



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 06:22 PM EDT

PDB ID : 2GXF  
Title : X-Ray Crystal Structure of Protein YybH from Bacillus subtilis. Northeast Structural Genomics Consortium Target SR506.  
Authors : Forouhar, F.; Abashidze, M.; Jayaraman, S.; Cunningham, K.; Fang, Y.; Ma, L.-C.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-05-08  
Resolution : 3.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

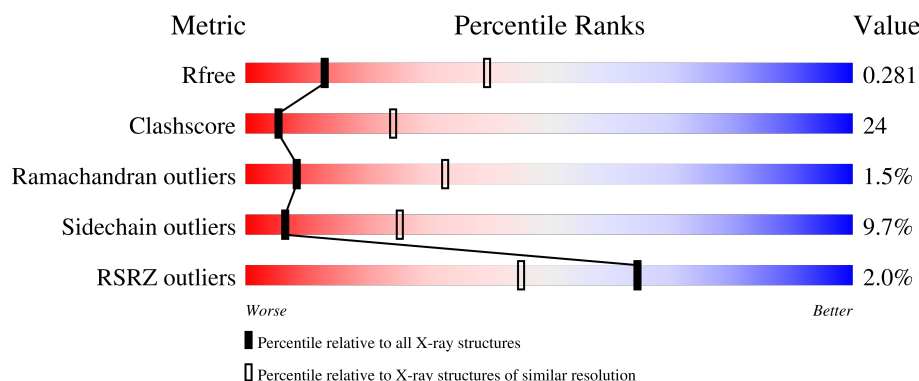
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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  $\geq 3$ , 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	142	<div> <div>2%</div> <div>47%</div> <div>31%</div> <div>5%</div> <div>16%</div> </div>
1	B	142	<div> <div>%</div> <div>47%</div> <div>31%</div> <div>6%</div> <div>16%</div> </div>
1	C	142	<div> <div>%</div> <div>51%</div> <div>27%</div> <div>•</div> <div>16%</div> </div>
1	D	142	<div> <div>%</div> <div>50%</div> <div>30%</div> <div>•</div> <div>16%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3845 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 Hypothetical protein yybH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	Se	0	0	0
			941	600	153	181	2	5			
1	B	119	Total	C	N	O	S	Se	0	0	0
			941	600	153	181	2	5			
1	C	119	Total	C	N	O	S	Se	0	0	0
			941	600	153	181	2	5			
1	D	119	Total	C	N	O	S	Se	0	0	0
			941	600	153	181	2	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P37496
A	25	MSE	MET	modified residue	UNP P37496
A	40	MSE	MET	modified residue	UNP P37496
A	70	MSE	MET	modified residue	UNP P37496
A	98	MSE	MET	modified residue	UNP P37496
A	130	MSE	-	cloning artifact	UNP P37496
A	131	ALA	-	cloning artifact	UNP P37496
A	132	GLY	-	cloning artifact	UNP P37496
A	133	ASP	-	cloning artifact	UNP P37496
A	134	PRO	-	cloning artifact	UNP P37496
A	135	LEU	-	cloning artifact	UNP P37496
A	136	GLU	-	cloning artifact	UNP P37496
A	137	HIS	-	expression tag	UNP P37496
A	138	HIS	-	expression tag	UNP P37496
A	139	HIS	-	expression tag	UNP P37496
A	140	HIS	-	expression tag	UNP P37496
A	141	HIS	-	expression tag	UNP P37496
A	142	HIS	-	expression tag	UNP P37496
B	1	MSE	MET	modified residue	UNP P37496
B	25	MSE	MET	modified residue	UNP P37496
B	40	MSE	MET	modified residue	UNP P37496

