wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 02:37 am GMT

PDB ID	:	2J4G
Title	:	Bacteroides thetaiotaomicron GH84 O-GlcNAcase in complex with n-butyl-thiazoline inhibitor
Authors	:	Dennis, R.J.; Davies, G.J.
Deposited on	:	2006-08-31
Resolution	:	2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

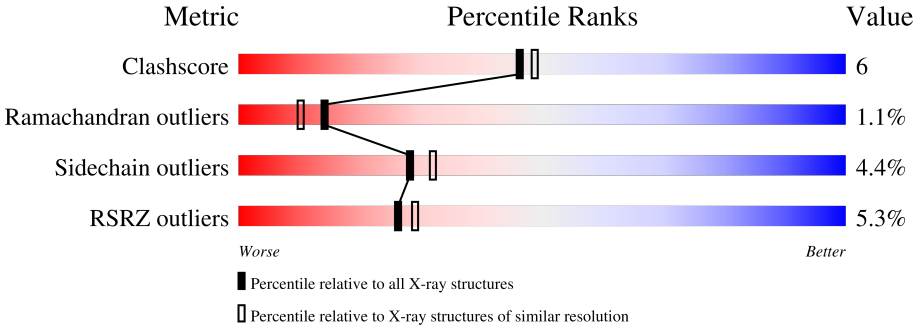
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	715	5% 69% 11% • 18%
1	B	715	4% 66% 13% • 19%

2 Entry composition (i)

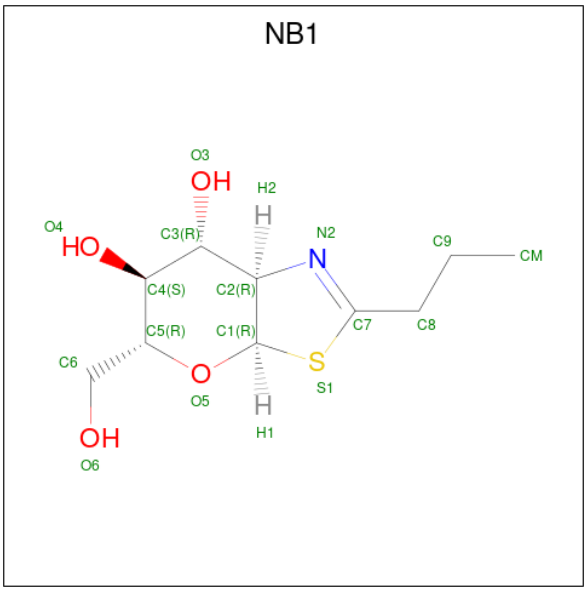
There are 5 unique types of molecules in this entry. The entry contains 10075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYALURONOGLUCOSAMINIDASE.

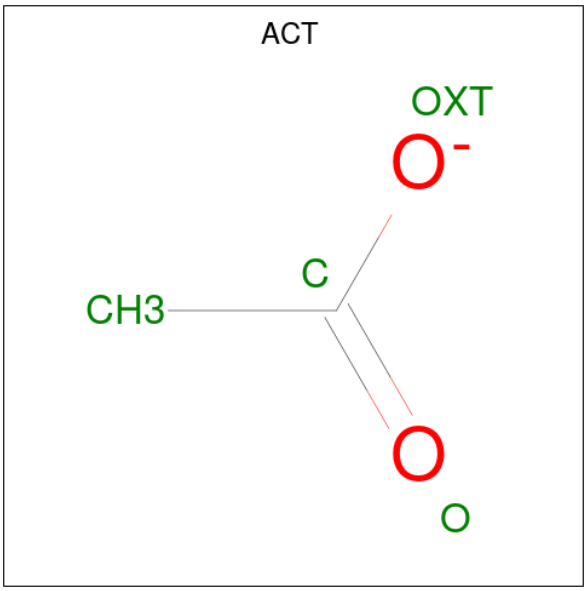
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	586	4759	3040	806	897	16	0	1	0
1	B	580	4706	3009	794	887	16	0	0	0

- Molecule 2 is (3AR,5R,6S,7R,7AR)-5-(HYDROXYMETHYL)-2-PROPYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D][1,3]THIAZOLE-6,7-DIOL (three-letter code: NB1) (formula: $C_{10}H_{17}NO_4S$).



