



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:58 AM GMT

PDB ID : 4AC5
Title : Lipidic sponge phase crystal structure of the Bl. viridis reaction centre solved using serial femtosecond crystallography
Authors : Johansson, L.C.; Arnlund, D.; White, T.A.; Katona, G.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Shoeman, R.L.; Lomb, L.; Malmerberg, E.; Davidsson, J.; Nass, K.; Liang, M.; Andreasson, J.; Aquila, A.; Bajt, S.; Barthelmess, M.; Barty, A.; Bogan, M.J.; Bostedt, C.; Bozek, J.D.; Caleman, C.; Coffee, R.; Coppola, N.; Ekeberg, T.; Epp, S.W.; Erk, B.; Fleckenstein, H.; Foucar, L.; Graafsma, H.; Gumprecht, L.; Hajdu, J.; Hampton, C.Y.; Hartmann, R.; Hartmann, A.; Hauser, G.; Hirsemann, H.; Holl, P.; Hunter, M.S.; Kassemeyer, S.; Kimmel, N.; Kirian, R.A.; Maia, F.R.N.C.; Marchesini, S.; Martin, A.V.; Reich, C.; Rolles, D.; Rudek, B.; Rudenko, A.; Schlichting, I.; Schulz, J.; Seibert, M.M.; Sierra, R.; Soltau, H.; Starodub, D.; Stellato, F.; Stern, S.; Struder, L.; Timneanu, N.; Ullrich, J.; Wahlgren, W.Y.; Wang, X.; Weidenspointner, G.; Wunderer, C.; Fromme, P.; Chapman, H.N.; Spence, J.C.H.; Neutze, R.
Deposited on : 2011-12-14
Resolution : 8.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

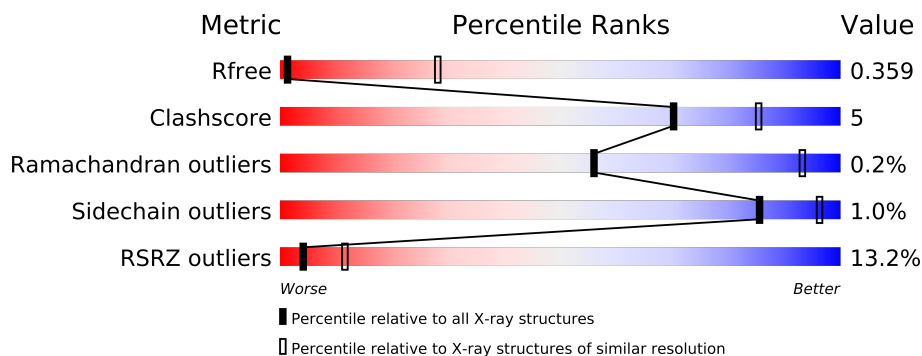
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)

1 Overall quality at a glance

The reported resolution of this entry is 8.20 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}	66092	1106 (11.50-3.50)
Clashscore	79885	1008 (12.70-3.54)
Ramachandran outliers	78287	1303 (12.70-3.50)
Sidechain outliers	78261	1277 (12.70-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	336	
2	H	258	
3	L	274	
4	M	324	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	NS5	M	1329	-	X
5	HEM	C	1334	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
6	BCB	L	1275	-	X
7	BPB	L	1276	-	X
7	BPB	M	1326	-	X
9	MQ7	M	1328	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9835 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2590	1632	464	476	18			

- Molecule 2 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	243	Total	C	N	O	S	0	0	0
			1886	1209	326	349	2			

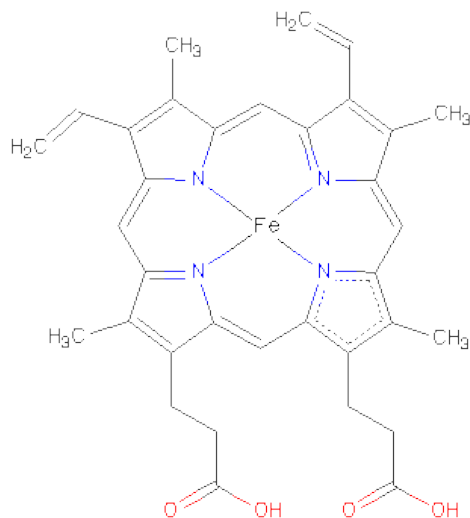
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	0	0
			2161	1452	350	352	7			

- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

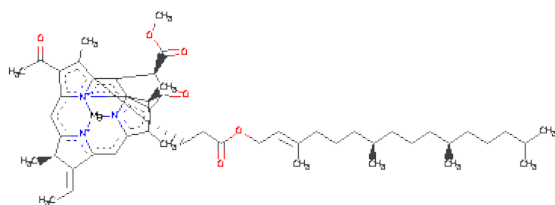
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

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



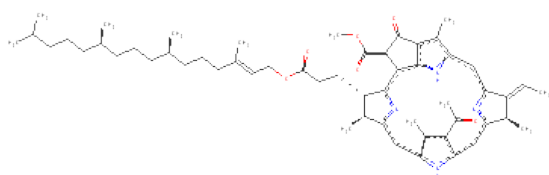
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
6	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
6	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).

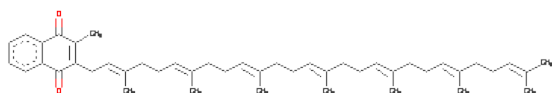


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

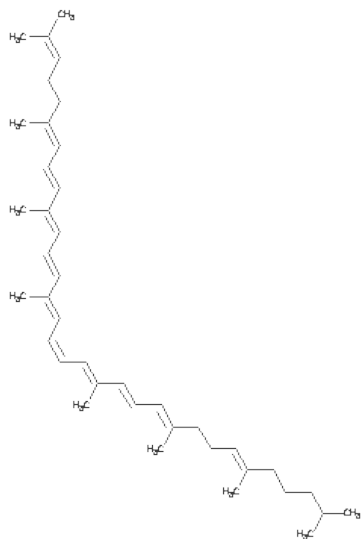
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 10 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).

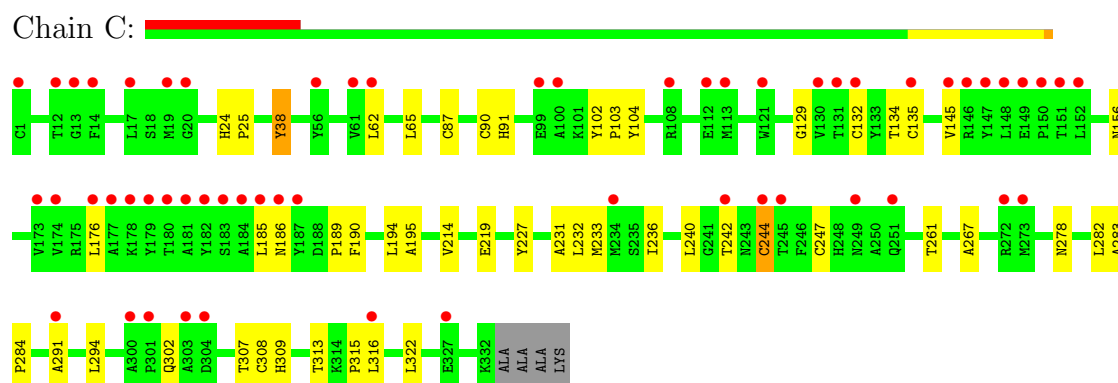


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	C	0	0
			40	40		

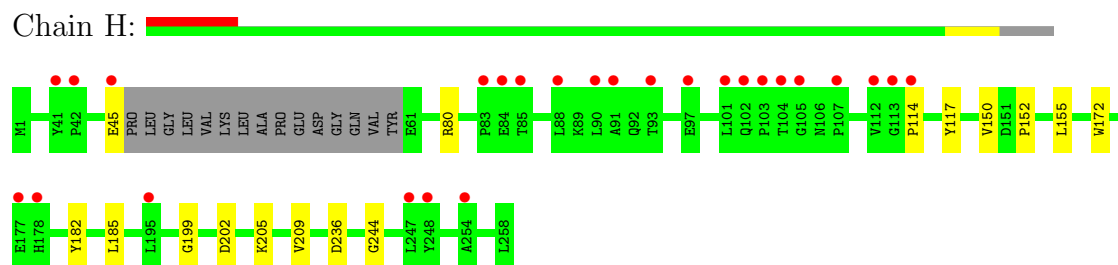
3 Residue-property plots

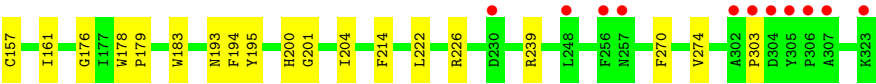
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



