



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:39 PM GMT

PDB ID : 1R2C
Title : PHOTOSYNTHETIC REACTION CENTER BLASTOCHLORIS VIRIDIS (ATCC)
Authors : Baxter, R.H.; Ponomarenko, N.; Pahl, R.; Srajer, V.; Moffat, K.; Norris, J.R.
Deposited on : 2003-09-26
Resolution : 2.86 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>

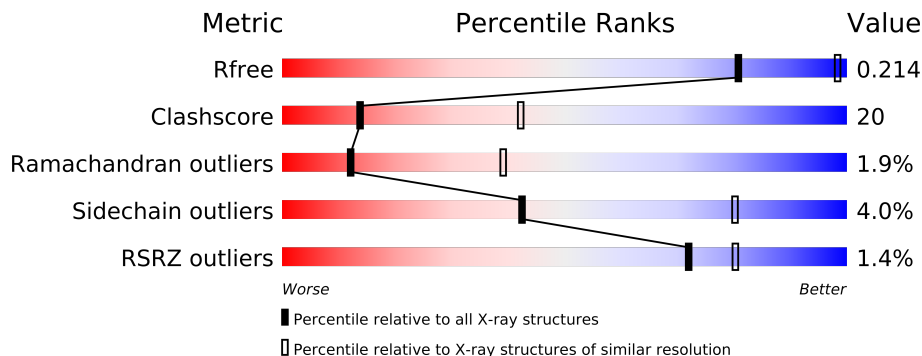
The following versions of software and data (see [references](#)) were used in the production of this report:

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)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.86 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	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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	L	273	
3	M	323	
4	H	258	

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	MQ7	M	501	-	X
11	UQ2	L	502	-	X
12	NS5	M	600	-	X
13	LDA	H	703	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	LDA	M	702	-	X
13	LDA	M	704	-	X
13	LDA	M	706	-	X
9	BPB	M	401	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 10140 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 precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	41	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	273	Total	C	N	O	S	10	0	0
			2171	1459	350	355	7			

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	323	Total	C	N	O	S	15	0	0
			2555	1702	419	423	11			

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	98	0	0
			2018	1292	344	380	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	MODIFIED RESIDUE	UNP P06008

- Molecule 5 is FE (II) ION (three-letter code: FE2) (formula: Fe).

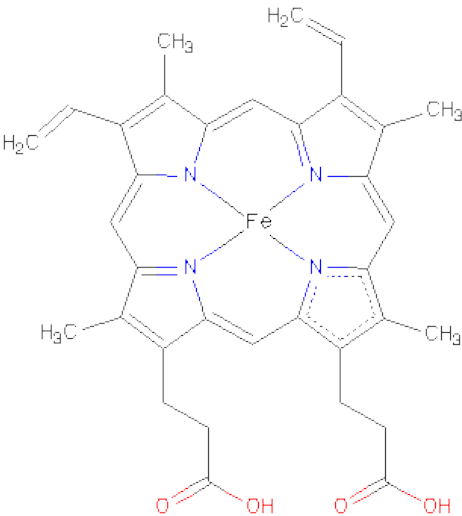
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Fe	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



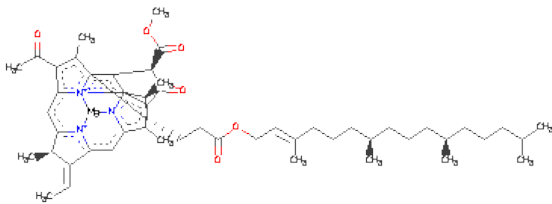
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



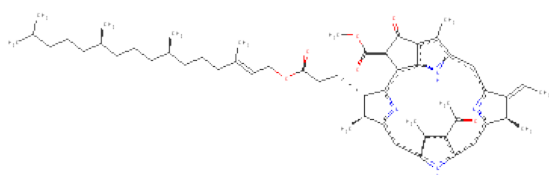
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



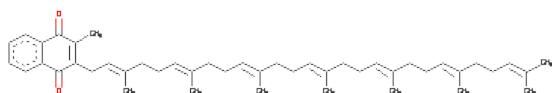
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	15	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



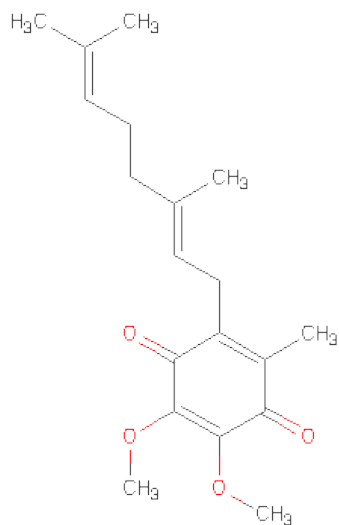
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



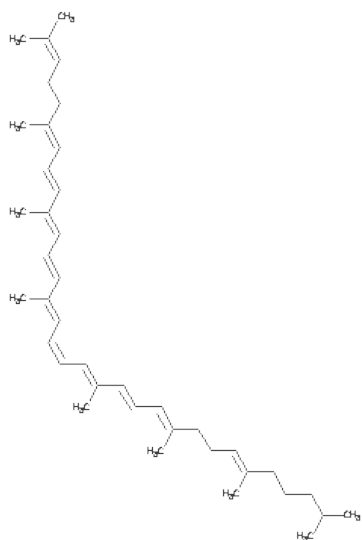
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	46	2		

- Molecule 11 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



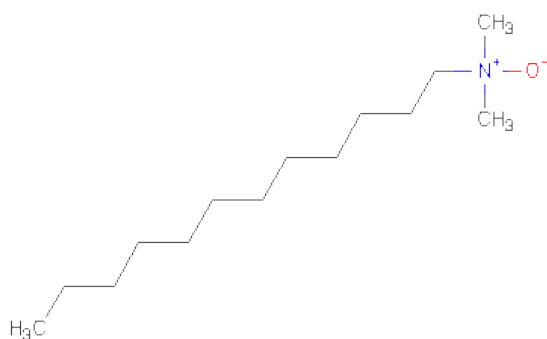
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 12 is 15-CIS-1,2-DIHYDRONEUROSPORENE (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C		11	0
			40	40			

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		

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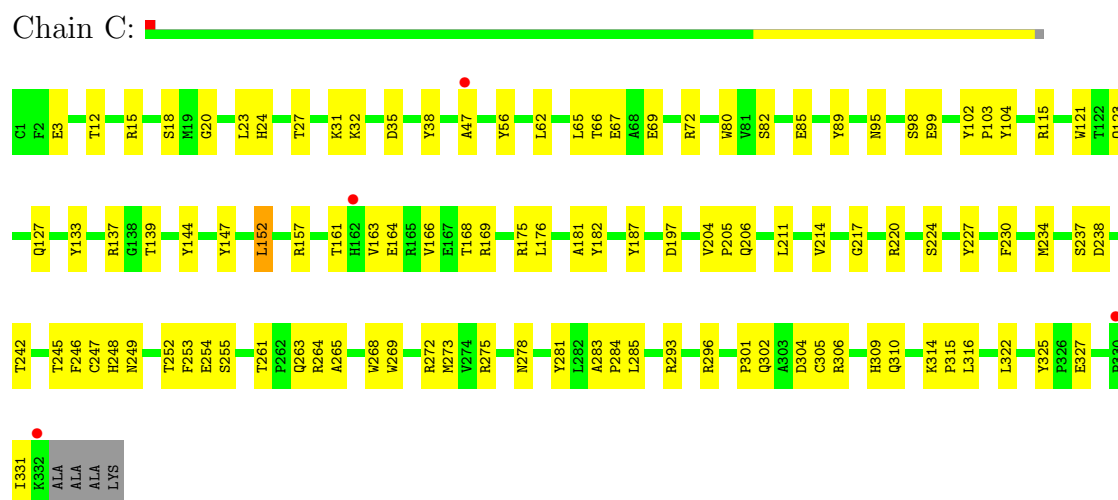
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	H	1	Total	C	N	O	0	0
			16	14	1	1		
13	M	1	Total	C	N	O	3	0
			16	14	1	1		
13	L	1	Total	C	N	O	3	0
			16	14	1	1		
13	M	1	Total	C	N	O	0	0
			16	14	1	1		

