



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 AM GMT

PDB ID : 2BVJ
Title : LIGAND-FREE STRUCTURE OF CYTOCHROME P450 PIKC
(CYP107L1)
Authors : Sherman, D.H.; Li, S.; Yermalitskaya, L.V.; Kim, Y.; Smith, J.A.; Waterman,
M.R.; Podust, L.M.
Deposited on : 2005-06-28
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

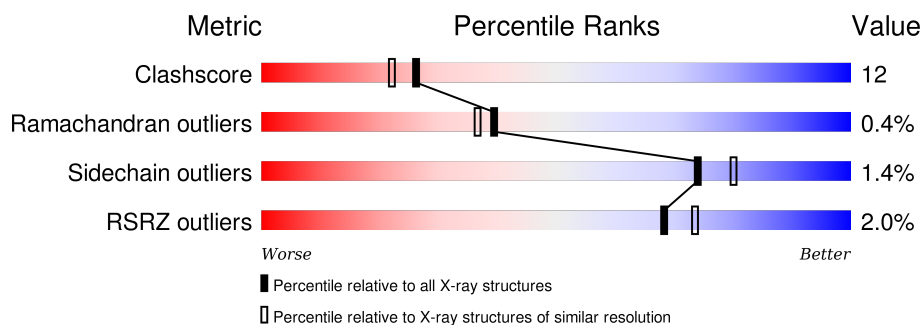
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	436	
1	B	436	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BME	A	1409	-	-	X	-
3	BME	B	1409	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	A	1410	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6463 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 P450 MONOOXYGENASE.

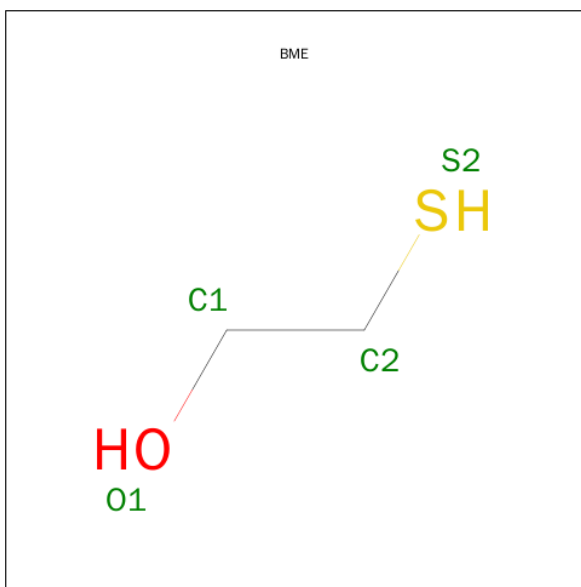
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	1
			3039	1916	549	561	13			
1	B	392	Total	C	N	O	S	0	0	1
			3007	1897	545	553	12			

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



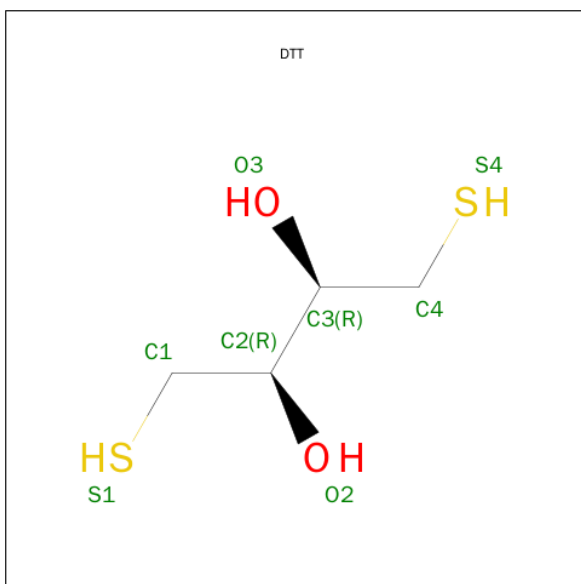
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $\text{C}_4\text{H}_{10}\text{O}_2\text{S}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

