



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2CHO
Title : Bacteroides thetaiotaomicron hexosaminidase with O-GlcNAcase activity
Authors : Dennis, R.J.; Taylor, E.J.; Macauley, M.S.; Stubbs, K.A.; Turkenburg, J.P.;
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Deposited on : 2006-03-16
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

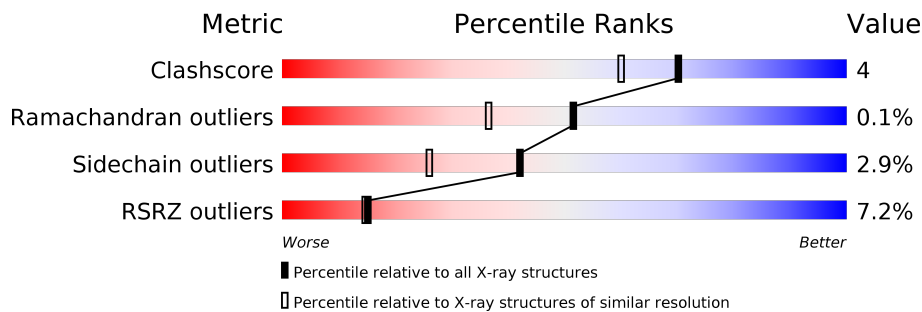
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	716	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 81% 7% • 10%</p>
1	B	716	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 79% 9% • 11%</p>
2	C	13	<div style="width: 100%; height: 10px; background-color: green;"></div> <p style="text-align: center;">100%</p>
2	D	13	<div style="width: 100%; height: 10px; background-color: green;"></div> <p style="text-align: center;">100%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11799 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			
1	A	641	5229	3358	879	974	18	0	4	0
1	B	639	5217	3350	876	973	18	0	5	0

- Molecule 2 is a protein called GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	13	65	39	13	13	0	0	0
2	D	13	65	39	13	13	0	0	0

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

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- 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	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	579	Total	O	0	0
			579	579		
6	B	602	Total	O	0	0
			602	602		
6	C	4	Total	O	0	0
			4	4		
6	D	4	Total	O	0	0
			4	4		

- Molecule 2: GLUCOSAMINIDASE

Chain C:  100%

There are no outlier residues recorded for this chain.

- 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, α , β , γ	51.69Å 93.45Å 98.83Å 75.51° 94.15° 77.15°	Depositor
Resolution (Å)	37.74 – 1.85 37.74 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.4 (37.74-1.85) 96.4 (37.74-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.220 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.059	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11799	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/5369	0.71	8/7276 (0.1%)
1	B	0.69	0/5357	0.72	5/7261 (0.1%)
All	All	0.67	0/10726	0.71	13/14537 (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	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	LEU	CA-CB-CG	-8.18	96.48	115.30
1	A	104	LEU	CA-CB-CG	-6.59	100.14	115.30
1	A	645	GLN	N-CA-C	5.98	127.14	111.00
1	A	615	LEU	CA-CB-CG	5.84	128.73	115.30
1	A	442	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	291	GLY	N-CA-C	-5.66	98.95	113.10
1	A	240	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	B	399	THR	CB-CA-C	-5.50	96.75	111.60
1	A	240	PHE	CB-CG-CD1	5.39	124.57	120.80
1	A	427	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	615	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	474	ARG	NE-CZ-NH2	-5.17	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CB-CG-OD2	-5.06	113.75	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	614	VAL	Peptide
1	A	644	ILE	Peptide
1	A	679	ARG	Peptide
1	B	644	ILE	Peptide
1	B	679	ARG	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	5229	0	5147	34	0
1	B	5217	0	5130	42	0
2	C	65	0	17	0	0
2	D	65	0	17	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	579	0	0	7	0
6	B	602	0	0	10	1
6	C	4	0	0	0	0
6	D	4	0	0	0	0
All	All	11799	0	10349	76	1

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 4.

