



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2025 – 10:17 pm BST

PDB ID : 9FZ9 / pdb_00009fz9
Title : Glycoside Hydrolase Family 157 from *Labilibaculum antarcticum*, wild type
SeMet derivative (LaGH157)
Authors : Bule, P.; Alves, V.D.; Carvalho, A.L.
Deposited on : 2024-07-04
Resolution : 2.44 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 ⓘ 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

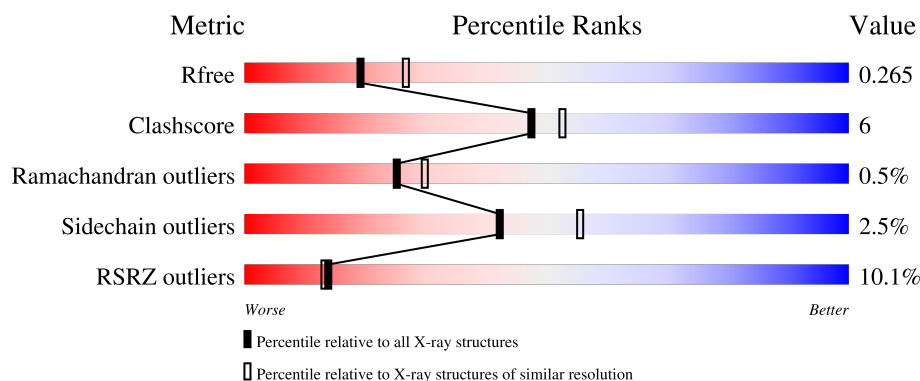
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	164625	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	537	<div> <div>5%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	537	<div> <div>8%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	537	<div> <div>18%</div> <div>83%</div> <div>13%</div> <div>...</div> </div>
1	D	537	<div> <div>8%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>

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	ACT	A	601	-	-	X	-
2	ACT	A	605	-	-	X	-
3	GOL	A	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17403 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 Glycoside hydrolase family 2 catalytic domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	Se	0	0	0
			4241	2713	684	829	4	11			
1	B	527	Total	C	N	O	S	Se	0	1	0
			4247	2717	685	830	4	11			
1	C	528	Total	C	N	O	S	Se	0	0	0
			4252	2721	685	831	4	11			
1	D	528	Total	C	N	O	S	Se	0	0	0
			4249	2719	685	830	4	11			

There are 36 discrepancies between the modelled and reference sequences:

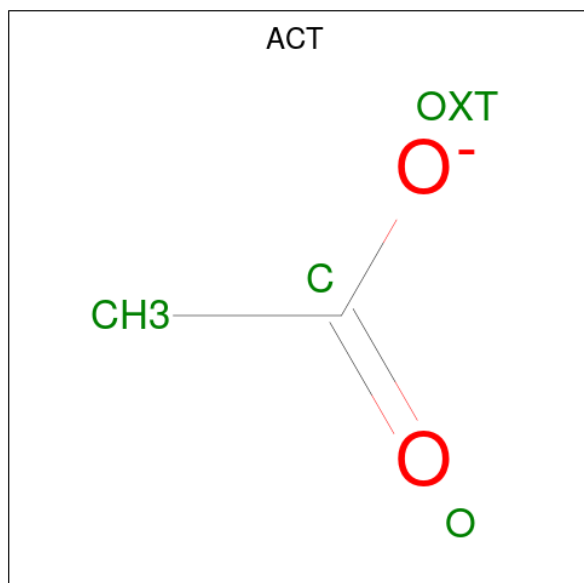
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP A0A1Y1CQ89
A	530	LEU	-	expression tag	UNP A0A1Y1CQ89
A	531	GLU	-	expression tag	UNP A0A1Y1CQ89
A	532	HIS	-	expression tag	UNP A0A1Y1CQ89
A	533	HIS	-	expression tag	UNP A0A1Y1CQ89
A	534	HIS	-	expression tag	UNP A0A1Y1CQ89
A	535	HIS	-	expression tag	UNP A0A1Y1CQ89
A	536	HIS	-	expression tag	UNP A0A1Y1CQ89
A	537	HIS	-	expression tag	UNP A0A1Y1CQ89
B	1	MSE	-	initiating methionine	UNP A0A1Y1CQ89
B	530	LEU	-	expression tag	UNP A0A1Y1CQ89
B	531	GLU	-	expression tag	UNP A0A1Y1CQ89
B	532	HIS	-	expression tag	UNP A0A1Y1CQ89
B	533	HIS	-	expression tag	UNP A0A1Y1CQ89
B	534	HIS	-	expression tag	UNP A0A1Y1CQ89
B	535	HIS	-	expression tag	UNP A0A1Y1CQ89
B	536	HIS	-	expression tag	UNP A0A1Y1CQ89
B	537	HIS	-	expression tag	UNP A0A1Y1CQ89
C	1	MSE	-	initiating methionine	UNP A0A1Y1CQ89
C	530	LEU	-	expression tag	UNP A0A1Y1CQ89

