Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:54 AM EDT

PDB ID	:	2CHN
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

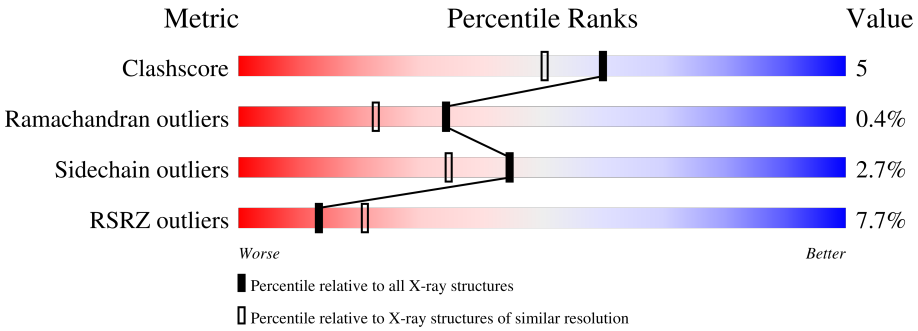
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 >=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 <=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	5% 79% 10% • 10%
1	B	716	8% 78% 10% • 11%
2	C	12	92% 8%
2	D	12	100%

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
1	A	642	Total	C	N	O	S	Se	0	4	0
			5235	3361	880	976	2	16			
1	B	639	Total	C	N	O	S	Se	0	7	0
			5227	3358	876	973	2	18			

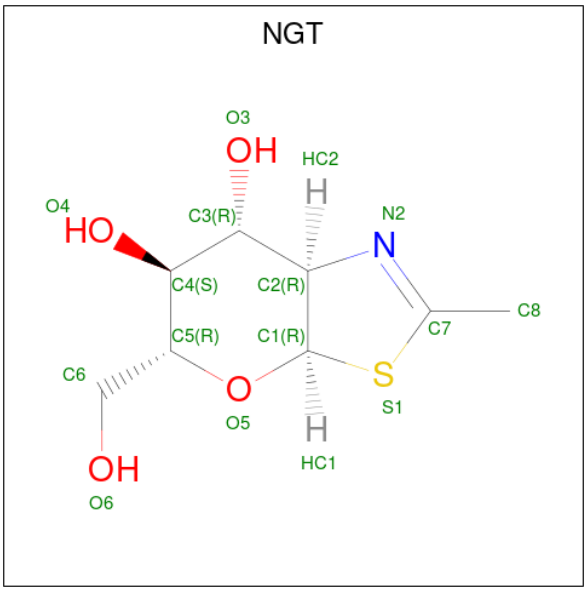
- Molecule 2 is a protein called GLUCOSAMINIDASE.

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

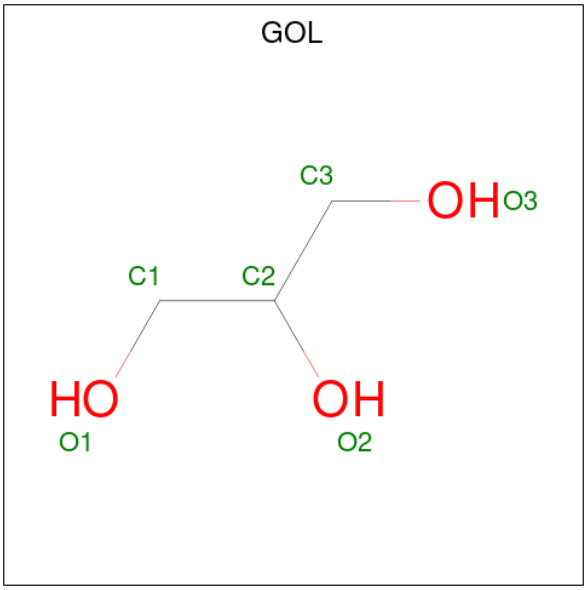
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is water.

