



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:37 PM GMT

PDB ID : 2B31
Title : Crystal structure of the complex formed between goat signalling protein with pentasaccharide at 3.1 Å resolution reveals large scale conformational changes in the residues of TIM barrel
Authors : Ethayathulla, A.S.; Kumar, J.; Srivastava, D.B.; Singh, N.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2005-09-19
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

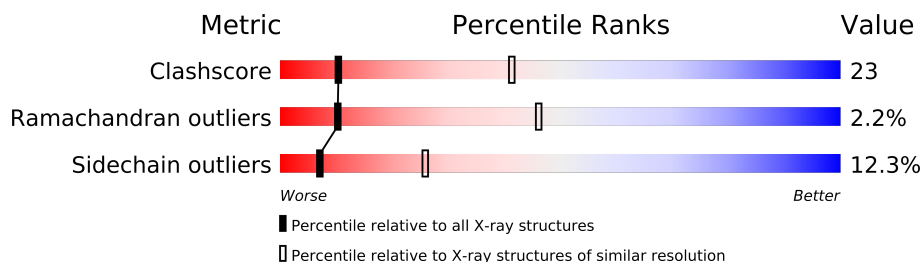
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3045 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Chitinase-3-like protein 1, SPG-40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2876	1836	508	523	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	GB 19526603
A	131	ALA	GLY	SEE REMARK 999	GB 19526603
A	205	ASN	GLN	SEE REMARK 999	GB 19526603
A	206	SER	GLU	SEE REMARK 999	GB 19526603
A	?	-	ASP	SEE REMARK 999	GB 19526603
A	361	ARG	GLU	SEE REMARK 999	GB 19526603

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			42	24	3	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	GB 19526603
A	131	ALA	GLY	SEE REMARK 999	GB 19526603
A	205	ASN	GLN	SEE REMARK 999	GB 19526603
A	206	SER	GLU	SEE REMARK 999	GB 19526603
A	?	-	ASP	SEE REMARK 999	GB 19526603
A	361	ARG	GLU	SEE REMARK 999	GB 19526603

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	GB 19526603
A	131	ALA	GLY	SEE REMARK 999	GB 19526603
A	205	ASN	GLN	SEE REMARK 999	GB 19526603
A	206	SER	GLU	SEE REMARK 999	GB 19526603
A	?	-	ASP	SEE REMARK 999	GB 19526603
A	361	ARG	GLU	SEE REMARK 999	GB 19526603

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	GB 19526603
A	131	ALA	GLY	SEE REMARK 999	GB 19526603
A	205	ASN	GLN	SEE REMARK 999	GB 19526603
A	206	SER	GLU	SEE REMARK 999	GB 19526603
A	?	-	ASP	SEE REMARK 999	GB 19526603
A	361	ARG	GLU	SEE REMARK 999	GB 19526603

- Molecule 5 is water.

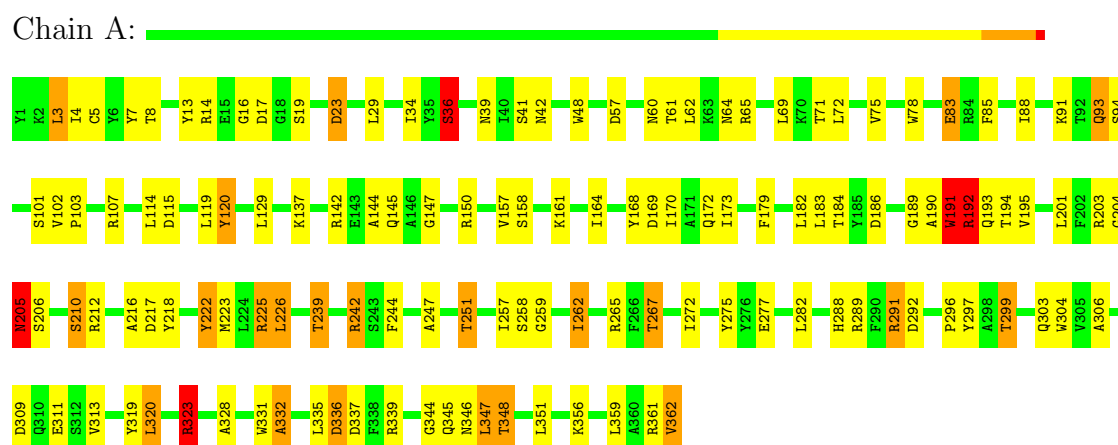
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: Chitinase-3-like protein 1, SPG-40



