	120.54
2	A	500	HEM	CHC-C4B-NB	4.68	129.50	124.42
4	B	800	S85	C05-C06-N01	-4.63	117.99	122.90
2	A	500	HEM	C4C-CHD-C1D	-4.63	116.08	126.06
2	A	500	HEM	CHD-C1D-ND	4.53	129.34	124.42
2	A	500	HEM	CHB-C1B-NB	4.37	129.77	124.37
2	A	500	HEM	C4A-CHB-C1B	-4.27	116.21	126.34
3	B	600	H4B	C2-N1-C8A	4.08	120.80	113.43
2	B	500	HEM	C1B-NB-C4B	4.03	109.23	105.07
2	B	500	HEM	CBA-CAA-C2A	-3.97	101.61	112.63
4	A	800	S85	C15-C14-C13	3.89	122.50	118.06
4	A	801	S85	C20-C21-N22	3.88	121.38	111.04
4	A	800	S85	C12-C13-C14	-3.71	118.83	123.52
2	A	500	HEM	C4C-NC-C1C	3.35	108.63	105.35
3	A	600	H4B	N3-C2-N1	-3.31	117.14	123.32
2	A	500	HEM	C1A-CHA-C4D	-3.30	118.52	126.34
4	A	800	S85	C14-C15-N18	-3.29	117.52	121.33
4	A	800	S85	F17-C13-C14	3.25	122.90	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	C4C-NC-C1C	3.24	108.52	105.35
2	A	500	HEM	C4B-C3B-C2B	-3.16	104.61	107.11
4	A	801	S85	C21-C20-N18	-3.16	100.85	112.31
4	A	800	S85	C05-C06-N01	-3.11	119.60	122.90
2	B	500	HEM	CHD-C1D-ND	3.10	127.78	124.42
4	B	800	S85	C12-C13-C14	-3.05	119.67	123.52
2	B	500	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
2	A	500	HEM	C2D-C1D-ND	2.90	113.36	109.88
2	A	500	HEM	CHB-C1B-C2B	-2.89	118.70	126.73
2	B	500	HEM	C4B-C3B-C2B	-2.87	104.84	107.11
4	B	800	S85	C09-C08-C06	2.81	119.30	112.99
4	A	800	S85	C09-C11-C16	2.79	125.12	120.54
2	B	500	HEM	O2D-CGD-CBD	2.78	122.97	114.03
2	B	500	HEM	O1D-CGD-CBD	-2.77	114.20	123.08
4	B	800	S85	C08-C06-N01	2.74	120.03	115.95
4	B	800	S85	C09-C11-C12	-2.73	116.05	120.54
2	B	500	HEM	CAD-C3D-C4D	2.73	129.44	124.66
4	A	800	S85	C16-C15-N18	2.73	124.48	121.33
2	B	500	HEM	CHA-C4D-C3D	-2.70	120.26	125.33
4	B	800	S85	F17-C13-C14	2.69	122.10	118.25
2	B	500	HEM	CHC-C4B-NB	2.60	127.24	124.42
2	A	500	HEM	C4D-ND-C1D	-2.56	102.43	105.07
2	A	500	HEM	CBD-CAD-C3D	2.56	119.74	112.63
3	B	600	H4B	C4A-C4-N3	2.50	119.76	112.31
2	A	500	HEM	C3D-C4D-ND	2.48	112.93	110.17
2	A	500	HEM	O2D-CGD-O1D	-2.43	117.23	123.30
4	A	801	S85	C05-C06-N01	-2.43	120.32	122.90
4	A	800	S85	C16-C11-C12	2.36	122.22	118.98
2	A	500	HEM	C1B-NB-C4B	2.33	107.48	105.07
3	B	600	H4B	N3-C2-N1	-2.32	119.00	123.32
4	B	800	S85	C14-C15-N18	-2.29	118.68	121.33
2	B	500	HEM	O2A-CGA-CBA	2.28	121.35	114.03
4	B	800	S85	C21-C20-N18	-2.24	104.17	112.31
2	B	500	HEM	C3D-C4D-ND	2.22	112.64	110.17
2	A	500	HEM	O2D-CGD-CBD	2.20	121.09	114.03
4	B	800	S85	C15-C14-C13	2.20	120.57	118.06
4	A	801	S85	C15-C14-C13	2.19	120.56	118.06
2	A	500	HEM	CMD-C2D-C1D	2.16	128.33	125.04
3	A	600	H4B	C4A-C4-N3	2.16	118.75	112.31
3	B	600	H4B	O4-C4-C4A	-2.16	122.28	127.24
2	B	500	HEM	C1A-CHA-C4D	-2.15	121.23	126.34
3	A	600	H4B	C4-C4A-N5	2.12	122.46	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C1D-C2D-C3D	-2.05	104.80	106.96
3	A	600	H4B	N2-C2-N3	2.01	120.98	116.71

