Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 12:23 AM GMT

PDB ID	:	3CBD
Title	:	Directed Evolution of cytochrome P450 BM3, to octane monoxygenase 139-3
Authors	:	Meharenna, Y.T.; Li, H.; Poulos, T.L.
Deposited on	:	2008-02-21
Resolution	:	2.65 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

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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)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.65 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		17
Ramachandran outliers		1.2%
Sidechain outliers		3.5%
RSRZ outliers		1.6%

Worse ⟵ ⟶ Better

∎ Percentile relative to all X-ray structures

∐ Percentile relative to X-ray structures of similar resolution
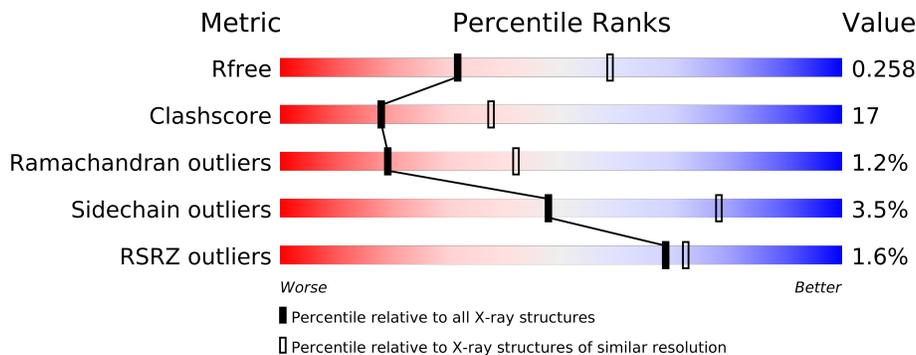
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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	A	455	
1	B	455	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	140	A	500	-	X
3	140	B	500	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7745 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 Bifunctional P-450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total 3667	C 2346	N 617	O 687	S 17	0	0	0
1	B	455	Total 3667	C 2346	N 617	O 687	S 17	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ALA	VAL	ENGINEERED	UNP P14779
A	138	TYR	HIS	ENGINEERED	UNP P14779
A	175	ILE	THR	ENGINEERED	UNP P14779
A	178	ILE	VAL	ENGINEERED	UNP P14779
A	184	VAL	ALA	ENGINEERED	UNP P14779
A	236	GLN	HIS	ENGINEERED	UNP P14779
A	252	GLY	GLU	ENGINEERED	UNP P14779
A	255	SER	ARG	ENGINEERED	UNP P14779
A	290	VAL	ALA	ENGINEERED	UNP P14779
A	295	THR	ALA	ENGINEERED	UNP P14779
A	353	VAL	LEU	ENGINEERED	UNP P14779
B	78	ALA	VAL	ENGINEERED	UNP P14779
B	138	TYR	HIS	ENGINEERED	UNP P14779
B	175	ILE	THR	ENGINEERED	UNP P14779
B	178	ILE	VAL	ENGINEERED	UNP P14779
B	184	VAL	ALA	ENGINEERED	UNP P14779
B	236	GLN	HIS	ENGINEERED	UNP P14779
B	252	GLY	GLU	ENGINEERED	UNP P14779
B	255	SER	ARG	ENGINEERED	UNP P14779
B	290	VAL	ALA	ENGINEERED	UNP P14779
B	295	THR	ALA	ENGINEERED	UNP P14779
B	353	VAL	LEU	ENGINEERED	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
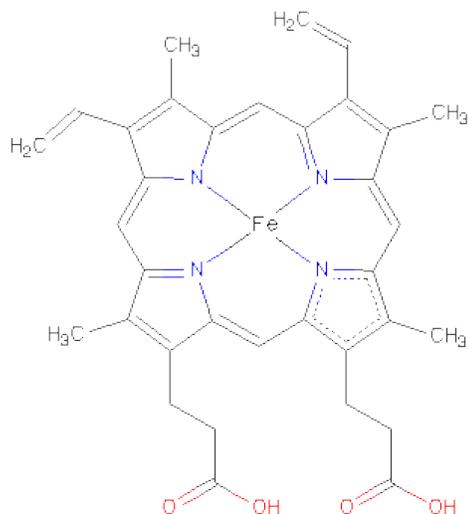
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is N-PALMITOYLGLYCINE (three-letter code: 140) (formula: $C_{18}H_{35}NO_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	18	1	3		
3	B	1	Total	C	N	O	0	0
			22	18	1	3		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total O 94 94		0	0
4	B	187	Total O 187 187		0	0

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: Bifunctional P-450/NADPH-P450 reductase

