



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2014 – 04:50 PM EDT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

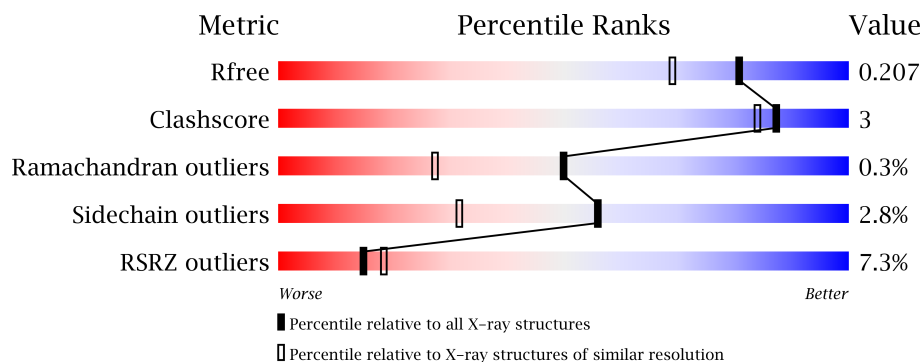
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MES	B	740	-	X
2	MES	B	741	-	X

2 Entry composition i

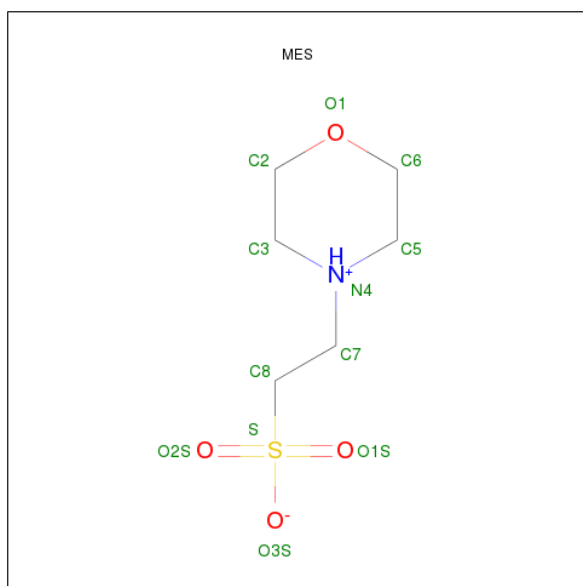
There are 3 unique types of molecules in this entry. The entry contains 10395 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Penicillin-binding protein 1a.

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

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (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		

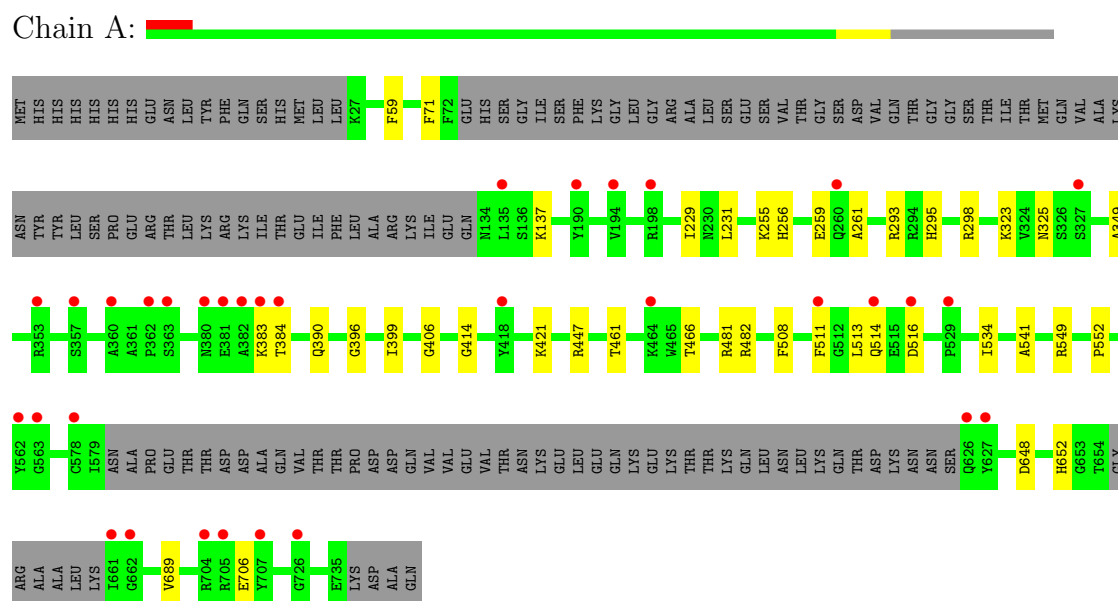
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	435	Total 435	O 435	0	0
3	B	489	Total 489	O 489	0	0