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.74Å 66.61Å 107.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.70 – 3.10	Depositor
% Data completeness (in resolution range)	98.2 (56.70-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.177 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3045	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG

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	0.98	2/2952 (0.1%)	0.95	8/4000 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	TYR	CE2-CZ	-5.41	1.31	1.38
1	A	222	TYR	CG-CD1	-5.19	1.32	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	TRP	N-CA-C	8.23	133.23	111.00
1	A	323	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	191	TRP	N-CA-CB	-6.03	99.75	110.60
1	A	336	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	191	TRP	CA-CB-CG	5.62	124.37	113.70
1	A	36	SER	C-N-CA	5.50	135.45	121.70
1	A	323	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	88	ILE	CB-CA-C	-5.03	101.53	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2876	0	2817	128	0
2	A	42	0	36	11	0
3	A	28	0	25	5	0
4	A	28	0	25	1	0
5	A	71	0	0	9	0
All	All	3045	0	2903	137	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:GLY:HA2	1:A:292:ASP:HB3	1.18	1.08
1:A:323:ARG:HG2	1:A:323:ARG:HH11	1.24	0.98
1:A:265:ARG:HD3	5:A:416:HOH:O	1.67	0.93
1:A:4:ILE:HD13	1:A:179:PHE:CE2	2.09	0.88
1:A:93:GLN:HB2	5:A:385:HOH:O	1.72	0.88
1:A:262:ILE:HD13	1:A:303:GLN:NE2	1.93	0.84
1:A:192:ARG:HA	1:A:192:ARG:NE	1.93	0.81
1:A:65:ARG:HD3	5:A:400:HOH:O	1.79	0.80
1:A:204:GLY:HA2	1:A:292:ASP:CB	2.08	0.79
1:A:361:ARG:O	1:A:362:VAL:HG12	1.83	0.78
1:A:137:LYS:HE3	1:A:150:ARG:NH2	2.00	0.76
1:A:23:ASP:HB3	5:A:374:HOH:O	1.84	0.76
1:A:323:ARG:NH1	1:A:323:ARG:HG2	1.96	0.75
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.68	0.74
1:A:289:ARG:HD3	5:A:395:HOH:O	1.87	0.74
1:A:169:ASP:OD2	1:A:172:GLN:HG3	1.87	0.74
1:A:4:ILE:CD1	1:A:179:PHE:CE2	2.71	0.74
1:A:204:GLY:O	1:A:206:SER:N	2.21	0.73
2:A:364:NDG:H6C2	2:A:365:NAG:N2	2.05	0.72
1:A:7:TYR:O	1:A:36:SER:HB2	1.92	0.70
1:A:195:VAL:HA	1:A:257:ILE:HD11	1.74	0.70
1:A:57:ASP:O	1:A:61:THR:HG23	1.91	0.69
1:A:164:ILE:CG2	1:A:170:ILE:HD11	2.23	0.69
1:A:267:THR:HB	1:A:277:GLU:OE1	1.93	0.69
1:A:320:LEU:CD1	1:A:328:ALA:HB2	2.22	0.68
1:A:291:ARG:HG3	1:A:292:ASP:N	2.07	0.68
1:A:323:ARG:CG	1:A:323:ARG:HH11	2.01	0.66
1:A:83:GLU:CD	1:A:83:GLU:H	1.97	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291:ARG:HG3	1:A:292:ASP:H	1.60	0.66