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Chain	Residue	Modelled	Actual	Comment	Reference
C	531	GLU	-	expression tag	UNP A0A1Y1CQ89
C	532	HIS	-	expression tag	UNP A0A1Y1CQ89
C	533	HIS	-	expression tag	UNP A0A1Y1CQ89
C	534	HIS	-	expression tag	UNP A0A1Y1CQ89
C	535	HIS	-	expression tag	UNP A0A1Y1CQ89
C	536	HIS	-	expression tag	UNP A0A1Y1CQ89
C	537	HIS	-	expression tag	UNP A0A1Y1CQ89
D	1	MSE	-	initiating methionine	UNP A0A1Y1CQ89
D	530	LEU	-	expression tag	UNP A0A1Y1CQ89
D	531	GLU	-	expression tag	UNP A0A1Y1CQ89
D	532	HIS	-	expression tag	UNP A0A1Y1CQ89
D	533	HIS	-	expression tag	UNP A0A1Y1CQ89
D	534	HIS	-	expression tag	UNP A0A1Y1CQ89
D	535	HIS	-	expression tag	UNP A0A1Y1CQ89
D	536	HIS	-	expression tag	UNP A0A1Y1CQ89
D	537	HIS	-	expression tag	UNP A0A1Y1CQ89

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



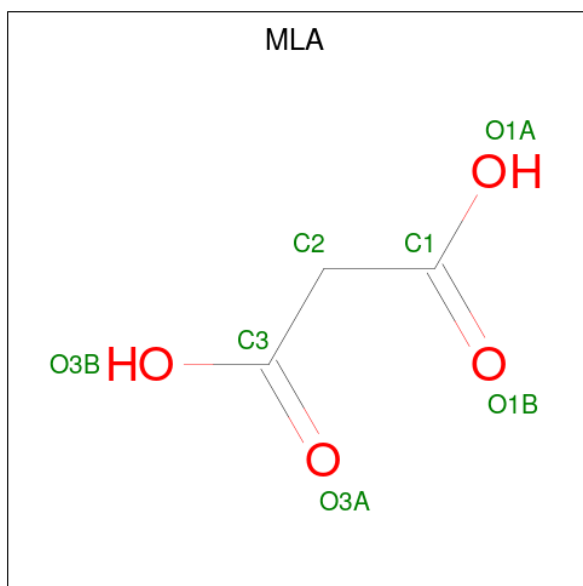
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		