Chain A:
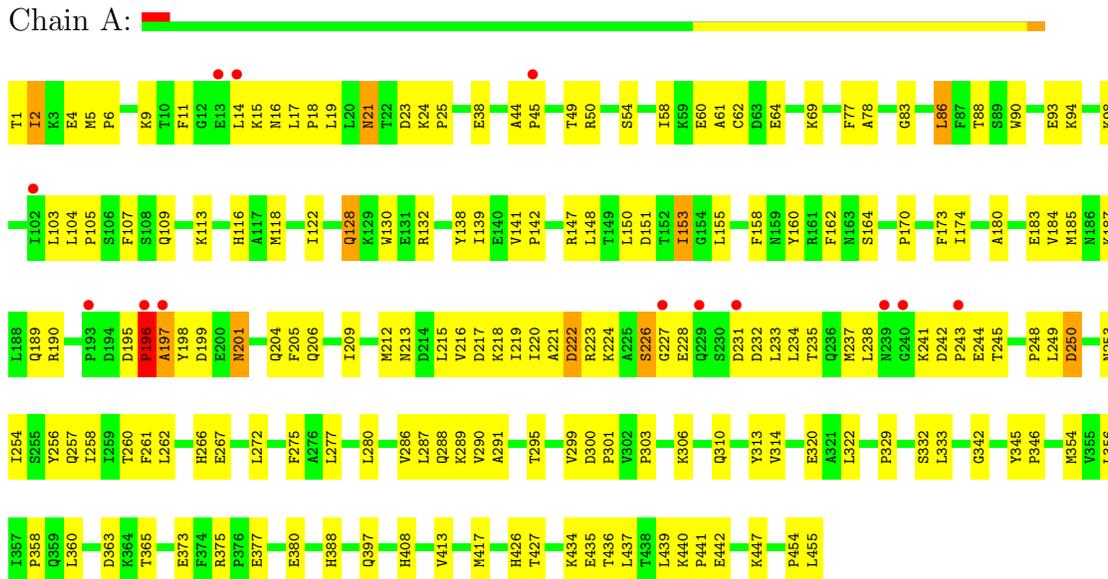
- Molecule 1: Bifunctional P-450/NADPH-P450 reductase

Chain B:
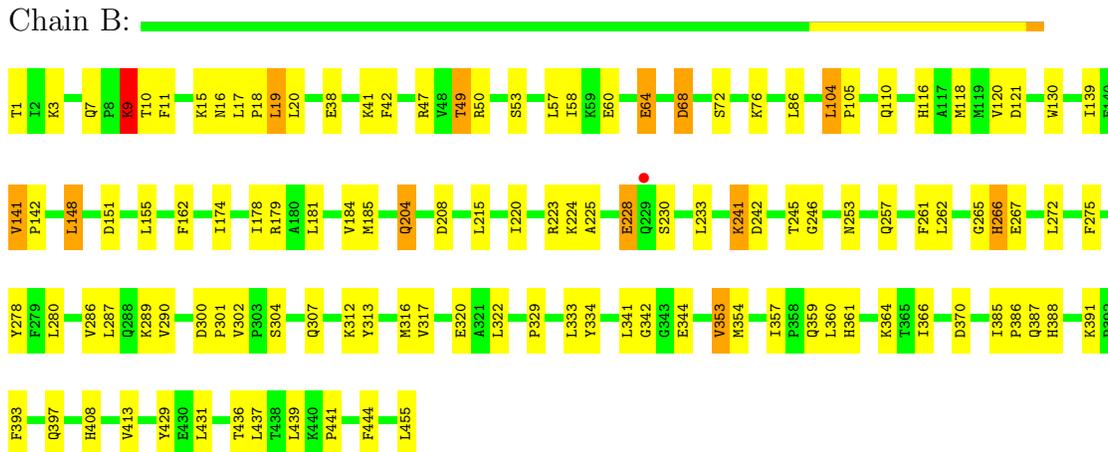
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.78Å 127.35Å 183.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.65 47.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.53-2.65) 97.8 (47.53-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.258 0.211 , 0.258	Depositor DCC
R_{free} test set	4241 reflections (11.23%)	DCC
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	1 of 41994 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7745	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 140

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	0.35	0/3751	0.60	0/5071
1	B	0.40	0/3751	0.64	0/5071
All	All	0.37	0/7502	0.62	0/10142

