



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:56 PM UTC

PDB ID : 4YYF / pdb_00004yyf
Title : The crystal structure of a glycosyl hydrolase of GH3 family member from [Mycobacterium smegmatis str. MC2 155]
Authors : Tan, K.; Hatzos-Skintges, C.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2015-03-23
Resolution : 1.92 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

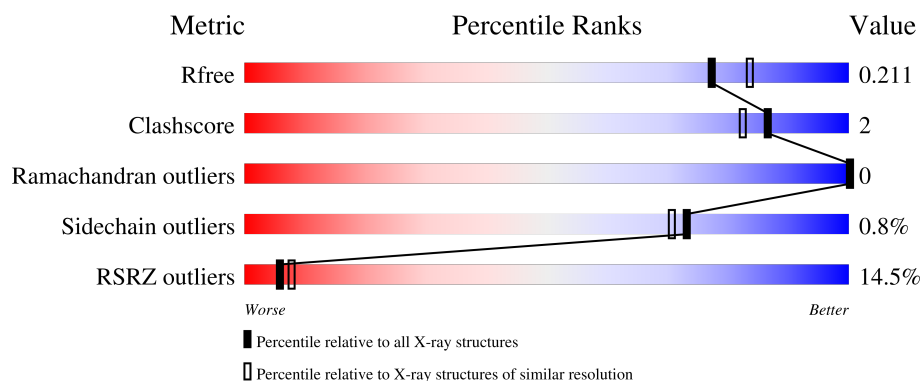
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	365	2% 88% 9%
1	B	365	2% 85% 5% 10%
1	C	365	34% 81% 7% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7645 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.

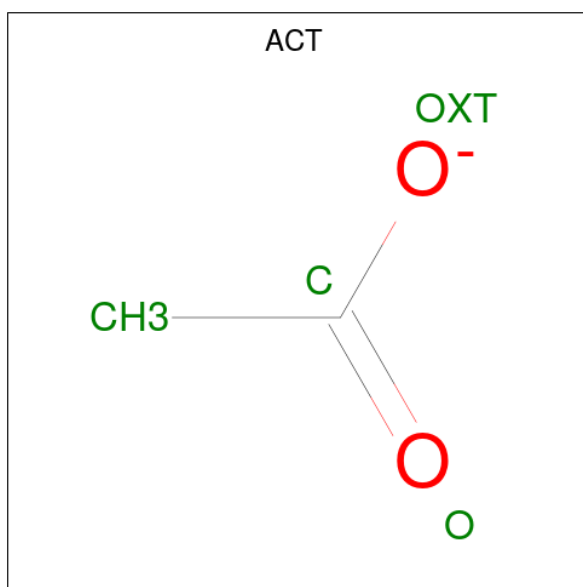
- Molecule 1 is a protein called Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	Se	0	1	0
			2387	1481	427	470	2	7			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2367	1469	422	468	1	7			
1	C	320	Total	C	N	O	S	Se	0	0	0
			2301	1430	412	451	2	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	-	expression tag	UNP A0QPD6
A	24	ASN	-	expression tag	UNP A0QPD6
A	25	ALA	-	expression tag	UNP A0QPD6
A	291	VAL	ALA	engineered mutation	UNP A0QPD6
B	23	SER	-	expression tag	UNP A0QPD6
B	24	ASN	-	expression tag	UNP A0QPD6
B	25	ALA	-	expression tag	UNP A0QPD6
B	291	VAL	ALA	engineered mutation	UNP A0QPD6
C	23	SER	-	expression tag	UNP A0QPD6
C	24	ASN	-	expression tag	UNP A0QPD6
C	25	ALA	-	expression tag	UNP A0QPD6
C	291	VAL	ALA	engineered mutation	UNP A0QPD6

