Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 03:33 PM EDT

PDB ID	:	3QJS
Title	:	The structure of and photolytic induced changes of carbon monoxide binding to the cytochrome ba3-oxidase from Thermus thermophilus
Authors	:	Liu, B.; Zhang, Y.; Sage, J.T.; Doukov, T.; Chen, Y.; Stout, C.D.; Fee, J.A.
Deposited on	:	2011-01-30
Resolution	:	2.80 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:

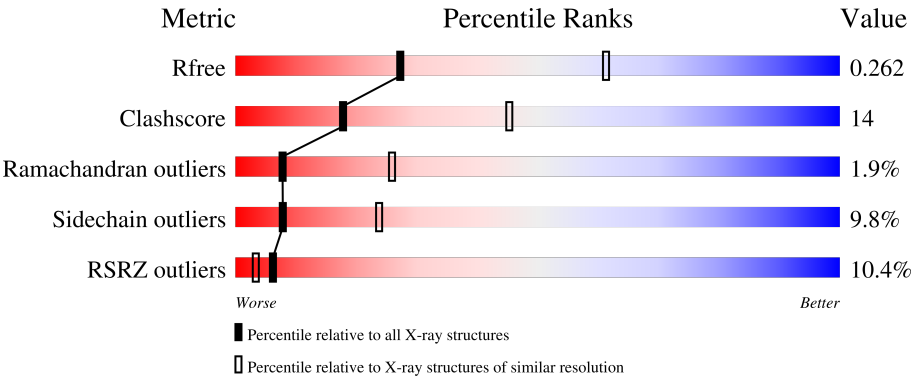
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	568	11% 69% 24% 5%
2	B	168	8% 72% 22% 5%
3	C	34	9% 76% 21%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6108 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4409	2985	709	699	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79
A	258	ARG	LYS	conflict	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	conflict	UNP Q5SJ80

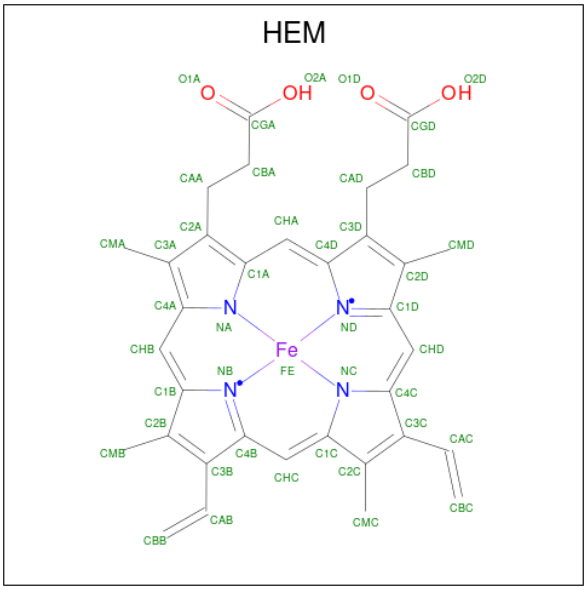
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

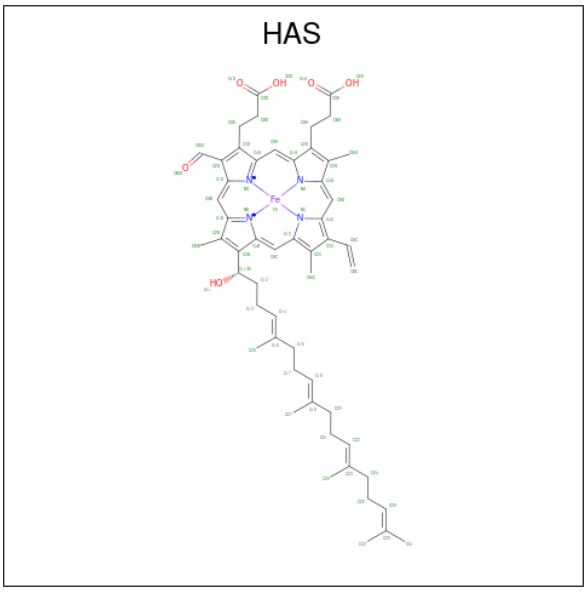
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



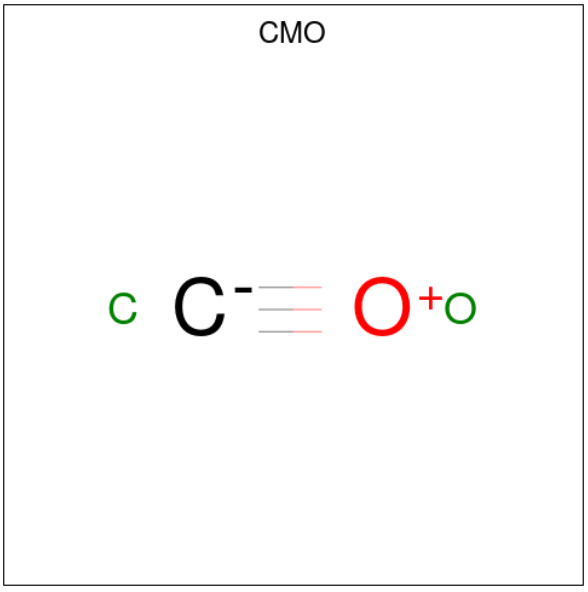
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



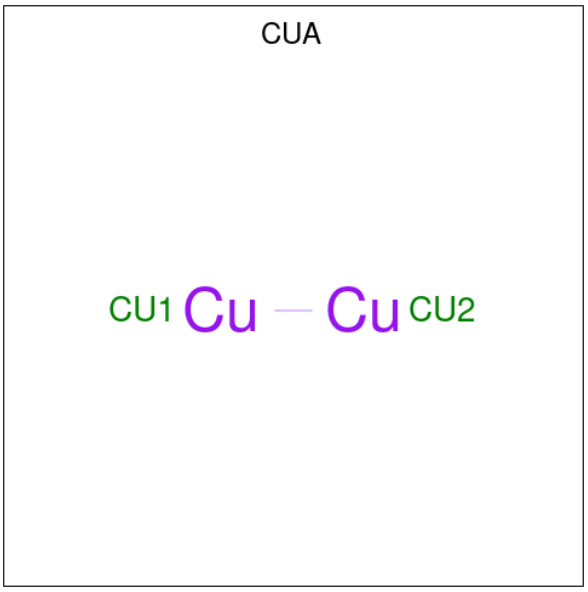
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cu 2 2	0	0

- Molecule 9 is water.