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	A	3667	0	3647	154	0
1	B	3667	0	3647	101	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	22	0	34	1	0
3	B	22	0	34	1	0
4	A	94	0	0	15	0
4	B	187	0	0	9	0
All	All	7745	0	7422	255	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 17.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:LYS:HG2	1:A:248:PRO:HG3	1.41	1.00
1:B:10:THR:HA	4:B:635:HOH:O	1.61	1.00
1:A:238:LEU:HD23	1:A:254:ILE:HD13	1.55	0.89
1:A:183:GLU:HG2	1:A:205:PHE:HD2	1.38	0.87
1:B:10:THR:HG23	1:B:11:PHE:H	1.38	0.87
1:B:286:VAL:O	1:B:290:VAL:HG23	1.77	0.84
1:B:181:LEU:O	1:B:184:VAL:HG22	1.79	0.83
1:A:204:GLN:HG3	4:A:564:HOH:O	1.80	0.82
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.60	0.81
1:A:78:ALA:HB1	4:A:554:HOH:O	1.81	0.81
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.63	0.81
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.63	0.80
1:A:2:ILE:HD12	1:A:2:ILE:H	1.46	0.80
1:A:223:ARG:HH21	1:A:234:LEU:HB3	1.47	0.79
1:A:301:PRO:HB3	1:A:455:LEU:HG	1.66	0.78
1:B:116:HIS:HD2	1:B:408:HIS:HE2	1.32	0.77
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.67	0.76
1:B:312:LYS:HB2	4:B:625:HOH:O	1.86	0.75
1:A:286:VAL:O	1:A:290:VAL:HG23	1.87	0.74
1:A:183:GLU:HG2	1:A:205:PHE:CD2	2.22	0.74
1:A:77:PHE:HB2	1:A:184:VAL:HG13	1.69	0.74
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.69	0.74
1:A:150:LEU:HD22	1:A:174:ILE:HD11	1.69	0.73
1:A:310:GLN:HG2	4:A:571:HOH:O	1.87	0.73
1:A:332:SER:HB3	1:A:354:MET:SD	2.28	0.73
1:B:86:LEU:H	1:B:257:GLN:HE22	1.37	0.73
1:A:205:PHE:CE1	1:A:209:ILE:HD11	2.23	0.73
1:B:10:THR:HG23	1:B:11:PHE:N	2.05	0.72
1:B:58:ILE:HD12	1:B:360:LEU:HD13	1.70	0.71
1:A:426:HIS:CD2	1:A:447:LYS:HG3	2.25	0.71
1:B:329:PRO:HG3	1:B:439:LEU:HG	1.73	0.69
1:A:94:LYS:HE3	1:A:98:LYS:HD2	1.76	0.68
1:A:58:ILE:HD12	1:A:360:LEU:HD13	1.76	0.68
1:B:174:ILE:O	1:B:178:ILE:HG12	1.94	0.67
1:A:262:LEU:O	1:A:266:HIS:HD2	1.77	0.66
1:A:201:ASN:HD22	1:A:201:ASN:N	1.92	0.65
1:B:118:MET:HB3	1:B:155:LEU:HD23	1.78	0.65
1:B:290:VAL:HG22	1:B:313:TYR:CE2	2.32	0.65
1:A:242:ASP:HB3	1:A:245:THR:OG1	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:LEU:N	1:A:105:PRO:HD2	2.12	0.64
1:A:190:ARG:HH11	1:A:190:ARG:HG2	1.62	0.64
1:A:9:LYS:HE2	1:A:11:PHE:HE1	1.61	0.63
1:B:242:ASP:OD2	1:B:245:THR:HG22	1.99	0.63
1:A:15:LYS:HG3	1:A:44:ALA:CA	2.29	0.63
1:A:223:ARG:HB3	4:A:567:HOH:O	1.99	0.63
1:A:116:HIS:HE1	1:A:303:PRO:O	1.82	0.63
1:B:120:VAL:HG11	1:B:302:VAL:HG23	1.81	0.62
1:A:436:THR:O	1:A:437:LEU:HB2	1.99	0.62
1:A:216:VAL:O	1:A:220:ILE:HG12	1.99	0.62
1:A:185:MET:HB2	1:A:437:LEU:HD12	1.82	0.62
