Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:46 AM EDT

PDB ID	:	6T7E
Title	:	PII-like protein CutA from Nostoc sp. PCC7120 in complex with MES
Authors	:	Selim, K.A.; Albrecht, R.; Forchhammer, K.; Hartmann, M.D.
Deposited on	:	2019-10-21
Resolution	:	2.45 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 (i) 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 (i)) were used in the production of this report:

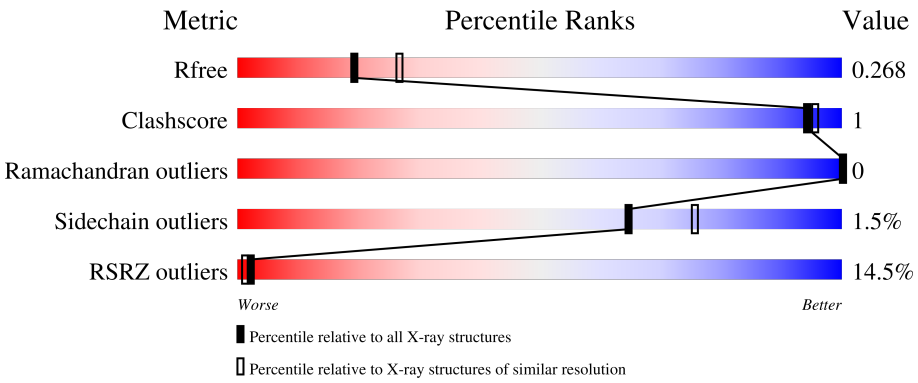
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	114	3% 81% 9% 11%
1	B	114	4% 88% • 10%
1	C	114	4% 87% • 11%
1	D	114	4% 82% 10% 9%
1	E	114	4% 88% • 9%

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Mol	Chain	Length	Quality of chain
1	F	114	61% 88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9838 atoms, of which 4900 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 Periplasmic divalent cation tolerance protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	102	1632	520	816	137	153	6	18	0	0
1	B	103	1649	527	825	137	154	6	19	0	0
1	C	102	1640	524	822	135	153	6	18	0	0
1	D	104	1658	533	830	134	155	6	20	0	0
1	E	104	1636	528	813	133	156	6	22	0	0
1	F	100	1507	484	742	130	147	4	26	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	-	expression tag	UNP Q8YL42
A	106	ALA	-	expression tag	UNP Q8YL42
A	107	TRP	-	expression tag	UNP Q8YL42
A	108	SER	-	expression tag	UNP Q8YL42
A	109	HIS	-	expression tag	UNP Q8YL42
A	110	PRO	-	expression tag	UNP Q8YL42
A	111	GLN	-	expression tag	UNP Q8YL42
A	112	PHE	-	expression tag	UNP Q8YL42
A	113	GLU	-	expression tag	UNP Q8YL42
A	114	LYS	-	expression tag	UNP Q8YL42
B	105	SER	-	expression tag	UNP Q8YL42
B	106	ALA	-	expression tag	UNP Q8YL42
B	107	TRP	-	expression tag	UNP Q8YL42
B	108	SER	-	expression tag	UNP Q8YL42
B	109	HIS	-	expression tag	UNP Q8YL42
B	110	PRO	-	expression tag	UNP Q8YL42
B	111	GLN	-	expression tag	UNP Q8YL42

