wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2023 – 09:27 PM EDT

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 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 (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:

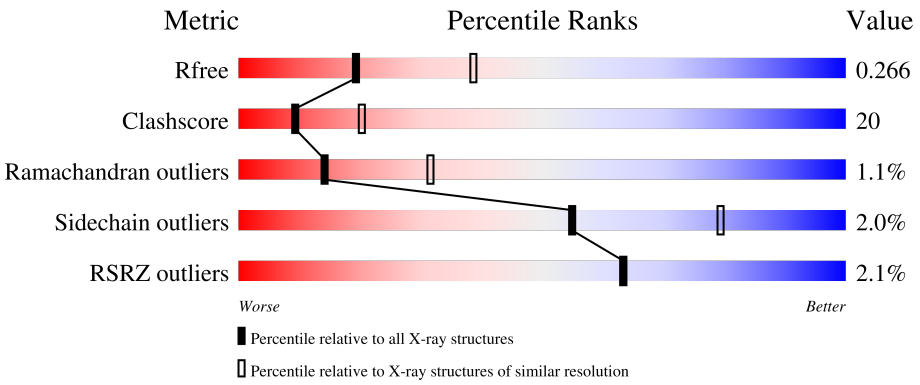
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.68 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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 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	263	73% 25% •
1	B	263	70% 29% •
1	C	263	2% 60% 38% •
1	D	263	% 68% 31%
1	E	263	8% 56% 39% •

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	CA	A	301	-	-	X	-

2 Entry composition (i)

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

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

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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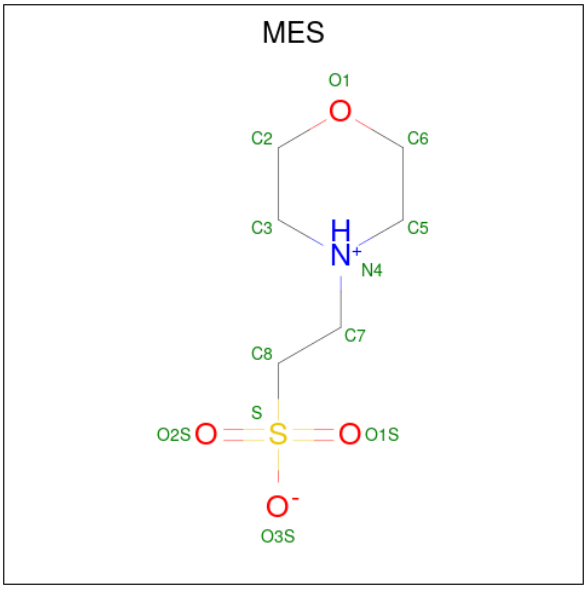
Chain	Residue	Modelled	Actual	Comment	Reference
C	201	ALA	LEU	engineered mutation	UNP P62593
C	265	MET	THR	engineered mutation	UNP P62593
D	42	GLY	ALA	engineered mutation	UNP P62593
D	52	ALA	ASN	engineered mutation	UNP P62593
D	120	GLY	ARG	engineered mutation	UNP P62593
D	182	THR	MET	engineered mutation	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).

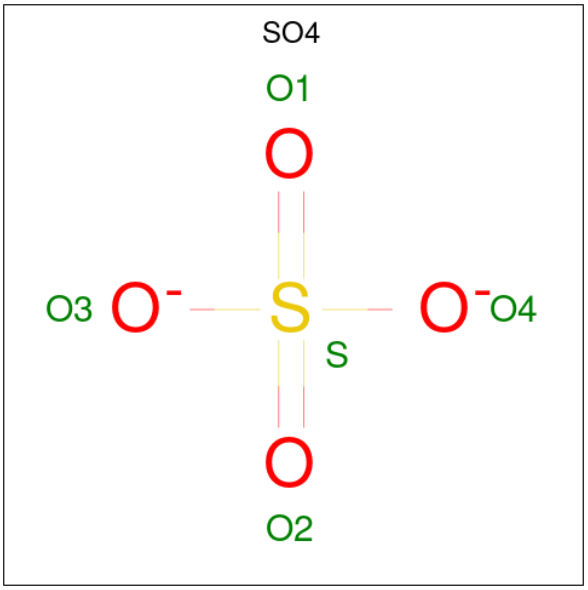
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