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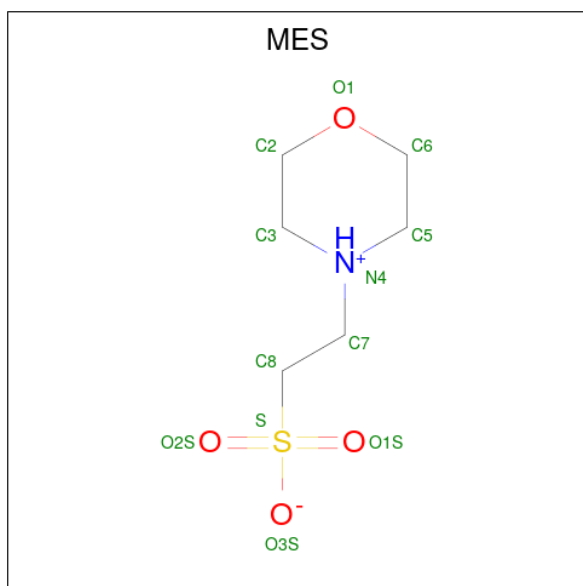
Chain	Residue	Modelled	Actual	Comment	Reference
B	70	MSE	MET	modified residue	UNP P37496
B	98	MSE	MET	modified residue	UNP P37496
B	130	MSE	-	cloning artifact	UNP P37496
B	131	ALA	-	cloning artifact	UNP P37496
B	132	GLY	-	cloning artifact	UNP P37496
B	133	ASP	-	cloning artifact	UNP P37496
B	134	PRO	-	cloning artifact	UNP P37496
B	135	LEU	-	cloning artifact	UNP P37496
B	136	GLU	-	cloning artifact	UNP P37496
B	137	HIS	-	expression tag	UNP P37496
B	138	HIS	-	expression tag	UNP P37496
B	139	HIS	-	expression tag	UNP P37496
B	140	HIS	-	expression tag	UNP P37496
B	141	HIS	-	expression tag	UNP P37496
B	142	HIS	-	expression tag	UNP P37496
C	1	MSE	MET	modified residue	UNP P37496
C	25	MSE	MET	modified residue	UNP P37496
C	40	MSE	MET	modified residue	UNP P37496
C	70	MSE	MET	modified residue	UNP P37496
C	98	MSE	MET	modified residue	UNP P37496
C	130	MSE	-	cloning artifact	UNP P37496
C	131	ALA	-	cloning artifact	UNP P37496
C	132	GLY	-	cloning artifact	UNP P37496
C	133	ASP	-	cloning artifact	UNP P37496
C	134	PRO	-	cloning artifact	UNP P37496
C	135	LEU	-	cloning artifact	UNP P37496
C	136	GLU	-	cloning artifact	UNP P37496
C	137	HIS	-	expression tag	UNP P37496
C	138	HIS	-	expression tag	UNP P37496
C	139	HIS	-	expression tag	UNP P37496
C	140	HIS	-	expression tag	UNP P37496
C	141	HIS	-	expression tag	UNP P37496
C	142	HIS	-	expression tag	UNP P37496
D	1	MSE	MET	modified residue	UNP P37496
D	25	MSE	MET	modified residue	UNP P37496
D	40	MSE	MET	modified residue	UNP P37496
D	70	MSE	MET	modified residue	UNP P37496
D	98	MSE	MET	modified residue	UNP P37496
D	130	MSE	-	cloning artifact	UNP P37496
D	131	ALA	-	cloning artifact	UNP P37496
D	132	GLY	-	cloning artifact	UNP P37496
D	133	ASP	-	cloning artifact	UNP P37496

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Chain	Residue	Modelled	Actual	Comment	Reference
D	134	PRO	-	cloning artifact	UNP P37496
D	135	LEU	-	cloning artifact	UNP P37496
D	136	GLU	-	cloning artifact	UNP P37496
D	137	HIS	-	expression tag	UNP P37496
D	138	HIS	-	expression tag	UNP P37496
D	139	HIS	-	expression tag	UNP P37496
D	140	HIS	-	expression tag	UNP P37496
D	141	HIS	-	expression tag	UNP P37496
D	142	HIS	-	expression tag	UNP P37496

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

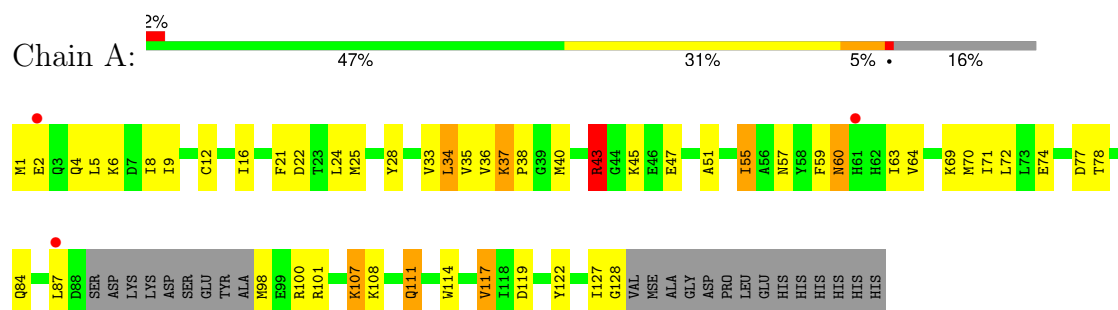
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	10	Total	O	0	0
			10	10		
3	C	8	Total	O	0	0
			8	8		
3	D	5	Total	O	0	0
			5	5		