1:B:333:LEU:HB2	1:B:353:VAL:HG23	1.81	0.62
1:B:300:ASP:HB3	1:B:301:PRO:HD2	1.81	0.61
1:A:201:ASN:ND2	1:A:201:ASN:N	2.49	0.61
1:B:47:ARG:NH1	3:B:500:140:O2	2.32	0.60
1:A:290:VAL:HG22	1:A:313:TYR:CD2	2.36	0.60
1:B:1:THR:HA	4:B:601:HOH:O	2.00	0.60
1:B:68:ASP:HB3	1:B:334:TYR:CE1	2.36	0.60
1:B:38:GLU:HG2	4:B:550:HOH:O	2.02	0.60
1:A:290:VAL:HG22	1:A:313:TYR:CE2	2.36	0.60
1:A:205:PHE:HE1	1:A:209:ILE:HD11	1.65	0.60
1:A:24:LYS:N	1:A:25:PRO:HD3	2.16	0.60
1:A:77:PHE:CB	1:A:184:VAL:HG13	2.31	0.59
1:B:10:THR:CG2	1:B:11:PHE:H	2.14	0.59
1:A:196:PRO:HA	1:A:199:ASP:OD1	2.03	0.59
1:A:1:THR:HG21	4:A:577:HOH:O	2.01	0.58
1:A:23:ASP:C	1:A:25:PRO:HD3	2.23	0.58
1:B:290:VAL:HG22	1:B:313:TYR:CD2	2.40	0.57
1:B:116:HIS:CD2	1:B:408:HIS:HE2	2.18	0.57
1:A:277:LEU:HD22	1:A:417:MET:HE1	1.87	0.57
1:B:233:LEU:HD21	1:B:261:PHE:CD2	2.39	0.57
1:B:304:SER:OG	1:B:307:GLN:HG3	2.05	0.57
1:B:228:GLU:HG2	1:B:230:SER:H	1.70	0.57
1:A:226:SER:O	1:A:228:GLU:N	2.37	0.57
1:A:15:LYS:HG3	1:A:44:ALA:HA	1.87	0.57
1:B:3:LYS:HD2	1:B:344:GLU:OE1	2.05	0.57
1:B:3:LYS:HE3	4:B:627:HOH:O	2.05	0.57
1:A:306:LYS:O	1:A:310:GLN:HG3	2.05	0.56
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.88	0.56
1:B:436:THR:O	1:B:437:LEU:HB2	2.05	0.56
1:B:184:VAL:HG21	1:B:437:LEU:HD11	1.86	0.56
1:A:237:MET:HE1	1:A:257:GLN:HB2	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:306:LYS:HG3	4:A:537:HOH:O	2.05	0.56
1:A:103:LEU:C	1:A:105:PRO:HD2	2.26	0.56
1:A:190:ARG:HD3	1:A:198:TYR:CD1	2.41	0.56
1:B:47:ARG:NH2	4:B:639:HOH:O	2.39	0.56
1:A:329:PRO:HG3	1:A:439:LEU:HG	1.87	0.56
1:B:141:VAL:HB	1:B:142:PRO:CD	2.36	0.56
1:B:262:LEU:O	1:B:266:HIS:HD2	1.88	0.56
1:A:249:LEU:HD22	1:A:253:ASN:OD1	2.05	0.55
1:A:299:VAL:HG23	1:A:300:ASP:OD2	2.06	0.55
1:B:393:PHE:CE1	2:B:460:HEM:HBB2	2.41	0.55
1:A:295:THR:HG22	4:A:569:HOH:O	2.05	0.55
1:B:120:VAL:HG11	1:B:302:VAL:CG2	2.37	0.55
1:B:179:ARG:HB3	1:B:208:ASP:OD2	2.07	0.54
1:A:220:ILE:C	4:A:567:HOH:O	2.45	0.54
1:B:228:GLU:HG2	1:B:230:SER:CB	2.38	0.54
1:A:50:ARG:N	1:A:50:ARG:HD2	2.23	0.54
1:A:107:PHE:HZ	1:A:261:PHE:HE2	1.54	0.53
1:B:10:THR:O	1:B:11:PHE:HB2	2.08	0.53
1:B:7:GLN:HG3	1:B:41:LYS:O	2.09	0.53
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.43	0.53
1:A:254:ILE:O	1:A:258:ILE:HG13	2.09	0.53
1:A:320:GLU:HA	1:A:320:GLU:OE2	2.09	0.53
1:B:104:LEU:N	1:B:105:PRO:HD2	2.24	0.52
1:A:109:GLN:O	1:A:113:LYS:HG3	2.09	0.52
1:B:312:LYS:HG2	1:B:316:MET:CE	2.39	0.52
1:A:237:MET:CE	1:A:257:GLN:HB2	2.40	0.52
1:A:5:MET:HE1	1:A:50:ARG:HG2	1.91	0.52
1:B:429:TYR:CE2	1:B:431:LEU:HA	2.44	0.52
1:A:301:PRO:HB3	1:A:455:LEU:CG	2.39	0.52
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.75	0.52
