Full wwPDB X-ray Structure Validation Report

May 18, 2020 – 07:15 am BST

PDB ID	:	3WRI
Title	:	Crystal structure of P450cam
Authors	:	Kishimoto, A.; Takagi, K.; Amano, A.; Sakurai, K.; Mizushima, T.; Shimada, H.
Deposited on	:	2014-02-25
Resolution	:	2.90 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:

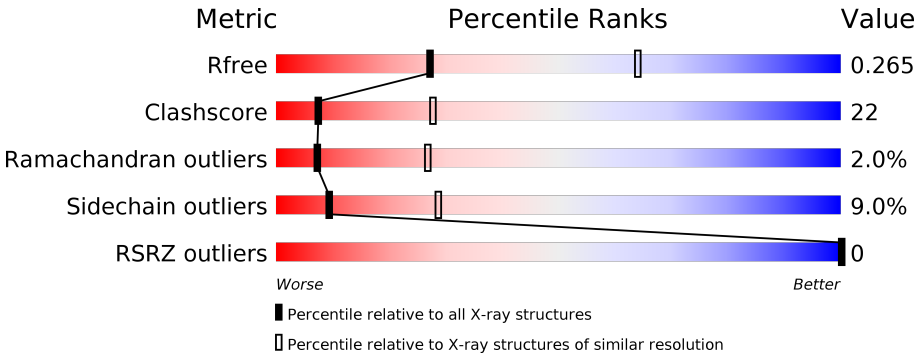
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	421	57% 34% 5% .
1	B	421	57% 34% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6577 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.

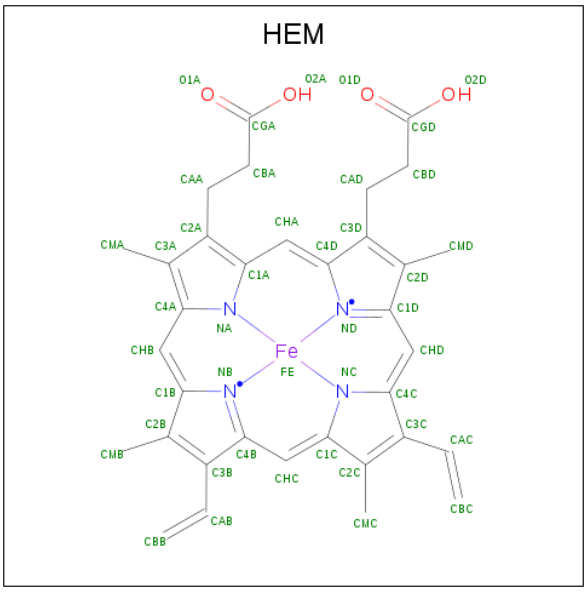
- Molecule 1 is a protein called Camphor 5-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	5	0
			3229	2050	569	591	19			
1	B	403	Total	C	N	O	S	0	8	0
			3231	2054	565	592	20			

There are 12 discrepancies between the modelled and reference sequences:

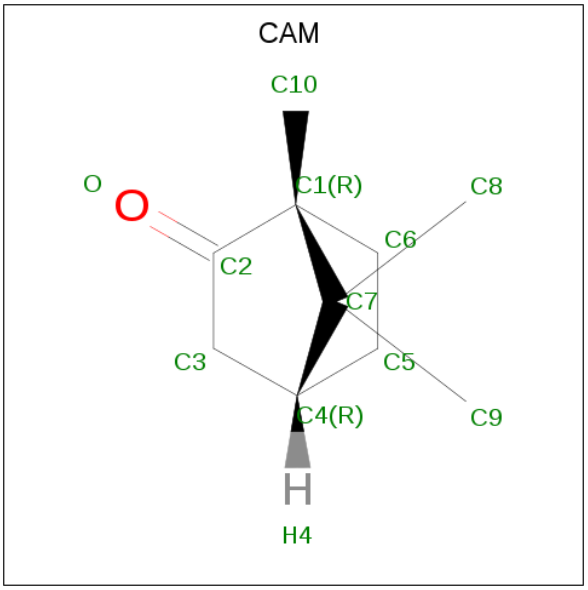
Chain	Residue	Modelled	Actual	Comment	Reference
A	415	HIS	-	EXPRESSION TAG	UNP P00183
A	416	HIS	-	EXPRESSION TAG	UNP P00183
A	417	HIS	-	EXPRESSION TAG	UNP P00183
A	418	HIS	-	EXPRESSION TAG	UNP P00183
A	419	HIS	-	EXPRESSION TAG	UNP P00183
A	420	HIS	-	EXPRESSION TAG	UNP P00183
B	415	HIS	-	EXPRESSION TAG	UNP P00183
B	416	HIS	-	EXPRESSION TAG	UNP P00183
B	417	HIS	-	EXPRESSION TAG	UNP P00183
B	418	HIS	-	EXPRESSION TAG	UNP P00183
B	419	HIS	-	EXPRESSION TAG	UNP P00183
B	420	HIS	-	EXPRESSION TAG	UNP P00183

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CAMPHOR (three-letter code: CAM) (formula: $C_{10}H_{16}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			11	10	1		

- Molecule 4 is water.

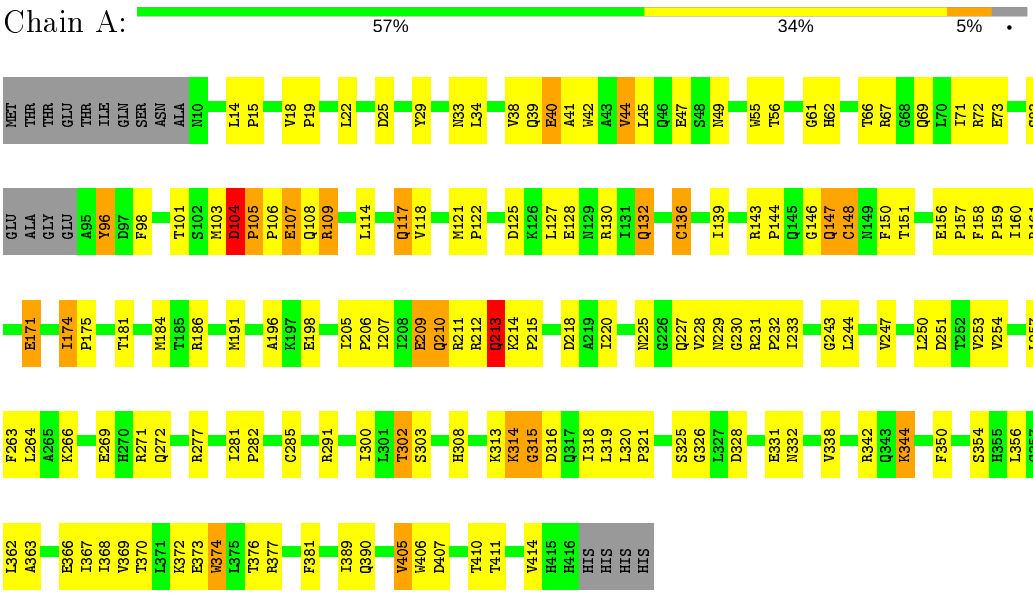
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	1	Total O 1 1	0	0

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.

