



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:37 AM UTC

PDB ID : 2CHN / pdb\_00002chn  
Title : Bacteroides thetaiotaomicron hexosaminidase with O-GlcNAcase activity-NAG-thiazoline complex  
Authors : Dennis, R.J.; Taylor, E.J.; Macauley, M.S.; Stubbs, K.A.; Turkenburg, J.P.; Hart, S.J.; Black, G.N.; Vocadlo, D.J.; Davies, G.J.  
Deposited on : 2006-03-15  
Resolution : 1.95 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

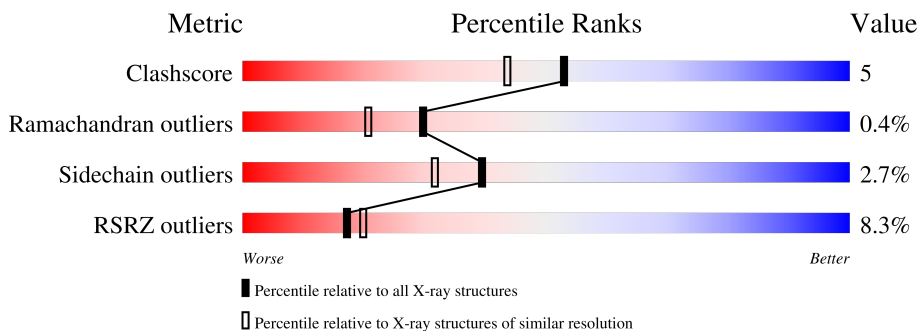
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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  $\geq 3$ , 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	716	
1	B	716	
2	C	12	
2	D	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	1720	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11738 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 GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	642	5235	3361	880	976	2	16	0	4	0
1	B	639	5227	3358	876	973	2	18	0	7	0

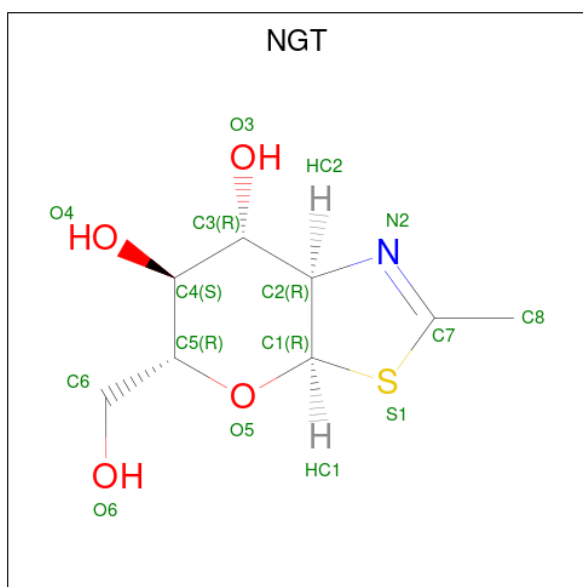
- Molecule 2 is a protein called GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	12	60	36	12	12	0	0	0
2	D	12	59	36	12	11	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TE TRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (CCD ID: NGT) (formula: C<sub>8</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
4	A	1	Total	14	8	1	4	1	0	0
4	B	1	Total	14	8	1	4	1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			
5	A	1	Total	6	3	3	0	0
5	B	1	Total	6	3	3	0	0

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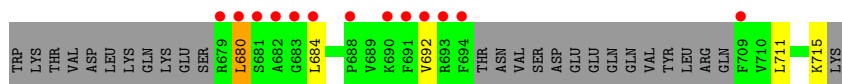
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	536	Total	O	0	0
			536	536		
6	B	557	Total	O	0	0
			557	557		
6	C	6	Total	O	0	0
			6	6		
6	D	4	Total	O	0	0
			4	4		