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2D-C3D-CAD-CBD
4	B	800	S85	N18-C20-C21-N22
4	A	801	S85	N18-C20-C21-N22
2	A	500	HEM	C4D-C3D-CAD-CBD
4	A	800	S85	C20-C21-N22-C23
3	B	600	H4B	C7-C6-C9-O9
3	B	600	H4B	C7-C6-C9-C10
4	A	800	S85	C06-C08-C09-C11
4	A	800	S85	C21-C20-N18-C19
4	A	801	S85	C21-C20-N18-C19
4	A	801	S85	C20-C21-N22-C23
2	A	500	HEM	CAD-CBD-CGD-O2D
4	B	800	S85	C06-C08-C09-C11
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAD-CBD-CGD-O1D
4	B	800	S85	C16-C15-N18-C19
2	A	500	HEM	CAA-CBA-CGA-O1A
3	B	600	H4B	N5-C6-C9-O9
2	B	500	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

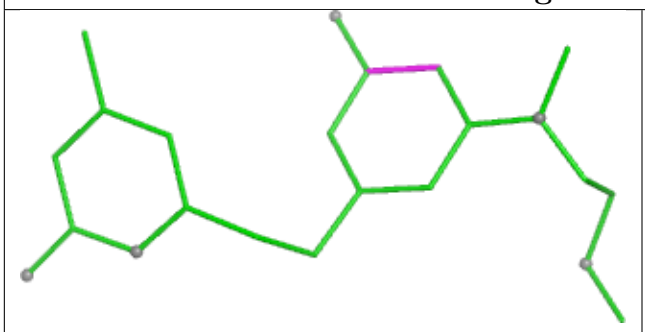
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	H4B	1	0
4	B	800	S85	2	0
3	B	600	H4B	1	0
4	A	800	S85	2	0
2	B	500	HEM	3	0
2	A	500	HEM	5	0
4	A	801	S85	1	0

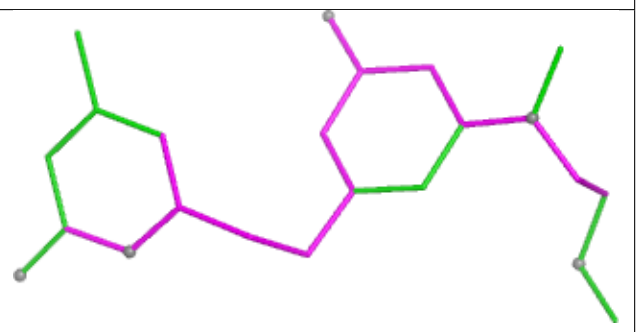
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 S85 B 800



Bond lengths



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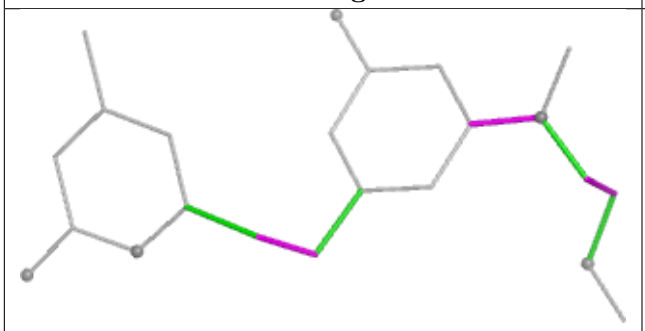
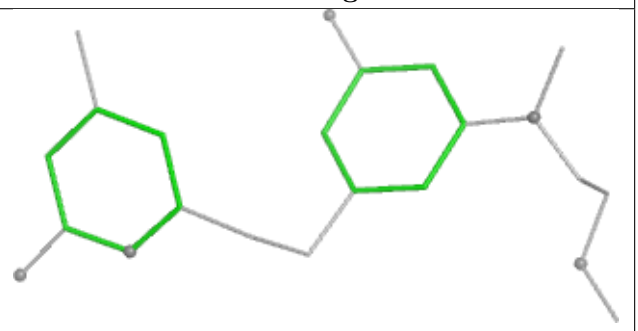
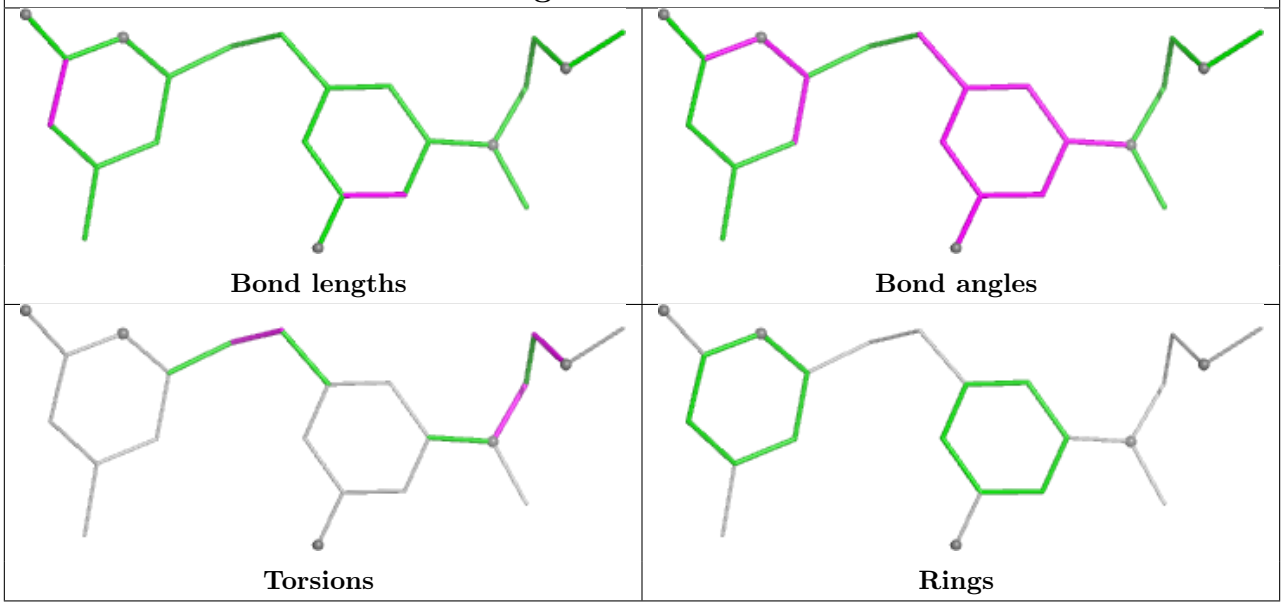