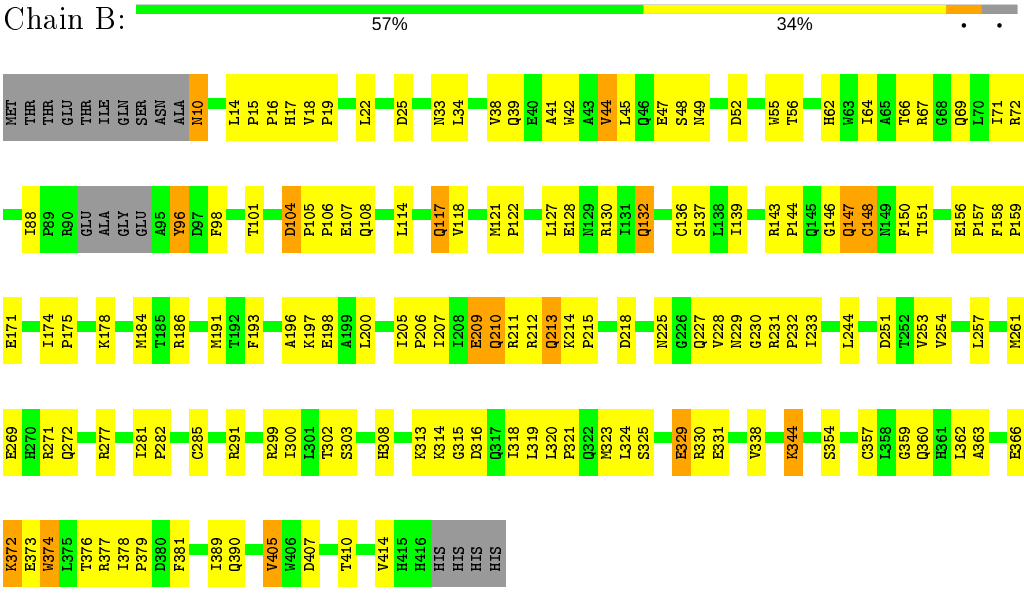
- Molecule 1: Camphor 5-monooxygenase

Chain A:



- Molecule 1: Camphor 5-monooxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.44Å 74.23Å 92.64Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	46.32 – 2.90 46.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.32-2.90) 99.8 (46.32-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117, PHENIX 1.7_650	Depositor
R, R_{free}	0.190 , 0.268 0.183 , 0.265	Depositor DCC
R_{free} test set	954 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 3.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6577	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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, CAM

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	0.62	3/3324 (0.1%)	0.72	1/4513 (0.0%)
1	B	0.62	2/3336 (0.1%)	0.72	1/4530 (0.0%)
All	All	0.62	5/6660 (0.1%)	0.72	2/9043 (0.0%)

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
1	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	TRP	CD2-CE2	5.71	1.48	1.41
1	A	374	TRP	CD2-CE2	5.49	1.48	1.41
1	B	55	TRP	CD2-CE2	5.35	1.47	1.41
1	A	406	TRP	CD2-CE2	5.35	1.47	1.41
1	A	55	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	10	ASN	CB-CA-C	5.31	121.03	110.40
1	A	104	ASP	C-N-CD	-5.23	109.10	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASP	Peptide
1	B	104	ASP	Peptide

