



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:19 AM EDT

PDB ID : 9LXL / pdb_00009lxl
Title : Crystal structure of GH29 family alpha-L-fucosidase from *Fusarium proliferatum* LE1
Authors : Korban, S.A.; Borshchevskiy, V.I.; Pospelov, V.A.; Bobrov, K.S.; Ivanova, D.N.; Kulminskaya, A.A.
Deposited on : 2025-02-18
Resolution : 2.19 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

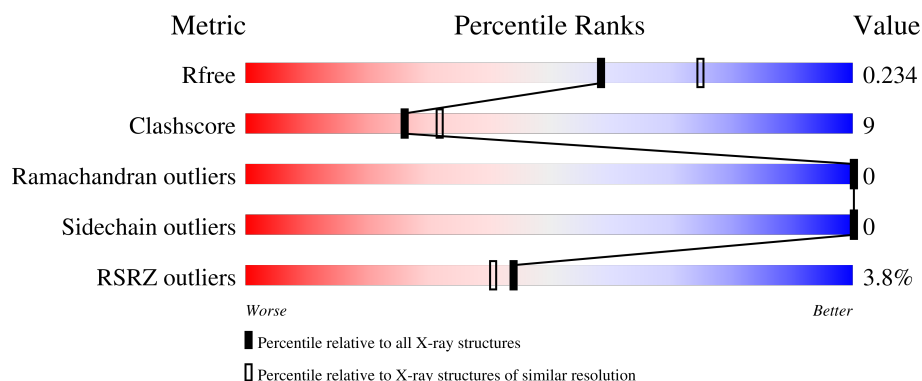
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	620	

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
6	AZI	A	708	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AZI	A	709	-	X	-	-
6	AZI	A	711	-	X	-	-
6	AZI	A	712	-	X	-	-
6	AZI	A	713	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4836 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 alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	6	0
			4512	2877	754	872	9			

There are 39 discrepancies between the modelled and reference sequences:

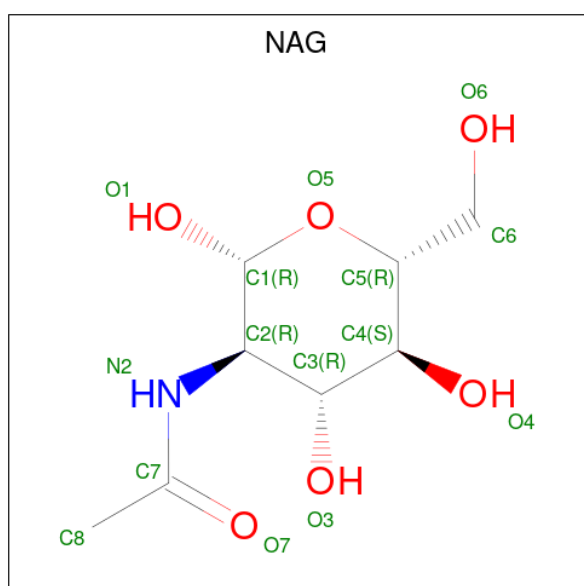
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	expression tag	UNP A0A365NIL9
A	2	THR	-	expression tag	UNP A0A365NIL9
A	456	ALA	THR	variant	UNP A0A365NIL9
A	479	LYS	GLN	variant	UNP A0A365NIL9
A	526	SER	ASN	variant	UNP A0A365NIL9
A	587	GLU	-	expression tag	UNP A0A365NIL9
A	588	ASN	-	expression tag	UNP A0A365NIL9
A	589	LEU	-	expression tag	UNP A0A365NIL9
A	590	TYR	-	expression tag	UNP A0A365NIL9
A	591	PHE	-	expression tag	UNP A0A365NIL9
A	592	GLN	-	expression tag	UNP A0A365NIL9
A	593	SER	-	expression tag	UNP A0A365NIL9
A	594	ALA	-	expression tag	UNP A0A365NIL9
A	595	ALA	-	expression tag	UNP A0A365NIL9
A	596	ALA	-	expression tag	UNP A0A365NIL9
A	597	SER	-	expression tag	UNP A0A365NIL9
A	598	PHE	-	expression tag	UNP A0A365NIL9
A	599	LEU	-	expression tag	UNP A0A365NIL9
A	600	GLU	-	expression tag	UNP A0A365NIL9
A	601	GLN	-	expression tag	UNP A0A365NIL9
A	602	LYS	-	expression tag	UNP A0A365NIL9
A	603	LEU	-	expression tag	UNP A0A365NIL9
A	604	ILE	-	expression tag	UNP A0A365NIL9
A	605	SER	-	expression tag	UNP A0A365NIL9
A	606	GLU	-	expression tag	UNP A0A365NIL9
A	607	GLU	-	expression tag	UNP A0A365NIL9
A	608	ASP	-	expression tag	UNP A0A365NIL9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	609	LEU	-	expression tag	UNP A0A365NIL9
A	610	ASN	-	expression tag	UNP A0A365NIL9
A	611	SER	-	expression tag	UNP A0A365NIL9
A	612	ALA	-	expression tag	UNP A0A365NIL9
A	613	VAL	-	expression tag	UNP A0A365NIL9
A	614	ASP	-	expression tag	UNP A0A365NIL9
A	615	HIS	-	expression tag	UNP A0A365NIL9
A	616	HIS	-	expression tag	UNP A0A365NIL9
A	617	HIS	-	expression tag	UNP A0A365NIL9
A	618	HIS	-	expression tag	UNP A0A365NIL9
A	619	HIS	-	expression tag	UNP A0A365NIL9
A	620	HIS	-	expression tag	UNP A0A365NIL9