• Molecule 2: REACTION CENTER PROTEIN H CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.50Å 84.60Å 375.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 8.20 56.84 – 8.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.10-8.20) 97.2 (56.84-8.20)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 8.36Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.351 , 0.384 0.352 , 0.359	Depositor DCC
R_{free} test set	95 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	-2.7	Xtriage
Anisotropy	-13.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 147.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 1992 reflections	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPB, BCB, FE2, MQ7, HEM, FME, NS5

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	C	0.31	0/2657	0.46	0/3624
2	H	0.32	0/1919	0.46	0/2621
3	L	0.34	0/2248	0.42	0/3069
4	M	0.33	0/2652	0.40	0/3630
All	All	0.33	0/9476	0.44	0/12944

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2590	0	2561	34	0
2	H	1886	0	1880	8	0
3	L	2161	0	2089	16	0
4	M	2548	0	2432	22	0
5	C	172	0	120	10	0
6	L	132	0	144	12	0
6	M	131	0	140	5	0
7	L	65	0	74	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	61	0	63	1	0
8	M	1	0	0	0	0
9	M	48	0	64	0	0
10	M	40	0	60	3	0
All	All	9835	0	9627	90	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:M:1325:BCB:HAA1	6:M:1325:BCB:HBD	1.62	0.80
1:C:247:CYS:SG	5:C:1335:HEM:HAC	2.24	0.78
1:C:308:CYS:SG	5:C:1336:HEM:HAC	2.25	0.76
7:L:1276:BPB:HHC	7:L:1276:BPB:HBBB	1.69	0.73
3:L:239:ASN:HA	3:L:242:LEU:HB2	1.76	0.66
4:M:176:GLY:H	10:M:1329:NS5:H14	1.60	0.65
1:C:176:LEU:HD21	1:C:186:ASN:HA	1.78	0.64
3:L:130:VAL:HA	3:L:134:PHE:HB2	1.80	0.62
1:C:278:ASN:HA	1:C:282:LEU:HB2	1.82	0.62
3:L:179:PHE:HA	3:L:182:VAL:HG12	1.81	0.62
6:M:1325:BCB:HAA1	6:M:1325:BCB:CBD	2.29	0.61
6:L:1275:BCB:OBD	4:M:201:GLY:HA2	1.99	0.61
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.82	0.61
1:C:244:CYS:SG	5:C:1335:HEM:HAB	2.41	0.61
3:L:132:GLN:OE1	3:L:145:ALA:HB1	2.03	0.57
4:M:77:VAL:HG13	4:M:91:LEU:HD21	1.89	0.55
1:C:236:ILE:CG2	5:C:1335:HEM:HBC2	2.37	0.55
1:C:195:ALA:HA	1:C:278:ASN:HD22	1.72	0.54
2:H:172:TRP:HB2	2:H:182:TYR:HB2	1.90	0.53
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.43	0.53
6:M:1325:BCB:HMB1	6:M:1325:BCB:HBB3	1.90	0.53
4:M:157:CYS:HA	4:M:161:ILE:HB	1.91	0.52
3:L:170:ASN:HB3	3:L:173:HIS:HB3	1.91	0.52
1:C:135:CYS:SG	5:C:1334:HEM:HAC	2.49	0.52
6:L:1275:BCB:HMD1	4:M:204:ILE:HD13	1.91	0.51
6:L:1274:BCB:HMB1	6:L:1274:BCB:HBB3	1.93	0.51
1:C:267:ALA:HB2	5:C:1336:HEM:HMA1	1.92	0.50
3:L:124:PRO:HB2	6:L:1274:BCB:H71	1.94	0.50
1:C:244:CYS:SG	3:L:162:TYR:HB3	2.52	0.49
4:M:270:PHE:O	4:M:274:VAL:HG23	2.13	0.49
3:L:250:ALA:HA	3:L:254:PHE:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:190:PHE:HZ	1:C:302:GLN:HB2	1.77	0.48
3:L:183:ASN:HD22	3:L:236:LEU:HB2	1.79	0.48
1:C:62:LEU:HB3	1:C:65:LEU:HD12	1.95	0.48
6:L:1275:BCB:HBB3	6:L:1275:BCB:HMB1	1.96	0.48
1:C:132:CYS:SG	5:C:1334:HEM:HAB	2.54	0.48
6:L:1275:BCB:HMD3	4:M:195:TYR:HE1	1.78	0.47
6:L:1274:BCB:H112	6:L:1275:BCB:HBB2	1.96	0.47
10:M:1329:NS5:H82	10:M:1329:NS5:H61	1.68	0.47
2:H:199:GLY:HA3	4:M:226:ARG:HG2	1.97	0.47
3:L:231:ARG:HA	4:M:222:LEU:HD11	1.97	0.47
2:H:152:PRO:HA	2:H:155:LEU:HD12	1.97	0.46
4:M:178:TRP:N	4:M:179:PRO:CD	2.78	0.46
1:C:240:LEU:HB3	1:C:313:THR:HA	1.97	0.46
6:L:1274:BCB:H122	7:L:1276:BPB:HAA	1.97	0.46
2:H:114:PRO:HG2	2:H:244:GLY:HA2	1.98	0.46
1:C:227:TYR:HH	4:M:183:TRP:HD1	1.62	0.46
1:C:38:TYR:CE2	1:C:316:LEU:HD13	2.51	0.46
1:C:190:PHE:HA	1:C:194:LEU:HB2	1.99	0.45
1:C:185:LEU:HD13	1:C:231:ALA:HA	1.98	0.45
3:L:42:ILE:HG12	7:L:1276:BPB:H6A	1.99	0.45
4:M:89:PHE:HB3	4:M:178:TRP:NE1	2.32	0.45
4:M:128:TRP:NE1	4:M:145:ALA:O	2.45	0.45
3:L:75:LEU:HA	3:L:142:TRP:CD1	2.52	0.45
2:H:150:VAL:HG11	2:H:205:LYS:HA	1.98	0.45
1:C:134:THR:HG23	1:C:316:LEU:HD12	1.99	0.45
1:C:283:ALA:H	1:C:284:PRO:HD3	1.82	0.45
1:C:91:HIS:CE1	1:C:104:TYR:HE2	2.35	0.44
1:C:247:CYS:HA	1:C:261:THR:OG1	2.17	0.44
1:C:145:VAL:HG22	1:C:156:ASN:HD22	1.82	0.44
2:H:117:TYR:HB2	2:H:236:ASP:HB3	1.99	0.44
4:M:120:MET:HA	6:M:1325:BCB:H202	1.98	0.44
1:C:233:MET:HB3	5:C:1335:HEM:C3B	2.53	0.44
6:M:1325:BCB:H3A	6:M:1325:BCB:HBA1	1.76	0.43
1:C:24:HIS:HA	1:C:25:PRO:HD3	1.85	0.43
7:L:1276:BPB:HHC	7:L:1276:BPB:CBB	2.42	0.43
1:C:90:CYS:SG	5:C:1333:HEM:CAC	3.06	0.43
1:C:189:PRO:CB	1:C:232:LEU:HA	2.49	0.43
3:L:63:ALA:HA	4:M:303:PRO:HB3	2.01	0.43
6:L:1275:BCB:CBB	6:L:1275:BCB:HMB1	2.49	0.43
1:C:214:VAL:HA	1:C:219:GLU:HB3	2.01	0.43
3:L:197:VAL:HG13	3:L:207:LYS:HB2	2.00	0.42
10:M:1329:NS5:H161	10:M:1329:NS5:H18	1.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:23:TRP:HZ2	4:M:133:SER:HB2	1.84	0.42
4:M:94:TYR:HA	4:M:95:PRO:HD3	1.93	0.42
6:L:1275:BCB:H93	6:L:1275:BCB:HAA2	2.00	0.41
4:M:105:PRO:HA	4:M:106:PRO:HD3	1.96	0.41
1:C:247:CYS:SG	5:C:1335:HEM:CAC	3.04	0.41
7:M:1326:BPB:H11A	7:M:1326:BPB:H9B	1.94	0.41
2:H:80:ARG:HG2	4:M:239:ARG:HH12	1.86	0.41
1:C:291:ALA:HA	1:C:294:LEU:HD12	2.01	0.41
3:L:168:HIS:CE1	6:L:1274:BCB:HMC2	2.56	0.40
4:M:92:GLY:HA3	4:M:179:PRO:HG2	2.03	0.40
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.56	0.40
3:L:60:ASP:O	3:L:64:ILE:HG13	2.21	0.40
1:C:102:TYR:N	1:C:103:PRO:CD	2.85	0.40
1:C:240:LEU:HB2	1:C:242:THR:HG22	2.04	0.40
6:L:1274:BCB:HBD	6:L:1274:BCB:HAA1	2.03	0.40
4:M:126:SER:HA	4:M:129:ILE:HD12	2.03	0.40
1:C:129:GLY:HA3	1:C:322:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	C	330/336 (98%)	311 (94%)	19 (6%)	0	100	100
2	H	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
3	L	271/274 (99%)	253 (93%)	17 (6%)	1 (0%)	43	90
4	M	321/324 (99%)	309 (96%)	11 (3%)	1 (0%)	50	91
All	All	1161/1192 (97%)	1102 (95%)	57 (5%)	2 (0%)	56	93