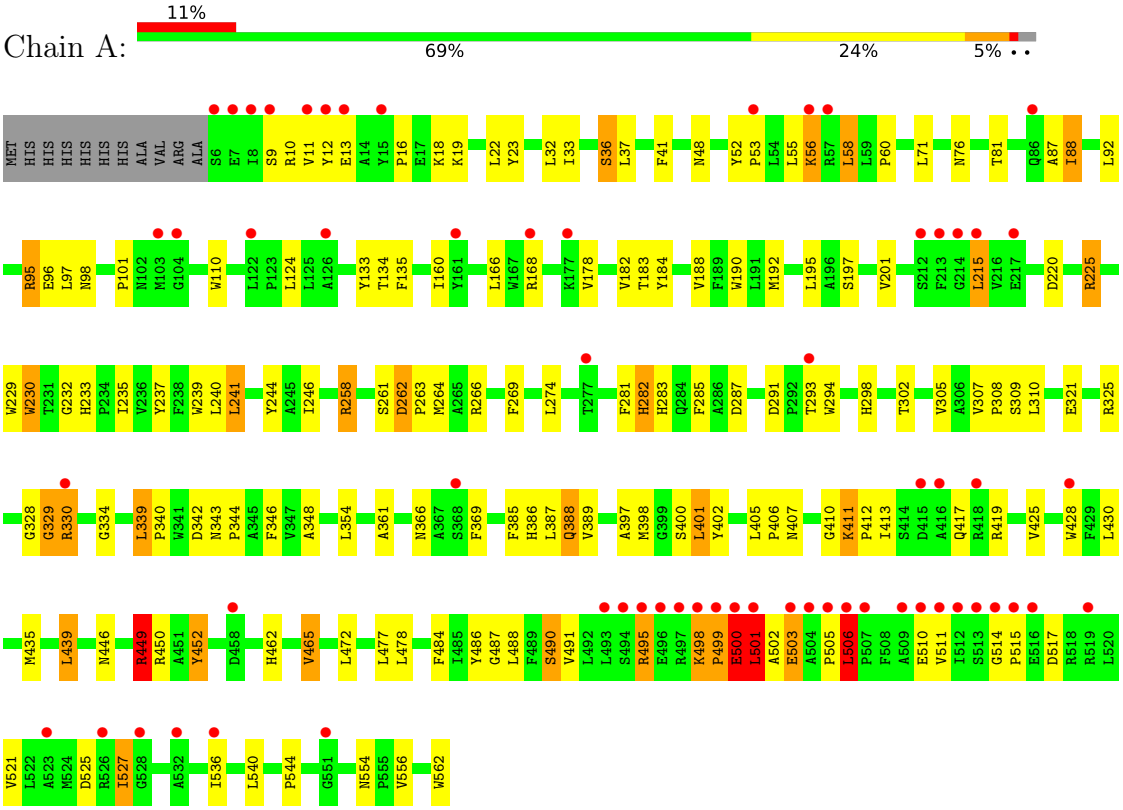
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	23	Total O 23 23	0	0
9	B	6	Total O 6 6	0	0

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.

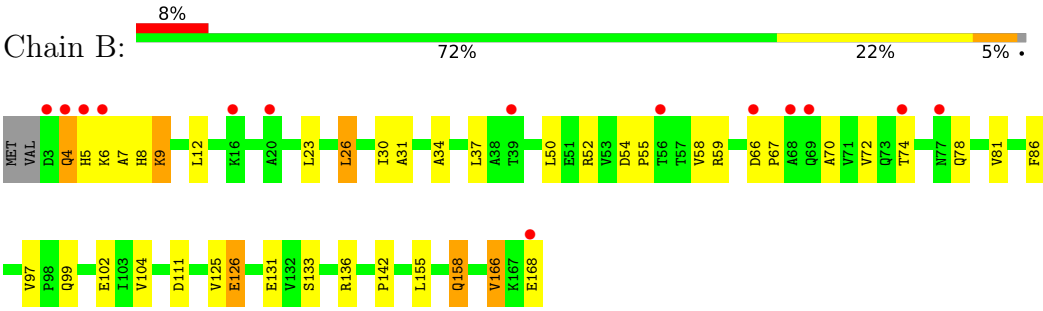
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



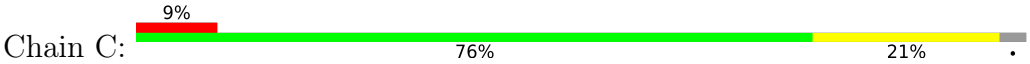
• Molecule 2: Cytochrome c oxidase subunit 2

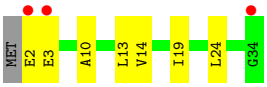
Chain B:



• Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.21Å 114.21Å 146.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 100.0 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.215 , 0.265 0.212 , 0.262	Depositor DCC
R_{free} test set	1251 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	81.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6108	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: HEM, HAS, CUA, CU1, CMO

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	0.81	1/4566 (0.0%)	0.84	5/6266 (0.1%)
2	B	0.86	3/1335 (0.2%)	0.81	0/1822
3	C	0.78	0/265	0.82	0/359
All	All	0.82	4/6166 (0.1%)	0.84	5/8447 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	PRO	CA-C	6.27	1.65	1.52
2	B	102	GLU	CG-CD	6.07	1.61	1.51
2	B	102	GLU	CB-CG	5.46	1.62	1.52
2	B	126	GLU	CG-CD	5.01	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	501	LEU	CA-CB-CG	7.94	133.56	115.30
1	A	449	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	A	499	PRO	N-CA-C	5.88	127.39	112.10
1	A	498	LYS	C-N-CD	-5.46	108.58	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	GLY	Peptide
2	B	87	ALA	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	4409	0	4516	146	1
2	B	1298	0	1282	25	0
3	C	259	0	279	3	0
4	A	1	0	0	0	0
5	A	43	0	30	9	0
6	A	65	0	61	10	0
7	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	23	0	0	10	0
9	B	6	0	0	0	0
All	All	6108	0	6168	166	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 14.