1:A:262:ILE:H	1:A:303:GLN:HE22	1.45	0.65
3:A:366:NAG:H61	3:A:367:NAG:HN2	1.63	0.64
1:A:239:THR:HG23	1:A:239:THR:O	1.96	0.64
1:A:244:PHE:CD1	1:A:257:ILE:HD13	2.34	0.63
1:A:320:LEU:HD11	1:A:328:ALA:HB2	1.80	0.62
2:A:364:NDG:C6	2:A:365:NAG:N2	2.63	0.61
1:A:251:THR:HG22	5:A:396:HOH:O	2.01	0.61
1:A:61:THR:O	1:A:64:ASN:HB2	2.00	0.61
1:A:239:THR:CG2	1:A:335:LEU:HB2	2.31	0.61
3:A:366:NAG:H61	3:A:367:NAG:N2	2.16	0.61
1:A:78:TRP:HZ3	1:A:120:TYR:CE2	2.19	0.60
1:A:272:ILE:HD12	2:A:364:NDG:H8C1	1.84	0.60
1:A:164:ILE:HG21	1:A:170:ILE:HD11	1.83	0.59
1:A:239:THR:CG2	1:A:239:THR:O	2.51	0.58
1:A:272:ILE:HD12	2:A:364:NDG:C8	2.33	0.58
1:A:91:LYS:HB2	1:A:94:SER:OG	2.04	0.57
1:A:212:ARG:HD2	1:A:212:ARG:O	2.04	0.57
1:A:336:ASP:OD1	1:A:337:ASP:N	2.36	0.57
1:A:320:LEU:HD23	1:A:320:LEU:C	2.25	0.57
1:A:210:SER:OG	1:A:210:SER:O	2.23	0.56
1:A:288:HIS:HD2	1:A:297:TYR:CE2	2.23	0.56
1:A:93:GLN:HG2	1:A:94:SER:N	2.20	0.55
2:A:364:NDG:H6C2	2:A:365:NAG:C7	2.37	0.55
1:A:191:TRP:CG	1:A:192:ARG:N	2.75	0.54
1:A:347:LEU:HD23	1:A:348:THR:H	1.73	0.54
1:A:145:GLN:C	1:A:147:GLY:H	2.11	0.54
1:A:17:ASP:HB3	1:A:339:ARG:HD2	1.89	0.53
1:A:186:ASP:OD2	1:A:242:ARG:NH1	2.41	0.52
1:A:39:ASN:HB2	1:A:48:TRP:CE3	2.43	0.52
1:A:191:TRP:CD1	1:A:192:ARG:HB2	2.45	0.52
2:A:364:NDG:H6C1	2:A:365:NAG:HN2	1.75	0.52
1:A:332:ALA:HB3	1:A:335:LEU:HD12	1.90	0.51
1:A:203:ARG:HB2	1:A:212:ARG:HH11	1.74	0.51
1:A:257:ILE:HG22	1:A:259:GLY:H	1.76	0.51
1:A:78:TRP:HZ3	1:A:120:TYR:CD2	2.28	0.51
1:A:60:ASN:ND2	1:A:71:THR:OG1	2.44	0.51
1:A:142:ARG:NH1	1:A:142:ARG:HB2	2.25	0.51
2:A:364:NDG:C6	2:A:365:NAG:HN2	2.24	0.51
3:A:366:NAG:H62	3:A:367:NAG:H83	1.94	0.50
1:A:101:SER:HB3	5:A:437:HOH:O	2.11	0.50
1:A:331:TRP:CE3	2:A:363:NAG:H83	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:GLY:C	1:A:206:SER:H	2.14	0.50
1:A:157:VAL:HG12	1:A:158:SER:N	2.27	0.49
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.93	0.49
1:A:217:ASP:HA	1:A:319:TYR:OH	2.13	0.49
1:A:203:ARG:HD3	1:A:212:ARG:HD3	1.94	0.49
1:A:275:TYR:CE2	1:A:351:LEU:HD13	2.48	0.49
1:A:119:LEU:HD11	2:A:363:NAG:H2	1.93	0.49
1:A:225:ARG:NE	1:A:225:ARG:O	2.45	0.49
1:A:247:ALA:HB2	1:A:258:SER:HB3	1.96	0.48
1:A:78:TRP:CZ3	1:A:120:TYR:CE2	3.00	0.48
1:A:189:GLY:O	1:A:191:TRP:N	2.47	0.47
1:A:137:LYS:HE3	1:A:150:ARG:CZ	2.44	0.47
1:A:114:LEU:HG	1:A:115:ASP:N	2.29	0.47
1:A:164:ILE:HA	1:A:168:TYR:HD2	1.79	0.47
1:A:288:HIS:CD2	1:A:297:TYR:CE2	3.02	0.47
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.50	0.47