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



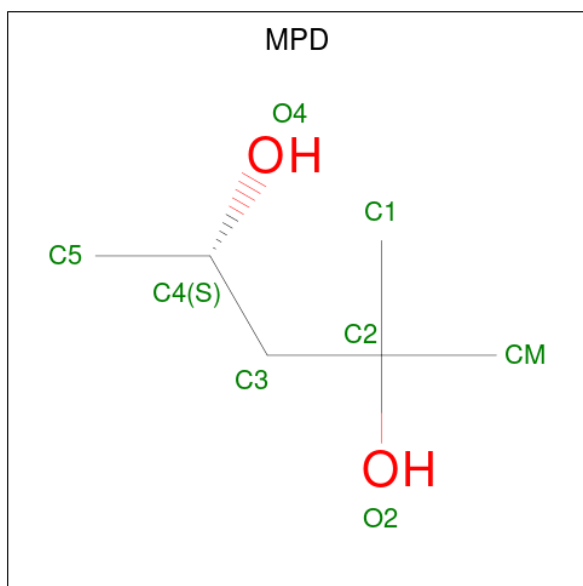
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).

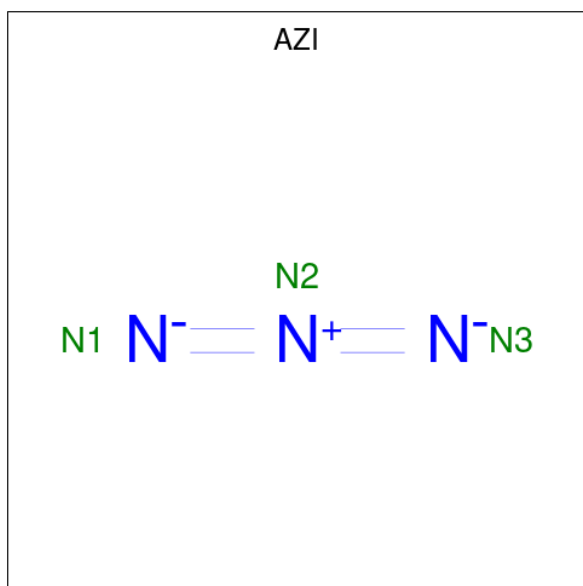


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

- 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 AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	N	0	0
			3	3		
6	A	1	Total	N	0	0
			3	3		
6	A	1	Total	N	0	0
			3	3		
6	A	1	Total	N	0	0
			3	3		
6	A	1	Total	N	0	0
			3	3		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

