



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:18 pm BST

PDB ID : 4CTZ
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with (S)-6-(2-amino-2-(3-(2-(4-methylpyridin-2-yl)ethyl)phenyl)ethyl)-4-methylpyridin-2-amine
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2014-03-15
Resolution : 2.01 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

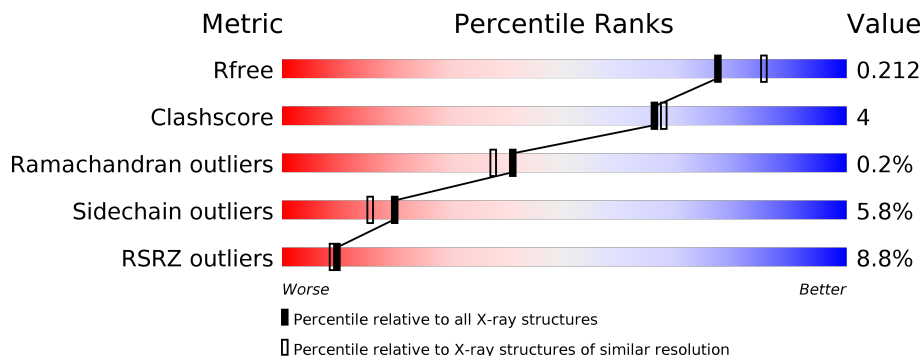
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	 9% 81% 9% • 9%
1	B	443	 7% 80% 9% • 9%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6923 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.

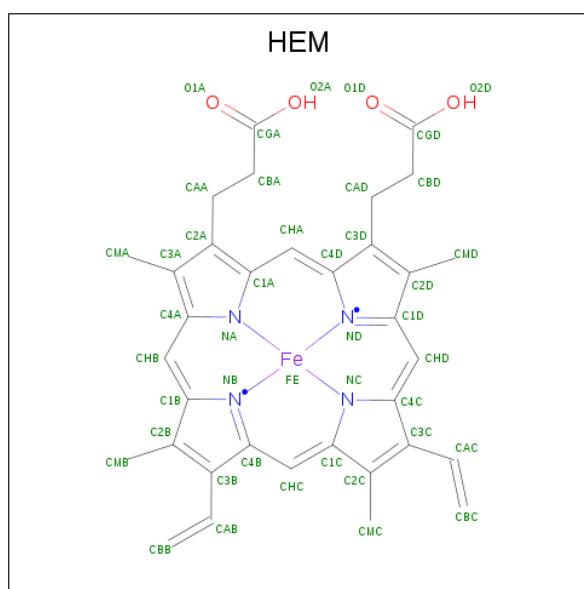
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	As	C	N	O				S
1	A	405	3223	1	2049	568	589	16	0	0	0
1	B	405	3229	1	2054	569	589	16	0	0	0

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



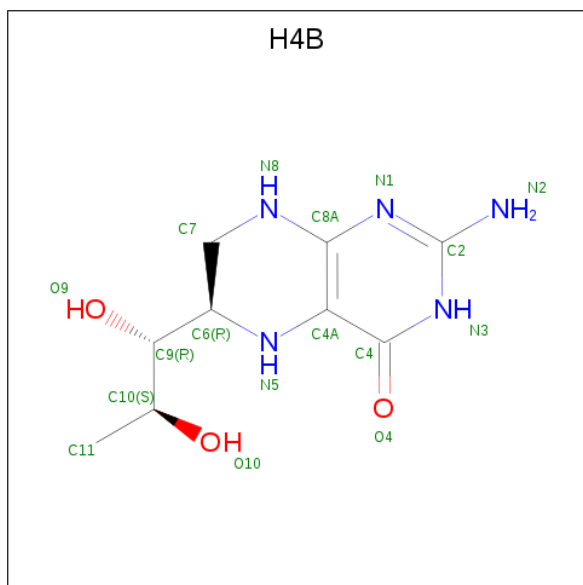
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0

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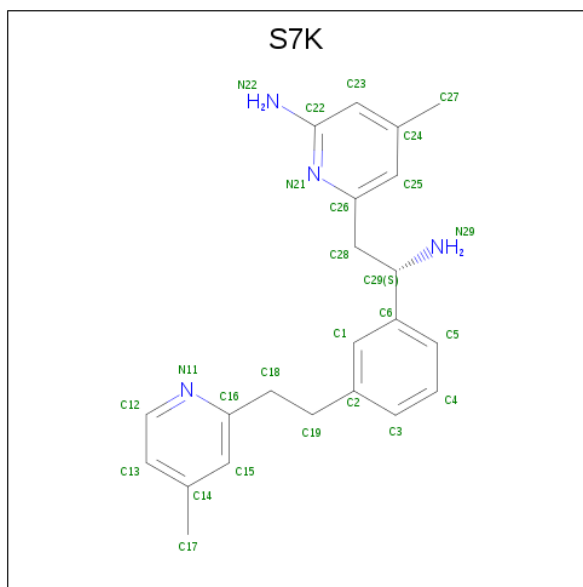
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	B	1	43	34	1	4	4	0	0

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



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

- Molecule 4 is (S)-6-(2-amino-2-(3-(2-(4-methylpyridin-2-yl)ethyl)phenyl)ethyl)-4-methylpyridin-2-amine (three-letter code: S7K) (formula: $C_{22}H_{26}N_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C N	0	0
			26	22 4		
4	B	1	Total	C N	0	0
			26	22 4		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



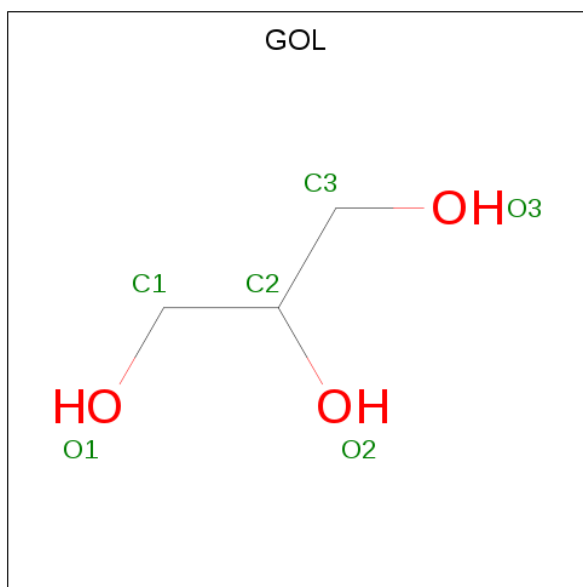
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			4	2 2		
5	A	1	Total	C O	0	0
			4	2 2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 (three-letter code: GOL) (formula: C₃H₈O₃).