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Chain	Residue	Modelled	Actual	Comment	Reference
B	112	PHE	-	expression tag	UNP Q8YL42
B	113	GLU	-	expression tag	UNP Q8YL42
B	114	LYS	-	expression tag	UNP Q8YL42
C	105	SER	-	expression tag	UNP Q8YL42
C	106	ALA	-	expression tag	UNP Q8YL42
C	107	TRP	-	expression tag	UNP Q8YL42
C	108	SER	-	expression tag	UNP Q8YL42
C	109	HIS	-	expression tag	UNP Q8YL42
C	110	PRO	-	expression tag	UNP Q8YL42
C	111	GLN	-	expression tag	UNP Q8YL42
C	112	PHE	-	expression tag	UNP Q8YL42
C	113	GLU	-	expression tag	UNP Q8YL42
C	114	LYS	-	expression tag	UNP Q8YL42
D	105	SER	-	expression tag	UNP Q8YL42
D	106	ALA	-	expression tag	UNP Q8YL42
D	107	TRP	-	expression tag	UNP Q8YL42
D	108	SER	-	expression tag	UNP Q8YL42
D	109	HIS	-	expression tag	UNP Q8YL42
D	110	PRO	-	expression tag	UNP Q8YL42
D	111	GLN	-	expression tag	UNP Q8YL42
D	112	PHE	-	expression tag	UNP Q8YL42
D	113	GLU	-	expression tag	UNP Q8YL42
D	114	LYS	-	expression tag	UNP Q8YL42
E	105	SER	-	expression tag	UNP Q8YL42
E	106	ALA	-	expression tag	UNP Q8YL42
E	107	TRP	-	expression tag	UNP Q8YL42
E	108	SER	-	expression tag	UNP Q8YL42
E	109	HIS	-	expression tag	UNP Q8YL42
E	110	PRO	-	expression tag	UNP Q8YL42
E	111	GLN	-	expression tag	UNP Q8YL42
E	112	PHE	-	expression tag	UNP Q8YL42
E	113	GLU	-	expression tag	UNP Q8YL42
E	114	LYS	-	expression tag	UNP Q8YL42
F	105	SER	-	expression tag	UNP Q8YL42
F	106	ALA	-	expression tag	UNP Q8YL42
F	107	TRP	-	expression tag	UNP Q8YL42
F	108	SER	-	expression tag	UNP Q8YL42
F	109	HIS	-	expression tag	UNP Q8YL42
F	110	PRO	-	expression tag	UNP Q8YL42
F	111	GLN	-	expression tag	UNP Q8YL42
F	112	PHE	-	expression tag	UNP Q8YL42
F	113	GLU	-	expression tag	UNP Q8YL42

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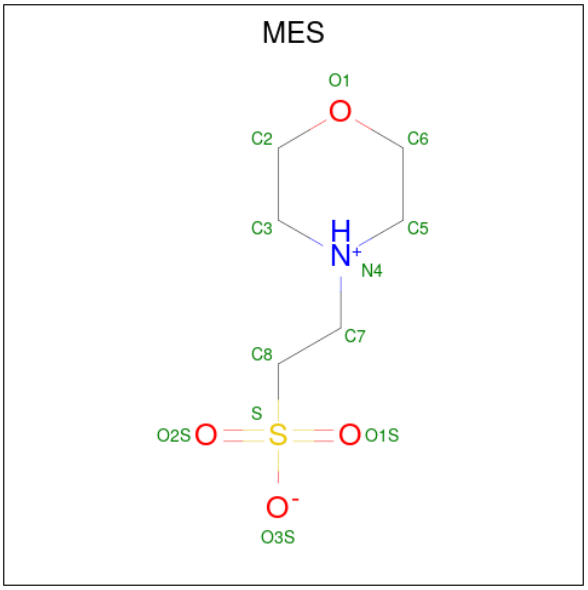
Chain	Residue	Modelled	Actual	Comment	Reference
F	114	LYS	-	expression tag	UNP Q8YL42

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	4	4	4	0	0
3	B	6	6	6	0	0
3	C	2	2	2	0	0
3	D	4	4	4	0	0

3 Residue-property plots (i)

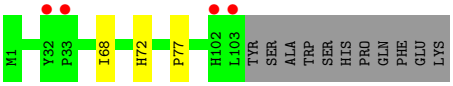
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Periplasmic divalent cation tolerance protein

Chain A:

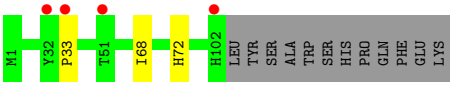
• Molecule 1: Periplasmic divalent cation tolerance protein

Chain B:



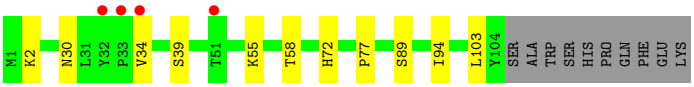
• Molecule 1: Periplasmic divalent cation tolerance protein

Chain C:



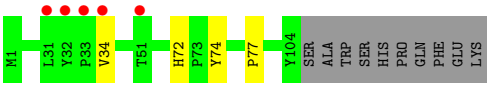
• Molecule 1: Periplasmic divalent cation tolerance protein

Chain D:



• Molecule 1: Periplasmic divalent cation tolerance protein

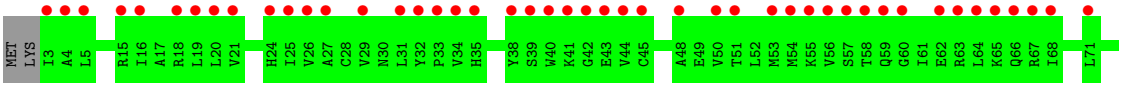
Chain E:

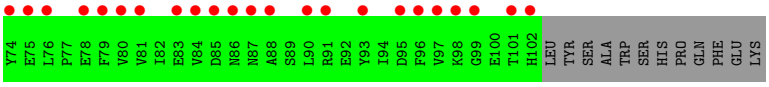


• Molecule 1: Periplasmic divalent cation tolerance protein

Chain F:

61%
88%
12%


MET LYS I3 A4 L5 R15 I16 A17 R18 L19 L20 V21 H24 I25 V26 A27 C28 V29 N30 L31 Y32 P33 V34 H35 Y38 S39 W40 K41 G42 E43 V44 C45 A48 E49 V50 T51 L52 M53 M54 K55 V56 S57 T58 Q59 G60 I61 E62 R63 L64 K65 Q66 R67 I68 L71


Y74 E75 L76 P77 E78 F79 V80 V81 I82 E83 V84 D85 N86 N87 A88 S89 L90 R91 E92 Y93 I94 D95 F96 V97 K98 G99 E100 T101 H102 LEU TYR SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.07Å 87.07Å 152.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.25 – 2.45 38.25 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.25-2.45) 99.8 (38.25-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049 2013/06/30	Depositor
R, R_{free}	0.222 , 0.271 0.224 , 0.268	Depositor DCC
R_{free} test set	1267 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9838	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/833	0.63	0/1132
1	B	0.43	0/841	0.68	0/1143
1	C	0.39	0/835	0.59	0/1133
1	D	0.43	0/846	0.58	0/1150
1	E	0.39	0/841	0.58	0/1145
1	F	0.29	0/781	0.47	0/1067
All	All	0.40	0/4977	0.59	0/6770

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	816	816	807	4	0
1	B	824	825	814	2	0
1	C	818	822	812	1	0
1	D	828	830	818	4	0
1	E	823	813	797	2	0
1	F	765	742	715	0	0
2	A	12	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	13	13	0	0
2	C	12	13	13	0	0
2	E	12	13	13	1	0
3	A	4	0	0	0	0
3	B	6	0	0	0	0
3	C	2	0	0	0	0
3	D	4	0	0	0	0
All	All	4938	4900	4815	13	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 1.

