



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:50 AM BST

PDB ID : 5VVU
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 : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

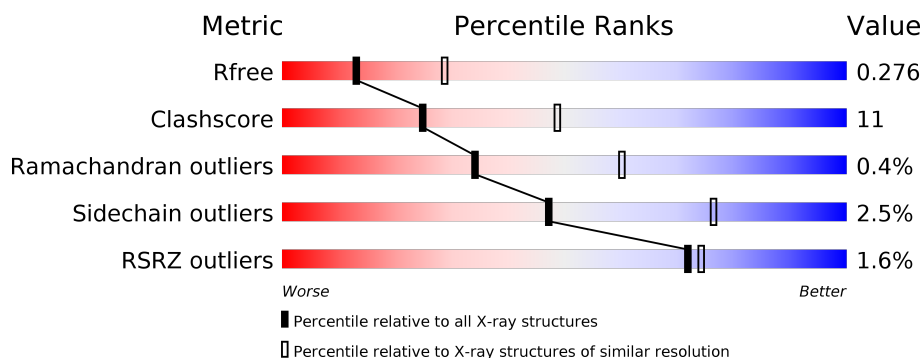
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	<div> <div></div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	504	<div> <div></div> <div> <div></div> <div>66%</div> <div>18%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	7	<div> <div>14%</div> <div> <div></div> <div>14%</div> <div>29%</div> <div>14%</div> <div>43%</div> </div> </div>
2	D	7	<div> <div>29%</div> <div> <div></div> <div>14%</div> <div>43%</div> <div>43%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7140 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	424	Total	C	N	O	S	0	0	0
			3480	2254	575	628	23			
1	C	429	Total	C	N	O	S	0	0	0
			3520	2279	581	636	24			

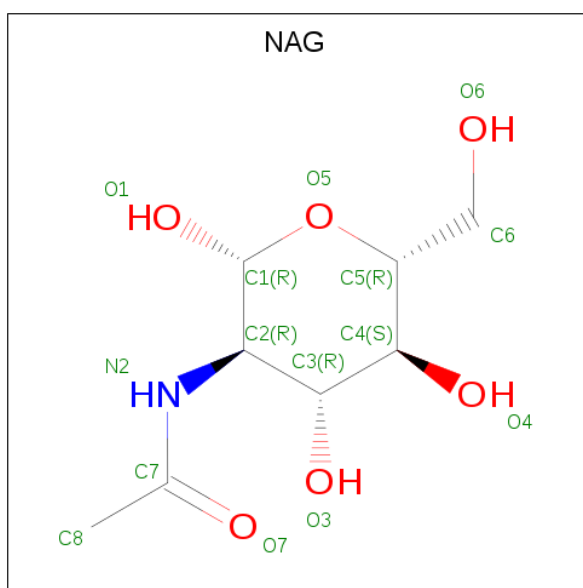
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	HIS	-	expression tag	UNP O60502
A	175	ASN	ASP	conflict	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	conflict	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 TAB1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	0	0	0
			31	20	4	7			
2	D	4	Total	C	N	O	0	0	0
			31	20	4	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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		

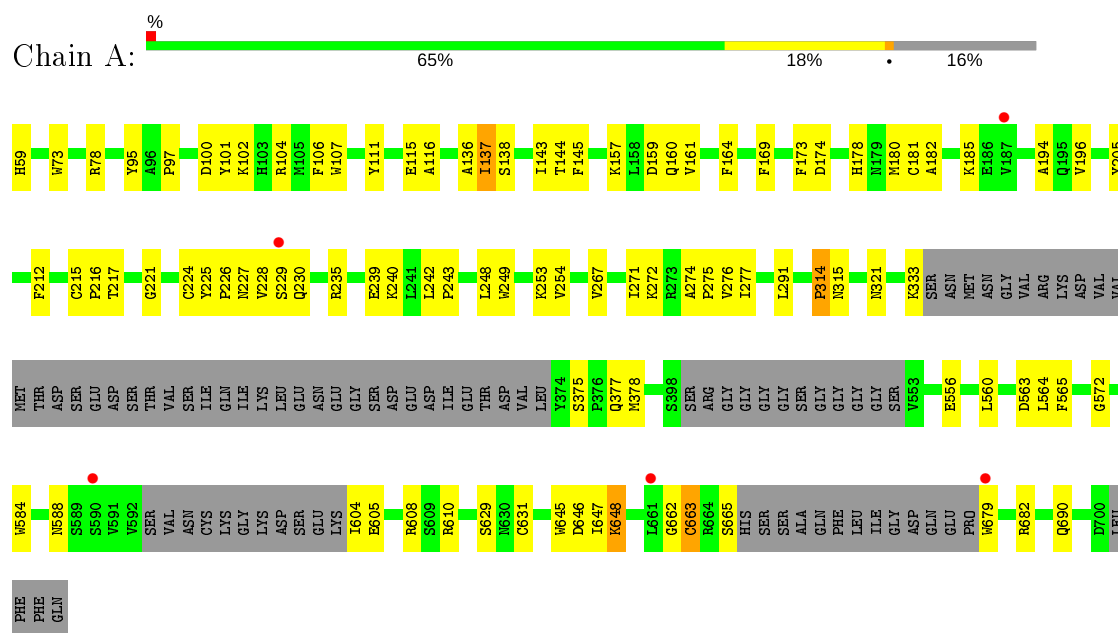
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	C	20	Total	O	0	0
			20	20		
4	D	1	Total	O	0	0
			1	1		

