



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:10 AM GMT

PDB ID : 2ZT9
Title : Crystal Structure of the Cytochrome b6f Complex from Nostoc sp. PCC 7120
Authors : Craner, W.A.; Baniulis D.; Yamashita E.
Deposited on : 2008-09-27
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

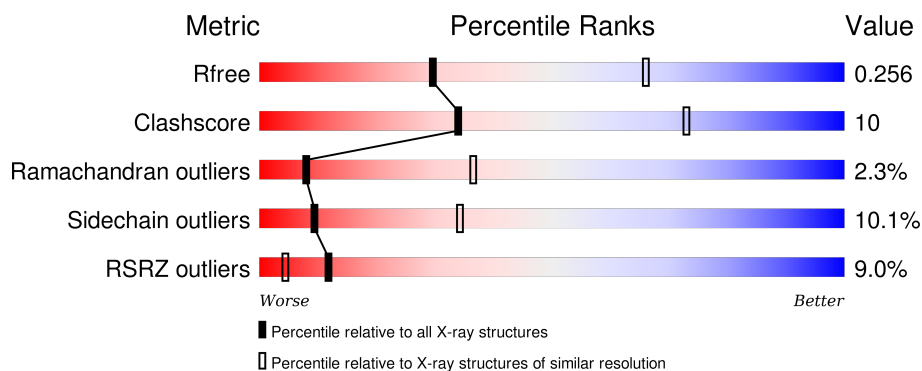
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>76%</div> <div>21%</div> <div>•</div> </div>
2	B	160	<div> <div>2%</div> <div>73%</div> <div>21%</div> <div>6%</div> <div>•</div> </div>
3	C	289	<div> <div>12%</div> <div>73%</div> <div>22%</div> <div>5%</div> </div>
4	D	179	<div> <div>25%</div> <div>76%</div> <div>16%</div> <div>•</div> <div>7%</div> </div>
5	E	31	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	34	
7	G	37	
8	H	29	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	UMQ	A	304	X	-	-	X
10	UMQ	A	305	X	-	-	X
10	UMQ	A	306	X	-	-	-
11	CLA	B	201	X	-	-	-
12	OPC	B	202	-	-	-	X
12	OPC	H	30	-	-	-	X
15	BCR	G	101	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7912 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1715	1144	272	288	11			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1239	830	195	208	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	289	Total	C	N	O	S	0	0	0
			2195	1396	364	429	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1249	791	213	239	6			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			227	157	35	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			231	156	36	38	1			

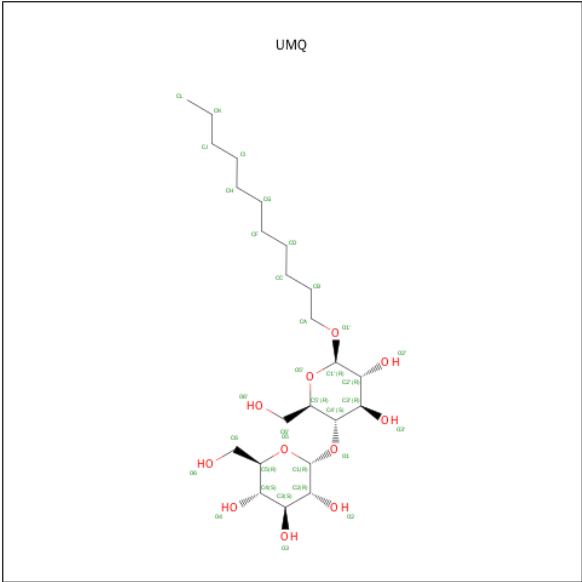
- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | G | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 281 | 188 | 44 | 48 | 1 | | | |

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | H | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 227 | 155 | 36 | 34 | 2 | | | |

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- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring. The structure includes various side chains and a central heme label.

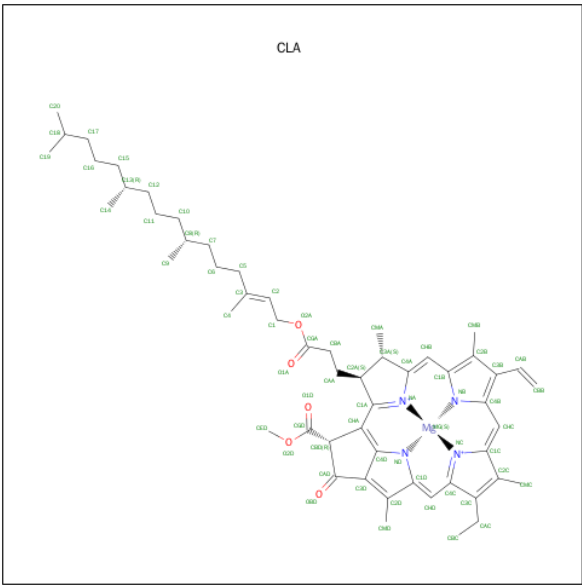
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK



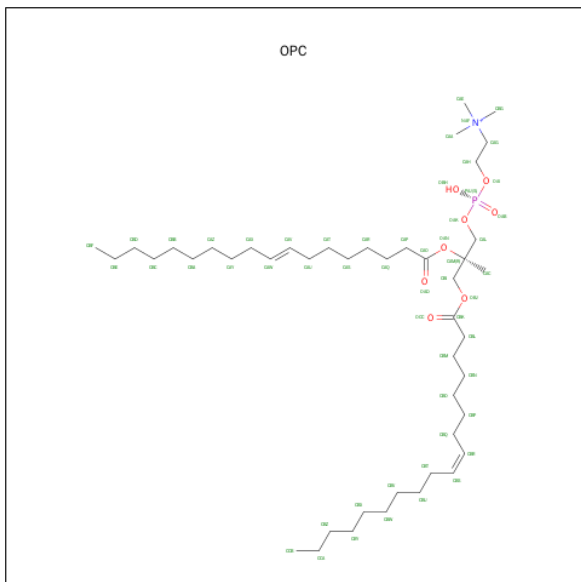
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O		0	0
			34	23	11			
10	A	1	Total	C	O		0	0
			34	23	11			
10	A	1	Total	C	O		0	0
			34	23	11			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



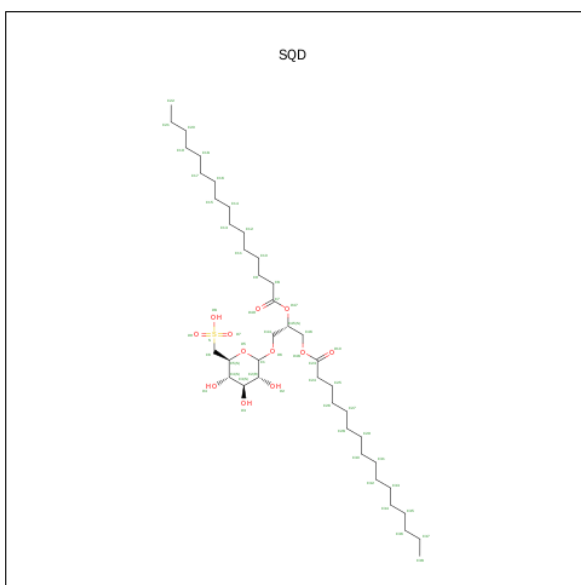
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 12 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).