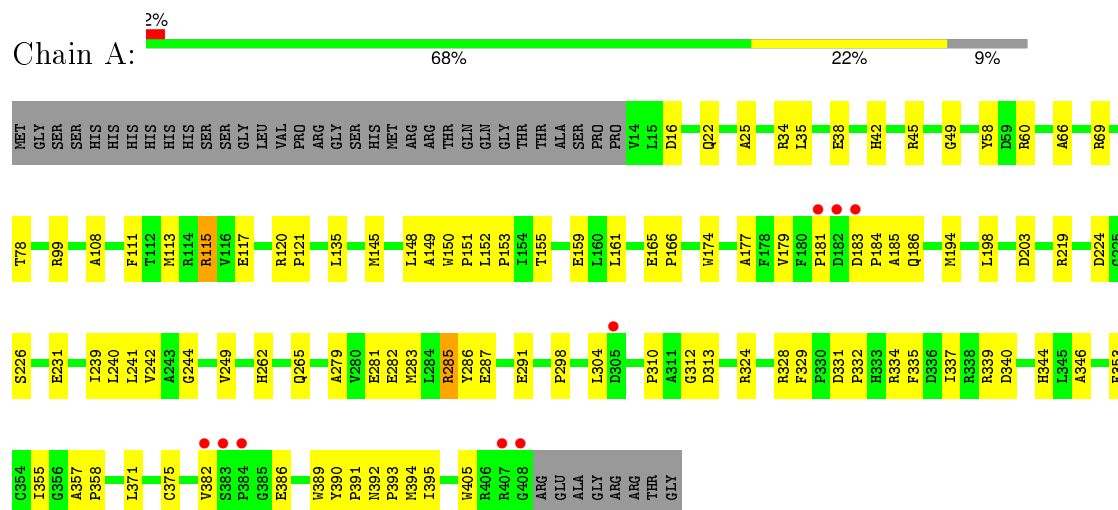
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total 144	O 144	0	0
5	B	171	Total 171	O 171	0	0

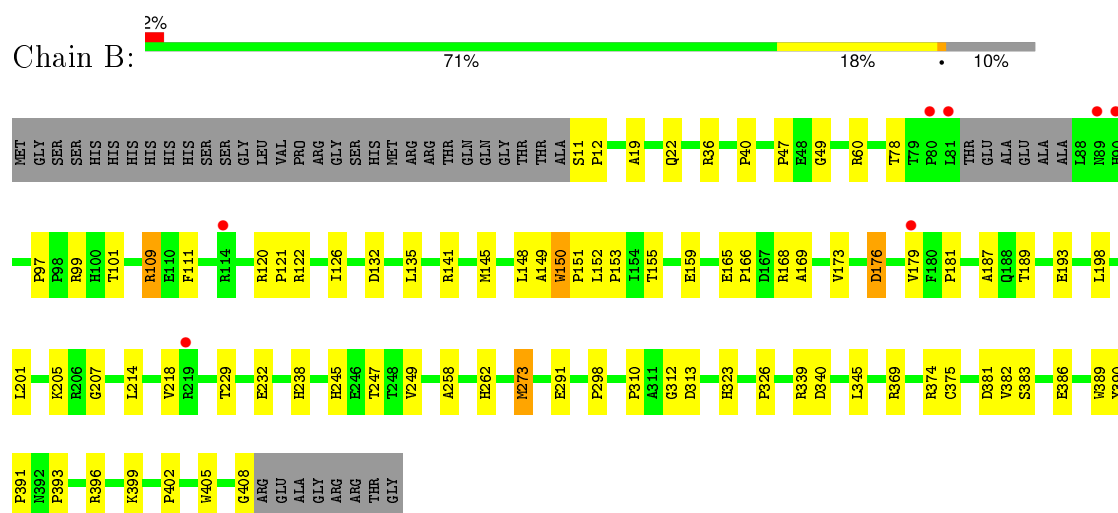
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 P450 MONOOXYGENASE