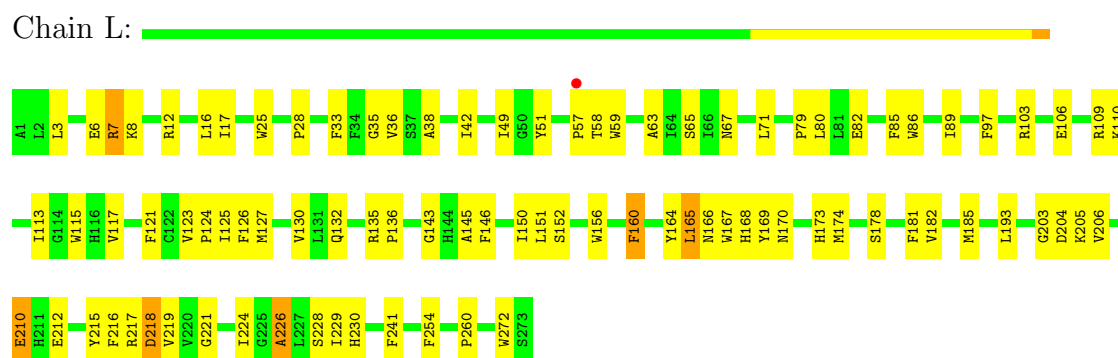
3 Residue-property plots

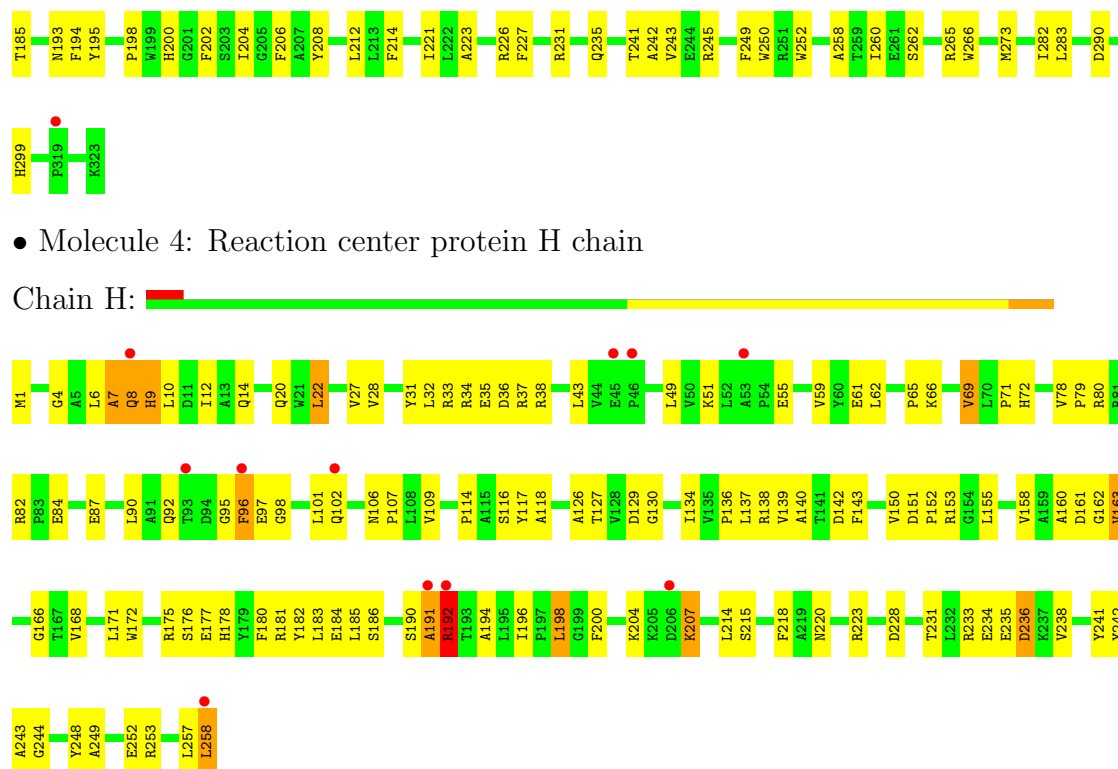
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 2: Reaction center protein L chain





• Molecule 4: Reaction center protein H chain

Chain H:

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50Å 223.50Å 112.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.86 48.83 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.83-2.86) 97.4 (48.83-2.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.228 0.190 , 0.214	Depositor DCC
R_{free} test set	6311 reflections (10.89%)	DCC
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 64248 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: LDA, BPB, BCB, FE2, SO4, MQ7, HEM, FME, UQ2, 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	0.35	0/2669	0.62	1/3637 (0.0%)
2	L	0.41	0/2259	0.60	0/3084
3	M	0.42	0/2659	0.58	0/3637
4	H	0.35	0/2055	0.62	0/2807
All	All	0.38	0/9642	0.61	1/13165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASN	N-CA-C	-6.50	93.44	111.00

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	2602	0	2579	74	0
2	L	2171	0	2098	90	0
3	M	2555	0	2452	112	0
4	H	2018	0	2020	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	1	0	0	0	0
6	H	5	0	0	0	0
6	M	15	0	0	0	0
7	C	172	0	120	7	0
8	L	132	0	144	22	0
8	M	132	0	143	29	0
9	L	65	0	74	12	0
9	M	65	0	74	22	0
10	M	48	0	64	0	0
11	L	23	0	26	4	0
12	M	40	0	60	5	0
13	H	16	0	31	4	0
13	L	16	0	31	2	0
13	M	64	0	124	11	0
All	All	10140	0	10040	393	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 20.