1:A:9:LYS:HE2	1:A:11:PHE:CE1	2.45	0.51
1:A:201:ASN:ND2	1:A:201:ASN:H	2.06	0.51
1:B:320:GLU:OE2	1:B:320:GLU:HA	2.10	0.51
1:A:104:LEU:HD23	1:A:104:LEU:C	2.31	0.51
1:B:275:PHE:CE1	1:B:441:PRO:HG3	2.46	0.51
1:B:329:PRO:CG	1:B:439:LEU:HG	2.40	0.51
1:A:160:TYR:OH	1:A:218:LYS:HE3	2.11	0.51
1:B:110:GLN:HA	1:B:110:GLN:HE21	1.76	0.50
1:B:49:THR:HG21	1:B:354:MET:HE3	1.93	0.50
1:B:49:THR:HG23	4:B:502:HOH:O	2.11	0.50
1:A:49:THR:HB	4:A:552:HOH:O	2.11	0.50
1:B:329:PRO:HG3	1:B:439:LEU:CG	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:ASN:O	1:A:19:LEU:HD23	2.12	0.50
1:A:196:PRO:O	1:A:199:ASP:OD1	2.30	0.50
1:A:153:ILE:O	1:A:153:ILE:HD13	2.12	0.49
1:A:222:ASP:O	1:A:226:SER:OG	2.31	0.49
1:B:16:ASN:O	1:B:19:LEU:HB2	2.12	0.49
1:B:289:LYS:HD3	1:B:313:TYR:CZ	2.47	0.49
1:A:170:PRO:HG3	4:A:532:HOH:O	2.12	0.49
1:A:363:ASP:OD1	1:A:365:THR:N	2.45	0.49
1:A:128:GLN:HG2	1:A:132:ARG:CZ	2.42	0.49
1:A:205:PHE:O	1:A:209:ILE:HG13	2.12	0.49
1:B:10:THR:O	1:B:15:LYS:O	2.30	0.49
1:B:49:THR:HG21	1:B:354:MET:CE	2.41	0.49
1:A:289:LYS:HD3	1:A:313:TYR:CZ	2.47	0.49
1:A:148:LEU:CD2	1:A:413:VAL:HG21	2.37	0.49
1:A:21:ASN:N	1:A:189:GLN:OE1	2.46	0.49
1:B:9:LYS:HB3	1:B:11:PHE:CE1	2.48	0.49
1:A:329:PRO:O	1:A:358:PRO:HD3	2.12	0.49
1:A:86:LEU:HD11	1:A:103:LEU:HD12	1.95	0.49
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.78	0.49
1:A:435:GLU:HG2	1:A:439:LEU:CD2	2.43	0.48
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.95	0.48
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.12	0.48
1:B:280:LEU:HB3	1:B:287:LEU:HD13	1.96	0.48
1:A:275:PHE:CE1	1:A:441:PRO:HG3	2.49	0.48
1:A:64:GLU:OE1	1:A:397:GLN:HG2	2.13	0.47
1:A:15:LYS:HG3	1:A:44:ALA:C	2.34	0.47
1:A:291:ALA:O	1:A:295:THR:HG23	2.15	0.47
1:A:60:GLU:OE2	1:A:342:GLY:HA2	2.14	0.47
1:A:17:LEU:N	1:A:18:PRO:HD2	2.28	0.47
1:B:130:TRP:CD2	1:B:139:ILE:HD13	2.50	0.47
1:A:180:ALA:O	1:A:184:VAL:HG23	2.15	0.47
1:A:266:HIS:CG	1:A:267:GLU:N	2.83	0.47
1:B:393:PHE:HE1	2:B:460:HEM:HBB2	1.79	0.47
1:A:130:TRP:CE2	1:A:139:ILE:HD13	2.50	0.47
1:A:83:GLY:HA3	1:A:256:TYR:CE1	2.50	0.47
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.96	0.47
1:B:241:LYS:HG2	1:B:246:GLY:O	2.15	0.47
1:B:266:HIS:CG	1:B:267:GLU:N	2.84	0.46
1:B:312:LYS:HG2	1:B:316:MET:HE3	1.97	0.46
1:A:9:LYS:O	1:A:19:LEU:HD21	2.14	0.46
1:A:221:ALA:O	1:A:224:LYS:HB2	2.15	0.46
1:A:301:PRO:CB	1:A:455:LEU:HG	2.42	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:LYS:HE3	2:A:460:HEM:O1A	2.16	0.46
1:A:150:LEU:HD22	1:A:174:ILE:CD1	2.42	0.46
1:B:110:GLN:HA	1:B:110:GLN:NE2	2.31	0.46
1:B:272:LEU:HD13	1:B:322:LEU:CD2	2.46	0.46
