



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:32 AM BST

PDB ID : 5VVV  
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](mailto: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.

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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

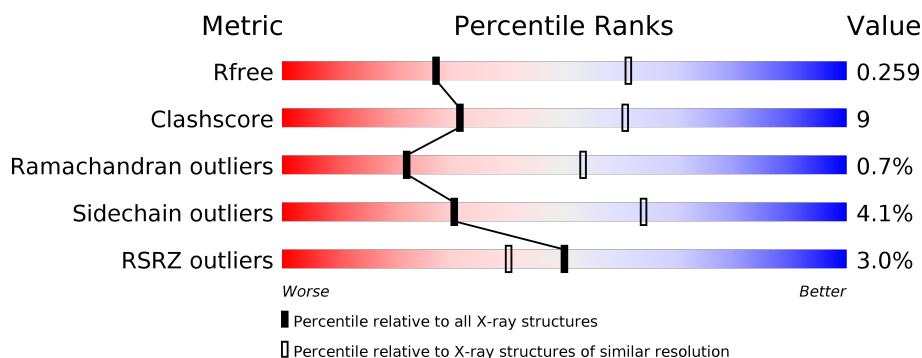
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>3%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	504	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	13	<div> <div>15%</div> <div>85%</div> </div>
2	D	13	<div> <div>8%</div> <div>31%</div> <div>62%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7015 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	416	Total	C	N	O	S	0	0	0
			3428	2227	563	616	22			
1	C	423	Total	C	N	O	S	0	0	0
			3477	2253	574	627	23			

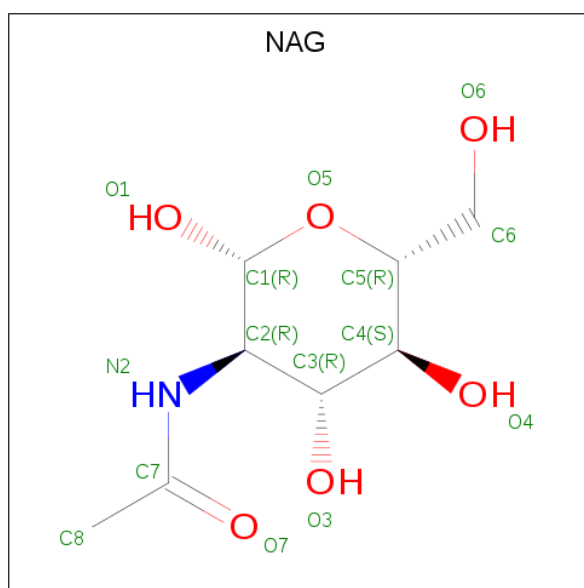
There are 24 discrepancies between the modelled and reference sequences:

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  $\alpha$ -crystallin B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			13	7	2	4			
2	D	5	Total	C	N	O	0	0	0
			34	20	5	9			

- 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		

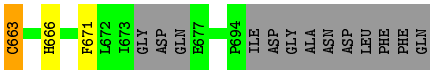
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	C	14	Total	O	0	0
			14	14		



- Molecule 1: Protein O-GlcNAcase





- Molecule 2: a-crystallin B



- Molecule 2: a-crystallin B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.08Å 96.26Å 89.81Å 90.00° 114.29° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 46.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.80) 99.9 (46.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.196 , 0.257 0.196 , 0.259	Depositor DCC
$R_{free}$ test set	1576 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.70	0/3522	0.83	2/4769 (0.0%)
1	C	0.67	0/3571	0.81	1/4832 (0.0%)
2	B	0.76	0/12	0.89	0/15
2	D	0.70	0/33	0.99	0/44
All	All	0.69	0/7138	0.82	3/9660 (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	104	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	C	287	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	628	LEU	CB-CG-CD2	-5.12	102.29	111.00