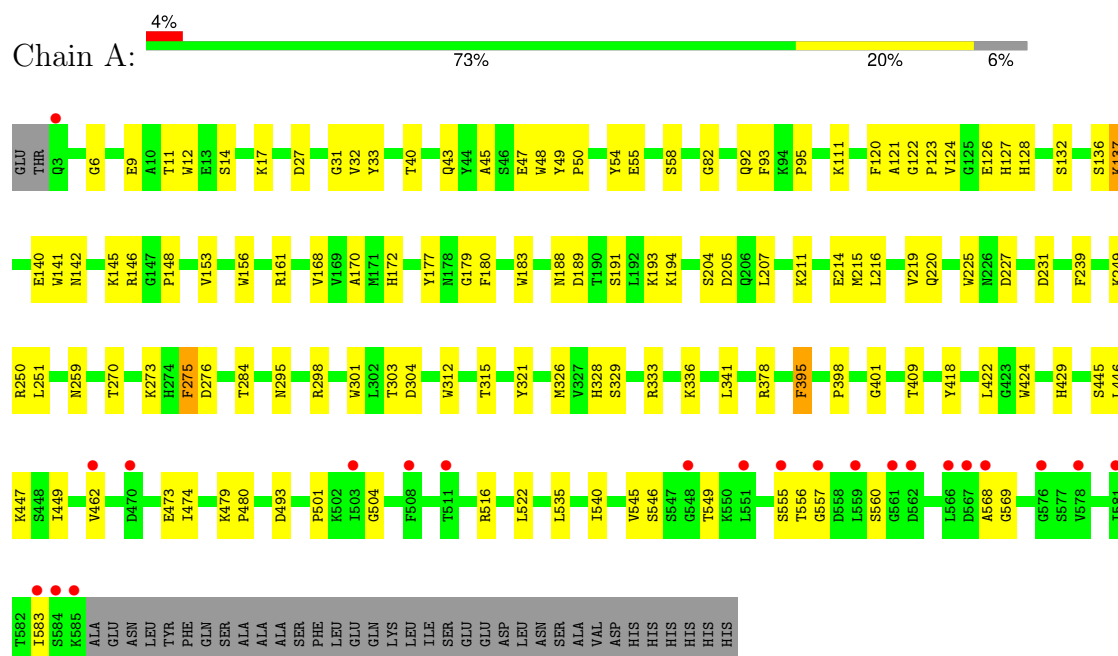
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	234	Total	O	0	0
			234	234		

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: alpha-L-fucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.76Å 76.76Å 225.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.44 – 2.19 63.44 – 2.19	Depositor EDS
% Data completeness (in resolution range)	68.0 (63.44-2.19) 68.0 (63.44-2.19)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.234 0.202 , 0.234	Depositor DCC
R_{free} test set	1233 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4836	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: TRS, AZI, MPD, NA, NAG, 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	0.73	0/4657	1.08	10/6344 (0.2%)

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	TRP	N-CA-C	-6.68	105.16	113.38
1	A	137	LYS	N-CA-C	-6.64	105.71	113.88
1	A	275	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	17	LYS	N-CA-C	-5.56	106.54	113.38
1	A	569	GLY	CA-C-O	-5.49	118.19	122.52
1	A	188	ASN	N-CA-C	-5.47	106.77	113.50
1	A	555	SER	N-CA-C	-5.45	106.63	113.28
1	A	304	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	395	PHE	CB-CA-C	5.09	118.96	111.73
1	A	557	GLY	N-CA-C	-5.04	107.45	115.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	ARG	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	4512	0	4180	81	0
2	A	42	0	39	1	0
3	A	8	0	12	2	0
4	A	16	0	28	2	0
5	A	1	0	0	0	0
6	A	15	0	0	0	0
7	A	8	0	6	0	0
8	A	234	0	0	3	0
All	All	4836	0	4265	83	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 9.