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 (three-letter code: ZN) (formula: Zn).

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

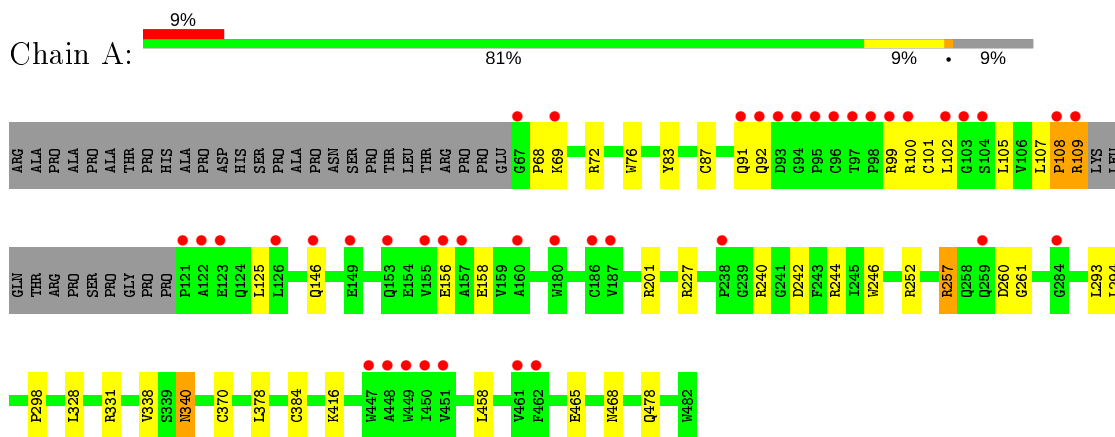
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	150	Total O 150 150	0	0
8	B	120	Total O 120 120	0	0

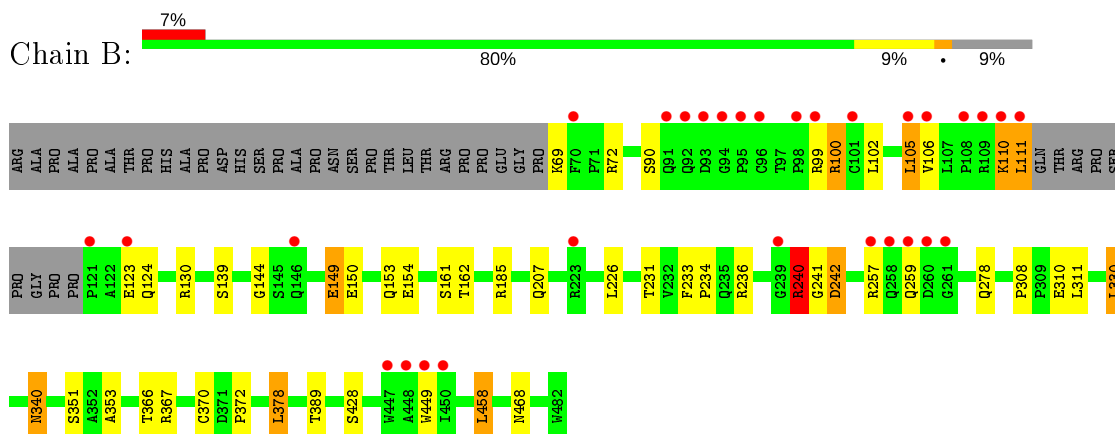
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.03Å 106.70Å 158.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.01 48.53 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.58-2.01) 98.1 (48.53-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.165 , 0.205 0.173 , 0.212	Depositor DCC
R_{free} test set	3280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CAS, S7K, ACT, 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	0.98	2/3303 (0.1%)	0.97	6/4497 (0.1%)
1	B	0.98	1/3308 (0.0%)	0.98	8/4502 (0.2%)
All	All	0.98	3/6611 (0.0%)	0.98	14/8999 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	428	SER	CB-OG	6.87	1.51	1.42
1	A	252	ARG	CZ-NH2	5.61	1.40	1.33
1	A	478	GLN	CD-OE1	-5.04	1.12	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-11.21	114.70	120.30
1	B	240	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	B	185	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	242	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	330	LEU	CB-CG-CD1	6.95	122.81	111.00
1	B	458	LEU	CB-CG-CD1	6.42	121.91	111.00
1	A	227	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	252	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	B	367	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	331	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	242	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	244	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	242	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	201	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	3223	0	3127	21	0
1	B	3229	0	3141	27	0
2	A	43	0	30	4	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	2	0
4	A	26	0	26	2	0
4	B	26	0	26	1	0
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	2	0
7	A	1	0	0	0	0
8	A	150	0	0	3	0
8	B	120	0	0	0	0
All	All	6923	0	6438	52	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 (52) 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:AS	1:A:384:CAS:SG	2.63	1.16
8:A:2011:HOH:O	1:B:100:ARG:HD2	1.75	0.86
1:B:236:ARG:HG2	1:B:236:ARG:HH11	1.54	0.72
1:B:236:ARG:NH1	1:B:242:ASP:OD1	2.28	0.66
1:A:384:CAS:CB	1:A:384:CAS:AS	3.05	0.64
1:B:236:ARG:HD2	1:B:351:SER:HB3	1.80	0.63
1:B:106:VAL:HG21	6:B:880:GOL:O3	1.98	0.63
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.34	0.61
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:CYS:HB2	8:A:2011:HOH:O	2.01	0.60
1:B:308:PRO:HD2	1:B:311:LEU:HD12	1.84	0.60
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.61	0.59
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.85	0.57
1:B:340:ASN:HD22	1:B:340:ASN:H	1.58	0.52
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.40	0.51
1:A:72:ARG:HD3	8:A:2002:HOH:O	2.10	0.51
1:B:236:ARG:HH11	1:B:236:ARG:CG	2.21	0.51
1:B:310:GLU:OE1	1:B:310:GLU:N	2.37	0.50
1:B:149:GLU:O	1:B:153:GLN:HG3	2.11	0.50
1:A:99:ARG:NH2	1:B:90:SER:O	2.45	0.50
1:B:150:GLU:O	1:B:154:GLU:HG3	2.13	0.49
1:A:384:CAS:SG	1:A:384:CAS:CE1	3.00	0.49
1:B:366:THR:O	1:B:370:CYS:HB2	2.13	0.48
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.42	0.48
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.44	0.47
1:B:449:TRP:HA	3:B:600:H4B:N1	2.29	0.47
2:B:500:HEM:HBD2	4:B:800:S7K:C3	2.44	0.47
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.97	0.47
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.81	0.46
1:B:259:GLN:OE1	1:B:259:GLN:N	2.48	0.46
1:B:110:LYS:O	1:B:111:LEU:C	2.53	0.45
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.98	0.45
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.56	0.45
3:B:600:H4B:O4	6:B:880:GOL:O2	2.27	0.45
2:A:500:HEM:HBD2	4:A:800:S7K:C3	2.47	0.44
1:B:236:ARG:HG2	1:B:236:ARG:NH1	2.29	0.44
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.47	0.44
1:B:240:ARG:HD2	1:B:241:GLY:O	2.17	0.43
1:B:123:GLU:HG2	1:B:124:GLN:N	2.33	0.43
1:A:340:ASN:HD22	1:A:340:ASN:H	1.67	0.43
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.86	0.43
1:A:109:ARG:NH1	1:A:109:ARG:HB2	2.34	0.43
1:B:161:SER:HB2	1:B:162:THR:HG23	2.00	0.43
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	2.00	0.42
2:A:500:HEM:HMC1	2:A:500:HEM:HBC2	2.02	0.42
1:A:260:ASP:OD1	1:A:261:GLY:N	2.52	0.42
1:A:101:CYS:HB3	1:B:468:ASN:HB3	2.03	0.41
1:A:465:GLU:OE1	1:B:105:LEU:HD13	2.20	0.41
1:B:231:THR:O	1:B:353:ALA:HA	2.20	0.41
1:A:68:PRO:HG2	1:A:83:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG23	4:A:800:S7K:H25	2.04	0.40
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.61	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	400/443 (90%)	392 (98%)	7 (2%)	1 (0%)	41	37
1	B	400/443 (90%)	384 (96%)	15 (4%)	1 (0%)	41	37
All	All	800/886 (90%)	776 (97%)	22 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	GLY
1	A	108	PRO

