



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:45 AM UTC

PDB ID : 5VVT / pdb_00005vvt
Title : Structural Investigations of the Substrate Specificity of Human O-GlcNAcase
Authors : Li, B.; Jiang, J.; Li, H.; Hu, C.-W.
Deposited on : 2017-05-20
Resolution : 2.80 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

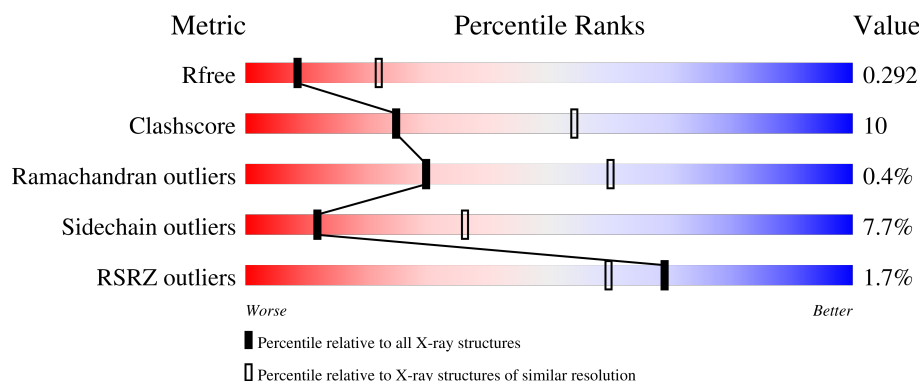
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	504	62% 20% 17%
1	C	504	59% 23% 16%
2	B	8	12% 12% 12% 75%
2	D	8	25% 12% 12% 12% 12% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7040 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 Protein O-GlcNAcase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3443	2232	567	621	23			
1	C	423	Total	C	N	O	S	0	0	0
			3477	2250	575	628	24			

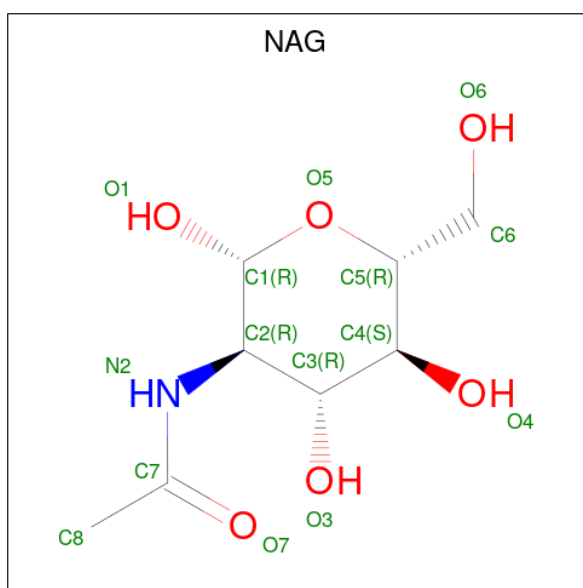
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	HIS	-	expression tag	UNP O60502
A	175	ASN	ASP	engineered mutation	UNP O60502
A	543	GLY	-	linker	UNP O60502
A	544	GLY	-	linker	UNP O60502
A	545	GLY	-	linker	UNP O60502
A	546	GLY	-	linker	UNP O60502
A	547	SER	-	linker	UNP O60502
A	548	GLY	-	linker	UNP O60502
A	549	GLY	-	linker	UNP O60502
A	550	GLY	-	linker	UNP O60502
A	551	GLY	-	linker	UNP O60502
A	552	SER	-	linker	UNP O60502
C	59	HIS	-	expression tag	UNP O60502
C	175	ASN	ASP	engineered mutation	UNP O60502
C	543	GLY	-	linker	UNP O60502
C	544	GLY	-	linker	UNP O60502
C	545	GLY	-	linker	UNP O60502
C	546	GLY	-	linker	UNP O60502
C	547	SER	-	linker	UNP O60502
C	548	GLY	-	linker	UNP O60502
C	549	GLY	-	linker	UNP O60502
C	550	GLY	-	linker	UNP O60502
C	551	GLY	-	linker	UNP O60502
C	552	SER	-	linker	UNP O60502