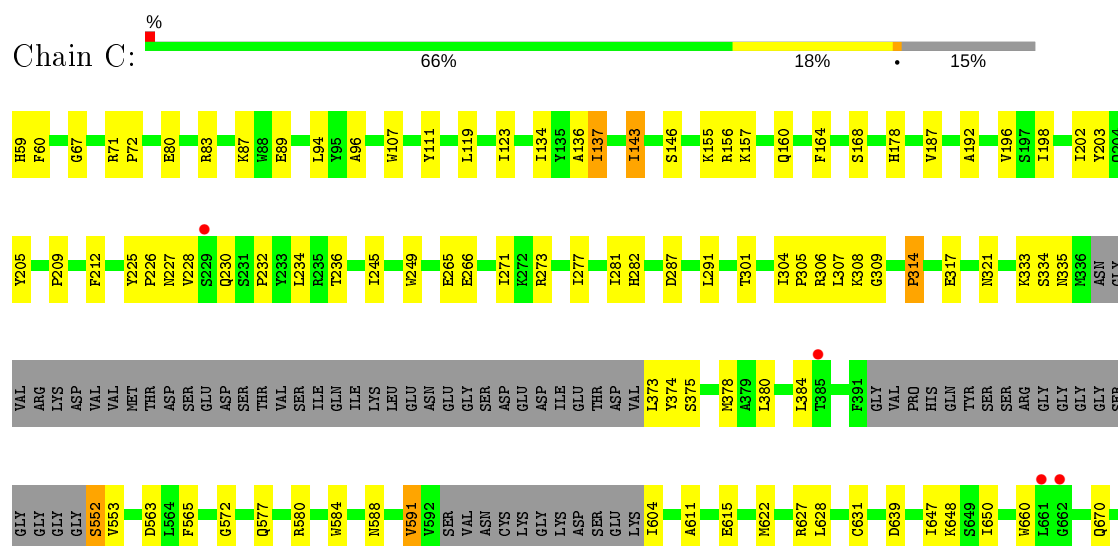
3 Residue-property plots

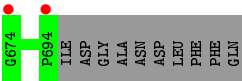
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein O-GlcNAcase

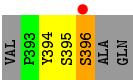


• Molecule 1: Protein O-GlcNAcase

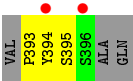




• Molecule 2: TAB1 peptide



• Molecule 2: TAB1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.51Å 96.06Å 88.97Å 90.00° 114.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 44.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 99.8 (44.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.208 , 0.275 0.208 , 0.276	Depositor DCC
R_{free} test set	1656 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	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	7140	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: 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	0.66	0/3574	0.79	1/4838 (0.0%)
1	C	0.63	0/3615	0.77	2/4893 (0.0%)
2	B	0.76	0/32	1.10	0/42
2	D	1.02	0/32	0.96	0/42
All	All	0.65	0/7253	0.78	3/9815 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	CYS	CA-CB-SG	5.90	124.61	114.00
1	C	287	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	287	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3480	0	3401	76	0
1	C	3520	0	3442	73	0
2	B	31	0	25	2	0
2	D	31	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	D	14	0	13	0	0
4	A	29	0	0	7	0
4	C	20	0	0	3	0
4	D	1	0	0	0	0
All	All	7140	0	6919	151	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 11.

