



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:36 PM GMT

PDB ID : 4TOB
Title : 1.95Å resolution structure of BfrB (Q151L) from *Pseudomonas aeruginosa*
Authors : Lovell, S.; Battaile, K.P.; Yao, H.; Kumar, R.; Eshelman, K.; Rivera, M.
Deposited on : 2014-06-05
Resolution : 1.95 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

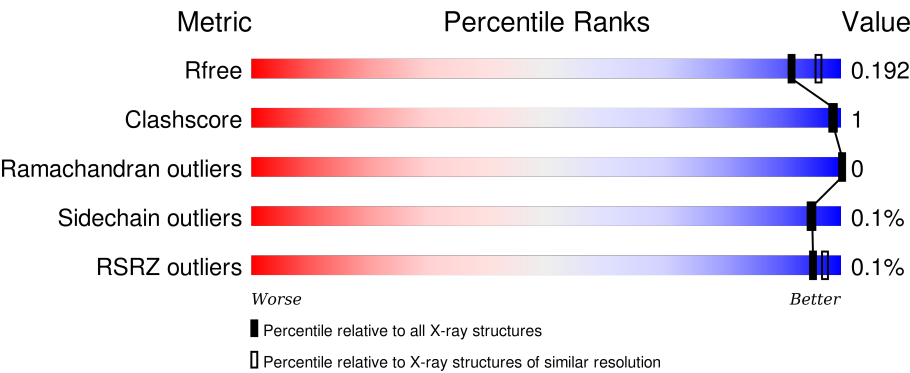
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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.




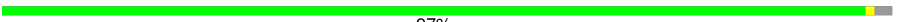













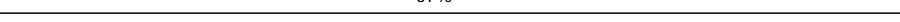
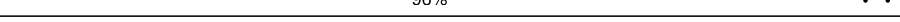
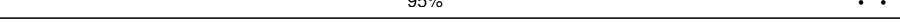
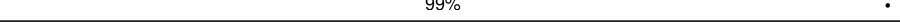
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	158	<div><div>%</div><div><div></div><div>97%</div><div>..</div></div></div>
1	B	158	<div><div></div><div>96%</div><div>..</div></div>
1	C	158	<div><div></div><div>96%</div><div>..</div></div>
1	D	158	<div><div></div><div>97%</div><div>..</div></div>
1	E	158	<div><div></div><div>96%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	158	 97% ..
1	G	158	 97% ..
1	H	158	 96% ..
1	I	158	 97% ..
1	J	158	 97% ..
1	K	158	 97% ..
1	L	158	 96% ..
1	M	158	 97% .
1	N	158	 96% ..
1	O	158	 96% ..
1	P	158	 96% ..
1	Q	158	 95% ..
1	R	158	 95% ...
1	S	158	 96% ..
1	T	158	 97% ..
1	U	158	 96% ..
1	V	158	 95% ..
1	W	158	 99% .
1	X	158	 98% .

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
2	MES	A	201	-	-	-	X
2	MES	B	202	-	-	-	X
2	MES	C	202	-	-	-	X
2	MES	D	201	-	-	-	X
2	MES	E	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	F	202	-	-	-	X
2	MES	G	201	-	-	-	X
2	MES	H	202	-	-	-	X
2	MES	I	201	-	-	-	X
2	MES	J	202	-	-	-	X
2	MES	K	202	-	-	-	X
2	MES	L	201	-	-	-	X
2	MES	M	201	-	-	-	X
2	MES	N	202	-	-	-	X
2	MES	O	202	-	-	-	X
2	MES	P	201	-	-	-	X
2	MES	Q	202	-	-	-	X
2	MES	R	201	-	-	-	X
2	MES	S	201	-	-	-	X
2	MES	T	202	-	-	-	X
2	MES	U	201	-	-	-	X
2	MES	V	202	-	-	-	X
2	MES	W	201	-	-	-	X
2	MES	X	202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34054 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1266	802	214	243	7			
1	B	155	Total	C	N	O	S	0	0	0
			1264	800	216	242	6			
1	C	155	Total	C	N	O	S	0	0	0
			1253	795	212	240	6			
1	D	155	Total	C	N	O	S	0	0	0
			1257	798	214	239	6			
1	E	155	Total	C	N	O	S	0	0	0
			1259	799	213	241	6			
1	F	156	Total	C	N	O	S	0	0	0
			1264	801	214	243	6			
1	G	155	Total	C	N	O	S	0	0	0
			1265	802	215	242	6			
1	H	155	Total	C	N	O	S	0	0	0
			1263	801	214	242	6			
1	I	155	Total	C	N	O	S	0	0	0
			1260	799	214	241	6			
1	J	155	Total	C	N	O	S	0	0	0
			1260	798	214	242	6			
1	K	155	Total	C	N	O	S	0	0	0
			1264	802	216	240	6			
1	L	154	Total	C	N	O	S	0	0	0
			1260	799	214	241	6			
1	M	154	Total	C	N	O	S	0	0	0
			1253	796	212	239	6			
1	N	156	Total	C	N	O	S	0	0	0
			1267	804	214	243	6			
1	O	155	Total	C	N	O	S	0	0	0
			1263	801	214	242	6			
1	P	155	Total	C	N	O	S	0	0	0
			1259	798	213	242	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total	C	N	O	S	0	0	0
			1259	799	213	241	6			
1	R	155	Total	C	N	O	S	0	0	0
			1261	800	214	241	6			
1	S	155	Total	C	N	O	S	0	0	0
			1258	798	213	241	6			
1	T	155	Total	C	N	O	S	0	0	0
			1259	797	214	242	6			
1	U	154	Total	C	N	O	S	0	0	0
			1255	796	214	239	6			
1	V	155	Total	C	N	O	S	0	0	0
			1251	795	213	237	6			
1	W	156	Total	C	N	O	S	0	0	0
			1272	806	217	243	6			
1	X	155	Total	C	N	O	S	0	0	0
			1260	800	214	240	6			

There are 24 discrepancies between the modelled and reference sequences:

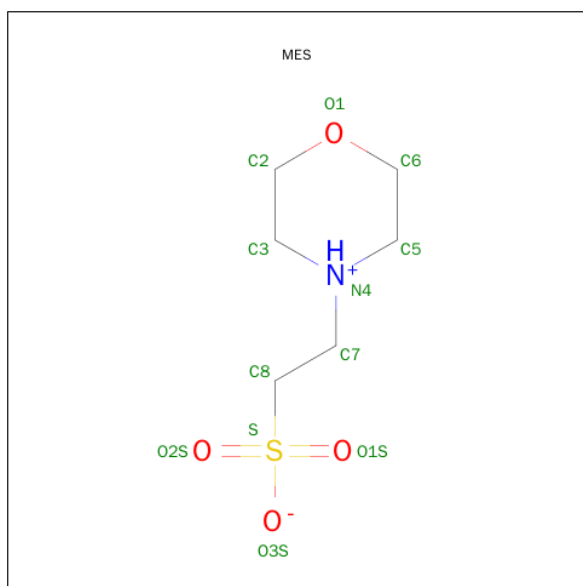
Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	GLN	engineered mutation	UNP Q9HY79
B	151	LEU	GLN	engineered mutation	UNP Q9HY79
C	151	LEU	GLN	engineered mutation	UNP Q9HY79
D	151	LEU	GLN	engineered mutation	UNP Q9HY79
E	151	LEU	GLN	engineered mutation	UNP Q9HY79
F	151	LEU	GLN	engineered mutation	UNP Q9HY79
G	151	LEU	GLN	engineered mutation	UNP Q9HY79
H	151	LEU	GLN	engineered mutation	UNP Q9HY79
I	151	LEU	GLN	engineered mutation	UNP Q9HY79
J	151	LEU	GLN	engineered mutation	UNP Q9HY79
K	151	LEU	GLN	engineered mutation	UNP Q9HY79
L	151	LEU	GLN	engineered mutation	UNP Q9HY79
M	151	LEU	GLN	engineered mutation	UNP Q9HY79
N	151	LEU	GLN	engineered mutation	UNP Q9HY79
O	151	LEU	GLN	engineered mutation	UNP Q9HY79
P	151	LEU	GLN	engineered mutation	UNP Q9HY79
Q	151	LEU	GLN	engineered mutation	UNP Q9HY79
R	151	LEU	GLN	engineered mutation	UNP Q9HY79
S	151	LEU	GLN	engineered mutation	UNP Q9HY79
T	151	LEU	GLN	engineered mutation	UNP Q9HY79
U	151	LEU	GLN	engineered mutation	UNP Q9HY79
V	151	LEU	GLN	engineered mutation	UNP Q9HY79
W	151	LEU	GLN	engineered mutation	UNP Q9HY79