All (393) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:152:PRO:HA	4:H:155:LEU:HD12	1.31	1.05
9:M:401:BPB:H14	9:M:401:BPB:H17	1.39	1.03
3:M:32:PRO:HG3	3:M:48:PRO:HD3	1.39	1.02
8:L:302:BCB:HBA1	8:L:302:BCB:HBD	1.46	0.94
9:L:402:BPB:HBBA	3:M:208:TYR:HB3	1.47	0.94
2:L:182:VAL:HG22	8:M:1301:BCB:H12	1.49	0.94
1:C:152:LEU:HD22	1:C:175:ARG:HA	1.53	0.90
2:L:226:ALA:HA	11:L:502:UQ2:H3M2	1.57	0.86
9:L:402:BPB:HBBB	9:L:402:BPB:HHC	1.57	0.86
2:L:42:ILE:HD13	9:L:402:BPB:H4A	1.58	0.85
13:M:701:LDA:HM22	4:H:33:ARG:HE	1.45	0.81
13:M:702:LDA:H11	4:H:14:GLN:NE2	1.95	0.81
9:L:402:BPB:HBB	3:M:208:TYR:CD2	2.16	0.81
4:H:6:LEU:HB2	4:H:10:LEU:HD12	1.62	0.81
4:H:152:PRO:HG2	4:H:171:LEU:HD11	1.65	0.79
8:L:302:BCB:CBA	8:L:302:BCB:HBD	2.12	0.79
1:C:47:ALA:O	1:C:66:THR:HG21	1.84	0.78
3:M:79:PHE:O	3:M:81:PRO:HD3	1.84	0.78
4:H:258:LEU:HD23	4:H:258:LEU:H	1.48	0.77
1:C:62:LEU:HB3	1:C:65:LEU:HD12	1.67	0.77
9:M:401:BPB:H9A	9:M:401:BPB:H5	1.65	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:212:GLU:OE1	11:L:502:UQ2:H3M3	1.86	0.76
8:L:302:BCB:HBA1	8:L:302:BCB:CBD	2.16	0.76
4:H:231:THR:OG1	4:H:234:GLU:HG3	1.87	0.75
2:L:182:VAL:HG22	8:M:1301:BCB:C1	2.17	0.74
2:L:8:LYS:HD2	4:H:116:SER:HB3	1.67	0.74
9:L:402:BPB:CBB	3:M:208:TYR:HB3	2.17	0.74
4:H:33:ARG:HH11	4:H:33:ARG:HA	1.51	0.74
4:H:138:ARG:HD2	4:H:228:ASP:OD1	1.86	0.73
2:L:230:HIS:CD2	3:M:221:ILE:HG13	2.24	0.72
4:H:80:ARG:NH2	4:H:82:ARG:HD2	2.05	0.72
4:H:106:ASN:ND2	4:H:109:VAL:HG23	2.04	0.71
2:L:181:PHE:CD2	9:M:401:BPB:HBB	2.25	0.71
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.55	0.71
4:H:114:PRO:HB2	4:H:244:GLY:HA2	1.74	0.70
3:M:200:HIS:CE1	3:M:204:ILE:HD11	2.27	0.70
1:C:254:GLU:N	1:C:254:GLU:OE1	2.24	0.69
1:C:152:LEU:CD2	1:C:175:ARG:HA	2.23	0.69
2:L:178:SER:O	2:L:182:VAL:HG23	1.93	0.69
4:H:160:ALA:HB3	4:H:214:LEU:HD23	1.75	0.69
2:L:182:VAL:CG2	8:M:1301:BCB:H12	2.24	0.68
3:M:29:VAL:CG1	3:M:51:LEU:HD13	2.22	0.68
3:M:231:ARG:HH22	4:H:235:GLU:CD	1.96	0.68
3:M:132:TYR:CE1	3:M:142:THR:HG21	2.29	0.68
3:M:241:THR:O	3:M:245:ARG:HG3	1.95	0.67
2:L:7:ARG:HD3	4:H:101:LEU:HD11	1.76	0.67
3:M:29:VAL:HG12	3:M:51:LEU:HD13	1.75	0.67
2:L:12:ARG:HD3	4:H:102:GLN:HE21	1.60	0.67
2:L:7:ARG:CD	4:H:101:LEU:HD11	2.25	0.66
1:C:95:ASN:ND2	1:C:98:SER:HB2	2.10	0.66
9:M:401:BPB:HBBB	9:M:401:BPB:HHC	1.78	0.66
2:L:226:ALA:O	2:L:229:ILE:HG22	1.96	0.65
2:L:80:LEU:HD12	2:L:80:LEU:H	1.62	0.65
3:M:159:GLY:HA3	12:M:600:NS5:H272	1.79	0.65
2:L:224:ILE:HG12	2:L:228:SER:HB3	1.79	0.64
3:M:299:HIS:HB3	13:M:702:LDA:H22	1.79	0.64
4:H:138:ARG:HH22	4:H:184:GLU:CD	2.01	0.64
1:C:247:CYS:HA	1:C:261:THR:OG1	1.98	0.63
4:H:163:VAL:HG13	4:H:215:SER:HB3	1.81	0.63
1:C:82:SER:HB2	1:C:85:GLU:HB2	1.82	0.62
3:M:235:GLN:NE2	3:M:242:ALA:HB3	2.14	0.62
2:L:132:GLN:O	2:L:136:PRO:HG2	2.00	0.62
3:M:12:ALA:HB2	4:H:180:PHE:CE2	2.35	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:M:1303:BCB:HMB1	8:M:1303:BCB:CBB	2.30	0.61
4:H:152:PRO:CG	4:H:171:LEU:HD11	2.30	0.61
8:L:304:BCB:HBB3	8:L:304:BCB:HMB1	1.82	0.61
3:M:162:HIS:HB3	3:M:163:PRO:HD3	1.83	0.60
1:C:169:ARG:HD2	3:M:78:HIS:CD2	2.35	0.60
2:L:35:GLY:CA	2:L:103:ARG:HD2	2.31	0.60
2:L:181:PHE:HB3	9:M:401:BPB:CBB	2.31	0.60
3:M:22:GLU:HB3	3:M:23:TRP:CE3	2.35	0.60
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.37	0.60
3:M:22:GLU:HB3	3:M:23:TRP:HE3	1.66	0.60
8:M:1303:BCB:HBA2	8:M:1303:BCB:HMA2	1.83	0.60
2:L:182:VAL:HG13	8:M:1301:BCB:H43	1.82	0.60
4:H:234:GLU:O	4:H:238:VAL:HG23	2.02	0.60
1:C:95:ASN:HD22	1:C:98:SER:HB2	1.67	0.60
4:H:190:SER:O	4:H:192:ARG:HG3	2.02	0.60
8:L:302:BCB:H2C	8:M:1303:BCB:H2C	1.83	0.60
3:M:258:ALA:HB1	3:M:262:SER:OG	2.02	0.60
4:H:185:LEU:HD23	4:H:194:ALA:O	2.02	0.60
1:C:217:GLY:O	1:C:220:ARG:HG2	2.01	0.60
3:M:226:ARG:HD3	4:H:200:PHE:CZ	2.37	0.60
3:M:243:VAL:HG11	3:M:260:ILE:HB	1.84	0.59
8:M:1303:BCB:HMB1	8:M:1303:BCB:HBB3	1.84	0.59
1:C:123:GLN:HG3	1:C:269:TRP:CD2	2.38	0.59
9:L:402:BPB:HBBB	9:L:402:BPB:CHC	2.32	0.59
3:M:95:PRO:HD3	3:M:174:PRO:HB3	1.84	0.59
2:L:173:HIS:HD2	8:L:302:BCB:HED2	1.66	0.59
13:M:701:LDA:CM2	4:H:33:ARG:HE	2.15	0.59
4:H:117:TYR:HB2	4:H:236:ASP:HB3	1.83	0.58
3:M:147:ASN:C	3:M:147:ASN:HD22	2.07	0.58
1:C:152:LEU:HD22	1:C:175:ARG:HG2	1.85	0.58
4:H:139:VAL:HG21	4:H:228:ASP:HB3	1.86	0.58
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.39	0.58
3:M:155:VAL:HG21	8:M:1303:BCB:H8	1.84	0.58
8:L:304:BCB:HMB1	8:L:304:BCB:CBB	2.34	0.58
9:M:401:BPB:C14	9:M:401:BPB:H17	2.25	0.58
8:L:302:BCB:HMB1	8:L:302:BCB:CBB	2.34	0.58
1:C:281:TYR:O	1:C:285:LEU:HG	2.04	0.58
8:L:302:BCB:HMB1	8:L:302:BCB:HBB3	1.86	0.58
4:H:33:ARG:HH11	4:H:33:ARG:CA	2.16	0.58
1:C:123:GLN:HG3	1:C:269:TRP:CE3	2.39	0.58
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.85	0.58
1:C:224:SER:HA	1:C:227:TYR:HD1	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:173:HIS:CD2	8:L:302:BCB:HED2	2.39	0.57
3:M:231:ARG:NH2	4:H:235:GLU:OE1	2.37	0.57
4:H:62:LEU:O	13:H:703:LDA:H11	2.05	0.57
4:H:151:ASP:OD1	4:H:153:ARG:HB2	2.04	0.57
3:M:195:TYR:CE2	8:M:1303:BCB:HMC2	2.40	0.56
7:C:1204:HEM:HHA	7:C:1204:HEM:HBD1	1.86	0.56
2:L:168:HIS:CE1	8:L:302:BCB:HMC2	2.41	0.56
3:M:160:CYS:C	3:M:163:PRO:HD2	2.26	0.56
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.05	0.56
3:M:107:LEU:HA	3:M:111:GLY:HA3	1.86	0.56
1:C:99:GLU:HG2	1:C:104:TYR:CD1	2.40	0.56
3:M:2:ASP:OD1	3:M:4:GLN:HB2	2.04	0.56
1:C:65:LEU:HD11	1:C:327:GLU:HG2	1.87	0.56
4:H:161:ASP:HB3	4:H:214:LEU:HD22	1.87	0.56
4:H:59:VAL:O	13:H:703:LDA:H21	2.05	0.56
3:M:202:PHE:CE2	4:H:20:GLN:HG2	2.41	0.56
1:C:314:LYS:HE2	7:C:1204:HEM:O1D	2.06	0.55
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.87	0.55
2:L:169:TYR:CG	2:L:260:PRO:HG3	2.41	0.55
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.41	0.55
3:M:66:ILE:HD12	9:M:401:BPB:H7	1.89	0.55
3:M:265:ARG:HH11	3:M:265:ARG:HG2	1.71	0.55
2:L:8:LYS:HE3	4:H:84:GLU:OE1	2.06	0.55
4:H:65:PRO:HG3	13:H:703:LDA:H92	1.89	0.54
2:L:80:LEU:H	2:L:80:LEU:CD1	2.20	0.54
3:M:127:TRP:O	3:M:131:VAL:HG23	2.07	0.54
2:L:42:ILE:CD1	9:L:402:BPB:H4A	2.34	0.54
2:L:166:ASN:OD1	2:L:168:HIS:HB2	2.07	0.54
4:H:192:ARG:HD3	4:H:192:ARG:O	2.07	0.54
9:M:401:BPB:HMC	9:M:401:BPB:H55	1.90	0.54
3:M:34:TYR:N	3:M:34:TYR:CD1	2.75	0.54
2:L:241:PHE:CE2	9:L:402:BPB:H43	2.42	0.54
3:M:69:ILE:HG21	12:M:600:NS5:H111	1.89	0.54
3:M:206:PHE:CD2	3:M:273:MET:HB3	2.43	0.54
2:L:167:TRP:HE1	2:L:173:HIS:CD2	2.27	0.53
2:L:38:ALA:O	2:L:42:ILE:HG13	2.08	0.53
3:M:66:ILE:CD1	9:M:401:BPB:H7	2.38	0.53
2:L:35:GLY:HA2	2:L:103:ARG:HD2	1.91	0.53
4:H:8:GLN:O	4:H:10:LEU:N	2.42	0.53
2:L:185:MET:CE	8:M:1301:BCB:H42	2.39	0.53
1:C:325:TYR:HA	1:C:327:GLU:OE2	2.09	0.53
3:M:37:TRP:HA	3:M:40:LYS:HG3	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:166:GLY:HA3	4:H:186:SER:O	2.09	0.53
2:L:79:PRO:HG2	2:L:82:GLU:HB2	1.91	0.53
2:L:7:ARG:NE	4:H:101:LEU:HD11	2.24	0.53
1:C:56:TYR:HB3	7:C:1201:HEM:O2A	2.08	0.53
8:M:1301:BCB:HHC	8:M:1301:BCB:HBB2	1.91	0.52
4:H:106:ASN:HD22	4:H:109:VAL:HG23	1.73	0.52
2:L:165:LEU:HD23	2:L:165:LEU:N	2.24	0.52
1:C:230:PHE:CE2	3:M:185:THR:HG21	2.44	0.52
4:H:134:ILE:N	4:H:134:ILE:HD12	2.24	0.52
4:H:204:LYS:HB2	4:H:207:LYS:O	2.10	0.52
2:L:164:TYR:O	2:L:166:ASN:N	2.34	0.52
8:M:1301:BCB:HBB3	8:M:1303:BCB:H62	1.92	0.52
3:M:235:GLN:OE1	3:M:235:GLN:HA	2.09	0.52
1:C:211:LEU:HD12	4:H:1:FME:O	2.09	0.52
4:H:28:VAL:O	4:H:33:ARG:HG2	2.09	0.52
9:L:402:BPB:HBB	3:M:208:TYR:CG	2.43	0.51
3:M:206:PHE:CE2	3:M:273:MET:HB3	2.45	0.51
1:C:3:GLU:O	2:L:254:PHE:HA	2.10	0.51
1:C:166:VAL:HG22	1:C:296:ARG:NH1	2.25	0.51
13:M:702:LDA:H11	4:H:14:GLN:HE21	1.75	0.51
3:M:160:CYS:SG	12:M:600:NS5:H322	2.50	0.51
3:M:243:VAL:CG1	3:M:260:ILE:HB	2.40	0.51
3:M:178:TRP:HA	3:M:178:TRP:CE3	2.46	0.51
3:M:124:LEU:HD21	8:M:1303:BCB:H142	1.92	0.51
1:C:272:ARG:N	1:C:272:ARG:HD2	2.25	0.51
3:M:17:ILE:HG22	3:M:18:THR:N	2.25	0.51
2:L:121:PHE:O	2:L:124:PRO:HG2	2.10	0.51
13:M:702:LDA:H11	4:H:14:GLN:HE22	1.74	0.51
3:M:73:MET:O	3:M:76:GLU:HB2	2.11	0.51
3:M:282:ILE:HD11	8:M:1303:BCB:OBD	2.11	0.51
9:M:401:BPB:C14	9:M:401:BPB:H10	2.41	0.51
4:H:258:LEU:CD2	4:H:258:LEU:H	2.21	0.51
4:H:192:ARG:NH2	4:H:223:ARG:HG2	2.26	0.51
4:H:249:ALA:HB3	4:H:253:ARG:NH1	2.26	0.50
4:H:183:LEU:HG	4:H:198:LEU:HD13	1.93	0.50
4:H:90:LEU:HD13	4:H:101:LEU:HD13	1.93	0.50
1:C:197:ASP:HB3	1:C:275:ARG:HD3	1.93	0.50
3:M:15:PRO:HD3	4:H:142:ASP:HB2	1.94	0.50
2:L:151:LEU:HD21	13:M:702:LDA:H123	1.93	0.50
2:L:210:GLU:OE1	4:H:176:SER:HB3	2.12	0.50
3:M:198:PRO:HG3	13:M:702:LDA:H112	1.92	0.50
1:C:56:TYR:OH	1:C:67:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:38:ARG:HA	4:H:79:PRO:HB3	1.94	0.50
4:H:220:ASN:HB2	4:H:241:TYR:OH	2.11	0.50
4:H:138:ARG:NH2	4:H:184:GLU:OE1	2.42	0.49
1:C:27:THR:HG22	1:C:31:LYS:HE2	1.93	0.49
3:M:241:THR:HG22	4:H:236:ASP:OD2	2.12	0.49
3:M:173:VAL:HG22	3:M:183:TRP:CE2	2.48	0.49
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.47	0.49