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	3229	0	3194	151	0
1	B	3231	0	3200	137	0
2	A	43	0	30	3	0
2	B	43	0	30	7	0
3	A	11	0	16	4	0
3	B	11	0	16	3	0
4	A	8	0	0	1	0
4	B	1	0	0	2	0
All	All	6577	0	6486	290	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 22.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HD2	1:B:344:LYS:O	1.37	1.24
1:A:344:LYS:HD3	1:A:344:LYS:O	1.51	1.10
1:A:105:PRO:N	1:A:106:PRO:HD2	1.67	1.08
1:A:14:LEU:HD11	1:A:18:VAL:HB	1.38	1.02
1:B:41:ALA:O	1:B:44:VAL:HG23	1.62	1.00
1:B:344:LYS:CD	1:B:344:LYS:O	2.13	0.95
1:A:105:PRO:CD	1:A:106:PRO:HD2	1.96	0.95
1:B:14:LEU:HD11	1:B:18:VAL:HB	1.48	0.95
1:A:372:LYS:O	1:A:376:THR:HG23	1.66	0.94
1:A:105:PRO:HD2	1:A:106:PRO:CD	1.98	0.94
1:A:125:ASP:HB3	1:B:48[A]:SER:HB2	1.50	0.94
1:A:125:ASP:HB3	1:B:48[B]:SER:HB2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLN:NE2	1:B:308:HIS:HE1	1.65	0.93
1:A:69:GLN:HE21	1:A:308:HIS:CE1	1.86	0.93
1:B:69:GLN:HE21	1:B:308:HIS:HE1	1.07	0.91
1:A:69:GLN:HE21	1:A:308:HIS:HE1	1.01	0.91
1:B:69:GLN:HE21	1:B:308:HIS:CE1	1.88	0.91
1:A:105:PRO:HD2	1:A:106:PRO:HD3	1.50	0.91
1:A:105:PRO:N	1:A:106:PRO:CD	2.32	0.91
1:A:105:PRO:CD	1:A:106:PRO:CD	2.50	0.90
1:A:69:GLN:NE2	1:A:308:HIS:HE1	1.70	0.89
1:B:372:LYS:O	1:B:376:THR:HG23	1.73	0.89
1:A:41:ALA:O	1:A:44:VAL:CG2	2.22	0.86
1:A:96:TYR:CE2	1:A:98:PHE:HD2	1.93	0.85
1:A:181:THR:HA	1:A:184:MET:CE	2.07	0.84
1:B:281:ILE:CG2	1:B:368:ILE:HG23	2.08	0.84
1:B:96:TYR:CE2	1:B:98:PHE:HD2	1.95	0.83
1:B:41:ALA:O	1:B:44:VAL:CG2	2.25	0.83
1:B:105:PRO:HD2	1:B:106:PRO:CD	2.09	0.82
1:B:281:ILE:HG22	1:B:368:ILE:HG23	1.64	0.77
1:B:105:PRO:HD2	1:B:106:PRO:HD2	1.66	0.77
1:B:14:LEU:HD12	1:B:15:PRO:CD	2.16	0.76
1:B:171:GLU:O	1:B:174:ILE:HG13	1.86	0.76
1:B:407:ASP:OD2	1:B:410:THR:HG23	1.86	0.76
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.68	0.75
1:B:62:HIS:CD2	1:B:88:ILE:HG21	2.22	0.74
1:A:104:ASP:C	1:A:106:PRO:HD2	2.08	0.74
1:A:281:ILE:CG2	1:A:368:ILE:HG23	2.17	0.74
1:A:291:ARG:HG2	1:A:338:VAL:HG22	1.70	0.74
1:A:14:LEU:HD12	1:A:15:PRO:CD	2.17	0.74
1:A:62:HIS:CD2	1:A:88:ILE:HG21	2.23	0.72
1:A:14:LEU:HD12	1:A:15:PRO:N	2.04	0.72
1:A:244:LEU:HD11	3:A:502:CAM:H103	1.71	0.72
1:B:136[A]:CYS:SG	1:B:377:ARG:NH1	2.63	0.72
1:A:407:ASP:OD2	1:A:410:THR:HG23	1.89	0.72
1:A:121:MET:N	1:A:122:PRO:HD2	2.06	0.71
1:A:181:THR:HA	1:A:184:MET:HE2	1.73	0.71
1:A:114:LEU:O	1:A:117:GLN:HB2	1.90	0.71
1:A:147:GLN:HB3	1:A:405:VAL:HG12	1.73	0.70
1:A:164:MET:HG3	1:A:174:ILE:HD13	1.74	0.70
1:A:319:LEU:HG	1:A:321:PRO:HG3	1.75	0.69
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.28	0.69
1:A:41:ALA:O	1:A:44:VAL:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:O	1:A:42:TRP:HD1	1.76	0.68
1:B:121:MET:N	1:B:122:PRO:HD2	2.08	0.68
1:B:105:PRO:CD	1:B:106:PRO:HD2	2.22	0.68
1:B:147:GLN:HB3	1:B:405:VAL:HG12	1.76	0.67
1:B:331:GLU:O	1:B:344:LYS:HE3	1.93	0.67
1:A:331:GLU:O	1:A:344:LYS:HE2	1.94	0.67
1:A:147:GLN:O	1:A:148:CYS:HB3	1.93	0.66
1:B:156:GLU:N	1:B:157:PRO:HD2	2.10	0.66
1:B:357:CYS:SG	2:B:501:HEM:FE	1.86	0.66
1:A:350:PHE:O	1:A:356:LEU:HD12	1.96	0.66
1:B:17:HIS:ND1	4:B:601:HOH:O	2.29	0.66
1:B:147:GLN:O	1:B:148:CYS:HB3	1.96	0.65
1:B:105:PRO:HD2	1:B:106:PRO:HD3	1.80	0.64
1:A:132:GLN:OE1	1:A:373:GLU:OE2	2.16	0.64
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.33	0.64
1:B:14:LEU:HD12	1:B:15:PRO:N	2.13	0.64
1:A:125:ASP:CB	1:B:48[A]:SER:HB2	2.26	0.63
1:A:125:ASP:CB	1:B:48[B]:SER:HB2	2.26	0.63
1:B:184[B]:MET:HG2	1:B:193:PHE:CE1	2.34	0.63
1:A:181:THR:HA	1:A:184:MET:HE3	1.81	0.62
1:B:38:VAL:O	1:B:42:TRP:HD1	1.82	0.62
2:B:501:HEM:NA	3:B:502:CAM:H51	2.14	0.62
1:A:156:GLU:N	1:A:157:PRO:HD2	2.14	0.62
1:A:263:PHE:CE1	1:A:338:VAL:HG21	2.35	0.62
1:A:344:LYS:CD	1:A:344:LYS:O	2.39	0.62
1:B:263:PHE:CE1	1:B:338:VAL:HG21	2.35	0.62
1:A:96:TYR:CD1	1:A:96:TYR:C	2.73	0.62
1:A:14:LEU:HD12	1:A:15:PRO:HD2	1.81	0.61
1:B:42:TRP:O	1:B:45:LEU:HD12	2.00	0.61
1:B:16:PRO:HG2	4:B:601:HOH:O	1.99	0.61
1:B:158:PHE:HB3	1:B:159:PRO:HD3	1.83	0.61
1:B:229:ASN:C	1:B:231:ARG:H	2.04	0.61
1:B:132:GLN:OE1	1:B:373:GLU:OE2	2.17	0.61
1:A:313:LYS:O	1:A:316:ASP:HB2	2.00	0.61
1:B:14:LEU:HD12	1:B:15:PRO:HD2	1.81	0.61
1:A:363:ALA:O	1:A:367:ILE:HD12	2.00	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.82	0.61
1:A:41:ALA:O	1:A:44:VAL:HG23	2.01	0.60
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.83	0.60
1:A:14:LEU:HD11	1:A:18:VAL:CB	2.24	0.60
1:B:191:MET:HE1	1:B:196:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:C1A	3:A:502:CAM:H51	2.37	0.60
1:B:96:TYR:CD1	1:B:96:TYR:C	2.74	0.60
1:B:344:LYS:CD	1:B:344:LYS:C	2.70	0.59
1:B:132:GLN:O	1:B:136[B]:CYS:SG	2.59	0.59
1:B:291:ARG:HG2	1:B:338:VAL:HG22	1.84	0.59
1:B:62:HIS:CD2	1:B:88:ILE:HD13	2.38	0.59
1:A:45:LEU:HB3	1:A:66:THR:HG22	1.84	0.58
1:B:319:LEU:HG	1:B:321:PRO:HG3	1.85	0.58
1:A:104:ASP:HB3	1:A:105:PRO:HD3	1.85	0.58
1:B:313:LYS:O	1:B:316:ASP:HB2	2.03	0.58
1:A:96:TYR:CE2	1:A:98:PHE:CD2	2.85	0.58
1:A:205:ILE:O	1:A:209:GLU:HG2	2.04	0.58
1:A:156:GLU:H	1:A:157:PRO:HD2	1.68	0.58
1:A:62:HIS:CD2	1:A:88:ILE:HD13	2.38	0.58
1:B:244:LEU:HD11	3:B:502:CAM:H103	1.86	0.58
1:A:132:GLN:O	1:A:136[B]:CYS:SG	2.60	0.57
2:B:501:HEM:C1A	3:B:502:CAM:H51	2.38	0.57
1:B:150:PHE:CE1	1:B:261:MET:HG3	2.38	0.57
1:B:363:ALA:O	1:B:367:ILE:HD12	2.04	0.57
1:A:229:ASN:C	1:A:231:ARG:H	2.06	0.57
1:A:300:ILE:HG13	1:A:316:ASP:O	2.05	0.57
1:B:206:PRO:O	1:B:210:GLN:HB2	2.03	0.57
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.85	0.57
1:B:14:LEU:HD11	1:B:18:VAL:CB	2.30	0.57
1:A:25:ASP:HA	1:A:56:THR:OG1	2.06	0.56
1:B:105:PRO:CD	1:B:106:PRO:CD	2.80	0.56
1:B:105:PRO:N	1:B:106:PRO:HD2	2.21	0.56
1:A:271:ARG:HD2	1:A:381:PHE:CE1	2.41	0.56
1:B:62:HIS:HD2	1:B:88:ILE:HG21	1.70	0.56
1:A:186:ARG:NH1	1:A:251:ASP:OD2	2.39	0.56
1:B:205:ILE:O	1:B:209:GLU:HG2	2.06	0.56
1:A:212:ARG:HA	1:A:225:ASN:HD21	1.71	0.55
1:A:213:GLN:OE1	1:A:213:GLN:HA	2.05	0.55
1:A:314:LYS:O	1:A:316:ASP:N	2.39	0.55
1:A:136[A]:CYS:SG	1:A:377:ARG:NH1	2.79	0.55
1:B:96:TYR:CE2	1:B:98:PHE:CD2	2.86	0.55
1:B:104:ASP:O	1:B:106:PRO:HD2	2.06	0.55
1:A:49:ASN:N	1:A:49:ASN:OD1	2.39	0.55
2:A:501:HEM:HBA1	3:A:502:CAM:H31	1.89	0.55
1:A:104:ASP:O	1:A:106:PRO:HD2	2.06	0.55
1:A:39:GLN:O	1:A:42:TRP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLN:NE2	1:B:308:HIS:CE1	2.56	0.55
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.89	0.54
1:B:25:ASP:HA	1:B:56:THR:HG1	1.71	0.54
1:B:212:ARG:HA	1:B:225:ASN:HD21	1.73	0.54
1:A:29:TYR:OH	1:A:88:ILE:O	2.21	0.54
1:A:171:GLU:O	1:A:174:ILE:HG12	2.08	0.54
1:B:369:VAL:O	1:B:370:THR:C	2.45	0.54
1:A:72:ARG:NH2	1:A:331:GLU:OE2	2.36	0.53
1:B:228:VAL:HG13	1:B:231:ARG:NH2	2.24	0.53
1:A:127:LEU:O	1:A:128:GLU:C	2.47	0.53
1:A:229:ASN:O	1:A:231:ARG:N	2.41	0.53
1:B:271:ARG:HD2	1:B:381:PHE:CE1	2.44	0.53
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.90	0.53