All (166) 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:233:HIS:NE2	1:A:237:TYR:CE2	1.77	1.44
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.87	1.37
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.62	1.16
1:A:506:LEU:H	1:A:506:LEU:CD2	1.65	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LEU:H	1:A:506:LEU:HD23	0.91	1.05
1:A:506:LEU:HD23	1:A:506:LEU:N	1.77	0.99
1:A:411:LYS:HE2	1:A:495:ARG:HH22	1.29	0.94
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.45	0.90
1:A:12:TYR:CD1	1:A:19:LYS:HB2	2.08	0.88
1:A:449:ARG:HH12	6:A:801:HAS:CGA	1.88	0.87
1:A:12:TYR:HD1	1:A:19:LYS:HB2	1.43	0.82
1:A:282:HIS:HA	9:A:570:HOH:O	1.78	0.82
1:A:12:TYR:HB3	1:A:19:LYS:HD2	1.64	0.79
2:B:86:PHE:O	2:B:88:PHE:N	2.16	0.78
1:A:52:TYR:N	1:A:53:PRO:HD2	1.99	0.78
1:A:330:ARG:H	1:A:334:GLY:HA3	1.49	0.77
1:A:386:HIS:HE1	5:A:800:HEM:C1A	2.05	0.74
1:A:281:PHE:O	9:A:570:HOH:O	2.06	0.72
1:A:291:ASP:OD2	1:A:293:THR:HB	1.90	0.71
1:A:96:GLU:OE1	1:A:182:VAL:HG23	1.91	0.70
2:B:74:THR:HG23	2:B:78:GLN:OE1	1.92	0.70
1:A:281:PHE:H	1:A:298:HIS:HD2	1.39	0.69
2:B:104:VAL:HG22	2:B:136:ARG:HG2	1.75	0.69
2:B:142:PRO:HG2	2:B:168:GLU:OE1	1.93	0.68
1:A:92:LEU:CD2	1:A:506:LEU:HD12	2.24	0.68
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.24	0.67
1:A:285:PHE:CG	9:A:570:HOH:O	2.48	0.67
1:A:92:LEU:CD2	1:A:506:LEU:CD1	2.73	0.67
1:A:282:HIS:CA	9:A:570:HOH:O	2.42	0.65
1:A:500:GLU:O	1:A:503:GLU:HG3	1.96	0.65
1:A:449:ARG:NH1	6:A:801:HAS:O2A	2.29	0.65
2:B:97:VAL:O	2:B:166:VAL:HA	1.96	0.65
1:A:9:SER:O	1:A:11:VAL:N	2.29	0.65
1:A:261:SER:HB3	1:A:264:MET:HB2	1.80	0.63
1:A:225:ARG:HD3	1:A:287:ASP:OD1	1.99	0.62
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.66	0.61
1:A:281:PHE:H	1:A:298:HIS:CD2	2.19	0.61
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.35	0.61
1:A:184:TYR:CD2	1:A:266:ARG:HG2	2.36	0.61
1:A:92:LEU:HD23	1:A:506:LEU:CD1	2.31	0.60
1:A:9:SER:C	1:A:11:VAL:H	2.04	0.60
3:C:10:ALA:O	3:C:14:VAL:HG23	2.01	0.60
1:A:282:HIS:C	9:A:570:HOH:O	2.40	0.60
1:A:397:ALA:O	1:A:400:SER:HB3	2.01	0.59
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:HA	1:A:16:PRO:HA	1.84	0.58
1:A:18:LYS:HE2	1:A:407:ASN:O	2.04	0.57
1:A:92:LEU:HD22	1:A:506:LEU:HD12	1.86	0.57
1:A:258:ARG:HD3	1:A:510:GLU:HB2	1.86	0.56
1:A:52:TYR:N	1:A:53:PRO:CD	2.68	0.56
1:A:385:PHE:HB3	6:A:801:HAS:C3A	2.36	0.56
1:A:411:LYS:HE2	1:A:495:ARG:NH2	2.11	0.56
2:B:50:LEU:HD23	2:B:131:GLU:OE1	2.05	0.56
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.88	0.55
1:A:500:GLU:CG	1:A:501:LEU:N	2.69	0.55
1:A:32:LEU:O	1:A:36:SER:HB2	2.07	0.55
1:A:330:ARG:HD2	1:A:330:ARG:N	2.22	0.55
1:A:500:GLU:CD	1:A:501:LEU:H	2.09	0.55
1:A:449:ARG:HD2	1:A:450:ARG:HD2	1.89	0.55
1:A:56:LYS:O	1:A:60:PRO:HA	2.06	0.54
1:A:12:TYR:CD1	1:A:19:LYS:CB	2.88	0.54
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.85	0.54
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.90	0.54
1:A:506:LEU:CD2	1:A:506:LEU:N	2.45	0.53
1:A:325:ARG:NH2	3:C:2:GLU:OE2	2.41	0.53
1:A:500:GLU:CD	1:A:501:LEU:N	2.61	0.53
1:A:446:ASN:ND2	9:A:572:HOH:O	2.42	0.53
1:A:462:HIS:HB2	9:A:586:HOH:O	2.08	0.53
1:A:517:ASP:O	1:A:521:VAL:HG23	2.09	0.53
1:A:95:ARG:HD3	1:A:506:LEU:HD21	1.91	0.52
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.91	0.52
2:B:125:VAL:HG21	2:B:133:SER:HB3	1.91	0.52
1:A:232:GLY:O	1:A:235:ILE:HG22	2.09	0.52
1:A:258:ARG:NH1	2:B:4:GLN:OE1	2.43	0.52
1:A:285:PHE:CD2	9:A:570:HOH:O	2.62	0.52
1:A:233:HIS:NE2	1:A:237:TYR:CD2	2.64	0.52
1:A:348:ALA:HB2	1:A:425:VAL:HG21	1.92	0.52
1:A:465:VAL:HG13	9:A:583:HOH:O	2.09	0.52
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.91	0.51
5:A:800:HEM:HBC2	5:A:800:HEM:HMC2	1.92	0.51
1:A:505:PRO:O	1:A:506:LEU:O	2.29	0.51
2:B:5:HIS:HA	2:B:8:HIS:HB3	1.91	0.51
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.46	0.50