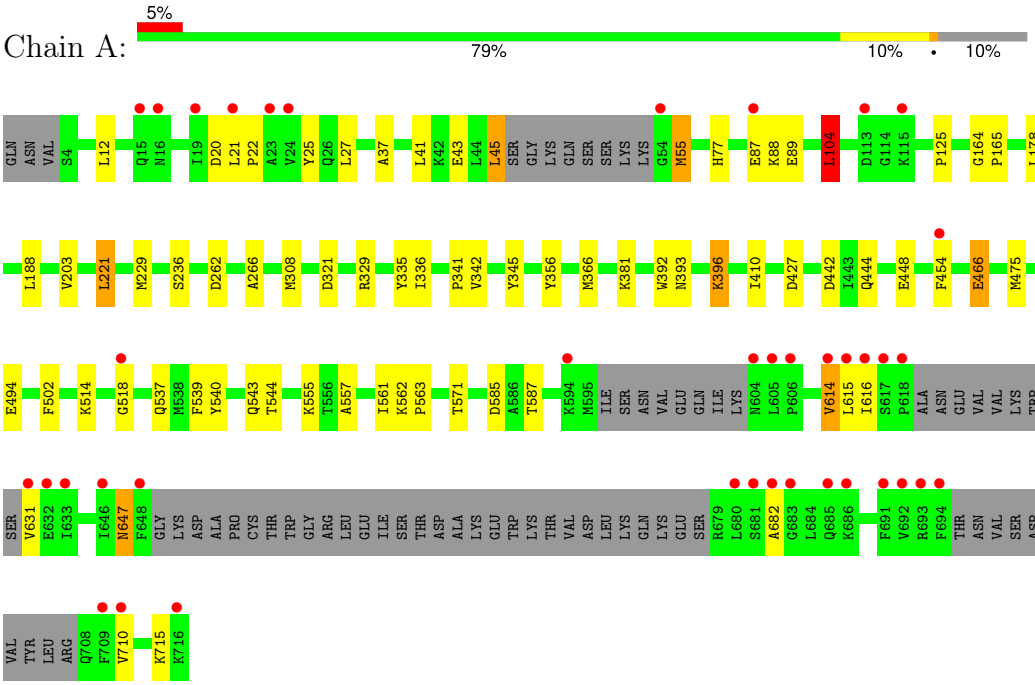
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	536	Total O 536 536	0	0
6	B	557	Total O 557 557	0	0
6	C	6	Total O 6 6	0	0
6	D	4	Total O 4 4	0	0

3 Residue-property plots (i)

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.

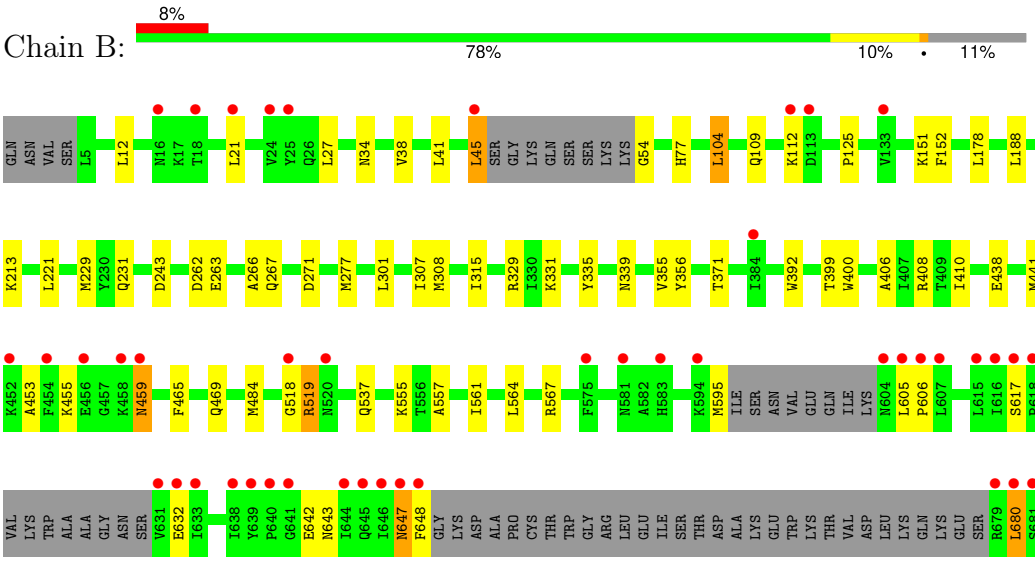
• Molecule 1: GLUCOSAMINIDASE

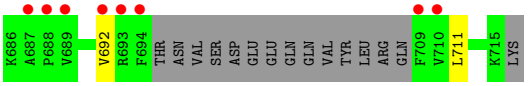
Chain A:



• Molecule 1: GLUCOSAMINIDASE

Chain B:



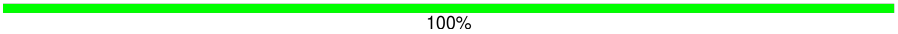


• Molecule 2: GLUCOSAMINIDASE

Chain C:

• Molecule 2: GLUCOSAMINIDASE

Chain D:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.71Å 94.54Å 99.48Å 75.34° 93.86° 77.07°	Depositor
Resolution (Å)	39.84 – 1.95 39.83 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.84-1.95) 96.7 (39.83-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.95Å)	Xtriage
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^2)	25.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11738	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, NGT

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	0.78	1/5359 (0.0%)	0.75	6/7236 (0.1%)
1	B	0.80	1/5357 (0.0%)	0.77	5/7233 (0.1%)
All	All	0.79	2/10716 (0.0%)	0.76	11/14469 (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	A	345	TYR	CD1-CE1	-5.26	1.31	1.39
1	B	263	GLU	CB-CG	5.14	1.61	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	LEU	CA-CB-CG	-6.61	100.11	115.30
1	A	104	LEU	CA-CB-CG	-6.06	101.36	115.30
1	A	442	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	427	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	329	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	329	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	221	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	277	MSE	CG-SE-CE	-5.06	87.78	98.90
1	B	519	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ASP	CB-CG-OD1	5.00	122.80	118.30
1	B	243	ASP	CB-CG-OD1	5.00	122.80	118.30

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 (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	5235	0	5152	45	0
1	B	5227	0	5148	53	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	2	0
6	A	536	0	0	7	0
6	B	557	0	0	12	0
6	C	6	0	0	0	0
6	D	4	0	0	0	0
All	All	11738	0	10390	96	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 (96) 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: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:45:LEU:HD23	1:A:45:LEU:C	2.21	0.60
1:A:484:MSE:HE3	1:B:537:GLN:HG2	1.82	0.60
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: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:615:LEU:HD23	1:A:616:ILE:C	2.28	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:540:TYR:CE1	1:A:544:THR:HG21	2.47	0.49
1:B:647:ASN:HD22	1:B:647:ASN:C	2.15	0.49
1:B:465:PHE:CD2	1:B:469:GLN:OE1	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:647:ASN:C	1:A:647:ASN:HD22	2.16	0.48
1:B:45:LEU:C	1:B:45:LEU:HD23	2.32	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:45:LEU:C	1:A:45:LEU:CD2	2.84	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:A:77:HIS:HB3	6:A:2132:HOH:O	2.17	0.44
1:A:341:PRO:O	1:A:342:VAL:C	2.56	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: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:B:315:ILE:HD12	1:B:339:ASN:HB3	2.01	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:438:GLU:OE1	1:B:441[A]:MSE:HE2	2.21	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:400:TRP:HZ2	5:D:1720:GOL:HO2	1.68	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%)	47	38
1	B	634/716 (88%)	611 (96%)	19 (3%)	4 (1%)	25	14
All	All	1268/1432 (88%)	1223 (96%)	40 (3%)	5 (0%)	34	22

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%)	552 (97%)	16 (3%)	43	33
1	B	568/614 (92%)	554 (98%)	14 (2%)	47	38
All	All	1136/1228 (92%)	1106 (97%)	30 (3%)	44	36

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

Mol	Chain	Res	Type
1	A	12	LEU
1	A	20	ASP
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	396	LYS
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
1	B	104	LEU
1	B	178	LEU
1	B	213	LYS
1	B	221	LEU
1	B	371	THR
1	B	459	ASN
1	B	632	GLU

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Mol	Chain	Res	Type
1	B	642	GLU
1	B	647	ASN
1	B	680	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	156	ASN
1	A	290	ASN
1	A	349	HIS
1	A	529	ASN
1	A	647	ASN
1	B	198	ASN
1	B	459	ASN
1	B	529	ASN
1	B	536	GLN
1	B	647	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

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	A	1719	-	5,5,5	0.50	0	5,5,5	0.58	0
4	NGT	A	1718	-	13,15,15	3.50	1 (7%)	14,22,22	1.48	1 (7%)
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%)
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%)

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	A	1719	-	-	0/4/4/4	-
4	NGT	A	1718	-	-	0/2/30/30	0/2/2/2
5	GOL	B	1718	-	-	2/4/4/4	-
4	NGT	B	1717	-	-	0/2/30/30	0/2/2/2
5	GOL	C	1720	-	-	3/4/4/4	-
5	GOL	D	1720	-	-	4/4/4/4	-