3:M:87:GLN:O	3:M:91:LEU:HG	2.13	0.49
3:M:17:ILE:HD11	4:H:175:ARG:O	2.12	0.49
2:L:28:PRO:O	3:M:252:TRP:HA	2.13	0.49
3:M:178:TRP:HA	3:M:178:TRP:HE3	1.77	0.49
3:M:24:GLY:HA3	3:M:50:TYR:HE1	1.78	0.49
2:L:224:ILE:HG12	2:L:228:SER:CB	2.42	0.49
1:C:65:LEU:HD21	1:C:327:GLU:CG	2.43	0.49
3:M:21:GLY:C	3:M:23:TRP:N	2.66	0.49
4:H:158:VAL:HG21	4:H:207:LYS:HD3	1.95	0.48
8:L:304:BCB:HMD2	8:M:1303:BCB:HBB3	1.93	0.48
1:C:144:TYR:CD2	1:C:310:GLN:HG2	2.48	0.48
4:H:181:ARG:HH11	4:H:181:ARG:HG2	1.78	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.48	0.48
8:M:1303:BCB:H143	9:M:401:BPB:CBA	2.44	0.48
8:L:302:BCB:HBA1	8:L:302:BCB:CHA	2.44	0.48
3:M:146:TRP:HA	3:M:146:TRP:CE3	2.47	0.48
1:C:253:PHE:CZ	7:C:1203:HEM:HMB3	2.48	0.48
1:C:206:GLN:OE1	1:C:206:GLN:HA	2.14	0.48
4:H:192:ARG:HD3	4:H:192:ARG:C	2.34	0.48
4:H:134:ILE:HG22	4:H:172:TRP:HE3	1.79	0.48
3:M:157:CYS:HA	3:M:161:ILE:HB	1.96	0.48
3:M:204:ILE:HG23	8:M:1303:BCB:HMB3	1.96	0.48
9:M:401:BPB:H14B	9:M:401:BPB:H10	1.96	0.47
4:H:27:VAL:O	4:H:31:TYR:HB3	2.14	0.47
8:M:1303:BCB:OBB	8:M:1303:BCB:HHC	2.14	0.47
3:M:59:PHE:HA	9:M:401:BPB:H4A	1.96	0.47
4:H:137:LEU:HA	4:H:140:ALA:HB3	1.97	0.47
2:L:3:LEU:HB2	2:L:6:GLU:HB2	1.95	0.47
4:H:10:LEU:O	4:H:10:LEU:HD12	2.14	0.47
1:C:65:LEU:HD21	1:C:327:GLU:HG2	1.96	0.47
1:C:12:THR:HG23	1:C:20:GLY:HA2	1.95	0.47
3:M:62:GLY:O	3:M:65:ALA:HB3	2.15	0.47
2:L:97:PHE:CE1	8:L:302:BCB:H101	2.50	0.47
3:M:69:ILE:O	3:M:73:MET:HG3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:127:THR:O	4:H:129:ASP:N	2.47	0.47
2:L:217:ARG:O	2:L:221:GLY:HA2	2.15	0.47
1:C:181:ALA:O	1:C:182:TYR:HB2	2.14	0.47
4:H:6:LEU:O	4:H:7:ALA:O	2.33	0.47
1:C:66:THR:OG1	1:C:69:GLU:HG3	2.15	0.47
1:C:18:SER:HB2	2:L:156:TRP:CD1	2.50	0.47
2:L:109:ARG:HD3	2:L:115:TRP:CZ2	2.50	0.47
3:M:212:LEU:C	3:M:212:LEU:HD23	2.35	0.47
8:L:302:BCB:OBB	8:L:302:BCB:HHC	2.14	0.46
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.97	0.46
2:L:193:LEU:HD13	2:L:216:PHE:CE2	2.50	0.46
9:M:401:BPB:H6A	9:M:401:BPB:H4	1.55	0.46
2:L:210:GLU:OE1	2:L:210:GLU:N	2.49	0.46
4:H:196:ILE:HA	4:H:242:TYR:CE2	2.51	0.46
2:L:80:LEU:HD12	2:L:80:LEU:N	2.29	0.46
1:C:252:THR:HG23	1:C:255:SER:HB2	1.97	0.46
1:C:247:CYS:HA	1:C:261:THR:HG1	1.80	0.46
2:L:85:PHE:O	2:L:89:ILE:HG13	2.16	0.46
2:L:123:VAL:N	2:L:124:PRO:HD2	2.30	0.46
8:M:1303:BCB:HAA2	8:M:1303:BCB:HBD	1.97	0.46
12:M:600:NS5:H29	12:M:600:NS5:H271	1.83	0.46
2:L:205:LYS:HA	4:H:69:VAL:HG13	1.96	0.46
13:L:705:LDA:HM22	13:L:705:LDA:H31	1.98	0.45
3:M:241:THR:N	4:H:118:ALA:HB2	2.31	0.45
3:M:21:GLY:C	3:M:23:TRP:H	2.18	0.45
4:H:107:PRO:HB2	4:H:248:TYR:CD2	2.51	0.45
2:L:117:VAL:HG11	3:M:249:PHE:CE2	2.52	0.45
4:H:248:TYR:O	4:H:249:ALA:C	2.54	0.45
3:M:29:VAL:HG11	3:M:51:LEU:HD13	1.98	0.45
2:L:65:SER:OG	2:L:67:ASN:OD1	2.28	0.45
8:L:304:BCB:HHC	8:L:304:BCB:OBB	2.16	0.45
3:M:195:TYR:CZ	8:M:1303:BCB:HMC2	2.52	0.45
2:L:165:LEU:H	2:L:165:LEU:HD23	1.82	0.45
4:H:66:LYS:HG2	4:H:78:VAL:HG23	1.97	0.45
9:L:402:BPB:HEDB	3:M:250:TRP:CZ3	2.52	0.45
2:L:168:HIS:HE2	8:L:302:BCB:HHC	1.82	0.45
2:L:212:GLU:HB3	11:L:502:UQ2:H2M3	1.98	0.44
4:H:33:ARG:O	4:H:37:ARG:HG3	2.17	0.44
3:M:227:PHE:CE1	4:H:243:ALA:HB2	2.52	0.44
4:H:215:SER:O	4:H:218:PHE:HB2	2.17	0.44
2:L:215:TYR:O	2:L:219:VAL:HG23	2.17	0.44
3:M:69:ILE:HG21	12:M:600:NS5:C11	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:52:GLY:O	3:M:56:ILE:HG13	2.17	0.44
1:C:293:ARG:NE	7:C:1202:HEM:O2A	2.49	0.44
2:L:146:PHE:HB3	2:L:156:TRP:CD2	2.53	0.44
2:L:206:VAL:O	4:H:71:PRO:HB3	2.17	0.44
9:M:401:BPB:CBC	9:M:401:BPB:HMC	2.47	0.44
9:L:402:BPB:CBB	3:M:208:TYR:CD2	2.95	0.44
1:C:204:VAL:HA	1:C:205:PRO:HD3	1.86	0.44
1:C:127:GLN:O	1:C:322:LEU:HD22	2.18	0.44
1:C:176:LEU:HD11	1:C:187:TYR:O	2.18	0.44
1:C:237:SER:HB3	1:C:242:THR:O	2.17	0.44
4:H:127:THR:C	4:H:129:ASP:N	2.71	0.44
4:H:8:GLN:O	4:H:9:HIS:C	2.55	0.43
4:H:143:PHE:CE1	4:H:175:ARG:HG2	2.53	0.43
1:C:147:TYR:CE1	1:C:301:PRO:HG3	2.53	0.43
1:C:245:THR:HA	1:C:248:HIS:O	2.18	0.43
3:M:184:LEU:HD21	8:M:1301:BCB:CAC	2.48	0.43
3:M:181:ILE:HD12	8:M:1301:BCB:CED	2.47	0.43
3:M:132:TYR:O	3:M:135:ALA:HB3	2.19	0.43
3:M:7:TYR:HB2	3:M:40:LYS:O	2.18	0.43
4:H:142:ASP:OD2	4:H:142:ASP:N	2.46	0.43
2:L:185:MET:HE3	8:M:1301:BCB:H42	2.00	0.43
3:M:2:ASP:OD1	3:M:5:THR:HG23	2.17	0.43
9:M:401:BPB:H19A	9:M:401:BPB:H15A	1.99	0.43
1:C:139:THR:HG23	1:C:157:ARG:NH2	2.33	0.43
4:H:22:LEU:HD22	4:H:22:LEU:HA	1.89	0.43
9:M:401:BPB:CHC	9:M:401:BPB:HBBB	2.48	0.43
2:L:218:ASP:O	3:M:50:TYR:HB3	2.18	0.43
2:L:86:TRP:CZ2	2:L:145:ALA:CB	3.01	0.43
8:L:304:BCB:HMD1	3:M:204:ILE:HD13	2.01	0.43
13:L:705:LDA:H32	13:M:701:LDA:HM11	1.99	0.43
3:M:55:GLY:O	3:M:59:PHE:HD1	2.01	0.43
1:C:247:CYS:HB3	1:C:264:ARG:HB2	1.99	0.43
3:M:1:ALA:O	3:M:3:TYR:N	2.52	0.43
3:M:77:VAL:HG21	3:M:84:PHE:HB2	2.00	0.43
2:L:135:ARG:CZ	2:L:160:PHE:CZ	3.01	0.43
3:M:11:GLN:O	4:H:180:PHE:HE2	2.01	0.43
3:M:265:ARG:NH1	3:M:265:ARG:HG2	2.32	0.43
3:M:62:GLY:HA3	9:M:401:BPB:H6	2.01	0.42
1:C:305:CYS:SG	7:C:1204:HEM:HMB2	2.59	0.42
2:L:113:ILE:HB	3:M:223:ALA:O	2.19	0.42
2:L:181:PHE:HD2	9:M:401:BPB:HBB	1.77	0.42
4:H:35:GLU:C	4:H:37:ARG:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:37:ARG:HD2	4:H:61:GLU:HB2	2.01	0.42
4:H:182:TYR:OH	4:H:235:GLU:HB3	2.19	0.42
4:H:180:PHE:O	4:H:198:LEU:HD23	2.19	0.42
4:H:136:PRO:HA	4:H:172:TRP:HA	2.01	0.42
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.19	0.42
4:H:152:PRO:O	4:H:168:VAL:HB	2.19	0.42
3:M:226:ARG:HD3	4:H:200:PHE:CE1	2.55	0.42
4:H:78:VAL:HA	4:H:79:PRO:C	2.39	0.42
2:L:58:THR:OG1	2:L:59:TRP:N	2.52	0.42
3:M:283:LEU:HD23	3:M:283:LEU:HA	1.88	0.42
1:C:115:ARG:NH1	1:C:331:ILE:HG13	2.35	0.42
8:L:304:BCB:H8	8:L:304:BCB:H51	1.92	0.42
2:L:150:ILE:O	8:L:304:BCB:HED1	2.19	0.42
8:M:1303:BCB:H143	9:M:401:BPB:HBA	2.02	0.42
4:H:4:GLY:O	4:H:12:ILE:HG12	2.20	0.42
2:L:25:TRP:O	4:H:98:GLY:HA3	2.20	0.42
2:L:167:TRP:NE1	2:L:173:HIS:CD2	2.88	0.42
8:M:1301:BCB:HBB3	8:M:1303:BCB:C6	2.49	0.42
4:H:72:HIS:CD2	4:H:126:ALA:HB3	2.55	0.42
3:M:38:LEU:HD22	3:M:46:ILE:HD11	2.01	0.42
1:C:246:PHE:CZ	1:C:263:GLN:HG2	2.55	0.42
4:H:106:ASN:HA	4:H:107:PRO:HD2	1.85	0.42
1:C:234:MET:SD	2:L:165:LEU:HB3	2.60	0.42
3:M:125:GLY:O	3:M:129:ILE:HG12	2.20	0.42
2:L:126:PHE:O	2:L:130:VAL:HG23	2.20	0.41
1:C:238:ASP:OD2	1:C:306:ARG:NH2	2.53	0.41
4:H:106:ASN:HD22	4:H:109:VAL:CG2	2.32	0.41
1:C:3:GLU:HB3	1:C:24:HIS:CE1	2.55	0.41
1:C:252:THR:HG23	1:C:252:THR:O	2.20	0.41
9:M:401:BPB:H44	9:M:401:BPB:HBA	1.56	0.41
4:H:6:LEU:HD11	4:H:12:ILE:HD13	2.02	0.41
3:M:29:VAL:HG22	3:M:30:GLY:N	2.34	0.41
1:C:163:VAL:HA	1:C:168:THR:HG21	2.03	0.41
2:L:33:PHE:O	2:L:36:VAL:HB	2.20	0.41
3:M:20:SER:HA	3:M:25:ASP:OD2	2.20	0.41
8:L:302:BCB:C1	8:L:304:BCB:H2C	2.50	0.41
2:L:215:TYR:OH	3:M:131:VAL:HG13	2.20	0.41
1:C:72:ARG:HG2	1:C:72:ARG:HH11	1.86	0.41
4:H:177:GLU:O	4:H:178:HIS:HB2	2.20	0.41
3:M:299:HIS:HB3	13:M:702:LDA:C2	2.46	0.41
3:M:258:ALA:HA	4:H:36:ASP:HB3	2.03	0.41
3:M:258:ALA:HB1	3:M:262:SER:HG	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:231:ARG:NH2	4:H:235:GLU:CD	2.68	0.41
3:M:155:VAL:HG22	8:M:1301:BCB:HBB1	2.01	0.41
4:H:6:LEU:HB2	4:H:10:LEU:CD1	2.41	0.41
2:L:12:ARG:HG3	2:L:12:ARG:HH11	1.86	0.41
2:L:58:THR:HG21	2:L:63:ALA:HB3	2.03	0.41
2:L:127:MET:CE	2:L:130:VAL:HB	2.50	0.41
1:C:265:ALA:O	1:C:268:TRP:HB3	2.21	0.41
3:M:10:ILE:HD13	4:H:152:PRO:HD3	2.03	0.41
3:M:183:TRP:CZ3	3:M:184:LEU:HD23	2.55	0.41
2:L:181:PHE:HB3	9:M:401:BPB:HBBB	2.03	0.41
3:M:124:LEU:CD2	8:M:1303:BCB:H142	2.50	0.41
2:L:110:LYS:O	4:H:114:PRO:HG3	2.20	0.41
4:H:65:PRO:CG	13:H:703:LDA:H92	2.50	0.41
3:M:266:TRP:CE3	4:H:32:LEU:HD13	2.56	0.41
2:L:16:LEU:HD13	2:L:106:GLU:HG2	2.03	0.41
1:C:65:LEU:HD22	1:C:69:GLU:HB3	2.03	0.41
8:L:302:BCB:H41	8:L:302:BCB:H62	1.90	0.40
1:C:137:ARG:CG	1:C:310:GLN:HE22	2.34	0.40
2:L:203:GLY:O	4:H:69:VAL:HG11	2.21	0.40
1:C:121:TRP:CE3	1:C:273:MET:HB2	2.56	0.40
2:L:121:PHE:CE2	2:L:125:ILE:HD11	2.56	0.40
4:H:181:ARG:HG2	4:H:181:ARG:NH1	2.36	0.40
3:M:71:PHE:CD2	13:M:706:LDA:H71	2.57	0.40
9:L:402:BPB:HHC	9:L:402:BPB:CBB	2.35	0.40
4:H:150:VAL:CG1	4:H:151:ASP:N	2.84	0.40
1:C:56:TYR:HB3	7:C:1201:HEM:CGA	2.51	0.40
3:M:178:TRP:N	3:M:179:PRO:CD	2.85	0.40
2:L:115:TRP:CD1	2:L:115:TRP:N	2.89	0.40
3:M:41:ILE:HD12	3:M:41:ILE:C	2.41	0.40
3:M:204:ILE:HG12	8:M:1303:BCB:CHB	2.51	0.40
2:L:224:ILE:HB	11:L:502:UQ2:H112	2.03	0.40
1:C:85:GLU:HG2	1:C:89:TYR:CD1	2.56	0.40
4:H:231:THR:O	4:H:234:GLU:N	2.55	0.40
4:H:191:ALA:O	4:H:192:ARG:HB3	2.21	0.40
1:C:304:ASP:C	1:C:304:ASP:OD1	2.60	0.40
2:L:170:ASN:O	2:L:174:MET:HG3	2.22	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%)	299 (91%)	30 (9%)	1 (0%)	50	84
2	L	271/273 (99%)	251 (93%)	17 (6%)	3 (1%)	21	57
3	M	321/323 (99%)	299 (93%)	19 (6%)	3 (1%)	25	62
4	H	256/258 (99%)	216 (84%)	25 (10%)	15 (6%)	2	6
All	All	1178/1190 (99%)	1065 (90%)	91 (8%)	22 (2%)	12	39