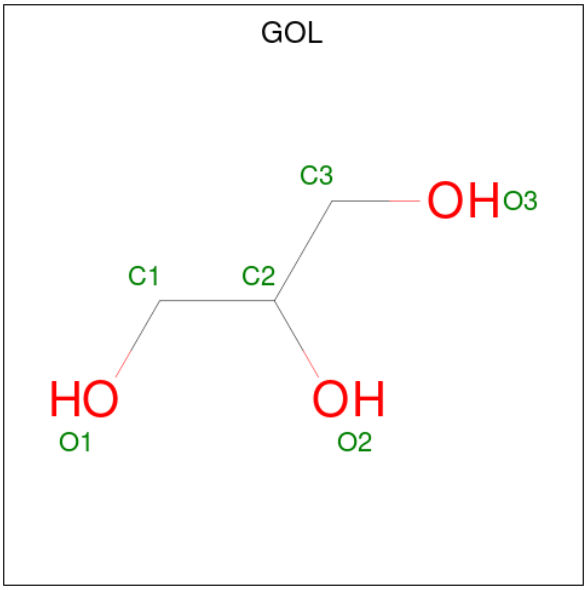
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	16	10	1	4	1	0	0
2	B	1	16	10	1	4	1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

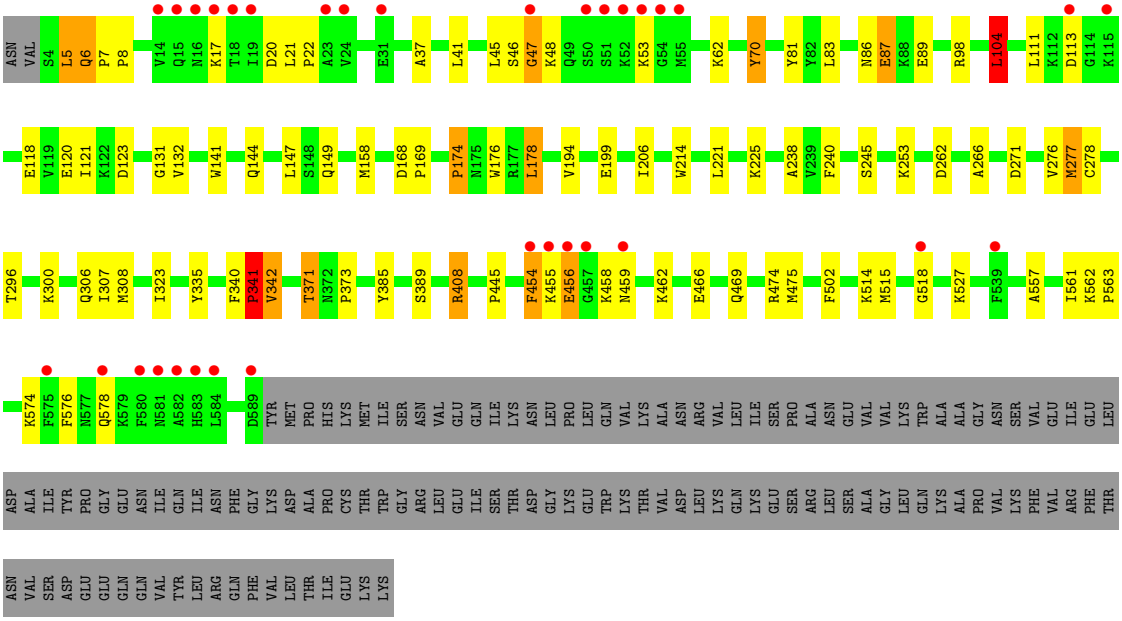
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	280	280	280	0	0
			Total	O		
5	B	278	278	278	0	0

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.