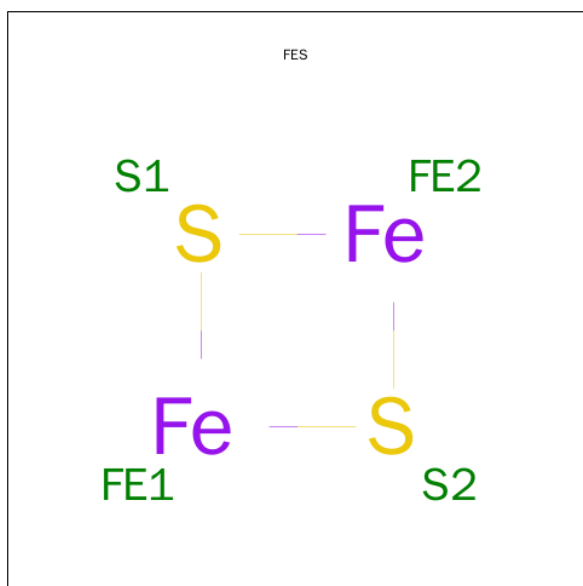
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 13 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



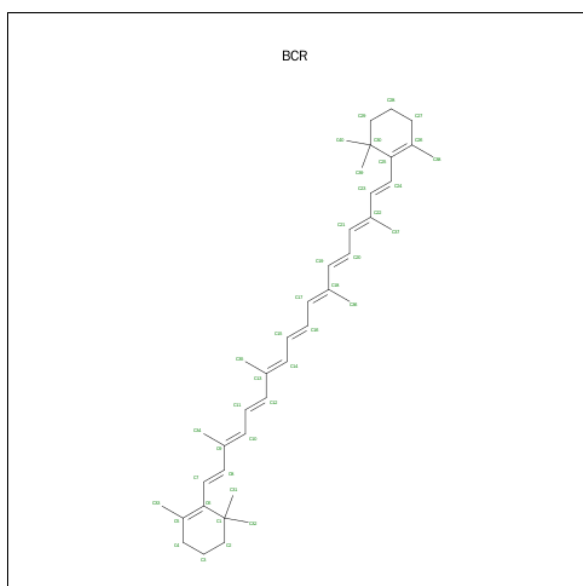
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total C 40 40	0	0

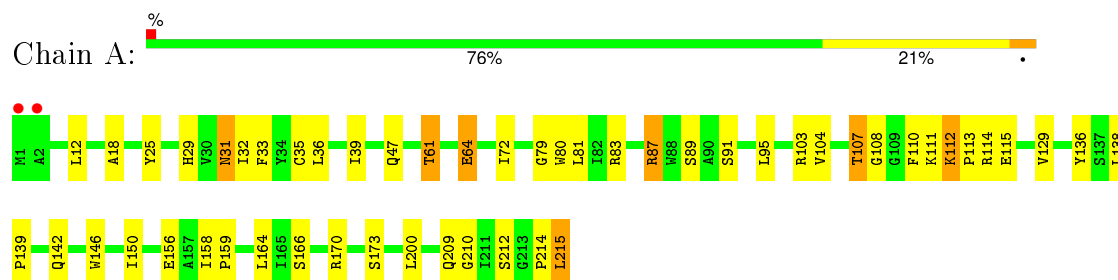
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 1 1	0	0
16	B	2	Total O 2 2	0	0

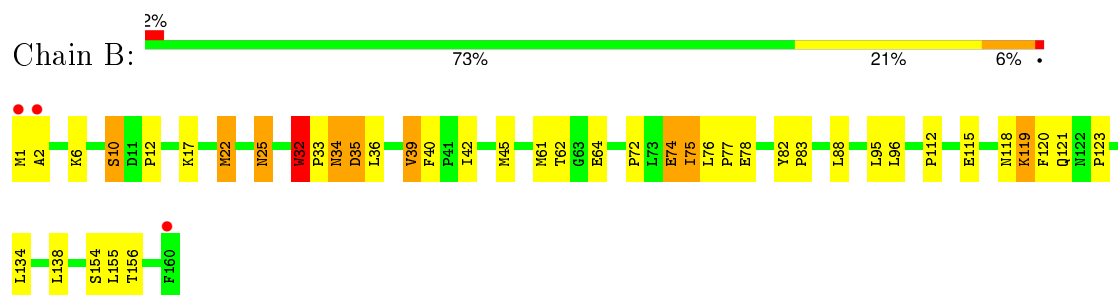
3 Residue-property plots

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.

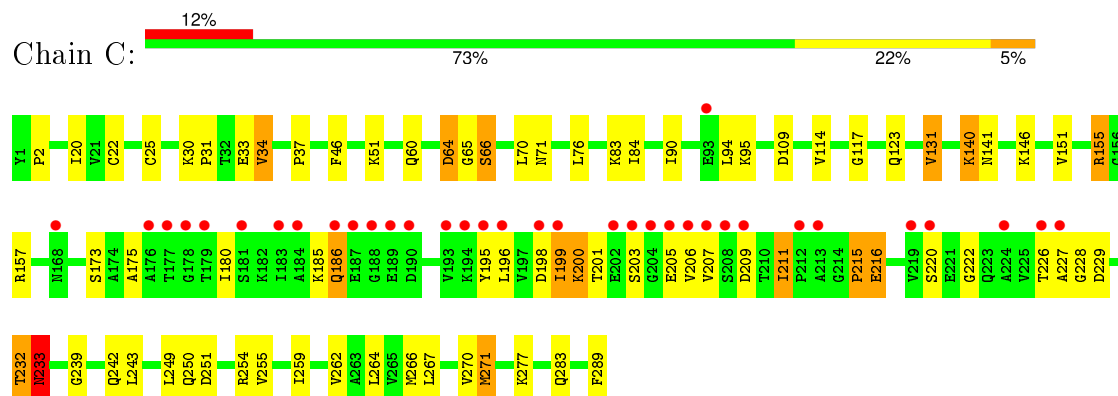
- Molecule 1: Cytochrome b6



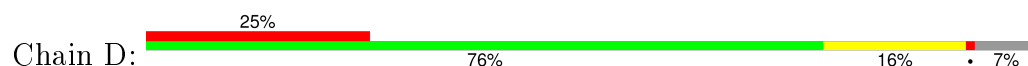
- Molecule 2: Cytochrome b6-f complex subunit 4

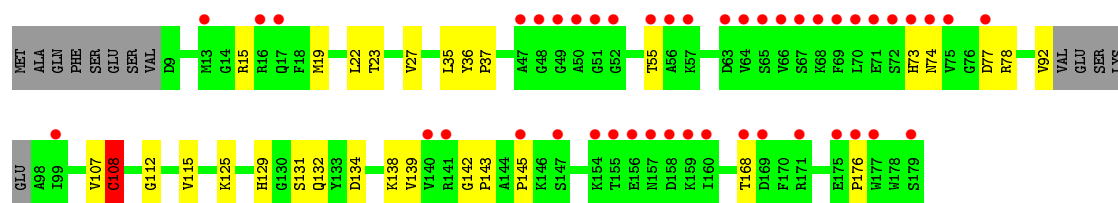


- Molecule 3: Apocytochrome f

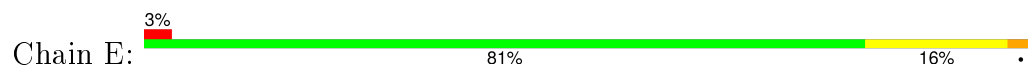


- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1





- Molecule 5: Cytochrome b6-f complex subunit 6



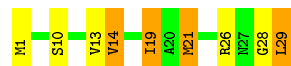
- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.22Å 159.22Å 365.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.69 – 3.00 45.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.69-3.00) 98.5 (45.68-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.259 0.228 , 0.256	Depositor DCC
R_{free} test set	2770 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54603 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, CLA, FES, OPC, HEM, BCR, SQD

