



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:50 PM UTC

PDB ID : 4Y68 / pdb_00004y68
Title : Structure of a lipoprotein from Streptococcus agalactiae
Authors : Khosa, S.; Hoepfner, A.; Smits, S.H.
Deposited on : 2015-02-12
Resolution : 2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

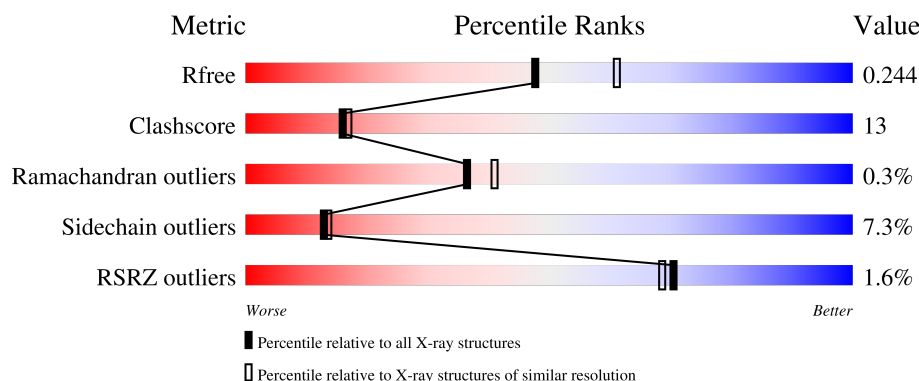
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	312	% 66% 23% • 8%
1	B	312	4% 63% 24% • 8%
1	C	312	79% 11% • 8%
1	D	312	71% 19% • 8%

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	C	401	-	-	X	-
2	MES	D	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9601 atoms, of which 13 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 Putative nisin-resistance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	287	Total	C	N	O	S	0	0	0
			2295	1450	408	431	6			
1	A	287	Total	C	N	O	S	0	0	0
			2251	1424	391	430	6			
1	B	286	Total	C	N	O	S	0	0	0
			2186	1378	379	423	6			
1	D	287	Total	C	N	O	S	0	0	0
			2285	1445	405	429	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	MET	-	expression tag	UNP Q3DLX7
C	10	GLY	-	expression tag	UNP Q3DLX7
C	11	SER	-	expression tag	UNP Q3DLX7
C	12	SER	-	expression tag	UNP Q3DLX7
C	13	HIS	-	expression tag	UNP Q3DLX7
C	14	HIS	-	expression tag	UNP Q3DLX7
C	15	HIS	-	expression tag	UNP Q3DLX7
C	16	HIS	-	expression tag	UNP Q3DLX7
C	17	HIS	-	expression tag	UNP Q3DLX7
C	18	HIS	-	expression tag	UNP Q3DLX7
C	19	HIS	-	expression tag	UNP Q3DLX7
C	20	HIS	-	expression tag	UNP Q3DLX7
C	21	SER	-	expression tag	UNP Q3DLX7
C	22	SER	-	expression tag	UNP Q3DLX7
C	23	GLY	-	expression tag	UNP Q3DLX7
C	24	LEU	-	expression tag	UNP Q3DLX7
C	25	VAL	-	expression tag	UNP Q3DLX7
C	26	PRO	-	expression tag	UNP Q3DLX7
C	27	ARG	-	expression tag	UNP Q3DLX7
C	28	GLY	-	expression tag	UNP Q3DLX7
C	29	SER	-	expression tag	UNP Q3DLX7