- Molecule 2: GLUCOSAMINIDASE

Chain C: 92% 8%



- Molecule 2: GLUCOSAMINIDASE

Chain D: 100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.71Å 94.54Å 99.48Å 75.34° 93.86° 77.07°	Depositor
Resolution (Å)	39.84 – 1.95 39.84 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.84-1.95) 96.7 (39.84-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.226 0.190 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: CA, NGT, GOL

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	0.95	0/5359	0.94	3/7236 (0.0%)
1	B	0.97	2/5357 (0.0%)	0.98	10/7233 (0.1%)
All	All	0.96	2/10716 (0.0%)	0.96	13/14469 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	ILE	C-O	-6.55	1.17	1.24
1	B	173	ALA	CA-CB	5.41	1.62	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	LEU	N-CA-C	6.71	118.60	111.28
1	A	89	GLU	N-CA-C	5.96	117.31	108.60
1	B	399	THR	N-CA-C	5.69	117.96	111.02
1	B	291	GLY	N-CA-C	-5.68	103.71	112.85
1	B	209	GLY	N-CA-C	5.53	120.77	113.37
1	B	89	GLU	N-CA-C	5.28	116.31	108.60
1	B	288	ASN	CA-C-N	-5.24	114.52	119.76
1	B	288	ASN	C-N-CA	-5.24	114.52	119.76
1	A	399	THR	N-CA-C	5.21	117.38	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	THR	CB-CA-C	-5.15	102.73	110.92
1	A	102	TYR	N-CA-C	5.08	116.89	111.36
1	B	277	MSE	CG-SE-CE	-5.07	87.78	98.92
1	B	560	VAL	CB-CA-C	-5.02	106.58	111.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5152	48	0
1	B	5227	0	5148	59	0
2	C	60	0	16	1	0
2	D	59	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
5	D	6	0	8	1	0
6	A	536	0	0	7	0
6	B	557	0	0	14	0
6	C	6	0	0	0	0
6	D	4	0	0	0	0
All	All	11738	0	10390	105	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 5.