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	3428	0	3357	48	0
1	C	3477	0	3403	70	0
2	B	13	0	10	1	0
2	D	34	0	33	10	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	21	0	0	1	0
4	C	14	0	0	1	0
All	All	7015	0	6829	124	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 (124) 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:220:CYS:HB3	1:C:250:THR:HG22	1.38	1.01
1:C:266:GLU:O	1:C:269:LYS:HG2	1.65	0.97
1:C:266:GLU:O	1:C:269:LYS:CG	2.14	0.95
2:D:41:SER:O	2:D:42:THR:OG1	1.86	0.92
1:C:264:ILE:HD13	1:C:307:LEU:HD21	1.57	0.85
2:D:42:THR:HG22	2:D:43:SER:H	1.40	0.85
1:A:173:PHE:O	1:A:217:THR:HG22	1.78	0.83
1:A:95:TYR:CD1	1:A:95:TYR:O	2.33	0.81
1:C:663:CYS:SG	1:C:666:HIS:NE2	2.54	0.79
1:C:234:LEU:HD22	1:C:271:ILE:HD11	1.65	0.78
1:C:663:CYS:SG	4:C:813:HOH:O	1.97	0.78
1:C:223:PHE:HZ	2:D:40:THR:HA	1.49	0.78
1:A:161:VAL:HA	1:A:164:PHE:CD2	2.20	0.76
1:A:622:MET:SD	1:A:648:LYS:HG2	2.26	0.76
1:A:215:CYS:HB2	1:A:248:LEU:HD12	1.70	0.73
1:A:80:GLU:OE1	1:A:83:ARG:NH1	2.23	0.72
2:D:42:THR:CG2	2:D:43:SER:H	2.03	0.72
1:C:83:ARG:HE	1:C:87:LYS:NZ	1.88	0.71
1:C:266:GLU:O	1:C:269:LYS:CD	2.38	0.70
1:C:266:GLU:O	1:C:269:LYS:HD2	1.91	0.69
1:A:682:ARG:O	1:A:691:ARG:NH2	2.26	0.68
1:C:553:VAL:HG11	1:C:628:LEU:HD23	1.76	0.68
1:C:230:GLN:HB3	1:C:235:ARG:NH1	2.08	0.67
1:C:266:GLU:HG2	1:C:269:LYS:HD2	1.77	0.67
1:C:230:GLN:CB	1:C:235:ARG:HH11	2.08	0.67
1:C:220:CYS:HB3	1:C:250:THR:CG2	2.19	0.66
1:A:692:LEU:O	1:C:586:ARG:NH1	2.29	0.66
1:C:314:PRO:HB2	1:C:321:ASN:OD1	1.97	0.64
2:D:42:THR:HG22	2:D:43:SER:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:THR:O	2:D:43:SER:HB2	1.98	0.62
2:B:41:SER:O	2:B:42:THR:HB	2.00	0.60
1:C:230:GLN:HB3	1:C:235:ARG:HH11	1.66	0.60
1:A:111:TYR:CE2	1:A:157:LYS:HE3	2.37	0.60
1:A:660:TRP:O	1:A:661:LEU:HD23	2.03	0.58
1:C:265:GLU:OE1	1:C:265:GLU:HA	2.02	0.58
1:C:625:PHE:CG	1:C:648:LYS:HD3	2.39	0.57
1:C:94:LEU:HD11	1:C:136:ALA:HB2	1.88	0.56
1:C:230:GLN:CG	1:C:235:ARG:HH11	2.18	0.56
1:A:560:LEU:O	1:A:564:LEU:HG	2.06	0.56
