



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:44 am BST

PDB ID : 3G66
Title : The crystal structure of Streptococcus pneumoniae Sortase C provides novel insights into catalysis as well as pilin substrate specificity
Authors : Neiers, F.; Madhurantakam, C.; Falker, S.; Manzano, C.; Dessen, A.; Normark, S.; Henriques-Normark, B.; Achour, A.
Deposited on : 2009-02-06
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 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 : 2.11
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) : 2.11

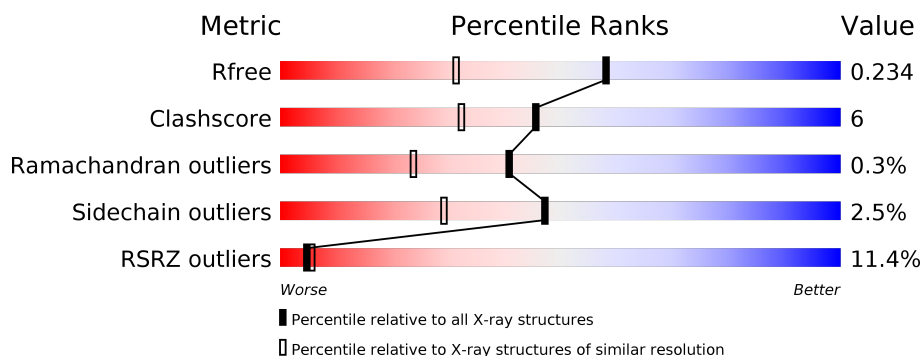
1 Overall quality at a glance

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 on 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	212	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>10%</div> </div> </div>
1	B	212	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3659 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 Sortase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	9	0
			1533	979	251	296	7			
1	B	196	Total	C	N	O	S	0	5	0
			1545	986	255	297	7			

There are 28 discrepancies between the modelled and reference sequences:

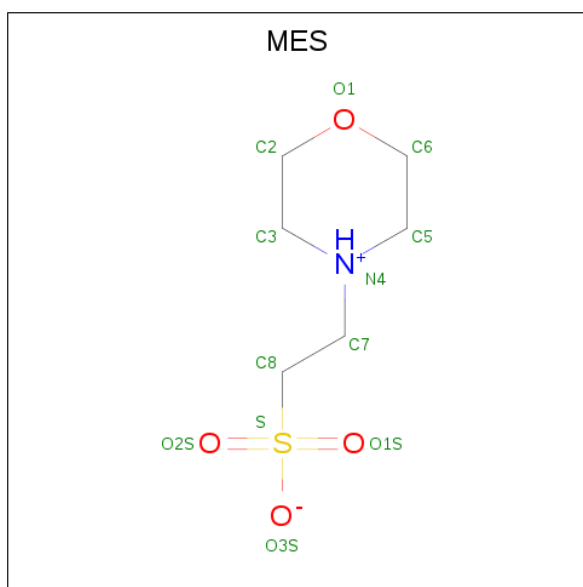
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	SER	-	EXPRESSION TAG	UNP A7KT63
A	245	ALA	-	EXPRESSION TAG	UNP A7KT63
A	246	GLU	-	EXPRESSION TAG	UNP A7KT63
A	247	ARG	-	EXPRESSION TAG	UNP A7KT63
A	248	ASN	-	EXPRESSION TAG	UNP A7KT63
A	249	ARG	-	EXPRESSION TAG	UNP A7KT63
A	250	ALA	-	EXPRESSION TAG	UNP A7KT63
A	251	VAL	-	EXPRESSION TAG	UNP A7KT63
A	252	ARG	-	EXPRESSION TAG	UNP A7KT63
A	253	GLU	-	EXPRESSION TAG	UNP A7KT63
A	254	ARG	-	EXPRESSION TAG	UNP A7KT63
A	255	GLY	-	EXPRESSION TAG	UNP A7KT63
A	256	GLN	-	EXPRESSION TAG	UNP A7KT63
A	257	PHE	-	EXPRESSION TAG	UNP A7KT63
B	46	SER	-	EXPRESSION TAG	UNP A7KT63
B	245	ALA	-	EXPRESSION TAG	UNP A7KT63
B	246	GLU	-	EXPRESSION TAG	UNP A7KT63
B	247	ARG	-	EXPRESSION TAG	UNP A7KT63
B	248	ASN	-	EXPRESSION TAG	UNP A7KT63
B	249	ARG	-	EXPRESSION TAG	UNP A7KT63
B	250	ALA	-	EXPRESSION TAG	UNP A7KT63
B	251	VAL	-	EXPRESSION TAG	UNP A7KT63
B	252	ARG	-	EXPRESSION TAG	UNP A7KT63
B	253	GLU	-	EXPRESSION TAG	UNP A7KT63
B	254	ARG	-	EXPRESSION TAG	UNP A7KT63