• Molecule 1: CYTOCHROME P450 MONOOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.19Å 64.17Å 73.59Å 90.00° 107.15° 90.00°	Depositor
Resolution (Å)	36.98 – 2.10 48.35 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (36.98-2.10) 94.4 (48.35-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.243 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55909 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6463	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, DTT, BME

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	0.31	0/3109	0.55	0/4245
1	B	0.31	0/3078	0.56	0/4203
All	All	0.31	0/6187	0.55	0/8448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3039	0	2998	91	0
1	B	3007	0	2949	64	0
2	A	43	0	30	4	0
2	B	43	0	30	0	0
3	A	4	0	6	3	1
3	B	4	0	6	4	1
4	A	8	0	10	0	0
5	A	144	0	0	6	0
5	B	171	0	0	8	0
All	All	6463	0	6029	150	2

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 12.

All (150) 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:334:ARG:HE	1:A:335:PHE:H	1.15	0.94
1:B:323:HIS:HE1	1:B:345:LEU:H	1.06	0.91
1:A:45:ARG:HE	1:A:49:GLY:HA2	1.34	0.90
1:B:22:GLN:HE22	1:B:389:TRP:H	1.26	0.83
1:A:334:ARG:HE	1:A:335:PHE:N	1.75	0.83
1:A:329:PHE:O	1:A:332:PRO:HG3	1.79	0.82
1:A:113:MET:HE2	5:B:2008:HOH:O	1.81	0.80
1:B:375:CYS:SG	3:B:1409:BME:S2	2.83	0.76
1:A:135:LEU:HD21	1:A:375:CYS:SG	2.26	0.76
1:B:323:HIS:HE1	1:B:345:LEU:N	1.84	0.74
1:A:334:ARG:HA	1:A:334:ARG:NE	2.05	0.71
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.73	0.71
1:B:323:HIS:CE1	1:B:345:LEU:H	1.99	0.70
1:A:262:HIS:NE2	1:A:334:ARG:NH2	2.40	0.70
1:A:183:ASP:HB3	1:A:186:GLN:HG2	1.73	0.69
1:B:145:MET:HA	1:B:149:ALA:HB3	1.75	0.69
1:B:135:LEU:HD13	3:B:1409:BME:H22	1.74	0.68
1:B:153:PRO:HB2	1:B:245:HIS:HD2	1.58	0.68
1:A:45:ARG:HE	1:A:49:GLY:CA	2.06	0.67
1:A:161:LEU:HD13	1:A:241:LEU:HG	1.75	0.67
1:A:344:HIS:HD2	1:A:346:ALA:H	1.44	0.66
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.78	0.66
1:B:165:GLU:HB3	1:B:166:PRO:HD3	1.77	0.65
1:B:141:ARG:HD3	1:B:381:ASP:OD2	1.96	0.65
1:A:224:ASP:OD1	1:A:226:SER:HB3	1.96	0.64
1:A:16:ASP:HA	1:A:45:ARG:HB3	1.79	0.64
1:A:334:ARG:NE	1:A:335:PHE:H	1.90	0.64
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.12	0.62
1:B:393:PRO:HG3	5:B:2163:HOH:O	1.99	0.62
1:A:115:ARG:CZ	1:B:181:PRO:HG2	2.30	0.62
1:B:11:SER:N	1:B:12:PRO:HD3	2.15	0.61
1:A:331:ASP:N	1:A:332:PRO:HD3	2.15	0.61
1:B:258:ALA:O	1:B:262:HIS:HD2	1.84	0.61
1:B:179:VAL:C	1:B:181:PRO:HD3	2.21	0.61
1:A:334:ARG:HD3	5:A:2118:HOH:O	2.02	0.58
1:A:183:ASP:OD2	1:A:185:ALA:HB3	2.03	0.58