Torsions

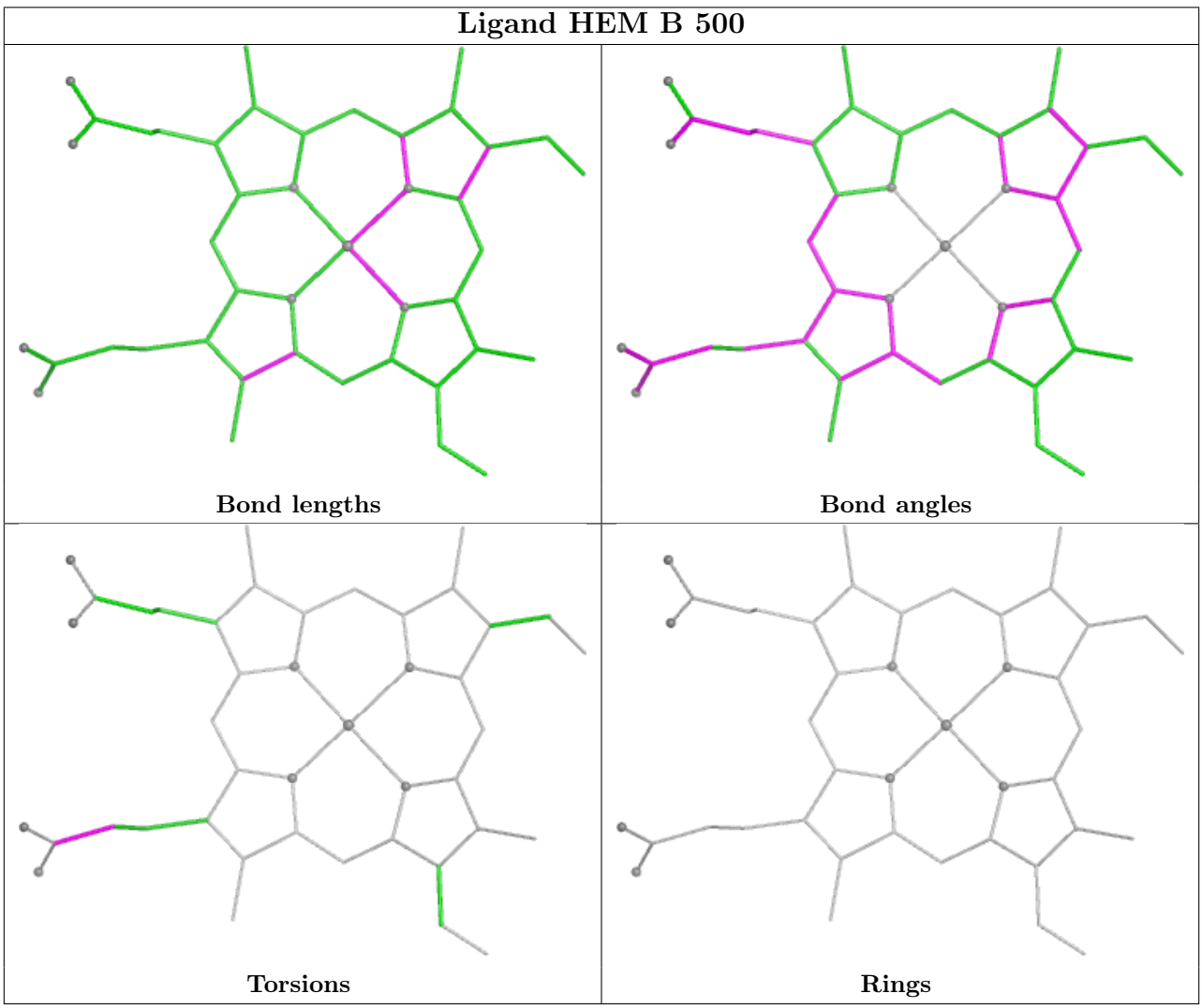


Rings

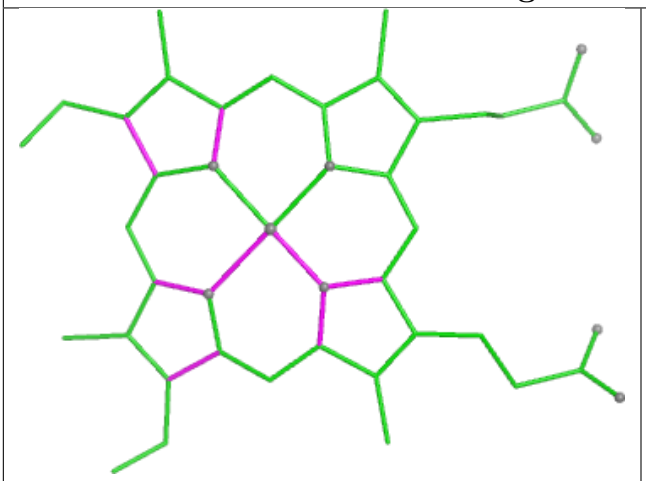
Ligand S85 A 800



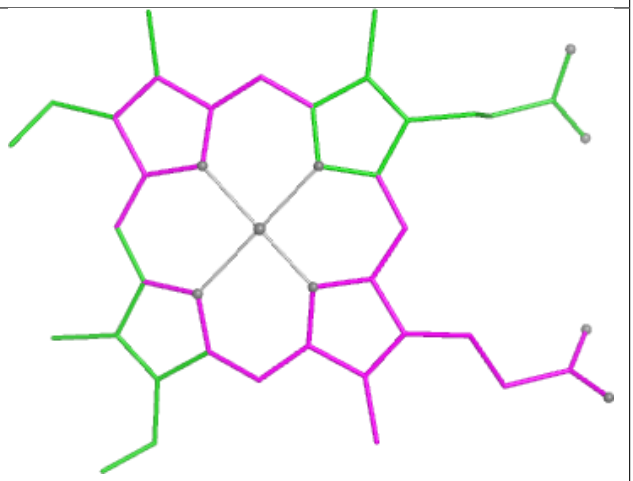
Ligand HEM B 500



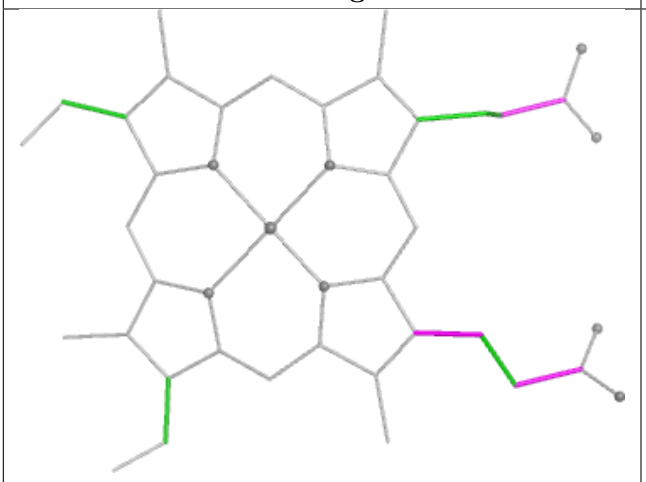
Ligand HEM A 500



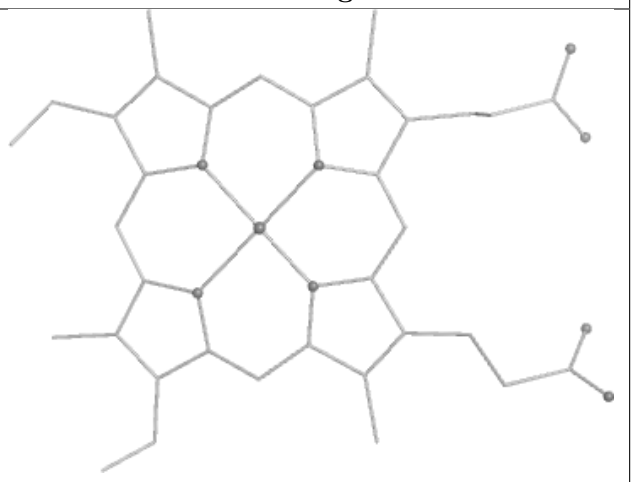
Bond lengths



Bond angles

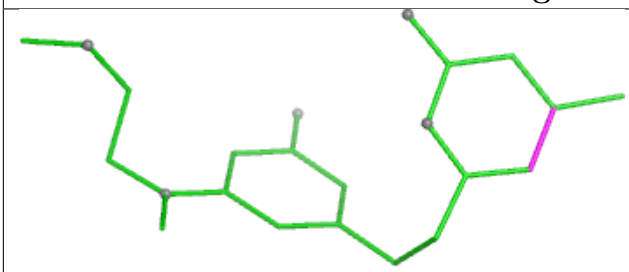


Torsions

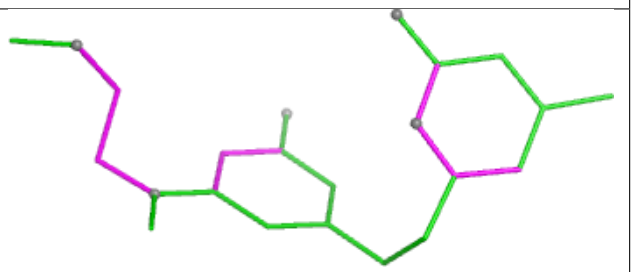


Rings

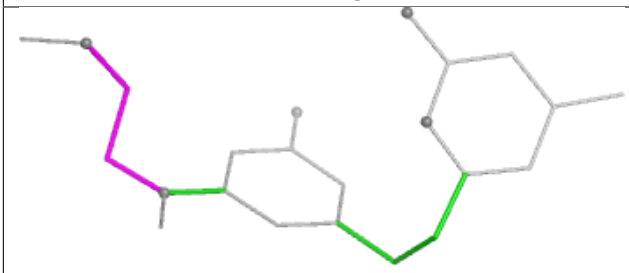
Ligand S85 A 801



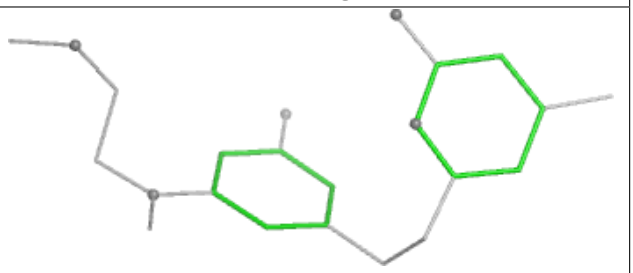
Bond lengths