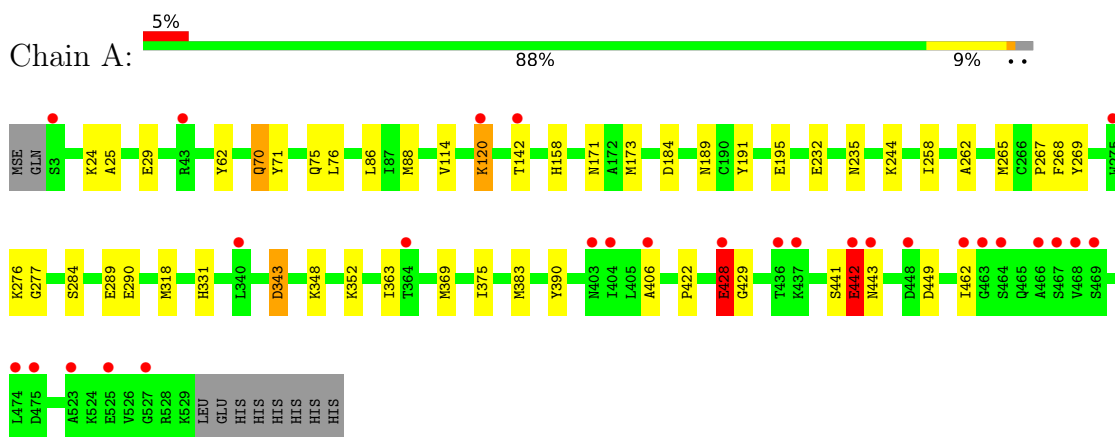
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total	O	0	0
			167	167		
5	B	144	Total	O	0	0
			144	144		
5	C	31	Total	O	0	0
			31	31		
5	D	35	Total	O	0	0
			35	35		

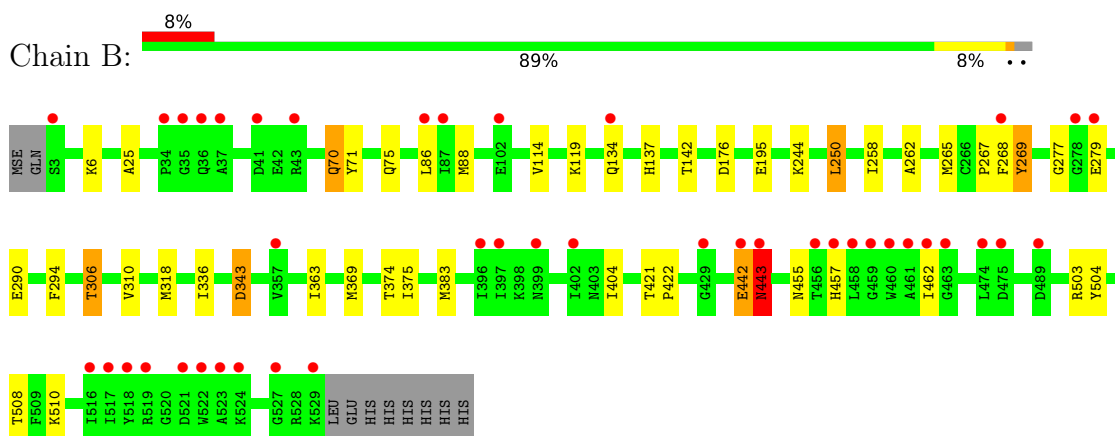
3 Residue-property plots

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.

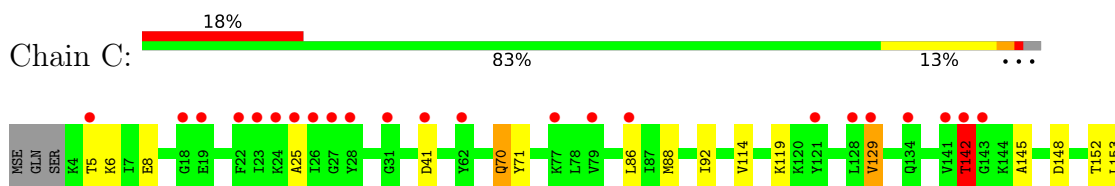
- Molecule 1: Glycoside hydrolase family 2 catalytic domain-containing protein