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

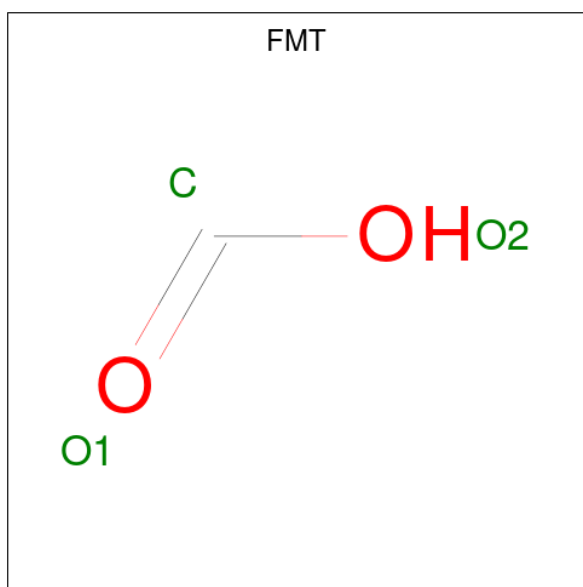


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

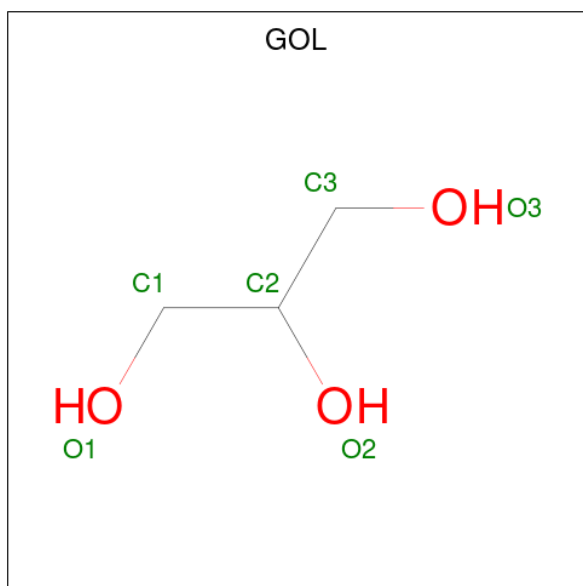
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	2	Total	Na	0	0
			2	2		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

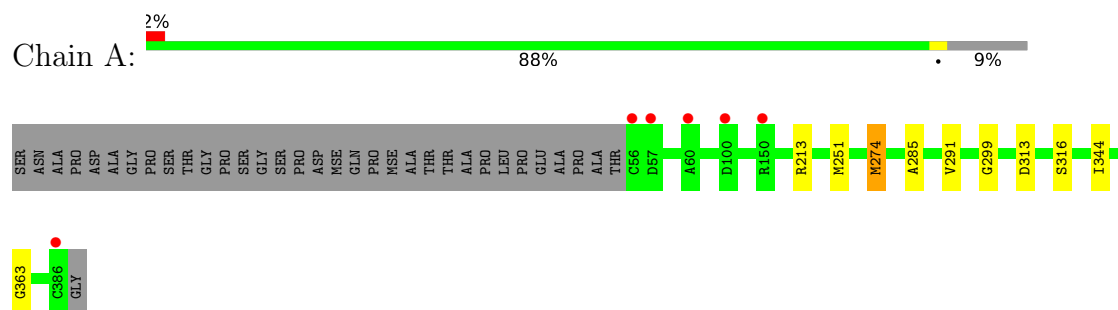
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total 236	O 236	0	0
6	B	227	Total 228	O 228	0	1
6	C	90	Total 90	O 90	0	0

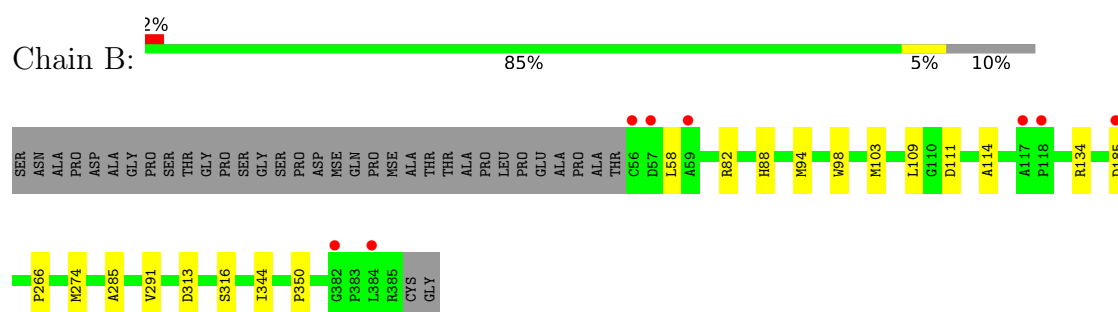
3 Residue-property plots [i](#)

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.