1:B:156:GLU:H	1:B:157:PRO:HD2	1.72	0.53
1:B:231:ARG:NH1	1:B:232:PRO:O	2.41	0.53
1:A:45:LEU:HB3	1:A:66:THR:CG2	2.39	0.52
1:A:132:GLN:OE1	1:A:373:GLU:CD	2.48	0.52
1:A:314:LYS:C	1:A:316:ASP:H	2.13	0.52
1:B:281:ILE:HG21	1:B:368:ILE:HG23	1.87	0.52
1:A:191:MET:HE1	1:A:196:ALA:HA	1.91	0.52
1:B:72:ARG:NH2	1:B:331:GLU:OE2	2.39	0.52
1:A:147:GLN:HB3	1:A:405:VAL:CG1	2.39	0.52
1:A:250:LEU:O	1:A:254:VAL:HG23	2.10	0.52
1:A:257:LEU:HD22	1:A:370:THR:HG21	1.92	0.51
1:A:67:ARG:O	1:A:71:ILE:HG13	2.10	0.51
1:B:300:ILE:HG13	1:B:316:ASP:O	2.10	0.51
1:A:164:MET:HG3	1:A:174:ILE:CD1	2.38	0.51
1:B:229:ASN:O	1:B:231:ARG:N	2.42	0.51
1:B:127:LEU:O	1:B:128:GLU:C	2.46	0.51
1:A:314:LYS:HG3	1:A:315:GLY:N	2.25	0.51
1:A:210:GLN:OE1	1:A:210:GLN:HA	2.11	0.51
1:B:121:MET:N	1:B:122:PRO:CD	2.74	0.51
1:B:156:GLU:N	1:B:157:PRO:CD	2.73	0.50
1:B:49:ASN:OD1	1:B:49:ASN:N	2.45	0.50
1:A:211:ARG:HH21	1:A:218:ASP:CG	2.15	0.50
1:A:121:MET:N	1:A:122:PRO:CD	2.74	0.50
1:A:150:PHE:CE1	1:A:261:MET:HG3	2.46	0.50
1:A:62:HIS:HD2	1:A:88:ILE:HG21	1.72	0.50
1:B:314:LYS:HG3	1:B:315:GLY:N	2.27	0.50
1:A:228:VAL:HG13	1:A:231:ARG:NH2	2.27	0.50
1:B:104:ASP:C	1:B:106:PRO:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PRO:O	1:A:161:ARG:HD2	2.11	0.50
1:A:231:ARG:NH1	1:A:232:PRO:O	2.45	0.50
1:A:211:ARG:O	1:A:214:LYS:O	2.30	0.49
1:B:45:LEU:HB3	1:B:66:THR:HG22	1.94	0.49
1:A:228:VAL:O	1:A:228:VAL:HG13	2.12	0.49
1:B:157:PRO:O	1:B:161:ARG:HD2	2.12	0.49
1:B:147:GLN:HE21	1:B:147:GLN:C	2.16	0.49
1:A:358:LEU:HD12	2:A:501:HEM:HMD1	1.94	0.49
1:B:143:ARG:HB3	1:B:144:PRO:HD3	1.94	0.49
1:B:207:ILE:O	1:B:211:ARG:HG3	2.12	0.49
1:A:42:TRP:O	1:A:45:LEU:HD12	2.12	0.48
1:A:114:LEU:O	1:A:117:GLN:CB	2.60	0.48
1:A:326:GLY:HA2	1:A:332:ASN:ND2	2.29	0.48
1:B:211:ARG:HH21	1:B:218:ASP:CG	2.16	0.48
1:B:25:ASP:HA	1:B:56:THR:OG1	2.13	0.48
1:A:171:GLU:O	1:A:174:ILE:CG1	2.62	0.48
1:B:19:PRO:HG2	1:B:22:LEU:HD12	1.95	0.48
1:A:314:LYS:HG3	1:A:315:GLY:H	1.79	0.47
1:A:139:ILE:HG12	1:A:374:TRP:CE3	2.50	0.47
1:A:160:ILE:HG23	1:A:161:ARG:N	2.30	0.47
1:B:263:PHE:CD2	1:B:263:PHE:C	2.87	0.47
1:B:45:LEU:HB3	1:B:66:THR:CG2	2.44	0.47
1:A:69:GLN:HG3	4:A:608:HOH:O	2.14	0.47
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.96	0.47
1:A:359:GLY:O	1:A:360:GLN:C	2.53	0.47
1:B:314:LYS:C	1:B:316:ASP:H	2.18	0.47
1:B:362:LEU:HG	1:B:366:GLU:OE1	2.14	0.47
1:B:67:ARG:O	1:B:71:ILE:HG13	2.14	0.47
1:B:233:ILE:O	1:B:233:ILE:HG23	2.15	0.47
1:A:331:GLU:O	1:A:344:LYS:CE	2.61	0.46
1:B:64:ILE:HG23	1:B:319:LEU:HD23	1.96	0.46
1:A:271:ARG:HD2	1:A:381:PHE:CZ	2.51	0.46
1:B:210:GLN:HA	1:B:210:GLN:OE1	2.15	0.46
1:B:33:ASN:O	1:B:34:LEU:C	2.54	0.46
1:A:243:GLY:O	1:A:247:VAL:HG13	2.15	0.46
1:A:108:GLN:HE22	1:A:354:SER:CB	2.28	0.46
1:B:318:ILE:HG12	1:B:320:LEU:HG	1.98	0.46
1:A:38:VAL:O	1:A:42:TRP:CD1	2.64	0.45
1:B:359:GLY:O	1:B:360:GLN:C	2.54	0.45
1:B:378:ILE:N	1:B:379:PRO:HD3	2.31	0.45
1:A:263:PHE:CD2	1:A:263:PHE:C	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:HD22	1:B:33:ASN:HA	1.56	0.45
1:B:146:GLY:O	1:B:405:VAL:HA	2.17	0.45
1:B:211:ARG:O	1:B:214:LYS:O	2.34	0.45
1:A:207:ILE:O	1:A:211:ARG:HG3	2.16	0.45
1:A:147:GLN:C	1:A:147:GLN:HE21	2.20	0.45
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.46	0.45
1:A:211:ARG:NH2	1:A:218:ASP:CG	2.70	0.45
1:B:186:ARG:NH1	1:B:251:ASP:OD2	2.50	0.45
1:B:96:TYR:HE2	1:B:98:PHE:HD2	1.58	0.45
1:B:108:GLN:HE22	1:B:354:SER:CB	2.30	0.45
1:A:156:GLU:N	1:A:157:PRO:CD	2.80	0.44
1:B:257:LEU:HD22	1:B:370:THR:HG21	1.99	0.44
1:A:318:ILE:HG12	1:A:320:LEU:HG	2.00	0.44
1:A:33:ASN:HD22	1:A:33:ASN:HA	1.59	0.44
1:B:209:GLU:H	1:B:209:GLU:HG2	1.56	0.44
1:B:227:GLN:HE22	1:B:232:PRO:HG3	1.83	0.44
1:A:105:PRO:O	1:A:109[A]:ARG:HG3	2.18	0.44
1:B:39:GLN:O	1:B:42:TRP:N	2.50	0.44
1:A:96:TYR:HE2	1:A:98:PHE:HD2	1.60	0.44
1:B:314:LYS:O	1:B:316:ASP:N	2.51	0.44
1:B:331:GLU:O	1:B:344:LYS:CE	2.63	0.43
1:A:253:VAL:O	1:A:254:VAL:C	2.57	0.43
1:A:281:ILE:HG21	1:A:368:ILE:HG23	1.97	0.43
1:B:303:SER:HA	1:B:314:LYS:HB2	2.00	0.43
1:A:14:LEU:C	1:A:14:LEU:HD12	2.38	0.43
1:A:262:GLU:HG2	1:A:266:LYS:HE3	2.01	0.43
1:A:39:GLN:O	1:A:41:ALA:N	2.52	0.43
1:B:114:LEU:O	1:B:117:GLN:HB2	2.19	0.43
1:B:213:GLN:OE1	1:B:213:GLN:HA	2.18	0.43
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.86	0.43
1:B:197:LYS:O	1:B:200:LEU:HB3	2.19	0.43
1:B:271:ARG:HD2	1:B:381:PHE:CZ	2.54	0.43
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.83	0.43
1:A:269:GLU:O	1:A:272:GLN:HB3	2.19	0.42
1:B:108:GLN:HE22	1:B:354:SER:HB2	1.83	0.42
1:A:174:ILE:O	1:A:175:PRO:C	2.57	0.42
1:B:114:LEU:O	1:B:117:GLN:CB	2.66	0.42
1:B:34:LEU:HD12	1:B:34:LEU:HA	1.64	0.42
1:B:160:ILE:HG23	1:B:161:ARG:N	2.34	0.42
1:B:52:ASP:OD1	1:B:330:ARG:NH2	2.51	0.42
1:A:362:LEU:HG	1:A:366:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLN:NE2	1:A:308:HIS:CE1	2.62	0.42
1:A:233:ILE:HG23	1:A:233:ILE:O	2.20	0.42
1:B:139:ILE:HG12	1:B:374:TRP:CE3	2.54	0.42
1:B:329:GLU:HG3	1:B:329:GLU:H	1.49	0.42
1:B:244:LEU:HD23	2:B:501:HEM:HMD3	2.01	0.42
1:A:39:GLN:O	1:A:40:GLU:C	2.58	0.42
1:A:143:ARG:NH1	1:A:411:THR:OG1	2.50	0.42
1:B:147:GLN:HB3	1:B:405:VAL:CG1	2.46	0.42
1:B:174:ILE:O	1:B:175:PRO:C	2.56	0.42
1:A:146:GLY:O	1:A:405:VAL:HA	2.19	0.42
1:A:369:VAL:O	1:A:370:THR:C	2.57	0.42
1:A:244:LEU:CD1	3:A:502:CAM:H103	2.43	0.41
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.62	0.41
1:B:82:SER:O	1:B:299:ARG:HB3	2.20	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.82	0.41
1:A:302:THR:O	1:A:303:SER:HB3	2.21	0.41
1:B:229:ASN:C	1:B:231:ARG:N	2.72	0.41
1:A:67:ARG:NH1	1:A:328:ASP:OD1	2.43	0.41
1:B:253:VAL:O	1:B:254:VAL:C	2.58	0.41
1:B:228:VAL:HG13	1:B:228:VAL:O	2.20	0.41
1:A:69:GLN:O	1:A:73:GLU:HB2	2.21	0.41
1:A:56:THR:O	1:A:61:GLY:HA2	2.21	0.41
1:A:107:GLU:H	1:A:107:GLU:HG2	1.58	0.41
1:B:69:GLN:O	1:B:73:GLU:HB2	2.21	0.41
1:A:227:GLN:HE22	1:A:232:PRO:HG3	1.85	0.40
1:A:218:ASP:OD2	1:A:220:ILE:N	2.55	0.40
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.82	0.40
1:A:260:SER:O	1:A:264:LEU:HG	2.22	0.40
1:A:332:ASN:HB3	1:A:342:ARG:NH1	2.37	0.40
1:B:269:GLU:O	1:B:272:GLN:HB3	2.21	0.40
1:B:132:GLN:OE1	1:B:373:GLU:CD	2.60	0.40
1:B:244:LEU:CD2	2:B:501:HEM:HMD3	2.52	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	404/421 (96%)	355 (88%)	39 (10%)	10 (2%)	5 21
1	B	407/421 (97%)	352 (86%)	49 (12%)	6 (2%)	10 34
All	All	811/842 (96%)	707 (87%)	88 (11%)	16 (2%)	7 27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	215	PRO
1	B	213	GLN
1	B	215	PRO
1	A	230	GLY
1	B	230	GLY
1	B	325	SER
1	A	40	GLU
1	A	148	CYS
1	A	171	GLU
1	A	314	LYS
1	A	315	GLY
1	B	148	CYS
1	B	282	PRO
1	A	282	PRO
1	A	105	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	354/365 (97%)	322 (91%)	32 (9%)	9 29
1	B	356/365 (98%)	323 (91%)	33 (9%)	9 27
All	All	710/730 (97%)	645 (91%)	65 (9%)	9 27

