



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:58 AM UTC

PDB ID : 6TXD / pdb_00006txd
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

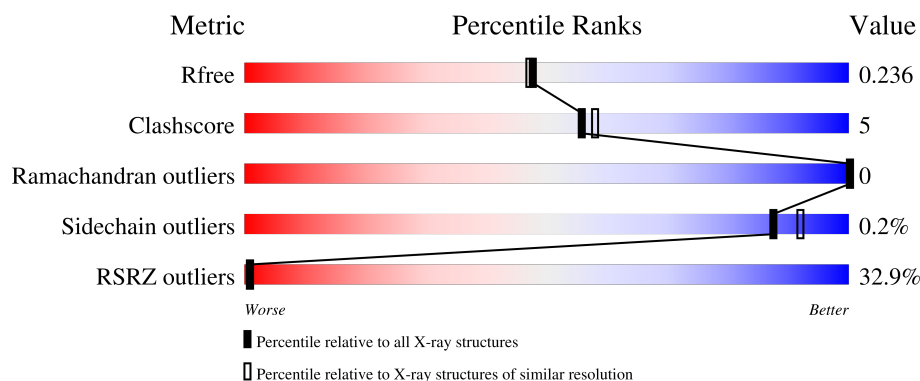
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	269	34% 87% 11%
1	B	269	31% 89% 10%
1	C	269	32% 89% 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
3	FMT	A	304	-	-	-	X

2 Entry composition [i](#)

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 (CCD ID: 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 (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

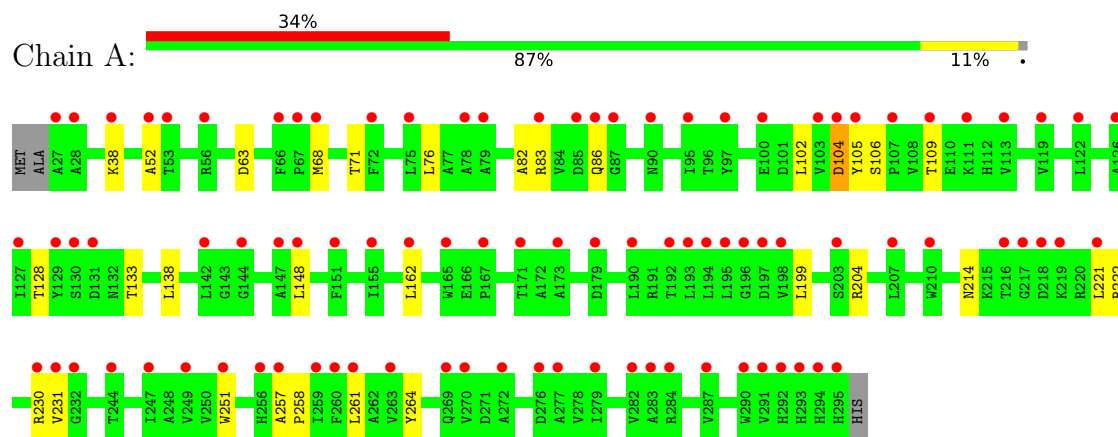
- Molecule 6 is water.

