Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:01 PM EDT

PDB ID	:	6TXD
Title	:	Variant W229D/F290W-12 of the last common ancestor of Gram-negative bacteria beta-lactamase class A (GNCA4)
Authors	:	Gavira, J.A.; Risso, V.; Sanchez-Ruiz, J.M.; Romero-Rivera, A.; Kamerlin, S.C.L.
Deposited on	:	2020-01-14
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 ⓘ 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 ⓘ) were used in the production of this report:

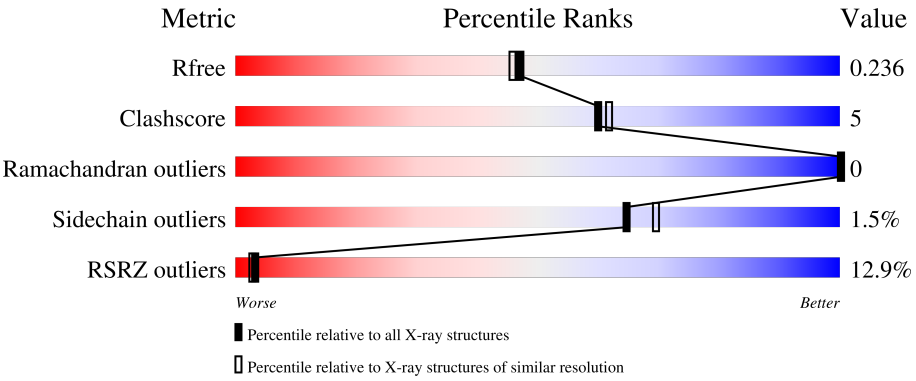
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	A	269	11% 86% 12%
1	B	269	11% 88% 10%
1	C	269	16% 88% 10%

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	C	404	-	-	-	X

2 Entry composition

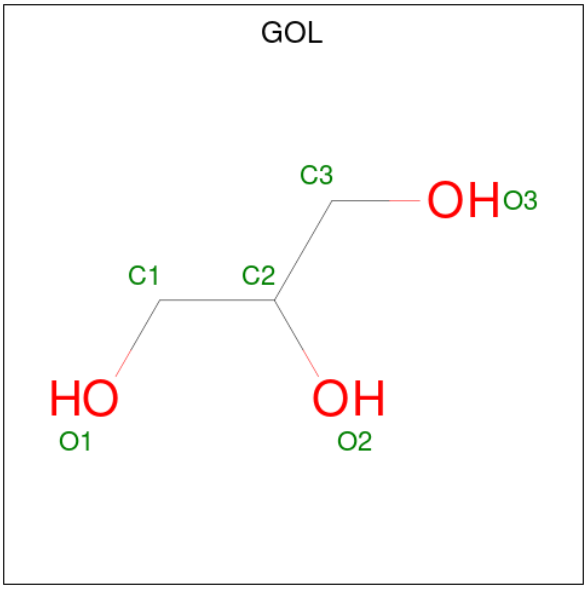
There are 6 unique types of molecules in this entry. The entry contains 6729 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (GNCA4-12).

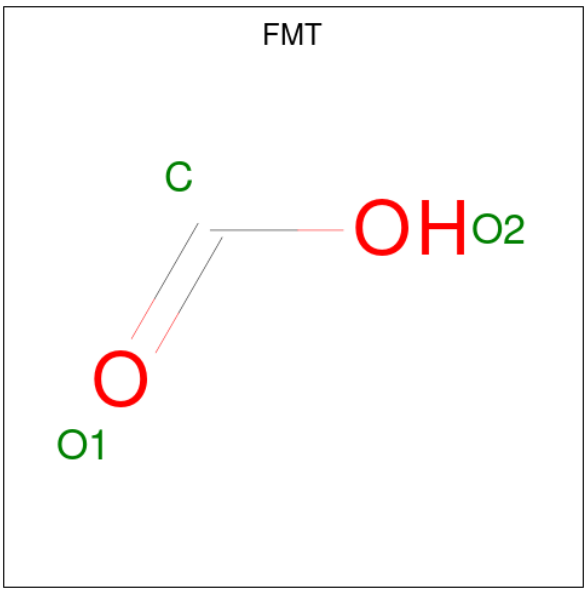
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	12	0
			2122	1318	389	410	5			
1	B	266	Total	C	N	O	S	0	8	0
			2081	1292	381	403	5			
1	C	265	Total	C	N	O	S	0	4	0
			2045	1271	368	401	5			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