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	47	GLU
1	A	83	SER
1	A	96	TYR
1	A	101	THR
1	A	103	MET
1	A	107	GLU
1	A	109[A]	ARG
1	A	109[B]	ARG
1	A	117	GLN
1	A	118	VAL
1	A	130	ARG
1	A	132	GLN
1	A	136[A]	CYS
1	A	136[B]	CYS
1	A	147	GLN
1	A	151	THR
1	A	166	LEU
1	A	174	ILE
1	A	198	GLU
1	A	209	GLU
1	A	210	GLN
1	A	213	GLN
1	A	277	ARG
1	A	285	CYS
1	A	302	THR
1	A	325	SER
1	A	344	LYS
1	A	389	ILE
1	A	390	GLN
1	A	405	VAL
1	A	414	VAL
1	B	10	ASN
1	B	44	VAL
1	B	47	GLU
1	B	84	GLU
1	B	96	TYR
1	B	101	THR
1	B	107	GLU
1	B	117	GLN
1	B	118	VAL
1	B	130	ARG

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Mol	Chain	Res	Type
1	B	132	GLN
1	B	137	SER
1	B	147	GLN
1	B	151	THR
1	B	161	ARG
1	B	166	LEU
1	B	178	LYS
1	B	198	GLU
1	B	209	GLU
1	B	210	GLN
1	B	263	PHE
1	B	267	SER
1	B	277	ARG
1	B	285	CYS
1	B	302	THR
1	B	323	MET
1	B	329	GLU
1	B	344	LYS
1	B	372	LYS
1	B	389	ILE
1	B	390	GLN
1	B	405	VAL
1	B	414	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	33	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN
1	A	145	GLN
1	A	147	GLN
1	A	225	ASN
1	A	227	GLN
1	A	255	ASN
1	A	308	HIS
1	A	317	GLN
1	B	30	ASN
1	B	33	ASN

