



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 10:34 AM EST

PDB ID : 3UDF
Title : Crystal structure of Apo PBP1a from Acinetobacter baumannii
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

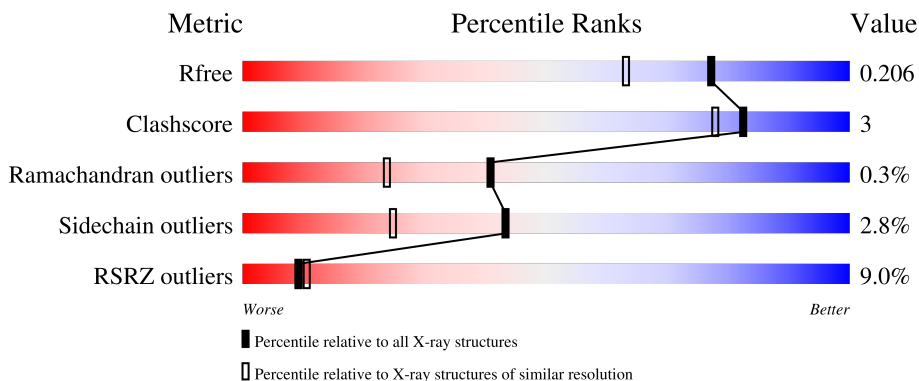
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	731	
1	B	731	

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	B	742	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10395 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 Penicillin-binding protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4703	2999	829	859	16	0	1	0
1	B	599	4720	3008	833	863	16	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

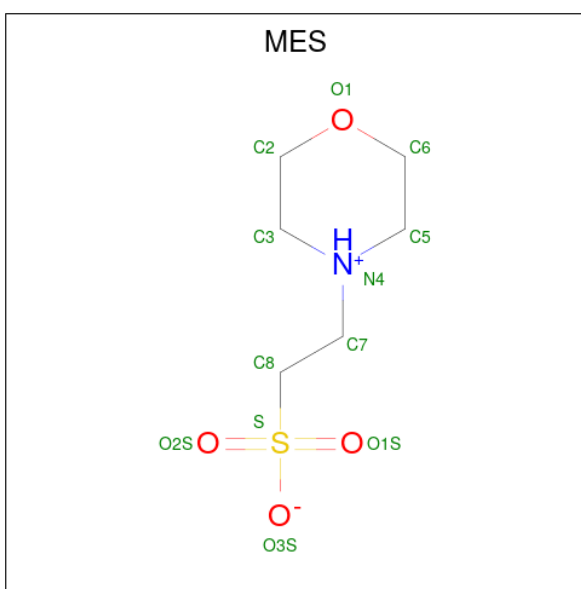
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP G1C794
A	10	HIS	-	expression tag	UNP G1C794
A	11	HIS	-	expression tag	UNP G1C794
A	12	HIS	-	expression tag	UNP G1C794
A	13	HIS	-	expression tag	UNP G1C794
A	14	HIS	-	expression tag	UNP G1C794
A	15	HIS	-	expression tag	UNP G1C794
A	16	GLU	-	expression tag	UNP G1C794
A	17	ASN	-	expression tag	UNP G1C794
A	18	LEU	-	expression tag	UNP G1C794
A	19	TYR	-	expression tag	UNP G1C794
A	20	PHE	-	expression tag	UNP G1C794
A	21	GLN	-	expression tag	UNP G1C794
A	22	SER	-	expression tag	UNP G1C794
A	23	HIS	-	expression tag	UNP G1C794
A	24	MET	-	expression tag	UNP G1C794
B	9	MET	-	expression tag	UNP G1C794
B	10	HIS	-	expression tag	UNP G1C794
B	11	HIS	-	expression tag	UNP G1C794
B	12	HIS	-	expression tag	UNP G1C794
B	13	HIS	-	expression tag	UNP G1C794
B	14	HIS	-	expression tag	UNP G1C794
B	15	HIS	-	expression tag	UNP G1C794
B	16	GLU	-	expression tag	UNP G1C794
B	17	ASN	-	expression tag	UNP G1C794