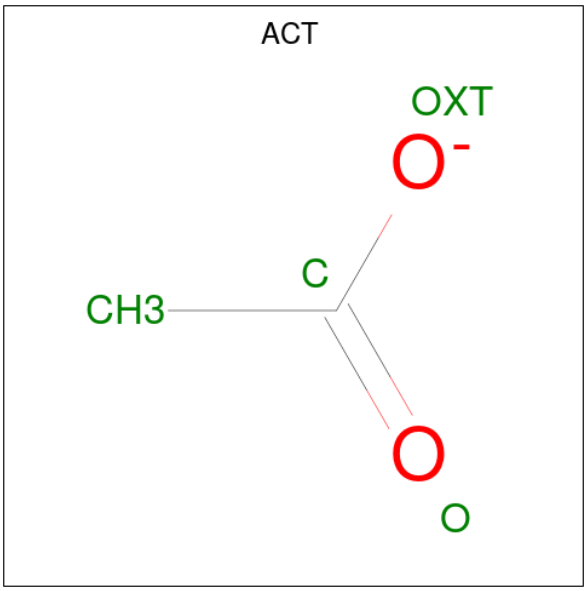
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

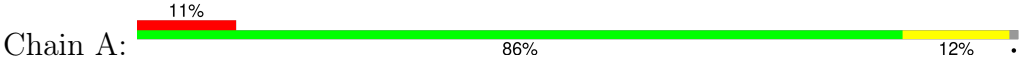
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	151	Total O 151 151	0	0
6	B	158	Total O 158 158	0	0
6	C	113	Total O 113 113	0	0

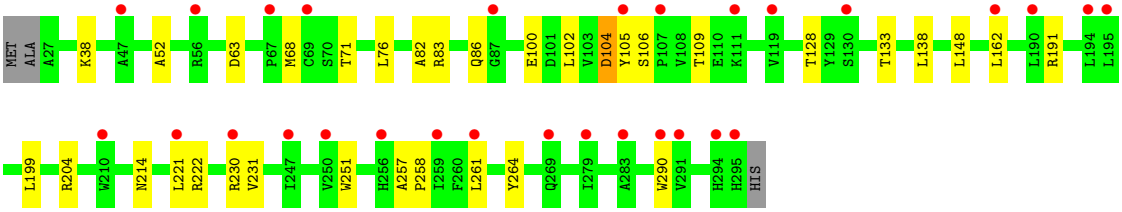
3 Residue-property plots (i)

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 (GNCA4-12)

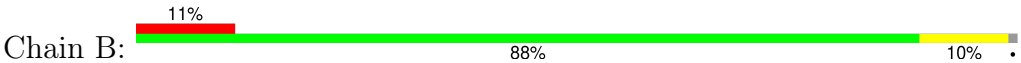
Chain A:

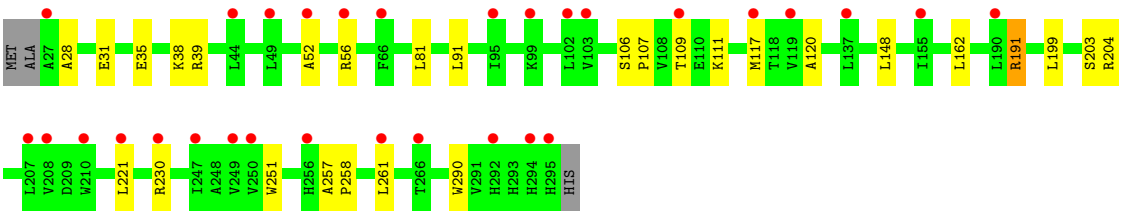




• Molecule 1: Beta lactamase (GNCA4-12)