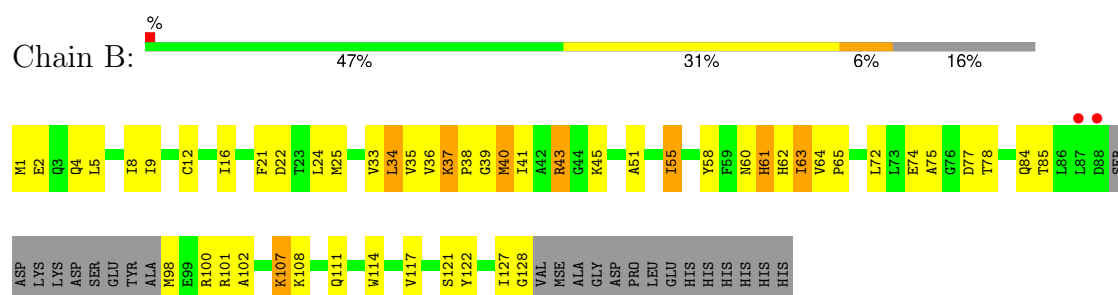
### 3 Residue-property plots [i](#)

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.

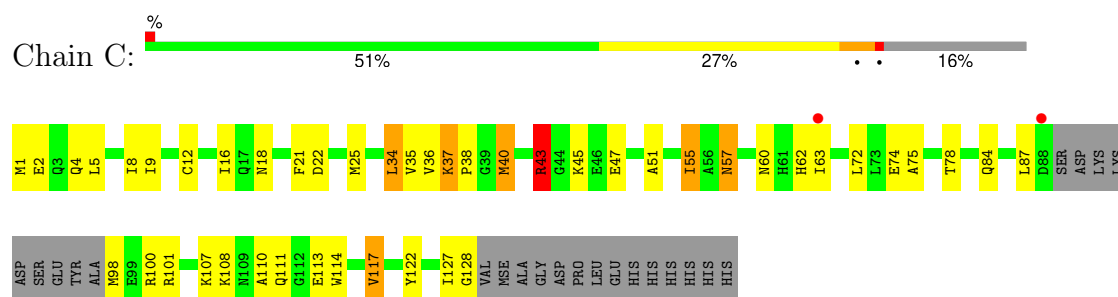
#### • Molecule 1: Hypothetical protein yybH



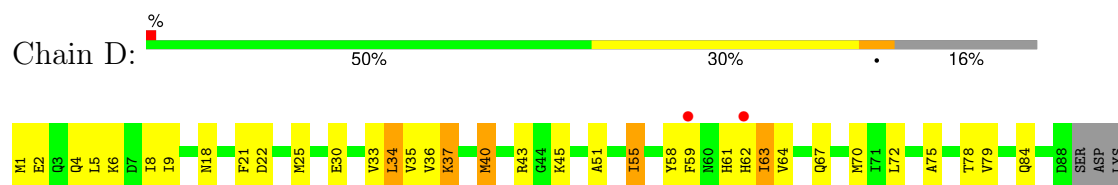
#### • Molecule 1: Hypothetical protein yybH



#### • Molecule 1: Hypothetical protein yybH



#### • Molecule 1: Hypothetical protein yybH



LYS	ASP	SER	GLU	TYR	ALA	K98	E99	R100	R101	A102	K107	K108	Q111	W114	V117	I118	D119	N120	S121	L126	I127	G128	VAL	MSF	ALA	GLY	ASP	PRO	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.25Å 88.25Å 82.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 3.10 29.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.42-3.10) 96.3 (29.42-3.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.286 0.264 , 0.281	Depositor DCC
$R_{free}$ test set	1110 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/951	1.17	6/1278 (0.5%)
1	B	0.46	0/951	0.91	5/1278 (0.4%)
1	C	0.45	0/951	0.89	5/1278 (0.4%)
1	D	0.45	0/951	0.91	5/1278 (0.4%)
All	All	0.46	0/3804	0.98	21/5112 (0.4%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH1	-20.04	110.28	120.30
1	A	100	ARG	NE-CZ-NH2	18.09	129.34	120.30
1	D	43	ARG	NE-CZ-NH2	-15.91	112.35	120.30
1	A	43	ARG	NE-CZ-NH1	-14.90	112.85	120.30
1	B	43	ARG	NE-CZ-NH2	-14.87	112.87	120.30
1	C	43	ARG	NE-CZ-NH1	-14.72	112.94	120.30
1	A	43	ARG	NE-CZ-NH2	14.44	127.52	120.30
1	B	43	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	D	43	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	C	43	ARG	NE-CZ-NH2	13.02	126.81	120.30
1	A	100	ARG	CD-NE-CZ	9.19	136.46	123.60
1	B	43	ARG	CD-NE-CZ	7.93	134.70	123.60
1	C	100	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	D	43	ARG	CD-NE-CZ	7.71	134.40	123.60
1	D	100	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	C	43	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	43	ARG	CD-NE-CZ	7.46	134.04	123.60
1	B	100	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	100	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	D	100	ARG	NE-CZ-NH1	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	NE-CZ-NH1	6.80	123.70	120.30