All (105) 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:B:459:ASN:H	1:B:459:ASN:HD22	1.05	1.00
1:B:555:LYS:HE3	6:B:2521:HOH:O	1.81	0.78
1:A:540:TYR:O	1:A:544:THR:HG23	1.84	0.77
1:B:459:ASN:HD22	1:B:459:ASN:N	1.83	0.77
1:A:22:PRO:HB3	1:A:55:MSE:HE3	1.68	0.75
1:B:459:ASN:H	1:B:459:ASN:ND2	1.86	0.69
1:A:631:VAL:HG11	6:A:2534:HOH:O	1.93	0.69
1:A:45:LEU:HD23	1:A:45:LEU:C	2.21	0.65
1:A:466:GLU:HB2	6:A:2438:HOH:O	1.97	0.64
1:A:37:ALA:HB1	1:A:104:LEU:HD13	1.78	0.64
1:B:408:ARG:HD2	6:B:2420:HOH:O	1.98	0.62
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.82	0.62
1:B:647:ASN:HD22	1:B:648:PHE:N	1.98	0.61
1:A:484:MSE:HE3	1:B:537:GLN:HG2	1.82	0.60
1:A:615:LEU:HD23	1:A:616:ILE:C	2.28	0.58
1:B:109:GLN:O	1:B:112:LYS:NZ	2.38	0.56
1:B:595:MSE:HE1	1:B:605:LEU:O	2.06	0.56
1:A:381:LYS:HB3	1:A:410[A]:ILE:HD11	1.87	0.55
1:A:356:TYR:CE2	5:C:1720:GOL:H31	2.42	0.55
1:A:615:LEU:HD23	1:A:616:ILE:N	2.22	0.54
1:B:647:ASN:HD22	1:B:647:ASN:C	2.15	0.54
1:B:680:LEU:HD12	1:B:680:LEU:N	2.22	0.54
1:B:408:ARG:CD	6:B:2420:HOH:O	2.53	0.54
1:B:438:GLU:HB2	1:B:441[B]:MSE:SE	2.57	0.54
1:B:152:PHE:CZ	1:B:410[A]:ILE:HD11	2.43	0.53
1:B:451:LEU:HD22	1:B:564:LEU:HD12	1.89	0.53
1:A:647:ASN:C	1:A:647:ASN:HD22	2.16	0.53
1:B:45:LEU:C	1:B:45:LEU:HD23	2.32	0.53
1:B:355:VAL:O	1:B:399:THR:HG23	2.09	0.53
1:B:331:LYS:HE3	6:B:2357:HOH:O	2.09	0.52
1:B:54:GLY:N	6:B:2039:HOH:O	2.41	0.52
1:B:445:PRO:HB2	6:B:2453:HOH:O	2.10	0.52
1:A:615:LEU:HD23	1:A:616:ILE:O	2.10	0.52
1:B:188:LEU:HD13	1:B:229:MSE:HE1	1.91	0.52
1:B:151:LYS:HG3	6:B:2161:HOH:O	2.11	0.51
1:A:466:GLU:CB	6:A:2438:HOH:O	2.58	0.51
1:A:188:LEU:HD13	1:A:229:MSE:HE1	1.93	0.51
1:B:606:PRO:O	1:B:617:SER:OG	2.25	0.50
1:A:41:LEU:HB2	1:A:104:LEU:HD21	1.93	0.50
1:B:125:PRO:HB3	1:B:392:TRP:CE3	2.46	0.50
1:A:45:LEU:C	1:A:45:LEU:CD2	2.84	0.50
1:A:540:TYR:CE1	1:A:544:THR:HG21	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:PHE:CD2	1:B:469:GLN:OE1	2.65	0.49
1:B:65:LYS:NZ	6:B:2058:HOH:O	2.46	0.49
1:A:555:LYS:HE3	6:A:2498:HOH:O	2.12	0.49
1:A:88:LYS:HG3	1:A:89:GLU:HG2	1.94	0.49
1:A:341:PRO:O	1:A:342:VAL:C	2.56	0.49
1:B:151:LYS:NZ	1:B:198:ASN:HD21	2.11	0.49
1:B:406:ALA:O	1:B:410[A]:ILE:HG12	2.13	0.48
1:A:203:VAL:HG22	1:A:236:SER:HB2	1.94	0.48
1:B:34:ASN:O	1:B:38:VAL:HG23	2.13	0.48
1:A:181:PRO:HG2	1:A:184:GLU:OE1	2.14	0.48
1:B:151:LYS:CE	6:B:2161:HOH:O	2.62	0.47
1:B:77:HIS:HB3	6:B:2129:HOH:O	2.14	0.47
1:A:562:LYS:HB3	1:A:563:PRO:HD3	1.97	0.46