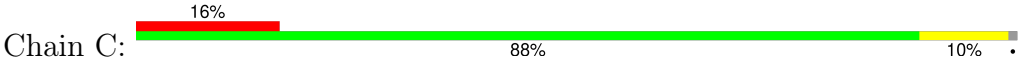
Chain B:

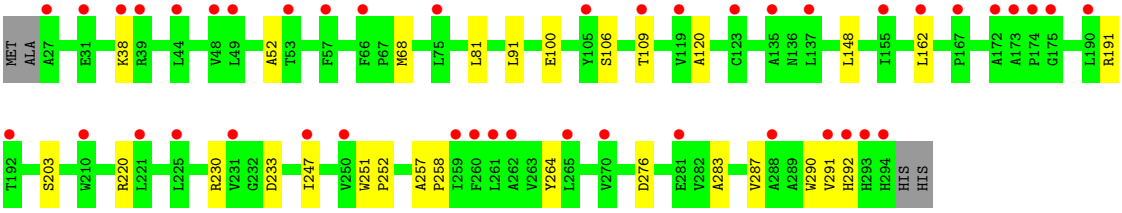




• Molecule 1: Beta lactamase (GNCA4-12)

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.31Å 148.23Å 245.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.74 – 2.00 74.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (71.74-2.00) 99.1 (74.11-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.212 , 0.235 0.211 , 0.236	Depositor DCC
R_{free} test set	4771 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	1.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6729	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: NA, FMT, GOL, ACT

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	0.24	0/2162	0.43	0/2940
1	B	0.24	0/2123	0.48	2/2889 (0.1%)
1	C	0.23	0/2080	0.43	0/2833
All	All	0.24	0/6365	0.45	2/8662 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	LYS	CD-CE-NZ	-7.46	94.54	111.70
1	B	38	LYS	CA-CB-CG	6.23	127.11	113.40

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	2122	0	2095	22	0
1	B	2081	0	2059	16	0
1	C	2045	0	2017	19	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	3	0	0
3	B	9	0	3	1	0
3	C	6	0	2	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	1	0
5	A	1	0	0	0	0
6	A	151	0	0	1	0
6	B	158	0	0	3	0
6	C	113	0	0	0	0
All	All	6729	0	6215	58	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 5.