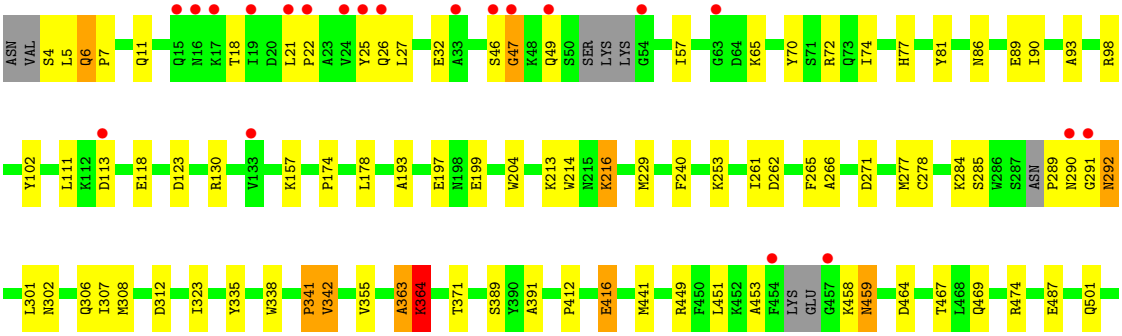
• Molecule 1: HYALURONOGLUCOSAMINIDASE

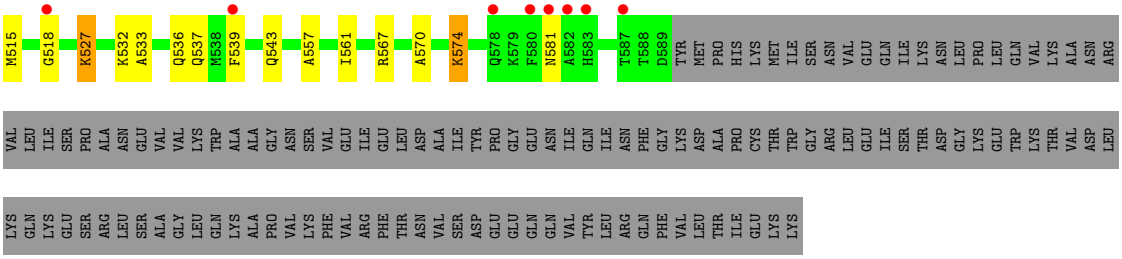
Chain A: 5% 69% 11% • 18%



• Molecule 1: HYALURONOGLUCOSAMINIDASE

Chain B: 4% 66% 13% • 19%




M515 G518 K527 K532 A533 Q536 Q537 M538 F539 Q543 A557 I561 R567 A570 K574 Q578 K579 F580 N581 A582 H583 T587 T588 D589 TYR MET PRO HIS LYS MET ILE SER ASN VAL GLU GLN ILE LYS ASN LEU PRO LEU GLN VAL LYS ALA ASN ARG
VAL LEU ILE SER PRO ALA ASN GLU VAL VAL LYS TRP ALA ALA GLY ASN SER VAL GLU ILE GLU LEU ASP ALA ILE TYR PRO GLY GLU ASN ILE GLN ILE ASN PHE GLY LYS ASP ALA PRO CYS THR TRP GLY ARG LEU GLU ILE SER THR ASP GLY LYS GLU TRP LYS THR VAL ASP LEU
LYS GLN LYS GLU SER ARG LEU SER ALA GLY LEU GLN LYS ALA PRO VAL LYS PHE VAL ARG PHE THR ASN VAL SER ASP GLU GLU GLN GLN VAL TYR LEU ARG GLN PHE VAL LEU THR ILE GLU LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.11Å 51.71Å 172.78Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	169.03 – 2.25 39.38 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (169.03-2.25) 99.6 (39.38-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.06 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.284 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.8	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	0.94	EDS
Total number of atoms	10075	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4882e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NB1, GOL, 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	0.70	0/4886	0.75	2/6626 (0.0%)
1	B	0.71	0/4827	0.76	6/6544 (0.1%)
All	All	0.70	0/9713	0.76	8/13170 (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	4
All	All	0	7

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	6	GLN	N-CA-C	9.37	136.29	111.00
1	B	364	LYS	N-CA-C	-8.90	86.96	111.00
1	A	5	LEU	C-N-CA	7.28	139.89	121.70
1	B	6	GLN	N-CA-CB	-5.63	100.47	110.60
1	B	342	VAL	N-CA-C	-5.57	95.97	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	341	PRO	Peptide
1	A	5	LEU	Peptide
1	B	174	PRO	Peptide
1	B	5	LEU	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	4759	0	4642	58	0
1	B	4706	0	4583	61	0
2	A	16	0	17	0	0
2	B	16	0	17	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	280	0	0	9	0
5	B	278	0	0	10	0
All	All	10075	0	9281	119	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 6.