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	343/375 (92%)	325 (95%)	18 (5%)	23	19
1	B	344/375 (92%)	322 (94%)	22 (6%)	17	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	687/750 (92%)	647 (94%)	40 (6%)	20	15

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	91	GLN
1	A	92	GLN
1	A	100	ARG
1	A	102	LEU
1	A	105	LEU
1	A	109	ARG
1	A	125	LEU
1	A	146	GLN
1	A	156	GLU
1	A	158	GLU
1	A	257	ARG
1	A	293	LEU
1	A	328	LEU
1	A	340	ASN
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	B	69	LYS
1	B	72	ARG
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	110	LYS
1	B	111	LEU
1	B	130	ARG
1	B	139	SER
1	B	149	GLU
1	B	207	GLN
1	B	226	LEU
1	B	240	ARG
1	B	257	ARG
1	B	278	GLN
1	B	330	LEU
1	B	340	ASN
1	B	372	PRO

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Mol	Chain	Res	Type
1	B	378	LEU
1	B	389	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	258	GLN
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	1.32	1 (20%)	1,9,11	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CAS	B	384	1	5,8,9	1.58	1 (20%)	1,9,11	0.23	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE1	2.68	2.03	1.96
1	A	384	CAS	AS-CE2	2.30	2.02	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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CAS	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
3	H4B	B	600	-	16,18,18	0.94	2 (12%)	11,26,26	2.19	7 (63%)
4	S7K	B	800	-	28,28,28	1.08	2 (7%)	34,38,38	2.30	11 (32%)
6	GOL	A	880	-	5,5,5	0.48	0	5,5,5	0.70	0
5	ACT	A	861	-	1,3,3	0.86	0	0,3,3	0.00	-
5	ACT	B	861	-	1,3,3	2.09	1 (100%)	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	1.73	0	0,3,3	0.00	-
5	ACT	A	860	-	1,3,3	1.25	0	0,3,3	0.00	-
6	GOL	B	880	-	5,5,5	0.63	0	5,5,5	0.97	0
3	H4B	A	600	-	16,18,18	1.19	2 (12%)	11,26,26	2.93	7 (63%)
4	S7K	A	800	-	28,28,28	1.45	3 (10%)	34,38,38	2.14	11 (32%)
2	HEM	A	500	1	27,50,50	1.36	3 (11%)	17,82,82	2.23	5 (29%)
2	HEM	B	500	1	27,50,50	1.47	7 (25%)	17,82,82	1.91	4 (23%)