All (58) 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:C:291:VAL:HG23	1:C:292:HIS:HD2	1.52	0.74
1:B:107:PRO:O	1:B:111:LYS:NZ	2.27	0.64
1:B:56:ARG:NH2	6:B:404:HOH:O	2.32	0.62
1:B:191[A]:ARG:NH1	6:B:403:HOH:O	2.32	0.62
1:B:39[A]:ARG:NH2	6:B:406:HOH:O	2.33	0.61
1:C:52:ALA:HB2	1:C:257:ALA:HB3	1.82	0.60
1:A:204:ARG:NH1	6:A:404:HOH:O	2.29	0.59
1:C:68:MET:HA	1:C:264:TYR:HE1	1.69	0.58
1:B:106:SER:HB3	1:B:109:THR:OG1	2.04	0.57
1:C:91:LEU:HB3	1:C:120:ALA:HB2	1.85	0.56
1:C:230:ARG:HB3	1:C:251:TRP:HB2	1.88	0.55
1:C:291:VAL:HG23	1:C:292:HIS:CD2	2.38	0.55
1:C:247:ILE:HD11	1:C:264:TYR:CZ	2.43	0.53
1:B:251:TRP:NE1	1:B:258:PRO:HG3	2.24	0.53
1:C:247:ILE:HD11	1:C:264:TYR:CE2	2.44	0.52
1:C:251:TRP:NE1	1:C:258:PRO:HG3	2.24	0.52
1:B:28:ALA:HA	1:B:31:GLU:OE2	2.11	0.50
1:A:104[B]:ASP:OD2	1:A:105[B]:TYR:N	2.44	0.50
1:C:283:ALA:O	1:C:287:VAL:HG23	2.11	0.50
1:A:52:ALA:HB2	1:A:257:ALA:HB3	1.93	0.49
1:A:106:SER:HB3	1:A:109:THR:OG1	2.13	0.49
1:A:230[A]:ARG:HB3	1:A:251:TRP:HB2	1.94	0.49
3:B:302:FMT:H	3:B:304:FMT:H	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD23	1:A:162:LEU:HD22	1.95	0.48
1:C:106:SER:HB3	1:C:109:THR:OG1	2.13	0.48
1:B:91:LEU:HB3	1:B:120:ALA:HB2	1.96	0.48
1:C:100[B]:GLU:H	1:C:100[B]:GLU:HG3	1.33	0.48
1:A:83:ARG:HA	1:A:86:GLN:HB2	1.96	0.48
1:A:68:MET:HA	1:A:264:TYR:HE1	1.79	0.48
1:B:199:LEU:O	1:B:204:ARG:NH1	2.48	0.47
1:C:81:LEU:HB3	1:C:203:SER:HB3	1.95	0.47
1:A:63:ASP:HB3	2:C:401:GOL:H32	1.98	0.46
1:A:251:TRP:HE1	1:A:258:PRO:HG3	1.81	0.46
1:C:220:ARG:NE	1:C:276:ASP:OD1	2.48	0.45
1:A:82:ALA:O	1:A:86:GLN:HG3	2.16	0.45
1:B:52:ALA:HB2	1:B:257:ALA:HB3	1.98	0.45
1:A:68:MET:HB2	1:A:71:THR:OG1	2.17	0.45
1:B:81:LEU:HB3	1:B:203:SER:HB3	2.00	0.44
1:A:251:TRP:NE1	1:A:258:PRO:HG3	2.32	0.44
1:C:148:LEU:HD23	1:C:162:LEU:HD22	1.99	0.44
1:B:148:LEU:HD23	1:B:162:LEU:HD22	1.99	0.44
1:B:221:LEU:HD22	1:B:261:LEU:HD21	1.99	0.44
1:C:251:TRP:HE1	1:C:258:PRO:HG3	1.82	0.44
1:A:76:LEU:HD21	1:A:138:LEU:HB2	1.99	0.43
1:B:109:THR:HA	1:B:117:MET:HE1	2.00	0.43
1:B:230[B]:ARG:HA	1:B:230[B]:ARG:HD2	1.68	0.43
1:A:102:LEU:HD23	1:A:133:THR:HG21	2.01	0.43
1:C:38:LYS:HB3	1:C:38:LYS:HE3	1.72	0.42
1:A:221:LEU:HD13	1:A:261:LEU:HD22	1.99	0.42
1:A:222:ARG:NH1	1:A:231:VAL:HG13	2.34	0.42
1:C:68:MET:HA	1:C:264:TYR:CE1	2.52	0.42
1:A:199:LEU:HB2	1:A:204:ARG:HG2	2.02	0.42
1:C:252:PRO:HG3	4:C:404:ACT:H3	2.00	0.42
1:A:38[B]:LYS:HB3	1:A:38[B]:LYS:HE3	1.73	0.41
1:A:128:THR:HA	1:A:214:ASN:HA	2.01	0.41
1:B:35[B]:GLU:HG3	1:B:39[B]:ARG:NH1	2.37	0.40
1:A:230[B]:ARG:HB3	1:A:251:TRP:HB2	2.03	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	A	276/269 (103%)	269 (98%)	7 (2%)	0	100	100
1	B	272/269 (101%)	269 (99%)	3 (1%)	0	100	100
1	C	268/269 (100%)	265 (99%)	3 (1%)	0	100	100
All	All	816/807 (101%)	803 (98%)	13 (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	A	218/208 (105%)	212 (97%)	6 (3%)	43	44
1	B	214/208 (103%)	211 (99%)	3 (1%)	67	72
1	C	210/208 (101%)	207 (99%)	3 (1%)	67	72
All	All	642/624 (103%)	630 (98%)	12 (2%)	65	61