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Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	EXPRESSION TAG	UNP A7KT63
B	256	GLN	-	EXPRESSION TAG	UNP A7KT63
B	257	PHE	-	EXPRESSION TAG	UNP A7KT63

- 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		

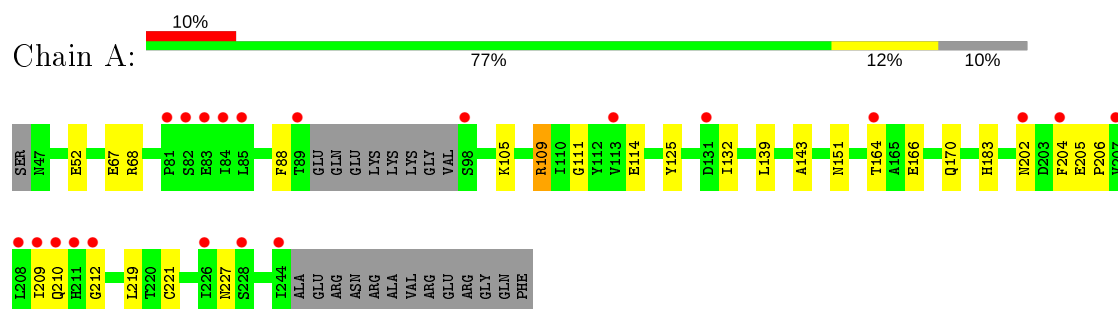
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	273	Total	O	0	0
			273	273		
3	B	284	Total	O	0	0
			284	284		

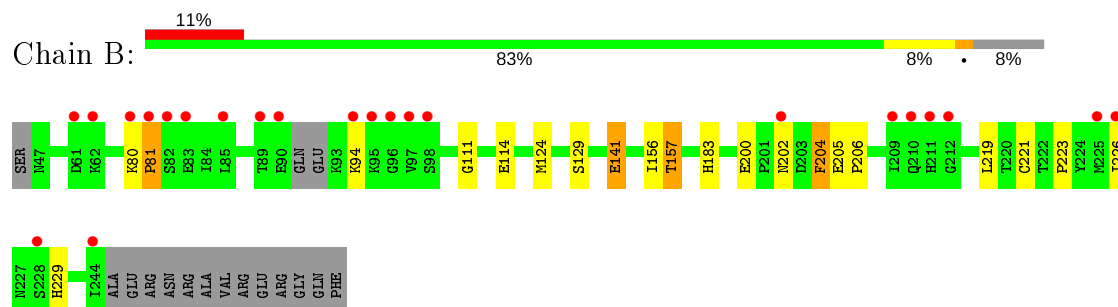
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Sortase C



• Molecule 1: Sortase C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.91Å 96.86Å 98.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 1.70 32.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.29-1.70) 99.7 (32.29-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.235 0.188 , 0.234	Depositor DCC
R_{free} test set	2669 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.069 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.65	0/1587	0.71	0/2158
1	B	0.68	0/1587	0.73	0/2158
All	All	0.67	0/3174	0.72	0/4316

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
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	80	LYS	Peptide

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	1533	0	1505	24	0
1	B	1545	0	1509	15	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
3	A	273	0	0	13	0
3	B	284	0	0	3	0
All	All	3659	0	3038	39	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 6.