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
3	H4B	B	600	-	-	1/8/17/17	0/2/2/2
4	S7K	B	800	-	-	5/13/13/13	0/3/3/3
6	GOL	A	880	-	-	1/4/4/4	-
6	GOL	B	880	-	-	2/4/4/4	-
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	S7K	A	800	-	-	2/13/13/13	0/3/3/3
2	HEM	A	500	1	-	0/6/54/54	-
2	HEM	B	500	1	-	1/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	S7K	C6-C29	-5.16	1.45	1.52
2	A	500	HEM	C3B-C2B	-4.15	1.34	1.40
2	A	500	HEM	C4D-C3D	3.28	1.50	1.42
2	B	500	HEM	C3C-C2C	-2.92	1.36	1.40
2	B	500	HEM	C3B-C2B	-2.86	1.36	1.40
4	A	800	S7K	C23-C22	2.73	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	S7K	C6-C29	-2.57	1.48	1.52
2	B	500	HEM	C2A-C3A	-2.53	1.30	1.37
3	A	600	H4B	C8A-N1	-2.39	1.30	1.34
2	A	500	HEM	C4B-NB	-2.37	1.31	1.36
2	B	500	HEM	CAA-C2A	-2.35	1.48	1.52
4	B	800	S7K	C16-N11	2.30	1.39	1.34
3	B	600	H4B	C4A-C8A	-2.27	1.37	1.41
2	B	500	HEM	C1B-C2B	-2.24	1.37	1.42
3	A	600	H4B	C4A-C8A	-2.20	1.37	1.41
2	B	500	HEM	CAD-C3D	2.20	1.56	1.52
2	B	500	HEM	CMB-C2B	2.12	1.56	1.51
5	B	861	ACT	CH3-C	2.09	1.51	1.48
3	B	600	H4B	C7-N8	-2.08	1.41	1.44
4	A	800	S7K	C26-N21	2.05	1.38	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	S7K	C18-C16-C15	-6.00	113.28	121.22
2	B	500	HEM	CBD-CAD-C3D	5.68	122.95	112.48
4	B	800	S7K	C25-C26-N21	-5.18	117.40	122.90
3	A	600	H4B	C4-C4A-N5	4.91	123.24	119.12
4	A	800	S7K	C24-C25-C26	4.67	123.38	120.32
2	A	500	HEM	CBA-CAA-C2A	-4.66	103.89	112.49
2	A	500	HEM	CAA-CBA-CGA	4.49	120.20	112.67
4	A	800	S7K	C18-C16-C15	-4.40	115.40	121.22
3	A	600	H4B	C4-C4A-C8A	4.29	118.39	114.57
3	A	600	H4B	N2-C2-N3	4.26	123.87	117.25
4	A	800	S7K	C13-C12-N11	-4.09	118.88	123.96
4	B	800	S7K	C22-N21-C26	3.94	121.08	118.10
4	B	800	S7K	C13-C12-N11	-3.93	119.07	123.96
4	B	800	S7K	C24-C25-C26	3.75	122.77	120.32
2	A	500	HEM	CMC-C2C-C3C	3.45	131.13	124.68
4	A	800	S7K	C25-C26-N21	-3.38	119.32	122.90
4	B	800	S7K	C18-C16-N11	3.33	123.74	116.91
4	A	800	S7K	C17-C14-C15	-3.27	116.09	120.94
3	B	600	H4B	N3-C2-N1	-3.27	120.30	125.42
3	A	600	H4B	N3-C2-N1	-3.20	120.40	125.42
4	A	800	S7K	C14-C15-C16	-3.17	118.24	120.32
3	B	600	H4B	C4-C4A-C8A	3.06	117.29	114.57
4	B	800	S7K	C17-C14-C15	-3.06	116.41	120.94
4	A	800	S7K	C12-N11-C16	3.04	121.58	117.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	S7K	C14-C15-C16	-3.04	118.33	120.32
3	B	600	H4B	C4A-N5-C6	-2.99	113.03	121.16
4	A	800	S7K	C18-C16-N11	2.92	122.90	116.91
2	B	500	HEM	CBA-CAA-C2A	-2.83	107.27	112.49
2	A	500	HEM	CBD-CAD-C3D	2.78	117.60	112.48
3	A	600	H4B	C2-N1-C8A	2.70	120.59	114.54
3	B	600	H4B	C2-N1-C8A	2.57	120.30	114.54
4	A	800	S7K	C19-C18-C16	-2.54	107.31	112.99
2	B	500	HEM	CAA-CBA-CGA	2.50	116.87	112.67
4	B	800	S7K	C5-C6-C29	-2.50	116.81	120.46
3	B	600	H4B	C4-C4A-N5	2.49	121.21	119.12
4	A	800	S7K	C19-C2-C3	-2.36	115.27	121.23
3	A	600	H4B	C4-N3-C2	2.35	119.66	115.93
4	A	800	S7K	C6-C1-C2	-2.34	117.69	120.94
3	A	600	H4B	C4A-N5-C6	-2.32	114.84	121.16
4	B	800	S7K	C28-C29-C6	-2.28	106.47	111.61
2	B	500	HEM	C3B-C4B-NB	-2.28	106.27	109.21
3	B	600	H4B	N2-C2-N1	2.17	120.63	117.25
2	A	500	HEM	CMB-C2B-C3B	2.16	128.72	124.68
4	B	800	S7K	C4-C5-C6	-2.14	118.00	120.65
3	B	600	H4B	C4-N3-C2	2.08	119.23	115.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

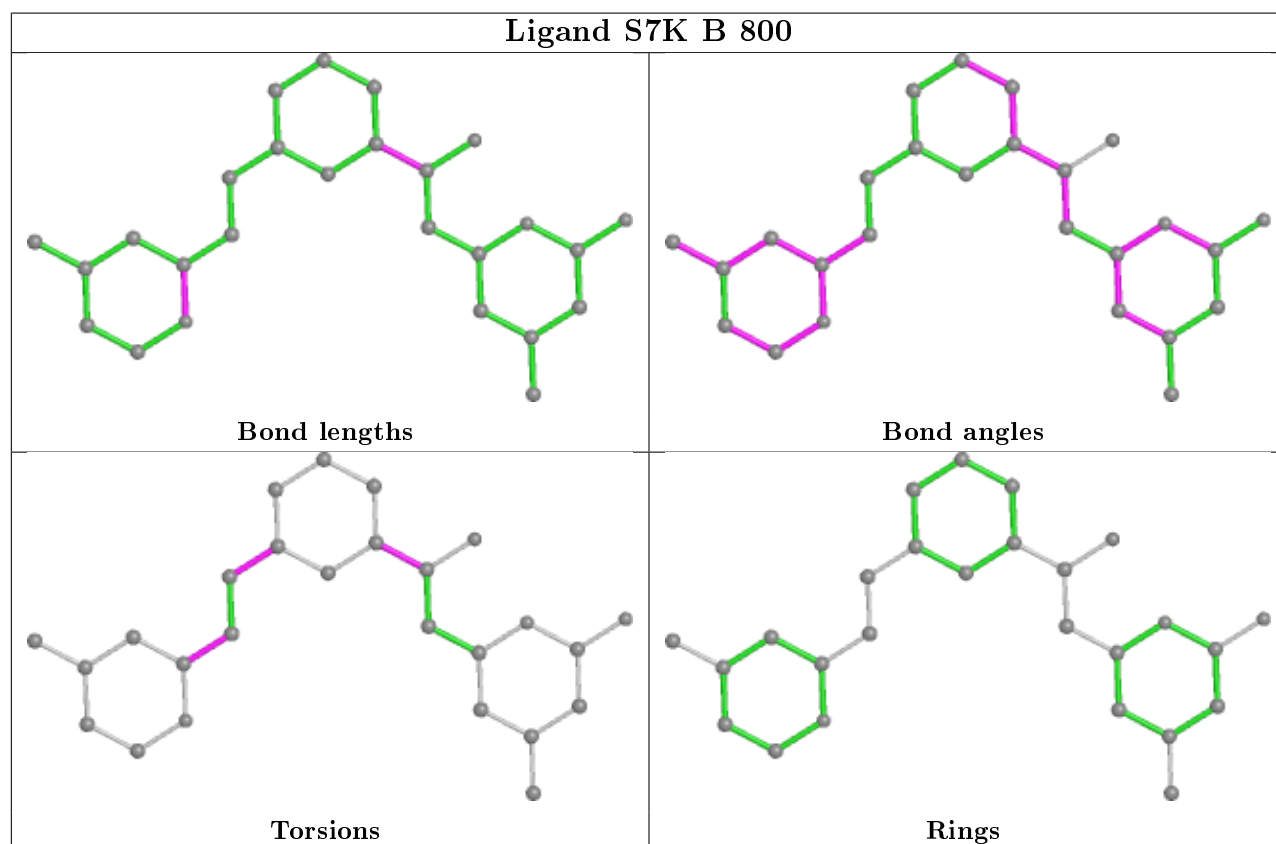
Mol	Chain	Res	Type	Atoms
6	B	880	GOL	O1-C1-C2-C3
4	B	800	S7K	N11-C16-C18-C19
4	B	800	S7K	C15-C16-C18-C19
2	B	500	HEM	C3A-C2A-CAA-CBA
4	A	800	S7K	C15-C16-C18-C19
4	A	800	S7K	N11-C16-C18-C19
4	B	800	S7K	C18-C19-C2-C1
4	B	800	S7K	C18-C19-C2-C3
6	B	880	GOL	O1-C1-C2-O2
6	A	880	GOL	C1-C2-C3-O3
3	B	600	H4B	N5-C6-C9-O9
4	B	800	S7K	N29-C29-C6-C5