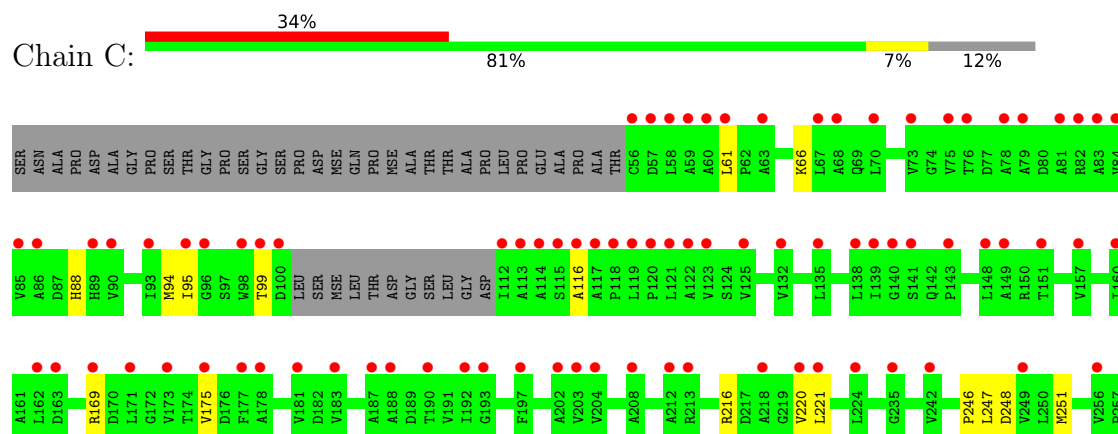
- Molecule 1: Beta-N-acetylhexosaminidase

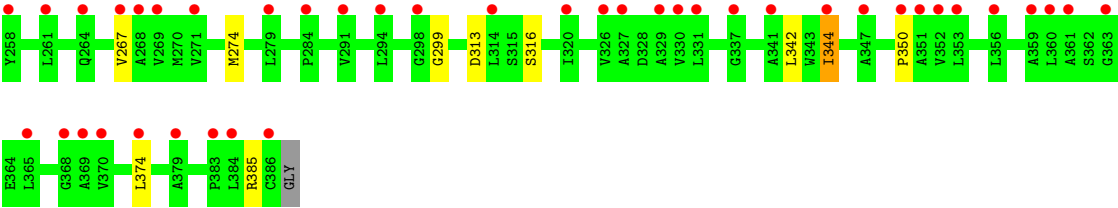


- Molecule 1: Beta-N-acetylhexosaminidase



- Molecule 1: Beta-N-acetylhexosaminidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.07Å 130.94Å 85.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.41 – 1.92 36.41 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.41-1.92) 99.0 (36.41-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.179 , 0.210 0.180 , 0.211	Depositor DCC
R_{free} test set	4378 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7645	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: FMT, NA, ACT, 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	0.50	0/2420	0.80	1/3290 (0.0%)
1	B	0.52	0/2400	0.79	0/3264
1	C	0.44	0/2334	0.77	1/3175 (0.0%)
All	All	0.49	0/7154	0.79	2/9729 (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	C	344	ILE	N-CA-C	5.82	117.76	112.29
1	A	344	ILE	N-CA-C	5.29	117.20	112.17

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	2387	0	2365	6	0
1	B	2367	0	2340	10	0
1	C	2301	0	2280	14	0
2	A	8	0	6	0	0
2	B	12	0	9	0	0
2	C	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	1	0	0
5	B	6	0	8	0	0
6	A	236	0	0	1	0
6	B	228	0	0	2	0
6	C	90	0	0	0	1
All	All	7645	0	7012	29	1