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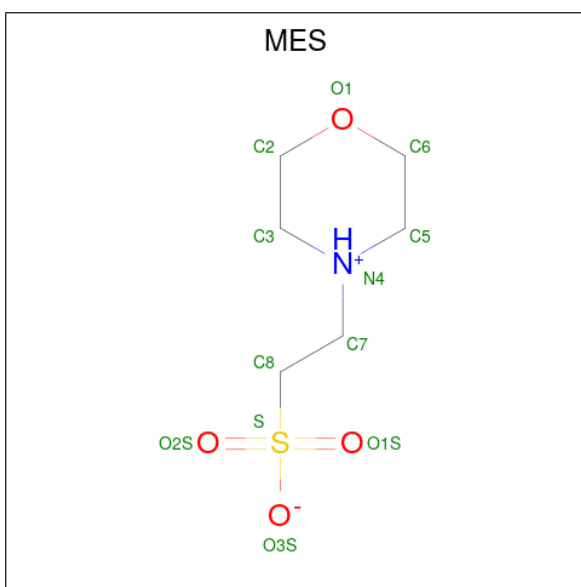
Chain	Residue	Modelled	Actual	Comment	Reference
C	30	HIS	-	expression tag	UNP Q3DLX7
A	9	MET	-	expression tag	UNP Q3DLX7
A	10	GLY	-	expression tag	UNP Q3DLX7
A	11	SER	-	expression tag	UNP Q3DLX7
A	12	SER	-	expression tag	UNP Q3DLX7
A	13	HIS	-	expression tag	UNP Q3DLX7
A	14	HIS	-	expression tag	UNP Q3DLX7
A	15	HIS	-	expression tag	UNP Q3DLX7
A	16	HIS	-	expression tag	UNP Q3DLX7
A	17	HIS	-	expression tag	UNP Q3DLX7
A	18	HIS	-	expression tag	UNP Q3DLX7
A	19	HIS	-	expression tag	UNP Q3DLX7
A	20	HIS	-	expression tag	UNP Q3DLX7
A	21	SER	-	expression tag	UNP Q3DLX7
A	22	SER	-	expression tag	UNP Q3DLX7
A	23	GLY	-	expression tag	UNP Q3DLX7
A	24	LEU	-	expression tag	UNP Q3DLX7
A	25	VAL	-	expression tag	UNP Q3DLX7
A	26	PRO	-	expression tag	UNP Q3DLX7
A	27	ARG	-	expression tag	UNP Q3DLX7
A	28	GLY	-	expression tag	UNP Q3DLX7
A	29	SER	-	expression tag	UNP Q3DLX7
A	30	HIS	-	expression tag	UNP Q3DLX7
B	9	MET	-	expression tag	UNP Q3DLX7
B	10	GLY	-	expression tag	UNP Q3DLX7
B	11	SER	-	expression tag	UNP Q3DLX7
B	12	SER	-	expression tag	UNP Q3DLX7
B	13	HIS	-	expression tag	UNP Q3DLX7
B	14	HIS	-	expression tag	UNP Q3DLX7
B	15	HIS	-	expression tag	UNP Q3DLX7
B	16	HIS	-	expression tag	UNP Q3DLX7
B	17	HIS	-	expression tag	UNP Q3DLX7
B	18	HIS	-	expression tag	UNP Q3DLX7
B	19	HIS	-	expression tag	UNP Q3DLX7
B	20	HIS	-	expression tag	UNP Q3DLX7
B	21	SER	-	expression tag	UNP Q3DLX7
B	22	SER	-	expression tag	UNP Q3DLX7
B	23	GLY	-	expression tag	UNP Q3DLX7
B	24	LEU	-	expression tag	UNP Q3DLX7
B	25	VAL	-	expression tag	UNP Q3DLX7
B	26	PRO	-	expression tag	UNP Q3DLX7
B	27	ARG	-	expression tag	UNP Q3DLX7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	GLY	-	expression tag	UNP Q3DLX7
B	29	SER	-	expression tag	UNP Q3DLX7
B	30	HIS	-	expression tag	UNP Q3DLX7
D	9	MET	-	expression tag	UNP Q3DLX7
D	10	GLY	-	expression tag	UNP Q3DLX7
D	11	SER	-	expression tag	UNP Q3DLX7
D	12	SER	-	expression tag	UNP Q3DLX7
D	13	HIS	-	expression tag	UNP Q3DLX7
D	14	HIS	-	expression tag	UNP Q3DLX7
D	15	HIS	-	expression tag	UNP Q3DLX7
D	16	HIS	-	expression tag	UNP Q3DLX7
D	17	HIS	-	expression tag	UNP Q3DLX7
D	18	HIS	-	expression tag	UNP Q3DLX7
D	19	HIS	-	expression tag	UNP Q3DLX7
D	20	HIS	-	expression tag	UNP Q3DLX7
D	21	SER	-	expression tag	UNP Q3DLX7
D	22	SER	-	expression tag	UNP Q3DLX7
D	23	GLY	-	expression tag	UNP Q3DLX7
D	24	LEU	-	expression tag	UNP Q3DLX7
D	25	VAL	-	expression tag	UNP Q3DLX7
D	26	PRO	-	expression tag	UNP Q3DLX7
D	27	ARG	-	expression tag	UNP Q3DLX7
D	28	GLY	-	expression tag	UNP Q3DLX7
D	29	SER	-	expression tag	UNP Q3DLX7
D	30	HIS	-	expression tag	UNP Q3DLX7