1:A:233:LEU:HD21	1:A:261:PHE:CD2	2.51	0.45
1:A:373:GLU:OE1	1:A:375:ARG:HD3	2.16	0.45
1:A:104:LEU:N	1:A:105:PRO:CD	2.80	0.45
1:A:5:MET:HA	1:A:6:PRO:HD3	1.75	0.45
1:B:253:ASN:O	1:B:257:GLN:HG2	2.15	0.45
1:A:231:ASP:HA	1:A:235:THR:HG21	1.96	0.45
1:B:9:LYS:HB3	1:B:11:PHE:HE1	1.80	0.45
1:A:158:PHE:CE1	1:A:258:ILE:HG23	2.52	0.45
1:A:235:THR:C	1:A:237:MET:H	2.20	0.45
1:A:272:LEU:HD13	1:A:322:LEU:CD2	2.47	0.45
1:B:312:LYS:HE2	1:B:316:MET:CE	2.46	0.45
1:B:228:GLU:HG2	1:B:230:SER:HB3	2.00	0.45
1:A:244:GLU:O	1:A:244:GLU:HG3	2.17	0.44
1:A:226:SER:HB3	4:A:568:HOH:O	2.16	0.44
1:A:209:ILE:HG22	1:A:213:ASN:ND2	2.33	0.44
1:A:290:VAL:CG1	1:A:314:VAL:HG22	2.47	0.44
1:A:130:TRP:CD2	1:A:139:ILE:HD13	2.51	0.44
1:B:313:TYR:O	1:B:317:VAL:HG23	2.17	0.44
1:A:223:ARG:N	4:A:567:HOH:O	2.49	0.44
1:A:69:LYS:HA	1:A:333:LEU:HD23	2.00	0.43
1:A:49:THR:CB	4:A:552:HOH:O	2.67	0.43
1:B:20:LEU:HG	1:B:42:PHE:CZ	2.53	0.43
1:A:454:PRO:O	1:A:455:LEU:HB2	2.18	0.43
1:A:280:LEU:HB3	1:A:287:LEU:HD13	2.00	0.43
1:A:83:GLY:HA3	1:A:256:TYR:CD1	2.53	0.43
1:B:17:LEU:HB3	1:B:18:PRO:HD3	2.00	0.43
1:B:151:ASP:OD1	1:B:162:PHE:HB2	2.18	0.43
1:A:262:LEU:O	1:A:266:HIS:CD2	2.64	0.43
1:B:290:VAL:HG22	1:B:313:TYR:HE2	1.81	0.43
1:B:179:ARG:NE	1:B:204:GLN:OE1	2.52	0.43
1:B:20:LEU:HG	1:B:42:PHE:HZ	1.83	0.43
1:A:205:PHE:CD1	1:A:209:ILE:HD11	2.54	0.43
1:A:196:PRO:O	1:A:197:ALA:C	2.57	0.43
1:A:277:LEU:HD22	1:A:417:MET:CE	2.48	0.43
1:B:455:LEU:N	1:B:455:LEU:HD22	2.33	0.43
1:B:184:VAL:HG23	1:B:185:MET:N	2.32	0.43
1:B:49:THR:HG22	1:B:50:ARG:H	1.84	0.42
1:A:212:MET:O	1:A:216:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:LYS:HA	1:A:190:ARG:HG3	2.00	0.42
1:A:190:ARG:NH1	4:A:546:HOH:O	2.53	0.42
1:B:266:HIS:HE1	4:B:620:HOH:O	2.01	0.42
1:A:130:TRP:CZ2	1:A:139:ILE:HG21	2.54	0.42
1:B:60:GLU:OE2	1:B:342:GLY:HA2	2.19	0.42
1:A:118:MET:HE1	1:A:155:LEU:HG	2.00	0.42
1:B:387:GLN:O	1:B:388:HIS:HB2	2.19	0.42
1:B:357:ILE:HG22	1:B:361:HIS:CE1	2.54	0.42
1:A:14:LEU:C	1:A:15:LYS:HG2	2.39	0.42
1:A:15:LYS:O	1:A:18:PRO:HD2	2.19	0.42
1:B:118:MET:O	1:B:121:ASP:HB3	2.20	0.42
1:A:426:HIS:CE1	1:A:427:THR:HG23	2.55	0.42
1:B:265:GLY:HA2	2:B:460:HEM:C3C	2.55	0.42
1:A:61:ALA:O	1:A:333:LEU:HD13	2.20	0.42
1:A:250:ASP:O	1:A:254:ILE:HG13	2.20	0.42
1:A:17:LEU:HD21	1:A:189:GLN:O	2.20	0.41
1:A:219:ILE:C	1:A:221:ALA:H	2.21	0.41
1:A:138:TYR:CD1	1:A:138:TYR:C	2.94	0.41
1:B:64:GLU:OE2	1:B:397:GLN:HG2	2.20	0.41
1:A:434:LYS:HB2	1:A:442:GLU:HB2	2.01	0.41
1:A:2:ILE:CD1	1:A:2:ILE:H	2.15	0.41
1:B:385:ILE:HA	1:B:386:PRO:HD3	1.95	0.41
1:A:62:CYS:HB3	1:A:388:HIS:CE1	2.55	0.41
1:B:312:LYS:HG2	1:B:316:MET:HE2	2.01	0.41
1:A:260:THR:HA	3:A:500:140:H181	2.01	0.41