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 (29) 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:B:313:ASP:OD2	1:B:316:SER:OG	2.23	0.56
1:C:88:HIS:NE2	1:C:350:PRO:HG3	2.23	0.54
1:A:213:ARG:NH2	6:A:505:HOH:O	2.40	0.53
1:C:246:PRO:HB2	1:C:248:ASP:OD1	2.10	0.52
1:C:247:LEU:HD11	1:C:251:MSE:HE2	1.92	0.52
1:C:313:ASP:OD2	1:C:316:SER:OG	2.22	0.51
1:B:82:ARG:NH1	6:B:503:HOH:O	2.33	0.51
1:B:94:MSE:HE1	1:B:344:ILE:HG22	1.92	0.51
1:B:285:ALA:O	1:B:291:VAL:HG21	2.12	0.50
1:A:363:GLY:HA3	1:B:114:ALA:HB2	1.92	0.50
1:C:66:LYS:HG2	1:C:374:LEU:HD22	1.94	0.49
1:C:251:MSE:HE1	1:C:299:GLY:O	2.11	0.49
1:C:94:MSE:HE2	1:C:342:LEU:HD21	1.95	0.49
1:A:285:ALA:O	1:A:291:VAL:HG21	2.14	0.48
1:B:88:HIS:CE1	1:B:350:PRO:HG3	2.49	0.47
1:C:95:ILE:HG23	1:C:99:THR:HG21	1.96	0.47
1:C:94:MSE:HE1	1:C:344:ILE:HG22	1.96	0.46
1:C:116:ALA:O	1:C:385:ARG:NH1	2.48	0.46
1:A:313:ASP:OD2	1:A:316:SER:OG	2.30	0.45
1:A:251:MSE:HE1	1:A:299:GLY:O	2.18	0.43
1:B:82:ARG:NH2	1:B:111:ASP:OD2	2.48	0.43
1:B:103:MSE:HE2	1:B:109:LEU:HD13	2.00	0.43
1:C:61:LEU:O	1:C:66:LYS:HE3	2.19	0.43
1:B:94:MSE:HE3	1:B:98:TRP:CZ2	2.54	0.42
1:C:175:VAL:HG22	1:C:221:LEU:HB3	2.01	0.41
1:C:169:ARG:HG2	1:C:220:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HG2	6:B:698[A]:HOH:O	2.21	0.41
1:A:274:MSE:SE	1:A:274:MSE:H	2.54	0.41
1:C:216:ARG:HH11	1:C:267:VAL:HB	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:588:HOH:O	6:C:588:HOH:O[2_755]	2.08	0.12

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	330/365 (90%)	322 (98%)	8 (2%)	0	100	100
1	B	328/365 (90%)	320 (98%)	8 (2%)	0	100	100
1	C	316/365 (87%)	308 (98%)	8 (2%)	0	100	100
All	All	974/1095 (89%)	950 (98%)	24 (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	244/258 (95%)	243 (100%)	1 (0%)	84	83
1	B	241/258 (93%)	237 (98%)	4 (2%)	53	41
1	C	234/258 (91%)	233 (100%)	1 (0%)	84	83
All	All	719/774 (93%)	713 (99%)	6 (1%)	73	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	MSE
1	B	58	LEU
1	B	134	ARG
1	B	185	ASP
1	B	274	MSE
1	C	274	MSE