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	0.50	0/1768	0.62	0/2411
2	B	0.50	0/1278	0.66	0/1752
3	C	0.44	0/2241	0.58	0/3053
4	D	0.40	0/1280	0.55	1/1745 (0.1%)
5	E	0.45	0/230	0.52	0/309
6	F	0.45	0/234	0.56	0/315
7	G	0.48	0/286	0.65	0/387
8	H	0.51	0/233	0.66	0/319
All	All	0.46	0/7550	0.60	1/10291 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	108	CYS	CA-CB-SG	5.66	124.18	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1715	0	1734	45	0
2	B	1239	0	1290	39	0
3	C	2195	0	2183	54	0
4	D	1249	0	1208	17	0
5	E	227	0	257	3	0
6	F	231	0	252	6	0
7	G	281	0	303	12	0
8	H	227	0	243	13	0
9	A	129	0	90	7	0
9	C	43	0	30	6	0
10	A	102	0	123	4	0
11	B	65	0	72	1	0
12	B	54	0	83	0	0
12	H	54	0	83	4	0
13	B	54	0	78	1	0
14	D	4	0	0	1	0
15	G	40	0	53	7	0
16	A	1	0	0	0	0
16	B	2	0	0	0	0
All	All	7912	0	8082	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:CYS:SG	9:A:303:HEM:HAB	1.79	1.22
1:A:35:CYS:HG	9:A:303:HEM:CAB	1.52	1.14
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.37	1.13
3:C:25:CYS:SG	9:C:301:HEM:HAC	1.93	1.09
2:B:34:ASN:HD22	2:B:34:ASN:H	1.13	0.96
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.45	0.96
3:C:22:CYS:HB2	9:C:301:HEM:HAB	1.46	0.95
3:C:250:GLN:HE21	3:C:251:ASP:H	0.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:303:HEM:HBD1	9:A:303:HEM:HHA	1.55	0.87
3:C:232:THR:O	3:C:233:ASN:HB3	1.75	0.87
1:A:32:ILE:HD11	15:G:101:BCR:H322	1.60	0.82
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.95	0.81
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.64	0.80
1:A:146:TRP:HB3	2:B:75:ILE:HD11	1.67	0.75
1:A:39:ILE:HD11	15:G:101:BCR:H312	1.70	0.74
3:C:250:GLN:HE21	3:C:251:ASP:N	1.81	0.73
2:B:22:MET:O	2:B:22:MET:HG2	1.88	0.73
4:D:131:SER:HA	4:D:142:GLY:HA3	1.71	0.73
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.21	0.72
2:B:34:ASN:ND2	2:B:34:ASN:H	1.84	0.70
3:C:60:GLN:HE22	3:C:157:ARG:H	1.38	0.70
1:A:112:LYS:O	1:A:115:GLU:OE1	2.10	0.70
8:H:28:GLY:C	8:H:29:LEU:HG	2.12	0.69
2:B:118:ASN:HD22	2:B:120:PHE:H	1.39	0.68
2:B:17:LYS:HB3	2:B:22:MET:O	1.93	0.68
1:A:103:ARG:O	1:A:107:THR:HB	1.94	0.67
3:C:226:THR:HG22	3:C:227:ALA:H	1.60	0.67
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.09	0.67
2:B:32:TRP:O	2:B:33:PRO:C	2.32	0.66
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.58	0.66
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.32	0.64
5:E:17:ILE:O	5:E:21:LEU:HB2	1.98	0.64
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.80	0.64
1:A:32:ILE:N	8:H:29:LEU:HD13	2.14	0.62
3:C:84:ILE:HD11	3:C:114:VAL:HG11	1.82	0.62
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.31	0.60
3:C:20:ILE:HD12	3:C:242:GLN:HG2	1.83	0.60
2:B:119:LYS:O	2:B:119:LYS:HG2	2.02	0.59
1:A:39:ILE:CD1	15:G:101:BCR:H312	2.33	0.59
10:A:304:UMQ:HB1	3:C:254:ARG:HA	1.85	0.58
4:D:108:CYS:HB3	4:D:115:VAL:HG22	1.86	0.57
4:D:15:ARG:NH1	5:E:28:ALA:O	2.37	0.56
2:B:34:ASN:HD21	3:C:283:GLN:HE22	1.51	0.56
3:C:262:VAL:HG13	8:H:14:VAL:HG13	1.86	0.56
3:C:200:LYS:HG3	3:C:206:VAL:HG22	1.86	0.56
3:C:175:ALA:HB2	3:C:209:ASP:OD2	2.06	0.56
3:C:30:LYS:HG2	3:C:239:GLY:HA3	1.87	0.56
3:C:155:ARG:HD2	3:C:155:ARG:H	1.72	0.55
6:F:20:TRP:CZ3	15:G:101:BCR:H19C	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:PRO:O	3:C:155:ARG:NH2	2.41	0.54
2:B:22:MET:CG	2:B:22:MET:O	2.54	0.54
1:A:29:HIS:HB2	7:G:28:GLN:HE22	1.72	0.54
1:A:114:ARG:NH1	1:A:210:GLY:O	2.41	0.54
2:B:45:MET:CE	4:D:27:VAL:HG13	2.37	0.54
4:D:131:SER:CA	4:D:142:GLY:HA3	2.37	0.53
1:A:209:GLN:HB3	2:B:22:MET:HE2	1.91	0.53
1:A:87:ARG:NH1	2:B:78:GLU:OE1	2.40	0.53
12:H:30:OPC:HAP2	12:H:30:OPC:HBL1	1.91	0.53
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.91	0.52
3:C:173:SER:HB2	3:C:228:GLY:HA2	1.90	0.52
3:C:255:VAL:O	3:C:259:ILE:HG12	2.09	0.52
3:C:34:VAL:HG23	3:C:243:LEU:HD12	1.92	0.52
1:A:32:ILE:H	8:H:29:LEU:HD13	1.72	0.52
1:A:83:ARG:HD2	9:A:301:HEM:O1A	2.09	0.52
1:A:111:LYS:O	1:A:113:PRO:HD2	2.09	0.52
1:A:146:TRP:HB3	2:B:75:ILE:CD1	2.38	0.52
3:C:270:VAL:HA	8:H:21:MET:HE2	1.90	0.52
3:C:22:CYS:HB2	9:C:301:HEM:CAB	2.31	0.51
8:H:10:SER:O	8:H:14:VAL:HG22	2.10	0.51
4:D:131:SER:CB	4:D:142:GLY:HA3	2.41	0.50
2:B:61:MET:HG3	3:C:146:LYS:HD3	1.93	0.50
3:C:140:LYS:N	3:C:140:LYS:HD3	2.25	0.50
1:A:31:ASN:HD22	1:A:33:PHE:H	1.58	0.50
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.94	0.50
2:B:25:ASN:ND2	2:B:25:ASN:H	2.08	0.50