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	57	PRO
4	H	7	ALA
4	H	8	GLN
4	H	9	HIS
4	H	96	PHE
4	H	257	LEU
2	L	165	LEU
3	M	2	ASP
3	M	177	ILE
4	H	49	LEU
4	H	130	GLY
4	H	162	GLY
4	H	163	VAL
2	L	226	ALA
4	H	55	GLU
4	H	191	ALA
4	H	95	GLY
4	H	192	ARG
4	H	51	LYS
3	M	193	ASN
4	H	43	LEU
1	C	214	VAL

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	281/282 (100%)	276 (98%)	5 (2%)	71	94
2	L	218/218 (100%)	209 (96%)	9 (4%)	41	79
3	M	249/249 (100%)	239 (96%)	10 (4%)	42	80
4	H	212/212 (100%)	198 (93%)	14 (7%)	24	55
All	All	960/961 (100%)	922 (96%)	38 (4%)	42	80

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	23	LEU
1	C	32	LYS
1	C	38	TYR
1	C	152	LEU
2	L	7	ARG
2	L	17	ILE
2	L	51	TYR
2	L	152	SER
2	L	160	PHE
2	L	204	ASP
2	L	210	GLU
2	L	218	ASP
2	L	272	TRP
3	M	22	GLU
3	M	27	ASP
3	M	34	TYR
3	M	51	LEU
3	M	147	ASN
3	M	178	TRP
3	M	181	ILE
3	M	194	PHE
3	M	214	PHE
3	M	290	ASP
4	H	22	LEU
4	H	34	ARG

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Mol	Chain	Res	Type
4	H	69	VAL
4	H	87	GLU
4	H	92	GLN
4	H	96	PHE
4	H	97	GLU
4	H	192	ARG
4	H	198	LEU
4	H	207	LYS
4	H	233	ARG
4	H	236	ASP
4	H	252	GLU
4	H	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	24	HIS
1	C	58	ASN
1	C	95	ASN
1	C	302	GLN
1	C	310	GLN
2	L	183	ASN
2	L	213	ASN
2	L	239	ASN
3	M	16	HIS
3	M	147	ASN
4	H	8	GLN
4	H	58	GLN
4	H	72	HIS
4	H	102	GLN
4	H	106	ASN
4	H	220	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	$\# Z > 2$
4	FME	H	1	4	9,9,10	5.82	2 (22%)	6,9,11	3.40	3 (50%)