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	165	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	M	193	ASN

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	C	278/282 (99%)	274 (99%)	4 (1%)	78	94
2	H	194/212 (92%)	192 (99%)	2 (1%)	85	96
3	L	216/219 (99%)	215 (100%)	1 (0%)	94	98
4	M	247/249 (99%)	245 (99%)	2 (1%)	89	97
All	All	935/962 (97%)	926 (99%)	9 (1%)	85	96

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

Mol	Chain	Res	Type
1	C	38	TYR
1	C	87	CYS
1	C	244	CYS
1	C	307	THR
2	H	45	GLU
2	H	185	LEU
3	L	272	TRP
4	M	194	PHE
4	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
4	M	72	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	FME	H	1	2	9,9,10	6.08	1 (11%)	6,9,11	3.48	2 (33%)

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	FME	H	1	2	-	1/7/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	O-C	18.11	1.23	1.11

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.79	110.09	122.97
2	H	1	FME	CE-SD-CG	2.80	110.70	100.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	HEM	C	1333	1	49,50,50	2.42	16 (32%)	46,82,82	2.07	6 (13%)
5	HEM	C	1334	1	49,50,50	2.32	15 (30%)	46,82,82	1.99	7 (15%)
5	HEM	C	1335	1	49,50,50	2.30	15 (30%)	46,82,82	2.07	9 (19%)
5	HEM	C	1336	1	49,50,50	2.41	16 (32%)	46,82,82	1.96	6 (13%)
6	BCB	L	1274	3	74,74,74	2.57	19 (25%)	94,115,115	3.06	32 (34%)
6	BCB	L	1275	-	74,74,74	2.57	19 (25%)	94,115,115	2.96	29 (30%)
7	BPB	L	1276	-	70,70,70	4.01	17 (24%)	93,101,101	2.54	27 (29%)
6	BCB	M	1324	-	73,73,74	2.57	21 (28%)	91,113,115	3.12	34 (37%)
6	BCB	M	1325	4	74,74,74	2.57	19 (25%)	94,115,115	3.04	31 (32%)
7	BPB	M	1326	-	66,66,70	4.24	20 (30%)	87,96,101	2.61	28 (32%)
9	MQ7	M	1328	-	49,49,49	1.33	2 (4%)	63,63,63	1.24	7 (11%)
10	NS5	M	1329	-	39,39,39	1.96	5 (12%)	46,46,46	2.51	16 (34%)

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	C	1333	1	-	0/14/114/114	0/0/8/8
5	HEM	C	1334	1	-	0/14/114/114	0/0/8/8
5	HEM	C	1335	1	-	0/14/114/114	0/0/8/8
5	HEM	C	1336	1	-	0/14/114/114	0/0/8/8
6	BCB	L	1274	3	-	1/41/137/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCB	L	1275	-	-	1/41/137/137	0/0/9/9
7	BPB	L	1276	-	-	1/52/105/105	0/0/6/6
6	BCB	M	1324	-	-	1/39/136/137	0/0/9/9
6	BCB	M	1325	4	-	1/41/137/137	0/0/9/9
7	BPB	M	1326	-	-	0/48/101/105	0/0/6/6
9	MQ7	M	1328	-	-	0/41/61/61	0/0/2/2
10	NS5	M	1329	-	-	0/43/43/43	0/0/0/0