3:C:266:MET:O	3:C:270:VAL:HG23	2.12	0.49
10:A:305:UMQ:HB2	13:B:203:SQD:O10	2.12	0.49
7:G:20:GLY:N	15:G:101:BCR:H363	2.26	0.49
1:A:215:LEU:HG	7:G:28:GLN:OE1	2.12	0.49
8:H:1:MET:HB3	12:H:30:OPC:HAE1	1.95	0.49
8:H:28:GLY:O	8:H:29:LEU:HG	2.13	0.49
3:C:199:ILE:O	3:C:200:LYS:CB	2.61	0.49
8:H:26:ARG:HH11	8:H:29:LEU:HD11	1.77	0.49
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.48	0.48
3:C:270:VAL:HG22	8:H:21:MET:HE2	1.96	0.48
7:G:26:TYR:CE2	7:G:30:LYS:HE2	2.49	0.48
3:C:250:GLN:NE2	3:C:251:ASP:H	1.85	0.48
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.95	0.48
4:D:77:ASP:N	4:D:77:ASP:OD2	2.46	0.48
6:F:11:LEU:HD21	12:H:30:OPC:HAV	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:SER:O	2:B:12:PRO:HD3	2.14	0.47
1:A:25:TYR:OH	3:C:289:PHE:O	2.24	0.47
4:D:129:HIS:HB2	14:D:200:FES:S1	2.54	0.47
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.49	0.47
1:A:129:VAL:HG21	11:B:201:CLA:H43	1.96	0.47
7:G:23:TYR:OH	7:G:27:LYS:HE3	2.15	0.47
3:C:22:CYS:CB	9:C:301:HEM:HAB	2.32	0.47
1:A:150:ILE:HD11	2:B:75:ILE:HG12	1.97	0.46
1:A:72:ILE:O	1:A:79:GLY:HA3	2.16	0.46
9:A:303:HEM:HBD1	9:A:303:HEM:CHA	2.32	0.46
15:G:101:BCR:H361	15:G:101:BCR:H20C	1.65	0.46
1:A:115:GLU:N	1:A:115:GLU:OE1	2.45	0.46
3:C:64:ASP:CG	3:C:65:GLY:H	2.19	0.46
4:D:168:THR:HA	4:D:176:PRO:HD3	1.98	0.46
3:C:271:MET:HG3	4:D:23:THR:HA	1.96	0.46
2:B:32:TRP:O	2:B:34:ASN:N	2.49	0.46
1:A:29:HIS:CB	7:G:28:GLN:HE22	2.30	0.45
4:D:134:ASP:HB2	4:D:138:LYS:H	1.81	0.45
3:C:155:ARG:HD2	3:C:155:ARG:N	2.31	0.45
3:C:270:VAL:HA	8:H:21:MET:CE	2.46	0.45
6:F:26:LEU:HA	6:F:29:ILE:HG23	1.97	0.45
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.97	0.45
1:A:138:LEU:N	1:A:139:PRO:CD	2.79	0.45
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.98	0.45
2:B:36:LEU:O	2:B:40:PHE:HB2	2.16	0.45
3:C:186:GLN:HE21	3:C:196:LEU:HG	1.82	0.45
3:C:37:PRO:HB3	12:H:30:OPC:HAH1	1.97	0.45
3:C:76:LEU:HD12	3:C:151:VAL:HG22	1.99	0.45
2:B:1:MET:HB3	2:B:2:ALA:H	1.61	0.45
3:C:199:ILE:O	3:C:200:LYS:HB2	2.16	0.45
2:B:74:GLU:OE1	7:G:1:MET:HA	2.17	0.45
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.98	0.44
1:A:61:THR:HG22	1:A:64:GLU:H	1.82	0.44
3:C:232:THR:O	3:C:233:ASN:CB	2.57	0.44
1:A:35:CYS:SG	9:A:303:HEM:C3B	2.91	0.44
15:G:101:BCR:H323	8:H:19:ILE:HG12	1.98	0.44
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.99	0.44
3:C:71:ASN:N	9:C:301:HEM:O2A	2.45	0.44
2:B:39:VAL:HA	2:B:42:ILE:HD12	1.99	0.44
2:B:35:ASP:HA	2:B:39:VAL:HG13	2.00	0.43
7:G:13:LEU:HA	7:G:16:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:HA3	2:B:121:GLN:HA	2.00	0.43
3:C:266:MET:SD	8:H:13:VAL:HG12	2.59	0.43
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.83	0.43
3:C:215:PRO:HB2	3:C:216:GLU:H	1.70	0.42
1:A:114:ARG:NH2	1:A:212:SER:HA	2.35	0.42
3:C:195:TYR:HB2	3:C:211:ILE:HG13	2.01	0.42
2:B:154:SER:C	2:B:156:THR:H	2.23	0.42
7:G:21:LEU:HA	7:G:21:LEU:HD12	1.91	0.42
6:F:5:LEU:HD21	7:G:11:LEU:HD12	2.00	0.42
4:D:78:ARG:HG2	4:D:92:VAL:HG22	2.02	0.42
4:D:131:SER:HB3	4:D:143:PRO:HD2	2.00	0.42
3:C:90:ILE:O	3:C:95:LYS:NZ	2.53	0.42
3:C:180:ILE:HA	3:C:198:ASP:O	2.20	0.42
1:A:209:GLN:O	2:B:22:MET:HB2	2.19	0.42
2:B:25:ASN:ND2	2:B:25:ASN:N	2.68	0.42
1:A:113:PRO:HB2	2:B:22:MET:CE	2.50	0.41
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.17	0.41
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.35	0.41
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.55	0.41
3:C:199:ILE:HD12	3:C:207:VAL:HG23	2.02	0.41
1:A:136:TYR:CE1	2:B:78:GLU:HG3	2.55	0.41
3:C:2:PRO:HG2	3:C:117:GLY:HA2	2.01	0.41
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.81	0.41
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.61	0.41
10:A:306:UMQ:HA2	2:B:32:TRP:NE1	2.36	0.40
1:A:111:LYS:HE2	2:B:115:GLU:O	2.22	0.40
5:E:15:THR:OG1	6:F:22:LEU:HD21	2.21	0.40
1:A:18:ALA:CB	10:A:306:UMQ:H6'1	2.52	0.40
3:C:180:ILE:O	3:C:222:GLY:HA2	2.21	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	213/215 (99%)	200 (94%)	12 (6%)	1 (0%)	34	76
2	B	158/160 (99%)	143 (90%)	10 (6%)	5 (3%)	5	27
3	C	287/289 (99%)	245 (85%)	31 (11%)	11 (4%)	4	22
4	D	162/179 (90%)	144 (89%)	16 (10%)	2 (1%)	16	56
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	5	26
7	G	35/37 (95%)	32 (91%)	1 (3%)	2 (6%)	2	12
8	H	27/29 (93%)	27 (100%)	0	0	100	100
All	All	941/974 (97%)	847 (90%)	72 (8%)	22 (2%)	8	36