All (76) 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:555:LYS:HE3	6:B:2544:HOH:O	1.55	1.05
1:B:459:ASN:H	1:B:459:ASN:HD22	0.97	0.97
1:B:459:ASN:N	1:B:459:ASN:HD22	1.76	0.83
1:B:647:ASN:HD22	1:B:648:PHE:N	1.77	0.82
1:B:459:ASN:H	1:B:459:ASN:ND2	1.79	0.81
1:B:355:VAL:O	1:B:399:THR:HG23	1.90	0.72
1:A:645:GLN:HB3	1:A:708:GLN:NE2	2.09	0.67
1:A:5:LEU:N	6:A:2004:HOH:O	2.28	0.66
1:A:151:LYS:NZ	1:A:198:ASN:HD21	1.94	0.65
1:B:408:ARG:HD2	6:B:2443:HOH:O	1.98	0.63
1:B:151:LYS:NZ	1:B:198:ASN:HD21	2.01	0.57
1:A:536:GLN:HG2	1:A:590:TYR:CD1	2.40	0.57
1:B:406:ALA:O	1:B:410[A]:ILE:HG12	2.04	0.57
1:A:151:LYS:HD3	1:A:198:ASN:ND2	2.20	0.56
1:B:445:PRO:HB2	6:B:2189:HOH:O	2.05	0.56
1:A:631:VAL:HG11	6:A:2577:HOH:O	2.07	0.55
1:B:151:LYS:HG3	6:B:2165:HOH:O	2.06	0.55
1:B:151:LYS:CG	6:B:2165:HOH:O	2.55	0.54
1:B:109:GLN:O	1:B:112:LYS:NZ	2.40	0.54
1:B:647:ASN:C	1:B:647:ASN:HD22	2.10	0.53
1:B:643:ASN:HA	1:B:684:LEU:HG	1.90	0.53
1:A:381:LYS:HB3	1:A:410[A]:ILE:HD11	1.92	0.52
1:A:37:ALA:HB1	1:A:104:LEU:HD13	1.92	0.51
1:B:271:ASP:N	1:B:271:ASP:OD1	2.41	0.51
1:A:45:LEU:HD23	1:A:45:LEU:C	2.31	0.51
1:A:540:TYR:O	1:A:544:THR:HG23	2.10	0.51
1:B:125:PRO:HB3	1:B:392:TRP:CE3	2.46	0.51
1:B:646:ILE:HG22	1:B:647:ASN:N	2.25	0.50
1:B:170:TYR:HB2	1:B:180:TYR:CE1	2.47	0.49
1:A:125:PRO:HB3	1:A:392:TRP:CE3	2.47	0.49
1:A:591:MET:HG3	1:A:593:HIS:O	2.12	0.49
1:B:45:LEU:C	1:B:45:LEU:HD23	2.33	0.48
1:B:452:LYS:O	1:B:453:ALA:C	2.52	0.48
1:A:646:ILE:HG22	1:A:647:ASN:N	2.28	0.48
1:B:356:TYR:HB3	1:B:399:THR:HG21	1.95	0.47
1:A:151:LYS:HD3	1:A:198:ASN:HD21	1.80	0.47
1:B:465:PHE:CD2	1:B:469:GLN:OE1	2.68	0.46
1:B:354:PRO:HB2	1:B:399:THR:HG22	1.97	0.46
1:B:301:LEU:HD12	1:B:307:ILE:HD11	1.97	0.46
1:B:189:GLN:NE2	6:B:2232:HOH:O	2.49	0.45
1:B:308:MET:HA	1:B:335:TYR:O	2.16	0.45
1:A:151:LYS:HG2	6:A:2169:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:VAL:HG21	1:B:711:LEU:HD22	1.98	0.45
1:B:438:GLU:CD	1:B:441:MET:HG3	2.37	0.45
1:A:540:TYR:CE1	1:A:544:THR:HG21	2.52	0.45
1:B:262:ASP:HA	1:B:266:ALA:HB3	1.99	0.45
1:A:308:MET:HA	1:A:335:TYR:O	2.18	0.44
1:B:151:LYS:HE2	1:B:194:VAL:HG13	1.98	0.44
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.52	0.44
1:A:445:PRO:HB2	6:A:2465:HOH:O	2.18	0.44
1:B:262:ASP:O	1:B:267:GLN:HG2	2.18	0.44
1:A:151:LYS:CG	6:A:2169:HOH:O	2.65	0.44
1:A:238:ALA:HA	1:A:276:VAL:O	2.18	0.44
1:A:444:GLN:NE2	1:A:448:GLU:OE2	2.48	0.44
1:B:532:LYS:HD2	1:B:532:LYS:HA	1.87	0.44
1:B:444:GLN:N	1:B:445:PRO:CD	2.81	0.43
1:B:183:LYS:HD2	6:B:2214:HOH:O	2.18	0.43
1:B:112:LYS:HE3	6:B:2121:HOH:O	2.19	0.43
1:B:591:MET:HG3	1:B:593:HIS:O	2.20	0.42
1:B:151:LYS:CE	6:B:2165:HOH:O	2.66	0.42
1:A:715:LYS:H	1:A:716:LYS:CA	2.33	0.42
1:A:715:LYS:H	1:A:716:LYS:HA	1.85	0.42
1:A:444:GLN:N	1:A:445:PRO:CD	2.83	0.42
1:A:644:ILE:HA	1:A:710:VAL:O	2.19	0.41
1:B:238:ALA:HA	1:B:276:VAL:O	2.20	0.41
1:A:151:LYS:CE	1:A:198:ASN:HD21	2.33	0.41
1:A:536:GLN:HG2	1:A:590:TYR:CG	2.56	0.41
1:B:11:GLN:NE2	6:B:2012:HOH:O	2.52	0.41
1:A:536:GLN:OE1	6:A:2518:HOH:O	2.22	0.41
1:A:444:GLN:HB3	1:A:445:PRO:HD3	2.03	0.41
1:A:141:TRP:CZ2	1:A:373:PRO:HG2	2.56	0.41
1:B:385:TYR:CD2	1:B:406:ALA:HB2	2.56	0.40
1:A:72:ARG:NH1	6:A:2082:HOH:O	2.54	0.40
1:B:562:LYS:N	1:B:563:PRO:CD	2.85	0.40
1:A:149:GLN:HB3	1:A:153:TYR:CZ	2.56	0.40
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2204:HOH:O	6:B:2482:HOH:O[1_455]	1.90	0.30