The worst 5 of 119 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:A:245:SER:HB3	5:A:2121:HOH:O	1.66	0.94
1:B:532:LYS:O	1:B:536:GLN:HG3	1.85	0.77
1:B:570:ALA:O	1:B:574:LYS:HE3	1.89	0.72
1:A:277:MET:CE	1:A:307:ILE:HG23	2.20	0.71
1:B:441:MET:HB2	5:B:2222:HOH:O	1.95	0.67

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	585/715 (82%)	553 (94%)	24 (4%)	8 (1%)	11 7
1	B	572/715 (80%)	544 (95%)	23 (4%)	5 (1%)	17 14
All	All	1157/1430 (81%)	1097 (95%)	47 (4%)	13 (1%)	14 10

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	47	GLY
1	A	342	VAL
1	B	47	GLY
1	A	455	LYS

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	513/629 (82%)	491 (96%)	22 (4%)	29 33
1	B	507/629 (81%)	483 (95%)	24 (5%)	26 29
All	All	1020/1258 (81%)	974 (96%)	46 (4%)	28 31

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	LYS

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Mol	Chain	Res	Type
1	B	292	ASN
1	B	72	ARG
1	B	213	LYS
1	B	342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	547	GLN
1	B	273	ASN
1	B	306	GLN
1	B	292	ASN
1	A	274	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACT	B	1591	-	3,3,3	0.82	0	3,3,3	1.43	0
2	NB1	A	1590	-	15,17,17	2.29	2 (13%)	14,24,24	2.40	4 (28%)
2	NB1	B	1590	-	15,17,17	2.67	2 (13%)	14,24,24	2.64	4 (28%)
4	GOL	A	1719	-	5,5,5	0.38	0	5,5,5	1.12	0
3	ACT	A	1591	-	3,3,3	0.83	0	3,3,3	1.37	0
4	GOL	B	1719	-	5,5,5	0.56	0	5,5,5	0.37	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
4	GOL	A	1719	-	-	0/4/4/4	-
4	GOL	B	1719	-	-	0/4/4/4	-
2	NB1	A	1590	-	-	0/5/33/33	0/2/2/2
2	NB1	B	1590	-	-	0/5/33/33	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1590	NB1	C7-N2	9.65	1.35	1.27
2	A	1590	NB1	C7-N2	7.57	1.34	1.27
2	A	1590	NB1	C7-S1	-3.41	1.70	1.76
2	B	1590	NB1	C7-S1	-2.73	1.71	1.76

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1590	NB1	C8-C7-S1	8.38	130.31	121.75
2	A	1590	NB1	C8-C7-S1	7.01	128.91	121.75
2	A	1590	NB1	C1-O5-C5	3.51	119.05	112.58
2	B	1590	NB1	C1-O5-C5	3.00	118.11	112.58
2	A	1590	NB1	C9-C8-C7	-2.89	110.00	115.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	586/715 (81%)	0.09	33 (5%)	24	26	13, 27, 63, 77	0
1	B	580/715 (81%)	0.13	29 (5%)	28	31	13, 26, 63, 78	0
All	All	1166/1430 (81%)	0.11	62 (5%)	26	29	13, 27, 63, 78	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	LYS	8.0
1	A	457	GLY	6.0
1	A	54	GLY	5.2
1	B	24	VAL	4.9
1	B	19	ILE	3.7

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(Å^2)	Q<0.9
3	ACT	B	1591	4/4	0.86	0.19	52,52,52,52	0
4	GOL	A	1719	6/6	0.91	0.13	25,31,32,36	0
4	GOL	B	1719	6/6	0.93	0.13	35,37,42,44	0
3	ACT	A	1591	4/4	0.94	0.10	56,56,56,56	0
2	NB1	B	1590	16/16	0.96	0.14	15,19,20,20	0
2	NB1	A	1590	16/16	0.98	0.14	14,18,19,21	0

6.5 Other polymers (i)

There are no such residues in this entry.