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1326	BPB	CHD-C4C	19.30	1.48	1.35
7	L	1276	BPB	CHD-C4C	18.52	1.47	1.35
7	L	1276	BPB	CAC-C3C	15.09	1.52	1.33
7	M	1326	BPB	CAC-C3C	15.01	1.52	1.33
6	L	1274	BCB	CAC-C3C	12.33	1.49	1.33
7	M	1326	BPB	C4B-CHC	12.29	1.49	1.35
6	M	1325	BCB	CAC-C3C	12.27	1.49	1.33
6	L	1275	BCB	CAC-C3C	12.23	1.48	1.33
7	L	1276	BPB	C4B-CHC	12.23	1.49	1.35
7	M	1326	BPB	C1B-CHB	12.22	1.49	1.35
6	M	1324	BCB	CAC-C3C	12.19	1.48	1.33
7	L	1276	BPB	C1B-CHB	11.91	1.48	1.35
6	M	1324	BCB	C1D-C2D	7.00	1.48	1.40
6	M	1325	BCB	C1D-C2D	7.00	1.48	1.40
10	M	1329	NS5	C29-C28	6.91	1.53	1.34
6	L	1275	BCB	C1D-C2D	6.83	1.48	1.40
6	L	1274	BCB	C1D-C2D	6.69	1.48	1.40
10	M	1329	NS5	C35-C36	6.38	1.53	1.32
6	L	1274	BCB	C4B-C3B	6.29	1.49	1.41
6	L	1275	BCB	C4B-C3B	6.16	1.49	1.41
7	L	1276	BPB	C4B-C3B	6.11	1.49	1.41
9	M	1328	MQ7	C3-C2	6.08	1.50	1.35
6	L	1274	BCB	C1A-CHA	6.07	1.49	1.37
6	M	1325	BCB	C4B-C3B	6.05	1.49	1.41
6	M	1325	BCB	C1A-CHA	6.02	1.49	1.37
5	C	1336	HEM	C3D-C2D	5.94	1.54	1.43
5	C	1333	HEM	C3D-C2D	5.93	1.54	1.43
5	C	1334	HEM	C3D-C2D	5.88	1.54	1.43
6	M	1324	BCB	C1A-CHA	5.83	1.48	1.37
6	L	1275	BCB	C1A-CHA	5.80	1.48	1.37
6	M	1324	BCB	C4B-C3B	5.78	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1335	HEM	C3D-C2D	5.72	1.53	1.43
9	M	1328	MQ7	C10-C5	5.72	1.49	1.40
7	M	1326	BPB	CHA-C1A	5.71	1.50	1.37
7	M	1326	BPB	C4B-C3B	5.64	1.48	1.41
7	L	1276	BPB	CHA-C1A	5.53	1.49	1.37
7	M	1326	BPB	C16-C15	-5.54	1.52	1.55
5	C	1336	HEM	C3C-C2C	-5.47	1.34	1.43
10	M	1329	NS5	C9-C8	-5.46	1.34	1.53
5	C	1334	HEM	C3C-C2C	-5.42	1.34	1.43
5	C	1335	HEM	C3B-C2B	-5.40	1.34	1.43
5	C	1335	HEM	C3C-C2C	-5.39	1.34	1.43
5	C	1333	HEM	C3B-C2B	-5.34	1.34	1.43
5	C	1334	HEM	C3B-C2B	-5.24	1.34	1.43
5	C	1336	HEM	C3B-C2B	-5.18	1.34	1.43
5	C	1333	HEM	C3C-C2C	-5.13	1.34	1.43
6	L	1274	BCB	O2D-CGD	5.01	1.46	1.33
7	L	1276	BPB	C4C-NC	-5.00	1.27	1.38
6	M	1325	BCB	O2D-CGD	4.97	1.46	1.33
6	L	1275	BCB	C1A-NA	-4.96	1.28	1.39
7	M	1326	BPB	C4C-NC	-4.95	1.27	1.38
7	M	1326	BPB	O2D-CGD	4.88	1.46	1.33
6	L	1275	BCB	O2D-CGD	4.87	1.46	1.33
7	L	1276	BPB	O2D-CGD	4.84	1.46	1.33
6	M	1324	BCB	O2D-CGD	4.84	1.46	1.33
5	C	1333	HEM	C3C-CAC	4.74	1.55	1.40
5	C	1336	HEM	C3B-CAB	4.74	1.55	1.40
6	M	1324	BCB	C1A-NA	-4.73	1.29	1.39
5	C	1333	HEM	C3B-CAB	4.68	1.55	1.40
6	M	1325	BCB	OBD-CAD	4.66	1.29	1.22
5	C	1334	HEM	C3B-CAB	4.65	1.55	1.40
5	C	1336	HEM	C3C-CAC	4.64	1.55	1.40
7	M	1326	BPB	OBD-CAD	4.63	1.29	1.22
5	C	1334	HEM	C3C-CAC	4.63	1.55	1.40
5	C	1335	HEM	C3B-CAB	4.62	1.55	1.40
6	L	1274	BCB	OBD-CAD	4.61	1.29	1.22
5	C	1335	HEM	C3C-CAC	4.61	1.54	1.40
6	M	1324	BCB	OBD-CAD	4.59	1.29	1.22
7	L	1276	BPB	OBD-CAD	4.53	1.28	1.22
6	M	1325	BCB	C1A-NA	-4.50	1.29	1.39
6	L	1274	BCB	C1A-NA	-4.44	1.29	1.39
7	L	1276	BPB	C1A-NA	-4.37	1.27	1.37
5	C	1334	HEM	C4A-C3A	4.36	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1326	BPB	C1A-NA	-4.29	1.27	1.37
6	L	1274	BCB	O2A-CGA	4.29	1.46	1.33
6	L	1275	BCB	OBD-CAD	4.29	1.28	1.22
5	C	1336	HEM	C4A-C3A	4.26	1.45	1.40
5	C	1335	HEM	C4A-C3A	4.24	1.45	1.40
6	L	1275	BCB	O2A-CGA	4.20	1.46	1.33
5	C	1334	HEM	C2B-C1B	4.20	1.45	1.44
5	C	1333	HEM	FE-ND	4.18	2.13	1.97
5	C	1333	HEM	C4A-C3A	4.18	1.45	1.40
5	C	1333	HEM	C2B-C1B	4.11	1.45	1.44
6	M	1325	BCB	O2A-CGA	4.09	1.46	1.33
7	M	1326	BPB	O2A-CGA	4.07	1.46	1.33
5	C	1336	HEM	C2D-C1D	4.06	1.45	1.44
7	L	1276	BPB	O2A-CGA	4.06	1.46	1.33
6	M	1324	BCB	O2A-CGA	4.05	1.46	1.33
5	C	1333	HEM	C3D-C4D	3.94	1.45	1.44
5	C	1336	HEM	C2B-C1B	3.90	1.45	1.44
6	L	1275	BCB	CHD-C4C	3.85	1.48	1.35