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

Mol	Chain	Res	Type
1	A	340	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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z > 2$
2	ACT	B	403	-	3,3,3	0.79	0	3,3,3	1.34	0
2	ACT	C	401	-	3,3,3	0.78	0	3,3,3	1.42	0
2	ACT	A	402	-	3,3,3	0.83	0	3,3,3	1.44	0
2	ACT	B	404	-	3,3,3	0.81	0	3,3,3	1.39	0
2	ACT	A	401	-	3,3,3	0.85	0	3,3,3	1.30	0
2	ACT	B	402	-	3,3,3	0.78	0	3,3,3	1.30	0
4	FMT	A	404	-	2,2,2	0.76	0	1,1,1	0.24	0
5	GOL	B	401	-	5,5,5	0.27	0	5,5,5	0.44	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
5	GOL	B	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	324/365 (88%)	-0.39	6 (1%) 66 73	13, 20, 35, 71	1 (0%)
1	B	323/365 (88%)	-0.39	8 (2%) 58 64	12, 20, 34, 78	0
1	C	314/365 (86%)	1.88	125 (39%) 1 0	36, 46, 66, 101	0
All	All	961/1095 (87%)	0.35	139 (14%) 6 8	12, 25, 57, 101	1 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	ILE	6.1
1	C	79	ALA	5.2
1	C	123	VAL	4.6
1	C	114	ALA	4.4
1	C	82	ARG	4.3
1	C	78	ALA	4.2
1	C	384	LEU	4.2
1	A	56	CYS	4.2
1	C	56	CYS	4.2
1	C	98	TRP	4.1
1	C	386	CYS	3.9
1	C	352	VAL	3.8
1	C	188	ALA	3.7
1	B	56	CYS	3.7
1	C	187	ALA	3.6
1	C	264	GLN	3.6
1	C	93	ILE	3.6
1	C	90	VAL	3.5
1	C	121	LEU	3.5
1	C	58	LEU	3.5
1	C	143	PRO	3.5
1	C	203	VAL	3.5
1	B	384	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	95	ILE	3.3
1	C	162	LEU	3.3
1	B	118	PRO	3.3
1	C	383	PRO	3.3
1	C	116	ALA	3.3
1	C	119	LEU	3.3
1	C	135	LEU	3.3
1	A	386	CYS	3.3
1	C	61	LEU	3.2
1	C	331	LEU	3.2
1	C	160	ILE	3.2
1	C	171	LEU	3.2
1	C	139	ILE	3.1
1	C	224	LEU	3.1
1	C	60	ALA	3.1
1	C	122	ALA	3.1
1	C	115	SER	3.1
1	C	379	ALA	3.1
1	C	360	LEU	3.1
1	C	59	ALA	3.0
1	C	117	ALA	3.0
1	B	382	GLY	2.9
1	C	351	ALA	2.9
1	C	370	VAL	2.9
1	C	368	GLY	2.9
1	C	84	VAL	2.8
1	C	202	ALA	2.8
1	C	261	LEU	2.8
1	C	249	VAL	2.8
1	C	326	VAL	2.8
1	C	363	GLY	2.7
1	C	173	VAL	2.7
1	C	86	ALA	2.7
1	C	113	ALA	2.7
1	C	208	ALA	2.7
1	C	99	THR	2.7
1	C	218	ALA	2.7
1	C	148	LEU	2.7
1	C	140	GLY	2.6
1	C	235	GLY	2.6
1	A	57	ASP	2.6
1	C	353	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	183	VAL	2.6
1	C	63	ALA	2.6
1	C	347	ALA	2.6
1	C	220	VAL	2.6
1	C	267	VAL	2.6
1	B	57	ASP	2.6
1	C	344	ILE	2.6
1	C	83	ALA	2.6
1	C	132	VAL	2.6
1	C	327	ALA	2.6
1	C	329	ALA	2.6
1	C	89	HIS	2.5
1	C	284	PRO	2.5
1	C	177	PHE	2.5
1	C	314	LEU	2.5
1	C	204	VAL	2.5
1	C	70	LEU	2.5
1	C	294	LEU	2.5
1	C	81	ALA	2.5
1	C	100	ASP	2.5
1	C	138	LEU	2.5
1	C	193	GLY	2.5
1	C	365	LEU	2.5
1	C	242	VAL	2.5
1	C	76	THR	2.4
1	A	100	ASP	2.4
1	C	279	LEU	2.4
1	C	256	VAL	2.4
1	C	320	ILE	2.4
1	C	268	ALA	2.4
1	C	125	VAL	2.3
1	C	141	SER	2.3
1	C	330	VAL	2.3
1	C	57	ASP	2.3
1	B	59	ALA	2.3
1	C	221	LEU	2.3
1	C	151	THR	2.3
1	C	350	PRO	2.3
1	C	361	ALA	2.3
1	C	356	LEU	2.3
1	C	178	ALA	2.2
1	C	73	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	374	LEU	2.2
1	C	298	GLY	2.2
1	A	60	ALA	2.2
1	C	75	VAL	2.2
1	C	157	VAL	2.2
1	B	117	ALA	2.2
1	C	212	ALA	2.2
1	C	213	ARG	2.2
1	C	181	VAL	2.2
1	C	118	PRO	2.2
1	C	85	VAL	2.1
1	C	67	LEU	2.1
1	C	149	ALA	2.1
1	C	341	ALA	2.1
1	C	359	ALA	2.1
1	C	258	TYR	2.1
1	B	185	ASP	2.1
1	C	269	VAL	2.1
1	C	163	ASP	2.1
1	C	192	ILE	2.1
1	C	120	PRO	2.1
1	C	68	ALA	2.1
1	C	96	GLY	2.0
1	C	337	GLY	2.0
1	C	369	ALA	2.0
1	C	197	PHE	2.0
1	C	190	THR	2.0
1	A	150	ARG	2.0
1	C	169	ARG	2.0
1	C	175	VAL	2.0
1	C	271	VAL	2.0
1	C	291	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 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(Å ²)	Q<0.9
2	ACT	B	404	4/4	0.73	0.20	54,55,57,60	0
2	ACT	B	403	4/4	0.79	0.25	49,53,57,65	0
4	FMT	A	404	3/3	0.85	0.16	53,53,54,55	0
2	ACT	A	402	4/4	0.88	0.16	28,30,35,38	0
5	GOL	B	401	6/6	0.94	0.09	23,32,33,33	0
2	ACT	C	401	4/4	0.95	0.16	31,32,32,33	0
3	NA	B	405	1/1	0.96	0.05	33,33,33,33	0
2	ACT	A	401	4/4	0.97	0.06	21,21,21,22	0
2	ACT	B	402	4/4	0.97	0.06	18,21,21,23	0
3	NA	A	403	1/1	0.98	0.06	20,20,20,20	0
3	NA	B	406	1/1	0.99	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.