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	633/716 (88%)	617 (98%)	16 (2%)	0	100	100
1	B	632/716 (88%)	608 (96%)	23 (4%)	1 (0%)	47	33
All	All	1265/1432 (88%)	1225 (97%)	39 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	GLY

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	567/630 (90%)	551 (97%)	16 (3%)	43	27
1	B	566/630 (90%)	549 (97%)	17 (3%)	41	24
All	All	1133/1260 (90%)	1100 (97%)	33 (3%)	42	26

All (33) 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

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Mol	Chain	Res	Type
1	A	55	MET
1	A	87	GLU
1	A	104	LEU
1	A	178	LEU
1	A	221	LEU
1	A	300	LYS
1	A	371	THR
1	A	396	LYS
1	A	466	GLU
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	87	GLU
1	B	104	LEU
1	B	178	LEU
1	B	213	LYS
1	B	221	LEU
1	B	323	ILE
1	B	371	THR
1	B	399	THR
1	B	459	ASN
1	B	541	ILE
1	B	632	GLU
1	B	642	GLU
1	B	647	ASN

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

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

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Mol	Chain	Res	Type
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 monosaccharides 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	B	1719	-	5,5,5	0.43	0	5,5,5	0.22	0
5	GOL	B	1717	-	5,5,5	0.53	0	5,5,5	0.48	0
5	GOL	A	1719	-	5,5,5	0.30	0	5,5,5	0.42	0
4	ACT	A	1718	-	1,3,3	0.37	0	0,3,3	0.00	-
5	GOL	A	1720	-	5,5,5	0.44	0	5,5,5	0.39	0
4	ACT	B	1718	-	1,3,3	1.42	0	0,3,3	0.00	-

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	1720	-	-	1/4/4/4	-
5	GOL	B	1719	-	-	0/4/4/4	-
5	GOL	A	1719	-	-	0/4/4/4	-
5	GOL	B	1717	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1720	GOL	O1-C1-C2-C3

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	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	5.26
1	D	891:UNK	C	899:UNK	N	5.02