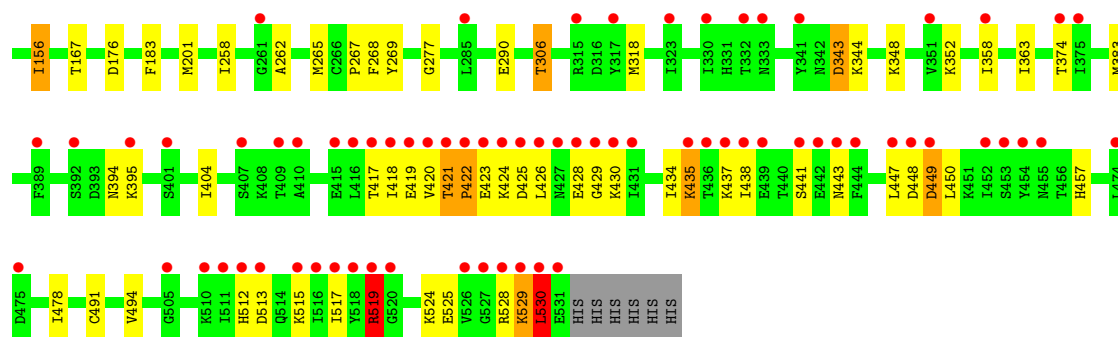


- Molecule 1: Glycoside hydrolase family 2 catalytic domain-containing protein

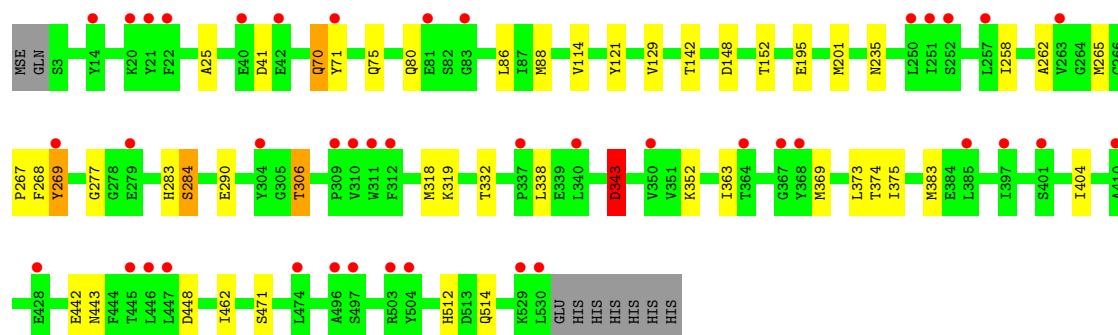


- Molecule 1: Glycoside hydrolase family 2 catalytic domain-containing protein





- Molecule 1: Glycoside hydrolase family 2 catalytic domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 112.58Å 251.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.44 49.41 – 2.44	Depositor EDS
% Data completeness (in resolution range)	93.5 (49.41-2.44) 93.4 (49.41-2.44)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.249 , 0.262 0.250 , 0.265	Depositor DCC
R_{free} test set	5365 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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

5.1 Standard geometry

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

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	0.58	0/4329	0.97	5/5835 (0.1%)
1	B	0.56	0/4338	0.96	3/5847 (0.1%)
1	C	0.58	0/4340	1.01	9/5850 (0.2%)
1	D	0.53	0/4337	0.95	4/5846 (0.1%)
All	All	0.56	0/17344	0.97	21/23378 (0.1%)

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	A	0	1
1	B	0	3
1	C	0	4
1	D	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	530	LEU	N-CA-CB	17.07	139.33	110.49
1	A	70	GLN	CB-CA-C	-7.53	97.58	109.70
1	C	530	LEU	N-CA-C	-7.49	94.84	110.80
1	C	343	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	70	GLN	CB-CA-C	-7.15	98.20	109.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	PHE	Peptide
1	B	268	PHE	Peptide
1	B	421	THR	Peptide
1	B	503	ARG	Sidechain
1	C	268	PHE	Peptide

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	4241	0	4128	59	0
1	B	4247	0	4136	41	0
1	C	4252	0	4140	51	0
1	D	4249	0	4139	42	0
2	A	12	0	9	8	0
3	A	6	0	8	14	0
3	B	12	0	16	0	0
4	A	7	0	2	1	0
5	A	167	0	0	4	0
5	B	144	0	0	7	0
5	C	31	0	0	4	0
5	D	35	0	0	1	0
All	All	17403	0	16578	186	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 6.

