



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:15 AM GMT

PDB ID : 4IBX
Title : Crystal structure of stabilized TEM-1 beta-lactamase variant v.13
Authors : Dellus-Gur, E.; Toth-Petroczy, A.; Elias, M.; Tawfik, D.S.
Deposited on : 2012-12-09
Resolution : 2.68 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>

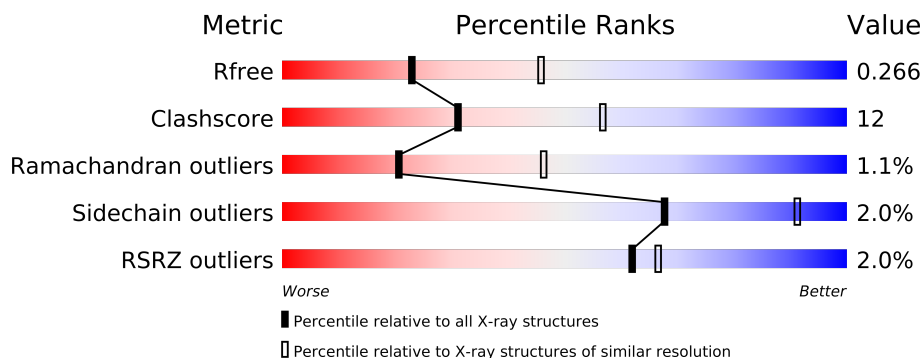
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.68 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	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)

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	263	
1	B	263	
1	C	263	
1	D	263	
1	E	263	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MES	A	302	-	X
3	MES	B	301	-	X
3	MES	D	301	-	X
4	SO4	C	302	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10281 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 Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	2	0
			2028	1267	358	392	11			
1	B	263	Total	C	N	O	S	0	2	0
			2030	1270	356	393	11			
1	C	263	Total	C	N	O	S	0	3	0
			2033	1271	358	393	11			
1	D	263	Total	C	N	O	S	0	2	0
			2028	1267	359	391	11			
1	E	263	Total	C	N	O	S	0	1	0
			2023	1263	359	390	11			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	ALA	ENGINEERED MUTATION	UNP P62593
A	52	ALA	ASN	ENGINEERED MUTATION	UNP P62593
A	120	GLY	ARG	ENGINEERED MUTATION	UNP P62593
A	182	THR	MET	ENGINEERED MUTATION	UNP P62593
A	184	VAL	ALA	CONFLICT	UNP P62593
A	201	ALA	LEU	ENGINEERED MUTATION	UNP P62593
A	265	MET	THR	ENGINEERED MUTATION	UNP P62593
B	42	GLY	ALA	ENGINEERED MUTATION	UNP P62593
B	52	ALA	ASN	ENGINEERED MUTATION	UNP P62593
B	120	GLY	ARG	ENGINEERED MUTATION	UNP P62593
B	182	THR	MET	ENGINEERED MUTATION	UNP P62593
B	184	VAL	ALA	CONFLICT	UNP P62593
B	201	ALA	LEU	ENGINEERED MUTATION	UNP P62593
B	265	MET	THR	ENGINEERED MUTATION	UNP P62593
C	42	GLY	ALA	ENGINEERED MUTATION	UNP P62593
C	52	ALA	ASN	ENGINEERED MUTATION	UNP P62593
C	120	GLY	ARG	ENGINEERED MUTATION	UNP P62593
C	182	THR	MET	ENGINEERED MUTATION	UNP P62593
C	184	VAL	ALA	CONFLICT	UNP P62593

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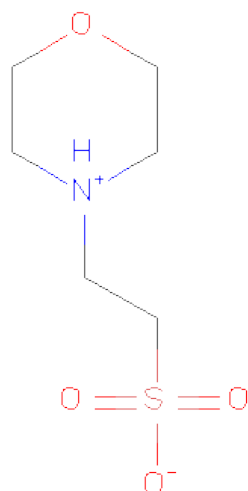
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Chain	Residue	Modelled	Actual	Comment	Reference
C	201	ALA	LEU	ENGINEERED MUTATION	UNP P62593
C	265	MET	THR	ENGINEERED MUTATION	UNP P62593
D	42	GLY	ALA	ENGINEERED MUTATION	UNP P62593
D	52	ALA	ASN	ENGINEERED MUTATION	UNP P62593
D	120	GLY	ARG	ENGINEERED MUTATION	UNP P62593
D	182	THR	MET	ENGINEERED MUTATION	UNP P62593
D	184	VAL	ALA	CONFLICT	UNP P62593
D	201	ALA	LEU	ENGINEERED MUTATION	UNP P62593
D	265	MET	THR	ENGINEERED MUTATION	UNP P62593
E	42	GLY	ALA	ENGINEERED MUTATION	UNP P62593
E	52	ALA	ASN	ENGINEERED MUTATION	UNP P62593
E	120	GLY	ARG	ENGINEERED MUTATION	UNP P62593
E	182	THR	MET	ENGINEERED MUTATION	UNP P62593
E	184	VAL	ALA	CONFLICT	UNP P62593
E	201	ALA	LEU	ENGINEERED MUTATION	UNP P62593
E	265	MET	THR	ENGINEERED MUTATION	UNP P62593