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

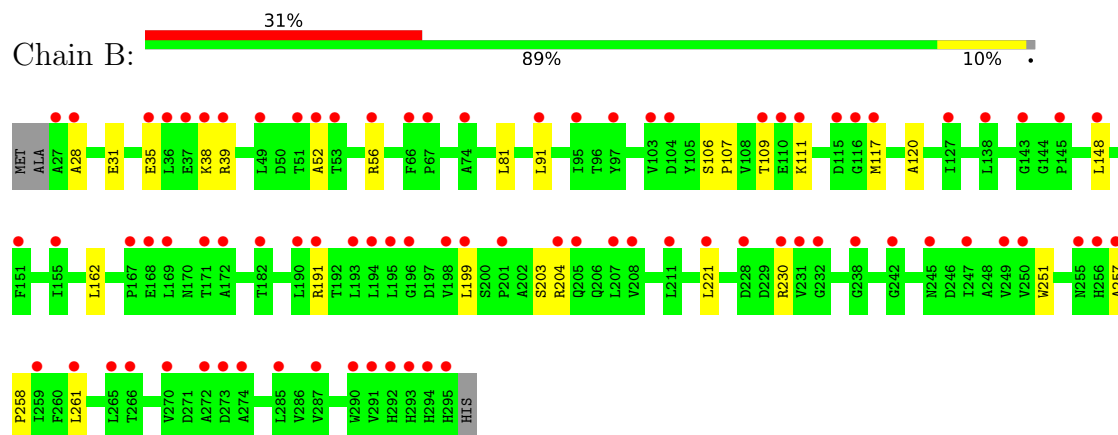
3 Residue-property plots

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.

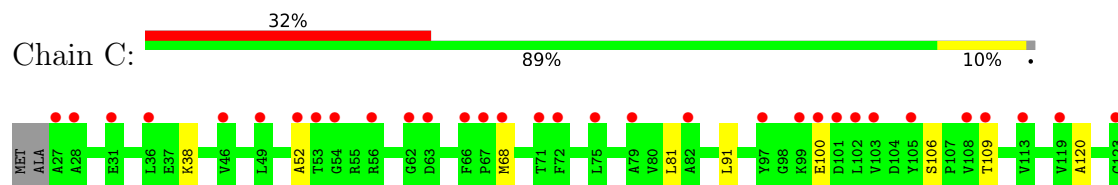
• Molecule 1: Beta lactamase (GNCA4-12)

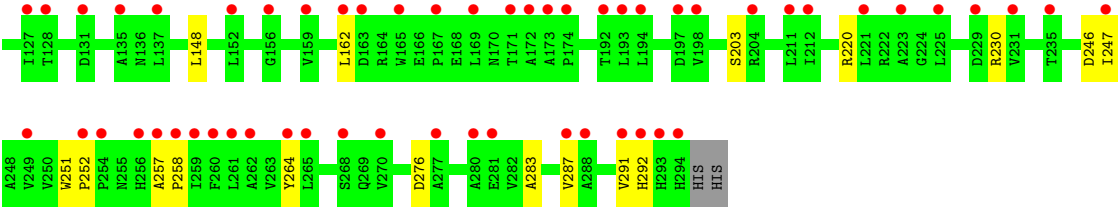


• Molecule 1: Beta lactamase (GNCA4-12)



• Molecule 1: Beta lactamase (GNCA4-12)





4 Data and refinement statistics

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 71.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (71.74-2.00) 99.1 (71.74-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.212 , 0.235 (Not available) , 0.236	Depositor DCC
R_{free} test set	4772 reflections (4.99%)	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 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ACT, FMT, GOL

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	0.14	0/2162	0.35	0/2940
1	B	0.13	0/2123	0.38	2/2889 (0.1%)
1	C	0.10	0/2080	0.30	0/2833
All	All	0.12	0/6365	0.35	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(°)	Ideal(°)
1	B	38	LYS	CA-CB-CG	6.50	127.11	114.10
1	B	38	LYS	CD-CE-NZ	-5.42	94.54	111.90

There are no chirality outliers.

There are no planarity outliers.

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	2122	0	2095	22	0
1	B	2081	0	2059	16	0
1	C	2045	0	2017	20	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	59	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 (59) 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:C:246:ASP:C	1:C:247:ILE:HD12	2.42	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: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:109:THR:HG22	1:B:117:MET:HE1	2.03	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

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	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