All (151) 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:622:MET:SD	1:C:648:LYS:CE	2.24	1.25
1:C:622:MET:SD	1:C:648:LYS:HE3	1.77	1.25
1:C:622:MET:CG	1:C:648:LYS:HE3	1.67	1.22
1:C:622:MET:SD	1:C:648:LYS:HE2	1.98	0.98
1:C:622:MET:HA	1:C:648:LYS:HE3	1.50	0.93
1:A:315:ASN:H	1:A:321:ASN:HD21	1.12	0.92
1:C:160:GLN:O	4:C:801:HOH:O	1.86	0.91
1:C:622:MET:CG	1:C:648:LYS:CE	2.49	0.89
1:C:622:MET:HA	1:C:648:LYS:CE	2.03	0.89
1:C:622:MET:HG3	1:C:648:LYS:HE3	1.57	0.85
1:A:604:ILE:HG23	1:A:605:GLU:OE1	1.76	0.84
1:A:78:ARG:HH12	1:A:95:TYR:HE2	1.25	0.81
1:C:622:MET:CA	1:C:648:LYS:HE3	2.13	0.77
1:A:101:TYR:CE1	1:A:106:PHE:CD2	2.74	0.76
1:C:156:ARG:NH2	1:C:205:TYR:OH	2.20	0.74
1:C:271:ILE:HG22	1:C:273:ARG:HG2	1.70	0.73
1:C:622:MET:HG3	1:C:648:LYS:CE	2.14	0.73
1:C:314:PRO:HB2	1:C:321:ASN:OD1	1.89	0.72
1:A:101:TYR:CE1	1:A:106:PHE:HD2	2.06	0.72
1:C:111:TYR:H	1:C:160:GLN:HE22	1.35	0.72
1:A:145:PHE:CD2	1:A:194:ALA:HB1	2.25	0.72
1:A:101:TYR:CZ	1:A:106:PHE:CD2	2.78	0.72
1:C:622:MET:CB	1:C:648:LYS:HE3	2.19	0.72
1:C:584:TRP:CE2	1:C:588:ASN:ND2	2.60	0.70
1:C:83:ARG:HG2	1:C:87:LYS:HE3	1.73	0.69
1:A:102:LYS:NZ	1:A:115:GLU:OE1	2.26	0.69
1:A:315:ASN:H	1:A:321:ASN:ND2	1.87	0.68
1:C:107:TRP:HB2	1:C:137:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:TRP:HB3	1:A:682:ARG:HB2	1.76	0.67
1:C:622:MET:HA	1:C:648:LYS:CD	2.24	0.67
1:A:78:ARG:NH1	1:A:95:TYR:HE2	1.93	0.67
1:A:230:GLN:HA	1:A:235:ARG:HH22	1.59	0.67
1:C:107:TRP:CH2	1:C:143:ILE:HD12	2.31	0.65
1:A:161:VAL:HA	1:A:164:PHE:HD2	1.61	0.65
1:A:333:LYS:O	4:A:801:HOH:O	2.15	0.65
1:A:315:ASN:N	1:A:321:ASN:HD21	1.90	0.65
1:A:145:PHE:HD2	1:A:194:ALA:HB1	1.62	0.64
1:A:116:ALA:HA	1:A:164:PHE:CZ	2.36	0.61
1:C:164:PHE:N	4:C:801:HOH:O	2.33	0.61
1:A:174:ASP:HA	4:A:802:HOH:O	2.01	0.61
1:A:217:THR:HA	4:A:802:HOH:O	2.00	0.61
1:C:111:TYR:N	1:C:160:GLN:HE22	2.00	0.60
1:A:375:SER:HB3	1:A:378:MET:HB2	1.82	0.60
1:A:216:PRO:O	4:A:802:HOH:O	2.17	0.60
1:A:161:VAL:HA	1:A:164:PHE:CD2	2.37	0.60
1:C:291:LEU:O	1:C:565:PHE:HB3	2.02	0.60
1:C:155:LYS:HD3	1:C:205:TYR:CD2	2.40	0.56
1:A:230:GLN:HA	1:A:235:ARG:NH2	2.20	0.56
1:A:230:GLN:CD	1:A:235:ARG:HH22	2.10	0.55
2:D:393:PRO:O	2:D:394:TYR:HD1	1.89	0.55
1:C:232:PRO:O	1:C:236:THR:HG23	2.07	0.54
1:C:304:ILE:HD12	1:C:335:ASN:HB3	1.89	0.54
1:A:111:TYR:HB2	1:A:160:GLN:HE22	1.72	0.54
1:C:553:VAL:HG21	1:C:628:LEU:HD23	1.90	0.54
1:A:107:TRP:HB2	1:A:137:ILE:HD11	1.90	0.53
2:B:394:TYR:O	2:B:396:SER:N	2.42	0.53
1:A:556:GLU:H	1:A:556:GLU:CD	2.12	0.53
1:C:622:MET:SD	1:C:648:LYS:CD	2.96	0.53
1:C:591:VAL:O	1:C:591:VAL:HG12	2.09	0.52
1:C:234:LEU:HD22	1:C:271:ILE:HD11	1.91	0.52
1:A:159:ASP:OD1	1:A:205:TYR:HE2	1.93	0.52
1:A:564:LEU:HD13	1:A:647:ILE:HG12	1.91	0.51
1:A:663:CYS:SG	1:A:665:SER:O	2.66	0.51
1:A:101:TYR:OH	1:A:106:PHE:CD2	2.62	0.50
1:A:314:PRO:HB2	1:A:321:ASN:ND2	2.26	0.50
1:C:552:SER:O	1:C:627:ARG:HD2	2.12	0.50
1:C:212:PHE:HD1	1:C:245:ILE:HG23	1.76	0.50
1:C:304:ILE:HB	1:C:305:PRO:HD3	1.93	0.50
1:C:375:SER:OG	1:C:378:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:ND2	1:A:229:SER:OG	2.45	0.50
1:A:584:TRP:CE2	1:A:588:ASN:ND2	2.80	0.50
1:A:216:PRO:C	4:A:802:HOH:O	2.49	0.49
1:A:196:VAL:HG11	1:A:240:LYS:HB3	1.94	0.49
1:C:563:ASP:HA	1:C:572:GLY:HA3	1.95	0.49
1:A:173:PHE:C	4:A:802:HOH:O	2.51	0.49