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Chain	Residue	Modelled	Actual	Comment	Reference
X	151	LEU	GLN	engineered mutation	UNP Q9HY79

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



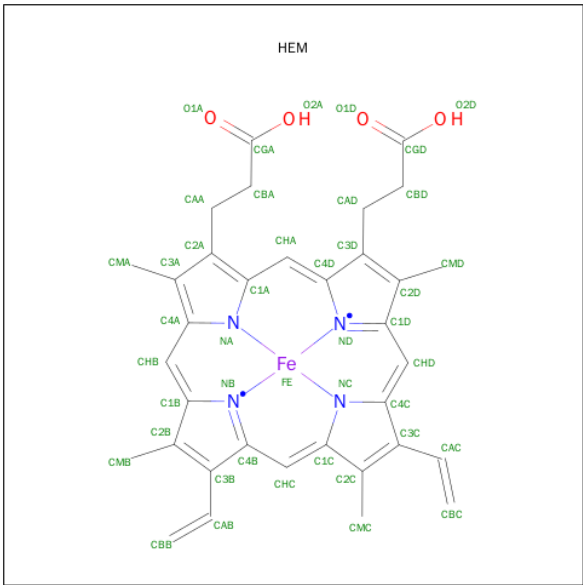
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	O	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	P	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	Q	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	R	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	S	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	T	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	W	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	119	Total O 119 119	0	0
4	B	136	Total O 136 136	0	0
4	C	141	Total O 141 141	0	0
4	D	134	Total O 134 134	0	0
4	E	94	Total O 94 94	0	0
4	F	119	Total O 119 119	0	0
4	G	141	Total O 141 141	0	0
4	H	146	Total O 146 146	0	0
4	I	117	Total O 117 117	0	0
4	J	130	Total O 130 130	0	0
4	K	130	Total O 130 130	0	0
4	L	129	Total O 129 129	0	0
4	M	110	Total O 110 110	0	0
4	N	130	Total O 130 130	0	0
4	O	132	Total O 132 132	0	0
4	P	123	Total O 123 123	0	0
4	Q	125	Total O 125 125	0	0
4	R	118	Total O 118 118	0	0
4	S	120	Total O 120 120	0	0
4	T	116	Total O 116 116	0	0
4	U	104	Total O 104 104	0	0
4	V	111	Total O 111 111	0	0

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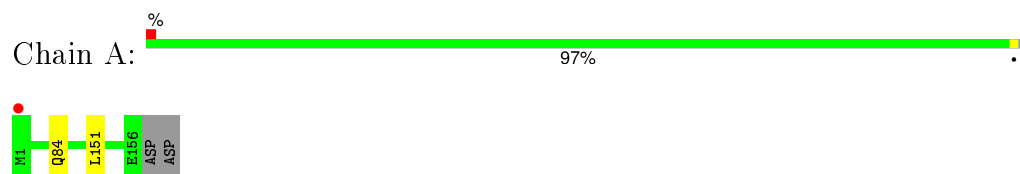
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	135	Total	O	0	0
			135	135		
4	X	138	Total	O	0	0
			138	138		

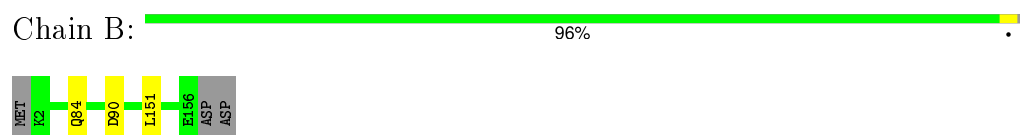
3 Residue-property plots

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.

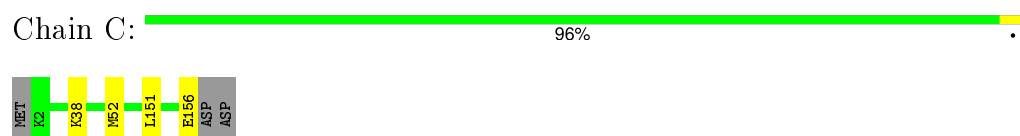
- Molecule 1: Bacterioferritin



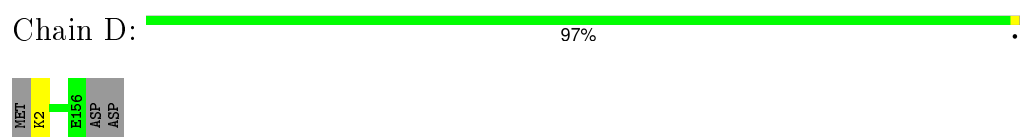
- Molecule 1: Bacterioferritin



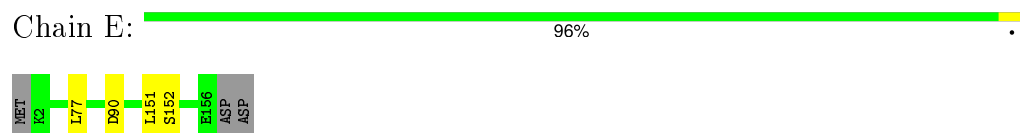
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin





- Molecule 1: Bacterioferritin

Chain G: 97% ..



- Molecule 1: Bacterioferritin

Chain H: 96% ..



- Molecule 1: Bacterioferritin

Chain I: 97% ..



- Molecule 1: Bacterioferritin

Chain J: 97% ..



- Molecule 1: Bacterioferritin

Chain K: 97% ..



- Molecule 1: Bacterioferritin

Chain L: 96% ..



- Molecule 1: Bacterioferritin

Chain M: 97% .



- Molecule 1: Bacterioferritin

Chain N:  96% ..



- Molecule 1: Bacterioferritin

Chain O:  96% ..



- Molecule 1: Bacterioferritin

Chain P:  96% ..



- Molecule 1: Bacterioferritin

Chain Q:  95% ..



- Molecule 1: Bacterioferritin

Chain R:  95% ...



- Molecule 1: Bacterioferritin

Chain S:  96% ..



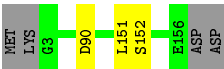
- Molecule 1: Bacterioferritin

Chain T:  97% ..



- Molecule 1: Bacterioferritin

Chain U:  96% ..