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	941	0	946	72	0
1	B	941	0	946	48	0
1	C	941	0	946	57	0
1	D	941	0	946	43	0
2	A	12	0	13	2	0
2	B	12	0	13	0	0
2	C	12	0	13	2	0
2	D	12	0	13	2	0
3	A	10	0	0	1	0
3	B	10	0	0	2	0
3	C	8	0	0	1	0
3	D	5	0	0	0	0
All	All	3845	0	3836	180	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 24.

All (180) 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:A:63:ILE:HD12	1:A:87:LEU:HD11	1.30	1.09
1:C:63:ILE:HD12	1:C:87:LEU:HD11	1.44	1.00
1:C:5:LEU:HD12	1:C:72:LEU:HD21	1.48	0.96
1:C:57:ASN:HD22	1:C:57:ASN:N	1.63	0.94
1:A:69:LYS:HZ1	1:C:108:LYS:CD	1.86	0.89
1:C:57:ASN:N	1:C:57:ASN:ND2	2.24	0.86
1:A:38:PRO:HD3	1:A:122:TYR:CE2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:LEU:HD12	1:D:72:LEU:HD21	1.62	0.81
1:A:63:ILE:HD12	1:A:87:LEU:CD1	2.10	0.79
1:B:39:GLY:HA2	1:C:113:GLU:HA	1.63	0.79
1:B:5:LEU:HD12	1:B:72:LEU:HD21	1.69	0.74
1:C:57:ASN:ND2	1:C:57:ASN:H	1.85	0.74
1:A:69:LYS:HZ1	1:C:108:LYS:HD2	1.55	0.71
1:A:5:LEU:HD12	1:A:72:LEU:HD21	1.71	0.71
1:B:65:PRO:HB2	1:B:85:THR:CG2	2.24	0.67
1:A:63:ILE:HG23	1:A:87:LEU:CD1	2.26	0.65
1:B:61:HIS:C	1:B:63:ILE:H	1.99	0.65
1:C:36:VAL:HB	1:C:40:MSE:HG2	1.78	0.65
1:C:62:HIS:O	1:C:63:ILE:HG12	1.97	0.64
1:C:117:VAL:HG12	1:D:75:ALA:HB1	1.79	0.64
1:B:39:GLY:CA	1:C:113:GLU:HA	2.28	0.63
1:C:128:GLY:HA3	1:D:101:ARG:NH2	2.14	0.63
1:D:36:VAL:HB	1:D:40:MSE:HG2	1.81	0.63
1:A:37:LYS:HA	1:A:122:TYR:OH	1.99	0.61
1:A:38:PRO:HD3	1:A:122:TYR:CZ	2.35	0.61
1:B:36:VAL:HB	1:B:40:MSE:HG2	1.81	0.61
1:A:107:LYS:HE3	1:B:77:ASP:OD1	2.01	0.60
1:C:101:ARG:NH2	1:D:128:GLY:HA3	2.16	0.60
1:A:5:LEU:O	1:A:9:ILE:HG12	2.02	0.59
1:B:5:LEU:O	1:B:9:ILE:HG12	2.03	0.58
1:B:25:MSE:HE2	1:B:45:LYS:O	2.04	0.58
1:D:6:LYS:HD2	1:D:67:GLN:HG2	1.85	0.58
1:D:25:MSE:HE2	1:D:45:LYS:O	2.03	0.58
1:A:51:ALA:O	1:A:55:ILE:HG12	2.04	0.58
1:C:101:ARG:HH22	1:D:128:GLY:HA3	1.69	0.58
1:C:127:ILE:HD13	1:D:84:GLN:HB2	1.85	0.58
1:A:37:LYS:HA	1:A:122:TYR:CZ	2.38	0.58
1:A:25:MSE:HE2	1:A:45:LYS:O	2.04	0.57
1:A:36:VAL:HB	1:A:40:MSE:HG2	1.85	0.57
1:A:71:ILE:HG23	1:C:110:ALA:O	2.04	0.57