1:B:132:ASP:OD1	1:B:374:ARG:NH2	2.36	0.58
1:A:120:ARG:HD3	5:A:2052:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLY:HA2	2:A:1408:HEM:HAC	1.85	0.57
1:A:58:TYR:CD2	1:A:328:ARG:HG3	2.40	0.57
1:B:201:LEU:O	1:B:205:LYS:HG2	2.05	0.56
1:B:214:LEU:O	1:B:218:VAL:HG23	2.06	0.56
1:A:405:TRP:CD1	3:A:1409:BME:H22	2.40	0.56
1:A:285:ARG:NH2	1:A:332:PRO:O	2.27	0.56
1:A:395:ILE:HD12	1:A:395:ILE:N	2.21	0.55
1:A:174:TRP:CE3	1:A:194:MET:HG3	2.42	0.55
1:A:334:ARG:CA	1:A:334:ARG:NE	2.69	0.55
1:A:375:CYS:HA	3:A:1409:BME:S2	2.47	0.55
1:A:244:GLY:HA2	2:A:1408:HEM:CAC	2.36	0.55
1:A:265:GLN:NE2	1:A:337:ILE:H	2.05	0.55
1:B:339:ARG:HG2	1:B:340:ASP:N	2.23	0.54
1:B:165:GLU:HA	1:B:168:ARG:HG2	1.89	0.53
1:A:66:ALA:HA	5:A:2128:HOH:O	2.08	0.53
1:B:148:LEU:O	1:B:151:PRO:HD2	2.09	0.53
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.91	0.53
1:B:36:ARG:HH12	1:B:326:PRO:HD3	1.73	0.53
1:A:22:GLN:HE22	1:A:389:TRP:H	1.57	0.53
1:A:111:PHE:CE2	2:A:1408:HEM:HBC1	2.44	0.52
1:A:265:GLN:NE2	1:A:337:ILE:HG12	2.23	0.52
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.74	0.52
1:B:122:ARG:NH1	1:B:159:GLU:OE1	2.43	0.52
1:B:383:SER:OG	1:B:386:GLU:HG3	2.09	0.52
1:A:194:MET:HE1	1:A:242:VAL:CG2	2.40	0.52
1:A:113:MET:HE3	5:B:2006:HOH:O	2.10	0.51
1:B:141:ARG:NH1	1:B:381:ASP:OD1	2.44	0.51
1:B:382:VAL:HG22	1:B:402:PRO:HG2	1.93	0.51
1:A:35:LEU:HB3	1:A:42:HIS:CD2	2.46	0.51
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.77	0.50
1:A:194:MET:HE2	1:A:198:LEU:HD11	1.92	0.50
1:B:179:VAL:O	1:B:181:PRO:HD3	2.12	0.50
1:B:150:TRP:CD1	1:B:249:VAL:HG11	2.46	0.50
1:A:310:PRO:HG2	1:A:313:ASP:CG	2.32	0.50
1:A:334:ARG:HA	1:A:334:ARG:CZ	2.42	0.50
1:A:34:ARG:O	1:A:38:GLU:HG3	2.12	0.50
1:B:40:PRO:CB	1:B:60:ARG:HG3	2.43	0.49
1:A:145:MET:HA	1:A:149:ALA:HB3	1.94	0.49
1:B:374:ARG:O	3:B:1409:BME:H21	2.12	0.49
1:B:291:GLU:OE2	1:B:396:ARG:HD2	2.12	0.48
1:B:122:ARG:HA	1:B:122:ARG:NE	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:THR:HG22	5:B:2060:HOH:O	2.12	0.48
1:A:155:THR:O	1:A:159:GLU:HG3	2.13	0.48
1:A:99:ARG:NH2	5:A:2031:HOH:O	2.46	0.48
1:A:45:ARG:NH1	1:A:45:ARG:HG2	2.28	0.48
1:B:78:THR:HG21	5:B:2123:HOH:O	2.13	0.48
1:A:177:ALA:O	1:A:181:PRO:HB3	2.14	0.48
1:A:60:ARG:HD2	1:A:304:LEU:HD22	1.96	0.47
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.95	0.47
1:A:183:ASP:OD1	1:A:184:PRO:HD2	2.13	0.47
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.95	0.47
1:A:174:TRP:CZ3	1:A:194:MET:HG3	2.48	0.47
1:B:78:THR:HG23	1:B:312:GLY:HA3	1.96	0.47
1:B:189:THR:O	1:B:193:GLU:HG3	2.14	0.47