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%)	216 (99%)	2 (1%)	70	78
1	B	214/208 (103%)	214 (100%)	0	100	100
1	C	210/208 (101%)	210 (100%)	0	100	100
All	All	642/624 (103%)	640 (100%)	2 (0%)	87	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104[A]	ASP
1	A	104[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	206	GLN
1	A	241	HIS
1	B	170	ASN
1	B	205	GLN
1	B	206	GLN
1	B	295	HIS
1	C	86	GLN
1	C	170	ASN
1	C	205	GLN
1	C	206	GLN
1	C	241	HIS
1	C	255	ASN
1	C	292	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	403	-	2,2,2	0.75	0	1,1,1	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	401	-	5,5,5	0.92	0	5,5,5	1.05	0
3	FMT	A	302	-	2,2,2	0.75	0	1,1,1	0.24	0
4	ACT	B	305	-	3,3,3	1.38	0	3,3,3	1.37	0
3	FMT	C	402	-	2,2,2	0.75	0	1,1,1	0.26	0
3	FMT	B	304	-	2,2,2	0.74	0	1,1,1	0.28	0
4	ACT	C	405	-	3,3,3	1.38	0	3,3,3	1.51	0
3	FMT	B	303	-	2,2,2	0.75	0	1,1,1	0.23	0
3	FMT	B	302	-	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
4	ACT	C	404	-	3,3,3	1.08	0	3,3,3	1.47	0
4	ACT	A	305	-	3,3,3	1.38	0	3,3,3	1.37	0
2	GOL	A	301	-	5,5,5	0.94	0	5,5,5	1.07	0
3	FMT	A	304	-	2,2,2	0.75	0	1,1,1	0.23	0
3	FMT	A	303	-	2,2,2	0.74	0	1,1,1	0.26	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
2	C	401	GOL	1	0
3	B	304	FMT	1	0
3	B	302	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, 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	266/269 (98%)	1.74	92 (34%)  	15, 29, 51, 95	12 (4%)
1	B	266/269 (98%)	1.62	83 (31%)  	13, 31, 53, 89	8 (3%)
1	C	265/269 (98%)	1.74	87 (32%)  	18, 43, 64, 111	4 (1%)
All	All	797/807 (98%)	1.70	262 (32%)  	13, 34, 58, 111	24 (3%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105[A]	TYR	8.3
1	C	119	VAL	7.1
1	B	27	ALA	6.8
1	A	87	GLY	6.4
1	C	99[A]	LYS	6.3
1	A	261	LEU	6.0
1	A	294	HIS	5.8
1	C	75	LEU	5.3
1	C	167	PRO	5.3
1	C	173	ALA	5.2
1	A	27	ALA	5.1
1	A	291	VAL	5.1
1	B	117	MET	5.0
1	A	295	HIS	5.0
1	C	27	ALA	5.0
1	B	295	HIS	4.9
1	A	283	ALA	4.9
1	C	294	HIS	4.8
1	C	171	THR	4.8
1	A	290	TRP	4.8
1	A	119	VAL	4.7
1	A	279	ILE	4.4
1	A	256	HIS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	172	ALA	4.4
1	A	104[A]	ASP	4.3
1	B	230[A]	ARG	4.3
1	C	137	LEU	4.2
1	A	67	PRO	4.2
1	B	56	ARG	4.1
1	B	39[A]	ARG	4.1
1	B	49	LEU	4.1
1	A	56[A]	ARG	4.0
1	B	256	HIS	4.0
1	A	103	VAL	4.0
1	A	197[A]	ASP	4.0
1	B	261	LEU	4.0
1	C	109	THR	4.0
1	B	104	ASP	3.8
1	B	231	VAL	3.8