1:A:173:PHE:CG	1:A:215:LEU:HD22	2.55	0.41
1:A:363:ASP:CG	4:A:553:HOH:O	2.58	0.41
1:B:364:LYS:C	1:B:366:ILE:H	2.24	0.41
1:B:278:TYR:HA	1:B:444:PHE:CZ	2.55	0.41
1:B:72:SER:O	1:B:76:LYS:HG3	2.21	0.41
1:A:345:TYR:HA	1:A:346:PRO:HD2	1.96	0.41
1:A:242:ASP:C	1:A:244:GLU:H	2.24	0.41
1:A:232:ASP:O	1:A:235:THR:HB	2.20	0.41
1:A:440:LYS:HA	1:A:441:PRO:HD3	1.83	0.41
1:B:220:ILE:HG13	4:B:562:HOH:O	2.20	0.41
1:B:302:VAL:HG13	1:B:302:VAL:O	2.21	0.41
1:B:57:LEU:HD22	1:B:341:LEU:HG	2.03	0.41
1:B:10:THR:CG2	1:B:11:PHE:N	2.75	0.40
1:A:147:ARG:HG2	1:A:164:SER:HB3	2.03	0.40
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.55	0.40
1:B:366:ILE:HD12	1:B:386:PRO:HG2	2.04	0.40
1:A:62:CYS:HB2	1:A:388:HIS:ND1	2.37	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:TRP:HB2	1:A:93:GLU:HG3	2.02	0.40
1:B:223:ARG:C	1:B:225:ALA:H	2.24	0.40
1:A:377:GLU:O	1:A:380:GLU:HB2	2.20	0.40
1:A:16:ASN:C	1:A:18:PRO:HD2	2.42	0.40
1:A:190:ARG:HD3	1:A:198:TYR:CE1	2.57	0.40
1:B:272:LEU:HD13	1:B:322:LEU:HG	2.02	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	A	453/455 (100%)	402 (89%)	45 (10%)	6 (1%)	18	39
1	B	453/455 (100%)	421 (93%)	27 (6%)	5 (1%)	21	45
All	All	906/910 (100%)	823 (91%)	72 (8%)	11 (1%)	19	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	227	GLY
1	B	9	LYS
1	A	197	ALA
1	A	243	PRO
1	B	370	ASP
1	B	224	LYS
1	A	196	PRO
1	B	64	GLU
1	B	141	VAL
1	A	45	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	400/400 (100%)	383 (96%)	17 (4%)	40	70
1	B	400/400 (100%)	389 (97%)	11 (3%)	56	84
All	All	800/800 (100%)	772 (96%)	28 (4%)	48	78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	GLU
1	A	21	ASN
1	A	88	THR
1	A	128	GLN
1	A	151	ASP
1	A	153	ILE
1	A	195	ASP
1	A	196	PRO
1	A	201	ASN
1	A	206	GLN
1	A	217	ASP
1	A	222	ASP
1	A	226	SER
1	A	250	ASP
1	A	288	GLN
1	A	356	LEU
1	B	9	LYS
1	B	19	LEU
1	B	49	THR
1	B	68	ASP
1	B	104	LEU
1	B	148	LEU
1	B	204	GLN
1	B	228	GLU
1	B	241	LYS
1	B	266	HIS
1	B	353	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	7	GLN
1	A	21	ASN
1	A	100	HIS
1	A	116	HIS
1	A	201	ASN
1	A	213	ASN
1	A	229	GLN
1	A	257	GLN
1	A	266	HIS
1	A	288	GLN
1	A	388	HIS
1	A	403	GLN
1	A	426	HIS
1	B	21	ASN
1	B	95	ASN
1	B	110	GLN
1	B	116	HIS
1	B	189	GLN
1	B	201	ASN
1	B	213	ASN
1	B	257	GLN
1	B	266	HIS
1	B	288	GLN
1	B	359	GLN
1	B	388	HIS
1	B	403	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	#$|Z| > 2$
2	HEM	A	460	1	49,50,50	2.74	18 (36%)	46,82,82	1.29	4 (8%)
3	140	A	500	-	21,21,21	0.91	1 (4%)	22,22,22	0.79	0
2	HEM	B	460	1	49,50,50	2.08	14 (28%)	46,82,82	1.51	8 (17%)
3	140	B	500	-	21,21,21	1.55	2 (9%)	22,22,22	1.07	1 (4%)