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Mol	Chain	Res	Type
1	B	59	ASN
1	B	69	GLN
1	B	108	GLN
1	B	110	GLN
1	B	145	GLN
1	B	147	GLN
1	B	225	ASN
1	B	227	GLN
1	B	255	ASN
1	B	308	HIS
1	B	317	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CAM	A	502	-	12,12,12	1.02	1 (8%)	20,21,21	1.25	2 (10%)
2	HEM	B	501	-	27,50,50	2.43	10 (37%)	17,82,82	2.62	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CAM	B	502	-	12,12,12	1.00	1 (8%)	20,21,21	1.00	0
2	HEM	A	501	1	27,50,50	2.30	9 (33%)	17,82,82	2.79	6 (35%)

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	CAM	A	502	-	-	-	0/3/2/2
2	HEM	B	501	-	-	0/6/54/54	-
3	CAM	B	502	-	-	-	0/3/2/2
2	HEM	A	501	1	-	0/6/54/54	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1A-NA	5.79	1.48	1.36
2	A	501	HEM	C1A-NA	5.57	1.47	1.36
2	A	501	HEM	C3C-C2C	5.51	1.48	1.40
2	B	501	HEM	C3C-C2C	5.31	1.47	1.40
2	B	501	HEM	C3B-C2B	4.84	1.47	1.40
2	B	501	HEM	C4A-NA	4.61	1.45	1.36
2	A	501	HEM	C3B-C2B	4.44	1.46	1.40
2	A	501	HEM	C4A-NA	3.75	1.43	1.36
2	B	501	HEM	C1B-C2B	3.05	1.49	1.42
2	A	501	HEM	C1C-C2C	2.97	1.49	1.42
2	B	501	HEM	C1C-C2C	2.90	1.49	1.42
2	A	501	HEM	C2A-C3A	2.87	1.46	1.37
2	B	501	HEM	C2A-C3A	2.86	1.46	1.37
2	A	501	HEM	C3D-C2D	2.83	1.46	1.37
2	B	501	HEM	C4D-C3D	2.81	1.48	1.42
2	B	501	HEM	C3D-C2D	2.81	1.46	1.37
2	A	501	HEM	C4D-C3D	2.39	1.48	1.42
2	B	501	HEM	C1D-CHD	2.33	1.47	1.41
2	A	501	HEM	C1B-C2B	2.26	1.47	1.42
3	A	502	CAM	C7-C1	-2.14	1.50	1.56
3	B	502	CAM	C7-C1	-2.01	1.50	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1D-C2D-C3D	-6.68	102.35	107.00
2	B	501	HEM	C3B-C4B-NB	5.54	116.37	109.21
2	B	501	HEM	C1D-C2D-C3D	-5.38	103.26	107.00
2	A	501	HEM	C3B-C4B-NB	4.96	115.63	109.21
2	A	501	HEM	CMB-C2B-C3B	4.07	132.29	124.68
2	B	501	HEM	CMC-C2C-C3C	3.86	131.90	124.68
2	A	501	HEM	CAA-CBA-CGA	-3.67	106.51	112.67
2	A	501	HEM	CMC-C2C-C3C	3.62	131.46	124.68
2	B	501	HEM	CMB-C2B-C3B	3.55	131.32	124.68
2	B	501	HEM	C4A-C3A-C2A	-3.41	104.63	107.00
3	A	502	CAM	C9-C7-C8	2.85	114.81	107.62
2	B	501	HEM	CBA-CAA-C2A	-2.47	107.92	112.49
3	A	502	CAM	C10-C1-C2	2.14	117.81	108.99
2	A	501	HEM	C4A-C3A-C2A	-2.09	105.55	107.00

There are no chirality outliers.

There are no torsion outliers.

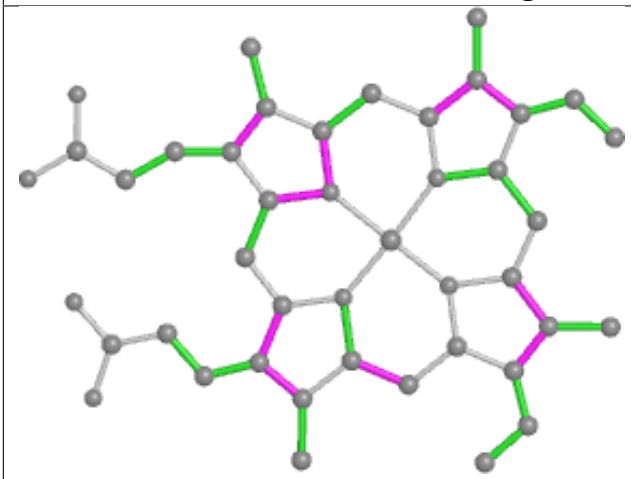
There are no ring outliers.