1:A:77:ASP:OD1	1:B:107:LYS:HE3	2.04	0.57
1:B:4:GLN:O	1:B:8:ILE:HG13	2.05	0.57
1:C:127:ILE:HG21	1:D:84:GLN:HB2	1.87	0.57
1:A:2:GLU:OE1	1:C:110:ALA:HB2	2.04	0.56
1:A:2:GLU:HA	1:A:72:LEU:HD22	1.87	0.56
1:C:4:GLN:O	1:C:8:ILE:HG13	2.05	0.56
1:C:5:LEU:O	1:C:9:ILE:HG12	2.04	0.56
1:C:25:MSE:HE2	1:C:45:LYS:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:HG13	1:D:64:VAL:O	2.05	0.56
1:B:39:GLY:HA2	1:C:113:GLU:CA	2.35	0.56
1:A:47:GLU:HG2	3:A:206:HOH:O	2.07	0.55
1:A:63:ILE:HG23	1:A:87:LEU:HD12	1.89	0.55
1:A:127:ILE:HD13	1:B:84:GLN:HB2	1.89	0.55
1:A:108:LYS:HE3	1:A:114:TRP:CZ2	2.41	0.55
1:C:128:GLY:HA3	1:D:101:ARG:HH22	1.72	0.54
1:A:34:LEU:HD23	1:A:119:ASP:CG	2.27	0.54
1:A:63:ILE:HG23	1:A:87:LEU:HD11	1.88	0.54
1:D:4:GLN:O	1:D:8:ILE:HG13	2.06	0.54
1:A:28:TYR:OH	2:A:201:MES:H52	2.08	0.53
1:B:108:LYS:HE3	1:B:114:TRP:CZ2	2.43	0.53
1:A:37:LYS:O	1:A:40:MSE:HB3	2.08	0.52
1:A:5:LEU:HD12	1:A:72:LEU:CD2	2.40	0.52
1:B:108:LYS:HE3	1:B:114:TRP:CE2	2.44	0.52
1:D:119:ASP:OD1	2:D:201:MES:H82	2.08	0.52
1:A:69:LYS:NZ	1:C:108:LYS:CD	2.67	0.52
1:D:5:LEU:O	1:D:9:ILE:HG12	2.10	0.52
1:C:84:GLN:HB2	1:D:127:ILE:HG21	1.90	0.52
1:A:34:LEU:HD23	1:A:119:ASP:HB3	1.91	0.52
1:A:69:LYS:HZ1	1:C:108:LYS:NZ	2.08	0.52
1:A:69:LYS:NZ	1:C:108:LYS:NZ	2.58	0.52
1:A:1:MSE:HE3	1:A:2:GLU:HB3	1.91	0.52
1:B:98:MSE:N	3:B:210:HOH:O	2.42	0.51
1:C:51:ALA:O	1:C:55:ILE:HG12	2.10	0.51
1:C:75:ALA:HB1	1:D:117:VAL:HG12	1.91	0.51
1:A:108:LYS:HE3	1:A:114:TRP:CE2	2.45	0.51
1:C:9:ILE:CD1	2:C:201:MES:H61	2.41	0.51
1:C:108:LYS:HE3	1:C:114:TRP:CZ2	2.45	0.51
1:D:1:MSE:HE3	1:D:2:GLU:HB3	1.93	0.51
1:B:63:ILE:O	1:B:63:ILE:HG22	2.10	0.51
1:C:60:ASN:HD21	1:C:63:ILE:HG21	1.76	0.51
1:D:51:ALA:O	1:D:55:ILE:HG12	2.10	0.51
1:A:69:LYS:HZ1	1:C:108:LYS:HD3	1.74	0.50
1:B:21:PHE:O	1:B:25:MSE:HG2	2.12	0.50
1:B:108:LYS:HB2	1:B:114:TRP:CE2	2.47	0.50
1:A:4:GLN:O	1:A:8:ILE:HG13	2.11	0.50
1:B:38:PRO:HD3	1:B:122:TYR:CE2	2.46	0.50
1:B:65:PRO:HB2	1:B:85:THR:HG22	1.91	0.50
1:C:9:ILE:HD12	2:C:201:MES:H61	1.93	0.50
1:B:37:LYS:HG3	1:B:40:MSE:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:LYS:HG3	1:D:40:MSE:HG2	1.94	0.49