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	460	1	-	0/14/114/114	0/0/8/8
3	140	A	500	-	-	0/20/20/20	0/0/0/0
2	HEM	B	460	1	-	0/14/114/114	0/0/8/8
3	140	B	500	-	-	0/20/20/20	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HEM	C3D-C4D	12.94	1.47	1.44
2	B	460	HEM	C2B-C1B	7.18	1.46	1.44
2	A	460	HEM	C2B-C1B	7.06	1.46	1.44
3	B	500	140	C2-C1	5.42	1.60	1.51
2	B	460	HEM	C3B-C2B	-4.57	1.35	1.43
2	A	460	HEM	CHB-C1B	4.21	1.41	1.35
2	B	460	HEM	C4A-C3A	4.11	1.45	1.40
2	A	460	HEM	CHA-C4D	3.75	1.41	1.35
2	A	460	HEM	C4A-C3A	3.72	1.44	1.40
2	B	460	HEM	CHD-C4C	3.57	1.42	1.36
3	B	500	140	C4-C3	3.47	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HEM	C3C-C2C	-3.31	1.38	1.43
2	B	460	HEM	C3C-C2C	-3.26	1.38	1.43
3	A	500	140	C2-C1	3.21	1.56	1.51
2	B	460	HEM	C3D-C2D	-3.19	1.38	1.43
2	A	460	HEM	C3D-C2D	-2.95	1.38	1.43
2	B	460	HEM	CHA-C4D	2.77	1.39	1.35
2	A	460	HEM	C3B-C2B	-2.76	1.38	1.43
2	B	460	HEM	CMC-C2C	2.66	1.55	1.47
2	B	460	HEM	CHB-C1B	2.55	1.39	1.35
2	B	460	HEM	C2D-C1D	2.55	1.45	1.44
2	B	460	HEM	CHC-C1C	2.52	1.40	1.36
2	B	460	HEM	FE-NA	2.37	2.02	1.92
2	A	460	HEM	CHC-C1C	2.36	1.40	1.36
2	A	460	HEM	CMB-C2B	2.29	1.54	1.47
2	A	460	HEM	C2D-C1D	2.29	1.45	1.44
2	A	460	HEM	C1A-C2A	2.24	1.47	1.43
2	A	460	HEM	CMC-C2C	2.21	1.54	1.47
2	A	460	HEM	C4A-NA	2.18	1.40	1.36
2	A	460	HEM	C1A-NA	2.16	1.40	1.36
2	A	460	HEM	CMD-C2D	2.11	1.54	1.47
2	B	460	HEM	CMB-C2B	2.11	1.53	1.47
2	B	460	HEM	C1A-NA	2.08	1.40	1.36
2	A	460	HEM	CHD-C4C	2.06	1.40	1.36
2	A	460	HEM	C1C-NC	2.02	1.40	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	HEM	C3B-C4B-NB	-5.71	109.91	114.00
2	A	460	HEM	C3B-C4B-NB	-4.39	110.86	114.00
3	B	500	140	C5-C4-C3	3.07	122.03	113.31
2	A	460	HEM	C3A-C4A-NA	3.01	111.68	109.41
2	B	460	HEM	C4A-CHB-C1B	-2.72	123.89	127.47
2	B	460	HEM	CMA-C3A-C4A	-2.67	124.51	128.62
2	B	460	HEM	CHC-C1C-NC	-2.65	122.43	124.73
2	B	460	HEM	C3A-C4A-NA	2.64	111.40	109.41
2	B	460	HEM	C4A-NA-C1A	-2.48	103.49	106.76
2	B	460	HEM	C1A-CHA-C4D	-2.24	124.53	127.47
2	B	460	HEM	C2D-C1D-ND	-2.15	110.39	112.93
2	A	460	HEM	C4A-NA-C1A	-2.04	104.08	106.76
2	A	460	HEM	C1A-CHA-C4D	-2.03	124.80	127.47

There are no chirality outliers.

There are no torsion outliers.

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	A	455/455 (100%)	-0.03	13 (2%)	49	53	35, 64, 114, 133	0
1	B	455/455 (100%)	-0.45	1 (0%)	93	96	33, 47, 68, 102	0
All	All	910/910 (100%)	-0.24	14 (1%)	68	73	33, 54, 102, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	4.1
1	A	229	GLN	4.0
1	A	102	ILE	3.9
1	B	229	GLN	3.7
1	A	14	LEU	3.7
1	A	197	ALA	3.0
1	A	196	PRO	2.7
1	A	193	PRO	2.6
1	A	240	GLY	2.4
1	A	45	PRO	2.4
1	A	239	ASN	2.3
1	A	231	ASP	2.2
1	A	13	GLU	2.2
1	A	243	PRO	2.0

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. 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
3	140	B	500	22/22	0.26	4.16	38,60,85,86	0
3	140	A	500	22/22	0.40	3.63	61,66,95,96	0
2	HEM	B	460	43/43	0.16	0.45	35,39,41,42	0
2	HEM	A	460	43/43	0.14	-0.73	54,58,62,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.