4 monomers are involved in 13 short contacts:

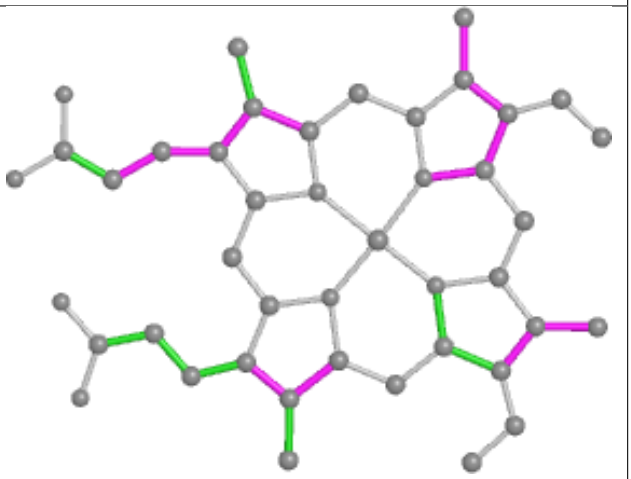
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CAM	4	0
2	B	501	HEM	7	0
3	B	502	CAM	3	0
2	A	501	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

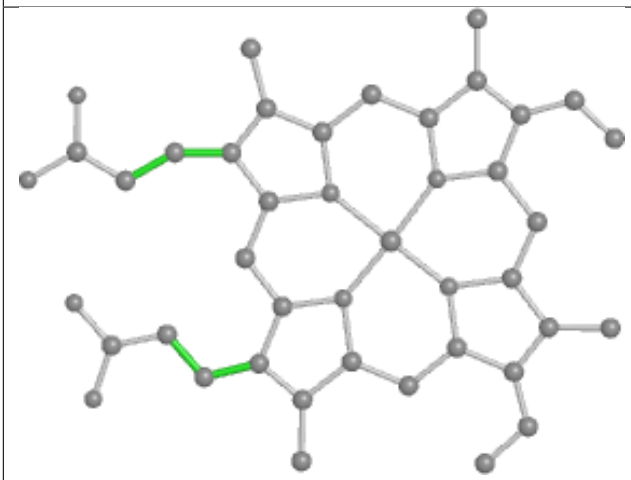
Ligand HEM B 501



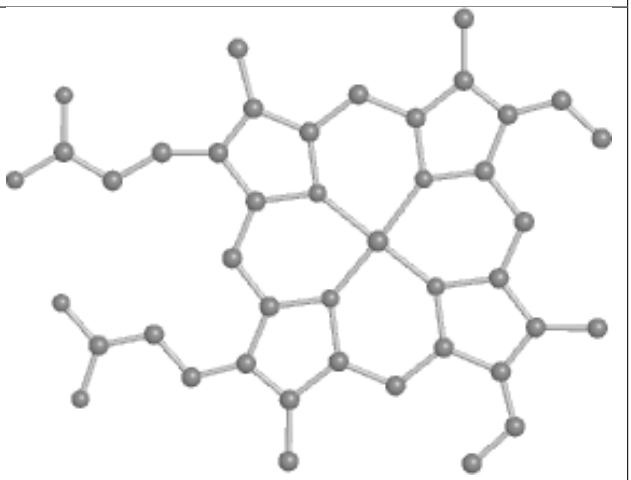
Bond lengths



Bond angles

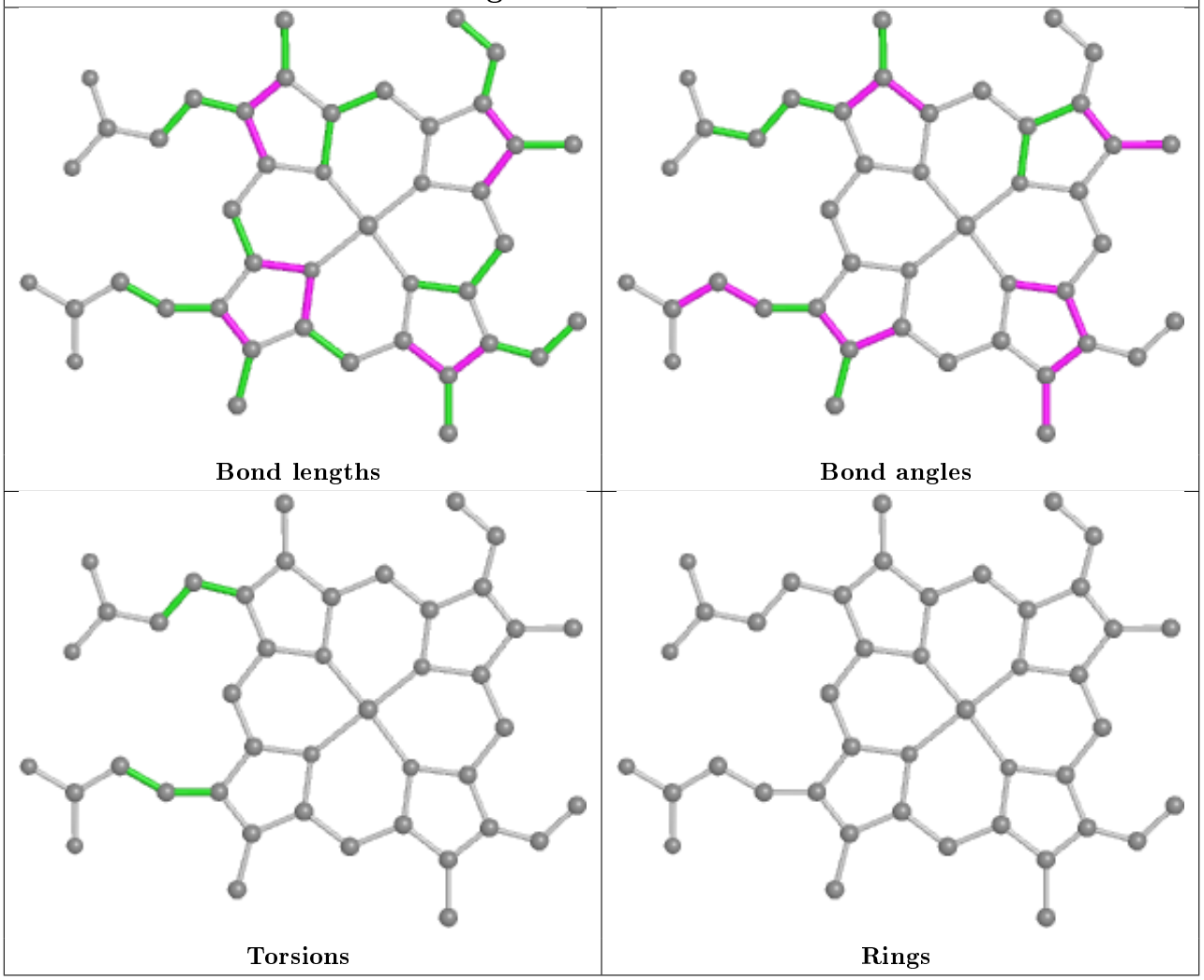


Torsions



Rings

Ligand HEM A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	403/421 (95%)	-0.70	0	100	100	15, 35, 63, 95	0
1	B	403/421 (95%)	-0.70	0	100	100	16, 34, 64, 94	0
All	All	806/842 (95%)	-0.70	0	100	100	15, 35, 64, 95	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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.