1:C:195:GLN:O	1:C:199:THR:OG1	2.24	0.56
1:A:95:TYR:HD1	1:A:95:TYR:O	1.86	0.55
1:C:230:GLN:HG2	1:C:235:ARG:HH11	1.71	0.55
1:C:273:ARG:NH1	1:C:274:ALA:HB3	2.21	0.55
1:A:161:VAL:O	1:A:164:PHE:HB2	2.07	0.54
1:A:173:PHE:O	1:A:217:THR:CG2	2.55	0.54
1:A:622:MET:CE	1:A:648:LYS:HD3	2.38	0.54
1:A:567:LEU:HB3	1:A:568:PRO:HD2	1.88	0.54
1:A:604:ILE:HG23	1:A:605:GLU:N	2.23	0.53
1:A:119:LEU:HD21	1:A:123:ILE:HD11	1.91	0.52
1:A:270:ILE:O	1:A:270:ILE:HG13	2.10	0.52
1:A:105:MET:CE	1:A:105:MET:HA	2.41	0.51
1:C:566:TYR:HB3	1:C:570:GLU:O	2.10	0.51
1:A:615:GLU:CD	1:A:659:GLN:HE21	2.13	0.51
1:C:291:LEU:O	1:C:565:PHE:HB3	2.10	0.51
1:C:158:LEU:HD22	1:C:169:PHE:HD2	1.75	0.51
1:A:120:MET:HG3	1:A:164:PHE:CD1	2.46	0.51
1:C:269:LYS:HG3	1:C:270:ILE:N	2.26	0.50
1:C:273:ARG:HH11	1:C:274:ALA:H	1.59	0.50
1:C:625:PHE:HD1	1:C:644:VAL:HG23	1.77	0.50
1:C:384:LEU:HD22	1:C:558:LEU:HB3	1.93	0.49
1:A:249:TRP:O	1:A:277:ILE:HA	2.12	0.49
1:C:83:ARG:HE	1:C:87:LYS:HZ1	1.57	0.49
1:C:319:GLU:HB3	1:C:636:ILE:HG12	1.93	0.49
1:A:119:LEU:HD22	1:A:164:PHE:CD2	2.48	0.48
2:D:42:THR:CG2	2:D:43:SER:N	2.72	0.47
1:A:102:LYS:NZ	1:A:115:GLU:OE1	2.47	0.47
1:C:225:TYR:HD1	1:C:226:PRO:HA	1.79	0.47
1:C:102:LYS:NZ	1:C:115:GLU:OE1	2.45	0.47
1:A:264:ILE:HA	1:A:267:VAL:HG12	1.97	0.47
1:C:259:ILE:CG2	1:C:264:ILE:HD12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:GLU:O	1:A:585:LEU:HG	2.15	0.47
2:D:41:SER:O	2:D:42:THR:CB	2.63	0.46
1:C:266:GLU:O	1:C:269:LYS:CB	2.64	0.46
2:D:41:SER:C	2:D:42:THR:HG1	2.01	0.46
1:A:101:TYR:CE1	1:C:634:ARG:HG3	2.51	0.46
1:A:215:CYS:HB2	1:A:248:LEU:CD1	2.43	0.45
1:A:137:ILE:HG23	1:A:171:LEU:HD23	1.98	0.45
1:C:248:LEU:HA	1:C:276:VAL:O	2.17	0.45
1:C:225:TYR:HA	1:C:226:PRO:HA	1.82	0.45
1:A:659:GLN:C	1:A:661:LEU:H	2.20	0.45
1:C:304:ILE:HD12	1:C:335:ASN:HB2	1.99	0.45
1:C:374:TYR:HE1	1:C:379:ALA:HB2	1.81	0.44
1:C:223:PHE:CZ	2:D:40:THR:HA	2.40	0.44
1:A:147:ASN:OD1	1:A:149:LYS:HB3	2.17	0.44
1:C:557:ASP:OD1	1:C:627:ARG:NH2	2.42	0.44