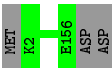
● Molecule 1: Bacterioferritin



● Molecule 1: Bacterioferritin



● Molecule 1: Bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.67Å 203.15Å 207.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.95 49.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.34-1.95) 100.0 (49.34-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1450)	Depositor
R, R_{free}	0.156 , 0.188 0.162 , 0.192	Depositor DCC
R_{free} test set	19331 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.0	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 384135 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34054	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.48	0/1287	0.58	0/1737
1	B	0.50	0/1285	0.59	1/1733 (0.1%)
1	C	0.46	0/1274	0.56	0/1721
1	D	0.50	0/1278	0.56	0/1724
1	E	0.45	0/1280	0.58	1/1727 (0.1%)
1	F	0.49	0/1285	0.57	0/1735
1	G	0.50	0/1286	0.57	1/1734 (0.1%)
1	H	0.53	0/1284	0.57	0/1732
1	I	0.47	0/1281	0.57	0/1728
1	J	0.48	0/1281	0.55	0/1729
1	K	0.47	0/1285	0.57	1/1732 (0.1%)
1	L	0.47	0/1281	0.57	0/1727
1	M	0.45	0/1274	0.56	0/1719
1	N	0.49	0/1288	0.58	0/1738
1	O	0.48	0/1284	0.57	1/1732 (0.1%)
1	P	0.46	0/1280	0.57	1/1728 (0.1%)
1	Q	0.44	0/1280	0.55	0/1726
1	R	0.46	0/1282	0.54	0/1729
1	S	0.45	0/1279	0.55	1/1726 (0.1%)
1	T	0.45	0/1280	0.55	0/1728
1	U	0.47	0/1276	0.55	1/1721 (0.1%)
1	V	0.46	0/1272	0.56	0/1717
1	W	0.48	0/1293	0.57	0/1743
1	X	0.49	0/1281	0.57	0/1728
All	All	0.47	0/30756	0.56	8/41494 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	90	ASP	CB-CG-OD1	5.98	123.68	118.30
1	E	90	ASP	CB-CG-OD1	5.80	123.52	118.30
1	S	90	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	90	ASP	CB-CG-OD1	5.62	123.36	118.30
1	U	90	ASP	CB-CG-OD1	5.60	123.34	118.30
1	K	90	ASP	CB-CG-OD1	5.39	123.15	118.30
1	O	90	ASP	CB-CG-OD1	5.33	123.09	118.30
1	G	90	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1266	0	1226	2	0
1	B	1264	0	1235	2	0
1	C	1253	0	1205	3	0
1	D	1257	0	1224	1	0
1	E	1259	0	1221	3	0
1	F	1264	0	1218	3	0
1	G	1265	0	1234	0	0
1	H	1263	0	1227	3	0
1	I	1260	0	1226	1	0
1	J	1260	0	1221	1	0
1	K	1264	0	1239	1	0
1	L	1260	0	1232	3	0
1	M	1253	0	1216	0	0
1	N	1267	0	1227	5	0
1	O	1263	0	1227	2	0
1	P	1259	0	1216	3	0
1	Q	1259	0	1227	4	0
1	R	1261	0	1228	5	0
1	S	1258	0	1219	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1259	0	1219	2	0
1	U	1255	0	1226	2	0
1	V	1251	0	1213	5	0
1	W	1272	0	1243	0	0
1	X	1260	0	1225	0	0
2	A	12	0	13	0	0
2	B	12	0	13	0	0
2	C	12	0	13	0	0
2	D	12	0	13	0	0
2	E	12	0	13	0	0
2	F	12	0	13	0	0
2	G	12	0	13	0	0
2	H	12	0	13	0	0
2	I	12	0	13	0	0
2	J	12	0	13	0	0
2	K	12	0	13	0	0
2	L	12	0	13	0	0
2	M	12	0	13	0	0
2	N	12	0	13	0	0
2	O	12	0	13	0	0
2	P	12	0	13	0	0
2	Q	12	0	13	0	0
2	R	12	0	13	0	0
2	S	12	0	13	0	0
2	T	12	0	13	0	0
2	U	12	0	13	0	0
2	V	12	0	13	0	0
2	W	12	0	13	0	0
2	X	12	0	13	0	0
3	B	43	0	30	0	0
3	C	43	0	30	2	0
3	F	43	0	30	2	0
3	H	43	0	30	1	0
3	J	43	0	30	1	0
3	K	43	0	30	3	0
3	N	43	0	30	1	0
3	O	43	0	30	2	0
3	Q	43	0	30	4	0
3	T	43	0	30	0	0
3	V	43	0	30	0	0
3	X	43	0	30	1	0
4	A	119	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	136	0	0	1	0
4	C	141	0	0	0	0
4	D	134	0	0	1	0
4	E	94	0	0	0	0
4	F	119	0	0	0	0
4	G	141	0	0	0	0
4	H	146	0	0	1	1
4	I	117	0	0	1	0
4	J	130	0	0	0	0
4	K	130	0	0	0	0
4	L	129	0	0	1	0
4	M	110	0	0	0	0
4	N	130	0	0	4	1
4	O	132	0	0	0	0
4	P	123	0	0	3	0
4	Q	125	0	0	1	0
4	R	118	0	0	3	0
4	S	120	0	0	1	0
4	T	116	0	0	1	0
4	U	104	0	0	0	0
4	V	111	0	0	2	0
4	W	135	0	0	0	0
4	X	138	0	0	0	0
All	All	34054	0	30066	51	1

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 1.