7	M	1326	BPB	C4D-ND	3.82	1.40	1.36
6	M	1324	BCB	CHD-C4C	3.80	1.48	1.35
7	L	1276	BPB	C4D-ND	3.79	1.40	1.36
5	C	1336	HEM	FE-ND	3.78	2.11	1.97
6	L	1274	BCB	C2C-C3C	-3.74	1.46	1.52
6	M	1325	BCB	CHD-C4C	3.73	1.48	1.35
6	L	1274	BCB	CHD-C4C	3.65	1.47	1.35
5	C	1335	HEM	FE-NA	3.64	2.08	1.92
5	C	1335	HEM	FE-ND	3.59	2.10	1.97
6	M	1324	BCB	C4D-ND	3.58	1.39	1.34
6	M	1324	BCB	C2C-C3C	-3.57	1.46	1.52
6	M	1325	BCB	C2C-C3C	-3.53	1.46	1.52
5	C	1334	HEM	FE-NA	3.51	2.07	1.92
5	C	1333	HEM	FE-NA	3.49	2.07	1.92
6	L	1275	BCB	C2C-C3C	-3.43	1.46	1.52
5	C	1336	HEM	FE-NA	3.39	2.07	1.92
5	C	1335	HEM	C2B-C1B	3.35	1.45	1.44
6	L	1274	BCB	C4D-ND	3.35	1.38	1.34
6	L	1275	BCB	C4D-ND	3.33	1.38	1.34
6	M	1325	BCB	C4C-NC	-3.28	1.35	1.38
6	M	1325	BCB	C4B-CHC	3.27	1.48	1.38
6	L	1275	BCB	C4B-CHC	3.27	1.48	1.38
6	M	1324	BCB	C4B-CHC	3.25	1.48	1.38
6	L	1274	BCB	C4B-CHC	3.24	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1275	BCB	C4C-NC	-3.20	1.35	1.38
5	C	1336	HEM	C3D-C4D	3.17	1.45	1.44
6	M	1325	BCB	C4D-ND	3.14	1.38	1.34
6	M	1324	BCB	C4C-NC	-3.14	1.35	1.38
5	C	1334	HEM	FE-ND	3.07	2.09	1.97
6	M	1325	BCB	C1D-CHD	3.05	1.48	1.39
6	L	1275	BCB	C1D-CHD	3.05	1.48	1.39
6	L	1274	BCB	C4C-NC	-3.04	1.35	1.38
6	L	1275	BCB	C1B-CHB	2.99	1.47	1.38
6	L	1275	BCB	CHC-C1C	2.99	1.48	1.39
6	M	1324	BCB	C1D-CHD	2.98	1.48	1.39
7	L	1276	BPB	CHB-C4A	-2.93	1.34	1.41
6	M	1325	BCB	CHC-C1C	2.92	1.48	1.39
6	L	1274	BCB	C1D-CHD	2.87	1.47	1.39
7	M	1326	BPB	C1D-C2D	2.83	1.49	1.42
6	L	1274	BCB	CHC-C1C	2.83	1.48	1.39
5	C	1333	HEM	FE-NB	2.82	2.08	1.97
6	M	1324	BCB	CHC-C1C	2.79	1.48	1.39
6	M	1325	BCB	C3D-C2D	2.79	1.48	1.40
6	M	1324	BCB	C3D-C2D	2.79	1.48	1.40
6	L	1275	BCB	C3D-C2D	2.78	1.48	1.40
7	M	1326	BPB	C3D-C2D	2.78	1.48	1.40
7	L	1276	BPB	CHC-C1C	-2.77	1.34	1.41
6	L	1274	BCB	C3D-C2D	2.77	1.48	1.40
7	M	1326	BPB	CHB-C4A	-2.77	1.34	1.41
10	M	1329	NS5	C28-C26	2.72	1.51	1.45
6	L	1274	BCB	C1B-CHB	2.71	1.46	1.38
6	L	1275	BCB	C3B-C2B	2.71	1.48	1.40
10	M	1329	NS5	C29-C30	2.70	1.51	1.43
7	M	1326	BPB	CHC-C1C	-2.69	1.34	1.41
5	C	1333	HEM	C2D-C1D	2.68	1.45	1.44
6	M	1325	BCB	C1B-CHB	2.66	1.46	1.38
7	L	1276	BPB	C3D-C2D	2.65	1.48	1.40
7	L	1276	BPB	C1D-C2D	2.63	1.48	1.42
6	L	1274	BCB	C3B-C2B	2.59	1.48	1.40
6	M	1324	BCB	C1B-CHB	2.57	1.46	1.38
5	C	1336	HEM	FE-NC	2.57	2.07	1.97
6	M	1325	BCB	C3B-C2B	2.56	1.48	1.40
5	C	1336	HEM	FE-NB	2.55	2.07	1.97
5	C	1333	HEM	CMB-C2B	2.54	1.55	1.47
5	C	1333	HEM	CMC-C2C	2.54	1.55	1.47
5	C	1334	HEM	CMB-C2B	2.52	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1336	HEM	CMB-C2B	2.51	1.55	1.47
5	C	1335	HEM	FE-NB	2.51	2.07	1.97
5	C	1334	HEM	CMC-C2C	2.49	1.55	1.47
6	L	1275	BCB	MG-NA	-2.48	1.99	2.07
5	C	1335	HEM	CMC-C2C	2.48	1.55	1.47
5	C	1336	HEM	CMD-C2D	2.47	1.55	1.47
5	C	1336	HEM	CMC-C2C	2.46	1.55	1.47
5	C	1335	HEM	CMB-C2B	2.46	1.55	1.47
5	C	1333	HEM	CMD-C2D	2.45	1.55	1.47
7	L	1276	BPB	C3B-C2B	2.45	1.47	1.40
5	C	1334	HEM	CMD-C2D	2.45	1.55	1.47
5	C	1334	HEM	FE-NB	2.42	2.06	1.97
5	C	1333	HEM	FE-NC	2.40	2.06	1.97
5	C	1334	HEM	C3D-C4D	2.39	1.45	1.44
7	M	1326	BPB	C3B-C2B	2.36	1.47	1.40
5	C	1335	HEM	FE-NC	2.33	2.06	1.97
7	M	1326	BPB	C3D-CAD	2.22	1.51	1.47
5	C	1335	HEM	C3D-C4D	2.22	1.45	1.44
6	M	1324	BCB	C3B-C2B	2.22	1.47	1.40
7	M	1326	BPB	C4D-CHA	2.18	1.47	1.45
5	C	1335	HEM	CMD-C2D	2.16	1.54	1.47
6	M	1325	BCB	MG-NA	-2.13	2.00	2.07
6	M	1324	BCB	C19-C18	2.08	1.52	1.49
5	C	1334	HEM	FE-NC	2.06	2.05	1.97
6	M	1324	BCB	MG-NA	-2.03	2.01	2.07
6	L	1274	BCB	MG-NA	-2.04	2.01	2.07
6	M	1324	BCB	CHB-C4A	-2.01	1.32	1.39

