WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2017 – 03:19 PM EST

PDB ID	:	5CXY
Title	:	Structure of a Glycosyltransferase in Complex with Inhibitor
Authors	:	Volkers, G.; Strynadka, N.C.J.
Deposited on	:	unknown
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.15 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		4.4%
RSRZ outliers		3.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
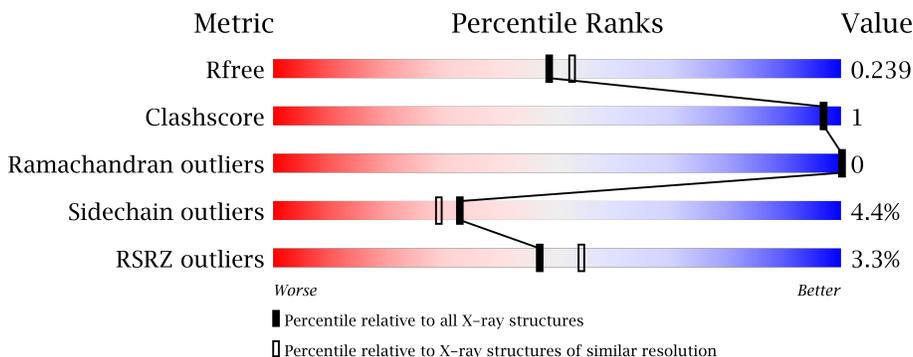
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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. 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	323	2% ▬ 84% 6% 10%
1	B	323	4% ▬ 82% 8% · 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5229 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 Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total 2395	C 1546	N 418	O 421	S 10	0	0	0
1	B	292	Total 2410	C 1558	N 420	O 422	S 10	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	-	expression tag	UNP O43173
A	59	PRO	-	expression tag	UNP O43173
A	60	GLU	-	expression tag	UNP O43173
A	61	HIS	-	expression tag	UNP O43173
A	62	HIS	-	expression tag	UNP O43173
A	63	HIS	-	expression tag	UNP O43173
A	64	HIS	-	expression tag	UNP O43173
A	65	HIS	-	expression tag	UNP O43173
A	66	HIS	-	expression tag	UNP O43173
A	67	ASP	-	expression tag	UNP O43173
A	68	TYR	-	expression tag	UNP O43173
A	69	ASP	-	expression tag	UNP O43173
A	70	ILE	-	expression tag	UNP O43173
A	71	PRO	-	expression tag	UNP O43173
A	72	THR	-	expression tag	UNP O43173
A	73	THR	-	expression tag	UNP O43173
A	74	GLU	-	expression tag	UNP O43173
A	75	ASN	-	expression tag	UNP O43173
A	76	LEU	-	expression tag	UNP O43173
A	77	TYR	-	expression tag	UNP O43173
A	78	PHE	-	expression tag	UNP O43173
A	79	GLN	-	expression tag	UNP O43173
A	80	GLY	-	expression tag	UNP O43173
B	58	ALA	-	expression tag	UNP O43173

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Chain	Residue	Modelled	Actual	Comment	Reference
B	59	PRO	-	expression tag	UNP O43173
B	60	GLU	-	expression tag	UNP O43173
B	61	HIS	-	expression tag	UNP O43173
B	62	HIS	-	expression tag	UNP O43173
B	63	HIS	-	expression tag	UNP O43173
B	64	HIS	-	expression tag	UNP O43173
B	65	HIS	-	expression tag	UNP O43173
B	66	HIS	-	expression tag	UNP O43173
B	67	ASP	-	expression tag	UNP O43173
B	68	TYR	-	expression tag	UNP O43173
B	69	ASP	-	expression tag	UNP O43173
B	70	ILE	-	expression tag	UNP O43173
B	71	PRO	-	expression tag	UNP O43173
B	72	THR	-	expression tag	UNP O43173
B	73	THR	-	expression tag	UNP O43173
B	74	GLU	-	expression tag	UNP O43173
B	75	ASN	-	expression tag	UNP O43173
B	76	LEU	-	expression tag	UNP O43173
B	77	TYR	-	expression tag	UNP O43173
B	78	PHE	-	expression tag	UNP O43173
B	79	GLN	-	expression tag	UNP O43173
B	80	GLY	-	expression tag	UNP O43173