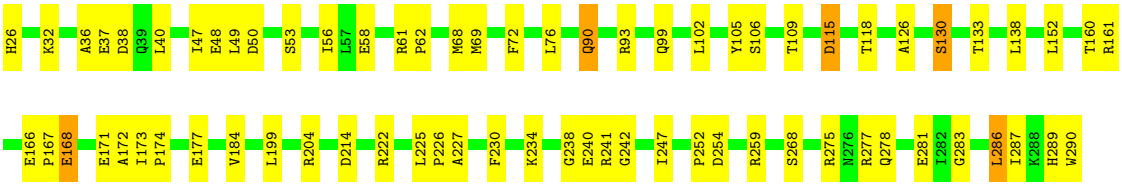
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	34	34	34	0	0
5	B	30	30	30	0	0
5	C	11	11	11	0	0
5	D	10	10	10	0	0
5	E	11	11	11	0	0

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.

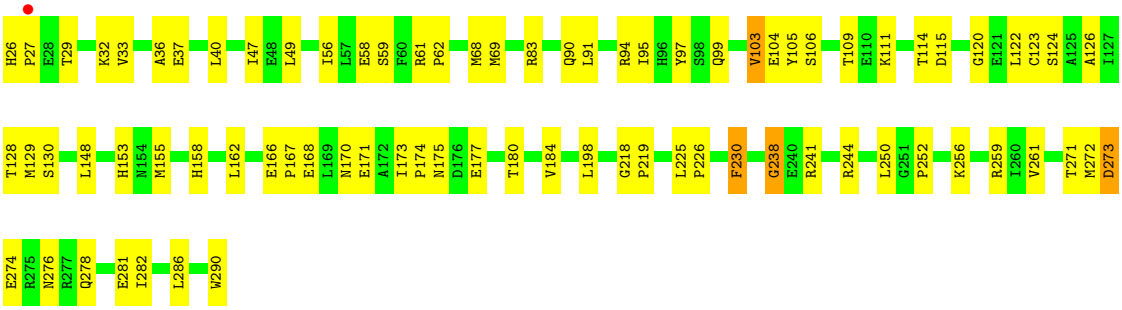
• Molecule 1: Beta-lactamase TEM

Chain A: 73% 25%



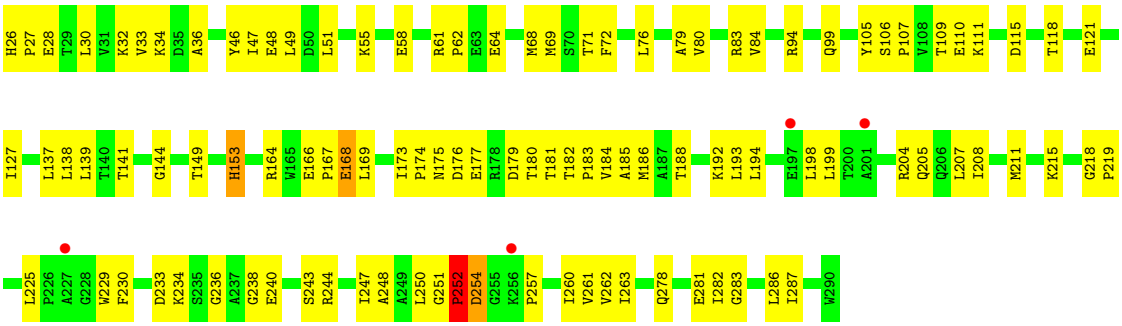
• Molecule 1: Beta-lactamase TEM

Chain B: 70% 29%



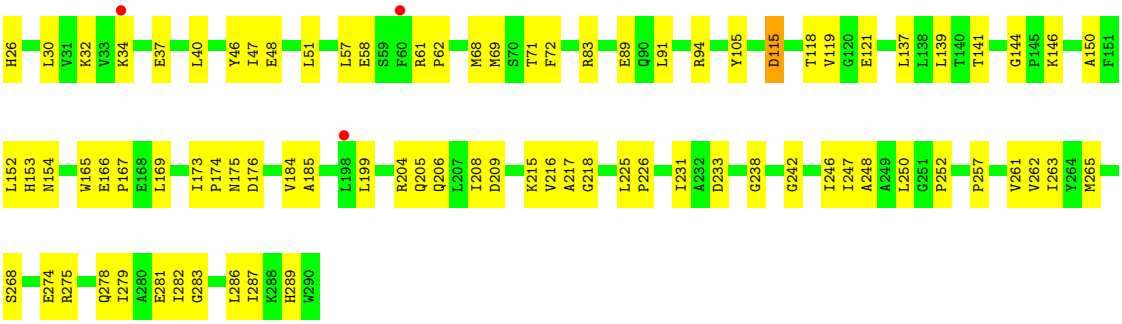
• Molecule 1: Beta-lactamase TEM

Chain C: 2% 60% 38%



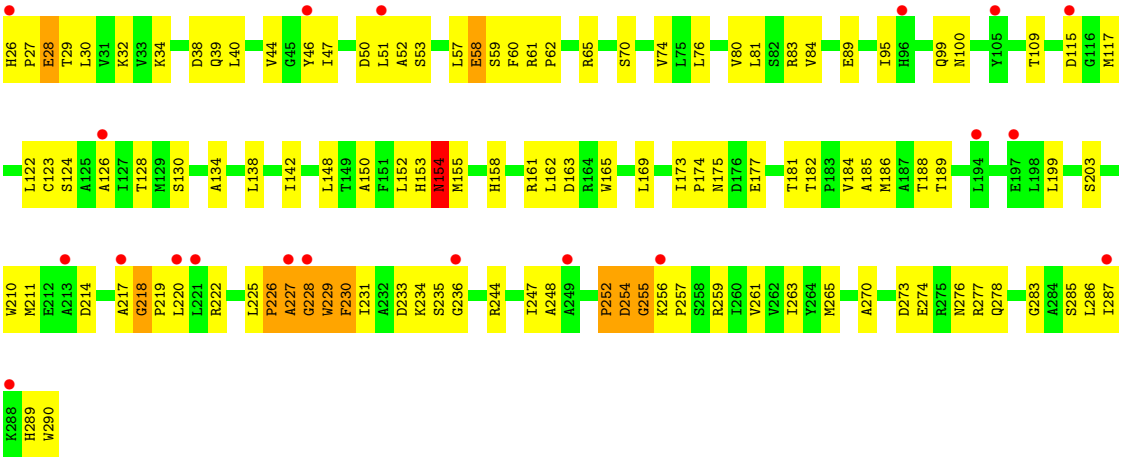
• Molecule 1: Beta-lactamase TEM

Chain D:



- Molecule 1: Beta-lactamase TEM

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
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 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[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: SO4, MES, CA

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

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	252	PRO	Mainchain

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	2028	0	2032	55	0
1	B	2030	0	2034	63	0
1	C	2033	0	2046	94	1
1	D	2028	0	2034	64	0
1	E	2023	0	2032	130	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	2	0
4	C	5	0	0	1	0
5	A	34	0	0	4	0
5	B	30	0	0	1	0
5	C	11	0	0	4	0
5	D	10	0	0	3	0
5	E	11	0	0	0	0
All	All	10281	0	10214	404	2

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 20.