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	-	expression tag	UNP G1C794
B	19	TYR	-	expression tag	UNP G1C794
B	20	PHE	-	expression tag	UNP G1C794
B	21	GLN	-	expression tag	UNP G1C794
B	22	SER	-	expression tag	UNP G1C794
B	23	HIS	-	expression tag	UNP G1C794
B	24	MET	-	expression tag	UNP G1C794

- 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	B	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	435	Total	O	0	0
			435	435		

Continued on next page...

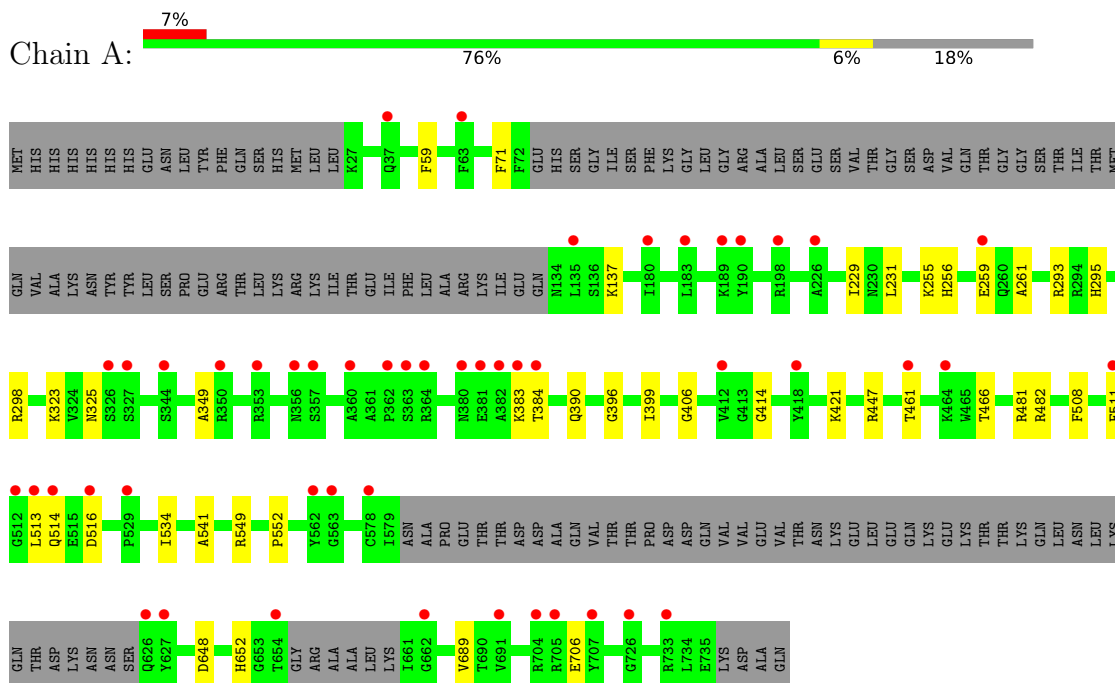
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	489	Total	O	0	0
			489	489		