1:A:21:PHE:O	1:A:25:MSE:HG2	2.13	0.49
1:A:59:PHE:CD2	1:A:60:ASN:N	2.81	0.49
1:D:21:PHE:O	1:D:25:MSE:HG2	2.11	0.49
1:D:108:LYS:HE3	1:D:114:TRP:CZ2	2.48	0.49
1:A:1:MSE:HE3	1:A:2:GLU:CB	2.43	0.48
1:A:108:LYS:HB2	1:A:114:TRP:CE2	2.48	0.48
1:B:1:MSE:HE3	1:B:2:GLU:HB3	1.96	0.48
1:A:127:ILE:HG21	1:B:84:GLN:HB2	1.94	0.48
1:C:74:GLU:O	1:D:33:VAL:HG11	2.13	0.48
1:C:108:LYS:HE3	1:C:114:TRP:CE2	2.49	0.47
1:C:37:LYS:HG3	1:C:40:MSE:HG2	1.95	0.47
1:D:2:GLU:HG2	1:D:2:GLU:O	2.15	0.47
1:B:51:ALA:O	1:B:55:ILE:HG12	2.15	0.47
1:A:60:ASN:HB3	1:A:63:ILE:HG13	1.96	0.47
1:C:117:VAL:HG12	1:D:75:ALA:CB	2.43	0.47
1:A:60:ASN:HB3	1:A:63:ILE:CG1	2.45	0.47
1:B:2:GLU:O	1:B:2:GLU:HG2	2.15	0.47
1:C:21:PHE:O	1:C:25:MSE:HG2	2.14	0.47
1:A:119:ASP:OD2	2:A:201:MES:H52	2.15	0.47
1:A:6:LYS:HD3	1:A:70:MSE:SE	2.65	0.46
1:A:64:VAL:HG13	1:A:64:VAL:O	2.16	0.46
1:C:108:LYS:HB2	1:C:114:TRP:CE2	2.50	0.46
1:A:117:VAL:HG12	1:B:75:ALA:HB1	1.97	0.46
1:A:128:GLY:HA3	1:B:101:ARG:NH2	2.31	0.46
1:D:108:LYS:HB2	1:D:114:TRP:CE2	2.50	0.46
1:D:108:LYS:HE3	1:D:114:TRP:CE2	2.50	0.46
1:C:1:MSE:HE3	1:C:2:GLU:HB3	1.98	0.45
1:A:33:VAL:HG22	1:B:75:ALA:HB2	1.98	0.45
1:A:87:LEU:HB3	1:A:98:MSE:HB3	1.99	0.45
1:A:69:LYS:NZ	1:C:108:LYS:HD3	2.31	0.45
1:A:63:ILE:CD1	1:A:87:LEU:HD11	2.21	0.45
1:C:87:LEU:HD22	3:C:208:HOH:O	2.17	0.45
1:A:2:GLU:HG2	1:A:2:GLU:O	2.17	0.45
1:A:34:LEU:HD23	1:A:119:ASP:CB	2.47	0.45
1:D:1:MSE:HE3	1:D:2:GLU:CB	2.47	0.45
1:A:34:LEU:HD22	1:A:35:VAL:N	2.32	0.44
1:A:33:VAL:HG11	1:B:74:GLU:O	2.18	0.44
1:B:1:MSE:HE3	1:B:2:GLU:CB	2.48	0.44
1:B:61:HIS:C	1:B:63:ILE:N	2.67	0.44
1:D:37:LYS:O	1:D:40:MSE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:CYS:O	1:A:16:ILE:HG13	2.18	0.44
1:A:128:GLY:HA3	1:B:101:ARG:HH22	1.83	0.44
1:A:37:LYS:HD2	1:A:40:MSE:HE2	1.99	0.43
1:B:102:ALA:HB1	1:B:121:SER:HA	2.00	0.43
1:D:63:ILE:H	1:D:63:ILE:HD12	1.82	0.43
1:A:69:LYS:NZ	1:C:108:LYS:HZ2	2.17	0.43
1:B:37:LYS:O	1:B:40:MSE:HB3	2.18	0.43
1:D:121:SER:HB3	2:D:201:MES:H81	2.00	0.43
1:B:37:LYS:HA	1:B:122:TYR:OH	2.19	0.43
1:C:63:ILE:HG23	1:C:87:LEU:HD11	2.00	0.43