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.99	0.50
2:B:26:LEU:O	2:B:30:ILE:HG13	2.11	0.50
1:A:487:GLY:O	1:A:491:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:O	1:A:527:ILE:HD12	2.11	0.49
2:B:4:GLN:H	2:B:7:ALA:HB3	1.77	0.49
1:A:328:GLY:O	1:A:330:ARG:HG3	2.13	0.49
1:A:554:ASN:HD22	2:B:52:ARG:HG3	1.78	0.49
1:A:33:ILE:HD11	1:A:488:LEU:HD23	1.94	0.49
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.47	0.49
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.27	0.49
1:A:97:LEU:HD11	1:A:183:THR:HG21	1.93	0.49
1:A:302:THR:O	1:A:305:VAL:HG12	2.14	0.48
1:A:307:VAL:N	1:A:308:PRO:HD2	2.28	0.48
1:A:449:ARG:HD2	1:A:450:ARG:CD	2.44	0.48
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.44	0.48
2:B:5:HIS:HA	2:B:8:HIS:CB	2.43	0.48
1:A:262:ASP:N	1:A:263:PRO:HD2	2.29	0.47
1:A:386:HIS:HE1	5:A:800:HEM:CHA	2.27	0.47
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.95	0.47
1:A:188:VAL:HG21	1:A:269:PHE:HB3	1.95	0.47
1:A:88:ILE:HG13	1:A:246:ILE:HD11	1.97	0.47
1:A:330:ARG:H	1:A:330:ARG:HD2	1.79	0.47
1:A:12:TYR:CB	1:A:19:LYS:HD2	2.38	0.47
1:A:435:MET:HG2	1:A:439:LEU:HD22	1.97	0.47
1:A:501:LEU:HD22	1:A:501:LEU:O	2.15	0.47
1:A:428:TRP:CH2	5:A:800:HEM:HBB1	2.50	0.47
1:A:514:GLY:HA2	2:B:5:HIS:CE1	2.50	0.47
1:A:366:ASN:CB	6:A:801:HAS:HMD	2.45	0.46
1:A:515:PRO:HD2	2:B:9:LYS:HE3	1.97	0.46
1:A:282:HIS:C	1:A:282:HIS:CD2	2.88	0.46
1:A:388:GLN:NE2	1:A:388:GLN:HA	2.30	0.46
1:A:92:LEU:HB3	1:A:182:VAL:HG11	1.97	0.46
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.98	0.46
1:A:220:ASP:OD2	2:B:52:ARG:NH1	2.49	0.46
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.50	0.46
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.97	0.46
1:A:321:GLU:OE1	1:A:325:ARG:NH1	2.49	0.45
1:A:366:ASN:C	6:A:801:HAS:HMD	2.37	0.45
1:A:477:LEU:HD12	5:A:800:HEM:HMB3	1.98	0.45
1:A:386:HIS:HE1	5:A:800:HEM:C4D	2.34	0.45
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.79	0.45
1:A:413:ILE:HG23	1:A:417:GLN:HB3	1.97	0.45
1:A:58:LEU:O	1:A:60:PRO:HD3	2.17	0.44
1:A:71:LEU:HD21	1:A:124:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HB	1:A:239:TRP:CD1	2.51	0.44
1:A:562:TRP:HA	2:B:155:LEU:HG	1.99	0.44
1:A:385:PHE:O	1:A:389:VAL:HG12	2.17	0.44
1:A:388:GLN:HE21	1:A:388:GLN:CA	2.31	0.44
1:A:398:MET:O	1:A:401:LEU:HB2	2.17	0.43
1:A:361:ALA:HB1	3:C:19:ILE:HA	1.99	0.43
1:A:410:GLY:O	1:A:411:LYS:C	2.57	0.43
2:B:66:ASP:OD1	2:B:67:PRO:HD2	2.19	0.43
1:A:240:LEU:HD21	1:A:244:TYR:CZ	2.54	0.42
1:A:342:ASP:OD1	1:A:342:ASP:N	2.41	0.42
5:A:800:HEM:HBC2	5:A:800:HEM:CMC	2.49	0.42
1:A:92:LEU:CD2	1:A:506:LEU:HD13	2.48	0.42
1:A:33:ILE:O	1:A:37:LEU:HG	2.20	0.42
1:A:495:ARG:HD3	1:A:495:ARG:HA	1.44	0.42
1:A:554:ASN:ND2	2:B:52:ARG:HG3	2.34	0.42
1:A:307:VAL:HA	1:A:310:LEU:HD12	2.02	0.41
1:A:101:PRO:HA	1:A:166:LEU:HD21	2.01	0.41
1:A:230:TRP:C	1:A:230:TRP:CD1	2.93	0.41
1:A:388:GLN:HA	1:A:388:GLN:HE21	1.85	0.41
1:A:486:TYR:O	1:A:490:SER:HB3	2.20	0.41
1:A:386:HIS:CE1	5:A:800:HEM:C4D	3.08	0.41
1:A:452:TYR:HB3	2:B:158:GLN:HG3	2.02	0.41
1:A:197:SER:O	1:A:201:VAL:HG23	2.20	0.41
1:A:398:MET:HG2	1:A:484:PHE:CE1	2.55	0.41
1:A:402:TYR:O	1:A:406:PRO:HG2	2.21	0.41
1:A:385:PHE:CB	6:A:801:HAS:C3A	2.98	0.41
1:A:285:PHE:N	9:A:570:HOH:O	2.54	0.41
1:A:412:PRO:HD3	1:A:498:LYS:HD2	2.03	0.41
1:A:500:GLU:O	1:A:502:ALA:N	2.54	0.41
2:B:54:ASP:HA	2:B:55:PRO:HD2	1.95	0.41
2:B:70:ALA:O	2:B:81:VAL:HA	2.21	0.41
1:A:329:GLY:HA2	1:A:330:ARG:HD2	2.03	0.41
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.92	0.40
1:A:134:THR:O	1:A:135:PHE:C	2.59	0.40
2:B:31:ALA:O	2:B:34:ALA:HB3	2.21	0.40
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.87	0.40
1:A:388:GLN:NE2	1:A:388:GLN:CA	2.85	0.40
6:A:801:HAS:HMB1	6:A:801:HAS:H11	1.96	0.40
1:A:192:MET:C	1:A:192:MET:SD	3.00	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:A:498:LYS:O	1:A:500:GLU:N[7_555]	1.93	0.27