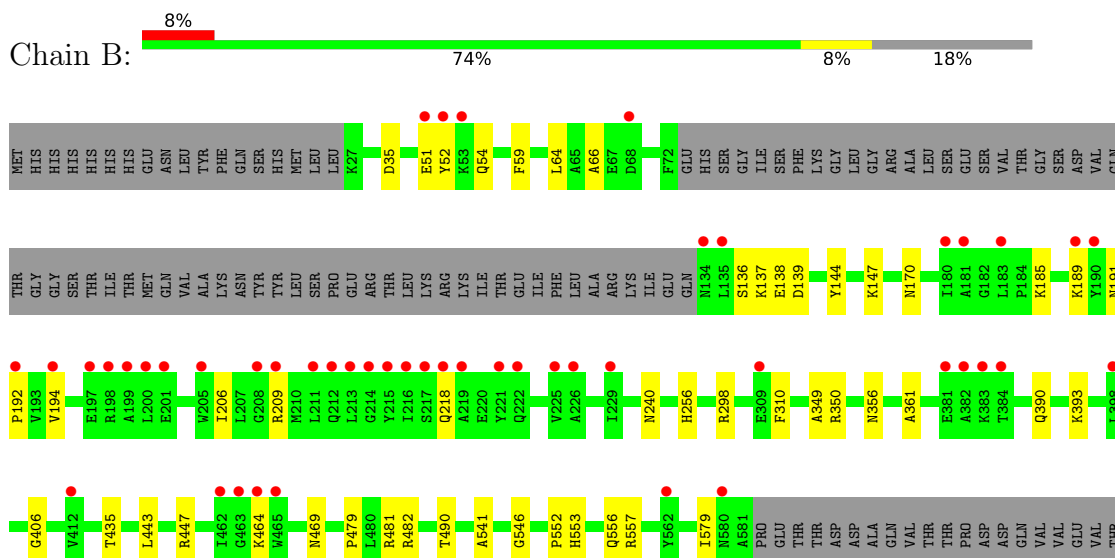
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Penicillin-binding protein 1a



- Molecule 1: Penicillin-binding protein 1a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.87Å 243.00Å 49.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 1.70 24.58 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (24.89-1.70) 96.7 (24.58-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.70Å)	Xtrriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.177 , 0.199 0.181 , 0.206	Depositor DCC
R_{free} test set	7659 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.187	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10395	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/4815	0.61	0/6530
1	B	0.54	0/4829	0.63	0/6548
All	All	0.51	0/9644	0.62	0/13078

There are no bond length outliers.

There are no bond angle outliers.

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	4703	0	4689	21	0
1	B	4720	0	4702	34	0
2	A	12	0	12	1	0
2	B	36	0	36	10	0
3	A	435	0	0	1	0
3	B	489	0	0	0	0
All	All	10395	0	9439	48	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 3.