1:C:125:ALA:HA	1:C:128:GLU:HB3	1.99	0.44
1:C:625:PHE:CZ	1:C:648:LYS:HE2	2.53	0.44
1:C:83:ARG:HE	1:C:87:LYS:HZ2	1.64	0.44
1:C:259:ILE:HG21	1:C:264:ILE:HD12	1.99	0.43
1:C:269:LYS:CG	1:C:270:ILE:N	2.81	0.43
1:C:60:PHE:CD1	1:C:332:TYR:HE1	2.37	0.43
1:C:67:GLY:HA2	1:C:96:ALA:O	2.18	0.43
1:A:83:ARG:HG3	1:A:129:TYR:CZ	2.54	0.43
1:A:584:TRP:CE2	1:A:588:ASN:ND2	2.87	0.43
1:A:333:LYS:C	4:A:807:HOH:O	2.56	0.43
1:A:563:ASP:HA	1:A:572:GLY:HA3	2.01	0.43
1:C:198:ILE:O	1:C:202:ILE:HG12	2.18	0.43
1:C:260:PRO:HG2	1:C:263:SER:HB3	1.99	0.43
1:A:101:TYR:CD1	1:C:634:ARG:HG3	2.53	0.43
1:A:95:TYR:O	1:A:95:TYR:CG	2.72	0.42
1:C:671:PHE:O	1:C:671:PHE:CG	2.72	0.42
1:C:158:LEU:HD22	1:C:169:PHE:CD2	2.53	0.42
1:C:225:TYR:HD1	1:C:226:PRO:CA	2.32	0.42
1:C:584:TRP:CE2	1:C:588:ASN:ND2	2.85	0.42
1:A:102:LYS:HA	1:A:106:PHE:O	2.19	0.42
1:A:159:ASP:OD2	1:A:205:TYR:HE2	2.02	0.42
1:A:170:ALA:HA	1:A:213:LEU:O	2.19	0.42
1:C:304:ILE:HD12	1:C:335:ASN:CB	2.49	0.42
1:A:225:TYR:HA	1:A:226:PRO:HA	1.78	0.42
1:A:145:PHE:CD2	1:A:194:ALA:HB1	2.54	0.41
1:A:248:LEU:HA	1:A:276:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:VAL:O	1:A:591:VAL:HG12	2.21	0.41
1:A:303:LEU:O	1:A:307:LEU:HG	2.20	0.41
1:C:234:LEU:HA	1:C:234:LEU:HD23	1.83	0.41
1:A:231:SER:HA	1:A:232:PRO:HD2	1.91	0.41
1:C:161:VAL:HA	1:C:164:PHE:CD2	2.56	0.41
1:C:263:SER:O	1:C:267:VAL:HG23	2.20	0.41
1:C:238:GLY:HA3	1:C:272:LYS:HD3	2.02	0.41
1:A:584:TRP:CZ2	1:A:588:ASN:ND2	2.89	0.41
1:C:564:LEU:HD13	1:C:647:ILE:HG12	2.03	0.40
1:C:192:ALA:O	1:C:196:VAL:HG22	2.21	0.40
1:C:249:TRP:O	1:C:277:ILE:HA	2.21	0.40
1:C:657:PHE:HA	1:C:671:PHE:CE1	2.56	0.40
1:C:62:CYS:O	1:C:90:LEU:HB3	2.21	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	406/504 (81%)	371 (91%)	33 (8%)	2 (0%)	29	61
1	C	413/504 (82%)	389 (94%)	22 (5%)	2 (0%)	29	61
2	D	3/13 (23%)	1 (33%)	0	2 (67%)	0	0
All	All	822/1021 (80%)	761 (93%)	55 (7%)	6 (1%)	22	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	43	SER
1	A	140	GLY
2	D	42	THR
1	A	314	PRO