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
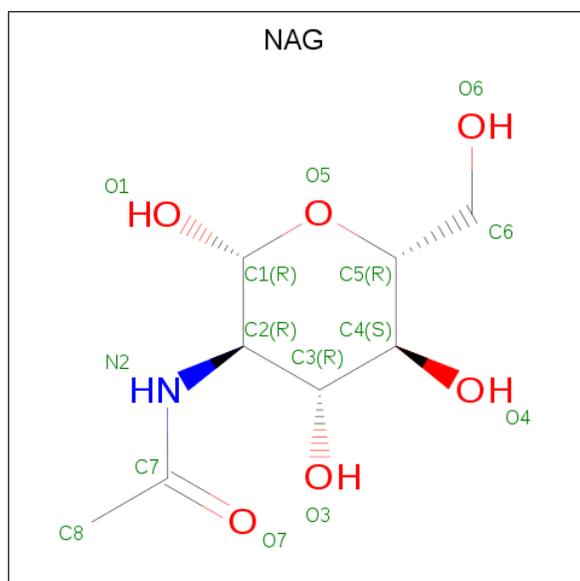
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

BMA
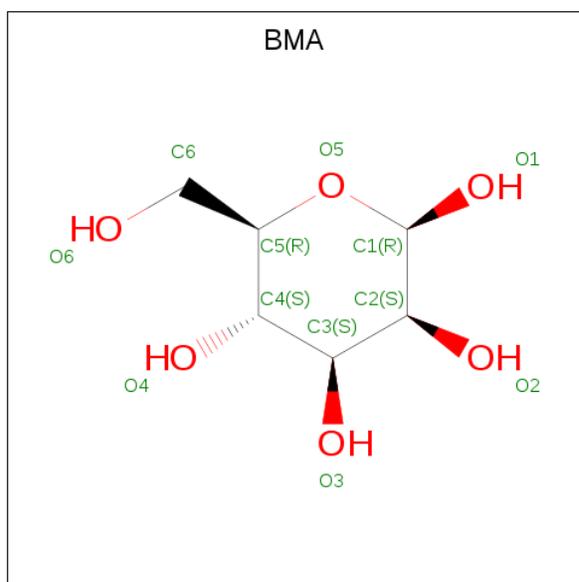
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

FUC
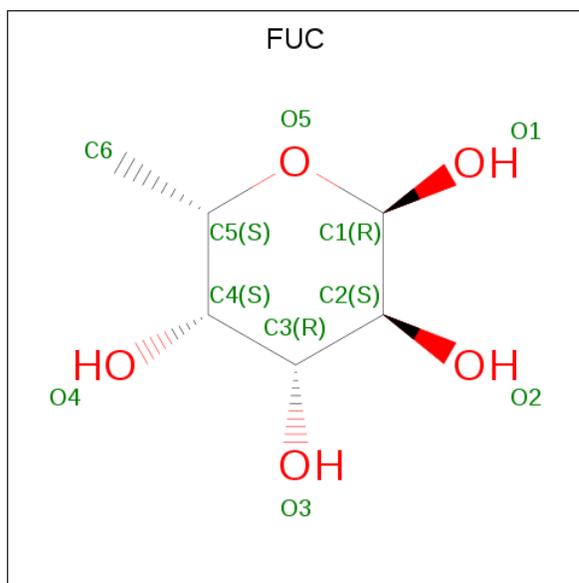
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 5'-O-[(R)-[(S)-[3-(acetylamino)phenyl](phosphono)methoxy](hydroxy)phosphoryl]cytidine (three-letter code: 55T) (formula: $C_{18}H_{24}N_4O_{12}P_2$).
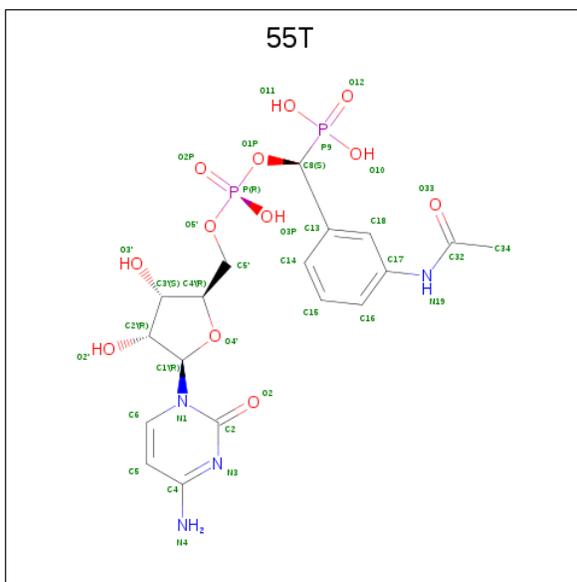
55T

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			36	18	4	12	2		
5	B	1	Total	C	N	O	P	0	0
			36	18	4	12	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total	O	0	0
			82	82		
6	B	53	Total	O	0	0
			53	53		