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

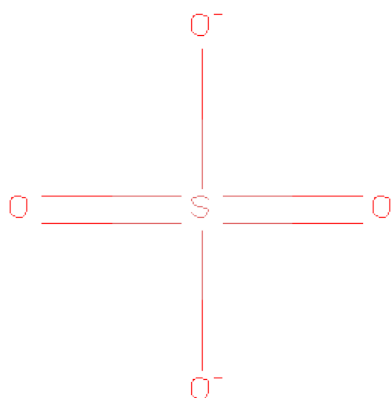
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

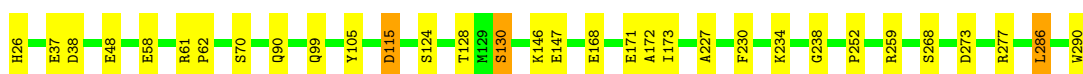
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total	O	0	0
			34	34		
5	B	30	Total	O	0	0
			30	30		
5	C	11	Total	O	0	0
			11	11		
5	D	10	Total	O	0	0
			10	10		
5	E	11	Total	O	0	0
			11	11		

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: Beta-lactamase TEM

Chain A: 



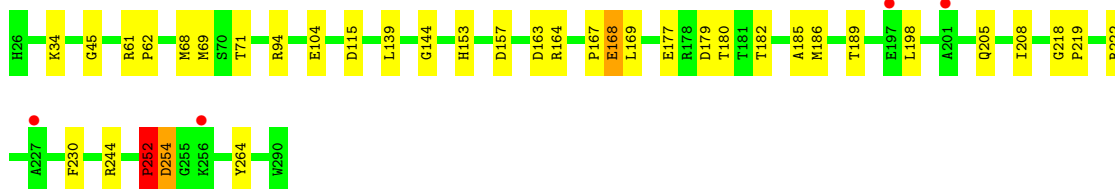
• Molecule 1: Beta-lactamase TEM

Chain B: 



• Molecule 1: Beta-lactamase TEM

Chain C: 



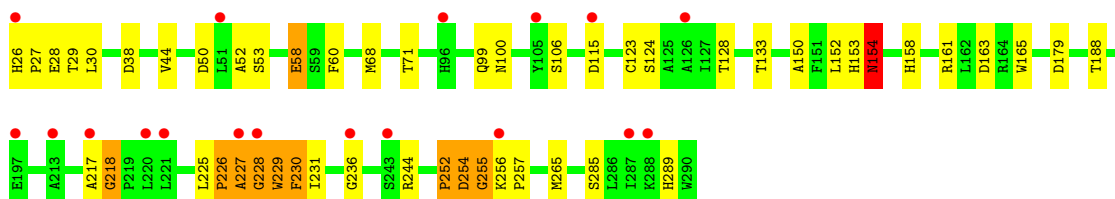
• Molecule 1: Beta-lactamase TEM

Chain D: 