All (48) 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:B:482:ARG:HH11	2:B:742:MES:H31	1.29	0.97
1:B:356:ASN:HD21	1:B:704:ARG:H	1.14	0.94
1:B:298:ARG:H	1:B:390:GLN:HE22	1.17	0.89
1:A:298:ARG:H	1:A:390:GLN:HE22	1.18	0.86
1:B:393:LYS:HE2	2:B:740:MES:H82	1.58	0.86
1:B:481:ARG:HH21	2:B:742:MES:H61	1.47	0.79
1:B:556:GLN:HE22	1:B:557:ARG:HH11	1.34	0.74
1:B:356:ASN:ND2	1:B:704:ARG:H	1.88	0.69
1:A:137:LYS:NZ	1:B:256:HIS:HD2	1.92	0.68
1:A:648:ASP:OD1	1:A:652:HIS:HD2	1.79	0.64
1:A:261:ALA:HA	1:B:144:TYR:CE1	2.37	0.59
1:A:323:LYS:HE3	1:A:325:ASN:HD21	1.68	0.59
1:A:482:ARG:NE	2:A:740:MES:O1S	2.34	0.58
1:B:469:ASN:HD21	1:B:490:THR:H	1.52	0.57
1:B:481:ARG:NH2	2:B:742:MES:H61	2.19	0.56
1:A:508:PHE:HB3	1:A:513:LEU:HD12	1.88	0.55
1:B:479:PRO:HG2	2:B:742:MES:H51	1.89	0.54
1:B:481:ARG:HE	2:B:742:MES:C6	2.21	0.54
1:B:66:ALA:HA	1:B:206:ILE:HG12	1.88	0.54
1:B:546:GLY:HA2	1:B:640:TYR:CE1	2.42	0.54
1:A:298:ARG:H	1:A:390:GLN:NE2	1.99	0.53
1:B:482:ARG:NH1	2:B:742:MES:H31	2.10	0.53
1:A:71:PHE:O	1:B:553:HIS:HA	2.10	0.51
1:A:293:ARG:NH2	3:A:1074:HOH:O	2.29	0.51
1:B:443:LEU:O	1:B:447:ARG:HG2	2.10	0.50
1:A:137:LYS:HZ2	1:B:256:HIS:HD2	1.59	0.50
1:B:541:ALA:HA	1:B:689:VAL:HG21	1.93	0.50
1:B:310:PHE:CD1	2:B:741:MES:H82	2.47	0.49
1:B:700:THR:HG21	2:B:740:MES:H61	1.96	0.47
1:B:350:ARG:HG2	1:B:361:ALA:HA	1.96	0.47
1:B:298:ARG:H	1:B:390:GLN:NE2	1.99	0.46
1:B:700:THR:HG21	2:B:740:MES:H22	1.98	0.46
1:A:541:ALA:HA	1:A:689:VAL:HG21	1.97	0.45
1:A:229:ILE:HG22	1:A:231:LEU:HG	1.98	0.44
1:B:191:ASN:HB3	1:B:194:VAL:HG12	1.98	0.44
1:B:579:ILE:CD1	1:B:626:GLN:N	2.80	0.44
1:A:399:ILE:HG12	1:A:534:ILE:HD13	1.98	0.44
1:B:52:TYR:OH	1:B:138:GLU:HG3	2.17	0.44
1:B:406:GLY:O	1:B:552:PRO:HA	2.18	0.43
1:A:295:HIS:HE1	1:A:706:GLU:OE2	2.01	0.43
1:A:137:LYS:HZ1	1:B:256:HIS:HD2	1.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:THR:HG22	1:A:466:THR:OG1	2.19	0.42
1:A:406:GLY:O	1:A:552:PRO:HA	2.20	0.41
1:B:51:GLU:HB2	1:B:54:GLN:HG3	2.02	0.41
1:B:191:ASN:HA	1:B:192:PRO:HD3	1.98	0.41
1:A:396:GLY:O	1:A:414:GLY:HA2	2.21	0.41
1:A:256:HIS:HD2	1:B:137:LYS:NZ	2.19	0.40
1:A:255:LYS:HG3	1:B:185:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

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	589/731 (81%)	575 (98%)	12 (2%)	2 (0%)	41 24
1	B	591/731 (81%)	573 (97%)	16 (3%)	2 (0%)	41 24
All	All	1180/1462 (81%)	1148 (97%)	28 (2%)	4 (0%)	41 24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	LYS
1	B	627	TYR
1	A	349	ALA
1	B	349	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/608 (80%)	479 (98%)	10 (2%)	55	38
1	B	490/608 (81%)	473 (96%)	17 (4%)	36	17
All	All	979/1216 (80%)	952 (97%)	27 (3%)	43	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	259	GLU
1	A	384	THR
1	A	421	LYS
1	A	447	ARG
1	A	481	ARG
1	A	511	PHE
1	A	514	GLN
1	A	516	ASP
1	A	549	ARG
1	B	35	ASP
1	B	59	PHE
1	B	64	LEU
1	B	136	SER
1	B	139	ASP
1	B	147	LYS
1	B	170	ASN
1	B	189	LYS
1	B	209	ARG
1	B	218	GLN
1	B	240	ASN
1	B	435	THR
1	B	464	LYS
1	B	650	ILE
1	B	705	ARG
1	B	718	ASN
1	B	733	ARG