1:A:170:ILE:HD13	1:A:223:MET:SD	2.55	0.46
1:A:222:TYR:CE2	1:A:226:LEU:HD21	2.51	0.46
1:A:8:THR:HA	1:A:36:SER:HB2	1.99	0.45
1:A:203:ARG:O	1:A:203:ARG:HG2	2.16	0.45
1:A:161:LYS:HE2	1:A:218:TYR:OH	2.15	0.45
1:A:75:VAL:HG23	1:A:114:LEU:HD11	1.99	0.45
1:A:201:LEU:HD12	1:A:216:ALA:HB3	1.98	0.45
1:A:144:ALA:HB2	1:A:150:ARG:HG3	1.99	0.45
1:A:75:VAL:CG2	1:A:114:LEU:HD11	2.46	0.45
4:A:369:NDG:H8C1	4:A:369:NDG:H2	1.56	0.44
1:A:23:ASP:CB	5:A:374:HOH:O	2.54	0.44
1:A:195:VAL:CG1	1:A:304:TRP:CE2	3.01	0.44
1:A:39:ASN:HB2	1:A:48:TRP:HE3	1.81	0.44
1:A:142:ARG:HB2	1:A:142:ARG:HH11	1.83	0.44
1:A:262:ILE:H	1:A:303:GLN:NE2	2.12	0.44
1:A:195:VAL:HG13	1:A:304:TRP:CH2	2.53	0.44
1:A:195:VAL:HG11	1:A:304:TRP:CE2	2.52	0.44
1:A:332:ALA:HB1	1:A:335:LEU:HG	2.00	0.44
1:A:195:VAL:CG1	1:A:304:TRP:CZ2	3.01	0.44
1:A:205:ASN:O	1:A:205:ASN:CG	2.56	0.44
1:A:120:TYR:CD1	1:A:120:TYR:N	2.78	0.43
1:A:157:VAL:CG1	1:A:158:SER:N	2.81	0.43
1:A:34:ILE:HG12	1:A:72:LEU:HB2	2.00	0.43
1:A:362:VAL:OXT	1:A:362:VAL:HG13	2.19	0.43
1:A:137:LYS:CE	1:A:150:ARG:NH2	2.78	0.43
1:A:14:ARG:O	1:A:19:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:ILE:CD1	2:A:364:NDG:H8C1	2.48	0.42
1:A:288:HIS:HB2	1:A:297:TYR:CZ	2.53	0.42
1:A:347:LEU:HD23	1:A:348:THR:N	2.34	0.42
1:A:164:ILE:HG23	1:A:170:ILE:HD11	1.98	0.42
1:A:3:LEU:HD22	1:A:5:CYS:SG	2.60	0.42
1:A:289:ARG:NH2	1:A:309:ASP:OD2	2.51	0.42
1:A:304:TRP:CZ3	1:A:306:ALA:HB2	2.54	0.42
1:A:62:LEU:C	1:A:64:ASN:H	2.22	0.42
1:A:13:TYR:CD2	3:A:366:NAG:H4	2.55	0.42
1:A:239:THR:HG22	1:A:335:LEU:CB	2.42	0.42
1:A:83:GLU:CD	1:A:83:GLU:N	2.71	0.41
1:A:362:VAL:CG1	1:A:362:VAL:OXT	2.68	0.41
1:A:157:VAL:HG12	1:A:158:SER:O	2.20	0.41
1:A:319:TYR:CE1	1:A:323:ARG:HD2	2.56	0.41
1:A:299:THR:HG23	1:A:304:TRP:HA	2.03	0.41
1:A:29:LEU:HD12	1:A:356:LYS:HD2	2.02	0.41
1:A:91:LYS:HD3	1:A:93:GLN:HE22	1.84	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.61	0.41
1:A:262:ILE:N	1:A:303:GLN:HE22	2.16	0.41
1:A:16:GLY:HA3	5:A:373:HOH:O	2.20	0.41
1:A:183:LEU:CD2	2:A:363:NAG:H82	2.51	0.41
1:A:251:THR:HG23	1:A:251:THR:O	2.20	0.40
1:A:13:TYR:CE2	3:A:366:NAG:H4	2.57	0.40
1:A:41:SER:O	1:A:42:ASN:HB2	2.21	0.40
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.98	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	359/361 (99%)	326 (91%)	25 (7%)	8 (2%)	10	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ALA
1	A	191	TRP
1	A	192	ARG
1	A	205	ASN
1	A	345	GLN
1	A	120	TYR
1	A	332	ALA
1	A	344	GLY