All (51) 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)
3:Q:201:HEM:HHC	3:Q:201:HEM:HBB2	1.71	0.73
3:F:201:HEM:HBB2	3:F:201:HEM:HHC	1.74	0.70
1:E:77:LEU:H	1:F:72:GLN:HE22	1.41	0.67
1:Q:72:GLN:HE22	1:R:77:LEU:H	1.45	0.65
1:S:84:GLN:NE2	4:S:392:HOH:O	2.31	0.62
1:Q:84:GLN:NE2	4:Q:348:HOH:O	2.32	0.62
1:A:84:GLN:NE2	4:A:334:HOH:O	2.33	0.61
4:R:353:HOH:O	1:V:121:LYS:CG	2.52	0.57
1:R:2:LYS:N	4:R:352:HOH:O	2.38	0.56
1:P:94:GLU:OE2	4:P:342:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:84:GLN:NE2	4:V:336:HOH:O	2.42	0.52
1:H:54:HIS:HD2	4:H:446:HOH:O	1.93	0.52
1:R:118:ASP:HB2	4:R:353:HOH:O	2.10	0.51
1:I:84:GLN:NE2	4:I:328:HOH:O	2.45	0.49
1:P:2:LYS:N	4:P:409:HOH:O	2.45	0.49
3:O:201:HEM:HBC2	3:O:201:HEM:HMC2	1.94	0.49
1:D:2:LYS:N	4:D:346:HOH:O	2.47	0.48
4:N:430:HOH:O	1:O:2:LYS:HD2	2.15	0.47
1:N:84:GLN:NE2	4:N:361:HOH:O	2.47	0.47
1:V:103:GLU:CG	4:V:408:HOH:O	2.63	0.46
3:C:201:HEM:HMC2	3:C:201:HEM:HBC2	1.97	0.46
1:T:2:LYS:N	4:T:327:HOH:O	2.48	0.46
3:X:201:HEM:HBC2	3:X:201:HEM:HMC1	1.98	0.45
1:O:52:MET:HB3	3:O:201:HEM:CHD	2.47	0.45
1:E:152:SER:OG	1:V:151:LEU:CD1	2.65	0.44
1:K:52:MET:HB3	3:K:201:HEM:CHD	2.48	0.44
1:B:84:GLN:NE2	4:B:354:HOH:O	2.50	0.44
1:Q:151:LEU:CD1	1:V:152:SER:OG	2.67	0.43
1:N:110:GLN:CG	4:N:302:HOH:O	2.67	0.43
1:F:152:SER:OG	1:H:151:LEU:CD1	2.67	0.43
1:N:81:GLU:HG2	1:N:85:GLU:OE2	2.19	0.43
1:P:84:GLN:NE2	4:P:325:HOH:O	2.52	0.42
3:K:201:HEM:HBC2	3:K:201:HEM:HMC1	2.00	0.42
1:B:151:LEU:CD1	1:H:152:SER:OG	2.68	0.42
3:Q:201:HEM:HBC2	3:Q:201:HEM:HMC2	2.01	0.42
1:C:52:MET:HB3	3:C:201:HEM:CHD	2.50	0.42
1:C:151:LEU:CD1	1:U:152:SER:OG	2.68	0.42
1:F:52:MET:HB3	3:F:201:HEM:CHB	2.50	0.42
1:A:151:LEU:CD1	1:L:152:SER:OG	2.68	0.42
1:Q:52:MET:HB3	3:Q:201:HEM:CHD	2.50	0.41
1:R:152:SER:OG	1:T:151:LEU:CD1	2.68	0.41
3:K:201:HEM:CHB	1:L:52:MET:HB3	2.50	0.41
1:E:151:LEU:CD1	1:J:152:SER:OG	2.69	0.41
1:S:152:SER:OG	1:U:151:LEU:CD1	2.69	0.41
1:N:52:MET:HB3	3:N:201:HEM:CHB	2.51	0.41
3:J:201:HEM:HMC2	3:J:201:HEM:HBC2	2.02	0.41
1:N:110:GLN:HG3	4:N:302:HOH:O	2.21	0.40
1:C:38:LYS:HB3	1:C:156:GLU:HG3	2.04	0.40
3:Q:201:HEM:CHB	1:R:52:MET:HB3	2.51	0.40
1:L:54:HIS:HD2	4:L:429:HOH:O	2.04	0.40
3:H:201:HEM:HBC2	3:H:201:HEM:HMC2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:311:HOH:O	4:N:302:HOH:O[3_455]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	154/158 (98%)	154 (100%)	0	0	100	100
1	B	153/158 (97%)	153 (100%)	0	0	100	100
1	C	153/158 (97%)	153 (100%)	0	0	100	100
1	D	153/158 (97%)	153 (100%)	0	0	100	100
1	E	153/158 (97%)	153 (100%)	0	0	100	100
1	F	154/158 (98%)	154 (100%)	0	0	100	100
1	G	153/158 (97%)	153 (100%)	0	0	100	100
1	H	153/158 (97%)	153 (100%)	0	0	100	100
1	I	153/158 (97%)	153 (100%)	0	0	100	100
1	J	153/158 (97%)	153 (100%)	0	0	100	100
1	K	153/158 (97%)	153 (100%)	0	0	100	100
1	L	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	M	152/158 (96%)	152 (100%)	0	0	100	100
1	N	154/158 (98%)	154 (100%)	0	0	100	100
1	O	153/158 (97%)	153 (100%)	0	0	100	100
1	P	153/158 (97%)	153 (100%)	0	0	100	100
1	Q	152/158 (96%)	152 (100%)	0	0	100	100
1	R	153/158 (97%)	153 (100%)	0	0	100	100
1	S	153/158 (97%)	153 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	153/158 (97%)	153 (100%)	0	0	100	100
1	U	152/158 (96%)	152 (100%)	0	0	100	100
1	V	153/158 (97%)	153 (100%)	0	0	100	100
1	W	154/158 (98%)	154 (100%)	0	0	100	100
1	X	153/158 (97%)	153 (100%)	0	0	100	100
All	All	3672/3792 (97%)	3671 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	135/144 (94%)	135 (100%)	0	100	100
1	B	137/144 (95%)	137 (100%)	0	100	100
1	C	132/144 (92%)	132 (100%)	0	100	100
1	D	134/144 (93%)	134 (100%)	0	100	100
1	E	134/144 (93%)	134 (100%)	0	100	100
1	F	134/144 (93%)	134 (100%)	0	100	100
1	G	136/144 (94%)	136 (100%)	0	100	100
1	H	135/144 (94%)	134 (99%)	1 (1%)	88	88
1	I	135/144 (94%)	135 (100%)	0	100	100
1	J	135/144 (94%)	135 (100%)	0	100	100
1	K	136/144 (94%)	136 (100%)	0	100	100
1	L	136/144 (94%)	136 (100%)	0	100	100
1	M	133/144 (92%)	133 (100%)	0	100	100
1	N	134/144 (93%)	134 (100%)	0	100	100
1	O	135/144 (94%)	135 (100%)	0	100	100
1	P	134/144 (93%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	135/144 (94%)	135 (100%)	0	100	100
1	R	135/144 (94%)	134 (99%)	1 (1%)	88	88
1	S	134/144 (93%)	134 (100%)	0	100	100
1	T	135/144 (94%)	135 (100%)	0	100	100
1	U	135/144 (94%)	135 (100%)	0	100	100
1	V	132/144 (92%)	132 (100%)	0	100	100
1	W	137/144 (95%)	137 (100%)	0	100	100
1	X	134/144 (93%)	134 (100%)	0	100	100
All	All	3232/3456 (94%)	3230 (100%)	2 (0%)	95	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	85	GLU
1	R	77	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	HIS
1	A	84	GLN
1	B	9	GLN
1	B	33	ASN
1	B	46	HIS
1	B	54	HIS
1	B	84	GLN
1	C	33	ASN
1	C	54	HIS
1	C	148	ASN
1	D	33	ASN
1	D	54	HIS
1	E	46	HIS
1	E	148	ASN
1	F	33	ASN
1	F	54	HIS
1	F	72	GLN
1	F	84	GLN

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Mol	Chain	Res	Type
1	G	33	ASN
1	G	46	HIS
1	G	54	HIS
1	H	33	ASN
1	H	54	HIS
1	H	84	GLN
1	I	33	ASN
1	I	46	HIS
1	I	54	HIS
1	I	84	GLN
1	I	148	ASN
1	J	33	ASN
1	J	46	HIS
1	J	54	HIS
1	J	84	GLN
1	K	33	ASN
1	L	33	ASN
1	L	54	HIS
1	M	33	ASN
1	N	33	ASN
1	N	84	GLN
1	O	33	ASN
1	O	43	HIS
1	O	54	HIS
1	P	33	ASN
1	P	84	GLN
1	P	148	ASN
1	Q	33	ASN
1	Q	54	HIS
1	Q	72	GLN
1	Q	84	GLN
1	R	33	ASN
1	S	33	ASN
1	S	54	HIS
1	T	33	ASN
1	T	54	HIS
1	U	10	HIS
1	U	33	ASN
1	U	54	HIS
1	V	9	GLN
1	V	33	ASN
1	V	46	HIS