All (83) 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:A:142:ASN:HD21	1:A:145:LYS:HD2	1.44	0.82
1:A:522:LEU:HD23	1:A:583:ILE:HG22	1.68	0.74
1:A:329:SER:O	1:A:333:ARG:HG2	1.95	0.66
1:A:11:THR:HG23	1:A:14:SER:H	1.62	0.64
1:A:504:GLY:N	1:A:549:THR:HG21	2.14	0.62
1:A:55:GLU:HB3	1:A:58:SER:HB3	1.79	0.62
1:A:137:LYS:HG2	1:A:214:GLU:OE2	2.01	0.60
1:A:49:TYR:N	1:A:50:PRO:HD2	2.17	0.59
1:A:170:ALA:HA	1:A:225:TRP:HB3	1.88	0.56
1:A:45:ALA:O	1:A:315:THR:HG21	2.05	0.55
1:A:326:MET:HA	1:A:326:MET:HE2	1.88	0.55
1:A:136:SER:O	1:A:145:LYS:NZ	2.38	0.55
1:A:328:HIS:CE1	1:A:422:LEU:HB3	2.43	0.54
1:A:462:VAL:HG21	1:A:474:ILE:HG23	1.90	0.54
1:A:50:PRO:HG2	1:A:180:PHE:HZ	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ARG:HG3	1:A:535:LEU:HD13	1.90	0.54
1:A:124:VAL:HG22	1:A:170:ALA:HB3	1.90	0.53
1:A:522:LEU:HD23	1:A:583:ILE:CG2	2.36	0.53
1:A:12:TRP:CD2	1:A:251:LEU:HD21	2.45	0.51
1:A:9:GLU:HG3	1:A:11:THR:HG22	1.93	0.51
1:A:47:GLU:HG2	1:A:48:TRP:HD1	1.76	0.51
1:A:132:SER:O	1:A:142:ASN:HA	2.11	0.51
1:A:556:THR:CB	1:A:560:SER:H	2.23	0.50
1:A:225:TRP:CZ2	1:A:273:LYS:HE3	2.46	0.50
1:A:395:PHE:HZ	3:A:703:TRS:H32	1.76	0.50
1:A:142:ASN:ND2	1:A:145:LYS:HD2	2.21	0.49
1:A:295:ASN:CG	2:A:706:NAG:HN2	2.20	0.49
1:A:395:PHE:CZ	3:A:703:TRS:H32	2.48	0.49
1:A:275:PHE:HE1	8:A:802:HOH:O	1.96	0.49
1:A:270:THR:HG23	1:A:284:THR:HG23	1.95	0.48
1:A:231:ASP:N	1:A:276:ASP:OD1	2.33	0.48
1:A:40:THR:O	1:A:43:GLN:HG3	2.14	0.47
1:A:303:THR:HG21	1:A:333:ARG:NH1	2.29	0.47
1:A:82:GLY:HA2	1:A:92:GLN:HB2	1.95	0.47
1:A:127:HIS:CD2	1:A:128:HIS:H	2.32	0.47
1:A:447:LYS:HG2	1:A:493:ASP:HB2	1.97	0.47
1:A:177:TYR:CG	1:A:204:SER:HB3	2.51	0.46
1:A:111:LYS:HE2	1:A:111:LYS:HB3	1.73	0.46
1:A:189:ASP:O	1:A:193:LYS:HG3	2.15	0.46
1:A:31:GLY:HA3	1:A:120:PHE:CE2	2.51	0.45
1:A:120:PHE:CE2	1:A:341:LEU:HD13	2.51	0.45
1:A:32:VAL:O	1:A:121:ALA:HA	2.16	0.45
1:A:126:GLU:OE1	1:A:211:LYS:HD3	2.17	0.45
1:A:545:VAL:CG1	1:A:568:ALA:HA	2.46	0.45
1:A:120:PHE:HE2	1:A:341:LEU:HD13	1.80	0.45
1:A:447:LYS:HA	1:A:447:LYS:HD2	1.72	0.45
1:A:321:TYR:CE1	1:A:398:PRO:HG2	2.51	0.45
1:A:250:ARG:NH1	8:A:808:HOH:O	2.41	0.45
1:A:153:VAL:HG12	1:A:219:VAL:HG11	1.98	0.45
1:A:33:TYR:CD1	1:A:341:LEU:HG	2.52	0.44
1:A:545:VAL:HG12	1:A:546:SER:O	2.18	0.44
1:A:122:GLY:HA3	1:A:168:VAL:O	2.17	0.44