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 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: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase
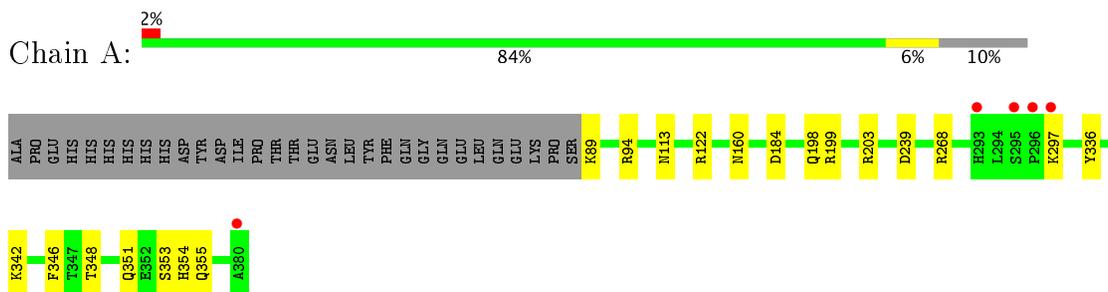
• Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase
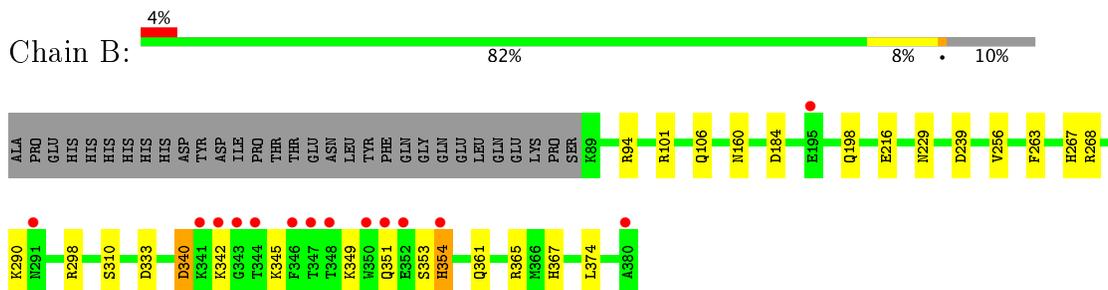
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.84Å　96.64Å　124.78Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	52.72　–　2.15 52.72　–　2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.72-2.15) 100.0 (52.72-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.37 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.198　,　0.235 0.205　,　0.239	Depositor DCC
R_{free} test set	2407 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5229	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 55T, BMA, NAG, FUC

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	0.89	0/2464	0.97	10/3338 (0.3%)
1	B	0.84	0/2481	0.93	8/3360 (0.2%)
All	All	0.86	0/4945	0.95	18/6698 (0.3%)

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	B	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	A	94	ARG	NE-CZ-NH1	13.79	127.20	120.30
1	B	268	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	239	ASP	CB-CG-OD1	7.85	125.37	118.30
1	B	268	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	340	ASP	CB-CG-OD2	7.63	125.16	118.30
1	A	268	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	340	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	94	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	354	HIS	N-CA-C	6.28	127.94	111.00
1	B	333	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	199	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	239	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	268	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	365	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	94	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	94	ARG	CG-CD-NE	-5.11	101.08	111.80
1	A	122	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	353	SER	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	2395	0	2331	4	0
1	B	2410	0	2349	7	0
2	A	112	0	98	0	0
2	B	84	0	76	0	0
3	A	11	0	10	0	0
4	A	10	0	10	0	0
5	A	36	0	0	2	0
5	B	36	0	0	1	0
6	A	82	0	0	0	0
6	B	53	0	0	0	0
All	All	5229	0	4874	11	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 1.

All (11) 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:367:HIS:HD2	1:B:374:LEU:H	1.41	0.69
1:B:340:ASP:O	1:B:340:ASP:OD2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:HD3	1:B:310:SER:O	2.09	0.53
1:B:263:PHE:O	1:B:267:HIS:HD2	1.95	0.49
1:A:336:TYR:OH	5:A:411:55T:C15	2.61	0.48
1:B:354:HIS:NE2	5:B:407:55T:O11	2.37	0.47
1:A:354:HIS:NE2	5:A:411:55T:O11	2.49	0.44
1:B:367:HIS:CD2	1:B:374:LEU:H	2.28	0.44
1:B:160:ASN:HB3	1:B:184:ASP:OD2	2.20	0.42
1:A:160:ASN:HB3	1:A:184:ASP:OD2	2.20	0.41
1:A:336:TYR:HD2	1:A:346:PHE:CE2	2.39	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	290/323 (90%)	284 (98%)	6 (2%)	0	100	100
1	B	290/323 (90%)	280 (97%)	10 (3%)	0	100	100
All	All	580/646 (90%)	564 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	261/294 (89%)	251 (96%)	10 (4%)	38	35
1	B	263/294 (90%)	250 (95%)	13 (5%)	29	24
All	All	524/588 (89%)	501 (96%)	23 (4%)	33	29