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100[A]	GLU
1	A	100[B]	GLU
1	A	104[A]	ASP
1	A	104[B]	ASP
1	A	191	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	TRP
1	B	191[A]	ARG
1	B	191[B]	ARG
1	B	290	TRP
1	C	191	ARG
1	C	233	ASP
1	C	290	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	292	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	FMT	A	303	-	2,2,2	0.74	0	1,1,1	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	C	405	-	3,3,3	1.38	0	3,3,3	1.51	0
4	ACT	A	305	-	3,3,3	1.38	0	3,3,3	1.37	0
3	FMT	B	302	-	2,2,2	0.75	0	1,1,1	0.25	0
3	FMT	A	304	-	2,2,2	0.75	0	1,1,1	0.23	0
3	FMT	C	403	-	2,2,2	0.75	0	1,1,1	0.25	0
2	GOL	B	301	-	5,5,5	0.92	0	5,5,5	1.06	0
3	FMT	B	303	-	2,2,2	0.75	0	1,1,1	0.23	0
2	GOL	C	401	-	5,5,5	0.92	0	5,5,5	1.05	0
4	ACT	B	305	-	3,3,3	1.38	0	3,3,3	1.37	0
3	FMT	B	304	-	2,2,2	0.74	0	1,1,1	0.28	0
3	FMT	A	302	-	2,2,2	0.75	0	1,1,1	0.24	0
2	GOL	A	301	-	5,5,5	0.94	0	5,5,5	1.07	0
3	FMT	C	402	-	2,2,2	0.75	0	1,1,1	0.26	0
4	ACT	C	404	-	3,3,3	1.08	0	3,3,3	1.47	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	GOL	A	301	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	C	401	GOL	C1-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
2	A	301	GOL	C1-C2-C3-O3
2	C	401	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O2-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	FMT	1	0
2	C	401	GOL	1	0
3	B	304	FMT	1	0
4	C	404	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	266/269 (98%)	1.07	29 (10%)	5 5	21, 30, 51, 95	0
1	B	266/269 (98%)	1.02	30 (11%)	5 4	21, 31, 53, 89	0
1	C	265/269 (98%)	1.13	44 (16%)	1 1	28, 43, 64, 111	0
All	All	797/807 (98%)	1.07	103 (12%)	3 3	21, 35, 58, 111	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	VAL	5.1
1	A	105[A]	TYR	5.0
1	C	27	ALA	4.7
1	A	87	GLY	4.6
1	C	265	LEU	4.4
1	A	261	LEU	4.4
1	C	75	LEU	4.4
1	C	162	LEU	4.1
1	C	291	VAL	4.0
1	A	119	VAL	4.0
1	B	27	ALA	3.8
1	C	66	PHE	3.8
1	C	221	LEU	3.8
1	B	295	HIS	3.6
1	C	137	LEU	3.6
1	B	250	VAL	3.6
1	B	247	ILE	3.6
1	B	102	LEU	3.6
1	B	95	ILE	3.4
1	A	162	LEU	3.4
1	A	294	HIS	3.4
1	B	256	HIS	3.4