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
4	FME	H	1	4	-	0/7/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	FME	O-C	17.19	1.23	1.11
4	H	1	FME	CA-C	2.56	1.53	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	CA-N-CN	-6.79	111.74	122.97
4	H	1	FME	O1-CN-N	-3.39	114.75	125.12
4	H	1	FME	CE-SD-CG	-3.00	89.07	100.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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$
7	HEM	C	1201	1	49,50,50	2.08	11 (22%)	46,82,82	1.26	4 (8%)
7	HEM	C	1202	1	49,50,50	1.96	11 (22%)	46,82,82	1.35	3 (6%)
7	HEM	C	1203	1	49,50,50	1.97	12 (24%)	46,82,82	1.32	6 (13%)
7	HEM	C	1204	1	49,50,50	2.25	13 (26%)	46,82,82	1.53	8 (17%)
13	LDA	H	703	-	15,15,15	4.87	3 (20%)	17,17,17	1.50	1 (5%)
6	SO4	H	801	-	4,4,4	0.79	0	6,6,6	0.35	0
8	BCB	L	302	2	74,74,74	1.72	13 (17%)	94,115,115	2.09	25 (26%)
8	BCB	L	304	2	74,74,74	1.72	14 (18%)	94,115,115	1.90	17 (18%)
9	BPB	L	402	-	70,70,70	1.74	11 (15%)	93,101,101	2.45	23 (24%)
11	UQ2	L	502	-	23,23,23	1.73	5 (21%)	31,31,31	1.26	3 (9%)
13	LDA	L	705	-	15,15,15	4.14	2 (13%)	17,17,17	2.65	1 (5%)
8	BCB	M	1301	3	74,74,74	1.71	12 (16%)	94,115,115	1.70	15 (15%)
8	BCB	M	1303	3	74,74,74	1.77	14 (18%)	94,115,115	1.75	19 (20%)
9	BPB	M	401	-	70,70,70	1.80	12 (17%)	93,101,101	2.12	24 (25%)
10	MQ7	M	501	-	49,49,49	1.73	13 (26%)	63,63,63	1.55	8 (12%)
12	NS5	M	600	-	39,39,39	0.78	0	46,46,46	1.04	4 (8%)
13	LDA	M	701	-	15,15,15	4.71	3 (20%)	17,17,17	1.53	1 (5%)
13	LDA	M	702	-	15,15,15	4.27	1 (6%)	17,17,17	1.99	1 (5%)
13	LDA	M	704	-	15,15,15	4.81	4 (26%)	17,17,17	1.68	1 (5%)
13	LDA	M	706	-	15,15,15	4.61	2 (13%)	17,17,17	1.23	1 (5%)
6	SO4	M	802	-	4,4,4	1.13	0	6,6,6	0.42	0
6	SO4	M	803	-	4,4,4	1.04	0	6,6,6	0.07	0
6	SO4	M	804	-	4,4,4	1.11	0	6,6,6	0.27	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
7	HEM	C	1201	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1202	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1203	1	-	0/14/114/114	0/0/8/8
7	HEM	C	1204	1	-	0/14/114/114	0/0/8/8
13	LDA	H	703	-	-	0/13/13/13	0/0/0/0
6	SO4	H	801	-	-	0/0/0/0	0/0/0/0
8	BCB	L	302	2	-	0/41/137/137	0/0/9/9
8	BCB	L	304	2	1/1/21/26	0/41/137/137	0/0/9/9
9	BPB	L	402	-	-	0/52/105/105	0/0/6/6
11	UQ2	L	502	-	-	0/15/39/39	0/1/1/1
13	LDA	L	705	-	-	0/13/13/13	0/0/0/0
8	BCB	M	1301	3	-	0/41/137/137	0/0/9/9
8	BCB	M	1303	3	1/1/21/26	0/41/137/137	0/0/9/9
9	BPB	M	401	-	1/1/18/23	0/52/105/105	0/0/6/6
10	MQ7	M	501	-	-	0/41/61/61	0/0/2/2
12	NS5	M	600	-	-	0/43/43/43	0/0/0/0
13	LDA	M	701	-	-	0/13/13/13	0/0/0/0
13	LDA	M	702	-	-	0/13/13/13	0/0/0/0
13	LDA	M	704	-	-	0/13/13/13	0/0/0/0
13	LDA	M	706	-	-	0/13/13/13	0/0/0/0
6	SO4	M	802	-	-	0/0/0/0	0/0/0/0
6	SO4	M	803	-	-	0/0/0/0	0/0/0/0
6	SO4	M	804	-	-	0/0/0/0	0/0/0/0

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	H	703	LDA	O1-N1	-18.37	1.22	1.39
13	M	704	LDA	O1-N1	-18.07	1.22	1.39
13	M	701	LDA	O1-N1	-17.72	1.22	1.39
13	M	706	LDA	O1-N1	-17.48	1.22	1.39
13	M	702	LDA	O1-N1	-16.30	1.24	1.39
13	L	705	LDA	O1-N1	-15.55	1.24	1.39
8	M	1303	BCB	C4D-CHA	-7.61	1.35	1.45
9	L	402	BPB	CHD-C4C	7.31	1.40	1.35
9	M	401	BPB	CHD-C4C	6.38	1.39	1.35
8	L	302	BCB	C4D-CHA	-6.25	1.37	1.45
7	C	1204	HEM	C3D-C4D	5.90	1.46	1.44
8	L	304	BCB	C4D-CHA	-5.59	1.38	1.45
9	M	401	BPB	CAC-C3C	5.58	1.40	1.33
8	M	1301	BCB	C4D-CHA	-5.37	1.38	1.45
11	L	502	UQ2	C7-C8	-5.21	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1204	HEM	C3B-C2B	-4.95	1.35	1.43
8	M	1301	BCB	C1D-C2D	4.92	1.46	1.40
7	C	1204	HEM	C3C-C2C	-4.88	1.35	1.43
8	M	1303	BCB	C1D-C2D	4.86	1.46	1.40
7	C	1202	HEM	C3C-C2C	-4.82	1.35	1.43
9	L	402	BPB	CAC-C3C	4.80	1.39	1.33
7	C	1204	HEM	C3D-C2D	-4.79	1.35	1.43
7	C	1203	HEM	C3B-C2B	-4.75	1.35	1.43
7	C	1201	HEM	C3D-C2D	-4.73	1.35	1.43
9	M	401	BPB	C4B-CHC	4.67	1.40	1.35
7	C	1201	HEM	C3B-C2B	-4.65	1.35	1.43
7	C	1203	HEM	C3D-C2D	-4.64	1.35	1.43
7	C	1201	HEM	C3C-C2C	-4.63	1.35	1.43
7	C	1202	HEM	C3D-C2D	-4.63	1.35	1.43
8	M	1301	BCB	CAC-C3C	4.60	1.39	1.33
7	C	1202	HEM	C3B-C2B	-4.52	1.35	1.43
8	L	304	BCB	C1D-C2D	4.52	1.45	1.40
7	C	1203	HEM	C3C-C2C	-4.48	1.35	1.43
7	C	1204	HEM	CBC-CAC	4.45	1.54	1.28
8	L	304	BCB	O2A-CGA	4.45	1.47	1.33
7	C	1201	HEM	C3B-CAB	4.44	1.54	1.40
7	C	1202	HEM	CBC-CAC	4.33	1.54	1.28
7	C	1204	HEM	CBB-CAB	4.28	1.53	1.28
7	C	1203	HEM	CBC-CAC	4.26	1.53	1.28
7	C	1204	HEM	C3B-CAB	4.25	1.53	1.40
8	L	302	BCB	O2D-CGD	4.24	1.44	1.33
9	L	402	BPB	C4B-CHC	4.23	1.40	1.35
9	L	402	BPB	C1B-CHB	4.15	1.40	1.35
7	C	1202	HEM	CBB-CAB	4.14	1.53	1.28
9	M	401	BPB	C1B-CHB	4.13	1.40	1.35
8	L	304	BCB	CAC-C3C	4.12	1.38	1.33
7	C	1201	HEM	CBB-CAB	4.11	1.52	1.28
7	C	1203	HEM	C3B-CAB	4.11	1.53	1.40
7	C	1201	HEM	C4A-C3A	4.09	1.45	1.40
7	C	1201	HEM	CBC-CAC	4.07	1.52	1.28
8	L	302	BCB	C1D-C2D	4.07	1.45	1.40
7	C	1203	HEM	CBB-CAB	4.06	1.52	1.28
8	L	302	BCB	C4B-C3B	4.05	1.46	1.41
8	M	1303	BCB	C4B-C3B	4.02	1.46	1.41
7	C	1204	HEM	C3C-CAC	3.99	1.53	1.40
8	M	1301	BCB	MG-NA	3.92	2.18	2.07
8	L	304	BCB	C4B-C3B	3.89	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1203	HEM	C3C-CAC	3.86	1.52	1.40
7	C	1202	HEM	C3B-CAB	3.79	1.52	1.40
8	M	1303	BCB	C4C-NC	3.73	1.40	1.38
8	L	302	BCB	CAC-C3C	3.70	1.37	1.33
8	L	304	BCB	C4C-NC	3.69	1.40	1.38
8	M	1301	BCB	C4B-C3B	3.67	1.46	1.41
8	M	1303	BCB	CAC-C3C	3.67	1.37	1.33
7	C	1202	HEM	C3C-CAC	3.66	1.51	1.40
7	C	1201	HEM	C3C-CAC	3.62	1.51	1.40
9	M	401	BPB	C4B-C3B	3.55	1.46	1.41
8	M	1301	BCB	C4C-NC	3.48	1.40	1.38
8	M	1301	BCB	O2A-CGA	3.44	1.44	1.33
9	M	401	BPB	C4D-CHA	-3.42	1.40	1.45
8	L	304	BCB	O2D-CGD	3.39	1.42	1.33
10	M	501	MQ7	C12-C13	3.38	1.39	1.32
8	M	1301	BCB	C2-C3	3.38	1.39	1.32
10	M	501	MQ7	C37-C38	3.38	1.39	1.32
9	M	401	BPB	C2-C3	3.31	1.39	1.32
8	M	1301	BCB	C4A-NA	3.25	1.39	1.32
7	C	1202	HEM	C4A-C3A	3.24	1.44	1.40
8	M	1303	BCB	C4A-NA	3.24	1.39	1.32
8	L	304	BCB	C4A-NA	3.23	1.39	1.32
9	L	402	BPB	C2-C3	3.22	1.39	1.32
9	L	402	BPB	O2D-CED	-3.21	1.37	1.45
8	M	1303	BCB	O2D-CGD	3.20	1.41	1.33
10	M	501	MQ7	C26-C27	-3.19	1.41	1.50
11	L	502	UQ2	C8-C9	3.18	1.39	1.32
10	M	501	MQ7	C22-C23	3.15	1.39	1.32
9	M	401	BPB	O2A-CGA	3.15	1.43	1.33
8	L	302	BCB	C2-C3	3.13	1.39	1.32
8	L	304	BCB	C2-C3	3.12	1.39	1.32
9	M	401	BPB	O2D-CED	-3.12	1.37	1.45
9	L	402	BPB	O2D-CGD	3.11	1.41	1.33
8	L	304	BCB	O2D-CED	-3.09	1.37	1.45
10	M	501	MQ7	C27-C28	3.09	1.39	1.32
9	M	401	BPB	O2D-CGD	3.08	1.41	1.33
7	C	1204	HEM	C4A-C3A	3.08	1.44	1.40
7	C	1204	HEM	CHA-C4D	3.05	1.40	1.35
10	M	501	MQ7	C11-C12	-3.04	1.45	1.50
8	L	304	BCB	MG-NA	3.04	2.16	2.07
7	C	1203	HEM	C4A-C3A	3.04	1.44	1.40
9	L	402	BPB	C4B-C3B	3.01	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	402	BPB	C4D-CHA	-3.00	1.41	1.45
13	M	701	LDA	CM2-N1	-2.98	1.44	1.49
8	M	1303	BCB	C2-C3	2.98	1.38	1.32
8	M	1301	BCB	O2D-CED	-2.96	1.37	1.45
7	C	1204	HEM	C2D-C1D	2.94	1.45	1.44
8	L	302	BCB	C4C-NC	2.93	1.40	1.38
10	M	501	MQ7	C32-C33	2.93	1.38	1.32
8	L	302	BCB	MG-NA	2.92	2.15	2.07
8	L	302	BCB	C1C-NC	2.92	1.38	1.32
8	M	1303	BCB	O2D-CED	-2.90	1.38	1.45
8	L	304	BCB	C1C-NC	2.88	1.38	1.32
8	L	302	BCB	C4A-NA	2.85	1.38	1.32
8	M	1301	BCB	C1C-NC	2.85	1.38	1.32
13	H	703	LDA	C1-N1	-2.84	1.46	1.51
8	L	302	BCB	MG-ND	-2.82	1.98	2.05
8	M	1303	BCB	C1C-NC	2.81	1.38	1.32
8	M	1303	BCB	O2A-CGA	2.79	1.42	1.33
7	C	1201	HEM	CHA-C4D	2.78	1.39	1.35
8	M	1301	BCB	C1D-ND	2.77	1.38	1.34
10	M	501	MQ7	C17-C18	2.76	1.38	1.32
13	L	705	LDA	C1-N1	-2.74	1.46	1.51
8	L	302	BCB	O2D-CED	-2.74	1.38	1.45
8	L	304	BCB	C1D-ND	2.72	1.38	1.34
8	M	1303	BCB	MG-ND	-2.72	1.99	2.05
13	H	703	LDA	CM1-N1	-2.69	1.45	1.49
13	M	701	LDA	CM1-N1	-2.63	1.45	1.49
13	M	704	LDA	CM2-N1	-2.61	1.45	1.49
13	M	704	LDA	CM1-N1	-2.53	1.45	1.49
11	L	502	UQ2	O3-CM3	-2.52	1.39	1.45
9	M	401	BPB	C3D-C4D	2.52	1.44	1.40
10	M	501	MQ7	C42-C43	2.52	1.40	1.32
7	C	1201	HEM	CHB-C1B	2.48	1.39	1.35
7	C	1202	HEM	CHA-C4D	2.48	1.39	1.35
9	L	402	BPB	C1-C2	-2.48	1.40	1.49
13	M	704	LDA	C1-N1	-2.46	1.46	1.51
13	M	706	LDA	C1-N1	-2.46	1.46	1.51
8	M	1303	BCB	MG-NA	2.41	2.14	2.07
11	L	502	UQ2	O2-CM2	-2.41	1.39	1.45
7	C	1202	HEM	FE-NA	2.36	2.02	1.92
8	L	302	BCB	C1D-ND	2.34	1.37	1.34
7	C	1203	HEM	CMC-C2C	2.30	1.54	1.47
8	M	1303	BCB	C1D-ND	2.26	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	502	UQ2	C13-C14	2.24	1.39	1.32
7	C	1203	HEM	CHA-C4D	2.22	1.39	1.35
9	M	401	BPB	C1-C2	-2.22	1.41	1.49
10	M	501	MQ7	C10-C5	-2.22	1.37	1.40
7	C	1201	HEM	C2B-C1B	2.22	1.45	1.44
10	M	501	MQ7	C31-C32	-2.15	1.44	1.50
7	C	1204	HEM	FE-NA	2.10	2.01	1.92
8	L	304	BCB	MG-ND	-2.10	2.00	2.05
7	C	1203	HEM	CMD-C2D	2.09	1.53	1.47
9	L	402	BPB	C3D-C4D	2.08	1.43	1.40
7	C	1203	HEM	CHD-C4C	2.08	1.40	1.36
10	M	501	MQ7	C24-C23	2.08	1.56	1.50
10	M	501	MQ7	C21-C22	-2.07	1.44	1.50
7	C	1204	HEM	CHB-C1B	2.02	1.38	1.35
7	C	1202	HEM	CMD-C2D	2.01	1.53	1.47

