Full wwPDB X-ray Structure Validation Report (i)

Jul 4, 2022 – 04:34 pm BST

PDB ID	:	7QOR
Title	:	Structure of beta-lactamase TEM-171
Authors	:	Hakanpaa, J.; Petrova, T.; Samygina, V.R.; Chojnowski, G.; Lamzin, V.; Egorov, A.M.
Deposited on	:	2021-12-28
Resolution	:	2.00 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:

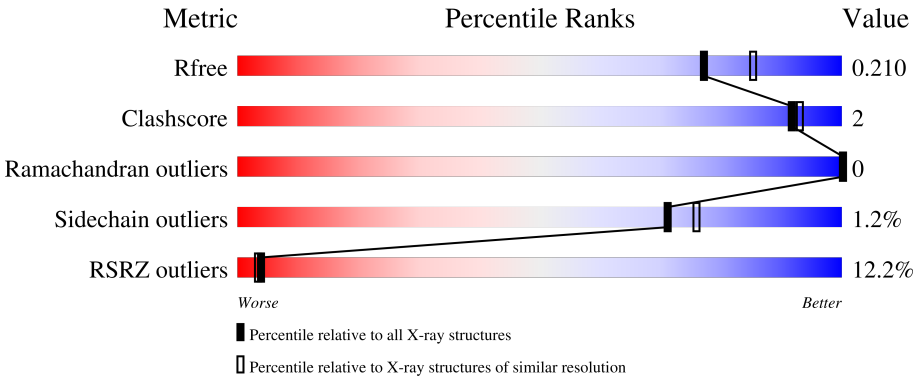
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	AAA	263	4% 95% 5%
1	BBB	263	17% 97% .
1	CCC	263	3% 95% 5%
1	DDD	263	3% 95% 5%
1	EEE	263	3% 96% .

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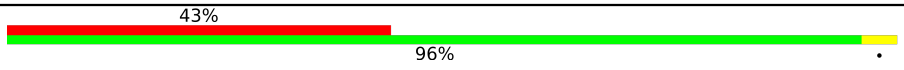
Mol	Chain	Length	Quality of chain
1	FFF	263	

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
4	ACT	DDD	401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13109 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.

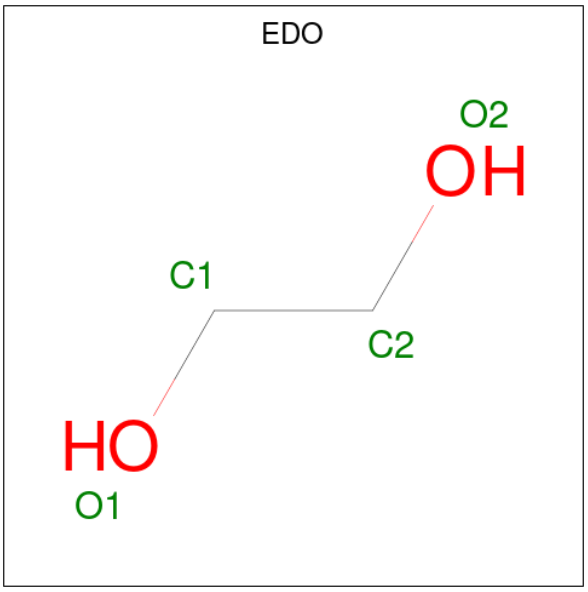
- Molecule 1 is a protein called Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	263	Total	C	N	O	S	0	1	0
			2034	1270	360	393	11			
1	BBB	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	CCC	263	Total	C	N	O	S	0	2	0
			2039	1275	362	391	11			
1	DDD	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	EEE	263	Total	C	N	O	S	0	2	0
			2045	1276	365	393	11			
1	FFF	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			

There are 6 discrepancies between the modelled and reference sequences:

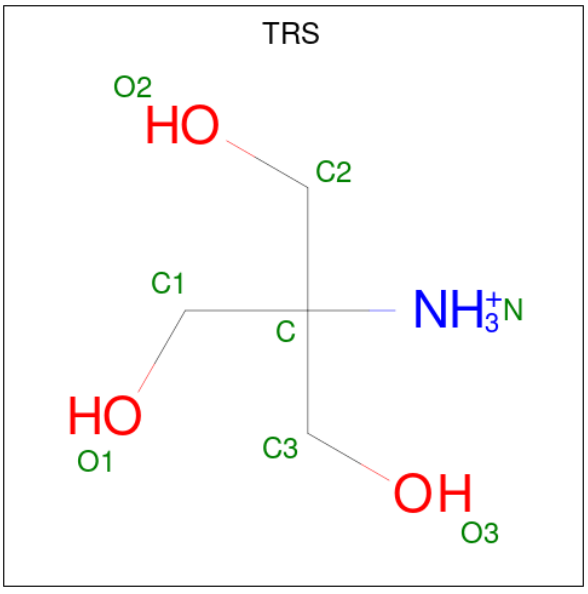
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	84	ILE	VAL	engineered mutation	UNP P62593
BBB	84	ILE	VAL	engineered mutation	UNP P62593
CCC	84	ILE	VAL	engineered mutation	UNP P62593
DDD	84	ILE	VAL	engineered mutation	UNP P62593
EEE	84	ILE	VAL	engineered mutation	UNP P62593
FFF	84	ILE	VAL	engineered mutation	UNP P62593

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



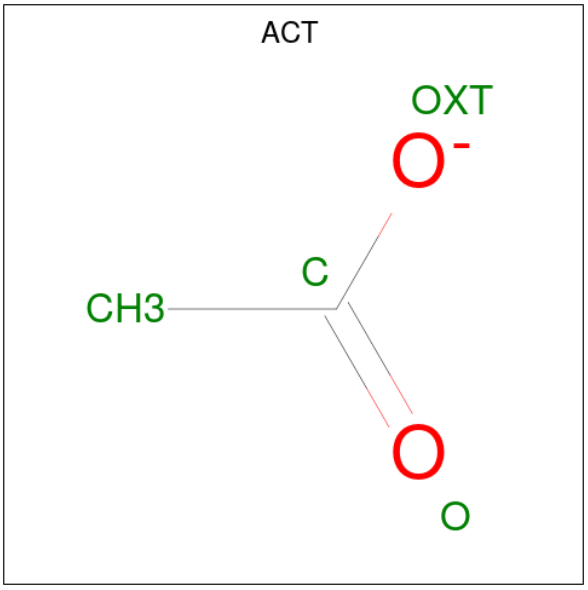
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

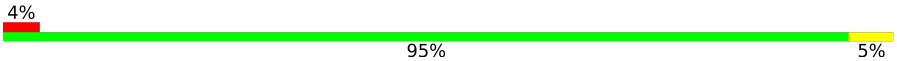
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	238	Total O 238 238	0	0
5	BBB	47	Total O 47 47	0	0
5	CCC	231	Total O 231 231	0	0
5	DDD	155	Total O 155 155	0	0
5	EEE	187	Total O 187 187	0	0
5	FFF	17	Total O 17 17	0	0

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.

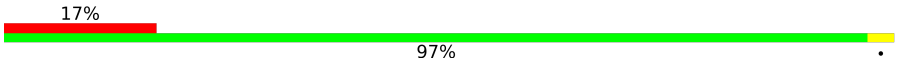
• Molecule 1: Beta-lactamase TEM

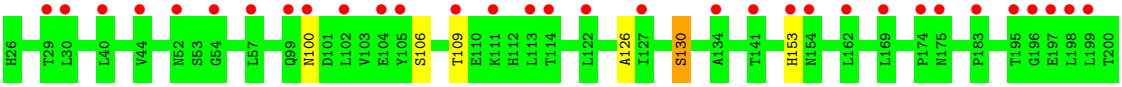
Chain AAA:

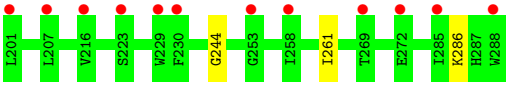


• Molecule 1: Beta-lactamase TEM

Chain BBB:

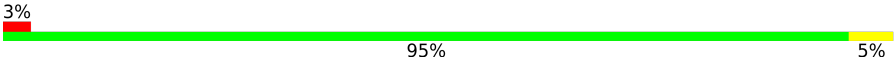


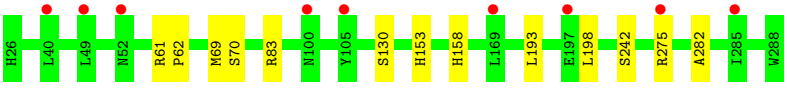




• Molecule 1: Beta-lactamase TEM

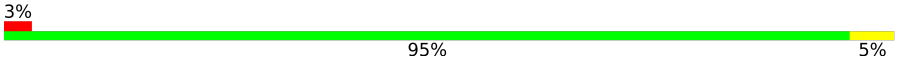
Chain CCC:

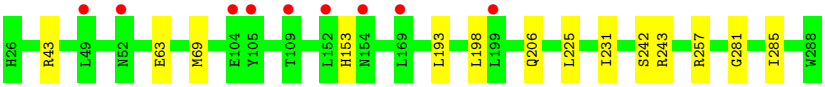




• Molecule 1: Beta-lactamase TEM

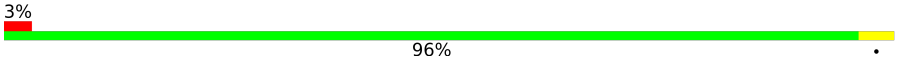
Chain DDD:

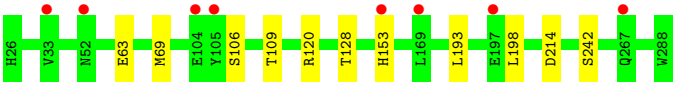




• Molecule 1: Beta-lactamase TEM

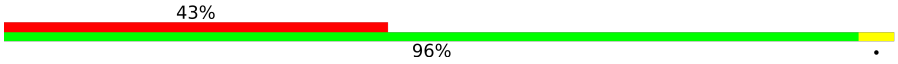
Chain EEE:

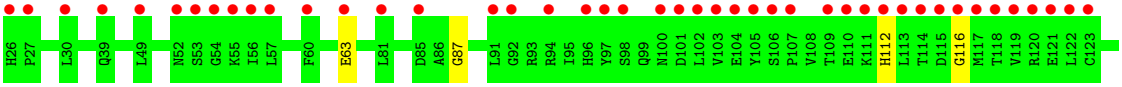


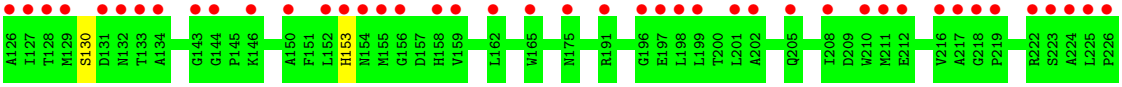


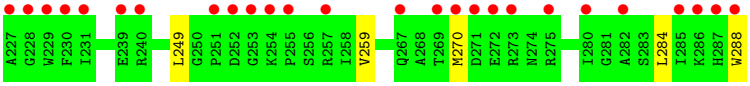
• Molecule 1: Beta-lactamase TEM

Chain FFF:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.19Å 88.19Å 499.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 14.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.00) 98.1 (14.95-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.190 , 0.211 0.201 , 0.210	Depositor DCC
R_{free} test set	6653 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, TRS, EDO