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	555/568 (98%)	515 (93%)	30 (5%)	10 (2%)	8	28
2	B	164/168 (98%)	154 (94%)	7 (4%)	3 (2%)	8	28
3	C	31/34 (91%)	28 (90%)	2 (6%)	1 (3%)	4	13
All	All	750/770 (97%)	697 (93%)	39 (5%)	14 (2%)	8	26

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	401	LEU
1	A	499	PRO
1	A	500	GLU
1	A	506	LEU
2	B	87	ALA
2	B	88	PHE
1	A	501	LEU
1	A	503	GLU
2	B	4	GLN
3	C	3	GLU
1	A	13	GLU
1	A	87	ALA
1	A	411	LYS

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	453/462 (98%)	410 (90%)	43 (10%)	8 25
2	B	136/138 (99%)	121 (89%)	15 (11%)	6 19
3	C	26/27 (96%)	24 (92%)	2 (8%)	13 35
All	All	615/627 (98%)	555 (90%)	60 (10%)	8 24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	48	ASN
1	A	56	LYS
1	A	58	LEU
1	A	88	ILE
1	A	95	ARG
1	A	98	ASN
1	A	133	TYR
1	A	168	ARG
1	A	178	VAL
1	A	195	LEU
1	A	215	LEU
1	A	225	ARG
1	A	230	TRP
1	A	241	LEU
1	A	258	ARG
1	A	262	ASP
1	A	274	LEU
1	A	282	HIS
1	A	309	SER
1	A	330	ARG
1	A	339	LEU
1	A	340	PRO
1	A	354	LEU
1	A	369	PHE
1	A	388	GLN

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Mol	Chain	Res	Type
1	A	405	LEU
1	A	419	ARG
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	452	TYR
1	A	465	VAL
1	A	472	LEU
1	A	478	LEU
1	A	490	SER
1	A	495	ARG
1	A	500	GLU
1	A	501	LEU
1	A	506	LEU
1	A	527	ILE
1	A	536	ILE
1	A	540	LEU
2	B	6	LYS
2	B	9	LYS
2	B	12	LEU
2	B	23	LEU
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	59	ARG
2	B	72	VAL
2	B	91	GLN
2	B	99	GLN
2	B	111	ASP
2	B	126	GLU
2	B	158	GLN
2	B	166	VAL
3	C	13	LEU
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS

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Mol	Chain	Res	Type
1	A	388	GLN
1	A	446	ASN
2	B	117	HIS
2	B	122	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	HEM	A	800	1	41,50,50	2.01	8 (19%)	45,82,82	1.73	11 (24%)
7	CMO	A	563	4	0,1,1	-	-	-		
6	HAS	A	801	1	57,72,72	2.97	14 (24%)	48,109,109	2.25	13 (27%)
8	CUA	B	802	2	0,1,1	-	-	-		

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	HEM	A	800	1	-	4/12/54/54	-
6	HAS	A	801	1	-	8/40/122/122	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C2D-C3D	11.76	1.47	1.36
5	A	800	HEM	C3D-C2D	8.21	1.54	1.36
6	A	801	HAS	CHC-C4B	7.81	1.50	1.37
6	A	801	HAS	CHA-C4D	6.38	1.48	1.37
6	A	801	HAS	C3C-CAC	-6.31	1.35	1.47
6	A	801	HAS	CHD-C4A	5.44	1.49	1.39
6	A	801	HAS	CHB-C1B	5.42	1.49	1.39
6	A	801	HAS	CHD-C4C	4.90	1.48	1.39
6	A	801	HAS	C2A-C3A	4.81	1.51	1.37
6	A	801	HAS	CHC-C1C	4.68	1.50	1.40
6	A	801	HAS	CHB-C1D	4.53	1.47	1.39
5	A	800	HEM	C3C-C2C	-4.50	1.34	1.40
6	A	801	HAS	C3C-C2C	4.28	1.46	1.40
6	A	801	HAS	CHA-C1A	3.99	1.48	1.40
5	A	800	HEM	C3C-CAC	3.85	1.55	1.47
6	A	801	HAS	C3B-C2B	3.69	1.43	1.34
5	A	800	HEM	FE-NB	2.96	2.11	1.96
5	A	800	HEM	FE-ND	2.45	2.09	1.96
5	A	800	HEM	CMB-C2B	2.21	1.55	1.50
6	A	801	HAS	O2D-CGD	-2.10	1.23	1.30
5	A	800	HEM	C2C-C1C	2.10	1.47	1.42
5	A	800	HEM	CAB-C3B	2.04	1.53	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	801	HAS	CBA-CAA-C2A	5.95	122.63	112.60
6	A	801	HAS	CAD-CBD-CGD	-5.43	101.91	113.60
6	A	801	HAS	CHB-C1D-C2D	-5.10	118.51	126.66
6	A	801	HAS	C4B-C3B-C2B	-5.01	103.64	108.79
6	A	801	HAS	OMD-CMD-C2D	-4.55	117.74	125.03
5	A	800	HEM	C4D-ND-C1D	4.11	109.32	105.07
6	A	801	HAS	CAA-CBA-CGA	-4.07	102.34	113.76
6	A	801	HAS	C27-C19-C20	3.75	121.58	115.27
5	A	800	HEM	C1B-NB-C4B	3.63	108.82	105.07
5	A	800	HEM	C4B-CHC-C1C	3.49	127.16	122.56
5	A	800	HEM	C4B-C3B-C2B	3.28	109.72	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CBA-CAA-C2A	-2.99	107.52	112.62
6	A	801	HAS	CMA-C3A-C2A	-2.95	119.38	124.94
5	A	800	HEM	CBB-CAB-C3B	-2.91	113.14	127.62
5	A	800	HEM	CHC-C4B-C3B	2.85	128.93	124.57
5	A	800	HEM	CAD-C3D-C4D	2.66	129.31	124.66
6	A	801	HAS	C20-C19-C18	-2.53	116.00	121.12
6	A	801	HAS	CMC-C2C-C3C	2.52	129.40	124.68
5	A	800	HEM	O1D-CGD-CBD	-2.45	115.20	123.08
6	A	801	HAS	C25-C23-C24	2.44	119.37	115.27
6	A	801	HAS	C32-C30-C31	2.42	119.94	114.60
5	A	800	HEM	C4D-C3D-C2D	-2.19	103.70	106.90
6	A	801	HAS	O1A-CGA-CBA	-2.13	116.24	123.08
5	A	800	HEM	O1A-CGA-CBA	-2.09	116.37	123.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C3A-C2A-CAA-CBA
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	C3D-C2D-CMD-OMD
6	A	801	HAS	C23-C24-C28-C29
5	A	800	HEM	C2B-C3B-CAB-CBB
5	A	800	HEM	C4B-C3B-CAB-CBB
5	A	800	HEM	C2A-CAA-CBA-CGA
6	A	801	HAS	CAD-CBD-CGD-O1D
6	A	801	HAS	CAA-CBA-CGA-O1A
6	A	801	HAS	CAA-CBA-CGA-O2A
6	A	801	HAS	CAD-CBD-CGD-O2D
5	A	800	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