- Molecule 2 is a protein called ELK1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			15	10	2	3			
2	D	4	Total	C	N	O	0	0	0
			28	18	4	6			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

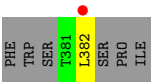
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	C	21	Total	O	0	0
			21	21		

- Molecule 1: Protein O-GlcNAcase

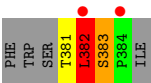
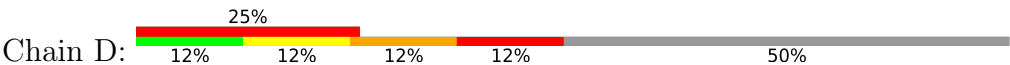




• Molecule 2: ELK1 peptide



• Molecule 2: ELK1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.36Å 95.79Å 89.32Å 90.00° 114.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.80) 99.9 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.211 , 0.291 0.211 , 0.292	Depositor DCC
R_{free} test set	1484 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7040	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: NAG

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	0.80	0/3537	1.12	5/4788 (0.1%)
1	C	0.74	0/3571	1.06	3/4831 (0.1%)
2	B	1.32	0/14	1.79	0/18
2	D	1.52	0/28	2.15	2/38 (5.3%)
All	All	0.77	0/7150	1.10	10/9675 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	381	THR	CB-CA-C	8.52	127.84	109.10
1	A	242	LEU	CA-C-N	7.89	129.70	119.84
1	A	242	LEU	C-N-CA	7.89	129.70	119.84
1	C	682	ARG	N-CA-C	6.54	119.65	109.52
1	A	391	PHE	CB-CA-C	-6.13	102.74	112.05
1	C	228	VAL	N-CA-C	5.36	115.56	110.42
1	C	304	ILE	N-CA-CB	5.35	114.10	110.52
2	D	382	LEU	N-CA-C	5.06	116.21	108.42
1	A	169	PHE	N-CA-C	5.06	116.88	109.24
1	A	309	GLY	N-CA-C	5.04	118.92	110.56

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	3443	0	3360	63	0
1	C	3477	0	3396	73	0
2	B	15	0	16	0	0
2	D	28	0	28	3	0
3	B	14	0	13	0	0
3	D	14	0	13	1	0
4	A	28	0	0	2	0
4	C	21	0	0	3	0
All	All	7040	0	6826	135	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 10.