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Mol	Chain	Res	Type
1	V	54	HIS
1	V	84	GLN
1	V	148	ASN
1	W	33	ASN
1	W	84	GLN
1	W	148	ASN
1	X	33	ASN
1	X	112	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MES	A	201	-	11,12,12	0.80	0	14,16,16	2.86	4 (28%)
3	HEM	B	201	1	30,50,50	2.23	8 (26%)	24,82,82	2.61	11 (45%)
2	MES	B	202	-	11,12,12	0.85	0	14,16,16	2.03	5 (35%)
3	HEM	C	201	1	30,50,50	2.05	6 (20%)	24,82,82	2.69	11 (45%)
2	MES	C	202	-	11,12,12	0.80	0	14,16,16	2.09	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	D	201	-	11,12,12	0.81	0	14,16,16	1.24	3 (21%)
2	MES	E	201	-	11,12,12	0.84	0	14,16,16	1.76	4 (28%)
3	HEM	F	201	1	30,50,50	2.02	7 (23%)	24,82,82	2.57	11 (45%)
2	MES	F	202	-	11,12,12	0.73	0	14,16,16	1.38	3 (21%)
2	MES	G	201	-	11,12,12	0.79	0	14,16,16	1.75	3 (21%)
3	HEM	H	201	1	30,50,50	2.03	5 (16%)	24,82,82	2.52	8 (33%)
2	MES	H	202	-	11,12,12	0.79	0	14,16,16	1.88	3 (21%)
2	MES	I	201	-	11,12,12	0.89	0	14,16,16	1.71	3 (21%)
3	HEM	J	201	1	30,50,50	2.06	6 (20%)	24,82,82	2.53	10 (41%)
2	MES	J	202	-	11,12,12	0.85	0	14,16,16	2.06	4 (28%)
3	HEM	K	201	1	30,50,50	1.95	5 (16%)	24,82,82	2.56	10 (41%)
2	MES	K	202	-	11,12,12	0.81	0	14,16,16	2.39	2 (14%)
2	MES	L	201	-	11,12,12	0.86	0	14,16,16	1.36	2 (14%)
2	MES	M	201	-	11,12,12	0.81	0	14,16,16	1.49	2 (14%)
3	HEM	N	201	1	30,50,50	2.29	6 (20%)	24,82,82	2.61	10 (41%)
2	MES	N	202	-	11,12,12	0.93	0	14,16,16	2.18	3 (21%)
3	HEM	O	201	1	30,50,50	2.09	7 (23%)	24,82,82	2.54	10 (41%)
2	MES	O	202	-	11,12,12	0.89	0	14,16,16	1.58	1 (7%)
2	MES	P	201	-	11,12,12	0.87	0	14,16,16	1.82	4 (28%)
3	HEM	Q	201	1	30,50,50	2.03	8 (26%)	24,82,82	2.60	11 (45%)
2	MES	Q	202	-	11,12,12	0.78	0	14,16,16	2.49	4 (28%)
2	MES	R	201	-	11,12,12	0.76	0	14,16,16	1.31	3 (21%)
2	MES	S	201	-	11,12,12	0.72	0	14,16,16	2.21	2 (14%)
3	HEM	T	201	1	30,50,50	2.04	7 (23%)	24,82,82	2.61	10 (41%)
2	MES	T	202	-	11,12,12	0.75	0	14,16,16	1.52	1 (7%)
2	MES	U	201	-	11,12,12	0.80	0	14,16,16	1.78	1 (7%)
3	HEM	V	201	1	30,50,50	2.15	7 (23%)	24,82,82	2.56	11 (45%)
2	MES	V	202	-	11,12,12	0.82	0	14,16,16	2.26	3 (21%)
2	MES	W	201	-	11,12,12	0.87	0	14,16,16	1.96	4 (28%)
3	HEM	X	201	1	30,50,50	2.22	6 (20%)	24,82,82	2.58	9 (37%)
2	MES	X	202	-	11,12,12	0.87	0	14,16,16	1.87	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	A	201	-	-	0/6/14/14	0/1/1/1
3	HEM	B	201	1	-	0/10/54/54	0/0/8/8
2	MES	B	202	-	-	0/6/14/14	0/1/1/1
3	HEM	C	201	1	-	0/10/54/54	0/0/8/8
2	MES	C	202	-	-	0/6/14/14	0/1/1/1
2	MES	D	201	-	-	0/6/14/14	0/1/1/1
2	MES	E	201	-	-	0/6/14/14	0/1/1/1
3	HEM	F	201	1	-	0/10/54/54	0/0/8/8
2	MES	F	202	-	-	0/6/14/14	0/1/1/1
2	MES	G	201	-	-	0/6/14/14	0/1/1/1
3	HEM	H	201	1	-	0/10/54/54	0/0/8/8
2	MES	H	202	-	-	0/6/14/14	0/1/1/1
2	MES	I	201	-	-	0/6/14/14	0/1/1/1
3	HEM	J	201	1	-	0/10/54/54	0/0/8/8
2	MES	J	202	-	-	0/6/14/14	0/1/1/1
3	HEM	K	201	1	-	0/10/54/54	0/0/8/8
2	MES	K	202	-	-	0/6/14/14	0/1/1/1
2	MES	L	201	-	-	0/6/14/14	0/1/1/1
2	MES	M	201	-	-	0/6/14/14	0/1/1/1
3	HEM	N	201	1	-	0/10/54/54	0/0/8/8
2	MES	N	202	-	-	0/6/14/14	0/1/1/1
3	HEM	O	201	1	-	0/10/54/54	0/0/8/8
2	MES	O	202	-	-	0/6/14/14	0/1/1/1
2	MES	P	201	-	-	0/6/14/14	0/1/1/1
3	HEM	Q	201	1	-	0/10/54/54	0/0/8/8
2	MES	Q	202	-	-	0/6/14/14	0/1/1/1
2	MES	R	201	-	-	0/6/14/14	0/1/1/1
2	MES	S	201	-	-	0/6/14/14	0/1/1/1
3	HEM	T	201	1	-	0/10/54/54	0/0/8/8
2	MES	T	202	-	-	0/6/14/14	0/1/1/1
2	MES	U	201	-	-	0/6/14/14	0/1/1/1
3	HEM	V	201	1	-	0/10/54/54	0/0/8/8
2	MES	V	202	-	-	0/6/14/14	0/1/1/1
2	MES	W	201	-	-	0/6/14/14	0/1/1/1
3	HEM	X	201	1	-	0/10/54/54	0/0/8/8
2	MES	X	202	-	-	0/6/14/14	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	201	HEM	C3B-C4B	-8.25	1.44	1.51
3	X	201	HEM	C3B-C4B	-7.71	1.45	1.51
3	B	201	HEM	C3B-C4B	-7.64	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	201	HEM	C3B-C4B	-7.32	1.45	1.51
3	O	201	HEM	C3B-C4B	-7.25	1.45	1.51
3	J	201	HEM	C3B-C4B	-7.11	1.45	1.51
3	C	201	HEM	C3B-C4B	-6.78	1.45	1.51
3	K	201	HEM	C3B-C4B	-6.61	1.46	1.51
3	H	201	HEM	C3B-C4B	-6.39	1.46	1.51
3	T	201	HEM	C3B-C4B	-6.15	1.46	1.51
3	Q	201	HEM	C3B-C4B	-5.72	1.46	1.51
3	X	201	HEM	C3D-C4D	-5.71	1.44	1.51
3	F	201	HEM	C3B-C4B	-5.46	1.47	1.51
3	F	201	HEM	C3D-C4D	-5.18	1.44	1.51
3	Q	201	HEM	C3D-C4D	-5.17	1.44	1.51
3	C	201	HEM	C3D-C4D	-4.93	1.45	1.51
3	N	201	HEM	C3D-C4D	-4.82	1.45	1.51
3	J	201	HEM	C3D-C4D	-4.81	1.45	1.51
3	O	201	HEM	C3D-C4D	-4.74	1.45	1.51
3	B	201	HEM	C3D-C4D	-4.73	1.45	1.51
3	T	201	HEM	C3D-C4D	-4.72	1.45	1.51
3	H	201	HEM	C3D-C4D	-4.71	1.45	1.51
3	V	201	HEM	C3D-C4D	-4.49	1.45	1.51
3	K	201	HEM	C3D-C4D	-4.43	1.45	1.51
3	F	201	HEM	C2C-C1C	-4.42	1.44	1.52
3	N	201	HEM	C2C-C1C	-4.42	1.44	1.52
3	H	201	HEM	C2C-C1C	-4.33	1.44	1.52
3	B	201	HEM	C2C-C1C	-4.32	1.44	1.52
3	X	201	HEM	C2C-C1C	-4.31	1.44	1.52
3	V	201	HEM	C2C-C1C	-4.25	1.44	1.52
3	Q	201	HEM	C2C-C1C	-4.22	1.44	1.52
3	C	201	HEM	C2C-C1C	-3.80	1.45	1.52
3	K	201	HEM	C2C-C1C	-3.70	1.45	1.52
3	J	201	HEM	C2C-C1C	-3.67	1.45	1.52
3	T	201	HEM	C2C-C1C	-3.65	1.45	1.52
3	O	201	HEM	C2C-C1C	-2.90	1.47	1.52
3	Q	201	HEM	C2D-C1D	-2.69	1.43	1.51
3	B	201	HEM	C2B-C1B	-2.26	1.44	1.51
3	K	201	HEM	C2D-C1D	-2.25	1.44	1.51
3	O	201	HEM	C2D-C1D	-2.25	1.44	1.51
3	N	201	HEM	C2D-C1D	-2.22	1.44	1.51
3	X	201	HEM	C2D-C1D	-2.21	1.44	1.51
3	O	201	HEM	C2B-C1B	-2.21	1.44	1.51
3	J	201	HEM	C2D-C1D	-2.16	1.44	1.51
3	Q	201	HEM	C2B-C1B	-2.14	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	HEM	C2D-C1D	-2.09	1.45	1.51
3	X	201	HEM	C2B-C1B	-2.09	1.45	1.51
3	C	201	HEM	C2B-C1B	-2.08	1.45	1.51
3	N	201	HEM	C2B-C1B	-2.04	1.45	1.51
3	V	201	HEM	C2D-C1D	-2.04	1.45	1.51
3	Q	201	HEM	FE-ND	2.01	2.08	1.97
3	F	201	HEM	FE-NC	2.04	2.03	1.95
3	B	201	HEM	CAA-C2A	2.04	1.55	1.52
3	H	201	HEM	FE-ND	2.05	2.08	1.97
3	Q	201	HEM	C3B-CAB	2.06	1.55	1.51
3	J	201	HEM	FE-NC	2.06	2.03	1.95
3	K	201	HEM	C3B-CAB	2.07	1.55	1.51
3	O	201	HEM	C1C-NC	2.08	1.38	1.36
3	C	201	HEM	C1C-NC	2.13	1.38	1.36
3	F	201	HEM	C1C-NC	2.14	1.38	1.36
3	T	201	HEM	C3B-CAB	2.14	1.55	1.51
3	Q	201	HEM	C1C-NC	2.15	1.38	1.36
3	X	201	HEM	FE-ND	2.18	2.09	1.97
3	H	201	HEM	FE-NC	2.19	2.04	1.95
3	V	201	HEM	FE-ND	2.23	2.09	1.97
3	V	201	HEM	C1C-NC	2.25	1.38	1.36
3	C	201	HEM	FE-ND	2.27	2.09	1.97
3	T	201	HEM	FE-NC	2.29	2.04	1.95
3	V	201	HEM	CAA-C2A	2.34	1.56	1.52
3	J	201	HEM	C1C-NC	2.37	1.38	1.36
3	F	201	HEM	C3C-CAC	2.39	1.55	1.51
3	B	201	HEM	FE-ND	2.41	2.10	1.97
3	F	201	HEM	C3B-CAB	2.48	1.56	1.51
3	O	201	HEM	C4C-NC	2.53	1.39	1.36
3	T	201	HEM	FE-ND	2.58	2.11	1.97
3	B	201	HEM	FE-NC	2.59	2.06	1.95
3	T	201	HEM	C1C-NC	3.18	1.39	1.36
3	N	201	HEM	C1C-NC	3.44	1.40	1.36