1:B:441[B]:MSE:HE3	1:B:441[B]:MSE:HA	1.97	0.46
1:B:643:ASN:HA	1:B:684:LEU:HG	1.98	0.46
1:B:680:LEU:CD1	1:B:680:LEU:H	2.28	0.46
1:A:475:MSE:HE3	1:A:502:PHE:CE1	2.51	0.45
1:B:151:LYS:CG	6:B:2161:HOH:O	2.64	0.45
1:B:356:TYR:CE2	5:D:1720:GOL:H12	2.50	0.45
1:A:514:LYS:NZ	6:A:2468:HOH:O	2.48	0.45
1:B:308:MSE:HA	1:B:335:TYR:O	2.17	0.45
1:A:262:ASP:HA	1:A:266:ALA:HB3	1.98	0.45
1:A:490:PRO:O	1:A:494:GLU:HG3	2.17	0.45
1:A:444:GLN:NE2	1:A:448:GLU:OE2	2.47	0.45
1:B:580:PHE:O	1:B:581:ASN:C	2.59	0.44
1:A:77:HIS:HB3	6:A:2132:HOH:O	2.17	0.44
1:B:341:PRO:O	1:B:342:VAL:C	2.60	0.44
1:B:465:PHE:CE2	1:B:469:GLN:OE1	2.71	0.44
1:B:262:ASP:HA	1:B:266:ALA:HB3	2.01	0.43
1:B:15:GLN:O	1:B:16:ASN:C	2.61	0.43
1:B:41:LEU:O	1:B:45:LEU:HD22	2.18	0.43
1:B:262:ASP:O	1:B:267:GLN:HG2	2.18	0.43
1:B:680:LEU:HD12	1:B:680:LEU:H	1.83	0.43
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.99	0.43
1:B:680:LEU:N	1:B:680:LEU:CD1	2.81	0.43
1:A:308:MSE:HA	1:A:335:TYR:O	2.19	0.43
1:A:557:ALA:HB1	1:A:561:ILE:HB	2.00	0.43
1:A:585:ASP:OD1	1:A:587:THR:HG23	2.19	0.43
1:A:83:LEU:C	1:A:83:LEU:HD23	2.43	0.43
1:B:315:ILE:HD12	1:B:339:ASN:HB3	2.01	0.43
1:B:452:LYS:O	1:B:453:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.53	0.43
1:B:271:ASP:N	1:B:271:ASP:OD1	2.50	0.43
1:A:25:TYR:CE1	1:A:45:LEU:HG	2.54	0.42
1:A:336:ILE:HG13	1:A:366:MSE:HE2	2.01	0.42
1:A:393:ASN:OD1	1:A:396:LYS:HD3	2.19	0.42
1:A:682:ALA:HB2	2:C:904:UNK:O	2.19	0.42
1:A:22:PRO:CB	1:A:55:MSE:HE3	2.44	0.42
1:A:615:LEU:HG	1:A:710:VAL:HG22	2.02	0.42
1:A:539:PHE:O	1:A:543:GLN:HG2	2.20	0.42
1:B:231:GLN:NE2	6:B:2281:HOH:O	2.44	0.42
1:A:164:GLY:N	1:A:165:PRO:HD3	2.34	0.42
1:A:631:VAL:CG1	6:A:2534:HOH:O	2.61	0.41
1:B:151:LYS:HE2	1:B:194:VAL:HG13	2.02	0.41
1:A:537:GLN:HG2	1:B:484:MSE:HE3	2.02	0.41
1:A:615:LEU:HD23	1:A:615:LEU:C	2.45	0.41
1:B:438:GLU:OE1	1:B:441[A]:MSE:HE2	2.21	0.41
1:B:517:GLU:O	1:B:518:GLY:C	2.63	0.41
1:B:567:ARG:HD2	6:B:2534:HOH:O	2.21	0.41
1:A:454:PHE:CE2	1:A:571:THR:CG2	3.04	0.41
1:B:692:VAL:HG21	1:B:711:LEU:HD22	2.03	0.41
1:B:595:MSE:C	6:B:2545:HOH:O	2.65	0.40
1:A:293:TYR:CD2	1:A:293:TYR:C	2.99	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	634/716 (88%)	612 (96%)	21 (3%)	1 (0%)	43 36
1	B	634/716 (88%)	611 (96%)	19 (3%)	4 (1%)	21 12
All	All	1268/1432 (88%)	1223 (96%)	40 (3%)	5 (0%)	30 21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	GLY
1	B	518	GLY
1	B	519	ARG
1	B	455	LYS
1	B	453	ALA