All (135) 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:132:GLU:OE1	1:C:211:THR:HG21	1.58	1.01
1:C:663:CYS:HA	1:C:666:HIS:CE1	1.98	0.99
1:C:663:CYS:SG	4:C:819:HOH:O	2.21	0.96
1:C:663:CYS:SG	1:C:666:HIS:NE2	2.08	0.94
1:A:101:TYR:HE1	1:A:106:PHE:HB2	1.39	0.87
1:C:234:LEU:HD22	1:C:271:ILE:HD11	1.63	0.81
1:A:180:MET:HE2	1:A:191:PHE:HA	1.64	0.80
1:A:101:TYR:CE1	1:A:106:PHE:HB2	2.17	0.79
1:A:152:SER:HB3	1:A:156:ARG:HH11	1.49	0.78
1:C:132:GLU:OE1	1:C:211:THR:CG2	2.34	0.76
1:C:314:PRO:HB2	1:C:321:ASN:OD1	1.85	0.76
1:C:375:SER:H	1:C:378:MET:HE3	1.52	0.75
1:C:663:CYS:HG	1:C:666:HIS:CD2	2.00	0.70
1:C:108:ARG:NH1	1:C:142:ASP:OD2	2.20	0.68
1:A:108:ARG:NH2	1:A:142:ASP:OD1	2.27	0.67
1:C:155:LYS:HD2	1:C:205:TYR:CD2	2.31	0.65
1:A:554:THR:OG1	1:A:556:GLU:OE1	2.14	0.64
1:C:123:ILE:HD13	1:C:166:CYS:HB2	1.79	0.64
1:A:224:CYS:SG	1:A:228:VAL:HG12	2.38	0.64
1:A:584:TRP:CE2	1:A:588:ASN:ND2	2.67	0.63
1:C:67:GLY:HA2	1:C:96:ALA:O	2.01	0.61
1:C:264:ILE:HA	1:C:267:VAL:HG12	1.83	0.59
1:C:304:ILE:HD12	1:C:335:ASN:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HA	1:A:164:PHE:CD2	2.37	0.58
1:A:553:VAL:N	4:A:801:HOH:O	2.36	0.58
1:C:204:GLN:HA	1:C:208:GLU:HG3	1.85	0.58
1:A:101:TYR:HD1	1:A:102:LYS:N	2.01	0.58
1:A:152:SER:C	1:A:156:ARG:HD3	2.29	0.57
1:A:554:THR:HG22	1:A:557:ASP:OD2	2.05	0.57
3:D:401:NAG:O7	3:D:401:NAG:H3	2.06	0.56
2:D:382:LEU:HG	2:D:383:SER:N	2.21	0.56
1:C:277:ILE:HB	1:C:310:VAL:HG23	1.86	0.55
1:C:663:CYS:SG	1:C:666:HIS:CE1	2.96	0.55
1:C:145:PHE:HE1	1:C:198:ILE:HD11	1.72	0.54
1:A:200:ASN:ND2	1:A:242:LEU:HG	2.22	0.54
1:A:584:TRP:CD2	1:A:610:ARG:NH2	2.75	0.54
1:A:578:MET:HE3	1:A:617:MET:HB3	1.90	0.54
1:C:670:GLN:OE1	1:C:671:PHE:N	2.41	0.53
1:A:152:SER:HB3	1:A:156:ARG:NH1	2.22	0.53
1:C:193:HIS:CD2	1:C:236:THR:HG21	2.44	0.52
1:A:80:GLU:OE1	1:A:83:ARG:NH2	2.41	0.52
1:C:145:PHE:CE1	1:C:198:ILE:HD11	2.44	0.52
1:A:107:TRP:O	1:A:157:LYS:HD2	2.09	0.52
1:A:66:GLU:HG2	1:A:97:PRO:HB3	1.92	0.51
1:A:108:ARG:NH1	1:A:150:GLU:OE2	2.44	0.51
1:C:580:ARG:HA	1:C:583:GLN:OE1	2.11	0.50
1:C:169:PHE:O	1:C:212:PHE:HA	2.12	0.50
1:C:606:GLU:O	1:C:609:SER:HB3	2.12	0.50
1:A:264:ILE:HA	1:A:267:VAL:HG12	1.93	0.50
1:C:102:LYS:NZ	1:C:115:GLU:OE2	2.43	0.50
1:C:120:MET:HE2	1:C:164:PHE:HD1	1.77	0.50
1:A:567:LEU:HB3	1:A:568:PRO:HD2	1.93	0.49
1:C:120:MET:HG3	1:C:164:PHE:O	2.12	0.49
1:C:155:LYS:HG2	1:C:202:ILE:HD13	1.94	0.49
1:C:284:ASN:ND2	1:C:316:CYS:H	2.10	0.49
1:A:300:SER:OG	1:A:302:GLU:HG3	2.13	0.48
1:A:560:LEU:O	1:A:564:LEU:HG	2.13	0.48
1:A:200:ASN:HD22	1:A:242:LEU:HG	1.78	0.48
1:C:175:ASN:HB3	2:D:382:LEU:O	2.12	0.48
1:C:284:ASN:HD22	1:C:315:ASN:HA	1.78	0.48
1:A:152:SER:O	1:A:156:ARG:HD3	2.14	0.48
1:A:249:TRP:O	1:A:277:ILE:HA	2.14	0.47
1:A:627:ARG:NH2	4:A:802:HOH:O	2.45	0.47
1:C:561:LEU:HD22	1:C:628:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TRP:C	1:A:333:LYS:H	2.23	0.47
1:C:560:LEU:O	1:C:564:LEU:HG	2.14	0.47
1:A:74:VAL:O	1:A:78:ARG:HG3	2.14	0.47
1:A:136:ALA:HA	1:A:170:ALA:O	2.15	0.47
1:A:242:LEU:HA	1:A:243:PRO:HD2	1.78	0.47
1:A:653:MET:HE3	1:A:653:MET:HB2	1.75	0.46
1:A:267:VAL:O	1:A:271:ILE:HG12	2.16	0.46
1:A:95:TYR:O	1:A:136:ALA:HB3	2.16	0.46
1:C:231:SER:O	1:C:235:ARG:HB2	2.16	0.46