1:C:111:TYR:HB2	1:C:160:GLN:NE2	2.28	0.49
1:A:608:ARG:HH21	1:A:662:GLY:HA2	1.78	0.48
1:A:95:TYR:O	1:A:136:ALA:HB3	2.13	0.48
1:A:560:LEU:O	1:A:564:LEU:HG	2.13	0.48
2:D:393:PRO:C	2:D:394:TYR:HD1	2.17	0.48
1:A:254:VAL:HG11	2:B:395:SER:HB3	1.95	0.48
1:C:380:LEU:HD12	1:C:384:LEU:HD13	1.94	0.48
1:C:80:GLU:OE2	1:C:83:ARG:NH2	2.46	0.48
1:C:604:ILE:N	4:C:808:HOH:O	2.47	0.48
1:A:104:ARG:HG3	1:A:138:SER:HB2	1.96	0.47
1:C:227:ASN:OD1	1:C:230:GLN:N	2.47	0.47
1:A:144:THR:HG23	1:A:181:CYS:SG	2.54	0.47
1:A:291:LEU:O	1:A:565:PHE:HB3	2.14	0.47
1:C:134:ILE:HG12	1:C:168:SER:HB2	1.95	0.47
1:A:224:CYS:SG	1:A:228:VAL:HG22	2.54	0.47
1:C:60:PHE:HE2	1:C:307:LEU:O	1.96	0.47
1:C:660:TRP:HZ2	1:C:670:GLN:HA	1.80	0.47
1:C:134:ILE:HG12	1:C:168:SER:CB	2.45	0.47
1:C:146:SER:HB2	1:C:187:VAL:HG21	1.97	0.47
1:C:234:LEU:HA	1:C:234:LEU:HD23	1.82	0.47
1:A:221:GLY:HA2	1:A:228:VAL:CG2	2.44	0.46
1:C:265:GLU:CD	1:C:306:ARG:HD3	2.35	0.46
1:A:78:ARG:NH1	1:A:95:TYR:CE2	2.77	0.46
1:A:73:TRP:O	1:A:78:ARG:NH2	2.48	0.46
1:A:225:TYR:HA	1:A:226:PRO:HA	1.81	0.46
1:C:67:GLY:HA2	1:C:96:ALA:O	2.16	0.46
1:A:161:VAL:O	1:A:164:PHE:HB2	2.16	0.46
1:C:111:TYR:H	1:C:160:GLN:NE2	2.08	0.45
1:C:198:ILE:O	1:C:202:ILE:HG12	2.16	0.45
1:A:249:TRP:O	1:A:277:ILE:HA	2.17	0.45
1:C:611:ALA:O	1:C:615:GLU:HG3	2.17	0.45
1:C:373:LEU:HB3	1:C:374:TYR:H	1.53	0.45
1:A:107:TRP:CH2	1:A:143:ILE:HD12	2.52	0.45
1:A:584:TRP:CD2	1:A:610:ARG:NH2	2.81	0.44
1:C:111:TYR:CE1	1:C:157:LYS:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HD11	1:C:136:ALA:HB2	1.99	0.44
1:A:230:GLN:CD	1:A:235:ARG:NH2	2.71	0.44
1:C:203:TYR:CD1	1:C:209:PRO:HD2	2.53	0.44
1:C:622:MET:HG3	1:C:648:LYS:NZ	2.32	0.44
1:C:59:HIS:O	1:C:59:HIS:CG	2.71	0.43
1:C:192:ALA:O	1:C:196:VAL:HG23	2.18	0.43
1:A:111:TYR:CE2	1:A:157:LYS:HE3	2.53	0.43
1:A:645:TRP:CZ3	2:D:394:TYR:HD2	2.37	0.43
1:A:104:ARG:O	1:A:107:TRP:HD1	2.01	0.43
1:A:648:LYS:HB3	1:A:648:LYS:HE3	1.82	0.43
1:A:239:GLU:HG2	1:A:272:LYS:HE2	1.99	0.43
1:A:563:ASP:HA	1:A:572:GLY:HA3	2.00	0.43
1:A:248:LEU:HA	1:A:276:VAL:O	2.19	0.43
1:A:267:VAL:O	1:A:271:ILE:HG12	2.18	0.43
1:C:225:TYR:HA	1:C:226:PRO:HA	1.87	0.43
1:A:690:GLN:OE1	1:C:650:ILE:HD11	2.19	0.43
1:A:174:ASP:CA	4:A:802:HOH:O	2.64	0.42
1:C:577:GLN:HA	1:C:580:ARG:NH1	2.33	0.42
1:A:116:ALA:HA	1:A:164:PHE:CE1	2.55	0.42
1:A:180:MET:O	1:A:185:LYS:HE3	2.20	0.42
1:C:317:GLU:HB3	1:C:639:ASP:HB3	2.02	0.42
1:A:315:ASN:HD22	1:A:321:ASN:ND2	2.17	0.42
1:A:169:PHE:O	1:A:212:PHE:HA	2.19	0.42
1:A:584:TRP:CE2	1:A:610:ARG:NH2	2.88	0.42
1:C:281:ILE:HG23	1:C:282:HIS:ND1	2.35	0.42
1:C:314:PRO:HB2	1:C:321:ASN:CG	2.40	0.41
1:C:60:PHE:CZ	1:C:309:GLY:HA2	2.55	0.41
1:A:97:PRO:HG2	1:A:100:ASP:HB2	2.01	0.41
1:A:102:LYS:O	1:A:107:TRP:HA	2.21	0.41
1:A:221:GLY:HA2	1:A:228:VAL:HG21	2.03	0.41
1:A:182:ALA:HA	1:A:185:LYS:HG3	2.03	0.41
1:C:228:VAL:HG13	1:C:266:GLU:OE2	2.20	0.41
1:A:274:ALA:HA	1:A:275:PRO:HD3	1.94	0.41
1:C:265:GLU:HA	1:C:265:GLU:OE1	2.21	0.41
1:C:89:GLU:HB2	1:C:333:LYS:HD3	2.03	0.41
1:A:242:LEU:HA	1:A:243:PRO:HD3	1.93	0.41
1:C:249:TRP:O	1:C:277:ILE:HA	2.21	0.41
1:C:119:LEU:O	1:C:123:ILE:HG13	2.20	0.40
1:C:60:PHE:HA	1:C:308:LYS:HE3	2.02	0.40
1:A:215:CYS:HB2	1:A:248:LEU:HD12	2.04	0.40
1:C:71:ARG:HA	1:C:72:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