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	641/716 (89%)	0.17	51 (7%) 12 12	9, 21, 54, 74	0
1	B	639/716 (89%)	0.20	41 (6%) 19 18	8, 20, 54, 74	0
2	C	0/13	-	-	-	-
2	D	0/13	-	-	-	-
All	All	1280/1458 (87%)	0.19	92 (7%) 15 15	8, 21, 54, 74	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	605	LEU	6.8
1	B	648	PHE	6.7
1	A	694	PHE	6.7
1	B	679	ARG	6.4
1	A	679	ARG	6.3
1	B	680	LEU	5.9
1	B	646	ILE	5.3
1	B	631	VAL	5.3
1	A	113	ASP	5.1
1	B	605	LEU	5.1
1	B	16	ASN	5.0
1	A	631	VAL	5.0
1	B	694	PHE	4.6
1	B	682	ALA	4.5
1	B	606	PRO	4.4
1	A	16	ASN	4.3
1	B	618	PRO	4.3
1	B	693	ARG	4.2
1	B	583	HIS	4.2
1	B	581	ASN	4.1
1	A	604	ASN	4.1
1	A	23	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	18	THR	3.9
1	A	54	GLY	3.9
1	B	709	PHE	3.8
1	B	647	ASN	3.8
1	B	683	GLY	3.8
1	A	518	GLY	3.7
1	A	693	ARG	3.7
1	B	458	LYS	3.6
1	B	617	SER	3.6
1	B	638	ILE	3.6
1	B	113	ASP	3.6
1	B	24	VAL	3.6
1	A	581	ASN	3.5
1	B	710	VAL	3.5
1	B	604	ASN	3.4
1	A	715	LYS	3.4
1	A	681	SER	3.3
1	A	716	LYS	3.3
1	B	54	GLY	3.2
1	A	583	HIS	3.2
1	B	685	GLN	3.2
1	A	45	LEU	3.2
1	A	606	PRO	3.2
1	A	680	LEU	3.1
1	A	87	GLU	3.1
1	B	645	GLN	3.1
1	A	618	PRO	3.1
1	B	462	LYS	3.0
1	B	45	LEU	3.0
1	B	518	GLY	3.0
1	A	24	VAL	3.0
1	A	112	LYS	2.9
1	A	454	PHE	2.8
1	A	594	LYS	2.8
1	A	632	GLU	2.7
1	A	115	LYS	2.7
1	A	17	LYS	2.7
1	A	648	PHE	2.7
1	B	632	GLU	2.7
1	A	15	GLN	2.7
1	A	710	VAL	2.6
1	A	638	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLU	2.6
1	A	21	LEU	2.6
1	A	19	ILE	2.6
1	B	112	LYS	2.5
1	A	595	MET	2.5
1	A	20	ASP	2.5
1	B	519	ARG	2.4
1	A	691	PHE	2.4
1	B	31	GLU	2.4
1	B	692	VAL	2.4
1	A	692	VAL	2.4
1	A	617	SER	2.3
1	A	682	ALA	2.3
1	A	456	GLU	2.3
1	A	519	ARG	2.3
1	A	252	GLN	2.3
1	B	684	LEU	2.3
1	B	25	TYR	2.2
1	A	55	MET	2.2
1	A	685	GLN	2.2
1	A	114	GLY	2.2
1	A	22	PRO	2.2
1	A	88	LYS	2.2
1	A	452	LYS	2.1
1	B	114	GLY	2.1
1	B	595	MET	2.1
1	B	18	THR	2.1
1	B	459	ASN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	1717	6/6	0.91	0.12	24,29,32,35	0
3	CA	A	1717	1/1	0.93	0.12	38,38,38,38	0
5	GOL	A	1720	6/6	0.93	0.10	26,32,34,37	0
3	CA	B	1716	1/1	0.96	0.08	34,34,34,34	0
5	GOL	A	1719	6/6	0.97	0.08	18,19,20,20	0
4	ACT	A	1718	4/4	0.97	0.12	15,16,16,17	0
4	ACT	B	1718	4/4	0.97	0.12	12,12,12,13	0
5	GOL	B	1719	6/6	0.98	0.08	15,16,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.