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).

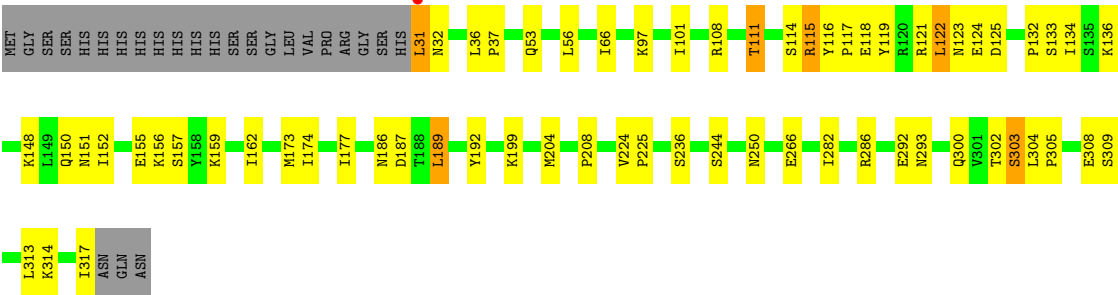


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	C	1	Total 12	C 6	N 1	O 4	S 1	0	0	
2	C	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
2	A	1	Total 12	C 6	N 1	O 4	S 1	0	0	
2	D	1	Total 12	C 6	N 1	O 4	S 1	0	0	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	193	Total	O	0	0
			193	193		
3	A	110	Total	O	0	0
			110	110		
3	B	73	Total	O	0	0
			73	73		
3	D	147	Total	O	0	0
			147	147		

● Molecule 1: Putative nisin-resistance protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.81Å 137.24Å 164.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.36 – 2.21 55.36 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (55.36-2.21) 99.6 (55.36-2.21)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.194 , 0.243 0.199 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9601	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

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	0.48	0/2291	0.83	4/3100 (0.1%)
1	B	0.44	0/2224	0.86	2/3018 (0.1%)
1	C	0.61	0/2335	0.84	1/3149 (0.0%)
1	D	0.58	1/2325 (0.0%)	0.82	0/3137
All	All	0.53	1/9175 (0.0%)	0.84	7/12404 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	PRO	CA-C	5.17	1.54	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	PRO	O-C-N	6.44	124.27	121.31
1	A	36	LEU	CA-C-N	6.13	124.14	119.66
1	A	36	LEU	C-N-CA	6.13	124.14	119.66
1	B	174	ILE	CB-CA-C	-5.93	108.07	113.70
1	B	126	ILE	N-CA-C	5.92	116.63	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2251	0	2272	70	0
1	B	2186	0	2138	81	0
1	C	2295	0	2366	40	0
1	D	2285	0	2351	59	0
2	A	12	0	12	0	0
2	C	24	13	24	8	0
2	D	12	0	12	9	0
3	A	110	0	0	10	0
3	B	73	0	0	8	0
3	C	193	0	0	13	1
3	D	147	0	0	7	1
All	All	9588	13	9175	241	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 13.