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
3	C	64	ASP
3	C	66	SER
3	C	200	LYS
3	C	215	PRO
3	C	233	ASN
4	D	145	PRO
3	C	220	SER
6	F	2	SER
2	B	74	GLU
2	B	155	LEU
3	C	199	ILE
3	C	216	GLU
3	C	201	THR
3	C	205	GLU
7	G	27	LYS
3	C	203	SER
4	D	74	ASN
2	B	75	ILE
7	G	36	GLY
2	B	77	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	169 (92%)	15 (8%)	14	46
2	B	134/134 (100%)	118 (88%)	16 (12%)	6	26
3	C	238/238 (100%)	216 (91%)	22 (9%)	11	40
4	D	133/145 (92%)	124 (93%)	9 (7%)	20	56
5	E	21/21 (100%)	18 (86%)	3 (14%)	4	19
6	F	22/24 (92%)	16 (73%)	6 (27%)	0	2
7	G	29/29 (100%)	25 (86%)	4 (14%)	4	20
8	H	24/24 (100%)	20 (83%)	4 (17%)	3	13
All	All	785/799 (98%)	706 (90%)	79 (10%)	9	34

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	31	ASN
1	A	36	LEU
1	A	61	THR
1	A	64	GLU
1	A	81	LEU
1	A	87	ARG
1	A	91	SER
1	A	95	LEU
1	A	107	THR
1	A	156	GLU
1	A	164	LEU
1	A	173	SER
1	A	200	LEU
1	A	215	LEU
2	B	6	LYS
2	B	10	SER
2	B	22	MET
2	B	25	ASN
2	B	34	ASN
2	B	35	ASP
2	B	39	VAL
2	B	62	THR

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Mol	Chain	Res	Type
2	B	64	GLU
2	B	76	LEU
2	B	88	LEU
2	B	95	LEU
2	B	96	LEU
2	B	119	LYS
2	B	134	LEU
2	B	138	LEU
3	C	34	VAL
3	C	66	SER
3	C	70	LEU
3	C	83	LYS
3	C	94	LEU
3	C	109	ASP
3	C	123	GLN
3	C	131	VAL
3	C	140	LYS
3	C	141	ASN
3	C	155	ARG
3	C	185	LYS
3	C	186	GLN
3	C	211	ILE
3	C	229	ASP
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	277	LYS
4	D	19	MET
4	D	22	LEU
4	D	35	LEU
4	D	55	THR
4	D	73	HIS
4	D	108	CYS
4	D	125	LYS
4	D	132	GLN
4	D	139	VAL
5	E	8	ILE
5	E	10	PHE
5	E	21	LEU

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Mol	Chain	Res	Type
6	F	6	LEU
6	F	10	LEU
6	F	22	LEU
6	F	25	LEU
6	F	29	ILE
6	F	30	GLN
7	G	6	LEU
7	G	16	VAL
7	G	21	LEU
7	G	30	LYS
8	H	14	VAL
8	H	19	ILE
8	H	21	MET
8	H	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	25	ASN
2	B	34	ASN
2	B	93	ASN
2	B	118	ASN
2	B	122	ASN
3	C	60	GLN
3	C	250	GLN
3	C	288	ASN
4	D	132	GLN
6	F	30	GLN
7	G	28	GLN
7	G	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

13 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	$\# Z > 2$
9	HEM	A	301	1	30,50,50	2.38	9 (30%)	24,82,82	2.39	8 (33%)
9	HEM	A	302	1	30,50,50	2.20	8 (26%)	24,82,82	2.28	8 (33%)
9	HEM	A	303	1	30,50,50	2.33	10 (33%)	24,82,82	2.45	10 (41%)
10	UMQ	A	304	-	35,35,35	1.39	3 (8%)	46,46,46	2.34	8 (17%)
10	UMQ	A	305	-	35,35,35	1.44	3 (8%)	46,46,46	2.38	7 (15%)
10	UMQ	A	306	-	35,35,35	1.47	3 (8%)	46,46,46	2.42	11 (23%)
11	CLA	B	201	16	55,73,73	1.83	12 (21%)	61,113,113	2.25	17 (27%)
12	OPC	B	202	-	53,53,54	2.01	14 (26%)	57,61,64	2.38	14 (24%)
13	SQD	B	203	-	53,54,54	1.28	3 (5%)	61,65,65	3.93	14 (22%)
9	HEM	C	301	3	30,50,50	2.05	9 (30%)	24,82,82	2.42	9 (37%)
14	FES	D	200	4	0,4,4	0.00	-	0,4,4	0.00	-
15	BCR	G	101	-	41,41,41	2.44	11 (26%)	56,56,56	5.34	16 (28%)
12	OPC	H	30	-	53,53,54	1.99	14 (26%)	57,61,64	2.35	16 (28%)

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
9	HEM	A	301	1	-	0/10/54/54	0/0/8/8
9	HEM	A	302	1	-	0/10/54/54	0/0/8/8
9	HEM	A	303	1	-	0/10/54/54	0/0/8/8
10	UMQ	A	304	-	2/2/10/10	0/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UMQ	A	305	-	2/2/10/10	0/20/60/60	0/2/2/2
10	UMQ	A	306	-	2/2/10/10	0/20/60/60	0/2/2/2
11	CLA	B	201	16	4/4/20/25	0/37/135/135	0/0/9/9
12	OPC	B	202	-	-	0/57/57/60	0/0/0/0
13	SQD	B	203	-	-	2/49/69/69	0/1/1/1
9	HEM	C	301	3	-	0/10/54/54	0/0/8/8
14	FES	D	200	4	-	0/0/4/4	0/1/1/1
15	BCR	G	101	-	-	0/29/63/63	0/2/2/2
12	OPC	H	30	-	-	0/57/57/60	0/0/0/0