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	HEM	CBA-CAA-C2A	-4.38	104.68	112.53
3	H	201	HEM	CBA-CAA-C2A	-4.38	104.68	112.53
3	O	201	HEM	CBA-CAA-C2A	-4.12	105.14	112.53
3	C	201	HEM	C3B-CAB-CBB	-3.99	118.34	124.46
3	Q	201	HEM	CBA-CAA-C2A	-3.86	105.61	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	201	HEM	CBA-CAA-C2A	-3.69	105.92	112.53
3	J	201	HEM	CBA-CAA-C2A	-3.65	105.99	112.53
3	F	201	HEM	CBA-CAA-C2A	-3.57	106.13	112.53
3	N	201	HEM	CBA-CAA-C2A	-3.51	106.23	112.53
3	B	201	HEM	CBD-CAD-C3D	-3.33	103.86	113.55
3	K	201	HEM	CBA-CAA-C2A	-3.33	106.56	112.53
3	K	201	HEM	CBD-CAD-C3D	-3.24	104.13	113.55
3	B	201	HEM	CBA-CAA-C2A	-3.22	106.76	112.53
3	B	201	HEM	CMA-C3A-C4A	-3.16	123.14	128.36
3	X	201	HEM	CMA-C3A-C4A	-3.11	123.22	128.36
3	H	201	HEM	CBD-CAD-C3D	-3.11	104.52	113.55
3	X	201	HEM	CBD-CAD-C3D	-3.05	104.69	113.55
3	X	201	HEM	CBA-CAA-C2A	-3.04	107.08	112.53
3	T	201	HEM	CBD-CAD-C3D	-2.94	104.98	113.55
3	Q	201	HEM	CMA-C3A-C4A	-2.86	123.63	128.36
3	V	201	HEM	CMA-C3A-C4A	-2.79	123.74	128.36
3	O	201	HEM	CBD-CAD-C3D	-2.79	105.44	113.55
3	V	201	HEM	C3B-CAB-CBB	-2.75	120.24	124.46
3	T	201	HEM	CBA-CAA-C2A	-2.68	107.73	112.53
3	J	201	HEM	CBD-CAD-C3D	-2.66	105.81	113.55
3	F	201	HEM	CBD-CAD-C3D	-2.65	105.84	113.55
3	N	201	HEM	CAA-C2A-C1A	-2.64	124.14	127.01
3	O	201	HEM	C3B-CAB-CBB	-2.63	120.43	124.46
3	K	201	HEM	CMA-C3A-C4A	-2.61	124.05	128.36
3	Q	201	HEM	CBD-CAD-C3D	-2.60	105.98	113.55
3	V	201	HEM	CBD-CAD-C3D	-2.60	105.98	113.55
3	C	201	HEM	CBD-CAD-C3D	-2.56	106.09	113.55
3	C	201	HEM	CMA-C3A-C4A	-2.52	124.19	128.36
2	Q	202	MES	O2S-S-O1S	-2.51	104.33	113.48
3	N	201	HEM	CMA-C3A-C4A	-2.44	124.32	128.36
3	F	201	HEM	CMA-C3A-C4A	-2.39	124.42	128.36
3	J	201	HEM	CMA-C3A-C4A	-2.38	124.43	128.36
2	F	202	MES	O3S-S-O2S	-2.35	106.14	111.61
3	F	201	HEM	C3B-C4B-NB	-2.34	107.15	111.63
3	J	201	HEM	C3B-CAB-CBB	-2.32	120.90	124.46
3	O	201	HEM	CMA-C3A-C4A	-2.24	124.66	128.36
3	N	201	HEM	CBD-CAD-C3D	-2.23	107.06	113.55
3	C	201	HEM	C3B-C4B-NB	-2.22	107.38	111.63
3	B	201	HEM	C3B-CAB-CBB	-2.22	121.06	124.46
2	P	201	MES	O3S-S-O1S	-2.20	106.50	111.61
3	Q	201	HEM	C3B-C4B-NB	-2.19	107.44	111.63
3	T	201	HEM	C3B-CAB-CBB	-2.18	121.11	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	HEM	C3B-C4B-NB	-2.14	107.54	111.63
3	T	201	HEM	CMA-C3A-C4A	-2.14	124.83	128.36
2	A	201	MES	O3S-S-O1S	-2.13	106.64	111.61
3	K	201	HEM	C3B-CAB-CBB	-2.12	121.20	124.46
3	V	201	HEM	C3B-C4B-NB	-2.05	107.70	111.63
2	B	202	MES	C6-C5-N4	-2.02	107.06	110.12
2	R	201	MES	C7-N4-C3	2.02	116.45	111.27
2	J	202	MES	C7-N4-C3	2.07	116.58	111.27
2	C	202	MES	C7-N4-C3	2.07	116.59	111.27
2	R	201	MES	O1S-S-C8	2.09	108.69	106.91
2	D	201	MES	C5-N4-C3	2.12	113.50	108.90
2	I	201	MES	C5-N4-C3	2.12	113.50	108.90
2	D	201	MES	O2S-S-C8	2.14	108.73	106.91
2	J	202	MES	O2S-S-C8	2.15	108.74	106.91
3	V	201	HEM	C2D-C3D-C4D	2.17	105.19	101.50
2	E	201	MES	C5-N4-C3	2.19	113.64	108.90
2	M	201	MES	C5-N4-C3	2.23	113.72	108.90
2	F	202	MES	C7-N4-C3	2.23	117.00	111.27
2	Q	202	MES	C5-N4-C3	2.24	113.75	108.90
2	W	201	MES	C5-N4-C3	2.24	113.75	108.90
2	S	201	MES	C5-N4-C3	2.25	113.78	108.90
2	E	201	MES	C7-N4-C3	2.26	117.06	111.27
2	N	202	MES	C5-N4-C3	2.27	113.81	108.90
2	X	202	MES	O2S-S-C8	2.27	108.84	106.91
3	J	201	HEM	C2D-C3D-C4D	2.28	105.36	101.50
3	K	201	HEM	C2D-C3D-C4D	2.29	105.38	101.50
3	Q	201	HEM	C2D-C3D-C4D	2.29	105.38	101.50
2	C	202	MES	C5-N4-C3	2.29	113.86	108.90
3	F	201	HEM	C2D-C3D-C4D	2.29	105.39	101.50
2	E	201	MES	O2S-S-C8	2.31	108.88	106.91
2	W	201	MES	C7-N4-C3	2.32	117.23	111.27
2	P	201	MES	O2S-S-C8	2.33	108.89	106.91
2	D	201	MES	C7-N4-C3	2.35	117.30	111.27
2	B	202	MES	O1-C2-C3	2.36	117.25	111.84
2	A	201	MES	O2S-S-C8	2.37	108.92	106.91
2	V	202	MES	C5-N4-C3	2.41	114.13	108.90
2	J	202	MES	C5-N4-C3	2.41	114.13	108.90
2	P	201	MES	C5-N4-C3	2.45	114.21	108.90
2	A	201	MES	C5-N4-C3	2.51	114.33	108.90
2	X	202	MES	C5-N4-C3	2.51	114.34	108.90
2	B	202	MES	C5-N4-C3	2.52	114.35	108.90
2	L	201	MES	C5-N4-C3	2.56	114.45	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	MES	O1S-S-C8	2.63	109.15	106.91
2	R	201	MES	C5-N4-C3	2.68	114.71	108.90
3	N	201	HEM	C2D-C3D-C4D	2.69	106.06	101.50
3	X	201	HEM	C2D-C3D-C4D	2.69	106.07	101.50
3	O	201	HEM	CMD-C2D-C3D	2.70	126.29	114.35
3	X	201	HEM	CMD-C2D-C3D	2.71	126.35	114.35
2	K	202	MES	C5-N4-C3	2.72	114.80	108.90
3	N	201	HEM	CMD-C2D-C3D	2.73	126.43	114.35
3	O	201	HEM	C2D-C3D-C4D	2.77	106.19	101.50
2	Q	202	MES	O2S-S-C8	2.79	109.28	106.91
3	H	201	HEM	CMD-C2D-C3D	2.79	126.68	114.35
3	F	201	HEM	CMD-C2D-C3D	2.82	126.84	114.35
3	Q	201	HEM	C3B-C4B-CHC	2.83	127.14	123.16
3	C	201	HEM	CMD-C2D-C3D	2.87	127.03	114.35
3	B	201	HEM	CMD-C2D-C3D	2.87	127.05	114.35
3	J	201	HEM	CMD-C2D-C3D	2.87	127.05	114.35
3	T	201	HEM	C2D-C3D-C4D	2.88	106.37	101.50
2	F	202	MES	O1S-S-C8	2.89	109.38	106.91
2	L	201	MES	O1S-S-C8	2.93	109.40	106.91
3	C	201	HEM	C2D-C3D-C4D	2.95	106.50	101.50
3	V	201	HEM	CMD-C2D-C3D	2.98	127.52	114.35
3	H	201	HEM	C2D-C3D-C4D	2.99	106.57	101.50
2	G	201	MES	O1S-S-C8	3.05	109.51	106.91
3	K	201	HEM	CMD-C2D-C3D	3.08	127.97	114.35
2	H	202	MES	C5-N4-C3	3.09	115.60	108.90
2	G	201	MES	C5-N4-C3	3.09	115.60	108.90