The worst 5 of 186 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:D:201:MSE:HE1	1:D:514:GLN:HB2	1.18	1.09
1:D:201:MSE:CE	1:D:514:GLN:HB2	1.86	1.04
1:A:24:LYS:HB3	1:A:318:MSE:HE3	1.36	1.03
1:A:173:MSE:HG2	3:A:602:GOL:C1	1.92	0.97
1:D:201:MSE:HE1	1:D:514:GLN:CB	1.93	0.97

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	525/537 (98%)	513 (98%)	11 (2%)	1 (0%)	44	53
1	B	526/537 (98%)	512 (97%)	10 (2%)	4 (1%)	16	18
1	C	526/537 (98%)	507 (96%)	15 (3%)	4 (1%)	16	18
1	D	526/537 (98%)	515 (98%)	10 (2%)	1 (0%)	44	53
All	All	2103/2148 (98%)	2047 (97%)	46 (2%)	10 (0%)	25	30

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	GLU
1	C	530	LEU
1	C	448	ASP
1	B	442	GLU
1	C	422	PRO

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	464/462 (100%)	455 (98%)	9 (2%)	52	65
1	B	465/462 (101%)	457 (98%)	8 (2%)	56	69
1	C	465/462 (101%)	444 (96%)	21 (4%)	23	32
1	D	465/462 (101%)	457 (98%)	8 (2%)	56	69
All	All	1859/1848 (101%)	1813 (98%)	46 (2%)	42	55

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	424	LYS
1	C	519	ARG
1	C	425	ASP
1	C	437	LYS
1	C	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	427	ASN
1	D	15	HIS
1	D	457	HIS
1	C	512	HIS
1	D	56	ASN

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](#)

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
3	GOL	A	602	-	5,5,5	0.41	0	5,5,5	0.95	0
3	GOL	B	601	-	5,5,5	0.14	0	5,5,5	0.43	0
4	MLA	A	604	-	6,6,6	1.84	2 (33%)	7,7,7	1.57	1 (14%)
3	GOL	B	602	-	5,5,5	0.07	0	5,5,5	0.23	0
2	ACT	A	601	-	3,3,3	1.04	0	3,3,3	0.93	0
2	ACT	A	603	-	3,3,3	1.05	0	3,3,3	0.92	0
2	ACT	A	605	-	3,3,3	1.84	1 (33%)	3,3,3	0.58	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	GOL	A	602	-	-	2/4/4/4	-
3	GOL	B	601	-	-	0/4/4/4	-
4	MLA	A	604	-	-	0/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	ACT	O-C	2.64	1.34	1.22
4	A	604	MLA	C2-C3	2.59	1.55	1.51
4	A	604	MLA	C2-C1	2.42	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	MLA	C3-C2-C1	3.27	124.33	112.87

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GOL	14	0
4	A	604	MLA	1	0
2	A	601	ACT	5	0
2	A	603	ACT	1	0
2	A	605	ACT	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	516/537 (96%)	0.11	28 (5%)	32 31	28, 40, 62, 104	0
1	B	516/537 (96%)	0.55	43 (8%)	19 18	27, 48, 71, 107	1 (0%)
1	C	517/537 (96%)	1.26	95 (18%)	4 4	51, 69, 92, 139	0
1	D	517/537 (96%)	0.85	42 (8%)	19 19	50, 66, 87, 105	0
All	All	2066/2148 (96%)	0.69	208 (10%)	14 13	27, 58, 85, 139	1 (0%)

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	429	GLY	7.3
1	A	443	ASN	7.2
1	C	424	LYS	6.6
1	D	530	LEU	6.6
1	C	419	GLU	6.6

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 oligosaccharides 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(\AA^2)	Q<0.9
2	ACT	A	605	4/4	0.79	0.17	34,38,45,61	0
2	ACT	A	603	4/4	0.84	0.19	33,45,45,48	0
4	MLA	A	604	7/7	0.85	0.17	56,64,77,81	0
2	ACT	A	601	4/4	0.86	0.13	32,43,45,48	0
3	GOL	A	602	6/6	0.87	0.36	46,63,76,79	0
3	GOL	B	602	6/6	0.88	0.15	50,57,58,67	0
3	GOL	B	601	6/6	0.93	0.12	37,44,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.