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	C3B-C4B	-8.46	1.44	1.51
15	G	101	BCR	C8-C9	-8.00	1.28	1.45
15	G	101	BCR	C23-C22	-7.87	1.28	1.45
9	A	302	HEM	C3B-C4B	-7.58	1.45	1.51
9	A	303	HEM	C3B-C4B	-7.02	1.45	1.51
9	C	301	HEM	C3B-C4B	-6.38	1.46	1.51
10	A	306	UMQ	C1'-C2'	-6.31	1.33	1.52
10	A	305	UMQ	C1'-C2'	-6.15	1.34	1.52
13	B	203	SQD	C6-S	-6.01	1.69	1.77
10	A	304	UMQ	C1'-C2'	-5.88	1.34	1.52
9	A	301	HEM	C3D-C4D	-5.47	1.44	1.51
12	B	202	OPC	CAG-CAH	-5.04	1.33	1.51
12	H	30	OPC	CBP-CBQ	-4.97	1.33	1.52
12	B	202	OPC	CAQ-CAP	-4.95	1.33	1.52
12	H	30	OPC	CAQ-CAP	-4.94	1.33	1.52
9	C	301	HEM	C3D-C4D	-4.92	1.45	1.51
9	A	303	HEM	C3D-C4D	-4.87	1.45	1.51
9	A	302	HEM	C3D-C4D	-4.74	1.45	1.51
12	H	30	OPC	CAG-CAH	-4.70	1.35	1.51
15	G	101	BCR	C24-C25	-4.48	1.29	1.45
12	B	202	OPC	CBP-CBQ	-4.48	1.35	1.52
15	G	101	BCR	C12-C13	-4.23	1.36	1.45
15	G	101	BCR	C19-C18	-4.07	1.36	1.45
10	A	306	UMQ	O2'-C2'	-4.04	1.33	1.43
9	A	303	HEM	C2C-C1C	-4.02	1.44	1.52
10	A	305	UMQ	O2'-C2'	-3.92	1.33	1.43
10	A	304	UMQ	O2'-C2'	-3.83	1.33	1.43
12	H	30	OPC	CBQ-CBR	-3.77	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	30	OPC	CBT-CBS	-3.71	1.33	1.50
9	A	302	HEM	C2C-C1C	-3.66	1.45	1.52
15	G	101	BCR	C7-C6	-3.65	1.32	1.45
9	A	301	HEM	C2C-C1C	-3.65	1.45	1.52
12	B	202	OPC	CBT-CBS	-3.59	1.34	1.50
12	B	202	OPC	CBQ-CBR	-3.58	1.34	1.50
9	C	301	HEM	C2C-C1C	-3.51	1.45	1.52
15	G	101	BCR	C24-C23	-3.26	1.23	1.33
12	H	30	OPC	CBP-CBO	-3.25	1.32	1.51
12	H	30	OPC	CAQ-CAR	-3.13	1.33	1.51
12	B	202	OPC	CAQ-CAR	-3.05	1.33	1.51
12	H	30	OPC	CAR-CAS	-3.01	1.34	1.51
12	B	202	OPC	CAR-CAS	-3.01	1.34	1.51
12	H	30	OPC	CBB-CBC	-3.00	1.34	1.51
12	B	202	OPC	CBC-CBD	-2.99	1.34	1.51
12	B	202	OPC	CBB-CBC	-2.97	1.34	1.51
12	B	202	OPC	CBP-CBO	-2.95	1.34	1.51
12	H	30	OPC	CBC-CBD	-2.94	1.34	1.51
15	G	101	BCR	C11-C10	-2.58	1.35	1.43
15	G	101	BCR	C20-C21	-2.47	1.36	1.43
12	B	202	OPC	CAG-NAF	-2.46	1.43	1.51
15	G	101	BCR	C15-C14	-2.38	1.36	1.43
15	G	101	BCR	C16-C17	-2.38	1.36	1.43
9	A	303	HEM	C2B-C1B	-2.24	1.44	1.51
9	A	301	HEM	C2D-C1D	-2.21	1.44	1.51
9	C	301	HEM	C2B-C1B	-2.20	1.44	1.51
12	H	30	OPC	CAG-NAF	-2.16	1.44	1.51
9	A	302	HEM	C2B-C1B	-2.10	1.45	1.51
9	C	301	HEM	C2D-C1D	-2.02	1.45	1.51
9	A	303	HEM	C3B-CAB	2.02	1.55	1.51
9	A	301	HEM	FE-NB	2.03	2.08	1.97
9	A	302	HEM	C3B-CAB	2.03	1.55	1.51
9	A	302	HEM	C1C-NC	2.05	1.38	1.36
9	A	302	HEM	C4C-NC	2.07	1.38	1.36
9	C	301	HEM	FE-NB	2.08	2.08	1.97
9	A	301	HEM	C3B-CAB	2.10	1.55	1.51
9	C	301	HEM	FE-NC	2.22	2.04	1.95
9	A	303	HEM	C1C-NC	2.22	1.38	1.36
9	C	301	HEM	C3B-CAB	2.35	1.55	1.51
9	C	301	HEM	C1C-NC	2.39	1.38	1.36
11	B	201	CLA	C4C-C3C	2.42	1.49	1.45
9	A	303	HEM	C4C-NC	2.45	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	CAA-C2A	2.46	1.56	1.52
9	A	303	HEM	C3C-CAC	2.48	1.56	1.51
11	B	201	CLA	C1B-CHB	2.49	1.46	1.39
11	B	201	CLA	C1C-C2C	2.52	1.49	1.44
9	A	301	HEM	C3C-CAC	2.64	1.56	1.51
11	B	201	CLA	C4B-CHC	2.67	1.47	1.39
11	B	201	CLA	C3D-C2D	2.79	1.46	1.40
11	B	201	CLA	CHD-C4C	2.99	1.48	1.41
9	A	302	HEM	FE-NC	3.00	2.07	1.95
9	A	303	HEM	FE-ND	3.03	2.13	1.97
10	A	304	UMQ	O1'-C1'	3.16	1.45	1.40
10	A	306	UMQ	O1'-C1'	3.37	1.46	1.40
10	A	305	UMQ	O1'-C1'	3.48	1.46	1.40
9	A	301	HEM	FE-NC	3.49	2.09	1.95
12	H	30	OPC	CAV-CAW	3.72	1.53	1.31
12	B	202	OPC	CAV-CAW	3.81	1.53	1.31
12	B	202	OPC	OAN-CAO	3.87	1.45	1.34
11	B	201	CLA	CHC-C1C	3.95	1.47	1.35
11	B	201	CLA	OBD-CAD	4.08	1.28	1.22
12	H	30	OPC	OAN-CAO	4.08	1.46	1.34
12	H	30	OPC	OBJ-CBK	4.28	1.46	1.33
11	B	201	CLA	O2A-CGA	4.31	1.46	1.33
13	B	203	SQD	O48-C23	4.33	1.46	1.33
13	B	203	SQD	O47-C7	4.36	1.47	1.34
11	B	201	CLA	O2D-CGD	4.48	1.44	1.33
9	A	303	HEM	FE-NC	4.66	2.14	1.95
11	B	201	CLA	C3C-C2C	4.83	1.47	1.36
12	B	202	OPC	OBJ-CBK	4.89	1.48	1.33
11	B	201	CLA	C3B-C2B	5.50	1.47	1.40