• Molecule 1: Beta-lactamase TEM

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	39.90Å 239.00Å 159.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.68 45.80 – 2.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.68-2.68) 98.4 (45.80-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.265 0.232 , 0.266	Depositor DCC
R_{free} test set	2187 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 13.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	2 of 43736 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10281	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2090e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: CA, SO4, 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	0.32	1/2069 (0.0%)	0.49	2/2801 (0.1%)
1	B	0.33	1/2071 (0.0%)	0.47	1/2804 (0.0%)
1	C	0.31	1/2076 (0.0%)	0.41	0/2809
1	D	0.34	1/2069 (0.0%)	0.47	2/2801 (0.1%)
1	E	0.29	1/2060 (0.0%)	0.47	1/2788 (0.0%)
All	All	0.32	5/10345 (0.0%)	0.46	6/14003 (0.0%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	252	PRO	C-N	9.84	1.56	1.34
1	B	252	PRO	C-N	8.52	1.53	1.34
1	C	252	PRO	C-N	8.01	1.52	1.34
1	A	252	PRO	C-N	7.16	1.50	1.34
1	E	252	PRO	C-N	6.15	1.48	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	252	PRO	C-N-CA	-7.55	102.82	121.70
1	D	238	GLY	O-C-N	6.74	133.49	122.70
1	A	238	GLY	O-C-N	6.02	132.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLY	C-N-CA	-5.61	107.67	121.70
1	D	238	GLY	CA-C-N	-5.40	105.32	117.20
1	B	238	GLY	C-N-CA	-5.30	108.46	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	252	PRO	Mainchain

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	2028	0	0	18	0
1	B	2030	0	0	21	0
1	C	2033	0	0	24	1
1	D	2028	0	0	15	0
1	E	2023	0	0	43	2
2	A	1	0	0	2	0
2	C	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
3	D	12	0	12	0	0
4	C	5	0	0	1	0
5	A	34	0	0	5	0
5	B	30	0	0	1	0
5	C	11	0	0	1	0
5	D	10	0	0	3	0
5	E	11	0	0	0	0
All	All	10281	0	36	120	2

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 12.