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	AAA	0.72	0/2071	0.87	1/2803 (0.0%)
1	BBB	0.68	0/2062	0.81	0/2791
1	CCC	0.76	0/2080	0.87	2/2816 (0.1%)
1	DDD	0.74	0/2062	0.86	2/2791 (0.1%)
1	EEE	0.71	0/2082	0.83	0/2817
1	FFF	0.70	0/2062	0.80	0/2791
All	All	0.72	0/12419	0.84	5/16809 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	83	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	AAA	257	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	DDD	257	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	CCC	83	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	DDD	243	ARG	NE-CZ-NH1	5.23	122.92	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	AAA	2034	0	2042	7	0
1	BBB	2028	0	2036	4	0
1	CCC	2039	0	2052	9	0
1	DDD	2028	0	2036	10	0
1	EEE	2045	0	2056	6	0
1	FFF	2028	0	2036	4	0
2	AAA	4	0	6	0	0
2	CCC	8	0	12	1	0
3	AAA	8	0	12	0	0
4	CCC	4	0	3	0	0
4	DDD	8	0	6	5	0
5	AAA	238	0	0	2	0
5	BBB	47	0	0	0	0
5	CCC	231	0	0	4	0
5	DDD	155	0	0	1	0
5	EEE	187	0	0	2	0
5	FFF	17	0	0	0	0
All	All	13109	0	12297	39	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 2.

All (39) 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:CCC:153[B]:HIS:CE1	5:CCC:504:HOH:O	2.03	1.11
1:AAA:196:GLY:HA3	5:AAA:538:HOH:O	1.72	0.88
1:DDD:43:ARG:HB2	4:DDD:401:ACT:H2	1.75	0.67
1:CCC:70:SER:OG	5:CCC:501:HOH:O	2.10	0.64
1:DDD:43:ARG:HD2	4:DDD:401:ACT:CH3	2.28	0.64
1:EEE:120[B]:ARG:NH2	5:EEE:305:HOH:O	2.32	0.62
1:AAA:70:SER:OG	5:AAA:501:HOH:O	2.13	0.61
1:CCC:275:ARG:NH2	5:CCC:505:HOH:O	2.33	0.61
1:DDD:43:ARG:CG	4:DDD:401:ACT:H2	2.30	0.61
1:DDD:43:ARG:CB	4:DDD:401:ACT:H2	2.33	0.59
1:CCC:153[B]:HIS:CD2	1:CCC:158:HIS:ND1	2.73	0.56
1:EEE:120[B]:ARG:HD3	5:EEE:302:HOH:O	2.04	0.56
1:DDD:43:ARG:HD2	4:DDD:401:ACT:H3	1.89	0.53
1:CCC:69:MET:SD	1:CCC:242:SER:HB3	2.49	0.52
1:FFF:249:LEU:HD11	1:FFF:288:TRP:CZ3	2.45	0.51
1:DDD:206:GLN:NE2	5:DDD:505:HOH:O	2.43	0.50
1:DDD:193:LEU:HD23	1:DDD:198:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:69:MET:SD	1:AAA:242:SER:HB3	2.54	0.48
1:CCC:153[B]:HIS:ND1	5:CCC:504:HOH:O	2.33	0.48
1:EEE:69:MET:SD	1:EEE:242:SER:HB3	2.57	0.45
1:BBB:286:LYS:HA	1:FFF:87:GLY:O	2.17	0.44
1:FFF:112:HIS:HB3	1:FFF:116:GLY:O	2.18	0.44
1:DDD:225:LEU:HD22	1:DDD:231:ILE:CG2	2.48	0.43
1:BBB:126:ALA:O	1:BBB:130:SER:HA	2.19	0.43
1:EEE:106:SER:HB3	1:EEE:109:THR:OG1	2.18	0.43
1:AAA:193:LEU:HD23	1:AAA:198:LEU:HD23	2.01	0.42
1:EEE:128:THR:HA	1:EEE:214:ASP:HA	2.01	0.42
1:CCC:61:ARG:N	1:CCC:62:PRO:CD	2.82	0.42
1:CCC:193:LEU:HD23	1:CCC:198:LEU:HD23	2.02	0.42
1:EEE:193:LEU:HD23	1:EEE:198:LEU:HD23	2.01	0.42
1:CCC:282:ALA:HB2	2:CCC:401:EDO:H21	2.01	0.42
1:DDD:69:MET:SD	1:DDD:242:SER:HB3	2.60	0.41
1:AAA:254:LYS:HB2	1:AAA:254:LYS:HE2	1.86	0.41
1:BBB:244:GLY:HA2	1:BBB:261:ILE:O	2.21	0.41
1:AAA:109:THR:OG1	1:AAA:133:THR:HB	2.21	0.41
1:BBB:106:SER:HB3	1:BBB:109:THR:OG1	2.20	0.41
1:FFF:259:VAL:HG21	1:FFF:284:LEU:HD21	2.04	0.40
1:DDD:281:GLY:O	1:DDD:285:ILE:HG12	2.21	0.40
1:AAA:113:LEU:HD23	1:AAA:113:LEU:HA	1.96	0.40