1	C	172	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	31[A]	GLU	3.4
1	C	173	ALA	3.3
1	B	261	LEU	3.3
1	C	167	PRO	3.3
1	C	135	ALA	3.2
1	C	250	VAL	3.2
1	A	256	HIS	3.1
1	A	291	VAL	3.1
1	B	230[A]	ARG	3.0
1	B	221	LEU	3.0
1	C	261	LEU	3.0
1	C	225	LEU	2.9
1	C	292	HIS	2.9
1	C	192	THR	2.9
1	B	210	TRP	2.9
1	C	109	THR	2.9
1	C	44	LEU	2.9
1	C	105	TYR	2.8
1	B	103	VAL	2.8
1	A	259	ILE	2.8
1	B	190	LEU	2.8
1	A	195	LEU	2.7
1	B	117	MET	2.7
1	C	259	ILE	2.7
1	C	294	HIS	2.7
1	B	137	LEU	2.7
1	C	123	CYS	2.7
1	A	210	TRP	2.6
1	A	295	HIS	2.6
1	B	266	THR	2.6
1	B	109	THR	2.5
1	A	190	LEU	2.5
1	B	44	LEU	2.5
1	C	155	ILE	2.5
1	A	283	ALA	2.4
1	C	288	ALA	2.4
1	A	56[A]	ARG	2.4
1	A	269	GLN	2.4
1	A	221	LEU	2.4
1	B	49	LEU	2.4
1	C	270	VAL	2.4
1	C	57	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	260	PHE	2.4
1	A	130	SER	2.4
1	B	56	ARG	2.4
1	C	53	THR	2.3
1	C	247	ILE	2.3
1	A	247	ILE	2.3
1	C	175	GLY	2.3
1	B	294	HIS	2.3
1	A	230[A]	ARG	2.3
1	B	155	ILE	2.3
1	B	292	HIS	2.2
1	C	39	ARG	2.2
1	A	67	PRO	2.2
1	C	49	LEU	2.2
1	C	174	PRO	2.2
1	A	47	ALA	2.2
1	C	190	LEU	2.1
1	A	250	VAL	2.1
1	B	249	VAL	2.1
1	A	111[A]	LYS	2.1
1	B	99	LYS	2.1
1	C	293	HIS	2.1
1	B	119	VAL	2.1
1	C	231	VAL	2.1
1	B	66	PHE	2.1
1	A	107	PRO	2.1
1	A	69	CYS	2.1
1	B	207	LEU	2.1
1	C	262	ALA	2.1
1	C	281	GLU	2.1
1	C	38	LYS	2.1
1	A	279	ILE	2.1
1	B	52	ALA	2.1
1	A	290	TRP	2.1
1	C	210	TRP	2.0
1	C	48	VAL	2.0
1	A	194	LEU	2.0
1	B	208	VAL	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	FMT	A	302	3/3	0.68	0.26	59,59,60,60	0
4	ACT	B	305	4/4	0.69	0.21	37,39,41,41	0
3	FMT	A	304	3/3	0.71	0.38	72,72,73,73	0
2	GOL	A	301	6/6	0.74	0.21	53,58,59,60	0
4	ACT	C	404	4/4	0.76	0.57	72,73,73,74	0
2	GOL	B	301	6/6	0.83	0.26	63,66,67,70	0
3	FMT	B	303	3/3	0.83	0.38	48,48,49,49	0
2	GOL	C	401	6/6	0.84	0.31	41,50,55,59	0
4	ACT	C	405	4/4	0.85	0.22	50,50,50,52	0
3	FMT	C	403	3/3	0.87	0.19	46,46,46,46	0
4	ACT	A	305	4/4	0.89	0.15	40,41,42,44	0
3	FMT	C	402	3/3	0.92	0.23	39,39,39,40	0
5	NA	A	306	1/1	0.93	0.20	35,35,35,35	0
3	FMT	B	304	3/3	0.94	0.17	30,30,34,36	0
3	FMT	B	302	3/3	0.94	0.14	31,31,32,32	0
3	FMT	A	303	3/3	0.95	0.15	34,34,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.