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C3D-C4D-ND	11.02	119.59	108.61
6	L	1274	BCB	C3D-C4D-ND	10.70	119.28	108.61
6	M	1325	BCB	C3D-C4D-ND	10.48	119.05	108.61
6	L	1275	BCB	C3D-C4D-ND	10.46	119.04	108.61
6	M	1324	BCB	C2C-C1C-NC	10.05	124.33	111.65
6	L	1274	BCB	C2C-C1C-NC	10.04	124.32	111.65
6	L	1274	BCB	C2B-C1B-NB	9.88	116.87	109.41
6	M	1324	BCB	C2B-C1B-NB	9.87	116.86	109.41
6	M	1325	BCB	C2B-C1B-NB	9.80	116.81	109.41
6	M	1325	BCB	C2C-C1C-NC	9.65	123.82	111.65
6	L	1275	BCB	C2C-C1C-NC	9.61	123.78	111.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C2C-C3C-CAC	-9.47	107.62	129.36
6	L	1275	BCB	C2C-C3C-CAC	-9.37	107.84	129.36
6	M	1325	BCB	C2C-C3C-CAC	-9.22	108.20	129.36
6	L	1274	BCB	C2C-C3C-CAC	-9.08	108.52	129.36
6	L	1275	BCB	C2B-C1B-NB	8.91	116.14	109.41
7	L	1276	BPB	CAC-C3C-C4C	-8.81	109.64	127.18
5	C	1333	HEM	C3B-C4B-NB	-8.75	107.74	114.00
5	C	1335	HEM	C3B-C4B-NB	-8.42	107.97	114.00
5	C	1334	HEM	C3B-C4B-NB	-8.39	108.00	114.00
5	C	1336	HEM	C3B-C4B-NB	-8.19	108.14	114.00
7	M	1326	BPB	CAC-C3C-C4C	-8.16	110.94	127.18
7	L	1276	BPB	C3D-C4D-ND	7.97	120.25	106.97
7	L	1276	BPB	C2C-C3C-CAC	-7.96	111.08	129.36
7	M	1326	BPB	C3D-C4D-ND	7.86	120.07	106.97
7	M	1326	BPB	C2C-C3C-CAC	-7.83	111.39	129.36
6	M	1324	BCB	C1B-C2B-C3B	-7.69	100.50	106.78
7	M	1326	BPB	CBC-CAC-C3C	-7.60	109.69	126.93
6	M	1325	BCB	C1B-C2B-C3B	-7.55	100.61	106.78
6	L	1274	BCB	C1B-C2B-C3B	-7.37	100.75	106.78
6	L	1275	BCB	C1B-C2B-C3B	-7.18	100.91	106.78
5	C	1335	HEM	C4D-ND-C1D	6.78	112.09	105.16
7	L	1276	BPB	CBC-CAC-C3C	-6.73	111.67	126.93
5	C	1333	HEM	C4D-ND-C1D	6.71	112.03	105.16
7	M	1326	BPB	C4D-C3D-C2D	-6.64	99.12	107.04
7	L	1276	BPB	C4D-C3D-C2D	-6.59	99.18	107.04
7	L	1276	BPB	C1B-C2B-C3B	-6.58	101.24	106.89
7	M	1326	BPB	C1B-C2B-C3B	-6.48	101.33	106.89
6	M	1324	BCB	C4D-C3D-C2D	-6.45	99.05	107.01
6	L	1274	BCB	C4D-C3D-C2D	-6.43	99.06	107.01
6	L	1275	BCB	C4D-C3D-C2D	-6.40	99.10	107.01
5	C	1334	HEM	C4D-ND-C1D	6.40	111.71	105.16
5	C	1336	HEM	C4D-ND-C1D	6.34	111.65	105.16
6	M	1325	BCB	C4D-C3D-C2D	-6.13	99.44	107.01
6	L	1275	BCB	C3D-CAD-CBD	6.00	116.08	107.60
6	M	1325	BCB	C3D-CAD-CBD	5.68	115.62	107.60
6	M	1324	BCB	C3D-CAD-CBD	5.55	115.44	107.60
6	M	1324	BCB	CAC-C3C-C4C	-5.50	116.23	127.18
6	L	1274	BCB	C3D-CAD-CBD	5.34	115.15	107.60
10	M	1329	NS5	C19-C20-C21	-5.26	119.71	127.29
6	L	1275	BCB	CAC-C3C-C4C	-5.24	116.75	127.18
6	M	1325	BCB	CAC-C3C-C4C	-5.15	116.93	127.18
10	M	1329	NS5	C18-C17-C15	-5.07	119.99	127.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	1329	NS5	C13-C12-C10	-5.00	123.12	127.91
6	M	1325	BCB	O2D-CGD-CBD	4.96	121.42	111.33
6	L	1275	BCB	CMD-C2D-C3D	-4.88	117.28	124.97
6	L	1274	BCB	CAC-C3C-C4C	-4.83	117.57	127.18
10	M	1329	NS5	C9-C8-C7	4.79	125.31	111.62
7	L	1276	BPB	C2C-C3C-C4C	-4.77	101.68	108.73
6	M	1324	BCB	CMD-C2D-C3D	-4.72	117.54	124.97
7	M	1326	BPB	CMD-C2D-C3D	-4.70	117.56	124.97
6	M	1325	BCB	CMD-C2D-C3D	-4.69	117.58	124.97
7	L	1276	BPB	CMD-C2D-C3D	-4.62	117.69	124.97
6	M	1324	BCB	O2D-CGD-CBD	4.56	120.63	111.33
7	L	1276	BPB	CMD-C2D-C1D	4.52	135.53	128.65
6	M	1325	BCB	CMD-C2D-C1D	4.48	135.52	128.62
7	M	1326	BPB	O2D-CGD-CBD	4.48	120.46	111.33
7	M	1326	BPB	CMD-C2D-C1D	4.48	135.46	128.65
10	M	1329	NS5	C29-C28-C26	-4.46	113.65	126.38
6	M	1324	BCB	CMD-C2D-C1D	4.43	135.44	128.62
6	L	1274	BCB	CMD-C2D-C3D	-4.40	118.04	124.97
10	M	1329	NS5	C30-C29-C28	-4.38	108.46	123.24
6	L	1275	BCB	CMD-C2D-C1D	4.37	135.35	128.62
7	L	1276	BPB	O2D-CGD-CBD	4.34	120.17	111.33
7	M	1326	BPB	C2C-C3C-C4C	-4.32	102.34	108.73
6	L	1275	BCB	O2D-CGD-CBD	4.32	120.13	111.33
7	L	1276	BPB	OBD-CAD-C3D	-4.30	119.78	127.96
6	L	1274	BCB	O2D-CGD-CBD	4.28	120.05	111.33
10	M	1329	NS5	C8-C9-C10	4.25	126.81	112.74
5	C	1335	HEM	C2D-C1D-ND	-4.23	107.94	112.93
7	M	1326	BPB	OBD-CAD-C3D	-4.17	120.02	127.96
6	L	1274	BCB	C4C-NC-C1C	-4.11	100.02	106.33
6	L	1275	BCB	C4D-C3D-CAD	-4.11	100.32	107.89
6	L	1274	BCB	CMD-C2D-C1D	4.09	134.91	128.62
6	L	1274	BCB	C3A-C4A-CHB	-4.07	117.90	122.11
10	M	1329	NS5	C34-C35-C36	-4.05	111.80	127.67
7	L	1276	BPB	OBD-CAD-CBD	-4.03	119.86	125.94
6	M	1325	BCB	C4D-C3D-CAD	-4.02	100.47	107.89
6	M	1325	BCB	CMB-C2B-C3B	3.98	131.24	124.97
7	M	1326	BPB	OBD-CAD-CBD	-3.93	120.00	125.94
6	M	1324	BCB	C4C-NC-C1C	-3.93	100.30	106.33
6	M	1325	BCB	CHC-C1C-NC	-3.89	120.25	125.86
6	L	1274	BCB	CMB-C2B-C3B	3.88	131.08	124.97
6	L	1274	BCB	C4D-C3D-CAD	-3.88	100.74	107.89
6	M	1325	BCB	C3D-C4D-CHA	3.87	114.55	108.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1325	BCB	C3A-C4A-CHB	-3.87	118.11	122.11
6	M	1324	BCB	C2C-C1C-CHC	-3.85	114.63	123.31
10	M	1329	NS5	C29-C30-C31	-3.85	124.22	127.91
6	L	1275	BCB	C3D-C4D-CHA	3.83	114.50	108.91
6	L	1274	BCB	CHC-C1C-NC	-3.80	120.37	125.86
6	M	1324	BCB	C4D-C3D-CAD	-3.79	100.89	107.89
6	L	1274	BCB	C3D-C4D-CHA	3.79	114.43	108.91
6	L	1275	BCB	CMB-C2B-C3B	3.79	130.93	124.97
6	L	1274	BCB	C4B-C3B-C2B	-3.75	104.38	106.84
6	M	1324	BCB	C3A-C4A-CHB	-3.74	118.25	122.11
6	M	1325	BCB	C4C-NC-C1C	-3.73	100.60	106.33
5	C	1333	HEM	C2D-C1D-ND	-3.70	108.56	112.93
6	L	1275	BCB	CHC-C1C-NC	-3.69	120.54	125.86
6	L	1275	BCB	C1D-CHD-C4C	-3.67	122.64	127.47
6	L	1274	BCB	C2C-C1C-CHC	-3.66	115.05	123.31
5	C	1336	HEM	C2D-C1D-ND	-3.61	108.67	112.93
6	L	1275	BCB	C4B-C3B-C2B	-3.57	104.50	106.84
6	L	1274	BCB	C4-C3-C5	3.56	120.80	115.39
6	L	1275	BCB	OBD-CAD-C3D	-3.52	121.27	127.96
6	L	1275	BCB	C4C-NC-C1C	-3.50	100.95	106.33
6	M	1324	BCB	C3D-C4D-CHA	3.50	114.00	108.91
5	C	1334	HEM	C2D-C1D-ND	-3.49	108.80	112.93
6	M	1325	BCB	C2C-C1C-CHC	-3.46	115.50	123.31