All (120) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:26:HIS:CE1	1:E:289:HIS:ND1	1.72	1.54
1:E:230:PHE:CD1	1:E:257:PRO:CD	2.13	1.30
1:E:230:PHE:CE1	1:E:257:PRO:CD	2.16	1.29
1:E:26:HIS:ND1	1:E:289:HIS:CG	2.02	1.26
1:E:26:HIS:ND1	1:E:289:HIS:CB	2.18	1.07
1:E:29:THR:OG1	1:E:285:SER:O	1.70	1.06
1:E:244:ARG:CB	1:E:265:MET:CE	2.36	1.04
1:E:153:HIS:O	1:E:154:ASN:CB	2.09	1.01
1:E:26:HIS:CE1	1:E:289:HIS:CE1	2.51	0.99
1:E:26:HIS:ND1	1:E:289:HIS:ND1	2.05	0.97
1:E:26:HIS:CE1	1:E:289:HIS:CG	2.53	0.88
1:E:230:PHE:CD1	1:E:257:PRO:N	2.44	0.86
1:E:252:PRO:O	1:E:254:ASP:CB	2.27	0.82
1:E:30:LEU:CD2	1:E:58:GLU:OE1	2.27	0.82
1:E:99:GLN:NE2	1:E:100:ASN:OD1	2.12	0.82
1:E:254:ASP:O	1:E:256:LYS:N	2.13	0.81
1:D:70:SER:OG	5:D:409:HOH:O	2.02	0.77
1:A:38:ASP:OD1	5:A:425:HOH:O	2.01	0.77
1:B:244:ARG:NH1	3:B:301:MES:O3S	2.19	0.75
1:E:29:THR:OG1	1:E:285:SER:OG	2.06	0.74
1:D:89:GLU:OE2	5:D:407:HOH:O	2.05	0.73
1:D:37:GLU:OE2	1:D:61:ARG:NH2	2.20	0.73
1:C:244:ARG:NH1	4:C:302:SO4:O2	2.22	0.72
1:B:103:VAL:CB	1:B:104[B]:GLU:OE1	2.38	0.72
1:E:150:ALA:O	1:E:153:HIS:O	2.08	0.70
1:A:99:GLN:OE1	1:A:99:GLN:N	2.24	0.70
1:B:103:VAL:C	1:B:104[B]:GLU:OE1	2.31	0.69
1:B:272:MET:O	1:B:273:ASP:CB	2.42	0.67
1:A:70:SER:OG	5:A:433:HOH:O	2.13	0.65
1:C:68:MET:O	1:C:71:THR:OG1	2.15	0.65
1:B:271:THR:OG1	1:B:274:GLU:CG	2.45	0.65
1:C:177:GLU:O	1:C:180:THR:OG1	2.15	0.65
1:C:68:MET:CE	1:C:186:MET:CE	2.75	0.64
1:E:225:LEU:O	1:E:226:PRO:O	2.15	0.64
1:C:252:PRO:O	1:C:254:ASP:CB	2.46	0.64
1:B:230:PHE:CD1	1:B:230:PHE:C	2.71	0.64
1:A:130:SER:OG	1:A:234:LYS:NZ	2.31	0.64
1:E:230:PHE:CE1	1:E:257:PRO:CG	2.81	0.62
1:B:103:VAL:CA	1:B:104[B]:GLU:OE1	2.47	0.62
1:B:272:MET:O	1:B:273:ASP:OD2	2.16	0.62
2:A:301:CA:CA	1:B:37:GLU:OE1	1.77	0.62
1:E:228:GLY:O	1:E:229:TRP:CB	2.47	0.62
1:C:164:ARG:NE	1:C:179:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:61:ARG:N	1:D:62:PRO:CD	2.63	0.60
1:A:37:GLU:OE1	2:A:301:CA:CA	1.79	0.60
1:E:29:THR:OG1	1:E:285:SER:C	2.40	0.60
1:D:68:MET:O	1:D:71:THR:OG1	2.19	0.60
1:C:139:LEU:O	1:C:144:GLY:N	2.35	0.60
1:D:139:LEU:O	1:D:144:GLY:N	2.36	0.59
1:E:236:GLY:O	1:E:244:ARG:NH1	2.35	0.59
1:C:167:PRO:O	1:C:169:LEU:N	2.36	0.59
1:E:254:ASP:O	1:E:255:GLY:C	2.42	0.58
1:E:231:ILE:CG2	1:E:231:ILE:O	2.51	0.58
1:B:124:SER:O	1:B:128:THR:OG1	2.21	0.58
1:A:48:GLU:OE2	1:A:259:ARG:NH1	2.37	0.57
1:E:230:PHE:CD1	1:E:256:LYS:CA	2.88	0.56
1:A:115:ASP:OD2	5:A:420:HOH:O	2.18	0.56
1:B:26:HIS:N	1:B:58:GLU:CG	2.69	0.56
1:C:205:GLN:NE2	1:C:208:ILE:CD1	2.69	0.56
1:D:115:ASP:OD1	1:D:115:ASP:N	2.38	0.56
1:C:182:THR:OG1	1:C:185:ALA:CB	2.53	0.56
1:C:168:GLU:N	1:C:168:GLU:OE1	2.38	0.56
1:A:230:PHE:C	1:A:230:PHE:CD1	2.79	0.55
1:B:61:ARG:N	1:B:62:PRO:CD	2.70	0.55
1:B:170:ASN:O	1:B:240:GLU:N	2.40	0.53
1:B:83:ARG:NH1	5:B:419:HOH:O	2.42	0.53
1:A:268:SER:CB	5:A:418:HOH:O	2.56	0.53
1:E:124:SER:O	1:E:128:THR:OG1	2.27	0.53
1:E:163:ASP:N	1:E:179:ASP:OD1	2.42	0.52
1:E:153:HIS:ND1	1:E:158:HIS:CD2	2.78	0.52
1:E:44:VAL:O	1:E:60:PHE:CD2	2.64	0.51
1:E:227:ALA:O	1:E:228:GLY:O	2.28	0.51
1:E:152:LEU:O	1:E:153:HIS:C	2.47	0.51
1:A:61:ARG:N	1:A:62:PRO:CD	2.73	0.51
1:C:222:ARG:N	5:C:409:HOH:O	2.44	0.51
1:C:45:GLY:N	1:C:264:TYR:O	2.45	0.49
1:E:50:ASP:OD2	1:E:53:SER:OG	2.31	0.49
1:A:286:LEU:CD1	1:A:290:TRP:CZ3	2.97	0.48
1:D:165:TRP:N	1:D:165:TRP:CD1	2.82	0.48
1:E:165:TRP:CD1	1:E:165:TRP:N	2.81	0.47
1:E:68:MET:O	1:E:71:THR:OG1	2.32	0.47
1:D:157:ASP:OD2	1:D:189:THR:OG1	2.33	0.46
1:B:94:ARG:NH1	1:B:115:ASP:O	2.48	0.46
1:D:83:ARG:NH1	5:D:407:HOH:O	2.49	0.46
1:C:167:PRO:C	1:C:169:LEU:N	2.69	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:GLY:N	1:B:219:PRO:CD	2.79	0.45
1:E:217:ALA:O	1:E:218:GLY:C	2.54	0.45
1:E:161:ARG:NH2	1:E:163:ASP:OD2	2.50	0.45
1:E:26:HIS:CD2	1:E:27:PRO:CD	2.99	0.45
1:D:168:GLU:OE1	1:D:168:GLU:N	2.50	0.45
1:C:218:GLY:N	1:C:219:PRO:CD	2.80	0.45
1:E:230:PHE:CD1	1:E:256:LYS:C	2.89	0.45
1:E:30:LEU:CB	1:E:58:GLU:OE1	2.64	0.45
1:B:65:ARG:NH2	1:B:159:VAL:O	2.49	0.45
1:A:146:LYS:NZ	1:A:147:GLU:OE2	2.50	0.45
1:B:105[B]:TYR:CE1	3:B:301:MES:H51	2.53	0.44
1:E:30:LEU:O	1:E:30:LEU:CD1	2.66	0.43
1:C:94:ARG:NH1	1:C:115:ASP:O	2.51	0.43
1:C:61:ARG:N	1:C:62:PRO:CD	2.81	0.43
1:C:230:PHE:C	1:C:230:PHE:CD1	2.91	0.43
1:E:106:SER:OG	1:E:133:THR:OG1	2.37	0.42
1:E:153:HIS:CE1	1:E:158:HIS:CD2	3.07	0.42
1:C:167:PRO:O	1:C:168:GLU:C	2.57	0.42
1:D:217:ALA:O	1:D:218:GLY:C	2.58	0.41
1:A:26:HIS:N	1:A:58:GLU:CG	2.84	0.41
1:A:172:ALA:N	5:A:429:HOH:O	2.52	0.41
1:C:198:LEU:CD2	1:C:198:LEU:N	2.84	0.41
1:A:227:ALA:O	1:D:83:ARG:NH2	2.54	0.41
1:C:163:ASP:N	1:C:179:ASP:OD1	2.53	0.41
1:A:273:ASP:O	1:A:277:ARG:N	2.54	0.41
1:B:97:TYR:CD1	1:B:97:TYR:N	2.89	0.41
1:B:65:ARG:NH1	1:B:180:THR:OG1	2.54	0.41
1:C:157:ASP:OD2	1:C:189:THR:OG1	2.39	0.41
1:A:124:SER:O	1:A:128:THR:OG1	2.40	0.40
1:A:171:GLU:OE2	1:A:173:ILE:CD1	2.70	0.40
1:D:164:ARG:NE	1:D:179:ASP:OD2	2.55	0.40