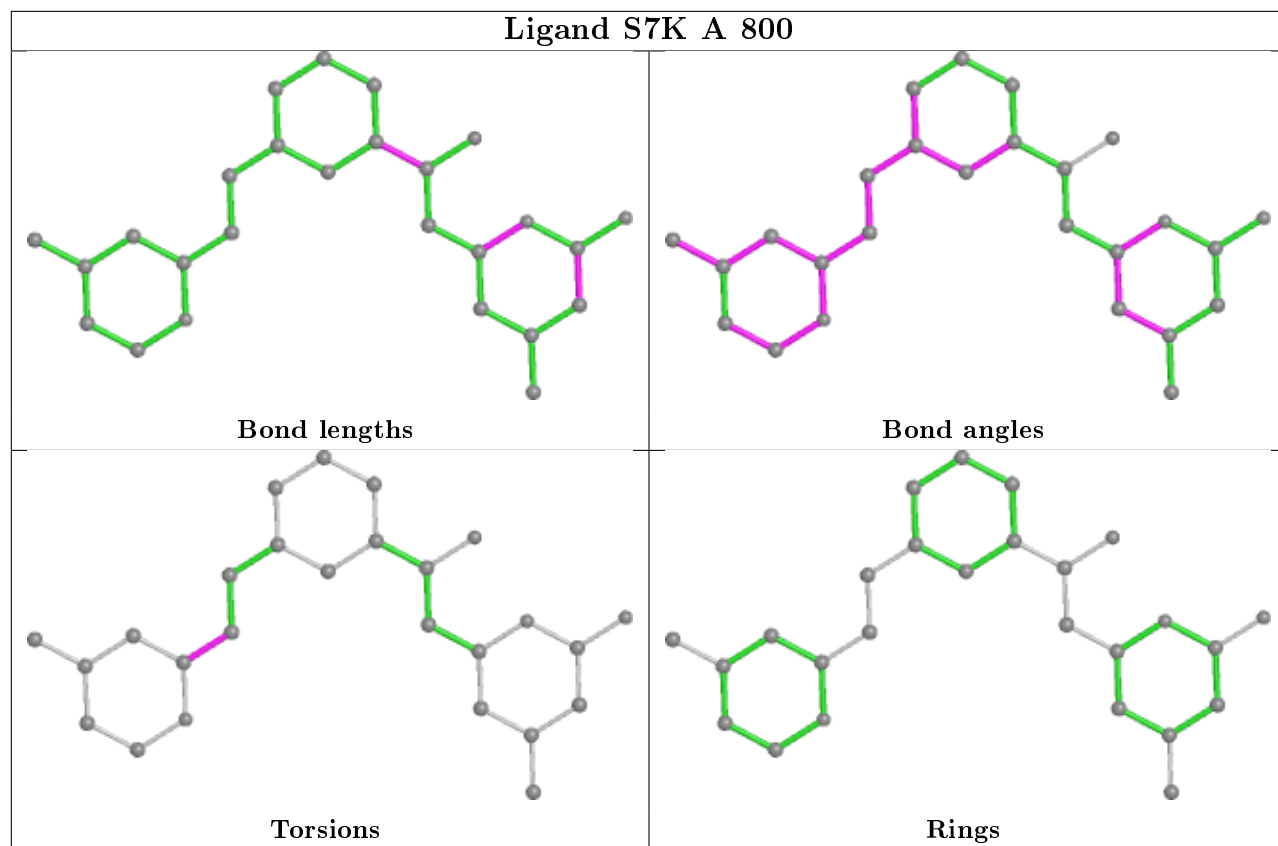
There are no ring outliers.

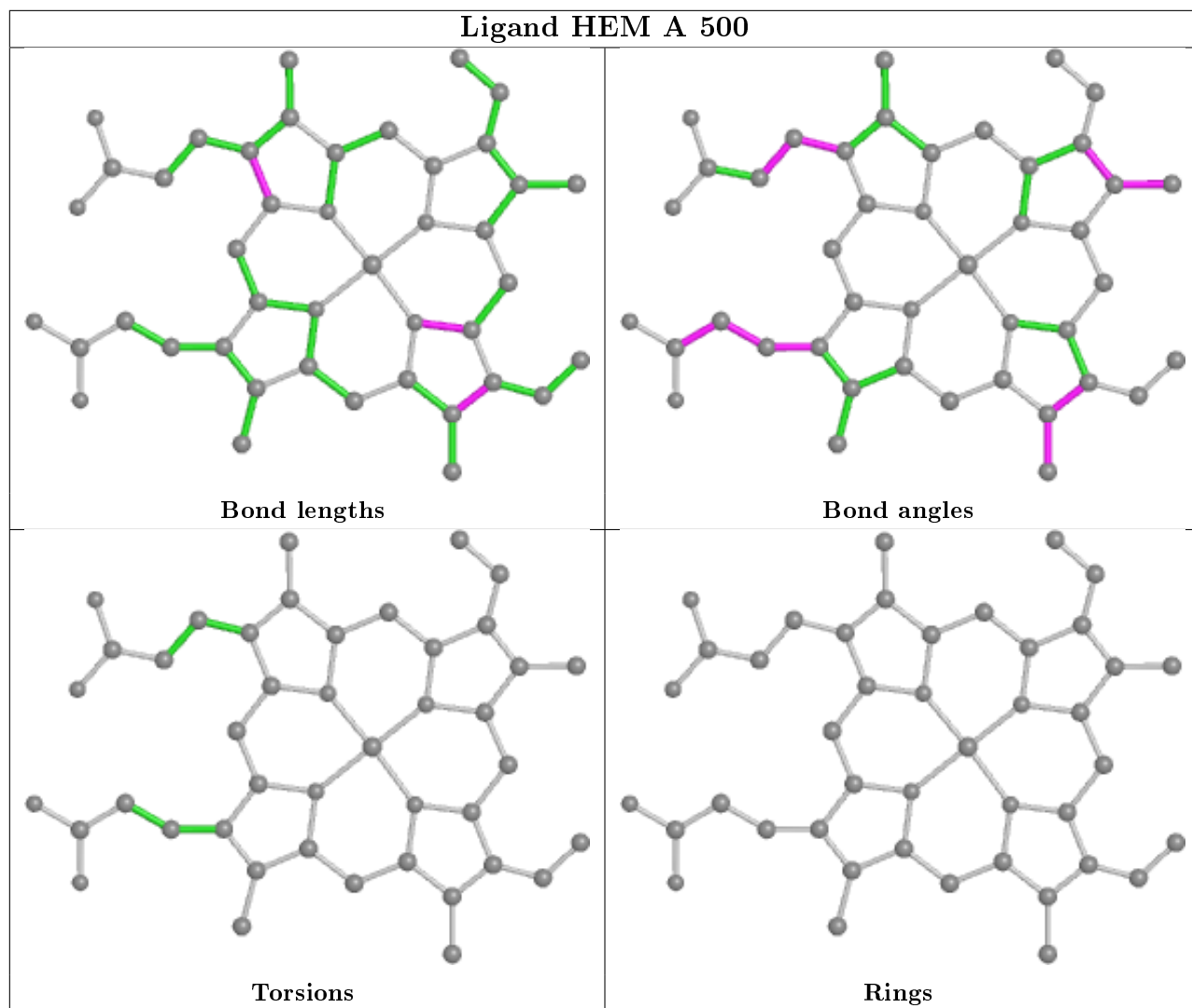
6 monomers are involved in 11 short contacts:

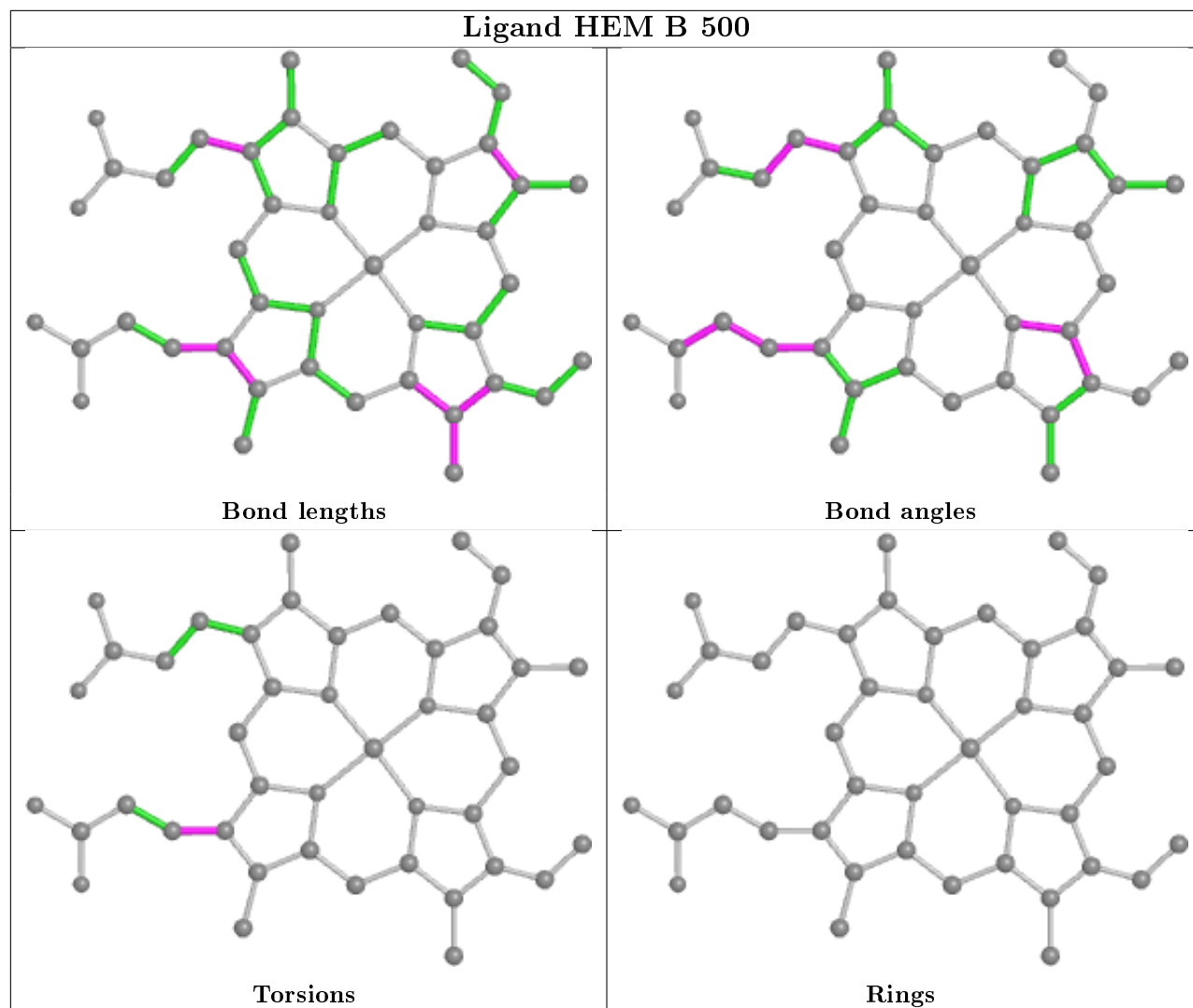
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	H4B	2	0
4	B	800	S7K	1	0
6	B	880	GOL	2	0
4	A	800	S7K	2	0
2	A	500	HEM	4	0
2	B	500	HEM	3	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/443 (91%)	0.47	41 (10%) 7 6	38, 52, 93, 128	0
1	B	404/443 (91%)	0.28	30 (7%) 14 13	39, 54, 94, 130	0
All	All	808/886 (91%)	0.38	71 (8%) 10 9	38, 53, 94, 130	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	LEU	14.6
1	B	110	LYS	8.8
1	A	91	GLN	6.2
1	A	93	ASP	5.9
1	B	94	GLY	5.5
1	B	109	ARG	5.2
1	A	69	LYS	5.2
1	A	98	PRO	5.1
1	A	123	GLU	5.0
1	A	67	GLY	4.7
1	A	97	THR	4.6
1	A	122	ALA	4.6
1	A	99	ARG	4.4
1	B	259	GLN	4.4
1	B	108	PRO	4.4
1	B	260	ASP	4.3
1	A	94	GLY	4.1
1	B	91	GLN	3.9
1	B	99	ARG	3.8
1	A	100	ARG	3.8
1	A	259	GLN	3.8
1	B	92	GLN	3.6
1	A	104	SER	3.6
1	A	450	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	451	VAL	3.5
1	A	95	PRO	3.4
1	A	121	PRO	3.3
1	A	447	TRP	3.2
1	A	96	CYS	3.1
1	A	108	PRO	3.1
1	A	160	ALA	3.1
1	A	448	ALA	3.0
1	A	449	TRP	2.9
1	A	109	ARG	2.9
1	A	186	CYS	2.9
1	B	447	TRP	2.9
1	B	105	LEU	2.9
1	B	106	VAL	2.8
1	B	146	GLN	2.8
1	B	261	GLY	2.8
1	A	126	LEU	2.7
1	B	98	PRO	2.7
1	B	70	PHE	2.7
1	A	102	LEU	2.6
1	A	238	PRO	2.6
1	B	93	ASP	2.6
1	A	92	GLN	2.6
1	A	155	VAL	2.5
1	A	461	VAL	2.5
1	B	257	ARG	2.5
1	B	223	ARG	2.5
1	B	448	ALA	2.4
1	A	180	TRP	2.4
1	A	187	VAL	2.3
1	A	146	GLN	2.3
1	B	239	GLY	2.3
1	A	284	GLY	2.3
1	B	95	PRO	2.3
1	A	103	GLY	2.3
1	B	123	GLU	2.3
1	B	449	TRP	2.2
1	B	450	ILE	2.2
1	A	156	GLU	2.2
1	A	153	GLN	2.2
1	B	258	GLN	2.2
1	B	101	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	121	PRO	2.2
1	A	157	ALA	2.1
1	A	462	PHE	2.0
1	A	149	GLU	2.0
1	B	96	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAS	B	384	9/10	0.96	0.08	52,61,87,88	0
1	CAS	A	384	9/10	0.97	0.08	49,52,71,78	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