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	AAA	262/263 (100%)	257 (98%)	5 (2%)	0	100	100
1	BBB	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
1	CCC	263/263 (100%)	257 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
1	EEE	263/263 (100%)	257 (98%)	6 (2%)	0	100	100
1	FFF	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
All	All	1571/1578 (100%)	1535 (98%)	36 (2%)	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	AAA	218/217 (100%)	215 (99%)	3 (1%)	67	72
1	BBB	217/217 (100%)	214 (99%)	3 (1%)	67	72
1	CCC	219/217 (101%)	218 (100%)	1 (0%)	88	92
1	DDD	217/217 (100%)	215 (99%)	2 (1%)	78	83
1	EEE	219/217 (101%)	217 (99%)	2 (1%)	78	83
1	FFF	217/217 (100%)	213 (98%)	4 (2%)	59	63
All	All	1307/1302 (100%)	1292 (99%)	15 (1%)	71	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	63	GLU
1	AAA	153	HIS
1	AAA	254	LYS
1	BBB	100	ASN
1	BBB	130	SER
1	BBB	153	HIS
1	CCC	130	SER
1	DDD	63	GLU
1	DDD	153	HIS
1	EEE	63	GLU

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Mol	Chain	Res	Type
1	EEE	153	HIS
1	FFF	63	GLU
1	FFF	130	SER
1	FFF	153	HIS
1	FFF	270	MET

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

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)

7 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	EDO	CCC	401	-	3,3,3	0.25	0	2,2,2	0.40	0
4	ACT	CCC	403	-	3,3,3	1.04	0	3,3,3	0.76	0
2	EDO	AAA	401	-	3,3,3	0.67	0	2,2,2	0.94	0
2	EDO	CCC	402	-	3,3,3	0.43	0	2,2,2	0.48	0
3	TRS	AAA	402	-	7,7,7	0.29	0	9,9,9	0.48	0
4	ACT	DDD	401	-	3,3,3	1.06	0	3,3,3	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	DDD	402	-	3,3,3	1.09	0	3,3,3	0.70	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
3	TRS	AAA	402	-	-	0/9/9/9	-
2	EDO	CCC	401	-	-	1/1/1/1	-
2	EDO	AAA	401	-	-	1/1/1/1	-
2	EDO	CCC	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	401	EDO	O1-C1-C2-O2
2	AAA	401	EDO	O1-C1-C2-O2
2	CCC	402	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	401	EDO	1	0
4	DDD	401	ACT	5	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