3	T	201	HEM	CMD-C2D-C3D	3.12	128.13	114.35
3	B	201	HEM	C2D-C3D-C4D	3.18	106.89	101.50
3	Q	201	HEM	CMD-C2D-C3D	3.31	129.00	114.35
2	H	202	MES	O2S-S-C8	3.31	109.73	106.91
2	I	201	MES	O1S-S-C8	3.49	109.89	106.91
3	F	201	HEM	C3B-C4B-CHC	3.58	128.20	123.16
2	M	201	MES	O1S-S-C8	3.67	110.04	106.91
2	C	202	MES	O2S-S-C8	3.79	110.14	106.91
2	W	201	MES	O2S-S-C8	3.83	110.18	106.91
2	T	202	MES	O2S-S-C8	3.92	110.25	106.91
2	I	201	MES	O2S-S-C8	3.94	110.27	106.91
2	G	201	MES	O2S-S-C8	3.95	110.28	106.91
3	B	201	HEM	CAD-C3D-C4D	4.00	126.58	112.47
3	X	201	HEM	CAD-C3D-C4D	4.01	126.61	112.47
3	H	201	HEM	CAD-C3D-C2D	4.01	124.74	113.22
3	F	201	HEM	CAD-C3D-C4D	4.08	126.85	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	201	HEM	CAD-C3D-C4D	4.12	126.98	112.47
3	Q	201	HEM	CAD-C3D-C4D	4.13	127.04	112.47
3	K	201	HEM	CAD-C3D-C2D	4.19	125.25	113.22
3	O	201	HEM	CAD-C3D-C4D	4.21	127.30	112.47
3	C	201	HEM	CAD-C3D-C4D	4.22	127.37	112.47
3	T	201	HEM	CAD-C3D-C2D	4.28	125.53	113.22
2	B	202	MES	O2S-S-C8	4.32	110.59	106.91
3	H	201	HEM	CMB-C2B-C3B	4.34	127.37	116.53
3	F	201	HEM	CMB-C2B-C3B	4.36	127.41	116.53
2	V	202	MES	O2S-S-C8	4.37	110.64	106.91
3	N	201	HEM	CAD-C3D-C2D	4.40	125.86	113.22
3	V	201	HEM	CAD-C3D-C4D	4.41	128.01	112.47
3	N	201	HEM	CAD-C3D-C4D	4.42	128.06	112.47
2	O	202	MES	O1S-S-C8	4.43	110.69	106.91
3	T	201	HEM	CAD-C3D-C4D	4.43	128.10	112.47
2	W	201	MES	O1S-S-C8	4.43	110.69	106.91
3	C	201	HEM	CAD-C3D-C2D	4.48	126.09	113.22
2	N	202	MES	O1S-S-C8	4.52	110.76	106.91
3	O	201	HEM	CAD-C3D-C2D	4.59	126.42	113.22
3	H	201	HEM	CAD-C3D-C4D	4.60	128.68	112.47
3	B	201	HEM	CAD-C3D-C2D	4.63	126.52	113.22
2	E	201	MES	O1S-S-C8	4.63	110.86	106.91
3	Q	201	HEM	CMB-C2B-C3B	4.69	128.25	116.53
3	V	201	HEM	CAD-C3D-C2D	4.73	126.81	113.22
3	K	201	HEM	CAD-C3D-C4D	4.77	129.29	112.47
3	V	201	HEM	CMB-C2B-C3B	4.77	128.45	116.53
3	K	201	HEM	CMB-C2B-C3B	4.78	128.47	116.53
3	B	201	HEM	CMB-C2B-C3B	4.81	128.54	116.53
2	H	202	MES	O1S-S-C8	4.83	111.03	106.91
3	X	201	HEM	CAD-C3D-C2D	4.91	127.32	113.22
3	C	201	HEM	CMB-C2B-C3B	4.91	128.78	116.53
3	O	201	HEM	CMB-C2B-C3B	4.93	128.83	116.53
3	T	201	HEM	CMC-C2C-C3C	4.94	128.85	116.53
3	Q	201	HEM	CAD-C3D-C2D	4.97	127.49	113.22
3	O	201	HEM	CMC-C2C-C3C	5.00	129.01	116.53
2	P	201	MES	O1S-S-C8	5.00	111.17	106.91
3	J	201	HEM	CAD-C3D-C2D	5.01	127.62	113.22
3	F	201	HEM	CAD-C3D-C2D	5.05	127.73	113.22
3	J	201	HEM	CMB-C2B-C3B	5.09	129.23	116.53
3	C	201	HEM	CMC-C2C-C3C	5.22	129.55	116.53
2	U	201	MES	O1S-S-C8	5.22	111.36	106.91
3	V	201	HEM	CMC-C2C-C3C	5.29	129.75	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	202	MES	O1S-S-C8	5.35	111.47	106.91
3	X	201	HEM	CMB-C2B-C3B	5.37	129.93	116.53
3	J	201	HEM	CMC-C2C-C3C	5.38	129.95	116.53
3	Q	201	HEM	CMC-C2C-C3C	5.40	130.00	116.53
2	C	202	MES	O1S-S-C8	5.47	111.58	106.91
3	B	201	HEM	CMC-C2C-C3C	5.53	130.34	116.53
2	N	202	MES	O2S-S-C8	5.54	111.63	106.91
3	N	201	HEM	CMC-C2C-C3C	5.58	130.45	116.53
3	F	201	HEM	CMC-C2C-C3C	5.59	130.50	116.53
3	X	201	HEM	CMC-C2C-C3C	5.63	130.57	116.53
3	N	201	HEM	CMB-C2B-C3B	5.69	130.73	116.53
2	V	202	MES	O1S-S-C8	5.82	111.87	106.91
3	H	201	HEM	CMC-C2C-C3C	5.83	131.08	116.53
3	K	201	HEM	CMC-C2C-C3C	5.84	131.11	116.53
3	T	201	HEM	CMB-C2B-C3B	6.03	131.59	116.53
2	J	202	MES	O1S-S-C8	6.15	112.15	106.91
2	S	201	MES	O1S-S-C8	7.13	112.99	106.91
2	K	202	MES	O1S-S-C8	7.64	113.42	106.91
2	Q	202	MES	O1S-S-C8	7.73	113.50	106.91
2	A	201	MES	O1S-S-C8	9.55	115.06	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	HEM	2	0
3	F	201	HEM	2	0
3	H	201	HEM	1	0
3	J	201	HEM	1	0
3	K	201	HEM	3	0
3	N	201	HEM	1	0
3	O	201	HEM	2	0
3	Q	201	HEM	4	0
3	X	201	HEM	1	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	156/158 (98%)	-0.40	1 (0%) 90 94	12, 18, 30, 43	0
1	B	155/158 (98%)	-0.45	0 100 100	12, 18, 29, 39	0
1	C	155/158 (98%)	-0.47	0 100 100	13, 19, 28, 42	0
1	D	155/158 (98%)	-0.51	0 100 100	13, 18, 27, 40	0
1	E	155/158 (98%)	-0.50	0 100 100	13, 18, 28, 43	0
1	F	156/158 (98%)	-0.48	0 100 100	13, 17, 27, 50	0
1	G	155/158 (98%)	-0.49	0 100 100	11, 17, 29, 40	0
1	H	155/158 (98%)	-0.46	0 100 100	10, 16, 26, 40	0
1	I	155/158 (98%)	-0.49	0 100 100	13, 18, 29, 41	0
1	J	155/158 (98%)	-0.50	0 100 100	14, 18, 29, 43	0
1	K	155/158 (98%)	-0.44	0 100 100	15, 20, 30, 41	0
1	L	154/158 (97%)	-0.45	0 100 100	14, 19, 28, 39	0
1	M	154/158 (97%)	-0.49	0 100 100	13, 19, 29, 42	0
1	N	156/158 (98%)	-0.44	1 (0%) 90 94	12, 18, 30, 47	0
1	O	155/158 (98%)	-0.50	0 100 100	12, 17, 26, 41	0
1	P	155/158 (98%)	-0.49	0 100 100	13, 19, 29, 42	0
1	Q	154/158 (97%)	-0.47	0 100 100	15, 19, 31, 43	0
1	R	155/158 (98%)	-0.50	0 100 100	15, 20, 30, 39	0
1	S	155/158 (98%)	-0.42	0 100 100	15, 20, 31, 42	0
1	T	155/158 (98%)	-0.49	0 100 100	15, 20, 30, 42	0
1	U	154/158 (97%)	-0.51	0 100 100	14, 19, 31, 40	0
1	V	155/158 (98%)	-0.51	0 100 100	14, 20, 31, 45	0
1	W	156/158 (98%)	-0.51	0 100 100	12, 17, 28, 52	0
1	X	155/158 (98%)	-0.56	0 100 100	12, 17, 28, 40	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3720/3792 (98%)	-0.48	2 (0%) 95 97	10, 19, 30, 52	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	1	MET	4.3
1	A	1	MET	2.1