1	B	238	GLY	3.8
1	C	131	ASP	3.8
1	C	66	PHE	3.8
1	B	257	ALA	3.7
1	C	123	CYS	3.7
1	C	67	PRO	3.7
1	B	38	LYS	3.7
1	A	272	ALA	3.7
1	C	135	ALA	3.7
1	B	250	VAL	3.6
1	A	171	THR	3.6
1	B	293	HIS	3.6
1	C	162	LEU	3.6
1	B	291	VAL	3.6
1	C	63	ASP	3.5
1	A	198	VAL	3.5
1	B	247	ILE	3.5
1	A	162	LEU	3.5
1	C	103	VAL	3.5
1	A	109	THR	3.5
1	C	288	ALA	3.5
1	C	198	VAL	3.5
1	A	79	ALA	3.4
1	B	221	LEU	3.4
1	C	113	VAL	3.4
1	A	53	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	105	TYR	3.4
1	C	247	ILE	3.4
1	C	225	LEU	3.3
1	A	130	SER	3.3
1	A	232	GLY	3.3
1	A	210	TRP	3.3
1	A	263	VAL	3.3
1	B	198	VAL	3.2
1	B	196	GLY	3.2
1	C	291	VAL	3.2
1	C	31[A]	GLU	3.2
1	A	221	LEU	3.1
1	C	221	LEU	3.1
1	A	85	ASP	3.1
1	B	274	ALA	3.1
1	B	211	LEU	3.1
1	C	163	ASP	3.1
1	A	231	VAL	3.1
1	A	276	ASP	3.0
1	A	259	ILE	3.0
1	B	167	PRO	3.0
1	A	284[A]	ARG	3.0
1	A	277	ALA	3.0
1	A	179	ASP	3.0
1	C	174	PRO	3.0
1	C	260	PHE	3.0
1	B	191[A]	ARG	2.9
1	B	207	LEU	2.9
1	C	252	PRO	2.9
1	A	230[A]	ARG	2.9
1	A	251	TRP	2.9
1	A	126	ALA	2.9
1	C	49	LEU	2.9
1	B	208	VAL	2.9
1	B	95	ILE	2.9
1	C	68	MET	2.9
1	A	257	ALA	2.9
1	B	242	GLY	2.9
1	C	256	HIS	2.9
1	C	261	LEU	2.8
1	A	113	VAL	2.8
1	B	37	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	292	HIS	2.8
1	C	223	ALA	2.8
1	A	122	LEU	2.8
1	A	190	LEU	2.8
1	B	103	VAL	2.8
1	A	155	ILE	2.8
1	C	127	ILE	2.8
1	A	66	PHE	2.8
1	A	147	ALA	2.8
1	B	292	HIS	2.8
1	B	272	ALA	2.8
1	C	193	LEU	2.8
1	A	293	HIS	2.7
1	B	294	HIS	2.7
1	C	281	GLU	2.7
1	A	131	ASP	2.7
1	A	111[A]	LYS	2.7
1	C	262	ALA	2.7
1	B	67	PRO	2.7
1	C	165	TRP	2.7
1	A	244	THR	2.7
1	B	190	LEU	2.7
1	B	195	LEU	2.7
1	C	102	LEU	2.7
1	A	107	PRO	2.7
1	B	97	TYR	2.7
1	B	249	VAL	2.7
1	A	195	LEU	2.6
1	A	216	THR	2.6
1	B	148	LEU	2.6
1	C	152	LEU	2.6
1	B	151	PHE	2.6
1	B	110[A]	GLU	2.6
1	B	115	ASP	2.6
1	C	194	LEU	2.6
1	B	204	ARG	2.6
1	A	95	ILE	2.6
1	A	192	THR	2.6
1	B	53	THR	2.6
1	B	265	LEU	2.6
1	A	151	PHE	2.5
1	C	264	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	192	THR	2.5
1	A	127	ILE	2.5
1	B	109	THR	2.5
1	C	268	SER	2.5
1	A	269	GLN	2.5
1	A	78	ALA	2.5
1	A	167	PRO	2.5
1	B	74	ALA	2.5
1	C	52	ALA	2.5
1	A	142	LEU	2.5
1	C	258	PRO	2.4
1	C	293	HIS	2.4
1	B	266	THR	2.4
1	B	169	LEU	2.4
1	C	100[A]	GLU	2.4
1	A	218	ASP	2.4
1	B	259	ILE	2.4
1	B	145	PRO	2.4
1	B	205	GLN	2.4
1	C	62	GLY	2.4
1	A	72	PHE	2.4
1	C	287	VAL	2.4
1	A	38[A]	LYS	2.4
1	B	182	THR	2.4
1	B	201	PRO	2.4
1	A	173	ALA	2.3
1	C	280	ALA	2.3