### 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	568/614 (92%)	554 (98%)	14 (2%)	42	34
1	B	568/614 (92%)	552 (97%)	16 (3%)	38	30
All	All	1136/1228 (92%)	1106 (97%)	30 (3%)	39	33

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	LEU
1	A	27	LEU
1	A	43	GLU
1	A	45	LEU
1	A	55	MSE
1	A	87	GLU
1	A	104	LEU
1	A	178	LEU
1	A	221	LEU
1	A	466	GLU
1	A	614	VAL
1	A	647	ASN
1	A	715	LYS
1	B	12	LEU
1	B	21	LEU
1	B	27	LEU
1	B	45	LEU

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	104	LEU
1	B	178	LEU
1	B	221	LEU
1	B	371	THR
1	B	459	ASN
1	B	541	ILE
1	B	632	GLU
1	B	642	GLU
1	B	647	ASN
1	B	680	LEU
1	B	715	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	73	GLN
1	A	144	GLN
1	A	339	ASN
1	A	372	ASN
1	A	529	ASN
1	A	608	GLN
1	A	643	ASN
1	A	647	ASN
1	B	73	GLN
1	B	77	HIS
1	B	95	ASN
1	B	144	GLN
1	B	198	ASN
1	B	273	ASN
1	B	339	ASN
1	B	372	ASN
1	B	401	GLN
1	B	425	ASN
1	B	459	ASN
1	B	529	ASN
1	B	536	GLN
1	B	647	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	C	1720	-	5,5,5	0.40	0	5,5,5	0.77	0
5	GOL	D	1720	-	5,5,5	0.35	0	5,5,5	1.43	2 (40%)
5	GOL	B	1718	-	5,5,5	0.47	0	5,5,5	0.61	0
4	NGT	B	1717	-	13,15,15	2.81	1 (7%)	14,22,22	1.50	2 (14%)
4	NGT	A	1718	-	13,15,15	3.50	1 (7%)	14,22,22	1.48	1 (7%)
5	GOL	A	1719	-	5,5,5	0.50	0	5,5,5	0.58	0

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
5	GOL	C	1720	-	-	3/4/4/4	-
5	GOL	D	1720	-	-	4/4/4/4	-
5	GOL	B	1718	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NGT	B	1717	-	-	0/2/30/30	0/2/2/2
4	NGT	A	1718	-	-	0/2/30/30	0/2/2/2
5	GOL	A	1719	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1718	NGT	C7-S1	-12.39	1.66	1.77
4	B	1717	NGT	C7-S1	-10.01	1.68	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1718	NGT	C8-C7-S1	3.85	124.76	118.96
4	B	1717	NGT	C8-C7-S1	3.81	124.69	118.96
4	B	1717	NGT	C3-C2-N2	-2.40	107.21	110.56
5	D	1720	GOL	O2-C2-C1	2.07	117.73	109.18
5	D	1720	GOL	O1-C1-C2	2.02	119.47	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1720	GOL	O1-C1-C2-C3
5	D	1720	GOL	O1-C1-C2-C3
5	D	1720	GOL	C1-C2-C3-O3
5	D	1720	GOL	O2-C2-C3-O3
5	C	1720	GOL	O1-C1-C2-O2
5	D	1720	GOL	O1-C1-C2-O2
5	C	1720	GOL	O2-C2-C3-O3
5	B	1718	GOL	O1-C1-C2-O2
5	B	1718	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1720	GOL	1	0
5	D	1720	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	891:UNK	C	899:UNK	N	5.34
1	D	891:UNK	C	899:UNK	N	5.17