All (2) 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	Distance(Å)	Clash(Å)
1:C:34[A]:LYS:CE	1:E:38:ASP:OD2[1_455]	1.96	0.24
1:E:99:GLN:OE1	1:E:158:HIS:NE2[1_455]	2.05	0.15

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	263/263 (100%)	252 (96%)	10 (4%)	1 (0%)	43	75
1	B	263/263 (100%)	247 (94%)	15 (6%)	1 (0%)	43	75
1	C	264/263 (100%)	251 (95%)	11 (4%)	2 (1%)	27	56
1	D	263/263 (100%)	249 (95%)	13 (5%)	1 (0%)	43	75
1	E	262/263 (100%)	235 (90%)	17 (6%)	10 (4%)	5	10
All	All	1315/1315 (100%)	1234 (94%)	66 (5%)	15 (1%)	21	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	226	PRO
1	E	227	ALA
1	E	255	GLY
1	C	168	GLU
1	C	254	ASP
1	E	154	ASN
1	E	218	GLY
1	E	228	GLY
1	E	229	TRP
1	D	105	TYR
1	E	58	GLU
1	E	254	ASP
1	A	105	TYR
1	E	52	ALA
1	B	103	VAL

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	217/215 (101%)	211 (97%)	6 (3%)	56	85
1	B	217/215 (101%)	210 (97%)	7 (3%)	51	81
1	C	218/215 (101%)	216 (99%)	2 (1%)	87	97
1	D	217/215 (101%)	215 (99%)	2 (1%)	87	97
1	E	216/215 (100%)	210 (97%)	6 (3%)	56	85
All	All	1085/1075 (101%)	1062 (98%)	23 (2%)	68	90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	115	ASP
1	A	130	SER
1	A	168[A]	GLU
1	A	168[B]	GLU
1	A	286	LEU
1	B	90	GLN
1	B	99	GLN
1	B	114	THR
1	B	123	CYS
1	B	230	PHE
1	B	256	LYS
1	B	273	ASP
1	C	69	MET
1	C	153	HIS
1	D	115	ASP
1	D	154	ASN
1	E	28	GLU
1	E	115	ASP
1	E	123	CYS
1	E	154	ASN
1	E	188	THR
1	E	230	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	MES	A	302	-	12,12,12	2.15	1 (8%)	16,16,16	2.65	6 (37%)
3	MES	B	301	-	12,12,12	2.14	1 (8%)	16,16,16	2.60	6 (37%)
4	SO4	C	302	-	4,4,4	0.28	0	6,6,6	0.07	0
3	MES	D	301	-	12,12,12	2.15	1 (8%)	16,16,16	2.64	6 (37%)