1:D:34:LEU:HD23	1:D:119:ASP:HB3	2.00	0.43
1:A:101:ARG:HH22	1:B:128:GLY:HA3	1.84	0.43
1:D:79:VAL:HG23	1:D:114:TRP:CH2	2.54	0.43
1:A:84:GLN:HB2	1:B:127:ILE:HD13	2.01	0.43
1:B:62:HIS:CE1	3:B:208:HOH:O	2.71	0.43
1:C:87:LEU:HB3	1:C:98:MSE:HB3	2.00	0.43
1:C:2:GLU:O	1:C:2:GLU:HG2	2.18	0.42
1:C:84:GLN:HB2	1:D:127:ILE:HD13	1.99	0.42
1:B:60:ASN:HD22	1:B:63:ILE:HD11	1.84	0.42
1:D:58:TYR:HD1	1:D:58:TYR:O	2.02	0.42
1:A:101:ARG:NH2	1:B:128:GLY:HA3	2.35	0.42
1:B:41:ILE:HD11	1:B:43:ARG:HD2	2.02	0.42
1:D:64:VAL:O	1:D:64:VAL:HG22	2.18	0.42
1:A:37:LYS:HG3	1:A:40:MSE:HG2	2.02	0.42
1:C:37:LYS:O	1:C:40:MSE:HB3	2.19	0.42
1:C:34:LEU:HD22	1:C:35:VAL:N	2.34	0.42
1:A:21:PHE:HA	1:A:24:LEU:HB3	2.02	0.42
1:A:74:GLU:O	1:B:33:VAL:HG11	2.19	0.42
1:C:12:CYS:O	1:C:16:ILE:HG13	2.19	0.42
1:B:12:CYS:O	1:B:16:ILE:HG13	2.20	0.42
1:D:30:GLU:HA	1:D:45:LYS:HG3	2.01	0.42
1:D:63:ILE:O	1:D:64:VAL:C	2.57	0.42
1:D:126:LEU:HD12	1:D:126:LEU:HA	1.89	0.41
1:A:87:LEU:HB3	1:A:98:MSE:CB	2.51	0.41
1:A:111:GLN:N	1:A:111:GLN:OE1	2.53	0.41
1:B:21:PHE:HA	1:B:24:LEU:HB3	2.02	0.41
1:A:43:ARG:NH1	1:B:74:GLU:O	2.51	0.41
1:A:64:VAL:O	1:A:87:LEU:O	2.39	0.41
1:A:69:LYS:HZ1	1:C:108:LYS:CE	2.34	0.41
1:C:18:ASN:N	1:C:18:ASN:HD22	2.18	0.41
1:C:43:ARG:O	1:C:47:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LYS:HD3	1:D:70:MSE:CE	2.51	0.41
1:A:63:ILE:HD12	1:A:87:LEU:CG	2.51	0.41
1:B:64:VAL:O	1:B:64:VAL:HG13	2.20	0.41
1:C:1:MSE:HE3	1:C:2:GLU:CB	2.51	0.41
1:D:102:ALA:HB1	1:D:121:SER:HA	2.02	0.40
1:D:34:LEU:HD22	1:D:35:VAL:N	2.36	0.40
1:C:38:PRO:HD3	1:C:122:TYR:CE2	2.56	0.40
1:D:18:ASN:N	1:D:18:ASN:HD22	2.19	0.40
1:B:34:LEU:HD22	1:B:35:VAL:N	2.37	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	115/142 (81%)	106 (92%)	8 (7%)	1 (1%)	14	45
1	B	115/142 (81%)	103 (90%)	9 (8%)	3 (3%)	4	21
1	C	115/142 (81%)	103 (90%)	11 (10%)	1 (1%)	14	45
1	D	115/142 (81%)	104 (90%)	9 (8%)	2 (2%)	7	30
All	All	460/568 (81%)	416 (90%)	37 (8%)	7 (2%)	8	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	HIS
1	D	61	HIS
1	B	63	ILE
1	A	55	ILE
1	B	55	ILE
1	C	55	ILE