1:A:353:PHE:CD2	1:B:49:GLY:HA3	2.50	0.47
1:B:323:HIS:HD2	5:B:2114:HOH:O	1.97	0.47
1:A:394:MET:HB2	1:A:395:ILE:HD12	1.97	0.47
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.95	0.47
1:B:126:ILE:HD13	1:B:155:THR:HG22	1.97	0.47
1:A:344:HIS:CD2	1:A:346:ALA:H	2.28	0.46
1:B:273:MET:HG2	1:B:369:ARG:NH1	2.30	0.46
1:A:282:GLU:OE1	1:A:285:ARG:HD3	2.16	0.46
1:A:113:MET:HE3	1:B:47:PRO:HB3	1.98	0.46
1:A:231:GLU:HG2	5:A:2025:HOH:O	2.16	0.45
1:B:245:HIS:HB3	5:B:2100:HOH:O	2.15	0.45
1:B:198:LEU:HD12	1:B:238:HIS:CE1	2.52	0.45
1:A:25:ALA:HB2	1:A:391:PRO:HA	1.99	0.45
1:A:334:ARG:NE	1:A:335:PHE:N	2.53	0.45
1:B:405:TRP:HB2	3:B:1409:BME:S2	2.57	0.45
1:A:265:GLN:HE21	1:A:337:ILE:H	1.63	0.45
1:A:148:LEU:C	1:A:151:PRO:HD2	2.37	0.44
1:A:150:TRP:HA	1:A:249:VAL:HG22	1.99	0.44
1:A:240:LEU:O	1:A:244:GLY:HA3	2.18	0.44
1:B:22:GLN:NE2	1:B:389:TRP:H	2.05	0.44
1:A:405:TRP:HB2	3:A:1409:BME:S2	2.58	0.44
1:B:310:PRO:HG2	1:B:313:ASP:OD2	2.18	0.44
1:A:194:MET:HE1	1:A:242:VAL:HG23	2.00	0.44
1:A:78:THR:HG23	1:A:312:GLY:HA3	1.99	0.44
1:B:390:TYR:CE1	1:B:399:LYS:HA	2.53	0.44
1:A:244:GLY:HA2	2:A:1408:HEM:C3C	2.53	0.43
1:B:408:GLY:N	5:B:2171:HOH:O	2.51	0.43
1:B:99:ARG:HH11	1:B:99:ARG:HG3	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HG23	1:A:240:LEU:N	2.33	0.43
1:A:382:VAL:CG2	1:A:386:GLU:HB2	2.48	0.43
1:B:298:PRO:HD2	1:B:313:ASP:O	2.19	0.43
1:B:40:PRO:HB3	1:B:60:ARG:HG3	2.00	0.43
1:B:109:ARG:O	1:B:109:ARG:HG2	2.17	0.43
1:A:291:GLU:HB3	1:A:393:PRO:O	2.18	0.43
1:B:148:LEU:C	1:B:151:PRO:HD2	2.39	0.42
1:B:150:TRP:HZ3	1:B:176:ASP:OD1	2.00	0.42
1:B:150:TRP:HD1	1:B:249:VAL:HG11	1.85	0.42
1:A:117:GLU:HG2	1:B:391:PRO:HD2	2.02	0.42
1:B:229:THR:OG1	1:B:232:GLU:HG3	2.20	0.42
1:A:281:GLU:HG3	1:B:19:ALA:HB1	2.02	0.42
1:A:161:LEU:CD1	1:A:241:LEU:HG	2.45	0.42
1:A:392:ASN:HB2	5:A:2142:HOH:O	2.19	0.41
1:A:281:GLU:OE1	1:A:344:HIS:HE1	2.03	0.41
1:A:324:ARG:HA	1:A:332:PRO:HB3	2.02	0.41
1:A:69:ARG:O	1:A:298:PRO:HA	2.21	0.41
1:A:339:ARG:HG2	1:A:340:ASP:N	2.34	0.41
1:A:331:ASP:N	1:A:332:PRO:CD	2.83	0.41
1:B:165:GLU:OE1	1:B:168:ARG:HG3	2.21	0.41
1:A:108:ALA:HA	1:A:355:ILE:HD11	2.02	0.41
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.86	0.41
1:A:390:TYR:HA	1:A:391:PRO:HD3	1.88	0.41
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.35	0.40
1:A:286:TYR:CD2	1:A:287:GLU:HG2	2.57	0.40
1:A:371:LEU:O	1:A:375:CYS:HB2	2.21	0.40
1:B:97:PRO:HB3	1:B:101:THR:OG1	2.20	0.40
1:A:279:ALA:O	1:A:283:MET:HG3	2.21	0.40
1:B:120:ARG:N	1:B:121:PRO:HD2	2.36	0.40
1:B:169:ALA:O	1:B:173:VAL:HG23	2.22	0.40