The worst 5 of 241 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:D:121:ARG:HE	2:D:401:MES:H52	1.09	1.16
1:C:42:ARG:NH2	3:C:607:HOH:O	1.89	1.03
1:A:53:GLN:HG2	1:A:54:ARG:HG2	1.47	0.96
1:C:49:ASP:OD2	3:C:607:HOH:O	1.83	0.95
1:C:80:TYR:H	2:C:401:MES:H51	1.27	0.95

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)
3:C:526:HOH:O	3:D:524:HOH:O[4_475]	2.04	0.16

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	285/312 (91%)	272 (95%)	13 (5%)	0	100	100
1	B	282/312 (90%)	264 (94%)	17 (6%)	1 (0%)	30	33
1	C	285/312 (91%)	278 (98%)	6 (2%)	1 (0%)	30	33
1	D	285/312 (91%)	277 (97%)	7 (2%)	1 (0%)	30	33
All	All	1137/1248 (91%)	1091 (96%)	43 (4%)	3 (0%)	36	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	ILE
1	D	236	SER
1	B	208	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/280 (89%)	225 (90%)	24 (10%)	8	7
1	B	234/280 (84%)	214 (92%)	20 (8%)	10	10
1	C	258/280 (92%)	243 (94%)	15 (6%)	18	21
1	D	256/280 (91%)	242 (94%)	14 (6%)	19	23
All	All	997/1120 (89%)	924 (93%)	73 (7%)	13	13

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	304	LEU
1	D	303	SER
1	D	31	LEU
1	D	118	GLU
1	A	122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	62	GLN
1	D	186	ASN
1	B	53	GLN
1	B	100	GLN
1	B	151	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 oligosaccharides 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	C	402	-	12,12,12	2.42	1 (8%)	15,16,16	2.17	7 (46%)
2	MES	D	401	-	12,12,12	2.35	1 (8%)	15,16,16	2.55	7 (46%)
2	MES	C	401	-	12,12,12	2.21	1 (8%)	15,16,16	2.44	7 (46%)
2	MES	A	401	-	12,12,12	2.22	1 (8%)	15,16,16	2.44	7 (46%)

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	C	402	-	-	6/6/14/14	0/1/1/1
2	MES	D	401	-	-	5/6/14/14	0/1/1/1
2	MES	C	401	-	-	6/6/14/14	0/1/1/1
2	MES	A	401	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	402	MES	C8-S	-7.97	1.66	1.77
2	D	401	MES	C8-S	-7.73	1.66	1.77
2	A	401	MES	C8-S	-7.36	1.67	1.77
2	C	401	MES	C8-S	-7.25	1.67	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	MES	C2-C3-N4	-5.40	101.91	110.12
2	A	401	MES	C5-N4-C3	5.01	119.62	108.84
2	C	401	MES	C6-C5-N4	-4.56	103.19	110.12
2	C	401	MES	C5-N4-C3	4.53	118.60	108.84
2	D	401	MES	C6-C5-N4	-3.83	104.30	110.12

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	MES	C8-C7-N4-C3
2	C	401	MES	N4-C7-C8-S
2	C	402	MES	C8-C7-N4-C3
2	C	402	MES	C8-C7-N4-C5
2	A	401	MES	C8-C7-N4-C3

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	MES	2	0
2	D	401	MES	9	0
2	C	401	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	287/312 (91%)	0.02	3 (1%) 79 78	28, 41, 58, 66	0
1	B	286/312 (91%)	0.57	14 (4%) 35 31	35, 52, 71, 81	0
1	C	287/312 (91%)	-0.42	0 100 100	19, 29, 44, 57	0
1	D	287/312 (91%)	-0.22	1 (0%) 90 89	20, 34, 54, 61	0
All	All	1147/1248 (91%)	-0.01	18 (1%) 70 68	19, 39, 61, 81	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	GLY	4.4
1	B	317	ILE	4.1
1	D	31	LEU	3.3
1	B	31	LEU	2.7
1	A	31	LEU	2.7

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MES	A	401	12/12	0.66	0.20	105,113,119,120	0
2	MES	D	401	12/12	0.78	0.15	58,68,81,88	0
2	MES	C	402	12/12	0.82	0.15	25,43,54,61	0
2	MES	C	401	12/12	0.86	0.14	34,44,60,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.