All (39) 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:141[A]:GLU:CD	1:B:141[A]:GLU:H	1.77	0.86
1:A:143:ALA:HB3	3:A:361:HOH:O	1.82	0.80
1:A:139:LEU:CD1	3:A:361:HOH:O	2.32	0.78
1:A:139:LEU:HD11	3:A:361:HOH:O	1.85	0.74
1:B:221[A]:CYS:SG	3:B:275:HOH:O	2.47	0.73
1:A:164:THR:HG22	3:A:354:HOH:O	1.93	0.68
1:B:94:LYS:HA	1:B:129:SER:HB2	1.76	0.68
1:B:183:HIS:HD2	3:B:12:HOH:O	1.84	0.60
1:B:200:GLU:OE2	1:B:229:HIS:NE2	2.36	0.59
1:A:205:GLU:N	1:A:206:PRO:HD3	2.19	0.58
1:A:166:GLU:OE2	1:A:170[B]:GLN:NE2	2.37	0.57
1:B:114:GLU:OE1	1:B:183:HIS:HE1	1.88	0.57
1:B:124:MET:CE	1:B:156:ILE:HG12	2.35	0.56
1:B:223:PRO:HG2	1:B:226:ILE:HB	1.87	0.56
1:B:124:MET:HE1	1:B:156:ILE:HG12	1.88	0.55
1:A:114:GLU:OE1	1:A:183:HIS:HE1	1.90	0.55
1:A:139:LEU:HD12	3:A:361:HOH:O	2.01	0.55
1:A:67[B]:GLU:HG3	3:A:355:HOH:O	2.08	0.54
1:A:205:GLU:N	1:A:206:PRO:CD	2.72	0.53
1:B:205:GLU:N	1:B:206:PRO:CD	2.71	0.53
1:B:205:GLU:N	1:B:206:PRO:HD3	2.25	0.52
1:A:227:ASN:ND2	3:A:563:HOH:O	2.42	0.51
1:A:183:HIS:HD2	3:A:27:HOH:O	1.94	0.51
1:A:221[B]:CYS:SG	3:A:289:HOH:O	2.60	0.49
1:B:157:THR:HB	1:B:219:LEU:HB3	1.95	0.48
1:A:52[B]:GLU:CD	1:A:109:ARG:HH22	2.19	0.45
1:A:114:GLU:OE2	2:A:5121:MES:H72	2.17	0.45
1:A:125:TYR:HB2	1:A:132:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:C	1:A:219:LEU:HD23	2.39	0.43
1:A:111:GLY:HA3	1:A:183:HIS:O	2.19	0.43
1:A:151:ASN:OD1	1:A:212:GLY:N	2.35	0.42
1:A:209:ILE:HD12	3:A:429:HOH:O	2.20	0.41
1:A:210:GLN:HB2	3:A:434:HOH:O	2.20	0.41
1:A:88:PHE:HE2	1:A:219:LEU:CD2	2.33	0.41
1:B:111:GLY:HA3	1:B:183:HIS:O	2.21	0.41
1:A:105:LYS:NZ	3:A:437:HOH:O	2.54	0.41
1:A:68:ARG:NH1	3:A:417:HOH:O	2.40	0.40
1:B:204:PHE:HB2	3:B:357:HOH:O	2.21	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	195/212 (92%)	187 (96%)	8 (4%)	0	100	100
1	B	197/212 (93%)	189 (96%)	7 (4%)	1 (0%)	29	13
All	All	392/424 (92%)	376 (96%)	15 (4%)	1 (0%)	41	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	81	PRO

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	167/184 (91%)	164 (98%)	3 (2%)	59	43
1	B	165/184 (90%)	159 (96%)	6 (4%)	35	16
All	All	332/368 (90%)	323 (97%)	9 (3%)	47	26