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

Mol	Chain	Res	Type
1	A	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	295	HIS
1	A	303	HIS
1	A	325	ASN
1	A	390	GLN
1	A	431	GLN
1	A	626	GLN
1	A	652	HIS
1	A	674	ASN
1	B	256	HIS
1	B	356	ASN
1	B	390	GLN
1	B	469	ASN
1	B	556	GLN
1	B	652	HIS
1	B	674	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	B	741	-	12,12,12	2.14	1 (8%)	14,16,16	2.55	7 (50%)
2	MES	B	740	-	12,12,12	1.77	1 (8%)	14,16,16	2.36	5 (35%)
2	MES	A	740	-	12,12,12	1.75	1 (8%)	14,16,16	2.19	5 (35%)
2	MES	B	742	-	12,12,12	2.19	1 (8%)	14,16,16	2.64	7 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	B	741	-	-	3/6/14/14	0/1/1/1
2	MES	B	740	-	-	3/6/14/14	0/1/1/1
2	MES	A	740	-	-	1/6/14/14	0/1/1/1
2	MES	B	742	-	-	6/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	742	MES	C8-S	-7.20	1.67	1.77
2	B	741	MES	C8-S	-7.09	1.67	1.77
2	A	740	MES	C8-S	-5.81	1.69	1.77
2	B	740	MES	C8-S	-5.48	1.69	1.77

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	740	MES	C5-N4-C3	6.06	122.47	108.83
2	A	740	MES	C5-N4-C3	5.19	120.52	108.83
2	B	741	MES	C7-N4-C3	4.45	122.61	111.23
2	B	742	MES	C7-N4-C5	4.37	122.42	111.23
2	B	742	MES	C5-N4-C3	4.35	118.62	108.83
2	B	741	MES	C5-N4-C3	4.22	118.33	108.83
2	B	741	MES	O2S-S-C8	3.79	111.48	106.92
2	B	742	MES	C6-C5-N4	-3.65	104.57	110.10
2	B	740	MES	C7-N4-C5	3.57	120.36	111.23
2	A	740	MES	C7-N4-C5	3.50	120.20	111.23
2	B	741	MES	C6-C5-N4	-3.35	105.02	110.10
2	B	742	MES	C2-C3-N4	-3.27	105.14	110.10
2	B	742	MES	O3S-S-C8	3.19	110.93	105.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	740	MES	C7-N4-C3	3.13	119.24	111.23
2	B	741	MES	C7-N4-C5	3.06	119.06	111.23
2	B	740	MES	O1S-S-C8	3.00	110.53	106.92
2	B	742	MES	C7-N4-C3	2.99	118.88	111.23
2	A	740	MES	O2S-S-C8	2.80	110.28	106.92
2	B	741	MES	C2-C3-N4	-2.75	105.94	110.10
2	B	742	MES	O2S-S-C8	2.50	109.93	106.92
2	A	740	MES	O3S-S-C8	2.37	109.60	105.77
2	B	740	MES	C7-N4-C3	2.29	117.10	111.23
2	B	741	MES	O3S-S-C8	2.28	109.45	105.77
2	B	740	MES	O2S-S-C8	-2.20	104.26	106.92

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	740	MES	C8-C7-N4-C3
2	B	741	MES	C8-C7-N4-C3
2	B	742	MES	N4-C7-C8-S
2	B	742	MES	C7-C8-S-O1S
2	B	742	MES	C7-C8-S-O3S
2	B	740	MES	C8-C7-N4-C3
2	B	742	MES	C8-C7-N4-C3
2	B	741	MES	C7-C8-S-O1S
2	B	742	MES	C7-C8-S-O2S
2	B	740	MES	C7-C8-S-O3S
2	B	741	MES	C7-C8-S-O3S
2	B	740	MES	C7-C8-S-O1S
2	B	742	MES	C8-C7-N4-C5