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	414/504 (82%)	388 (94%)	25 (6%)	1 (0%)	47	73
1	C	421/504 (84%)	403 (96%)	16 (4%)	2 (0%)	29	54
2	B	2/7 (29%)	0	2 (100%)	0	100	100
2	D	2/7 (29%)	0	2 (100%)	0	100	100
All	All	839/1022 (82%)	791 (94%)	45 (5%)	3 (0%)	34	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	PRO
1	C	314	PRO
1	C	591	VAL

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	375/442 (85%)	366 (98%)	9 (2%)	49	77
1	C	381/442 (86%)	373 (98%)	8 (2%)	53	80
2	B	4/6 (67%)	3 (75%)	1 (25%)	0	1
2	D	4/6 (67%)	3 (75%)	1 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	764/896 (85%)	745 (98%)	19 (2%)	47 76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	137	ILE
1	A	178	HIS
1	A	253	LYS
1	A	377	GLN
1	A	629	SER
1	A	631	CYS
1	A	646	ASP
1	A	648	LYS
2	B	396	SER
1	C	137	ILE
1	C	143	ILE
1	C	178	HIS
1	C	301	THR
1	C	334	SER
1	C	552	SER
1	C	631	CYS
1	C	647	ILE
2	D	395	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	227	ASN
1	A	321	ASN
1	C	160	GLN
1	C	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3.30	5 (35%)	17,19,21	2.89	9 (52%)
3	NAG	D	401	2	14,14,15	4.12	7 (50%)	17,19,21	2.81	10 (58%)