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, 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	403/443 (90%)	-0.50	4 (0%)	79	83	32, 45, 78, 109	0
1	B	402/443 (90%)	-0.41	1 (0%)	91	93	33, 49, 84, 119	0
All	All	805/886 (90%)	-0.46	5 (0%)	85	88	32, 47, 82, 119	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	3.6
1	A	122	ALA	2.9
1	A	107	LEU	2.8
1	A	121	PRO	2.3
1	B	91	GLN	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAS	B	384	9/10	0.92	0.12	55,60,112,112	0
1	CAS	A	384	9/10	0.95	0.10	39,42,80,81	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

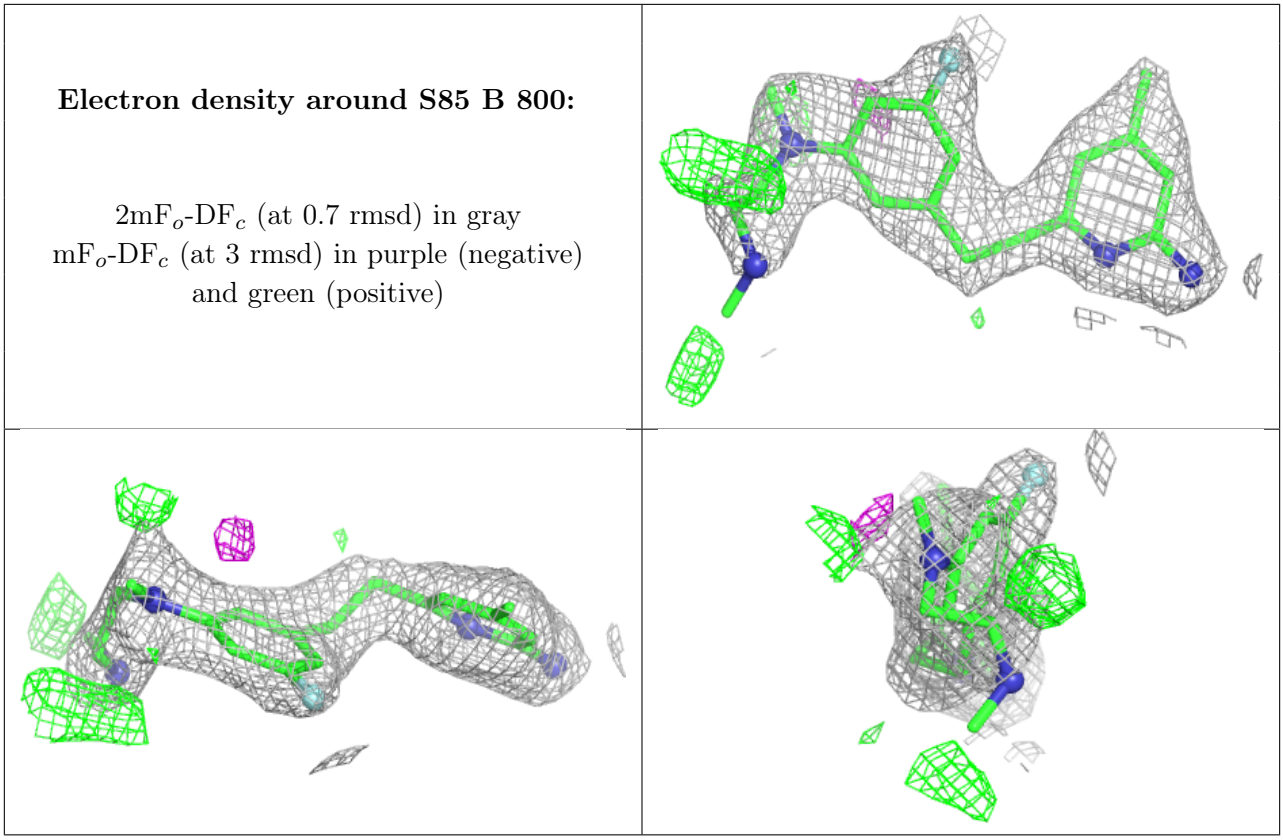
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	880	6/6	0.82	0.19	59,85,87,91	0
4	S85	B	800	23/23	0.89	0.15	44,60,95,109	0
4	S85	A	800	23/23	0.89	0.15	29,55,82,94	0
4	S85	A	801	23/23	0.90	0.13	42,68,75,76	0
6	GOL	B	880	6/6	0.90	0.15	69,76,78,79	0
5	ACT	B	861	4/4	0.94	0.09	43,45,51,54	0
5	ACT	A	860	4/4	0.95	0.08	40,47,47,53	0
3	H4B	A	600	17/17	0.96	0.06	40,49,53,55	0
3	H4B	B	600	17/17	0.96	0.07	43,47,55,57	0
5	ACT	A	861	4/4	0.96	0.09	41,44,47,49	0
5	ACT	B	860	4/4	0.97	0.09	46,50,52,53	0
2	HEM	B	500	43/43	0.98	0.06	35,41,52,64	0
2	HEM	A	500	43/43	0.98	0.07	22,30,65,72	0
7	ZN	A	1483	1/1	0.98	0.10	64,64,64,64	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.