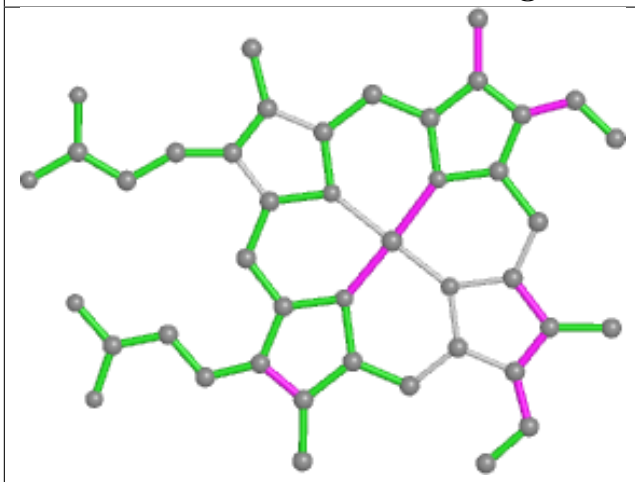
2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	9	0
6	A	801	HAS	10	0

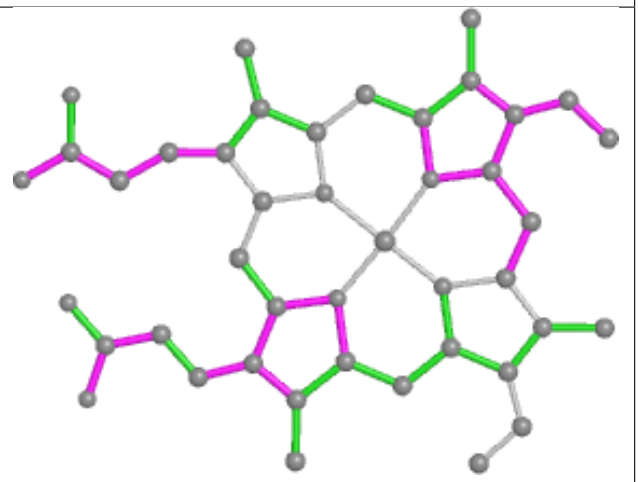
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