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	-	3/6/23/26	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	D	401	NAG	C1-C2	11.30	1.69	1.52
3	B	401	NAG	C1-C2	9.78	1.67	1.52
3	D	401	NAG	C4-C5	6.05	1.65	1.53
3	D	401	NAG	C3-C2	5.07	1.63	1.52
3	B	401	NAG	C3-C2	4.60	1.62	1.52
3	D	401	NAG	C7-N2	3.22	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAG	C2-N2	3.08	1.51	1.46
3	B	401	NAG	C8-C7	2.73	1.56	1.50
3	D	401	NAG	O5-C1	2.72	1.48	1.43
3	B	401	NAG	C6-C5	2.64	1.60	1.51
3	D	401	NAG	O5-C5	2.60	1.48	1.43
3	B	401	NAG	O5-C1	2.35	1.47	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAG	C1-O5-C5	5.41	119.52	112.19
3	D	401	NAG	C1-O5-C5	5.40	119.51	112.19
3	D	401	NAG	C3-C4-C5	-5.08	101.17	110.24
3	B	401	NAG	C8-C7-N2	4.47	123.66	116.10
3	B	401	NAG	C2-N2-C7	4.22	128.91	122.90
3	B	401	NAG	C3-C4-C5	-4.21	102.73	110.24
3	B	401	NAG	O3-C3-C2	-4.12	100.95	109.47
3	D	401	NAG	O5-C1-C2	4.03	117.65	111.29
3	D	401	NAG	C8-C7-N2	3.92	122.74	116.10
3	B	401	NAG	O5-C5-C4	-3.34	102.69	110.83
3	D	401	NAG	C2-N2-C7	3.23	127.50	122.90
3	B	401	NAG	O5-C1-C2	2.86	115.81	111.29
3	D	401	NAG	O7-C7-C8	-2.85	116.77	122.06
3	B	401	NAG	O7-C7-C8	-2.69	117.05	122.06
3	D	401	NAG	C1-C2-N2	2.57	114.89	110.49
3	D	401	NAG	O3-C3-C2	-2.54	104.22	109.47
3	B	401	NAG	O3-C3-C4	-2.48	104.61	110.35
3	D	401	NAG	O4-C4-C3	-2.29	105.06	110.35
3	D	401	NAG	C4-C3-C2	2.03	114.00	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	NAG	O5-C5-C6-O6
3	B	401	NAG	C1-C2-N2-C7
3	D	401	NAG	C3-C2-N2-C7
3	D	401	NAG	C1-C2-N2-C7
3	B	401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 ⓘ

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	424/504 (84%)	0.02	5 (1%) 79 80	34, 60, 97, 133	0
1	C	429/504 (85%)	0.06	6 (1%) 75 77	42, 70, 97, 125	0
2	B	4/7 (57%)	1.53	1 (25%) 0 0	72, 95, 110, 112	0
2	D	4/7 (57%)	1.73	2 (50%) 0 0	87, 101, 115, 121	0
All	All	861/1022 (84%)	0.05	14 (1%) 72 74	34, 67, 98, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	VAL	4.7
1	C	694	PRO	4.2
2	B	396	SER	3.7
1	A	590	SER	2.8
2	D	394	TYR	2.8
1	C	229	SER	2.5
1	A	661	LEU	2.4
2	D	396	SER	2.4
1	C	674	GLY	2.4
1	C	661	LEU	2.3
1	C	385	THR	2.3
1	A	229	SER	2.2
1	A	679	TRP	2.1
1	C	662	GLY	2.1

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 [i](#)

There are no monosaccharides 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
3	NAG	B	401	14/15	0.96	0.21	46,50,57,57	0
3	NAG	D	401	14/15	0.97	0.19	46,53,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.