1:A:111:TYR:H	1:A:160:GLN:HE22	1.63	0.46
1:A:232:PRO:O	1:A:235:ARG:HG2	2.16	0.46
1:C:196:VAL:HG12	1:C:241:LEU:HD13	1.97	0.46
1:A:78:ARG:O	1:A:81:LEU:HB3	2.16	0.45
1:C:120:MET:HE2	1:C:164:PHE:CD1	2.50	0.45
1:A:297:LYS:NZ	1:A:570:GLU:OE2	2.48	0.45
1:A:177:ASP:N	1:A:177:ASP:OD1	2.49	0.45
1:A:145:PHE:HB3	1:A:188:PHE:CE2	2.52	0.45
1:A:231:SER:HB3	1:A:234:LEU:HB2	1.99	0.45
1:C:584:TRP:CD2	1:C:610:ARG:NH1	2.84	0.45
1:C:663:CYS:CA	1:C:666:HIS:CE1	2.86	0.45
1:C:645:TRP:CD1	1:C:645:TRP:C	2.95	0.45
1:C:246:GLU:CD	1:C:308:LYS:HD2	2.42	0.45
1:A:79:LYS:HE3	1:A:79:LYS:HB2	1.89	0.44
1:C:204:GLN:HB2	4:C:808:HOH:O	2.17	0.44
1:C:271:ILE:HG23	1:C:273:ARG:HD2	1.99	0.44
1:C:584:TRP:CE2	1:C:610:ARG:NH1	2.85	0.44
1:A:107:TRP:CD1	1:A:139:PRO:HA	2.53	0.44
1:A:225:TYR:HD1	1:A:226:PRO:HA	1.81	0.44
1:A:248:LEU:HA	1:A:276:VAL:O	2.17	0.44
1:C:62:CYS:O	1:C:90:LEU:HB3	2.17	0.44
1:A:111:TYR:N	1:A:160:GLN:HE22	2.16	0.44
1:A:225:TYR:HA	1:A:226:PRO:HA	1.76	0.44
1:C:69:TYR:OH	2:D:382:LEU:HB3	2.18	0.44
1:A:569:TYR:CZ	1:C:678:PRO:HG3	2.53	0.44
1:C:193:HIS:HD2	1:C:236:THR:HG21	1.81	0.44
1:C:127:ARG:HE	1:C:127:ARG:HB2	1.62	0.44
1:C:381:LYS:NZ	4:C:804:HOH:O	2.51	0.44
1:C:248:LEU:HA	1:C:276:VAL:O	2.18	0.43
1:A:155:LYS:HB3	1:A:205:TYR:CE2	2.53	0.43
1:A:622:MET:HE2	1:A:652:SER:HA	1.99	0.43
1:C:264:ILE:HG13	1:C:307:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:THR:HB	1:C:335:ASN:HD22	1.83	0.43
1:A:70:GLY:HA2	1:C:641:TYR:CD2	2.54	0.43
1:A:648:LYS:HE3	1:A:648:LYS:HB3	1.68	0.43
1:C:216:PRO:HG2	1:C:219:TYR:HA	2.01	0.43
1:A:215:CYS:HB2	1:A:248:LEU:HD12	2.00	0.43
1:A:256:SER:HB3	1:A:258:GLU:O	2.18	0.43
1:C:107:TRP:CZ3	1:C:108:ARG:HG3	2.54	0.43
1:A:686:ALA:HB1	1:C:650:ILE:HD12	2.01	0.42
1:C:329:ALA:O	1:C:333:LYS:HG3	2.19	0.42
1:A:279:ASP:OD2	1:A:296:TYR:OH	2.26	0.42
1:C:200:ASN:HD21	1:C:241:LEU:HD12	1.85	0.42
1:C:180:MET:O	1:C:185:LYS:HE2	2.19	0.42
1:C:249:TRP:O	1:C:277:ILE:HA	2.19	0.42
1:C:651:MET:HA	1:C:651:MET:HE3	2.00	0.42
1:C:192:ALA:O	1:C:196:VAL:HG22	2.19	0.42
1:A:264:ILE:HG13	1:A:303:LEU:HD22	2.02	0.42
1:C:107:TRP:O	1:C:157:LYS:NZ	2.47	0.42
1:C:203:TYR:HB2	1:C:245:ILE:HD11	2.01	0.41
1:A:94:LEU:HD11	1:A:136:ALA:HB2	2.00	0.41
1:C:124:SER:HA	1:C:127:ARG:HH21	1.85	0.41
1:C:225:TYR:CD1	1:C:226:PRO:HA	2.55	0.41
1:C:147:ASN:HA	1:C:148:PRO:HD3	1.82	0.41
1:C:660:TRP:HZ2	1:C:670:GLN:HA	1.85	0.41
1:A:210:GLU:HG3	1:A:211:THR:N	2.36	0.41
1:A:614:PHE:HA	1:A:617:MET:HE3	2.02	0.41
1:A:108:ARG:HH12	1:A:150:GLU:CD	2.28	0.40
1:C:94:LEU:HD11	1:C:136:ALA:HB2	2.03	0.40
1:C:319:GLU:HG3	1:C:635:THR:HG22	2.03	0.40
1:C:107:TRP:CE2	1:C:139:PRO:HB3	2.56	0.40
1:C:239:GLU:OE2	1:C:272:LYS:HE2	2.20	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	409/504 (81%)	378 (92%)	29 (7%)	2 (0%)	24	55
1	C	413/504 (82%)	384 (93%)	28 (7%)	1 (0%)	43	72
2	D	2/8 (25%)	1 (50%)	1 (50%)	0	100	100
All	All	824/1016 (81%)	763 (93%)	58 (7%)	3 (0%)	30	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASP
1	A	314	PRO
1	C	314	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	370/442 (84%)	349 (94%)	21 (6%)	18	49
1	C	376/442 (85%)	342 (91%)	34 (9%)	9	28
2	B	2/8 (25%)	1 (50%)	1 (50%)	0	0
2	D	4/8 (50%)	2 (50%)	2 (50%)	0	0
All	All	752/900 (84%)	694 (92%)	58 (8%)	12	36