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(^{o})	Ideal(^{o})
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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1720	GOL	1	0
5	D	1720	GOL	2	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^{th} 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	626/716 (87%)	0.20	39 (6%) 20 29	12, 26, 63, 80	0
1	B	623/716 (87%)	0.29	57 (9%) 9 15	14, 27, 63, 80	0
2	C	0/12	-	-	-	-
2	D	0/12	-	-	-	-
All	All	1249/1456 (85%)	0.24	96 (7%) 13 21	12, 27, 63, 80	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	648	PHE	7.0
1	A	694	PHE	6.8
1	B	605	LEU	6.4
1	B	694	PHE	5.8
1	B	646	ILE	5.8
1	A	605	LEU	5.3
1	B	454	PHE	4.9
1	B	647	ASN	4.7
1	B	709	PHE	4.7
1	A	23	ALA	4.7
1	B	631	VAL	4.6
1	B	606	PRO	4.5
1	A	682	ALA	4.4
1	A	631	VAL	4.4
1	B	680	LEU	4.3
1	B	682	ALA	4.3
1	B	618	PRO	4.2
1	A	113	ASP	4.2
1	A	691	PHE	4.1
1	B	615	LEU	4.1
1	B	681	SER	4.0
1	A	680	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	616	ILE	4.0
1	B	638	ILE	4.0
1	B	617	SER	3.9
1	A	24	VAL	3.9
1	A	633	ILE	3.8
1	B	644	ILE	3.6
1	A	681	SER	3.6
1	A	615	LEU	3.5
1	A	632	GLU	3.5
1	A	604	ASN	3.5
1	B	688	PRO	3.5
1	A	709	PHE	3.5
1	B	633	ILE	3.4
1	B	518	GLY	3.4
1	B	452	LYS	3.4
1	A	21	LEU	3.3
1	B	687	ALA	3.3
1	A	16	ASN	3.3
1	A	618	PRO	3.3
1	A	693	ARG	3.3
1	B	683	GLY	3.3
1	B	456	GLU	3.2
1	B	16	ASN	3.2
1	A	616	ILE	3.2
1	A	685	GLN	3.1
1	B	685	GLN	3.1
1	A	54	GLY	3.1
1	A	606	PRO	3.1
1	A	594	LYS	3.0
1	B	692	VAL	3.0
1	A	15	GLN	3.0
1	B	607	LEU	3.0
1	B	113	ASP	3.0
1	A	518	GLY	3.0
1	B	693	ARG	3.0
1	B	21	LEU	3.0
1	B	458	LYS	2.9
1	B	604	ASN	2.9
1	B	640	PRO	2.9
1	B	581	ASN	2.8
1	A	716	LYS	2.8
1	A	692	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	641	GLY	2.7
1	A	87	GLU	2.7
1	A	617	SER	2.6
1	A	614	VAL	2.6
1	B	710	VAL	2.6
1	B	24	VAL	2.6
1	A	115	LYS	2.6
1	B	684	LEU	2.5
1	B	18	THR	2.5
1	B	639	TYR	2.5
1	B	645	GLN	2.5
1	B	45	LEU	2.5
1	A	646	ILE	2.4
1	B	594	LYS	2.4
1	B	451	LEU	2.4
1	A	710	VAL	2.4
1	B	679	ARG	2.4
1	B	25	TYR	2.4
1	B	575	PHE	2.3
1	A	19	ILE	2.3
1	B	632	GLU	2.3
1	A	683	GLY	2.3
1	B	133	VAL	2.3
1	B	689	VAL	2.3
1	B	112	LYS	2.3
1	A	648	PHE	2.2
1	A	686	LYS	2.1
1	B	583	HIS	2.1
1	B	384	ILE	2.1
1	B	459	ASN	2.1
1	A	454	PHE	2.0
1	B	520	ASN	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 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^{th} 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(Å^2)	Q<0.9
5	GOL	B	1718	6/6	0.87	0.15	42,48,50,51	0
5	GOL	D	1720	6/6	0.91	0.16	42,44,45,45	0
5	GOL	A	1719	6/6	0.92	0.16	32,42,44,47	0
5	GOL	C	1720	6/6	0.94	0.10	30,33,34,35	0
3	CA	A	1717	1/1	0.97	0.07	42,42,42,42	0
4	NGT	A	1718	14/14	0.98	0.11	15,17,19,20	0
4	NGT	B	1717	14/14	0.98	0.13	17,19,20,21	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.