1	B	36	LEU	2.3
1	B	232	GLY	2.3
1	B	273	ASP	2.3
1	C	259	ILE	2.3
1	A	270	VAL	2.3
1	C	231	VAL	2.3
1	C	82	ALA	2.3
1	C	257	ALA	2.3
1	C	101	ASP	2.3
1	C	197[A]	ASP	2.3
1	A	219[A]	LYS	2.3
1	B	168	GLU	2.3
1	C	277	ALA	2.3
1	A	100[A]	GLU	2.3
1	C	72	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	249	VAL	2.3
1	B	143	GLY	2.3
1	C	54	GLY	2.3
1	A	193	LEU	2.3
1	C	169	LEU	2.3
1	A	97	TYR	2.3
1	B	171	THR	2.2
1	B	270	VAL	2.2
1	C	270	VAL	2.2
1	B	111	LYS	2.2
1	B	228	ASP	2.2
1	B	28	ALA	2.2
1	B	172	ALA	2.2
1	B	194	LEU	2.2
1	B	285	LEU	2.2
1	A	292	HIS	2.2
1	C	56	ARG	2.2
1	B	116	GLY	2.2
1	A	52	ALA	2.2
1	A	194	LEU	2.2
1	C	204	ARG	2.2
1	C	71	THR	2.2
1	A	68	MET	2.2
1	C	254	PRO	2.2
1	C	229	ASP	2.2
1	A	282	VAL	2.2
1	C	108	VAL	2.2
1	B	52	ALA	2.2
1	C	79	ALA	2.2
1	A	207	LEU	2.2
1	B	138	LEU	2.2
1	B	193	LEU	2.2
1	C	235	THR	2.2
1	B	35[A]	GLU	2.1
1	C	212	ILE	2.1
1	A	287	VAL	2.1
1	A	196	GLY	2.1
1	A	217	GLY	2.1
1	C	28	ALA	2.1
1	A	203	SER	2.1
1	B	255	ASN	2.1
1	C	128	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	66	PHE	2.1
1	A	83	ARG	2.1
1	C	211	LEU	2.1
1	A	86	GLN	2.1
1	A	144	GLY	2.1
1	B	155	ILE	2.1
1	C	156	GLY	2.1
1	A	260	PHE	2.1
1	B	287	VAL	2.1
1	C	159	VAL	2.1
1	B	91	LEU	2.1
1	C	265	LEU	2.1
1	C	97	TYR	2.1
1	B	127	ILE	2.1
1	C	46	VAL	2.1
1	A	165	TRP	2.1
1	A	28	ALA	2.1
1	B	199	LEU	2.0
1	C	36	LEU	2.0
1	A	90[A]	ASN	2.0
1	C	53	THR	2.0
1	A	129	TYR	2.0
1	A	247	ILE	2.0
1	A	249	VAL	2.0
1	B	290	TRP	2.0
1	B	245	ASN	2.0
1	A	75	LEU	2.0
1	A	148	LEU	2.0
1	B	51	THR	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 oligosaccharides 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. 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
3	FMT	A	304	3/3	0.65	0.46	72,72,73,73	0
4	ACT	B	305	4/4	0.67	0.20	37,39,41,41	0
4	ACT	C	404	4/4	0.73	0.35	72,73,73,74	0
3	FMT	A	302	3/3	0.79	0.26	59,59,60,60	0
4	ACT	A	305	4/4	0.79	0.19	40,41,42,44	0
2	GOL	A	301	6/6	0.81	0.23	53,58,59,60	0
4	ACT	C	405	4/4	0.82	0.23	50,50,50,52	0
2	GOL	B	301	6/6	0.83	0.21	63,66,67,70	0
2	GOL	C	401	6/6	0.87	0.16	41,50,55,59	0
3	FMT	B	303	3/3	0.88	0.35	48,48,49,49	0
3	FMT	B	304	3/3	0.88	0.13	30,30,34,36	0
5	NA	A	306	1/1	0.89	0.20	35,35,35,35	0
3	FMT	C	402	3/3	0.90	0.13	39,39,39,40	0
3	FMT	C	403	3/3	0.91	0.13	46,46,46,46	0
3	FMT	B	302	3/3	0.92	0.10	31,31,32,32	0
3	FMT	A	303	3/3	0.92	0.12	34,34,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.