1:A:123:PRO:HB3	1:A:156:TRP:CD1	2.53	0.44
1:A:172:HIS:ND1	1:A:227:ASP:HB2	2.32	0.44
1:A:333:ARG:HD3	8:A:971:HOH:O	2.17	0.44
1:A:142:ASN:HD21	1:A:145:LYS:CD	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HG2	1:A:148:PRO:HB3	1.99	0.44
1:A:535:LEU:HD23	1:A:540:ILE:HG12	1.99	0.44
1:A:54:TYR:HB3	1:A:183:TRP:O	2.18	0.44
1:A:207:LEU:HG	1:A:211:LYS:HE3	2.00	0.44
1:A:429:HIS:CE1	1:A:473:GLU:HB3	2.52	0.43
1:A:445:SER:HB2	1:A:493:ASP:O	2.19	0.43
1:A:140:GLU:OE1	1:A:194:LYS:NZ	2.42	0.43
1:A:93:PHE:O	1:A:148:PRO:HD3	2.18	0.43
1:A:141:TRP:HA	1:A:146:ARG:HE	1.84	0.42
1:A:191:SER:O	1:A:194:LYS:HB3	2.19	0.42
1:A:479:LYS:HG3	1:A:480:PRO:HD2	2.01	0.42
1:A:249:LYS:HD3	1:A:249:LYS:HA	1.76	0.42
1:A:27:ASP:OD1	1:A:378:ARG:NH1	2.45	0.42
1:A:216:LEU:HD12	1:A:216:LEU:C	2.45	0.42
1:A:301:TRP:NE1	1:A:336:LYS:O	2.52	0.42
1:A:446:LEU:HD21	1:A:449:ILE:HD11	2.01	0.42
4:A:705:MPD:H11	4:A:705:MPD:H4	1.71	0.41
1:A:205:ASP:HB3	1:A:249:LYS:HG3	2.03	0.41
1:A:179:GLY:HA2	1:A:239:PHE:CD1	2.55	0.41
1:A:161:ARG:NH2	1:A:220:GLN:O	2.51	0.41
1:A:215:MET:HB3	1:A:215:MET:HE3	1.76	0.41
4:A:704:MPD:H11	4:A:704:MPD:H4	1.89	0.41
1:A:6:GLY:HA3	1:A:259:ASN:CG	2.45	0.41
1:A:424:TRP:CG	1:A:479:LYS:HD3	2.56	0.41
1:A:401:GLY:HA3	1:A:422:LEU:HD12	2.03	0.40
1:A:501:PRO:O	1:A:546:SER:OG	2.28	0.40
1:A:409:THR:OG1	1:A:418:TYR:HB2	2.21	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	587/620 (95%)	572 (97%)	15 (3%)	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	457/520 (88%)	457 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	388	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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	$\# Z > 2$
6	AZI	A	713	-	2,2,2	4.64	2 (100%)	0,1,1	-	-
4	MPD	A	705	-	7,7,7	0.23	0	9,10,10	0.30	0
7	ACT	A	714	-	3,3,3	1.03	0	3,3,3	0.84	0
6	AZI	A	709	-	2,2,2	3.11	2 (100%)	0,1,1	-	-
6	AZI	A	712	-	2,2,2	4.55	2 (100%)	0,1,1	-	-
4	MPD	A	704	-	7,7,7	0.23	0	9,10,10	0.32	0
6	AZI	A	708	-	2,2,2	3.07	2 (100%)	0,1,1	-	-
3	TRS	A	703	-	7,7,7	0.17	0	9,9,9	0.25	0
2	NAG	A	701	1	14,14,15	0.29	0	17,19,21	0.46	0
6	AZI	A	711	-	2,2,2	3.16	2 (100%)	0,1,1	-	-
2	NAG	A	702	1	14,14,15	0.30	0	17,19,21	0.43	0
7	ACT	A	710	-	3,3,3	1.10	0	3,3,3	0.79	0
2	NAG	A	706	1	14,14,15	0.33	0	17,19,21	1.17	2 (11%)