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	302/302 (100%)	265 (88%)	37 (12%)	7 26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	ASP
1	A	36	SER
1	A	69	LEU
1	A	83	GLU
1	A	85	PHE
1	A	93	GLN
1	A	107	ARG
1	A	129	LEU
1	A	173	ILE
1	A	184	THR
1	A	191	TRP
1	A	192	ARG
1	A	193	GLN
1	A	194	THR
1	A	205	ASN
1	A	210	SER
1	A	225	ARG
1	A	226	LEU
1	A	239	THR

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Mol	Chain	Res	Type
1	A	242	ARG
1	A	251	THR
1	A	262	ILE
1	A	267	THR
1	A	282	LEU
1	A	291	ARG
1	A	296	PRO
1	A	299	THR
1	A	311	GLU
1	A	313	VAL
1	A	320	LEU
1	A	323	ARG
1	A	346	ASN
1	A	347	LEU
1	A	348	THR
1	A	359	LEU
1	A	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	93	GLN
1	A	109	HIS
1	A	128	HIS
1	A	188	HIS
1	A	288	HIS
1	A	294	GLN
1	A	303	GLN
1	A	310	GLN
1	A	345	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

7 carbohydrates 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
2	NAG	A	363	2	12,14,15	1.18	1 (8%)	15,19,21	3.81	10 (66%)
2	NDG	A	364	2	12,14,15	0.81	0	15,19,21	3.28	7 (46%)
2	NAG	A	365	3,2	12,14,15	2.08	4 (33%)	15,19,21	3.27	7 (46%)
3	NAG	A	366	3,2	12,14,15	1.92	4 (33%)	15,19,21	5.29	9 (60%)
3	NAG	A	367	3	12,14,15	1.63	1 (8%)	15,19,21	3.96	8 (53%)
4	NAG	A	368	1,4	12,14,15	1.09	2 (16%)	15,19,21	2.22	6 (40%)
4	NDG	A	369	4	12,14,15	0.58	0	15,19,21	2.73	8 (53%)