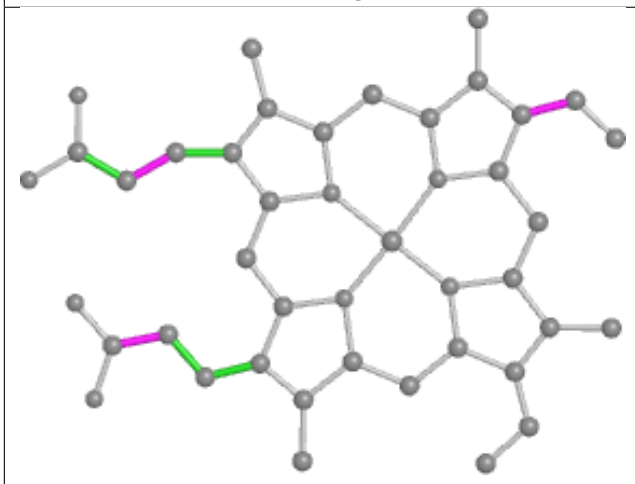
Ligand HEM A 800



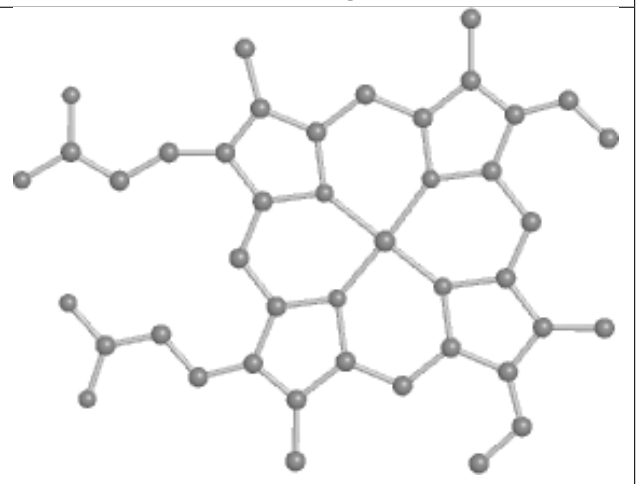
Bond lengths



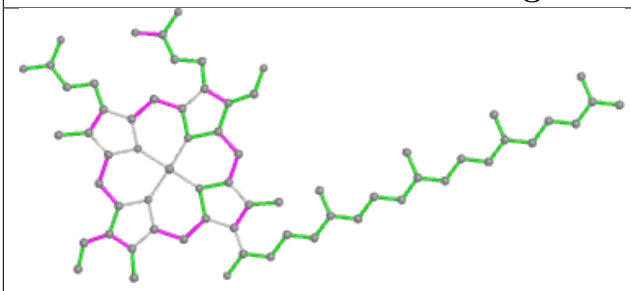
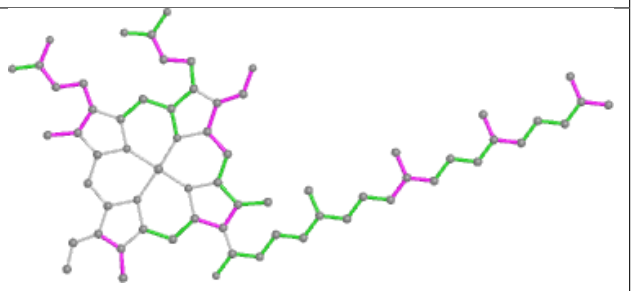
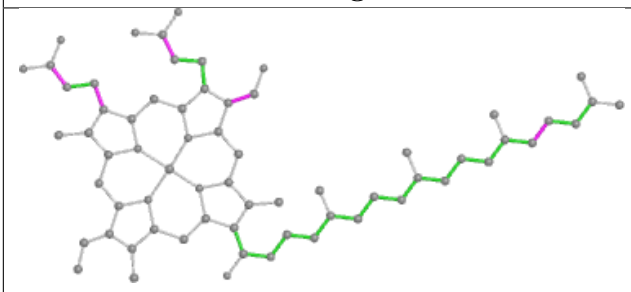
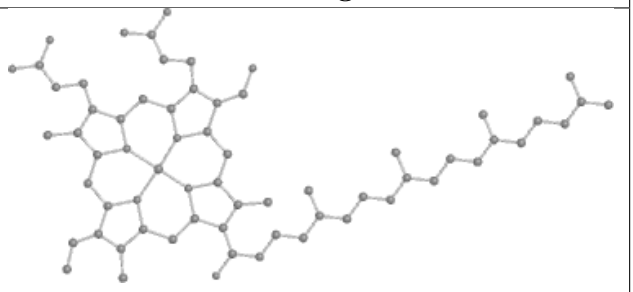
Bond angles



Torsions



Rings

Ligand HAS A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	557/568 (98%)	0.49	62 (11%) 5 3	42, 67, 100, 135	1 (0%)
2	B	166/168 (98%)	0.32	14 (8%) 11 5	47, 66, 112, 151	0
3	C	33/34 (97%)	0.30	3 (9%) 9 5	52, 61, 136, 167	0
All	All	756/770 (98%)	0.44	79 (10%) 6 3	42, 67, 102, 167	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	13.7
1	A	8	ILE	9.2
1	A	7	GLU	7.8
1	A	11	VAL	7.6
1	A	515	PRO	7.5
1	A	497	ARG	7.5
2	B	69	GLN	6.4
1	A	516	GLU	6.2
2	B	3	ASP	5.7
1	A	505	PRO	5.7
1	A	513	SER	5.7
1	A	514	GLY	5.7
3	C	2	GLU	5.6
1	A	495	ARG	5.3
1	A	214	GLY	5.1
1	A	504	ALA	4.9
1	A	418	ARG	4.8
1	A	9	SER	4.7
1	A	511	VAL	4.6
1	A	526	ARG	4.6
1	A	56	LYS	4.6
1	A	501	LEU	4.3
2	B	68	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	519	ARG	4.3
1	A	493	LEU	4.3
1	A	213	PHE	4.1
1	A	12	TYR	4.1
1	A	103	MET	4.0
2	B	4	GLN	4.0
1	A	415	ASP	4.0
1	A	104	GLY	4.0
1	A	215	LEU	3.8
1	A	13	GLU	3.7
1	A	496	GLU	3.7
1	A	536	ILE	3.6
1	A	416	ALA	3.5
2	B	6	LYS	3.5
1	A	177	LYS	3.4
1	A	330	ARG	3.4
1	A	500	GLU	3.3
1	A	509	ALA	3.3
1	A	512	ILE	3.3
2	B	5	HIS	3.2
3	C	3	GLU	3.2
1	A	57	ARG	3.2
1	A	528	GLY	3.2
1	A	458	ASP	3.2
3	C	34	GLY	3.1
1	A	122	LEU	3.1
1	A	494	SER	3.0
2	B	39	THR	3.0
1	A	293	THR	3.0
1	A	368	SER	2.9
1	A	532	ALA	2.9
2	B	20	ALA	2.9
1	A	499	PRO	2.8
1	A	277	THR	2.7
1	A	161	TYR	2.7
1	A	510	GLU	2.7
2	B	168	GLU	2.6
1	A	217	GLU	2.6
1	A	86	GLN	2.5
1	A	498	LYS	2.5
1	A	523	ALA	2.5
1	A	506	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	ARG	2.5
1	A	15	TYR	2.5
1	A	503	GLU	2.5
2	B	77	ASN	2.4
2	B	56	THR	2.3
1	A	53	PRO	2.2
1	A	126	ALA	2.2
1	A	507	PRO	2.2
1	A	212	SER	2.2
2	B	74	THR	2.2
1	A	551	GLY	2.2
1	A	428	TRP	2.1
2	B	16	LYS	2.1
2	B	66	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