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	120	MET
1	A	151	VAL
1	A	177	ASP
1	A	180	MET
1	A	202	ILE

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Mol	Chain	Res	Type
1	A	210	GLU
1	A	273	ARG
1	A	290	ARG
1	A	301	THR
1	A	307	LEU
1	A	314	PRO
1	A	330	THR
1	A	382	LEU
1	A	393	VAL
1	A	616	GLU
1	A	622	MET
1	A	629	SER
1	A	663	CYS
1	A	695	ILE
1	A	699	ASN
2	B	382	LEU
1	C	76	GLU
1	C	100	ASP
1	C	101	TYR
1	C	105	MET
1	C	113	VAL
1	C	119	LEU
1	C	137	ILE
1	C	141	LEU
1	C	153	THR
1	C	154	LEU
1	C	163	GLN
1	C	178	HIS
1	C	198	ILE
1	C	199	THR
1	C	208	GLU
1	C	210	GLU
1	C	211	THR
1	C	213	LEU
1	C	228	VAL
1	C	242	LEU
1	C	271	ILE
1	C	273	ARG
1	C	284	ASN
1	C	304	ILE
1	C	386	GLU
1	C	553	VAL

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Mol	Chain	Res	Type
1	C	586	ARG
1	C	589	SER
1	C	608	ARG
1	C	613	LYS
1	C	631	CYS
1	C	649	SER
1	C	682	ARG
1	C	688	GLU
2	D	382	LEU
2	D	383	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	178	HIS
1	A	227	ASN
1	C	86	GLN
1	C	175	ASN
1	C	200	ASN
1	C	335	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](#)