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
4	MPD	A	705	-	-	1/5/5/5	-
4	MPD	A	704	-	-	1/5/5/5	-
3	TRS	A	703	-	-	2/9/9/9	-
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	0/6/23/26	0/1/1/1
2	NAG	A	706	1	-	4/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	713	AZI	N1-N2	-4.66	1.13	1.23
6	A	713	AZI	N3-N2	-4.62	1.13	1.23
6	A	712	AZI	N3-N2	-4.61	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	712	AZI	N1-N2	-4.50	1.13	1.23
6	A	711	AZI	N1-N2	-3.18	1.16	1.23
6	A	711	AZI	N3-N2	-3.14	1.16	1.23
6	A	709	AZI	N1-N2	-3.11	1.16	1.23
6	A	709	AZI	N3-N2	-3.11	1.16	1.23
6	A	708	AZI	N1-N2	-3.08	1.16	1.23
6	A	708	AZI	N3-N2	-3.05	1.16	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	706	NAG	C1-O5-C5	-2.87	108.34	112.19
2	A	706	NAG	C2-N2-C7	2.29	125.97	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	706	NAG	C3-C2-N2-C7
2	A	706	NAG	C8-C7-N2-C2
2	A	706	NAG	O7-C7-N2-C2
3	A	703	TRS	N-C-C2-O2
2	A	706	NAG	O5-C5-C6-O6
3	A	703	TRS	C3-C-C2-O2
4	A	704	MPD	O2-C2-C3-C4
4	A	705	MPD	O2-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	MPD	1	0
4	A	704	MPD	1	0
3	A	703	TRS	2	0
2	A	706	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	583/620 (94%)	0.26	22 (3%) 44 41	22, 51, 112, 152	6 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	ILE	3.0
1	A	551	LEU	2.9
1	A	511	THR	2.9
1	A	548	GLY	2.9
1	A	585	LYS	2.8
1	A	462	VAL	2.8
1	A	584	SER	2.7
1	A	581	ILE	2.7
1	A	559	LEU	2.5
1	A	555	SER	2.4
1	A	578	VAL	2.3
1	A	562	ASP	2.2
1	A	567	ASP	2.2
1	A	557	GLY	2.2
1	A	3	GLN	2.2
1	A	503	ILE	2.1
1	A	566	LEU	2.1
1	A	576	GLY	2.1
1	A	508	PHE	2.1
1	A	470	ASP	2.0
1	A	568	ALA	2.0
1	A	561	GLY	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	NAG	A	706	14/15	0.43	0.17	93,109,124,131	0
6	AZI	A	713	3/3	0.70	0.20	63,63,75,80	0
6	AZI	A	709	3/3	0.72	0.19	53,53,69,76	0
3	TRS	A	703	8/8	0.77	0.19	42,54,58,61	8
2	NAG	A	701	14/15	0.78	0.14	56,77,87,92	0
7	ACT	A	714	4/4	0.79	0.12	48,67,76,84	0
4	MPD	A	705	8/8	0.83	0.17	53,63,77,81	0
6	AZI	A	712	3/3	0.85	0.34	56,56,65,71	0
2	NAG	A	702	14/15	0.86	0.12	47,52,64,72	0
6	AZI	A	708	3/3	0.87	0.12	56,56,67,75	0
7	ACT	A	710	4/4	0.88	0.10	58,60,64,69	0
5	NA	A	707	1/1	0.91	0.08	46,46,46,46	0
6	AZI	A	711	3/3	0.91	0.14	62,62,64,72	0
4	MPD	A	704	8/8	0.92	0.12	42,50,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.