All (13) 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:89:SER:HB2	1:D:94:ILE:HD11	1.82	0.60
1:D:2:LYS:HE2	1:D:58:THR:HG23	1.94	0.49
1:C:68:ILE:O	1:C:72:HIS:HB2	2.12	0.49
1:E:72:HIS:CG	1:E:77:PRO:HB3	2.50	0.47
1:B:72:HIS:CG	1:B:77:PRO:HB3	2.50	0.47
1:A:2:LYS:HD2	1:A:81:VAL:CG1	2.45	0.45
1:E:74:TYR:CD2	2:E:200:MES:H51	2.52	0.44
1:B:68:ILE:O	1:B:72:HIS:HB2	2.18	0.43
1:A:68:ILE:O	1:A:72:HIS:HB2	2.18	0.43
1:D:30:ASN:OD1	1:D:55:LYS:NZ	2.34	0.42
1:D:72:HIS:CG	1:D:77:PRO:HB3	2.54	0.42
1:A:72:HIS:CG	1:A:77:PRO:HB3	2.56	0.41
1:A:37:ILE:HA	1:A:45:CYS:O	2.21	0.41

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	100/114 (88%)	100 (100%)	0	0	100	100
1	B	101/114 (89%)	101 (100%)	0	0	100	100
1	C	100/114 (88%)	100 (100%)	0	0	100	100
1	D	102/114 (90%)	102 (100%)	0	0	100	100
1	E	102/114 (90%)	102 (100%)	0	0	100	100
1	F	98/114 (86%)	97 (99%)	1 (1%)	0	100	100
All	All	603/684 (88%)	602 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	91/104 (88%)	88 (97%)	3 (3%)	38	49
1	B	90/104 (86%)	90 (100%)	0	100	100
1	C	90/104 (86%)	89 (99%)	1 (1%)	73	82
1	D	91/104 (88%)	88 (97%)	3 (3%)	38	49
1	E	89/104 (86%)	88 (99%)	1 (1%)	73	82
1	F	80/104 (77%)	80 (100%)	0	100	100
All	All	531/624 (85%)	523 (98%)	8 (2%)	65	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	55	LYS
1	A	92	GLU
1	C	33	PRO
1	D	34	VAL
1	D	39	SER
1	D	103	LEU

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Mol	Chain	Res	Type
1	E	34	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	B	87	ASN
1	C	102	HIS
1	D	66	GLN
1	E	7	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	C	200	-	12,12,12	2.09	1 (8%)	15,16,16	1.45	4 (26%)
2	MES	E	200	-	12,12,12	2.28	1 (8%)	15,16,16	1.43	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MES	B	200	-	12,12,12	2.16	1 (8%)	15,16,16	1.37	2 (13%)
2	MES	A	200	-	12,12,12	2.27	1 (8%)	15,16,16	1.28	1 (6%)