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Mol	Chain	Res	Type
1	D	55	ILE

### 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	103/117 (88%)	93 (90%)	10 (10%)	6	25
1	B	103/117 (88%)	94 (91%)	9 (9%)	8	31
1	C	103/117 (88%)	93 (90%)	10 (10%)	6	25
1	D	103/117 (88%)	92 (89%)	11 (11%)	5	21
All	All	412/468 (88%)	372 (90%)	40 (10%)	6	25

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	34	LEU
1	A	37	LYS
1	A	43	ARG
1	A	57	ASN
1	A	60	ASN
1	A	78	THR
1	A	107	LYS
1	A	111	GLN
1	A	117	VAL
1	B	22	ASP
1	B	34	LEU
1	B	37	LYS
1	B	40	MSE
1	B	58	TYR
1	B	78	THR
1	B	107	LYS
1	B	111	GLN
1	B	117	VAL
1	C	22	ASP

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Mol	Chain	Res	Type
1	C	34	LEU
1	C	37	LYS
1	C	40	MSE
1	C	43	ARG
1	C	57	ASN
1	C	78	THR
1	C	107	LYS
1	C	111	GLN
1	C	117	VAL
1	D	22	ASP
1	D	34	LEU
1	D	37	LYS
1	D	40	MSE
1	D	59	PHE
1	D	62	HIS
1	D	63	ILE
1	D	78	THR
1	D	107	LYS
1	D	111	GLN
1	D	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	18	ASN
1	A	26	ASN
1	A	60	ASN
1	B	3	GLN
1	B	18	ASN
1	B	26	ASN
1	B	60	ASN
1	C	3	GLN
1	C	18	ASN
1	C	26	ASN
1	C	57	ASN
1	D	3	GLN
1	D	18	ASN
1	D	26	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	201	-	12,12,12	3.29	4 (33%)	15,16,16	0.89	0
2	MES	D	201	-	12,12,12	3.11	4 (33%)	15,16,16	1.02	0
2	MES	A	201	-	12,12,12	3.08	4 (33%)	15,16,16	1.03	0
2	MES	C	201	-	12,12,12	3.12	4 (33%)	15,16,16	1.05	0

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	201	-	-	3/6/14/14	0/1/1/1
2	MES	D	201	-	-	3/6/14/14	0/1/1/1
2	MES	A	201	-	-	5/6/14/14	0/1/1/1
2	MES	C	201	-	-	6/6/14/14	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	MES	O1S-S	9.03	1.70	1.45
2	D	201	MES	O1S-S	8.55	1.69	1.45
2	A	201	MES	O1S-S	8.32	1.68	1.45
2	C	201	MES	O1S-S	7.85	1.67	1.45
2	C	201	MES	O2S-S	5.08	1.59	1.45
2	B	201	MES	O2S-S	4.81	1.58	1.45
2	D	201	MES	O2S-S	4.70	1.58	1.45
2	A	201	MES	O2S-S	4.56	1.58	1.45
2	C	201	MES	O3S-S	3.00	1.58	1.47
2	A	201	MES	O3S-S	2.93	1.58	1.47
2	D	201	MES	O3S-S	2.80	1.57	1.47
2	B	201	MES	C5-N4	2.73	1.54	1.46
2	C	201	MES	C5-N4	2.66	1.54	1.46
2	A	201	MES	C5-N4	2.63	1.54	1.46
2	B	201	MES	O3S-S	2.54	1.56	1.47
2	D	201	MES	C5-N4	2.21	1.52	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	MES	N4-C7-C8-S
2	C	201	MES	N4-C7-C8-S
2	C	201	MES	C7-C8-S-O2S
2	D	201	MES	C8-C7-N4-C3
2	D	201	MES	C8-C7-N4-C5
2	C	201	MES	C7-C8-S-O3S
2	A	201	MES	C7-C8-S-O1S
2	C	201	MES	C7-C8-S-O1S
2	A	201	MES	N4-C7-C8-S
2	D	201	MES	N4-C7-C8-S
2	A	201	MES	C8-C7-N4-C3
2	A	201	MES	C8-C7-N4-C5
2	B	201	MES	C8-C7-N4-C3
2	C	201	MES	C8-C7-N4-C3
2	C	201	MES	C8-C7-N4-C5
2	A	201	MES	C7-C8-S-O3S
2	B	201	MES	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	MES	2	0
2	A	201	MES	2	0
2	C	201	MES	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	114/142 (80%)	0.12	3 (2%) 57 38	20, 52, 74, 89	0
1	B	114/142 (80%)	0.13	2 (1%) 67 49	21, 52, 79, 88	0
1	C	114/142 (80%)	0.06	2 (1%) 67 49	19, 52, 77, 94	0
1	D	114/142 (80%)	0.15	2 (1%) 67 49	21, 54, 90, 104	0
All	All	456/568 (80%)	0.11	9 (1%) 64 45	19, 52, 80, 104	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	HIS	2.7
1	A	61	HIS	2.6
1	A	2	GLU	2.5
1	B	87	LEU	2.5
1	D	59	PHE	2.5
1	C	63	ILE	2.3
1	B	88	ASP	2.3
1	A	87	LEU	2.3
1	C	88	ASP	2.2

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MES	D	201	12/12	0.91	0.13	58,60,69,69	0
2	MES	C	201	12/12	0.92	0.12	33,37,48,48	0
2	MES	B	201	12/12	0.93	0.11	28,31,34,34	0
2	MES	A	201	12/12	0.95	0.08	24,29,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.