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	203	SQD	O9-S-C6	-21.30	88.99	106.94
13	B	203	SQD	O8-S-O9	-12.30	82.97	111.61
13	B	203	SQD	O9-S-O7	-8.97	80.82	113.48
12	H	30	OPC	CAA-NAF-CAE	-8.77	86.43	108.98
12	H	30	OPC	CAA-NAF-CBG	-8.74	86.49	108.98
12	B	202	OPC	CAA-NAF-CBG	-8.56	86.96	108.98
12	B	202	OPC	CAA-NAF-CAE	-8.44	87.26	108.98
12	B	202	OPC	CAA-NAF-CAG	-5.64	87.46	109.90
12	H	30	OPC	CAA-NAF-CAG	-5.33	88.70	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	BCR	C30-C25-C26	-4.44	116.14	122.66
9	A	301	HEM	CBD-CAD-C3D	-4.41	100.73	113.55
15	G	101	BCR	C34-C9-C10	-4.21	116.68	122.90
13	B	203	SQD	O6-C44-C45	-4.01	101.46	110.99
11	B	201	CLA	C1C-C2C-C3C	-3.90	102.24	106.91
11	B	201	CLA	CHD-C4C-C3C	-3.82	119.04	124.94
11	B	201	CLA	C1C-NC-C4C	-3.54	101.97	106.27
11	B	201	CLA	O1D-CGD-CBD	-3.53	119.56	124.62
15	G	101	BCR	C27-C26-C25	-3.52	118.29	122.78
9	A	303	HEM	C3B-CAB-CBB	-3.24	119.49	124.46
9	A	303	HEM	CAA-C2A-C1A	-3.12	123.62	127.01
11	B	201	CLA	CAA-CBA-CGA	-3.05	104.39	113.32
9	A	303	HEM	CBA-CAA-C2A	-2.91	107.32	112.53
15	G	101	BCR	C38-C26-C25	-2.72	121.94	124.61
11	B	201	CLA	CAA-C2A-C3A	-2.65	105.58	113.22
13	B	203	SQD	O5-C1-C2	-2.64	104.86	110.28
11	B	201	CLA	C4C-C3C-C2C	-2.54	102.83	106.94
15	G	101	BCR	C32-C1-C6	-2.52	106.35	110.30
15	G	101	BCR	C28-C27-C26	-2.49	109.92	113.87
11	B	201	CLA	O2D-CGD-O1D	-2.47	118.68	123.79
13	B	203	SQD	C1-O5-C5	-2.41	109.06	113.75
12	B	202	OPC	CAM-OAN-CAO	-2.41	112.11	117.89
11	B	201	CLA	C3B-CAB-CBB	-2.35	121.51	126.32
15	G	101	BCR	C20-C21-C22	-2.25	123.95	127.20
11	B	201	CLA	CHC-C1C-C2C	-2.25	120.44	126.35
9	A	303	HEM	CAA-CBA-CGA	-2.24	108.63	112.75
9	A	301	HEM	CMA-C3A-C4A	-2.24	124.66	128.36
9	C	301	HEM	CBD-CAD-C3D	-2.23	107.06	113.55
9	A	302	HEM	CMA-C3A-C4A	-2.22	124.69	128.36
9	A	302	HEM	CBD-CAD-C3D	-2.18	107.20	113.55
12	H	30	OPC	OBJ-CBK-OCC	-2.16	117.91	123.49
13	B	203	SQD	C1-C2-C3	-2.15	105.72	109.97
10	A	304	UMQ	C1'-O5'-C5'	-2.14	109.59	113.75
13	B	203	SQD	C45-O47-C7	-2.11	112.83	117.89
9	C	301	HEM	C3B-CAB-CBB	-2.09	121.25	124.46
12	H	30	OPC	CAX-CAW-CAV	-2.02	111.31	125.34
15	G	101	BCR	C33-C5-C6	-2.00	122.64	124.61
12	H	30	OPC	CBG-NAF-CAG	2.13	118.36	109.90
15	G	101	BCR	C11-C10-C9	2.15	130.30	127.20
12	H	30	OPC	CAQ-CAR-CAS	2.16	125.70	114.53
9	A	303	HEM	C2D-C3D-C4D	2.17	105.17	101.50
9	A	302	HEM	C2D-C3D-C4D	2.26	105.33	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	203	SQD	C46-O48-C23	2.28	123.23	116.85
12	H	30	OPC	CBU-CBT-CBS	2.28	124.42	112.45
10	A	306	UMQ	C1'-O5'-C5'	2.32	118.25	113.75
12	H	30	OPC	CAR-CAS-CAT	2.35	126.66	114.53
12	B	202	OPC	CBI-OBJ-CBK	2.43	123.65	116.85
9	A	303	HEM	CMD-C2D-C3D	2.44	125.12	114.35
12	B	202	OPC	CBG-NAF-CAG	2.47	119.73	109.90
12	B	202	OPC	CAE-NAF-CAG	2.49	119.82	109.90
15	G	101	BCR	C30-C25-C24	2.50	122.83	115.82
11	B	201	CLA	CAC-C3C-C4C	2.63	128.65	124.83
9	C	301	HEM	C2D-C3D-C4D	2.63	105.96	101.50
10	A	306	UMQ	O5'-C5'-C4'	2.71	115.47	109.75
12	B	202	OPC	CBU-CBT-CBS	2.74	126.83	112.45
12	B	202	OPC	CBP-CBQ-CBR	2.77	126.98	112.45
11	B	201	CLA	CMB-C2B-C3B	2.79	130.54	125.09
13	B	203	SQD	O48-C23-C24	2.80	120.43	111.90
11	B	201	CLA	CMC-C2C-C1C	2.84	129.42	125.02
12	H	30	OPC	OBJ-CBK-CBL	2.86	120.61	111.90
12	B	202	OPC	OBJ-CBK-CBL	2.91	120.76	111.90
9	C	301	HEM	CMD-C2D-C3D	2.93	127.29	114.35
12	H	30	OPC	CBP-CBQ-CBR	2.93	127.83	112.45
9	A	302	HEM	CMD-C2D-C3D	2.94	127.34	114.35
12	H	30	OPC	CBO-CBP-CBQ	2.97	125.44	113.86
10	A	306	UMQ	O5-C5-C4	2.98	115.28	109.68
12	H	30	OPC	CAE-NAF-CAG	3.01	121.88	109.90
11	B	201	CLA	O2A-CGA-CBA	3.03	121.14	111.90
9	A	301	HEM	CMD-C2D-C3D	3.13	128.19	114.35
12	B	202	OPC	CBO-CBP-CBQ	3.20	126.35	113.86
12	H	30	OPC	CAH-CAG-NAF	3.29	126.61	116.03
12	H	30	OPC	OAN-CAO-CAP	3.29	118.68	111.53
15	G	101	BCR	C38-C26-C27	3.33	119.74	113.43
13	B	203	SQD	O8-S-O7	3.33	119.37	111.61
10	A	306	UMQ	C1-O5-C5	3.34	120.23	113.75
12	B	202	OPC	CAR-CAQ-CAP	3.36	125.62	113.29
9	A	301	HEM	C2D-C3D-C4D	3.50	107.43	101.50
10	A	304	UMQ	CA-O1'-C1'	3.55	120.14	113.94
10	A	304	UMQ	O5'-C1'-O1'	3.64	118.81	110.05
9	A	301	HEM	CAD-C3D-C4D	3.82	125.96	112.47
9	C	301	HEM	C3B-C4B-CHC	3.83	128.56	123.16
12	H	30	OPC	CBG-NAF-CAE	3.92	119.05	108.98
9	A	303	HEM	CAD-C3D-C2D	3.97	124.63	113.22
10	A	305	UMQ	O5'-C1'-C2'	3.98	118.44	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEM	CMC-C2C-C3C	3.98	126.48	116.53
10	A	306	UMQ	O5'-C1'-O1'	4.00	119.68	110.05
11	B	201	CLA	C3B-C4B-NB	4.05	114.45	109.21
9	C	301	HEM	CMC-C2C-C3C	4.08	126.72	116.53
10	A	304	UMQ	O2'-C2'-C3'	4.12	119.61	110.34
9	C	301	HEM	CAD-C3D-C4D	4.14	127.07	112.47
10	A	305	UMQ	O2'-C2'-C3'	4.16	119.70	110.34
9	A	301	HEM	CMB-C2B-C3B	4.16	126.93	116.53
10	A	306	UMQ	O2'-C2'-C3'	4.17	119.72	110.34
12	B	202	OPC	CBG-NAF-CAE	4.19	119.75	108.98
10	A	305	UMQ	O5'-C1'-O1'	4.21	120.19	110.05
12	B	202	OPC	OAN-CAO-CAP	4.22	120.71	111.53
9	A	302	HEM	CAD-C3D-C4D	4.28	127.56	112.47
9	A	302	HEM	CMC-C2C-C3C	4.36	127.42	116.53
9	A	303	HEM	CMB-C2B-C3B	4.38	127.46	116.53
10	A	306	UMQ	CA-O1'-C1'	4.47	121.76	113.94
9	A	301	HEM	CMC-C2C-C3C	4.48	127.71	116.53
15	G	101	BCR	C8-C9-C10	4.52	126.27	118.98
13	B	203	SQD	O47-C7-C8	4.61	121.54	111.53
9	A	302	HEM	CMB-C2B-C3B	4.62	128.07	116.53
9	A	301	HEM	CAD-C3D-C2D	4.64	126.54	113.22
10	A	306	UMQ	O2'-C2'-C1'	4.64	120.20	110.02
9	C	301	HEM	CMB-C2B-C3B	4.66	128.16	116.53
10	A	304	UMQ	O5'-C1'-C2'	4.73	119.98	110.28
13	B	203	SQD	O6-C1-C2	4.75	114.04	108.04
10	A	304	UMQ	O2'-C2'-C1'	4.75	120.43	110.02
9	C	301	HEM	CAD-C3D-C2D	4.78	126.97	113.22
9	A	302	HEM	CAD-C3D-C2D	4.83	127.10	113.22
10	A	305	UMQ	C1'-C2'-C3'	4.86	119.54	109.97
10	A	305	UMQ	O2'-C2'-C1'	4.90	120.76	110.02
10	A	306	UMQ	O5'-C1'-C2'	4.94	120.41	110.28
10	A	305	UMQ	CA-O1'-C1'	4.94	122.58	113.94
9	A	303	HEM	CAD-C3D-C4D	5.03	130.19	112.47
10	A	304	UMQ	C1'-C2'-C3'	5.06	119.95	109.97
10	A	306	UMQ	C1'-C2'-C3'	5.13	120.08	109.97
15	G	101	BCR	C8-C7-C6	6.29	146.21	127.32
11	B	201	CLA	O2D-CGD-CBD	7.62	121.75	111.30
11	B	201	CLA	C2C-C1C-NC	8.73	116.75	110.24
10	A	306	UMQ	O1'-C1'-C2'	9.40	119.91	108.04
10	A	304	UMQ	O1'-C1'-C2'	10.42	121.20	108.04
10	A	305	UMQ	O1'-C1'-C2'	10.56	121.38	108.04
13	B	203	SQD	O7-S-C6	11.21	116.39	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	BCR	C23-C24-C25	13.91	169.08	127.32
15	G	101	BCR	C7-C8-C9	18.66	154.66	126.22
15	G	101	BCR	C24-C23-C22	29.37	170.99	126.22