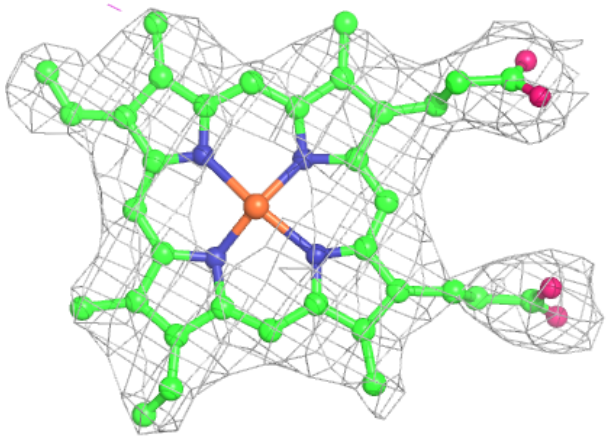
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CAM	A	502	11/11	0.94	0.30	18,19,25,30	11
3	CAM	B	502	11/11	0.95	0.28	17,20,29,31	11
2	HEM	A	501	43/43	0.98	0.13	9,16,25,31	0
2	HEM	B	501	43/43	0.99	0.15	7,16,25,27	0

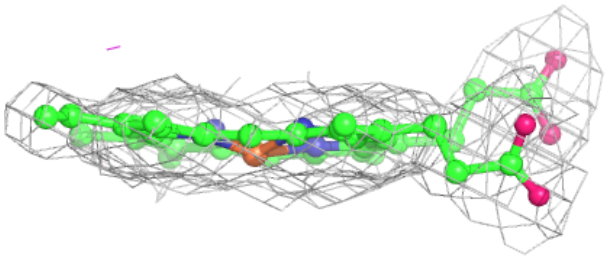
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

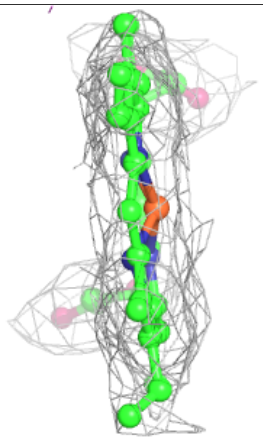
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 501:

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

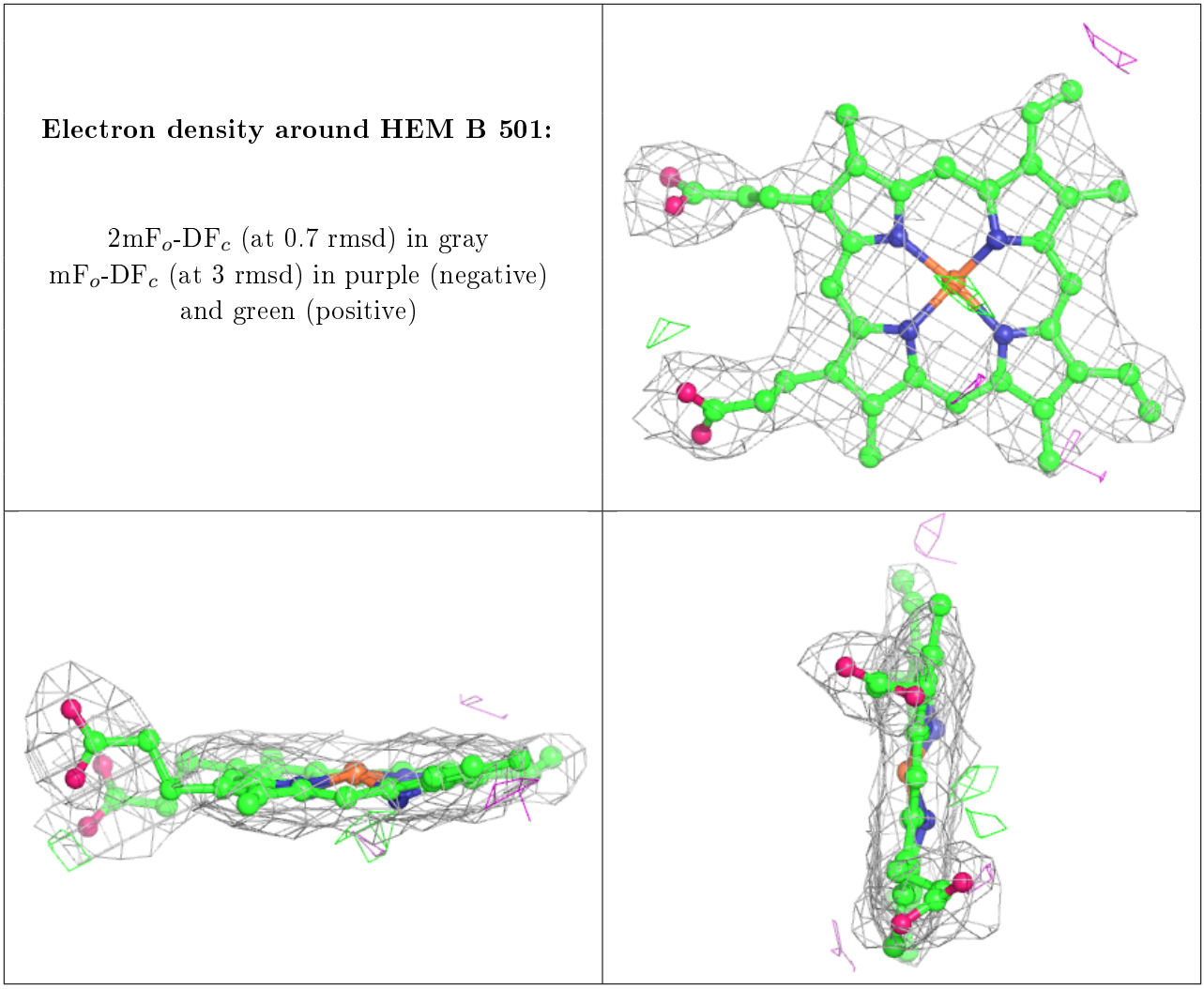






Electron density around HEM B 501:

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



6.5 Other polymers

There are no such residues in this entry.