All (2) 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)
3:A:1409:BME:C1	3:A:1409:BME:C1[2_556]	1.58	0.62
3:B:1409:BME:C1	3:B:1409:BME:C1[2_557]	1.77	0.43

5.3 Torsion angles

5.3.1 Protein backbone

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	393/436 (90%)	377 (96%)	15 (4%)	1 (0%)	46	45
1	B	388/436 (89%)	372 (96%)	14 (4%)	2 (0%)	34	30
All	All	781/872 (90%)	749 (96%)	29 (4%)	3 (0%)	39	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ALA
1	A	179	VAL
1	B	207	GLY

5.3.2 Protein sidechains

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	314/355 (88%)	310 (99%)	4 (1%)	76	82
1	B	309/355 (87%)	304 (98%)	5 (2%)	70	76
All	All	623/710 (88%)	614 (99%)	9 (1%)	74	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	203	ASP
1	A	219	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	ARG
1	B	109	ARG
1	B	111	PHE
1	B	150	TRP
1	B	176	ASP
1	B	273	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	238	HIS
1	A	265	GLN
1	A	344	HIS
1	B	22	GLN
1	B	124	GLN
1	B	238	HIS
1	B	245	HIS
1	B	262	HIS
1	B	323	HIS

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](#)

5 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
2	HEM	A	1408	1,5	30,50,50	2.86	12 (40%)	24,82,82	1.99	6 (25%)
3	BME	A	1409	-	3,3,3	0.92	0	2,2,2	0.86	0
4	DTT	A	1410	-	7,7,7	0.63	0	4,8,8	1.77	1 (25%)
2	HEM	B	1408	1,5	30,50,50	2.80	11 (36%)	24,82,82	2.10	6 (25%)
3	BME	B	1409	-	3,3,3	0.49	0	2,2,2	0.89	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
2	HEM	A	1408	1,5	-	0/10/54/54	0/0/8/8
3	BME	A	1409	-	-	0/1/1/1	0/0/0/0
4	DTT	A	1410	-	-	0/8/8/8	0/0/0/0
2	HEM	B	1408	1,5	-	0/10/54/54	0/0/8/8
3	BME	B	1409	-	-	0/1/1/1	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1408	HEM	C2D-C3D	-6.67	1.34	1.54
2	A	1408	HEM	C2D-C3D	-6.59	1.34	1.54
2	B	1408	HEM	C3B-C4B	-6.46	1.46	1.51
2	A	1408	HEM	C3C-CAC	-6.34	1.39	1.51
2	B	1408	HEM	C3C-CAC	-6.05	1.40	1.51
2	A	1408	HEM	C3B-CAB	-6.04	1.40	1.51
2	B	1408	HEM	C3B-CAB	-5.99	1.40	1.51
2	A	1408	HEM	C3B-C4B	-5.87	1.46	1.51
2	A	1408	HEM	C3D-C4D	-5.12	1.45	1.51
2	B	1408	HEM	C2C-C1C	-4.34	1.44	1.52