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, 95^{th} 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	AAA	263/263 (100%)	0.17	10 (3%) 40 39	33, 43, 59, 70	0
1	BBB	263/263 (100%)	0.90	44 (16%) 1 1	62, 77, 99, 111	0
1	CCC	263/263 (100%)	0.16	9 (3%) 45 44	32, 40, 55, 66	0
1	DDD	263/263 (100%)	0.19	9 (3%) 45 44	36, 48, 66, 78	0
1	EEE	263/263 (100%)	0.25	8 (3%) 50 49	35, 51, 72, 81	0
1	FFF	263/263 (100%)	2.20	113 (42%) 0 0	70, 105, 150, 170	0
All	All	1578/1578 (100%)	0.65	193 (12%) 4 3	32, 53, 124, 170	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	105	TYR	7.9
1	FFF	230	PHE	7.7
1	FFF	56	ILE	7.4
1	FFF	225	LEU	7.3
1	FFF	104	GLU	7.2
1	FFF	288	TRP	7.2
1	FFF	216	VAL	6.9
1	FFF	122	LEU	6.9
1	FFF	114	THR	6.8
1	FFF	229	TRP	6.5
1	FFF	223	SER	6.5
1	FFF	113	LEU	6.3
1	FFF	111	LYS	6.3
1	FFF	57	LEU	6.2
1	FFF	227	ALA	5.9
1	FFF	201	LEU	5.9
1	BBB	52	ASN	5.8
1	FFF	100	ASN	5.8
1	FFF	103	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	FFF	91	LEU	5.5
1	BBB	105	TYR	5.5
1	FFF	127	ILE	5.4
1	FFF	53	SER	5.3
1	FFF	52	ASN	5.3
1	BBB	230	PHE	5.3
1	FFF	222	ARG	5.3
1	FFF	109	THR	5.3
1	FFF	197	GLU	5.2
1	FFF	97	TYR	5.2
1	FFF	271	ASP	5.1
1	FFF	92	GLY	5.0
1	FFF	252	ASP	4.9
1	FFF	196	GLY	4.9
1	FFF	154	ASN	4.9
1	FFF	26	HIS	4.8
1	FFF	153	HIS	4.7
1	FFF	112	HIS	4.6
1	FFF	254	LYS	4.6
1	FFF	217	ALA	4.5
1	FFF	106	SER	4.5
1	FFF	239	GLU	4.5
1	FFF	110	GLU	4.4
1	FFF	210	TRP	4.4
1	FFF	85	ASP	4.4
1	FFF	133	THR	4.4
1	FFF	269	THR	4.4
1	FFF	270	MET	4.4
1	FFF	226	PRO	4.4
1	FFF	55	LYS	4.4
1	FFF	253	GLY	4.3
1	FFF	102	LEU	4.3
1	FFF	116	GLY	4.2
1	FFF	98	SER	4.2
1	BBB	104	GLU	4.2
1	FFF	175	ASN	4.2
1	BBB	127	ILE	4.1
1	BBB	201	LEU	4.0
1	FFF	96	HIS	3.9
1	FFF	218	GLY	3.9
1	FFF	129	MET	3.9
1	FFF	120	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	BBB	114	THR	3.8
1	FFF	128	THR	3.8
1	FFF	255	PRO	3.8
1	BBB	44	VAL	3.7
1	BBB	153	HIS	3.7
1	FFF	212	GLU	3.6
1	FFF	272	GLU	3.6
1	FFF	275	ARG	3.6
1	FFF	27	PRO	3.5
1	FFF	101	ASP	3.5
1	BBB	100	ASN	3.5
1	BBB	285	ILE	3.5
1	DDD	49	LEU	3.5
1	FFF	132	ASN	3.4
1	FFF	146	LYS	3.4
1	FFF	158	HIS	3.3
1	FFF	205	GLN	3.3
1	FFF	273	ARG	3.3
1	FFF	257	ARG	3.2
1	BBB	169	LEU	3.1
1	EEE	104	GLU	3.1
1	FFF	49	LEU	3.1
1	FFF	107	PRO	3.1
1	FFF	117	MET	3.1
1	BBB	196	GLY	3.1
1	FFF	94	ARG	3.0
1	EEE	169	LEU	3.0
1	FFF	156	GLY	3.0
1	DDD	105	TYR	3.0
1	FFF	280	ILE	2.9
1	CCC	169	LEU	2.9
1	FFF	231	ILE	2.9
1	BBB	109	THR	2.9
1	BBB	99	GLN	2.9