2 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	NAG	B	401	2	14,14,15	4.05	6 (42%)	17,19,21	3.23	9 (52%)
3	NAG	D	401	2	14,14,15	3.24	6 (42%)	17,19,21	2.94	9 (52%)

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	NAG	B	401	2	-	2/6/23/26	0/1/1/1
3	NAG	D	401	2	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAG	C1-C2	12.40	1.69	1.52
3	D	401	NAG	C1-C2	9.27	1.65	1.52
3	B	401	NAG	C3-C2	4.56	1.62	1.52
3	B	401	NAG	C8-C7	4.46	1.59	1.50
3	D	401	NAG	C3-C2	4.27	1.61	1.52
3	B	401	NAG	O5-C1	3.61	1.49	1.43
3	D	401	NAG	C7-N2	3.37	1.45	1.34
3	D	401	NAG	C8-C7	2.99	1.56	1.50
3	B	401	NAG	C6-C5	2.81	1.61	1.51
3	B	401	NAG	O5-C5	2.62	1.48	1.43
3	D	401	NAG	C4-C5	2.39	1.58	1.53
3	D	401	NAG	C6-C5	2.21	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	C1-O5-C5	7.44	122.16	112.19
3	D	401	NAG	C3-C4-C5	-6.97	97.59	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	C8-C7-N2	5.45	125.15	116.12
3	B	401	NAG	C3-C4-C5	-5.21	100.78	110.23
3	D	401	NAG	C8-C7-N2	4.73	123.96	116.12
3	B	401	NAG	O3-C3-C2	-4.26	100.55	109.40
3	D	401	NAG	O5-C1-C2	4.12	117.67	111.29
3	D	401	NAG	C1-O5-C5	3.95	117.48	112.19
3	B	401	NAG	O5-C5-C4	-3.43	102.49	110.83
3	D	401	NAG	O7-C7-C8	-2.78	117.11	122.05
3	B	401	NAG	O7-C7-C8	-2.68	117.27	122.05
3	D	401	NAG	C6-C5-C4	-2.63	106.57	113.02
3	B	401	NAG	O3-C3-C4	-2.58	104.30	110.38
3	D	401	NAG	O5-C5-C4	-2.55	104.61	110.83
3	B	401	NAG	O7-C7-N2	-2.50	117.57	121.98
3	B	401	NAG	C6-C5-C4	-2.45	107.00	113.02
3	D	401	NAG	O4-C4-C3	-2.43	104.65	110.38
3	D	401	NAG	O3-C3-C2	-2.25	104.73	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	C1-C2-N2-C7
3	D	401	NAG	C3-C2-N2-C7
3	B	401	NAG	C3-C2-N2-C7
3	D	401	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	NAG	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 [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	419/504 (83%)	-0.20	6 (1%) 73 64	29, 61, 105, 132	0
1	C	423/504 (83%)	-0.05	5 (1%) 76 68	42, 74, 101, 143	0
2	B	2/8 (25%)	2.07	1 (50%) 0 0	76, 76, 76, 90	0
2	D	4/8 (50%)	2.24	2 (50%) 0 0	93, 105, 112, 121	0
All	All	848/1024 (82%)	-0.11	14 (1%) 69 60	29, 70, 103, 143	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	382	LEU	4.4
1	C	59	HIS	3.6
1	A	604	ILE	3.6
1	C	373	LEU	3.4
2	B	382	LEU	3.4
1	A	101	TYR	3.3
1	C	178	HIS	2.9
1	A	679	TRP	2.8
2	D	384	PRO	2.8
1	A	695	ILE	2.3
1	A	696	ASP	2.3
1	C	671	PHE	2.2
1	A	113	VAL	2.1
1	C	134	ILE	2.1

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($\text{\AA}^2$)	Q<0.9
3	NAG	B	401	14/15	0.95	0.08	41,47,55,56	0
3	NAG	D	401	14/15	0.98	0.05	48,53,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.