10	M	1329	NS5	C11-C10-C9	3.43	120.60	115.39
6	M	1324	BCB	CHC-C1C-NC	-3.43	120.91	125.86
6	L	1275	BCB	C2C-C1C-CHC	-3.40	115.64	123.31
6	M	1325	BCB	C4B-C3B-C2B	-3.39	104.61	106.84
9	M	1328	MQ7	C14-C13-C15	3.38	120.53	115.39
10	M	1329	NS5	CM3-C36-C35	-3.36	111.63	122.62
10	M	1329	NS5	CM4-C36-C35	-3.32	111.75	122.62
6	M	1325	BCB	C1D-CHD-C4C	-3.30	123.14	127.47
6	L	1275	BCB	C2D-C3D-CAD	3.29	160.58	138.46
6	L	1274	BCB	C1D-CHD-C4C	-3.26	123.18	127.47
6	L	1274	BCB	C2D-C3D-CAD	3.23	160.19	138.46
6	M	1325	BCB	OBD-CAD-C3D	-3.22	121.83	127.96
6	M	1325	BCB	C2D-C3D-CAD	3.22	160.08	138.46
6	M	1324	BCB	C2D-C3D-CAD	3.21	160.06	138.46
6	M	1325	BCB	O2D-CGD-O1D	-3.20	117.29	123.79
6	M	1324	BCB	OBD-CAD-C3D	-3.13	122.01	127.96
7	L	1276	BPB	CMB-C2B-C3B	3.13	129.90	124.97
10	M	1329	NS5	C24-C25-C26	-3.06	122.88	127.29
6	L	1274	BCB	CBC-CAC-C3C	-3.03	120.05	126.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1276	BPB	C4D-ND-C1D	-3.02	101.79	108.72
6	L	1275	BCB	CBC-CAC-C3C	-3.02	120.08	126.93
6	M	1324	BCB	C2A-C1A-CHA	-3.02	119.55	125.47
7	M	1326	BPB	C4D-C3D-CAD	-2.98	105.23	108.14
5	C	1333	HEM	C1B-NB-C4B	2.94	108.17	105.16
6	L	1274	BCB	OBD-CAD-C3D	-2.94	122.37	127.96
7	M	1326	BPB	C3D-C4D-CHA	2.93	112.42	109.18
6	M	1324	BCB	CBC-CAC-C3C	-2.93	120.29	126.93
10	M	1329	NS5	C8-C7-C5	-2.89	121.57	127.80
6	L	1274	BCB	O2A-CGA-CBA	2.89	121.02	111.94
5	C	1334	HEM	C1B-NB-C4B	2.88	108.11	105.16
7	M	1326	BPB	C4D-ND-C1D	-2.79	102.32	108.72
6	M	1325	BCB	CBC-CAC-C3C	-2.79	120.60	126.93
6	M	1324	BCB	CMB-C2B-C3B	2.77	129.34	124.97
5	C	1336	HEM	C1B-NB-C4B	2.75	107.98	105.16
5	C	1335	HEM	C1B-NB-C4B	2.73	107.95	105.16
7	L	1276	BPB	C4D-C3D-CAD	-2.71	105.49	108.14
6	M	1325	BCB	C4-C3-C5	2.68	119.46	115.39
7	M	1326	BPB	CMB-C2B-C3B	2.68	129.19	124.97
6	M	1324	BCB	C1D-CHD-C4C	-2.66	123.97	127.47
9	M	1328	MQ7	C34-C33-C35	2.65	119.42	115.39
10	M	1329	NS5	C32-C31-C33	2.61	119.36	115.39
7	L	1276	BPB	C2B-C1B-NB	2.60	115.18	106.38
7	L	1276	BPB	C3C-C4C-NC	2.60	114.07	109.23
7	L	1276	BPB	C3D-C4D-CHA	2.59	112.05	109.18
6	M	1324	BCB	C4D-ND-C1D	-2.59	103.44	106.57
9	M	1328	MQ7	C19-C18-C20	2.58	119.31	115.39
7	M	1326	BPB	C4-C3-C5	2.56	119.28	115.39
7	M	1326	BPB	C2D-C3D-CAD	2.56	155.65	138.46
6	L	1274	BCB	CAA-C2A-C1A	2.55	118.00	111.62
6	M	1325	BCB	C2A-C1A-CHA	-2.55	120.47	125.47
6	L	1275	BCB	C4-C3-C5	2.55	119.26	115.39
5	C	1335	HEM	C4C-NC-C1C	2.54	108.18	105.53
6	L	1274	BCB	C3A-C4A-NA	2.52	114.43	111.79
7	L	1276	BPB	C2D-C3D-CAD	2.51	155.32	138.46
5	C	1333	HEM	C4C-NC-C1C	2.50	108.13	105.53
6	M	1325	BCB	O2A-CGA-CBA	2.49	119.78	111.94
7	M	1326	BPB	C2B-C1B-NB	2.47	114.74	106.38
7	L	1276	BPB	C1D-CHD-C4C	-2.46	125.12	129.92
6	L	1274	BCB	C1C-C2C-C3C	-2.46	93.11	100.28
10	M	1329	NS5	C6-C5-C4	2.45	119.12	115.39
6	M	1325	BCB	C1C-C2C-C3C	-2.44	93.17	100.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1324	BCB	C1C-C2C-C3C	-2.43	93.19	100.28
5	C	1334	HEM	C4C-NC-C1C	2.43	108.06	105.53
9	M	1328	MQ7	C24-C23-C25	2.42	119.08	115.39
7	M	1326	BPB	O2A-CGA-CBA	2.41	119.51	111.94
5	C	1336	HEM	C4C-NC-C1C	2.40	108.03	105.53
6	L	1275	BCB	O2A-CGA-CBA	2.40	119.49	111.94
6	M	1324	BCB	C4B-C3B-C2B	-2.39	105.27	106.84
6	M	1324	BCB	C4-C3-C5	2.38	119.01	115.39
5	C	1333	HEM	CMA-C3A-C4A	-2.38	124.96	128.62
9	M	1328	MQ7	C39-C38-C40	2.37	119.00	115.39
6	L	1275	BCB	C2A-C1A-CHA	-2.35	120.86	125.47
6	L	1275	BCB	C1C-C2C-C3C	-2.34	93.46	100.28
6	M	1325	BCB	C3A-C4A-NA	2.34	114.24	111.79
5	C	1335	HEM	CBD-CAD-C3D	-2.33	109.28	114.37
6	L	1274	BCB	C4D-ND-C1D	-2.31	103.78	106.57
7	L	1276	BPB	CHD-C4C-NC	-2.30	124.34	128.59
6	M	1324	BCB	O2A-CGA-CBA	2.30	119.17	111.94
9	M	1328	MQ7	C29-C28-C30	2.30	118.88	115.39
7	M	1326	BPB	C4C-NC-C1C	2.30	110.62	106.73
6	L	1274	BCB	OBD-CAD-CBD	-2.29	122.48	125.94
6	M	1325	BCB	OBD-CAD-CBD	-2.28	122.50	125.94
7	M	1326	BPB	CMB-C2B-C1B	2.26	129.48	125.81
5	C	1334	HEM	CMA-C3A-C4A	-2.26	125.14	128.62
6	M	1324	BCB	OBD-CAD-CBD	-2.24	122.56	125.94
6	L	1275	BCB	O1D-CGD-CBD	-2.23	119.86	124.42
7	L	1276	BPB	C4B-C3B-C2B	-2.22	105.36	106.92
5	C	1335	HEM	CMA-C3A-C4A	-2.22	125.21	128.62
7	M	1326	BPB	O1D-CGD-CBD	-2.21	119.89	124.42
6	L	1275	BCB	CED-O2D-CGD	2.18	121.21	116.02
6	M	1324	BCB	O1D-CGD-CBD	-2.17	119.97	124.42
6	L	1275	BCB	OBD-CAD-CBD	-2.18	122.66	125.94
5	C	1336	HEM	C3A-C4A-NA	-2.17	107.77	109.41
7	L	1276	BPB	CHD-C4C-C3C	-2.17	121.58	126.90
6	M	1324	BCB	O2D-CGD-O1D	-2.16	119.41	123.79
6	L	1274	BCB	O1D-CGD-CBD	-2.14	120.03	124.42
6	M	1324	BCB	C3A-C4A-NA	2.13	114.02	111.79
6	M	1325	BCB	CAA-C2A-C3A	-2.12	108.02	113.04
7	M	1326	BPB	C3C-C4C-NC	2.09	113.13	109.23
6	M	1324	BCB	C15-C16-C17	-2.09	110.54	114.68
9	M	1328	MQ7	C31-C32-C33	-2.09	123.30	127.80
7	M	1326	BPB	CHD-C4C-NC	-2.08	124.74	128.59
7	L	1276	BPB	O2A-CGA-CBA	2.08	118.47	111.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1276	BPB	C3B-C4B-NB	2.07	112.53	105.84
7	L	1276	BPB	O2D-CGD-O1D	-2.07	119.58	123.79
7	M	1326	BPB	C1D-CHD-C4C	-2.07	125.89	129.92
5	C	1334	HEM	CBD-CAD-C3D	-2.07	109.86	114.37
5	C	1335	HEM	CHD-C1D-ND	2.07	126.30	124.58
7	L	1276	BPB	O1D-CGD-CBD	-2.04	120.24	124.42
7	M	1326	BPB	O2D-CGD-O1D	-2.04	119.65	123.79
6	L	1274	BCB	C2A-C1A-CHA	-2.03	121.48	125.47
6	M	1324	BCB	CMB-C2B-C1B	2.03	130.17	126.16
7	M	1326	BPB	C3B-C4B-NB	2.02	112.35	105.84
5	C	1335	HEM	CBA-CAA-C2A	-2.00	109.17	112.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	1324	BCB	CBC-CAC-C3C-C2C
6	L	1275	BCB	CBC-CAC-C3C-C4C
6	M	1325	BCB	CBC-CAC-C3C-C2C
6	L	1274	BCB	CBC-CAC-C3C-C4C
7	L	1276	BPB	CBC-CAC-C3C-C4C