1	EEE	33	VAL	2.9
1	DDD	169	LEU	2.9
1	FFF	199	LEU	2.8
1	BBB	197	GLU	2.8
1	FFF	224	ALA	2.8
1	FFF	63	GLU	2.8
1	FFF	228	GLY	2.8
1	BBB	216	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	FFF	134	ALA	2.8
1	DDD	109	THR	2.8
1	FFF	118	THR	2.8
1	EEE	267	GLN	2.8
1	BBB	154	ASN	2.8
1	FFF	143	GLY	2.8
1	FFF	267	GLN	2.8
1	AAA	105	TYR	2.8
1	CCC	52	ASN	2.7
1	FFF	126	ALA	2.7
1	BBB	111	LYS	2.7
1	FFF	150	ALA	2.7
1	EEE	52	ASN	2.7
1	AAA	169	LEU	2.7
1	BBB	102	LEU	2.7
1	FFF	240	ARG	2.6
1	BBB	253	GLY	2.6
1	BBB	272	GLU	2.6
1	BBB	30	LEU	2.6
1	BBB	122	LEU	2.6
1	FFF	286	LYS	2.6
1	AAA	100	ASN	2.6
1	FFF	119	VAL	2.6
1	BBB	40	LEU	2.5
1	DDD	199	LEU	2.5
1	FFF	219	PRO	2.5
1	FFF	282	ALA	2.5
1	FFF	152	LEU	2.5
1	BBB	198	LEU	2.5
1	CCC	49	LEU	2.5
1	FFF	211	MET	2.5
1	FFF	285	ILE	2.5
1	FFF	115	ASP	2.5
1	FFF	165	TRP	2.5
1	FFF	198	LEU	2.5
1	FFF	54	GLY	2.4
1	FFF	123	CYS	2.4
1	CCC	100	ASN	2.4
1	BBB	223	SER	2.4
1	FFF	159	VAL	2.4
1	FFF	287	HIS	2.4
1	AAA	49	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	EEE	153	HIS	2.4
1	BBB	199	LEU	2.3
1	FFF	121	GLU	2.3
1	FFF	144	GLY	2.3
1	BBB	134	ALA	2.3
1	BBB	29	THR	2.3
1	DDD	154	ASN	2.3
1	DDD	52	ASN	2.3
1	BBB	288	TRP	2.3
1	FFF	155	MET	2.3
1	AAA	30	LEU	2.3
1	AAA	199	LEU	2.3
1	FFF	131	ASP	2.3
1	AAA	154	ASN	2.2
1	BBB	162	LEU	2.2
1	BBB	174	PRO	2.2
1	FFF	251	PRO	2.2
1	FFF	208	ILE	2.2
1	FFF	81	LEU	2.2
1	BBB	183	PRO	2.2
1	BBB	258	ILE	2.2
1	BBB	207	LEU	2.2
1	BBB	229	TRP	2.2
1	FFF	162	LEU	2.2
1	CCC	197	GLU	2.2
1	AAA	104[A]	GLU	2.2
1	BBB	57	LEU	2.2
1	DDD	152	LEU	2.2
1	FFF	30	LEU	2.2
1	BBB	195	THR	2.2
1	FFF	60	PHE	2.2
1	CCC	40	LEU	2.1
1	BBB	269	THR	2.1
1	CCC	285	ILE	2.1
1	FFF	39	GLN	2.1
1	DDD	104	GLU	2.1
1	EEE	197	GLU	2.1
1	FFF	191	ARG	2.1
1	AAA	197	GLU	2.1
1	AAA	29	THR	2.1
1	CCC	275	ARG	2.1
1	BBB	175	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	FFF	202	ALA	2.1
1	BBB	113	LEU	2.1
1	BBB	141	THR	2.0
1	BBB	54	GLY	2.0
1	CCC	105	TYR	2.0
1	EEE	105	TYR	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, 95^{th} 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
3	TRS	AAA	402	8/8	0.73	0.27	56,76,78,81	0
2	EDO	CCC	401	4/4	0.78	0.24	72,72,73,73	0
4	ACT	CCC	403	4/4	0.80	0.29	78,84,85,87	0
4	ACT	DDD	402	4/4	0.81	0.20	79,80,82,85	0
2	EDO	AAA	401	4/4	0.90	0.11	49,49,51,51	0
2	EDO	CCC	402	4/4	0.93	0.10	49,51,53,53	0
4	ACT	DDD	401	4/4	0.96	0.10	60,60,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.