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	202	ASN
1	A	204	PHE
1	B	81	PRO
1	B	141[A]	GLU
1	B	141[B]	GLU
1	B	157	THR
1	B	202	ASN
1	B	204	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	187	GLN
1	A	202	ASN
1	A	210	GLN
1	A	227	ASN
1	A	229	HIS
1	B	183	HIS
1	B	195	GLN
1	B	210	GLN

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

2 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	5121	-	12,12,12	1.32	1 (8%)	14,16,16	5.21	6 (42%)
2	MES	A	5121	-	12,12,12	1.33	1 (8%)	14,16,16	7.36	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	5121	-	-	1/6/14/14	0/1/1/1
2	MES	A	5121	-	-	5/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5121	MES	C8-S	-3.92	1.71	1.77
2	A	5121	MES	C8-S	-3.75	1.72	1.77

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5121	MES	O1S-S-C8	-18.86	84.20	106.92
2	A	5121	MES	O2S-S-C8	-14.20	89.82	106.92
2	B	5121	MES	O1S-S-C8	-11.87	92.62	106.92
2	B	5121	MES	O2S-S-C8	-10.37	94.43	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5121	MES	O3S-S-C8	-9.77	89.96	105.77
2	B	5121	MES	C5-N4-C3	7.00	124.59	108.83
2	A	5121	MES	C5-N4-C3	6.14	122.65	108.83
2	B	5121	MES	O3S-S-C8	-5.83	96.34	105.77
2	B	5121	MES	O3S-S-O1S	4.86	123.15	111.27
2	A	5121	MES	C7-N4-C5	4.70	123.25	111.23
2	A	5121	MES	O3S-S-O1S	4.58	122.45	111.27
2	A	5121	MES	O3S-S-O2S	3.99	121.01	111.27
2	B	5121	MES	C7-N4-C5	3.82	121.00	111.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5121	MES	C8-C7-N4-C5
2	A	5121	MES	C8-C7-N4-C5
2	A	5121	MES	C7-C8-S-O1S
2	A	5121	MES	C7-C8-S-O2S
2	A	5121	MES	C7-C8-S-O3S
2	A	5121	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5121	MES	1	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	190/212 (89%)	0.50	21 (11%) 5 6	8, 17, 40, 48	0
1	B	196/212 (92%)	0.70	23 (11%) 4 5	8, 17, 46, 59	0
All	All	386/424 (91%)	0.60	44 (11%) 5 5	8, 17, 42, 59	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	GLY	9.8
1	B	97	VAL	9.1
1	B	244	ILE	7.9
1	B	95	LYS	7.0
1	B	94	LYS	6.6
1	B	89	THR	6.1
1	B	81	PRO	5.5
1	B	226	ILE	5.1
1	A	83	GLU	4.9
1	A	89	THR	4.9
1	A	244	ILE	4.4
1	A	211	HIS	4.3
1	A	98	SER	4.3
1	B	202	ASN	4.2
1	A	209	ILE	3.9
1	A	226	ILE	3.9
1	B	211	HIS	3.9
1	B	90	GLU	3.8
1	B	80	LYS	3.7
1	B	98	SER	3.7
1	B	85	LEU	3.4
1	A	81	PRO	3.2
1	B	83	GLU	3.1
1	A	82	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	3.0
1	A	202	ASN	3.0
1	A	164	THR	3.0
1	A	212	GLY	3.0
1	A	131[A]	ASP	2.9
1	B	225	MET	2.9
1	B	61[A]	ASP	2.7
1	A	84	ILE	2.7
1	B	209	ILE	2.6
1	A	208	LEU	2.6
1	A	204	PHE	2.5
1	B	82	SER	2.5
1	A	228	SER	2.4
1	A	207	VAL	2.2
1	B	212	GLY	2.2
1	A	113	VAL	2.1
1	B	210	GLN	2.1
1	A	210	GLN	2.1
1	B	228	SER	2.0
1	B	62	LYS	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. 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(\AA^2)	Q<0.9
2	MES	A	5121	12/12	0.86	0.16	21,25,31,38	0
2	MES	B	5121	12/12	0.90	0.14	19,20,27,33	0

6.5 Other polymers

There are no such residues in this entry.