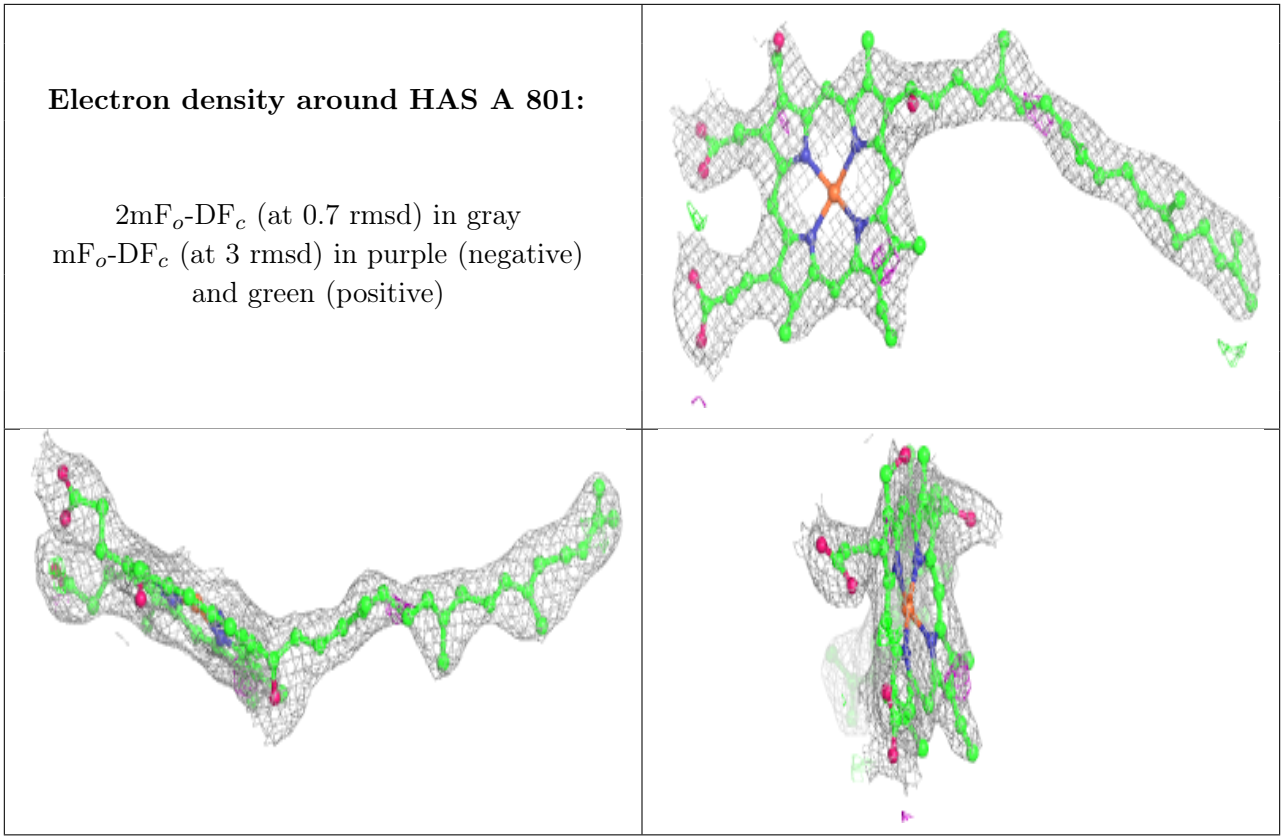
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	HAS	A	801	65/65	0.96	0.14	29,35,45,47	0
5	HEM	A	800	43/43	0.97	0.12	32,37,42,46	0
7	CMO	A	563	2/2	0.99	0.10	36,36,36,46	0
8	CUA	B	802	2/2	0.99	0.03	41,41,41,42	0
4	CU1	A	803	1/1	1.00	0.06	41,41,41,41	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.

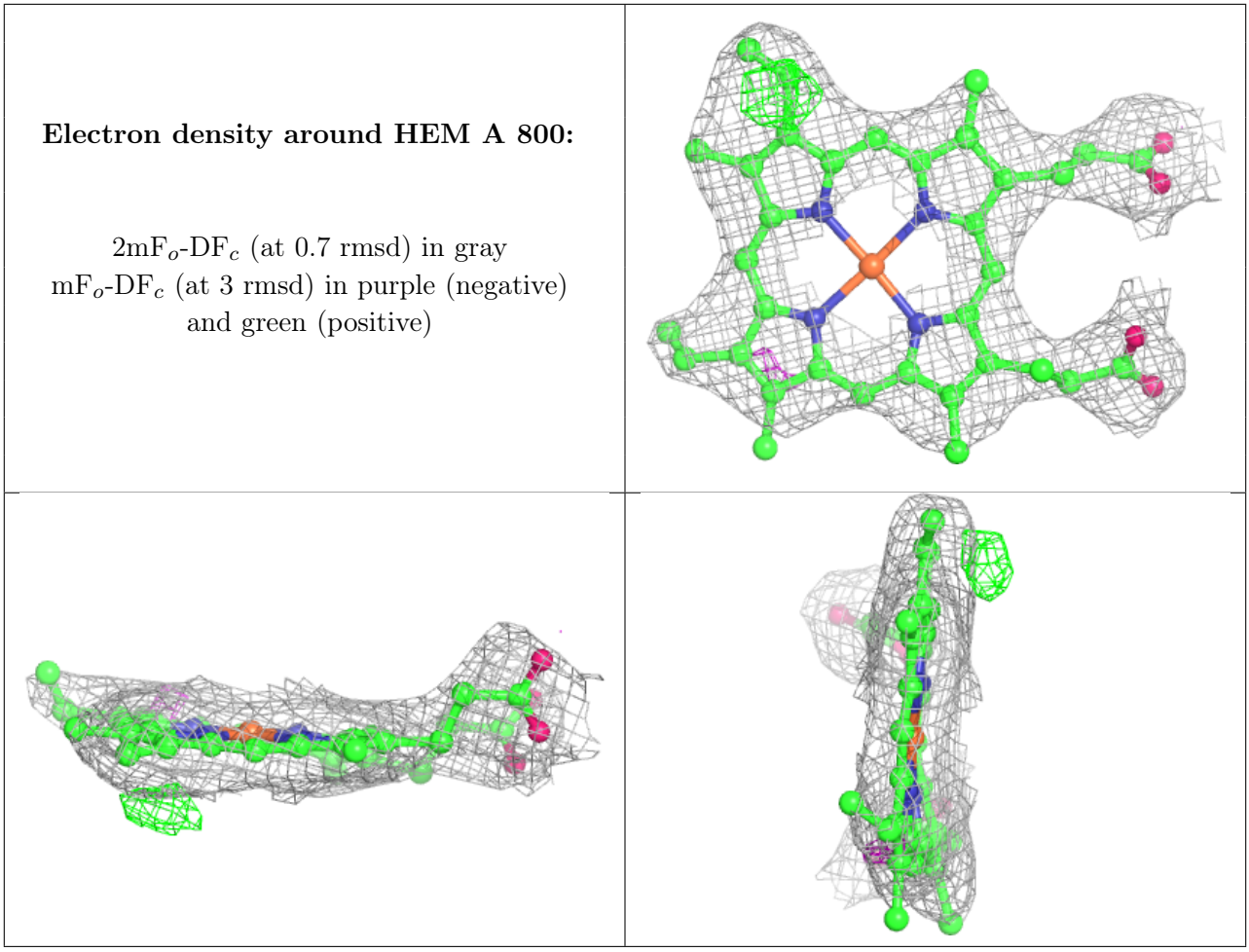
Electron density around HAS A 801:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.