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	200	-	-	0/6/14/14	0/1/1/1
2	MES	E	200	-	-	0/6/14/14	0/1/1/1
2	MES	B	200	-	-	0/6/14/14	0/1/1/1
2	MES	A	200	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	200	MES	C8-S	-7.48	1.67	1.77
2	A	200	MES	C8-S	-7.40	1.67	1.77
2	B	200	MES	C8-S	-7.02	1.67	1.77
2	C	200	MES	C8-S	-6.78	1.68	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	200	MES	O1S-S-C8	3.18	111.53	106.73
2	C	200	MES	O2S-S-C8	2.67	110.77	106.73
2	C	200	MES	O1S-S-C8	2.62	110.69	106.73
2	B	200	MES	O2S-S-C8	2.62	110.68	106.73
2	A	200	MES	O3S-S-C8	2.38	110.66	106.00
2	C	200	MES	O2S-S-O1S	-2.13	106.90	113.82
2	B	200	MES	O2S-S-O1S	-2.09	107.02	113.82
2	E	200	MES	C6-C5-N4	2.02	113.19	110.12
2	C	200	MES	O3S-S-C8	2.00	109.92	106.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	200	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 (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	102/114 (89%)	0.09	3 (2%)	51	47	33, 45, 61, 73	0
1	B	103/114 (90%)	0.03	4 (3%)	39	36	34, 43, 61, 104	0
1	C	102/114 (89%)	0.11	4 (3%)	39	36	33, 54, 68, 79	0
1	D	104/114 (91%)	0.02	4 (3%)	40	37	33, 43, 58, 64	0
1	E	104/114 (91%)	0.36	5 (4%)	30	28	40, 57, 73, 88	0
1	F	100/114 (87%)	3.28	69 (69%)	0	0	99, 128, 139, 142	0
All	All	615/684 (89%)	0.64	89 (14%)	2	1	33, 51, 133, 142	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	56	VAL	10.6
1	F	79	PHE	8.6
1	F	93	TYR	8.1
1	F	32	TYR	7.9
1	F	66	GLN	7.7
1	F	45	CYS	7.2
1	F	40	TRP	6.8
1	F	33	PRO	6.4
1	F	102	HIS	6.3
1	F	39	SER	6.1
1	F	88	ALA	6.1
1	F	62	GLU	5.9
1	F	25	ILE	5.6
1	F	96	PHE	5.5
1	F	64	LEU	5.4
1	F	3	ILE	5.3
1	F	20	LEU	5.2
1	F	27	ALA	5.1
1	F	78	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	44	VAL	5.0
1	F	26	VAL	4.9
1	F	57	SER	4.8
1	F	75	GLU	4.8
1	F	101	THR	4.6
1	F	55	LYS	4.6
1	F	59	GLN	4.6
1	F	54	MET	4.5
1	F	29	VAL	4.5
1	F	68	ILE	4.3
1	F	87	ASN	4.3
1	E	32	TYR	4.0
1	F	74	TYR	4.0
1	F	99	GLY	3.9
1	F	42	GLY	3.9
1	F	5	LEU	3.9
1	F	80	VAL	3.9
1	F	4	ALA	3.8
1	F	71	LEU	3.5
1	E	33	PRO	3.5
1	F	84	VAL	3.5
1	F	58	THR	3.5
1	F	21	VAL	3.5
1	B	103	LEU	3.4
1	F	24	HIS	3.4
1	F	81	VAL	3.3
1	F	34	VAL	3.3
1	F	48	ALA	3.3
1	F	43	GLU	3.3
1	F	38	TYR	3.2
1	F	91	ARG	3.2
1	F	31	LEU	3.1
1	F	63	ARG	3.0
1	F	35	HIS	3.0
1	F	18	ARG	3.0
1	D	32	TYR	3.0
1	C	102	HIS	2.9
1	F	53	MET	2.8
1	D	51	THR	2.8
1	F	15	ARG	2.8
1	F	41	LYS	2.8
1	B	102	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	60	GLY	2.7
1	F	50	VAL	2.7
1	F	16	ILE	2.7
1	C	32	TYR	2.7
1	F	19	LEU	2.6
1	A	43	GLU	2.6
1	D	33	PRO	2.5
1	F	90	LEU	2.5
1	E	51	THR	2.5
1	F	86	ASN	2.5
1	F	67	ARG	2.5
1	F	95	ASP	2.5
1	E	34	VAL	2.5
1	F	83	GLU	2.5
1	F	98	LYS	2.4
1	C	33	PRO	2.4
1	A	33	PRO	2.4
1	F	51	THR	2.3
1	F	65	LYS	2.3
1	F	97	VAL	2.3
1	B	32	TYR	2.2
1	C	51	THR	2.1
1	B	33	PRO	2.1
1	D	34	VAL	2.1
1	A	40	TRP	2.1
1	F	85	ASP	2.0
1	E	31	LEU	2.0
1	F	76	LEU	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	200	12/12	0.82	0.36	79,84,95,96	0
2	MES	C	200	12/12	0.86	0.27	87,90,93,94	0
2	MES	E	200	12/12	0.86	0.29	79,83,95,98	0
2	MES	A	200	12/12	0.90	0.26	73,78,82,85	0

6.5 Other polymers (i)

There are no such residues in this entry.