There are no ring outliers.

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, 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	C	332/336 (98%)	1.02	57 (17%) 2 8	12, 15, 19, 21	0
2	H	243/258 (94%)	0.71	26 (10%) 6 15	12, 16, 25, 26	0
3	L	273/274 (99%)	0.82	31 (11%) 6 14	10, 15, 21, 22	0
4	M	323/324 (99%)	0.75	37 (11%) 5 14	11, 15, 20, 20	0
All	All	1171/1192 (98%)	0.83	151 (12%) 4 12	10, 15, 21, 26	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	305	TYR	6.1
1	C	131	THR	5.6
2	H	84	GLU	5.3
3	L	223	SER	5.1
1	C	186	ASN	5.0
2	H	83	PRO	5.0
3	L	222	TYR	4.8
4	M	303	PRO	4.8
3	L	264	GLY	4.6
1	C	17	LEU	4.6
3	L	111	LEU	4.4
1	C	19	MET	4.3
1	C	179	TYR	4.1
1	C	187	TYR	4.0
4	M	306	PRO	3.9
1	C	150	PRO	3.9
2	H	45	GLU	3.8
3	L	13	GLY	3.8
1	C	301	PRO	3.8
4	M	16	HIS	3.8
2	H	107	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	145	VAL	3.7
1	C	176	LEU	3.7
1	C	303	ALA	3.7
1	C	132	CYS	3.6
1	C	146	ARG	3.6
1	C	177	ALA	3.6
3	L	27	GLY	3.6
4	M	47	GLY	3.5
2	H	91	ALA	3.5
4	M	30	GLY	3.5
1	C	182	TYR	3.4
1	C	14	PHE	3.4
1	C	178	LYS	3.4
4	M	45	GLN	3.4
1	C	149	GLU	3.4
4	M	43	ASP	3.3
3	L	57	PRO	3.2
4	M	31	LYS	3.2
4	M	76	GLU	3.2
1	C	99	GLU	3.2
2	H	104	THR	3.1
4	M	17	ILE	3.1
3	L	265	TRP	3.1
1	C	181	ALA	3.1
3	L	14	GLY	3.1
1	C	130	VAL	3.1
1	C	304	ASP	3.0
3	L	260	PRO	3.0
1	C	180	THR	3.0
4	M	248	LEU	3.0
1	C	173	VAL	3.0
4	M	32	PRO	2.9
4	M	48	PRO	2.9
2	H	90	LEU	2.9
3	L	155	ASP	2.9
4	M	73	MET	2.9
4	M	46	ILE	2.9
2	H	103	PRO	2.9
2	H	105	GLY	2.9
4	M	29	VAL	2.9
2	H	114	PRO	2.8
1	C	12	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	97	GLU	2.8
1	C	273	MET	2.8
3	L	110	LYS	2.8
1	C	244	CYS	2.8
1	C	1	CYS	2.8
2	H	102	GLN	2.7
2	H	41	TYR	2.7
1	C	184	ALA	2.7
1	C	108	ARG	2.7
3	L	221	GLY	2.7
1	C	183	SER	2.7
4	M	103	GLY	2.7
1	C	242	THR	2.7
3	L	213	ASN	2.7
1	C	151	THR	2.6
3	L	56	GLY	2.6
3	L	1	ALA	2.6
1	C	20	GLY	2.6
4	M	34	TYR	2.6
3	L	12	ARG	2.6
3	L	80	LEU	2.6
1	C	185	LEU	2.6
2	H	112	VAL	2.6
4	M	230	ASP	2.5
4	M	49	ILE	2.5
4	M	33	PHE	2.5
1	C	112	GLU	2.5
1	C	13	GLY	2.5
1	C	245	THR	2.5
4	M	12	ALA	2.5
2	H	254	ALA	2.5
2	H	178	HIS	2.4
1	C	147	TYR	2.4
4	M	92	GLY	2.4
2	H	88	LEU	2.4
2	H	113	GLY	2.4
4	M	257	ASN	2.4
3	L	214	GLN	2.4
3	L	263	TRP	2.4
2	H	195	LEU	2.4
3	L	202	ASP	2.4
1	C	251	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	174	VAL	2.4
4	M	302	ALA	2.4
3	L	220	VAL	2.4
1	C	300	ALA	2.4
1	C	327	GLU	2.4
3	L	81	LEU	2.4
1	C	61	VAL	2.3
4	M	307	ALA	2.3
3	L	107	ILE	2.3
1	C	56	TYR	2.2
4	M	104	ILE	2.2
3	L	166	ASN	2.2
2	H	85	THR	2.2
1	C	135	CYS	2.2
1	C	148	LEU	2.2
2	H	101	LEU	2.2
4	M	70	LEU	2.2
1	C	316	LEU	2.2
1	C	121	TRP	2.2
3	L	165	LEU	2.2
4	M	18	THR	2.2
4	M	304	ASP	2.2
2	H	247	LEU	2.2
2	H	42	PRO	2.2
1	C	100	ALA	2.2
1	C	113	MET	2.2
2	H	93	THR	2.2
1	C	249	ASN	2.2
2	H	177	GLU	2.1
1	C	272	ARG	2.1
3	L	152	SER	2.1
4	M	323	LYS	2.1
4	M	90	TRP	2.1
4	M	14	GLY	2.1
2	H	248	TYR	2.1
3	L	225	GLY	2.1
1	C	62	LEU	2.1
3	L	65	SER	2.1
4	M	15	PRO	2.1
3	L	217	ARG	2.1
1	C	234	MET	2.0
4	M	256	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	291	ALA	2.0
4	M	28	ARG	2.0
1	C	152	LEU	2.0
3	L	3	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	H	1	10/11	0.41	1.29	18,18,18,18	0

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	BCB	L	1275	66/66	0.55	2.07	19,20,21,21	0
7	BPB	L	1276	65/65	0.51	1.93	2,2,4,4	0
9	MQ7	M	1328	48/48	0.66	1.88	9,9,10,10	0
10	NS5	M	1329	40/40	0.63	1.88	27,28,30,30	0
6	BCB	L	1274	66/66	0.47	1.35	29,29,30,30	0
7	BPB	M	1326	61/65	0.54	1.26	26,26,27,27	0
6	BCB	M	1325	66/66	0.49	1.16	12,12,15,15	0
8	FE2	M	1327	1/1	0.42	1.05	2,2,2,2	0
6	BCB	M	1324	65/66	0.48	0.84	16,16,16,17	0
5	HEM	C	1334	43/43	0.62	0.51	2,2,2,2	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HEM	C	1336	43/43	0.40	0.00	2,2,2,2	0
5	HEM	C	1333	43/43	0.34	-0.13	15,16,16,16	0
5	HEM	C	1335	43/43	0.35	-0.25	4,4,4,4	0

6.5 Other polymers

There are no such residues in this entry.