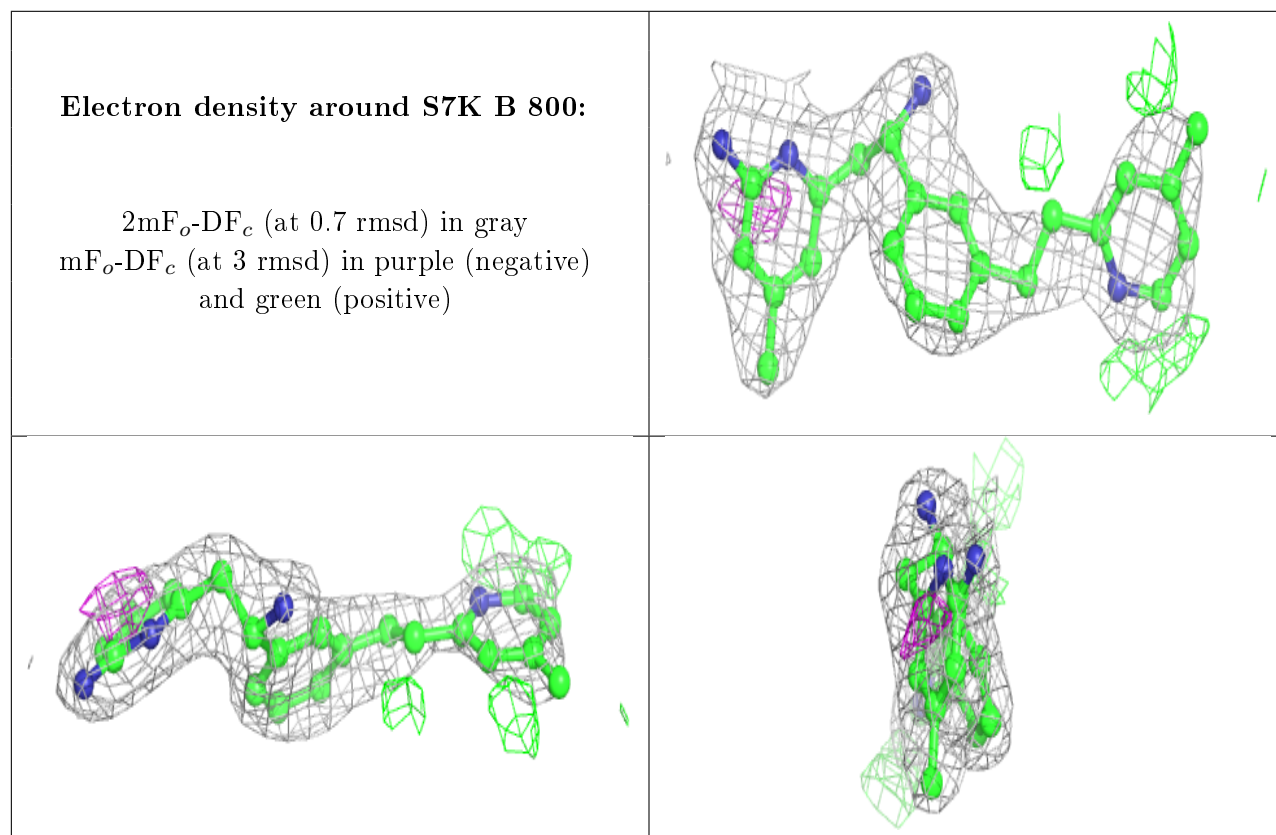
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	B	861	4/4	0.83	0.24	58,59,64,66	0
6	GOL	A	880	6/6	0.87	0.16	60,70,77,85	0
6	GOL	B	880	6/6	0.92	0.14	65,73,76,79	0
4	S7K	B	800	26/26	0.94	0.12	39,51,90,92	0
4	S7K	A	800	26/26	0.94	0.17	42,52,95,99	0
5	ACT	A	861	4/4	0.95	0.11	52,56,58,62	0
5	ACT	B	860	4/4	0.95	0.28	58,61,63,64	0
3	H4B	B	600	17/17	0.96	0.16	37,43,51,52	0
3	H4B	A	600	17/17	0.97	0.19	38,43,49,54	0
5	ACT	A	860	4/4	0.97	0.16	52,58,65,70	0
2	HEM	A	500	43/43	0.98	0.20	39,45,52,55	0

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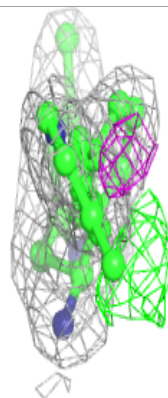
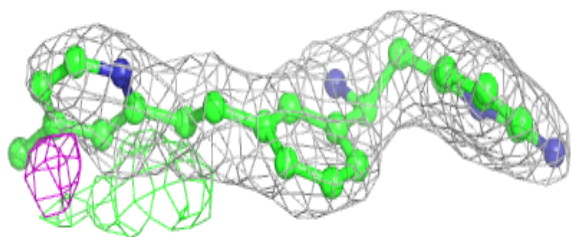
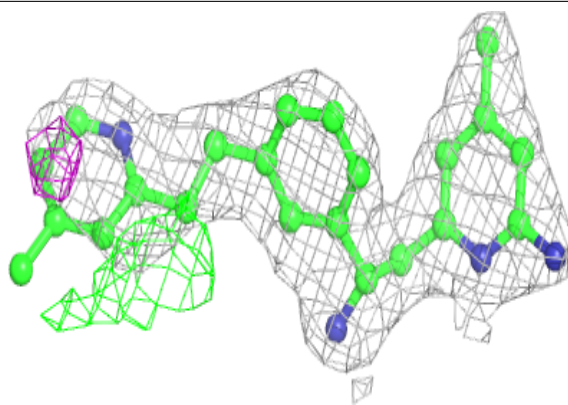
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	B	500	43/43	0.98	0.15	33,42,60,63	0
7	ZN	A	900	1/1	0.99	0.04	91,91,91,91	0

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.