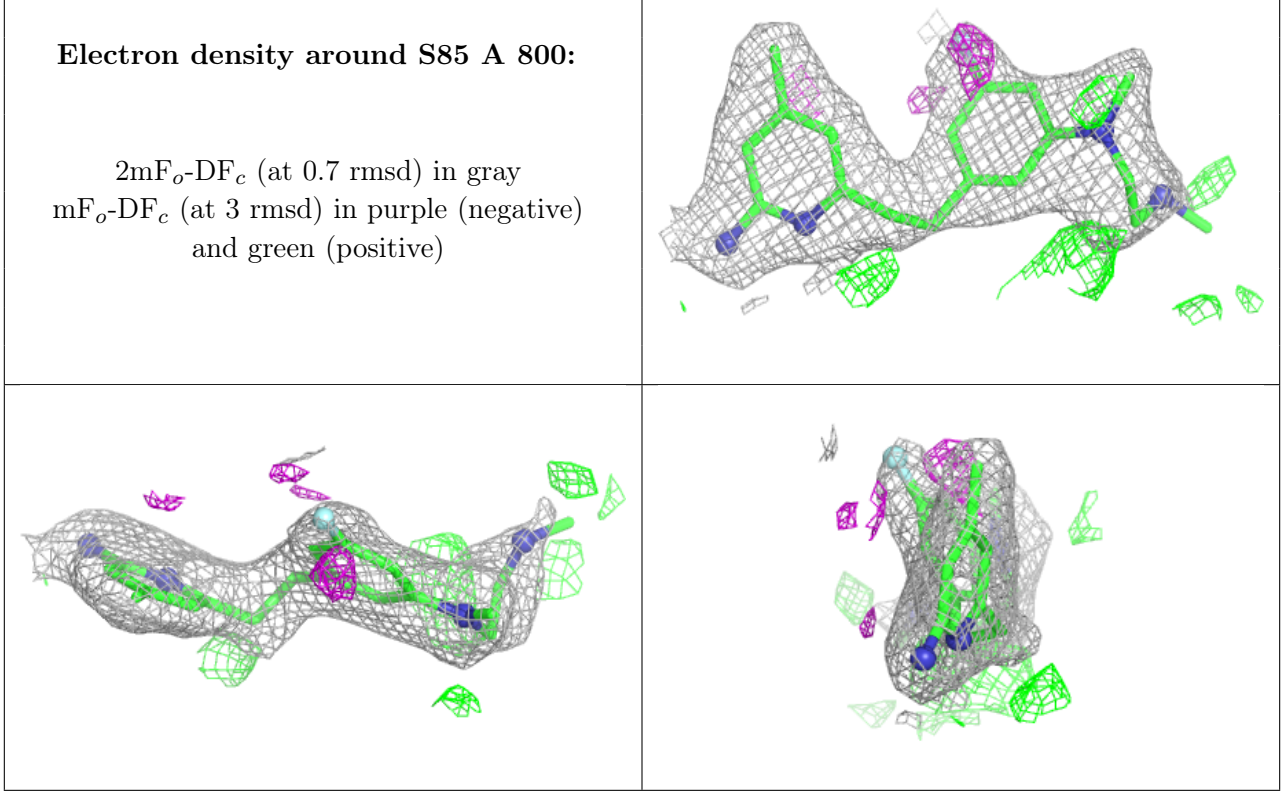
Electron density around S85 B 800:

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



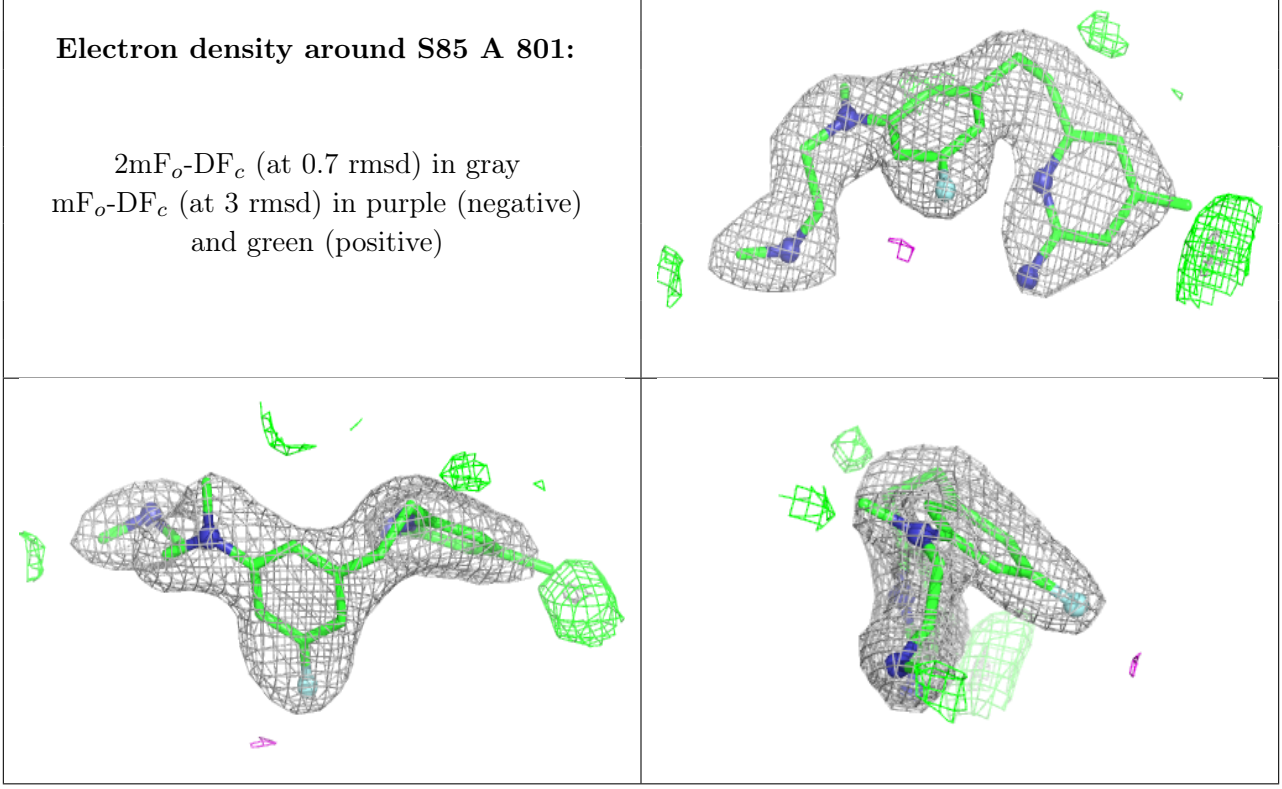
Electron density around S85 A 800:

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



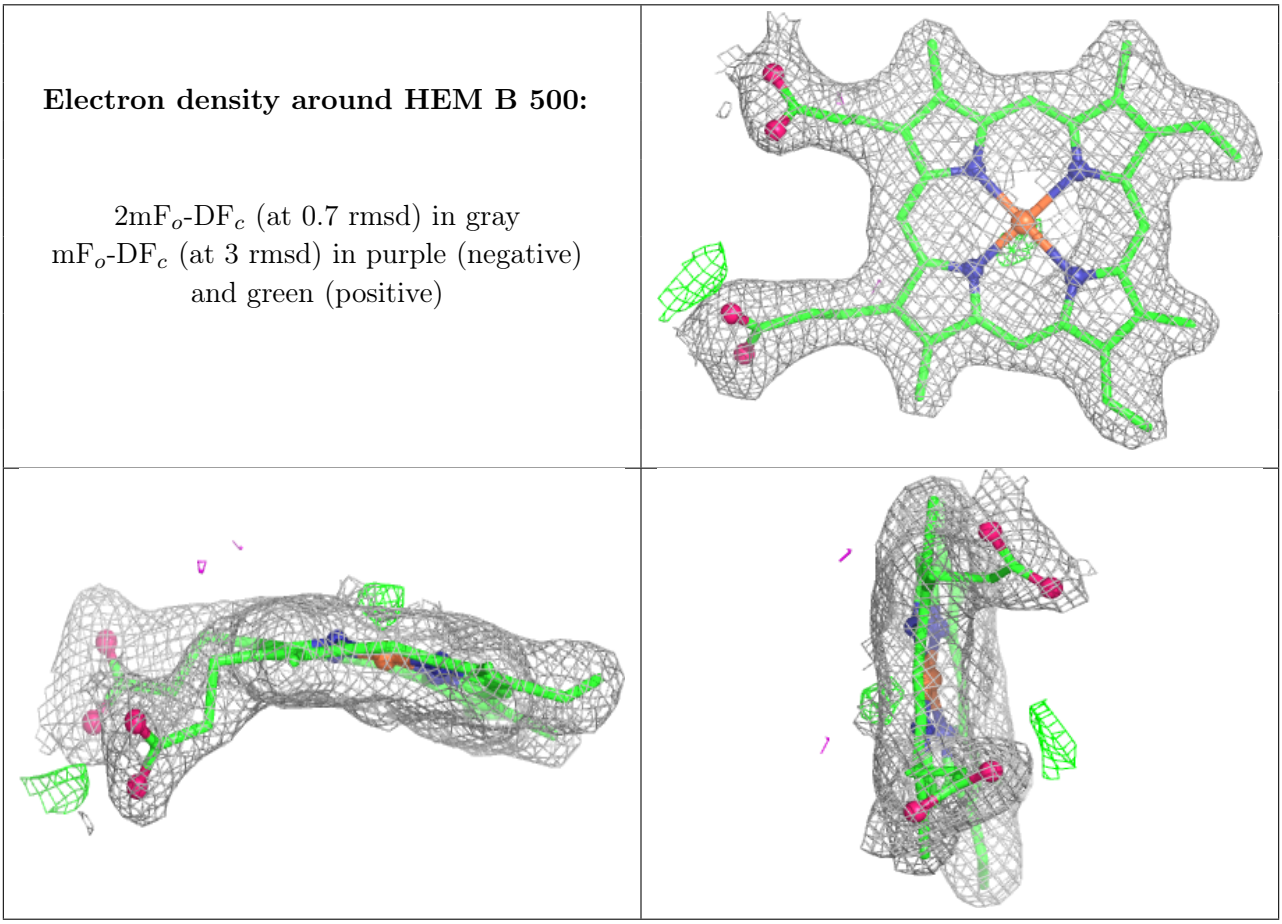
Electron density around S85 A 801:

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



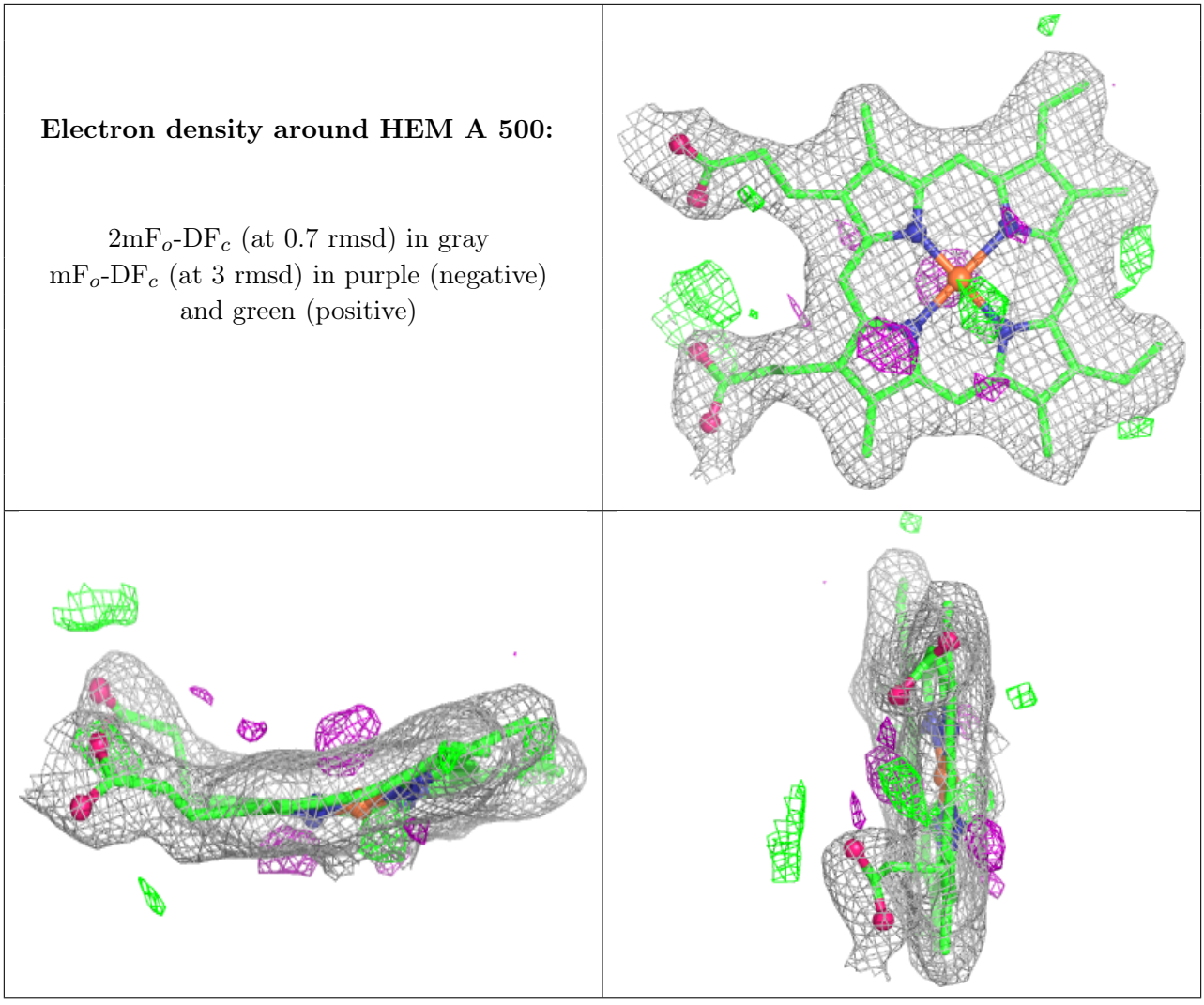
Electron density around HEM B 500:

$2mF_o$-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 500:

$2mF_o$-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.