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	741	MES	1	0
2	B	740	MES	3	0
2	A	740	MES	1	0
2	B	742	MES	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	596/731 (81%)	0.40	49 (8%) 11 13	16, 31, 60, 95	0
1	B	599/731 (81%)	0.41	58 (9%) 7 8	12, 27, 66, 100	0
All	All	1195/1462 (81%)	0.41	107 (8%) 9 10	12, 29, 62, 100	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	ALA	10.4
1	B	382	ALA	6.3
1	B	194	VAL	6.2
1	B	205	TRP	6.0
1	B	209	ARG	5.9
1	B	562	TYR	5.9
1	A	562	TYR	5.7
1	A	381	GLU	5.5
1	B	219	ALA	5.0
1	B	381	GLU	4.9
1	B	190	TYR	4.9
1	B	212	GLN	4.8
1	A	626	GLN	4.8
1	B	225	VAL	4.7
1	A	627	TYR	4.6
1	B	627	TYR	4.6
1	B	135	LEU	4.5
1	B	215	TYR	4.4
1	B	226	ALA	4.2
1	B	462	ILE	4.2
1	A	578	CYS	4.2
1	B	662	GLY	4.2
1	B	180	ILE	4.1
1	B	221	TYR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	211	LEU	4.0
1	B	626	GLN	4.0
1	B	53	LYS	4.0
1	A	384	THR	3.9
1	B	652	HIS	3.8
1	B	384	THR	3.7
1	B	189	LYS	3.6
1	B	463	GLY	3.4
1	B	198	ARG	3.4
1	B	197	GLU	3.4
1	A	516	ASP	3.4
1	B	737	ASP	3.4
1	B	465	TRP	3.3
1	B	707	TYR	3.3
1	A	514	GLN	3.2
1	B	68	ASP	3.2
1	B	653	GLY	3.2
1	A	360	ALA	3.2
1	B	213	LEU	3.2
1	B	218	GLN	3.1
1	B	661	ILE	3.1
1	B	200	LEU	3.1
1	A	226	ALA	3.1
1	B	199	ALA	3.0
1	B	217	SER	3.0
1	B	51	GLU	2.9
1	B	52	TYR	2.9
1	A	198	ARG	2.9
1	A	380	ASN	2.9
1	B	201	GLU	2.8
1	B	383	LYS	2.8
1	A	704	ARG	2.8
1	A	464	LYS	2.8
1	A	726	GLY	2.8
1	B	134	ASN	2.8
1	A	707	TYR	2.7
1	A	135	LEU	2.7
1	B	464	LYS	2.7
1	B	222	GLN	2.7
1	B	229	ILE	2.7
1	A	563	GLY	2.7
1	A	662	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	183	LEU	2.6
1	B	208	GLY	2.6
1	B	216	ILE	2.6
1	B	214	GLY	2.6
1	A	326	SER	2.5
1	B	192	PRO	2.5
1	A	357	SER	2.5
1	A	180	ILE	2.5
1	A	327	SER	2.5
1	A	705	ARG	2.4
1	B	309	GLU	2.4
1	A	364	ARG	2.3
1	A	511	PHE	2.3
1	B	181	ALA	2.3
1	A	353	ARG	2.3
1	A	362	PRO	2.3
1	A	418	TYR	2.3
1	A	691	VAL	2.3
1	A	350	ARG	2.3
1	A	529	PRO	2.2
1	A	190	TYR	2.2
1	A	412	VAL	2.2
1	A	37	GLN	2.2
1	B	705	ARG	2.2
1	A	363	SER	2.2
1	A	259	GLU	2.1
1	A	356	ASN	2.1
1	A	654	THR	2.1
1	B	398	LEU	2.1
1	A	344	SER	2.1
1	A	183	LEU	2.1
1	B	645	ILE	2.1
1	A	383	LYS	2.0
1	B	412	VAL	2.0
1	A	733	ARG	2.0
1	A	189	LYS	2.0
1	A	461	THR	2.0
1	A	512	GLY	2.0
1	A	63	PHE	2.0
1	A	513	LEU	2.0
1	B	580	ASN	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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	MES	B	742	12/12	0.72	0.25	67,69,73,73	0
2	MES	B	741	12/12	0.92	0.33	45,61,72,73	0
2	MES	B	740	12/12	0.92	0.17	22,31,34,36	0
2	MES	A	740	12/12	0.94	0.16	33,43,50,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.