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
2	NAG	A	363	2	-	0/6/23/26	0/1/1/1
2	NDG	A	364	2	-	0/6/23/26	0/1/1/1
2	NAG	A	365	3,2	-	0/6/23/26	0/1/1/1
3	NAG	A	366	3,2	-	0/6/23/26	0/1/1/1
3	NAG	A	367	3	-	0/6/23/26	0/1/1/1
4	NAG	A	368	1,4	-	0/6/23/26	0/1/1/1
4	NDG	A	369	4	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	365	NAG	C8-C7	4.34	1.59	1.50
3	A	367	NAG	O7-C7	3.93	1.31	1.23
3	A	366	NAG	C2-N2	3.80	1.50	1.46
3	A	366	NAG	O7-C7	3.63	1.31	1.23
2	A	365	NAG	C2-N2	-3.39	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	365	NAG	C4-C3	2.83	1.59	1.52
4	A	368	NAG	O5-C5	-2.52	1.40	1.45
2	A	365	NAG	O7-C7	2.37	1.28	1.23
4	A	368	NAG	C2-N2	-2.33	1.43	1.46
2	A	363	NAG	O7-C7	2.27	1.28	1.23
3	A	366	NAG	O5-C5	-2.16	1.41	1.45
3	A	366	NAG	O3-C3	2.12	1.48	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	367	NAG	C2-N2-C7	-11.69	103.45	123.09
3	A	366	NAG	O6-C6-C5	11.05	149.38	111.36
3	A	366	NAG	O5-C5-C6	10.07	117.54	106.98
2	A	363	NAG	C2-N2-C7	9.78	139.51	123.09
3	A	366	NAG	C2-N2-C7	8.58	137.50	123.09
2	A	365	NAG	O5-C5-C4	-7.92	100.60	110.65
2	A	364	NDG	O-C5-C6	7.24	114.58	106.98
4	A	369	NDG	O-C5-C6	7.00	114.33	106.98
2	A	364	NDG	O-C5-C4	5.81	118.03	110.65
3	A	367	NAG	O5-C5-C6	-5.80	100.90	106.98
2	A	363	NAG	C3-C2-N2	-5.79	102.94	111.76
2	A	365	NAG	O5-C5-C6	5.78	113.05	106.98
2	A	364	NDG	C2-N2-C7	-5.53	113.80	123.09
3	A	366	NAG	C3-C2-N2	5.49	120.12	111.76
3	A	366	NAG	C3-C4-C5	5.29	119.65	110.20
2	A	363	NAG	O5-C5-C4	5.02	117.03	110.65
4	A	368	NAG	C2-N2-C7	-4.73	115.15	123.09
3	A	366	NAG	O4-C4-C5	-4.22	98.16	109.28
3	A	366	NAG	C8-C7-N2	4.10	124.12	116.11
2	A	365	NAG	O7-C7-N2	-4.10	113.34	121.90
3	A	367	NAG	C3-C2-N2	3.94	117.76	111.76
2	A	363	NAG	O4-C4-C5	-3.87	99.08	109.28
2	A	365	NAG	C6-C5-C4	3.71	121.97	113.00
2	A	364	NDG	O7-C7-C8	-3.66	114.91	122.04
3	A	367	NAG	C8-C7-N2	-3.55	109.16	116.11
2	A	365	NAG	O7-C7-C8	3.54	128.96	122.04
4	A	369	NDG	O3-C3-C4	-3.48	102.55	110.35
2	A	363	NAG	C8-C7-N2	-3.32	109.62	116.11
3	A	366	NAG	O7-C7-N2	-3.26	115.10	121.90
4	A	368	NAG	C3-C2-N2	-3.15	106.97	111.76
4	A	368	NAG	C3-C4-C5	-3.14	104.60	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	366	NAG	O5-C5-C4	3.13	114.62	110.65
3	A	367	NAG	C4-C3-C2	-3.04	103.88	111.32
4	A	369	NDG	O-C5-C4	3.01	114.48	110.65
4	A	368	NAG	O5-C5-C6	3.00	110.13	106.98
2	A	364	NDG	C4-C3-C2	-2.78	104.51	111.32
4	A	369	NDG	C6-C5-C4	-2.78	106.29	113.00
4	A	369	NDG	O7-C7-C8	-2.71	116.76	122.04
4	A	369	NDG	C4-C3-C2	2.68	117.87	111.32
2	A	363	NAG	O7-C7-N2	2.67	127.48	121.90
3	A	367	NAG	C3-C4-C5	-2.56	105.63	110.20
4	A	368	NAG	O6-C6-C5	-2.55	102.57	111.36
2	A	365	NAG	O4-C4-C5	-2.50	102.71	109.28
4	A	369	NDG	C8-C7-N2	2.49	120.98	116.11
2	A	363	NAG	O3-C3-C2	2.45	114.22	109.09
2	A	365	NAG	O3-C3-C4	2.38	115.68	110.35
3	A	367	NAG	O4-C4-C5	2.34	115.44	109.28
2	A	363	NAG	C4-C3-C2	-2.30	105.68	111.32
2	A	363	NAG	C6-C5-C4	-2.27	107.53	113.00
4	A	369	NDG	O3-C3-C2	-2.20	104.48	109.09
2	A	363	NAG	O5-C5-C6	2.15	109.24	106.98
2	A	364	NDG	O4-C4-C5	-2.15	103.63	109.28
3	A	367	NAG	O6-C6-C5	-2.13	104.04	111.36
2	A	364	NDG	C6-C5-C4	-2.07	108.00	113.00
4	A	368	NAG	C8-C7-N2	2.02	120.05	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.