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	705	LDA	C2-C1-N1	10.58	132.03	113.80
9	L	402	BPB	C1-C2-C3	10.48	144.81	126.19
9	M	401	BPB	C1-C2-C3	9.55	143.17	126.19
9	L	402	BPB	C5-C3-C2	8.43	137.31	121.08
13	M	702	LDA	C2-C1-N1	7.87	127.37	113.80
10	M	501	MQ7	C11-C12-C13	7.23	138.98	126.76
8	L	304	BCB	C1-C2-C3	6.63	137.98	126.19
9	L	402	BPB	O2A-CGA-CBA	6.50	132.39	111.94
13	M	704	LDA	C2-C1-N1	6.45	124.92	113.80
9	M	401	BPB	C5-C3-C2	6.44	133.48	121.08
9	L	402	BPB	O2D-CGD-CBD	6.17	123.89	111.33
8	M	1301	BCB	C1-C2-C3	6.17	137.15	126.19
8	L	302	BCB	C1-C2-C3	-6.16	115.23	126.19
7	C	1202	HEM	C3B-C4B-NB	-5.98	109.72	114.00
8	L	304	BCB	O2D-CGD-CBD	5.90	123.34	111.33
9	L	402	BPB	O2A-CGA-O1A	-5.89	107.33	123.43
8	L	302	BCB	O2A-CGA-CBA	5.84	130.31	111.94
9	M	401	BPB	O2D-CGD-CBD	5.84	123.22	111.33
13	H	703	LDA	C2-C1-N1	5.77	123.74	113.80
8	M	1301	BCB	O2D-CGD-CBD	5.70	122.94	111.33
7	C	1204	HEM	C3B-C4B-NB	-5.65	109.96	114.00
8	L	302	BCB	O2D-CGD-CBD	5.55	122.63	111.33
7	C	1203	HEM	C3B-C4B-NB	-5.51	110.06	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	701	LDA	C2-C1-N1	5.41	123.12	113.80
7	C	1201	HEM	C3B-C4B-NB	-5.36	110.17	114.00
9	L	402	BPB	C4-C3-C2	-5.31	113.01	123.52
8	L	304	BCB	OBB-CAB-C3B	5.05	127.75	120.04
9	L	402	BPB	O1D-CGD-CBD	-4.97	114.23	124.42
8	M	1303	BCB	O2D-CGD-CBD	4.81	121.13	111.33
9	M	401	BPB	O1D-CGD-CBD	-4.78	114.63	124.42
8	L	304	BCB	O1D-CGD-CBD	-4.69	114.81	124.42
8	L	302	BCB	C3C-C4C-NC	4.66	113.15	109.98
13	M	706	LDA	C2-C1-N1	4.55	121.65	113.80
9	L	402	BPB	C3D-C4D-CHA	4.50	114.17	109.18
8	L	302	BCB	O2A-CGA-O1A	-4.49	111.16	123.43
9	M	401	BPB	C3D-C4D-CHA	4.49	114.15	109.18
8	L	302	BCB	O1D-CGD-CBD	-4.47	115.25	124.42
8	L	304	BCB	C6-C5-C3	4.42	123.30	112.78
8	M	1303	BCB	C3D-C4D-CHA	4.40	115.32	108.91
8	M	1301	BCB	O1D-CGD-CBD	-4.37	115.46	124.42
8	L	302	BCB	C3D-C4D-CHA	4.27	115.14	108.91
8	M	1301	BCB	C3D-C4D-CHA	4.24	115.09	108.91
9	L	402	BPB	CHD-C4C-NC	-4.15	120.93	128.59
8	L	304	BCB	C3D-C4D-CHA	4.13	114.93	108.91
10	M	501	MQ7	C40-C38-C37	4.12	129.00	121.08
7	C	1204	HEM	CAD-C3D-C4D	4.10	131.89	124.53
8	M	1303	BCB	C15-C13-C12	4.05	132.81	111.92
8	M	1303	BCB	C3A-C4A-CHB	3.99	126.24	122.11
8	L	302	BCB	CMD-C2D-C3D	3.95	131.19	124.97
9	M	401	BPB	C4-C3-C2	-3.91	115.77	123.52
8	M	1301	BCB	C3A-C4A-CHB	3.90	126.14	122.11
8	M	1303	BCB	O1D-CGD-CBD	-3.87	116.48	124.42
8	L	302	BCB	OBB-CAB-C3B	3.82	125.87	120.04
9	M	401	BPB	CHD-C4C-NC	-3.82	121.55	128.59
8	M	1303	BCB	O2A-CGA-CBA	3.79	123.85	111.94
9	L	402	BPB	C4-C3-C5	-3.76	109.67	115.39
9	L	402	BPB	OBD-CAD-CBD	-3.61	120.48	125.94
7	C	1201	HEM	CAD-C3D-C4D	3.61	131.02	124.53
11	L	502	UQ2	CM3-O3-C3	3.59	128.67	116.48
8	M	1303	BCB	OBD-CAD-CBD	-3.57	120.55	125.94
8	L	304	BCB	CBC-CAC-C3C	-3.56	118.85	126.93
8	M	1301	BCB	C4A-NA-C1A	3.56	110.58	106.13
9	M	401	BPB	C3C-C2C-C1C	3.55	105.28	101.05
9	L	402	BPB	C3C-C2C-C1C	3.52	105.25	101.05
8	L	302	BCB	CAA-C2A-C3A	-3.48	104.81	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	304	BCB	C4A-NA-C1A	3.48	110.48	106.13
8	M	1301	BCB	OBD-CAD-CBD	-3.42	120.78	125.94
10	M	501	MQ7	C39-C38-C40	-3.36	110.28	115.39
8	M	1303	BCB	C3A-C4A-NA	-3.35	108.28	111.79
8	L	302	BCB	OBD-CAD-CBD	-3.34	120.90	125.94
8	M	1303	BCB	C4A-NA-C1A	3.34	110.30	106.13
9	M	401	BPB	OBD-CAD-CBD	-3.33	120.91	125.94
8	L	302	BCB	C4A-NA-C1A	3.33	110.29	106.13
8	L	304	BCB	C3C-C4C-NC	3.30	112.23	109.98
8	L	304	BCB	CMB-C2B-C3B	3.30	130.16	124.97
12	M	600	NS5	C19-C18-C17	3.29	130.65	123.36
9	L	402	BPB	CMD-C2D-C3D	3.25	130.09	124.97
8	M	1303	BCB	OBB-CAB-C3B	3.23	124.97	120.04
8	L	302	BCB	CED-O2D-CGD	-3.19	108.42	116.02
8	M	1303	BCB	C3C-C4C-NC	3.17	112.14	109.98
8	L	304	BCB	C3A-C4A-CHB	3.16	125.38	122.11
8	L	302	BCB	CMB-C2B-C3B	3.13	129.90	124.97
8	M	1303	BCB	C2C-C1C-NC	-3.13	107.70	111.65
9	M	401	BPB	CMD-C2D-C3D	3.12	129.88	124.97
9	M	401	BPB	C3D-C2D-C1D	-3.11	105.15	107.01
7	C	1202	HEM	CAD-C3D-C4D	3.11	130.11	124.53
8	M	1303	BCB	C6-C5-C3	3.11	120.16	112.78
8	L	302	BCB	CAA-C2A-C1A	3.06	119.26	111.62
9	M	401	BPB	C4-C3-C5	-3.05	110.74	115.39
8	L	304	BCB	C3A-C4A-NA	-3.05	108.60	111.79
8	L	304	BCB	OBD-CAD-CBD	-3.05	121.34	125.94
8	M	1301	BCB	C3A-C4A-NA	-3.04	108.61	111.79
8	L	302	BCB	CMD-C2D-C1D	-3.02	123.97	128.62
9	L	402	BPB	CMD-C2D-C1D	-2.98	124.12	128.65
7	C	1204	HEM	CMA-C3A-C4A	-2.97	124.06	128.62
8	M	1301	BCB	CED-O2D-CGD	-2.96	108.96	116.02
8	M	1301	BCB	C2C-C1C-NC	-2.95	107.93	111.65
8	M	1301	BCB	C3C-C4C-NC	2.93	111.97	109.98
7	C	1203	HEM	CMA-C3A-C4A	-2.90	124.16	128.62
10	M	501	MQ7	C16-C17-C18	2.86	133.97	127.80
9	L	402	BPB	C2C-C3C-C4C	-2.85	104.53	108.73
7	C	1204	HEM	CAD-C3D-C2D	-2.84	120.91	127.25
8	M	1303	BCB	C2C-C3C-C4C	-2.83	104.55	108.73
9	M	401	BPB	C2C-C1C-NC	-2.82	108.20	113.50
9	M	401	BPB	C2C-C3C-C4C	-2.80	104.59	108.73
7	C	1203	HEM	CBD-CAD-C3D	-2.79	108.28	114.37
8	L	302	BCB	C2C-C1C-NC	-2.79	108.13	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	302	BCB	C2D-C1D-ND	2.79	111.51	109.41
8	M	1303	BCB	CMD-C2D-C3D	2.78	129.35	124.97
8	L	304	BCB	C2C-C1C-NC	-2.73	108.20	111.65
7	C	1204	HEM	CBA-CAA-C2A	-2.73	107.89	112.69
8	L	302	BCB	C2C-C3C-C4C	-2.72	104.71	108.73
8	L	302	BCB	CBC-CAC-C3C	-2.71	120.78	126.93
8	M	1303	BCB	C1-C2-C3	-2.71	121.37	126.19
8	L	302	BCB	C3A-C4A-CHB	2.70	124.91	122.11
7	C	1201	HEM	C2D-C1D-ND	-2.70	109.75	112.93
8	M	1301	BCB	C2C-C3C-C4C	-2.68	104.77	108.73
9	M	401	BPB	OB-BA-C3B	2.68	124.12	120.04
10	M	501	MQ7	C41-C42-C43	2.64	138.01	127.67
7	C	1203	HEM	C2D-C1D-ND	-2.62	109.84	112.93
7	C	1202	HEM	C2D-C1D-ND	-2.61	109.84	112.93
8	L	304	BCB	C2C-C3C-C4C	-2.61	104.87	108.73
8	M	1303	BCB	C3D-C4D-ND	2.60	111.20	108.61
10	M	501	MQ7	C26-C25-C23	-2.60	104.14	112.74
9	M	401	BPB	C3A-C4A-NA	-2.59	109.13	113.57
12	M	600	NS5	C16-C15-C14	-2.53	114.01	118.09
12	M	600	NS5	C18-C19-C20	2.53	128.95	123.36
9	L	402	BPB	OB-BA-C3B	2.52	123.89	120.04
7	C	1204	HEM	C2D-C1D-ND	-2.51	109.97	112.93
10	M	501	MQ7	C41-C40-C38	2.49	120.98	112.74
9	L	402	BPB	C3A-C4A-NA	-2.49	109.30	113.57
8	L	302	BCB	C2A-C3A-C4A	2.47	105.20	101.40
9	M	401	BPB	O2A-CGA-CBA	2.47	119.71	111.94
9	M	401	BPB	CMD-C2D-C1D	-2.42	124.96	128.65
9	L	402	BPB	C2C-C1C-NC	-2.42	108.95	113.50
8	M	1303	BCB	O2A-CGA-O1A	-2.42	116.83	123.43
8	L	302	BCB	C3D-C4D-ND	2.35	110.95	108.61
12	M	600	NS5	C14-C15-C17	2.34	122.56	118.97
7	C	1201	HEM	CAD-C3D-C2D	-2.32	122.08	127.25
8	M	1301	BCB	CMD-C2D-C3D	2.29	128.57	124.97
7	C	1204	HEM	CAA-C2A-C3A	-2.27	122.53	129.00
9	M	401	BPB	C6-C5-C3	-2.25	107.43	112.78
9	L	402	BPB	C3A-C2A-C1A	2.21	104.72	101.91
9	M	401	BPB	C3D-C4D-ND	2.21	110.65	106.97
9	L	402	BPB	C1D-CHD-C4C	-2.20	125.64	129.92
8	L	302	BCB	C3A-C2A-C1A	2.18	104.16	101.08
8	L	304	BCB	C3A-C2A-C1A	2.15	104.11	101.08
9	L	402	BPB	C3D-C4D-ND	2.14	110.53	106.97
8	L	302	BCB	C15-C13-C12	-2.13	100.91	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1303	BCB	C3A-C2A-C1A	2.13	104.09	101.08
9	M	401	BPB	C1D-CHD-C4C	-2.12	125.78	129.92
9	M	401	BPB	C3A-C2A-C1A	2.12	104.60	101.91
11	L	502	UQ2	C7-C8-C9	2.11	130.31	126.76
9	L	402	BPB	C3D-C2D-C1D	-2.10	105.75	107.01
8	M	1301	BCB	C3D-C4D-ND	2.09	110.69	108.61
7	C	1203	HEM	CBA-CAA-C2A	-2.08	109.02	112.69
8	L	304	BCB	CMB-C2B-C1B	-2.07	122.06	126.16
9	M	401	BPB	C3A-C4A-CHB	2.06	125.76	121.69
9	L	402	BPB	C3A-C4A-CHB	2.06	125.76	121.69
7	C	1204	HEM	CMA-C3A-C2A	2.05	128.82	124.94
8	M	1301	BCB	C3A-C2A-C1A	2.05	103.98	101.08
9	M	401	BPB	CED-O2D-CGD	2.05	120.89	116.02
7	C	1203	HEM	CMA-C3A-C2A	2.02	128.75	124.94
11	L	502	UQ2	O3-C3-C4	-2.02	110.22	116.54
10	M	501	MQ7	C14-C13-C15	-2.01	112.34	115.39