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
3	MES	A	302	-	-	0/6/14/14	1/1/1/1
3	MES	B	301	-	-	0/6/14/14	0/1/1/1
4	SO4	C	302	-	-	0/0/0/0	0/0/0/0
3	MES	D	301	-	-	0/6/14/14	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	MES	C8-S	-6.53	1.66	1.78
3	A	302	MES	C8-S	-6.51	1.66	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	MES	C8-S	-6.48	1.66	1.78

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	MES	C5-N4-C3	5.22	120.11	109.75
3	A	302	MES	C5-N4-C3	5.18	120.01	109.75
3	D	301	MES	C5-N4-C3	4.73	119.13	109.75
3	D	301	MES	C2-C3-N4	-4.73	103.90	109.96
3	A	302	MES	C8-C7-N4	-4.34	105.01	112.44
3	A	302	MES	C6-C5-N4	-4.14	104.65	109.96
3	B	301	MES	C8-C7-N4	-4.13	105.37	112.44
3	D	301	MES	C8-C7-N4	-4.08	105.46	112.44
3	B	301	MES	C2-C3-N4	-3.92	104.94	109.96
3	D	301	MES	C6-C5-N4	-3.71	105.20	109.96
3	A	302	MES	C2-C3-N4	-3.68	105.25	109.96
3	B	301	MES	C6-C5-N4	-3.53	105.44	109.96
3	D	301	MES	C7-N4-C5	3.42	120.60	111.66
3	D	301	MES	C7-N4-C3	3.29	120.27	111.66
3	A	302	MES	C7-N4-C5	3.21	120.05	111.66
3	B	301	MES	C7-N4-C5	3.19	120.00	111.66
3	A	302	MES	C7-N4-C3	3.17	119.94	111.66
3	B	301	MES	C7-N4-C3	3.15	119.89	111.66

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	MES	C2-C3-C5-C6-N4-O1
3	A	302	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

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	263/263 (100%)	-0.32	0 100 100	10, 20, 36, 44	0
1	B	263/263 (100%)	-0.30	0 100 100	9, 19, 31, 40	0
1	C	263/263 (100%)	0.01	4 (1%) 70 74	19, 35, 55, 68	0
1	D	263/263 (100%)	0.11	4 (1%) 70 74	21, 38, 62, 73	0
1	E	263/263 (100%)	0.65	18 (6%) 17 18	33, 49, 74, 88	0
All	All	1315/1315 (100%)	0.03	26 (1%) 62 66	9, 30, 63, 88	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	105	TYR	4.5
1	E	26	HIS	4.1
1	E	96	HIS	3.4
1	E	287	ILE	3.4
1	E	213	ALA	3.3
1	C	197	GLU	3.2
1	E	51	LEU	3.2
1	D	34	LYS	3.1
1	E	256	LYS	3.0
1	D	198	LEU	2.9
1	E	115	ASP	2.9
1	E	221	LEU	2.6
1	C	227	ALA	2.6
1	C	201	ALA	2.5
1	D	281	GLU	2.5
1	E	228	GLY	2.3
1	C	256	LYS	2.3
1	E	288	LYS	2.3
1	E	227	ALA	2.3
1	E	220	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	236	GLY	2.2
1	D	60	PHE	2.2
1	E	243	SER	2.1
1	E	126	ALA	2.0
1	E	197	GLU	2.0
1	E	217	ALA	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
3	MES	D	301	12/12	0.29	4.07	56,63,66,66	12
4	SO4	C	302	5/5	0.22	3.25	55,55,56,56	5
3	MES	A	302	12/12	0.24	3.09	52,59,60,61	12
3	MES	B	301	12/12	0.27	2.24	51,60,66,66	0
2	CA	C	301	1/1	0.08	-2.85	66,66,66,66	0
2	CA	A	301	1/1	0.07	-3.85	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.