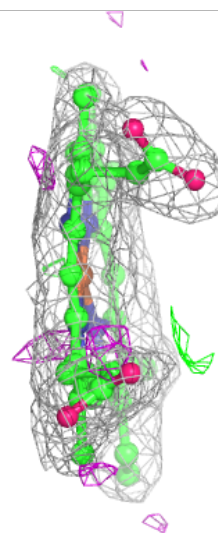
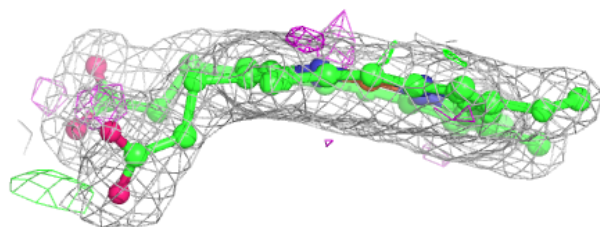
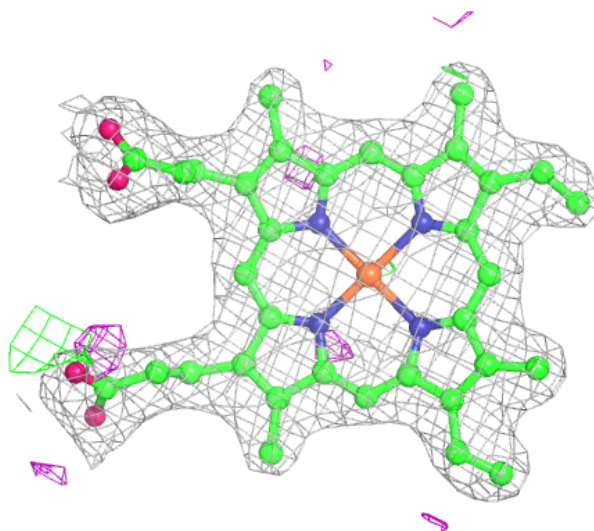
Electron density around S7K A 800:

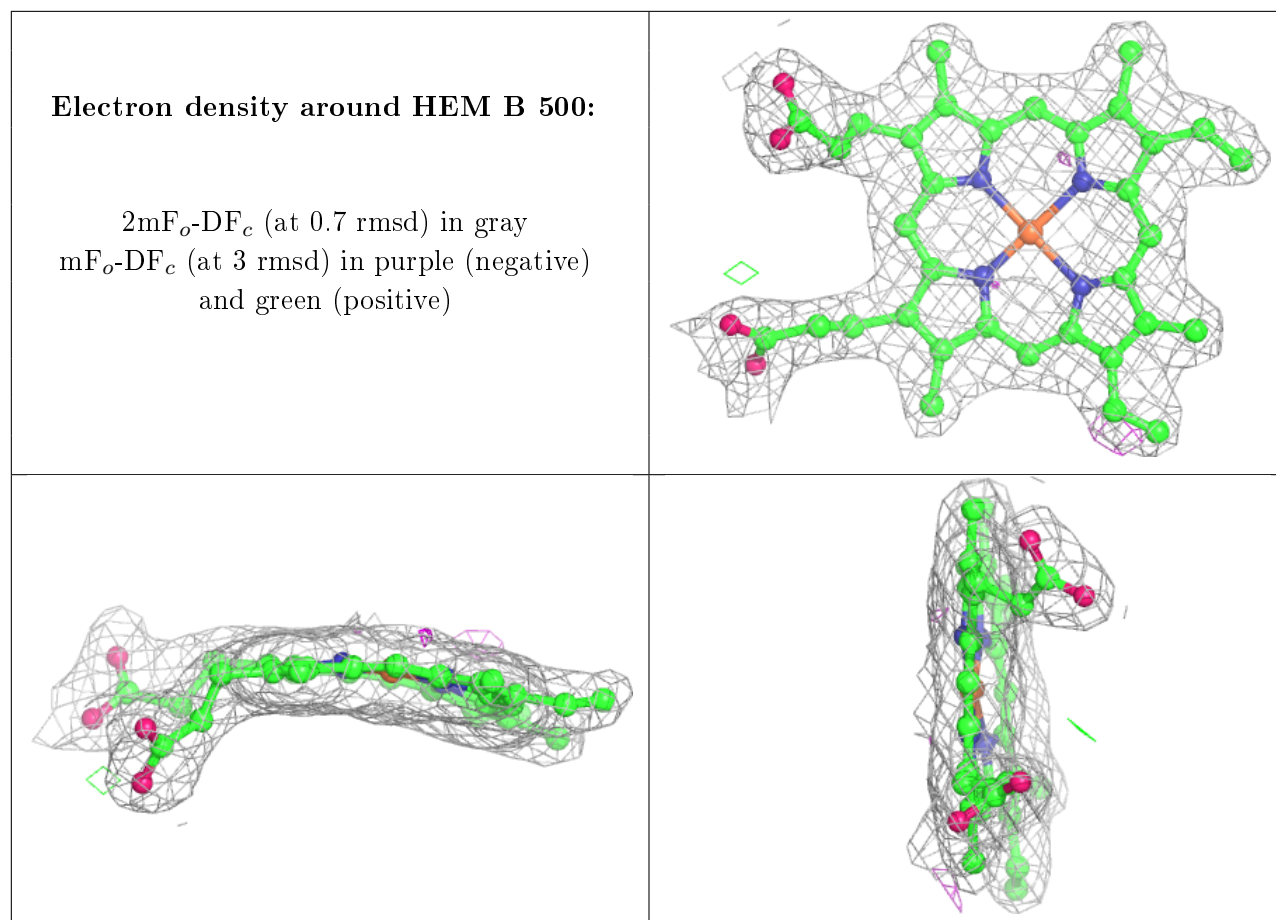
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.