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
2	MES	I	201	12/12	0.91	0.28	34.42	32,35,42,49	0
2	MES	X	202	12/12	0.90	0.27	25.13	31,36,40,48	0
2	MES	B	202	12/12	0.90	0.27	20.46	32,39,46,47	0
2	MES	S	201	12/12	0.95	0.22	20.34	29,36,41,45	0
2	MES	U	201	12/12	0.90	0.23	19.68	27,35,43,46	0
2	MES	F	202	12/12	0.94	0.22	18.87	26,34,40,42	0
2	MES	J	202	12/12	0.91	0.25	18.14	27,35,41,46	0
2	MES	O	202	12/12	0.94	0.18	16.03	29,32,37,43	0
2	MES	T	202	12/12	0.93	0.25	15.58	29,35,39,39	0
2	MES	V	202	12/12	0.93	0.24	15.18	31,37,45,47	0
2	MES	E	201	12/12	0.94	0.23	15.15	27,35,42,47	0
2	MES	L	201	12/12	0.93	0.23	14.37	27,35,39,41	0
2	MES	K	202	12/12	0.93	0.24	13.99	28,37,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MES	P	201	12/12	0.90	0.26	13.91	30,36,41,49	0
2	MES	G	201	12/12	0.92	0.20	13.29	29,35,40,42	0
2	MES	N	202	12/12	0.93	0.22	12.64	27,34,42,43	0
2	MES	R	201	12/12	0.92	0.18	11.76	27,33,49,50	0
2	MES	D	201	12/12	0.94	0.20	11.48	29,32,36,36	0
2	MES	Q	202	12/12	0.90	0.26	11.47	31,34,45,46	0
2	MES	W	201	12/12	0.92	0.24	11.44	29,33,42,46	0
2	MES	C	202	12/12	0.92	0.24	11.16	29,37,48,50	0
2	MES	A	201	12/12	0.94	0.16	9.78	25,31,35,43	0
2	MES	M	201	12/12	0.90	0.25	9.66	29,35,39,39	0
2	MES	H	202	12/12	0.95	0.17	7.72	22,26,33,34	0
3	HEM	X	201	43/43	0.98	0.09	1.11	12,15,26,33	0
3	HEM	V	201	43/43	0.98	0.09	1.06	13,17,25,31	0
3	HEM	Q	201	43/43	0.98	0.09	0.79	13,18,26,35	0
3	HEM	N	201	43/43	0.98	0.09	0.75	12,16,26,32	0
3	HEM	T	201	43/43	0.98	0.09	0.73	14,17,26,33	0
3	HEM	C	201	43/43	0.98	0.09	0.52	11,15,25,30	0
3	HEM	B	201	43/43	0.98	0.09	0.40	11,15,25,32	0
3	HEM	H	201	43/43	0.98	0.09	0.38	11,13,22,30	0
3	HEM	F	201	43/43	0.98	0.09	0.22	10,15,24,33	0
3	HEM	J	201	43/43	0.98	0.09	-0.00	12,16,26,31	0
3	HEM	O	201	43/43	0.98	0.09	-0.03	11,15,25,28	0
3	HEM	K	201	43/43	0.98	0.09	-0.06	14,17,29,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.