2	B	1408	HEM	C3D-C4D	-3.24	1.47	1.51
2	A	1408	HEM	C2C-C1C	-3.15	1.46	1.52
2	A	1408	HEM	C2D-C1D	-2.14	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1408	HEM	C2B-C1B	-2.02	1.45	1.51
2	B	1408	HEM	CHD-C4C	2.02	1.41	1.36
2	A	1408	HEM	CBB-CAB	2.42	1.43	1.29
2	B	1408	HEM	CBC-CAC	2.54	1.44	1.29
2	B	1408	HEM	CBB-CAB	2.68	1.44	1.29
2	B	1408	HEM	C4C-NC	2.72	1.39	1.36
2	A	1408	HEM	CBC-CAC	2.88	1.45	1.29
2	B	1408	HEM	C1C-NC	3.07	1.39	1.36
2	A	1408	HEM	C4C-NC	3.37	1.40	1.36
2	A	1408	HEM	C1C-NC	3.38	1.40	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1410	DTT	C2-C1-S1	-2.94	109.04	113.91
2	B	1408	HEM	CMD-C2D-C3D	2.66	126.11	114.35
2	B	1408	HEM	C2D-C3D-C4D	2.74	106.14	101.50
2	A	1408	HEM	CMD-C2D-C3D	3.08	127.99	114.35
2	A	1408	HEM	CMC-C2C-C3C	3.11	124.30	116.53
2	A	1408	HEM	C2D-C3D-C4D	3.37	107.21	101.50
2	A	1408	HEM	CAD-C3D-C4D	3.93	126.32	112.47
2	B	1408	HEM	CAD-C3D-C2D	4.17	125.20	113.22
2	A	1408	HEM	CMB-C2B-C3B	4.39	127.49	116.53
2	B	1408	HEM	CAD-C3D-C4D	4.54	128.48	112.47
2	B	1408	HEM	CMC-C2C-C3C	4.56	127.92	116.53
2	A	1408	HEM	CAD-C3D-C2D	4.59	126.40	113.22
2	B	1408	HEM	CMB-C2B-C3B	4.61	128.04	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1408	HEM	4	0
3	A	1409	BME	3	1
3	B	1409	BME	4	1

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	395/436 (90%)	0.06	9 (2%) 64 70	14, 27, 47, 65	0
1	B	392/436 (89%)	0.04	7 (1%) 71 76	15, 25, 50, 61	0
All	All	787/872 (90%)	0.05	16 (2%) 68 73	14, 26, 48, 65	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	GLY	5.8
1	A	181	PRO	3.6
1	A	384	PRO	3.5
1	B	81	LEU	3.2
1	A	407	ARG	2.8
1	A	383	SER	2.6
1	A	182	ASP	2.6
1	B	80	PRO	2.5
1	B	89	ASN	2.4
1	A	382	VAL	2.2
1	B	179	VAL	2.1
1	A	183	ASP	2.1
1	B	90	HIS	2.1
1	B	219	ARG	2.0
1	A	305	ASP	2.0
1	B	114	ARG	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	DTT	A	1410	8/8	0.53	0.30	10.78	48,52,58,69	0
3	BME	B	1409	4/4	0.53	0.19	4.98	58,60,62,67	0
2	HEM	A	1408	43/43	0.97	0.13	0.58	15,17,22,25	0
3	BME	A	1409	4/4	0.89	0.13	0.10	47,47,48,50	0
2	HEM	B	1408	43/43	0.97	0.11	0.07	12,16,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.