The worst 5 of 404 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:E:230:PHE:CE1	1:E:257:PRO:HD3	1.23	1.74
1:E:230:PHE:CD1	1:E:257:PRO:HD3	1.37	1.54
1:E:26:HIS:CE1	1:E:289:HIS:ND1	1.72	1.54
1:E:244:ARG:HB3	1:E:265:MET:CE	1.54	1.34
1:E:230:PHE:CD1	1:E:257:PRO:CD	2.13	1.30

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	Interatomic distance (Å)	Clash overlap (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 (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	263/263 (100%)	252 (96%)	10 (4%)	1 (0%)	34	58
1	B	263/263 (100%)	247 (94%)	15 (6%)	1 (0%)	34	58
1	C	264/263 (100%)	251 (95%)	11 (4%)	2 (1%)	19	40
1	D	263/263 (100%)	249 (95%)	13 (5%)	1 (0%)	34	58
1	E	262/263 (100%)	235 (90%)	17 (6%)	10 (4%)	3	6
All	All	1315/1315 (100%)	1234 (94%)	66 (5%)	15 (1%)	14	31

5 of 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

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Mol	Chain	Res	Type
1	C	254	ASP

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	217/215 (101%)	211 (97%)	6 (3%)	43	70
1	B	217/215 (101%)	210 (97%)	7 (3%)	39	65
1	C	218/215 (101%)	216 (99%)	2 (1%)	78	91
1	D	217/215 (101%)	215 (99%)	2 (1%)	78	91
1	E	216/215 (100%)	210 (97%)	6 (3%)	43	70
All	All	1085/1075 (101%)	1062 (98%)	23 (2%)	55	78

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	153	HIS
1	E	28	GLU
1	D	154	ASN
1	E	115	ASP
1	B	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	39	GLN
1	E	112	HIS
1	E	278	GLN
1	E	158	HIS
1	B	206	GLN

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)

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	B	301	-	12,12,12	2.26	1 (8%)	14,16,16	2.55	8 (57%)
4	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.07	0
3	MES	A	302	-	12,12,12	2.27	1 (8%)	14,16,16	2.56	8 (57%)
3	MES	D	301	-	12,12,12	2.28	1 (8%)	14,16,16	2.58	8 (57%)

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	B	301	-	-	5/6/14/14	0/1/1/1
3	MES	A	302	-	-	4/6/14/14	0/1/1/1
3	MES	D	301	-	-	5/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	MES	C8-S	-7.62	1.66	1.77
3	A	302	MES	C8-S	-7.60	1.66	1.77
3	B	301	MES	C8-S	-7.57	1.66	1.77

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	301	MES	C5-N4-C3	5.01	120.11	108.83
3	A	302	MES	C5-N4-C3	4.97	120.01	108.83
3	D	301	MES	C5-N4-C3	4.58	119.13	108.83
3	D	301	MES	C2-C3-N4	-4.09	103.90	110.10
3	D	301	MES	C7-N4-C5	3.66	120.60	111.23

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	MES	C8-C7-N4-C3
3	A	302	MES	N4-C7-C8-S
3	B	301	MES	N4-C7-C8-S
3	D	301	MES	C8-C7-N4-C5
3	D	301	MES	N4-C7-C8-S

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	MES	2	0
4	C	302	SO4	1	0
3	D	301	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, 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%)	-0.34	0	100	100	10, 20, 36, 44	0
1	B	263/263 (100%)	-0.31	1 (0%)	92	93	9, 19, 31, 40	0
1	C	263/263 (100%)	-0.02	4 (1%)	73	74	19, 35, 55, 68	0
1	D	263/263 (100%)	0.08	3 (1%)	80	81	21, 38, 62, 73	0
1	E	263/263 (100%)	0.64	20 (7%)	13	11	33, 49, 74, 88	0
All	All	1315/1315 (100%)	0.01	28 (2%)	63	63	9, 30, 63, 88	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	105	TYR	4.7
1	E	287	ILE	3.7
1	E	51	LEU	3.6
1	E	213	ALA	3.6
1	D	198	LEU	3.3

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
4	SO4	C	302	5/5	0.87	0.24	55,55,56,56	5
2	CA	C	301	1/1	0.88	0.07	66,66,66,66	0
3	MES	B	301	12/12	0.90	0.26	51,60,66,66	0
3	MES	A	302	12/12	0.90	0.24	52,59,60,61	12
3	MES	D	301	12/12	0.91	0.29	56,63,66,66	12
2	CA	A	301	1/1	0.91	0.09	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.