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	M	401	BPB	C13
8	M	1303	BCB	C13
8	L	304	BCB	C8

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	C	332/336 (98%)	-0.35	4 (1%) 75 83	23, 45, 67, 78	15 (4%)
2	L	273/273 (100%)	-0.51	1 (0%) 90 94	25, 43, 65, 76	6 (2%)
3	M	323/323 (100%)	-0.54	1 (0%) 91 95	25, 42, 68, 77	8 (2%)
4	H	252/258 (97%)	-0.07	11 (4%) 33 39	30, 56, 84, 93	19 (7%)
All	All	1180/1190 (99%)	-0.38	17 (1%) 72 80	23, 46, 71, 93	48 (4%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	8	GLN	4.6
4	H	46	PRO	4.2
4	H	258	LEU	4.1
4	H	191	ALA	3.6
4	H	93	THR	3.0
4	H	192	ARG	3.0
4	H	53	ALA	2.8
1	C	332	LYS	2.8
3	M	319	PRO	2.5
4	H	96	PHE	2.5
4	H	102	GLN	2.2
2	L	57	PRO	2.2
1	C	47	ALA	2.2
1	C	330	PRO	2.2
4	H	206	ASP	2.1
4	H	45	GLU	2.1
1	C	162	HIS	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
4	FME	H	1	10/11	0.27	2.37	53,55,63,65	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
13	LDA	M	704	16/16	0.43	8.37	79,82,83,84	3
13	LDA	M	702	16/16	0.47	7.82	73,87,100,101	0
13	LDA	M	706	16/16	0.50	5.74	99,105,114,114	0
11	UQ2	L	502	23/23	0.24	4.89	48,49,50,50	23
13	LDA	H	703	16/16	0.37	3.56	74,79,85,85	0
12	NS5	M	600	40/40	0.22	3.56	39,58,67,68	11
9	BPB	M	401	65/65	0.22	2.88	37,45,94,95	0
10	MQ7	M	501	48/48	0.20	2.31	36,45,67,70	0
9	BPB	L	402	65/65	0.18	1.79	31,41,45,47	0
13	LDA	L	705	16/16	0.31	1.60	71,78,94,95	3
8	BCB	L	304	66/66	0.17	0.39	23,29,54,57	0
7	HEM	C	1203	43/43	0.15	0.34	26,33,41,44	0
8	BCB	M	1303	66/66	0.17	0.33	17,25,46,48	0
8	BCB	L	302	66/66	0.16	0.13	10,20,42,43	0
8	BCB	M	1301	66/66	0.17	0.07	33,43,59,63	15
13	LDA	M	701	16/16	0.17	0.07	48,50,52,52	0
6	SO4	M	803	5/5	0.13	-0.08	102,102,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	HEM	C	1204	43/43	0.13	-0.23	32,36,48,53	0
7	HEM	C	1201	43/43	0.13	-0.49	47,51,61,65	0
7	HEM	C	1202	43/43	0.13	-0.55	39,43,55,58	0
6	SO4	M	804	5/5	0.11	-0.72	81,82,82,83	0
6	SO4	H	801	5/5	0.12	-0.86	73,76,76,77	0
6	SO4	M	802	5/5	0.10	-1.69	57,59,61,61	0
5	FE2	M	500	1/1	0.05	-3.28	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.