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	306	UMQ	C2'
10	A	306	UMQ	C1'
10	A	305	UMQ	C2'
10	A	305	UMQ	C1'
10	A	304	UMQ	C2'
10	A	304	UMQ	C1'
11	B	201	CLA	C8
11	B	201	CLA	NC
11	B	201	CLA	ND
11	B	201	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	203	SQD	C45-O47-C7-O49
13	B	203	SQD	C45-O47-C7-C8

There are no ring outliers.

11 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	2	0
9	A	303	HEM	5	0
10	A	304	UMQ	1	0
10	A	305	UMQ	1	0
10	A	306	UMQ	2	0
11	B	201	CLA	1	0
13	B	203	SQD	1	0
9	C	301	HEM	6	0
14	D	200	FES	1	0
15	G	101	BCR	7	0
12	H	30	OPC	4	0

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	215/215 (100%)	-0.37	2 (0%) 85 64	34, 47, 75, 102	0
2	B	160/160 (100%)	-0.17	3 (1%) 70 41	46, 63, 96, 108	0
3	C	289/289 (100%)	0.53	35 (12%) 6 2	48, 64, 136, 139	0
4	D	166/179 (92%)	1.23	45 (27%) 1 0	48, 111, 140, 143	0
5	E	31/31 (100%)	-0.27	1 (3%) 51 23	72, 78, 94, 95	0
6	F	32/34 (94%)	-0.43	0 100 100	60, 71, 88, 95	0
7	G	37/37 (100%)	-0.15	0 100 100	52, 63, 98, 99	0
8	H	29/29 (100%)	-0.34	0 100 100	57, 60, 69, 77	0
All	All	959/974 (98%)	0.22	86 (8%) 12 4	34, 64, 135, 143	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	179	SER	9.5
3	C	203	SER	7.2
2	B	1	MET	7.0
3	C	204	GLY	6.6
4	D	156	GLU	6.6
3	C	224	ALA	6.5
4	D	157	ASN	5.6
4	D	73	HIS	5.6
3	C	184	ALA	5.2
4	D	69	PHE	5.1
4	D	72	SER	5.0
3	C	186	GLN	4.9
4	D	49	GLY	4.8
4	D	50	ALA	4.8
3	C	194	LYS	4.7
4	D	56	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	160	PHE	4.7
3	C	189	GLU	4.5
4	D	70	LEU	4.4
3	C	206	VAL	4.4
4	D	175	GLU	4.3
3	C	220	SER	4.2
4	D	155	THR	4.2
3	C	199	ILE	4.1
3	C	219	VAL	4.1
3	C	183	ILE	4.0
3	C	177	THR	4.0
4	D	57	LYS	3.8
3	C	195	TYR	3.8
1	A	1	MET	3.8
3	C	181	SER	3.7
4	D	158	ASP	3.7
3	C	179	THR	3.7
4	D	160	ILE	3.7
3	C	196	LEU	3.5
4	D	74	ASN	3.5
4	D	77	ASP	3.5
3	C	178	GLY	3.5
4	D	67	SER	3.5
3	C	207	VAL	3.4
3	C	227	ALA	3.4
3	C	188	GLY	3.4
3	C	202	GLU	3.4
4	D	140	VAL	3.3
4	D	66	VAL	3.3
4	D	159	LYS	3.3
4	D	64	VAL	3.3
4	D	48	GLY	3.2
4	D	55	THR	3.1
3	C	190	ASP	2.9
4	D	63	ASP	2.9
1	A	2	ALA	2.9
3	C	205	GLU	2.9
3	C	213	ALA	2.8
4	D	71	GLU	2.7
3	C	198	ASP	2.7
3	C	226	THR	2.7
4	D	176	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	52	GLY	2.6
4	D	17	GLN	2.6
4	D	47	ALA	2.6
4	D	141	ARG	2.6
4	D	169	ASP	2.5
4	D	154	LYS	2.5
3	C	176	ALA	2.5
3	C	208	SER	2.5
3	C	168	ASN	2.5
4	D	13	MET	2.5
4	D	51	GLY	2.5
4	D	99	ILE	2.4
4	D	145	PRO	2.4
4	D	65	SER	2.4
5	E	31	LEU	2.4
3	C	187	GLU	2.4
4	D	168	THR	2.4
4	D	68	LYS	2.3
2	B	2	ALA	2.3
3	C	193	VAL	2.3
3	C	212	PRO	2.3
4	D	171	ARG	2.2
4	D	177	TRP	2.2
4	D	16	ARG	2.2
3	C	209	ASP	2.1
3	C	93	GLU	2.0
4	D	75	VAL	2.0
4	D	147	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
12	OPC	H	30	54/55	0.70	0.40	5.44	81,109,134,134	0
10	UMQ	A	304	34/34	0.80	0.36	4.65	72,103,110,111	0
15	BCR	G	101	40/40	0.83	0.30	4.07	57,66,76,77	0
12	OPC	B	202	54/55	0.90	0.41	3.25	75,82,110,111	0
10	UMQ	A	305	34/34	0.80	0.35	2.01	135,137,140,141	0
10	UMQ	A	306	34/34	0.87	0.28	1.44	95,100,104,104	0
11	CLA	B	201	65/65	0.94	0.23	1.25	59,64,88,89	0
13	SQD	B	203	54/54	0.85	0.33	0.77	79,105,121,121	0
9	HEM	A	302	43/43	0.98	0.21	0.65	40,43,52,54	0
9	HEM	A	301	43/43	0.99	0.20	0.37	38,40,44,45	0
9	HEM	A	303	43/43	0.98	0.18	0.06	54,56,60,64	0
9	HEM	C	301	43/43	0.97	0.23	-0.02	52,55,63,64	0
14	FES	D	200	4/4	0.97	0.09	-2.08	105,106,106,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.