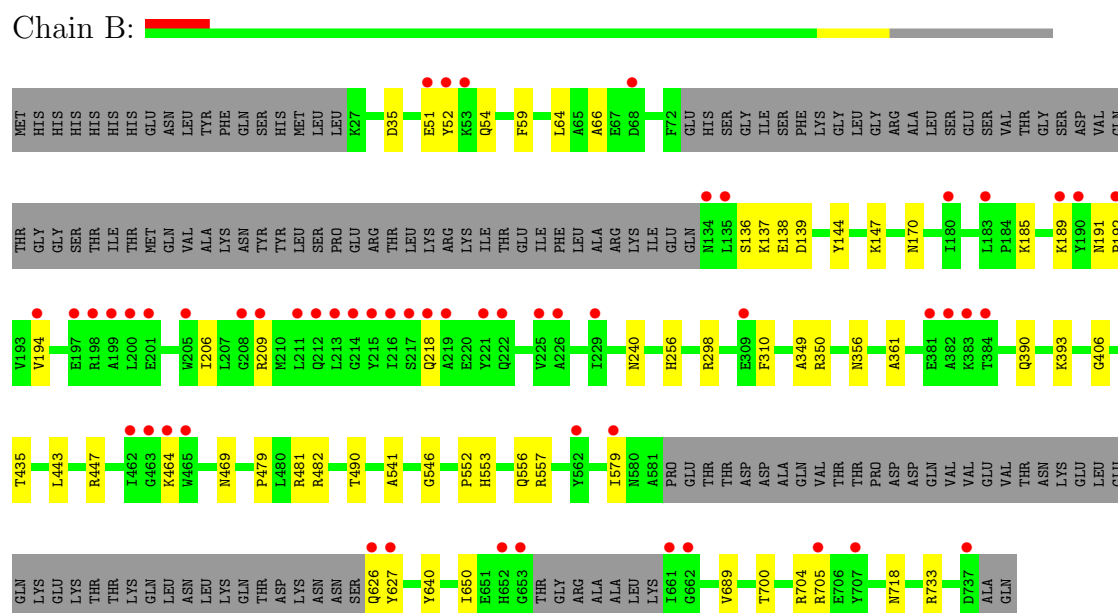
3 Residue-property plots

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: 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)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.177 , 0.199 0.182 , 0.207	Depositor DCC
R_{free} test set	7659 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 153066 reflections	Xtriage
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

Xtriage'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.

5 Model quality

5.1 Standard geometry

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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:546:GLY:HA2	1:B:640:TYR:CE1	2.42	0.54
1:B:66:ALA:HA	1:B:206:ILE:HG12	1.88	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
1:A:461:THR:HG22	1:A:466:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	589/731 (81%)	575 (98%)	12 (2%)	2 (0%)	50 27
1	B	591/731 (81%)	573 (97%)	16 (3%)	2 (0%)	50 27
All	All	1180/1462 (81%)	1148 (97%)	28 (2%)	4 (0%)	50 27

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 ⓘ

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/608 (80%)	479 (98%)	10 (2%)	68	47
1	B	490/608 (81%)	473 (96%)	17 (4%)	48	23
All	All	979/1216 (80%)	952 (97%)	27 (3%)	56	32

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

Some 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
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 ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	596/731 (81%)	0.31	33 (5%) 24 28	16, 31, 60, 95	0
1	B	599/731 (81%)	0.31	54 (9%) 10 12	12, 27, 66, 100	0
All	All	1195/1462 (81%)	0.31	87 (7%) 15 18	12, 29, 62, 100	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	ALA	10.5
1	B	194	VAL	6.0
1	B	382	ALA	5.8
1	B	205	TRP	5.5
1	A	562	TYR	5.3
1	A	381	GLU	5.1
1	B	562	TYR	5.0
1	B	209	ARG	4.9
1	B	627	TYR	4.6
1	A	626	GLN	4.6
1	B	381	GLU	4.5
1	B	225	VAL	4.2
1	B	662	GLY	4.2
1	B	462	ILE	4.1
1	B	219	ALA	4.1
1	B	190	TYR	4.0
1	B	211	LEU	4.0
1	B	215	TYR	4.0
1	B	212	GLN	4.0
1	B	53	LYS	3.8
1	B	626	GLN	3.8
1	A	627	TYR	3.8
1	B	221	TYR	3.8
1	B	198	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	180	ILE	3.6
1	B	135	LEU	3.6
1	B	737	ASP	3.5
1	A	384	THR	3.5
1	B	229	ILE	3.5
1	A	135	LEU	3.5
1	B	652	HIS	3.4
1	B	653	GLY	3.4
1	B	226	ALA	3.3
1	B	707	TYR	3.2
1	A	514	GLN	3.2
1	B	661	ILE	3.1
1	B	465	TRP	3.1
1	A	516	ASP	3.1
1	B	189	LYS	3.0
1	B	200	LEU	3.0
1	B	463	GLY	2.9
1	B	201	GLU	2.9
1	B	68	ASP	2.9
1	B	197	GLU	2.8
1	A	578	CYS	2.8
1	B	384	THR	2.8
1	B	464	LYS	2.8
1	B	199	ALA	2.8
1	B	208	GLY	2.8
1	A	380	ASN	2.8
1	A	198	ARG	2.8
1	B	218	GLN	2.8
1	B	52	TYR	2.8
1	B	217	SER	2.8
1	A	360	ALA	2.7
1	B	213	LEU	2.6
1	B	51	GLU	2.6
1	A	662	GLY	2.5
1	B	222	GLN	2.5
1	B	192	PRO	2.5
1	A	726	GLY	2.5
1	A	563	GLY	2.4
1	B	383	LYS	2.4
1	A	704	ARG	2.4
1	A	362	PRO	2.4
1	B	216	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	183	LEU	2.3
1	A	705	ARG	2.3
1	A	327	SER	2.3
1	B	309	GLU	2.3
1	A	464	LYS	2.3
1	A	707	TYR	2.3
1	B	705	ARG	2.3
1	A	357	SER	2.2
1	B	134	ASN	2.2
1	A	190	TYR	2.2
1	A	383	LYS	2.1
1	A	260	GLN	2.1
1	A	529	PRO	2.1
1	A	418	TYR	2.1
1	A	661	ILE	2.1
1	A	353	ARG	2.1
1	A	194	VAL	2.1
1	B	214	GLY	2.1
1	B	579	ILE	2.1
1	A	511	PHE	2.0
1	A	363	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MES	B	740	12/12	0.17	4.04	22,31,34,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MES	B	741	12/12	0.29	2.28	45,61,72,73	0
2	MES	B	742	12/12	0.24	1.83	67,69,73,73	0
2	MES	A	740	12/12	0.14	1.47	33,43,50,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.