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Mol	Chain	Res	Type
1	C	314	PRO
1	C	573	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%)	359 (97%)	11 (3%)	41	75
1	C	376/442 (85%)	358 (95%)	18 (5%)	25	58
2	B	2/13 (15%)	2 (100%)	0	100	100
2	D	5/13 (38%)	3 (60%)	2 (40%)	0	0
All	All	753/910 (83%)	722 (96%)	31 (4%)	30	64

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	120	MET
1	A	141	LEU
1	A	159	ASP
1	A	225	TYR
1	A	278	TRP
1	A	382	LEU
1	A	590	SER
1	A	608	ARG
1	A	635	THR
1	A	652	SER
1	C	100	ASP
1	C	113	VAL
1	C	137	ILE
1	C	171	LEU
1	C	199	THR
1	C	213	LEU
1	C	242	LEU
1	C	250	THR

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Mol	Chain	Res	Type
1	C	265	GLU
1	C	299	ARG
1	C	301	THR
1	C	334	SER
1	C	374	TYR
1	C	378	MET
1	C	553	VAL
1	C	624	MET
1	C	631	CYS
1	C	663	CYS
2	D	40	THR
2	D	41	SER

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

Mol	Chain	Res	Type
1	C	288	GLN

### 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 monosaccharides 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	D	101	2	14,14,15	2.88	5 (35%)	17,19,21	2.95	8 (47%)
3	NAG	B	101	2	14,14,15	2.66	3 (21%)	17,19,21	3.03	8 (47%)

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	D	101	2	-	1/6/23/26	0/1/1/1
3	NAG	B	101	2	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	NAG	C1-C2	7.55	1.63	1.52
3	B	101	NAG	C1-C2	7.45	1.63	1.52
3	D	101	NAG	C3-C2	4.89	1.62	1.52
3	B	101	NAG	C8-C7	4.24	1.59	1.50
3	B	101	NAG	C3-C2	3.53	1.60	1.52
3	D	101	NAG	C4-C5	2.90	1.59	1.53
3	D	101	NAG	C7-N2	2.77	1.43	1.34
3	D	101	NAG	C8-C7	2.31	1.55	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	101	NAG	C1-O5-C5	5.96	120.26	112.19
3	B	101	NAG	C3-C4-C5	-5.66	100.15	110.24
3	D	101	NAG	C3-C4-C5	-5.63	100.20	110.24
3	D	101	NAG	C1-O5-C5	5.51	119.66	112.19
3	D	101	NAG	O5-C1-C2	4.44	118.29	111.29
3	B	101	NAG	O5-C1-C2	4.39	118.23	111.29
3	B	101	NAG	O3-C3-C2	-4.13	100.93	109.47
3	D	101	NAG	C8-C7-N2	3.82	122.57	116.10
3	D	101	NAG	O4-C4-C3	-3.55	102.13	110.35
3	D	101	NAG	C2-N2-C7	3.46	127.83	122.90
3	B	101	NAG	C2-N2-C7	3.45	127.82	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	101	NAG	C8-C7-N2	3.43	121.90	116.10
3	B	101	NAG	O4-C4-C3	-3.28	102.77	110.35
3	D	101	NAG	O5-C5-C4	-2.85	103.89	110.83
3	D	101	NAG	O7-C7-C8	-2.72	117.00	122.06
3	B	101	NAG	C6-C5-C4	-2.32	107.57	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	101	NAG	C1-C2-N2-C7
3	D	101	NAG	C3-C2-N2-C7
3	B	101	NAG	C3-C2-N2-C7

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	416/504 (82%)	0.03	17 (4%) 37 27	34, 64, 107, 144	0
1	C	423/504 (83%)	0.00	8 (1%) 66 59	43, 78, 111, 146	0
2	B	2/13 (15%)	0.27	0 100 100	69, 69, 69, 106	0
2	D	5/13 (38%)	0.67	0 100 100	90, 100, 118, 132	0
All	All	846/1034 (81%)	0.02	25 (2%) 50 40	34, 73, 110, 146	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	VAL	5.6
1	A	145	PHE	4.6
1	A	591	VAL	4.2
1	A	225	TYR	4.0
1	A	607	TRP	3.7
1	A	679	TRP	3.6
1	C	374	TYR	3.5
1	A	224	CYS	3.3
1	A	606	GLU	3.1
1	C	235	ARG	3.0
1	A	228	VAL	2.9
1	A	180	MET	2.8
1	A	608	ARG	2.7
1	A	188	PHE	2.7
1	A	229	SER	2.7
1	C	608	ARG	2.7
1	C	230	GLN	2.6
1	A	183	ALA	2.5
1	C	167	ARG	2.4
1	C	166	CYS	2.3
1	A	592	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	607	TRP	2.2
1	A	230	GLN	2.2
1	C	273	ARG	2.2
1	A	186	GLU	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 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, 95<sup>th</sup> 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	101	14/15	0.97	0.17	43,50,58,59	0
3	NAG	D	101	14/15	0.98	0.19	41,52,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.