## 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	626/716 (87%)	0.27	50 (7%) 18 21	10, 26, 63, 80	4 (0%)
1	B	623/716 (87%)	0.34	54 (8%) 16 18	10, 27, 63, 80	5 (0%)
2	C	0/12	-	-	-	-
2	D	0/12	-	-	-	-
All	All	1249/1456 (85%)	0.30	104 (8%) 17 20	10, 27, 63, 80	9 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	631	VAL	6.6
1	A	648	PHE	5.0
1	A	631	VAL	4.6
1	B	680	LEU	4.5
1	A	694	PHE	4.5
1	A	454	PHE	4.5
1	B	454	PHE	4.3
1	B	682	ALA	4.0
1	A	682	ALA	3.8
1	A	633	ILE	3.8
1	A	680	LEU	3.7
1	B	618	PRO	3.7
1	A	679	ARG	3.6
1	A	605	LEU	3.5
1	B	679	ARG	3.5
1	B	606	PRO	3.5
1	B	648	PHE	3.5
1	B	605	LEU	3.5
1	A	646	ILE	3.4
1	A	684	LEU	3.3
1	B	694	PHE	3.2
1	A	618	PRO	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	709	PHE	3.1
1	B	616	ILE	3.1
1	B	582	ALA	3.1
1	B	646	ILE	3.0
1	B	451	LEU	3.0
1	B	457	GLY	3.0
1	A	15	GLN	3.0
1	A	644	ILE	2.9
1	A	716	LYS	2.9
1	B	644	ILE	2.9
1	B	45	LEU	2.9
1	A	683	GLY	2.9
1	A	692	VAL	2.9
1	A	23	ALA	2.9
1	A	457	GLY	2.9
1	A	606	PRO	2.8
1	B	588	THR	2.8
1	A	604	ASN	2.8
1	B	456	GLU	2.8
1	B	519	ARG	2.7
1	A	453	ALA	2.7
1	B	54	GLY	2.7
1	A	691	PHE	2.7
1	B	461	ASP	2.7
1	A	693	ARG	2.7
1	A	451	LEU	2.7
1	B	615	LEU	2.6
1	B	518	GLY	2.6
1	B	292	ASN	2.6
1	A	616	ILE	2.6
1	A	614	VAL	2.6
1	B	24	VAL	2.6
1	B	458	LYS	2.6
1	A	689	VAL	2.6
1	B	691	PHE	2.5
1	B	581	ASN	2.5
1	A	461	ASP	2.5
1	A	615	LEU	2.5
1	B	693	ARG	2.5
1	B	692	VAL	2.5
1	B	635	LEU	2.5
1	A	710	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	684	LEU	2.4
1	A	18	THR	2.4
1	B	252	GLN	2.4
1	B	688	PRO	2.4
1	A	456	GLU	2.4
1	A	588	THR	2.4
1	A	617	SER	2.4
1	B	681	SER	2.4
1	A	45	LEU	2.3
1	A	540	TYR	2.3
1	B	638	ILE	2.3
1	B	604	ASN	2.3
1	B	453	ALA	2.3
1	A	458	LYS	2.3
1	B	452	LYS	2.3
1	A	460	TYR	2.3
1	B	19	ILE	2.3
1	A	519	ARG	2.2
1	A	518	GLY	2.2
1	A	687	ALA	2.2
1	B	633	ILE	2.2
1	B	459	ASN	2.2
1	B	617	SER	2.2
1	B	583	HIS	2.2
1	A	711	LEU	2.2
1	A	685	GLN	2.2
1	B	21	LEU	2.2
1	A	72	ARG	2.1
1	A	459	ASN	2.1
1	B	173	ALA	2.1
1	B	637	ALA	2.1
1	B	683	GLY	2.1
1	B	447	ALA	2.1
1	A	642	GLU	2.1
1	A	713	ILE	2.0
1	B	594	LYS	2.0
1	A	641	GLY	2.0
1	B	462	LYS	2.0
1	B	690	LYS	2.0
1	A	709	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	GOL	D	1720	6/6	0.85	0.15	42,44,45,45	0
5	GOL	C	1720	6/6	0.89	0.13	30,33,34,35	0
5	GOL	B	1718	6/6	0.89	0.12	42,48,50,51	0
5	GOL	A	1719	6/6	0.94	0.10	32,42,44,47	0
4	NGT	A	1718	14/14	0.98	0.06	15,17,19,20	0
4	NGT	B	1717	14/14	0.98	0.04	17,19,20,21	0
3	CA	A	1717	1/1	0.98	0.08	42,42,42,42	0
3	CA	B	1716	1/1	0.99	0.08	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.