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	113	ASN
1	A	198	GLN
1	A	203	ARG
1	A	297	LYS
1	A	342	LYS
1	A	348	THR
1	A	351	GLN
1	A	353	SER
1	A	355	GLN
1	B	106	GLN
1	B	198	GLN
1	B	216	GLU
1	B	229	ASN
1	B	239	ASP
1	B	256	VAL
1	B	290	LYS
1	B	298	ARG
1	B	342	LYS
1	B	345	LYS
1	B	349	LYS
1	B	351	GLN
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	291	ASN
1	A	351	GLN
1	B	106	GLN
1	B	267	HIS
1	B	291	ASN
1	B	367	HIS

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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

18 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	#$|Z| > 2$
2	NAG	A	401	1,2	14,14,15	0.47	0	15,19,21	1.34	2 (13%)
2	NAG	A	402	3,2	14,14,15	0.64	0	15,19,21	1.02	1 (6%)
3	BMA	A	403	2	11,11,12	0.91	0	13,15,17	1.08	0
2	NAG	A	404	1,2	14,14,15	0.93	0	15,19,21	1.70	4 (26%)
2	NAG	A	405	2	14,14,15	0.45	0	15,19,21	1.34	2 (13%)
2	NAG	A	406	1,2,4	14,14,15	1.07	0	15,19,21	1.66	1 (6%)
2	NAG	A	407	2	14,14,15	1.35	2 (14%)	15,19,21	1.51	3 (20%)
4	FUC	A	408	2	9,10,11	0.55	0	13,14,16	0.67	0
2	NAG	A	409	1,2	14,14,15	1.07	2 (14%)	15,19,21	2.13	5 (33%)
2	NAG	A	410	2	14,14,15	0.72	0	15,19,21	1.45	5 (33%)
5	55T	A	411	-	33,38,38	1.09	2 (6%)	38,57,57	1.29	7 (18%)
2	NAG	B	401	1,2	14,14,15	0.81	0	15,19,21	1.81	5 (33%)
2	NAG	B	402	2	14,14,15	0.74	0	15,19,21	1.51	4 (26%)
2	NAG	B	403	1,2	14,14,15	0.71	0	15,19,21	1.69	2 (13%)
2	NAG	B	404	2	14,14,15	1.07	0	15,19,21	1.41	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|$ > 2	Counts	RMSZ	#$\|Z\|$ > 2
2	NAG	B	405	1	14,14,15	1.18	2 (14%)	15,19,21	2.99	10 (66%)
2	NAG	B	406	1	14,14,15	1.06	1 (7%)	15,19,21	2.12	4 (26%)
5	55T	B	407	-	33,38,38	1.18	4 (12%)	38,57,57	1.55	8 (21%)

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	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	402	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	403	2	-	0/2/19/22	0/1/1/1
2	NAG	A	404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	405	2	-	0/6/23/26	0/1/1/1
2	NAG	A	406	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	407	2	-	0/6/23/26	0/1/1/1
4	FUC	A	408	2	-	0/0/17/20	0/1/1/1
2	NAG	A	409	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	410	2	-	0/6/23/26	0/1/1/1
5	55T	A	411	-	-	0/21/45/45	0/3/3/3
2	NAG	B	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	402	2	-	0/6/23/26	0/1/1/1
2	NAG	B	403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	404	2	-	0/6/23/26	0/1/1/1
2	NAG	B	405	1	-	0/6/23/26	0/1/1/1
2	NAG	B	406	1	-	0/6/23/26	0/1/1/1
5	55T	B	407	-	-	0/21/45/45	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	NAG	C8-C7	-2.76	1.44	1.50
2	A	409	NAG	C2-N2	-2.25	1.42	1.46
2	B	405	NAG	C4-C5	2.07	1.57	1.53
5	B	407	55T	C18-C13	2.08	1.42	1.39
5	A	411	55T	C18-C17	2.09	1.43	1.39
2	A	407	NAG	C3-C2	2.22	1.57	1.52
5	B	407	55T	O4'-C1'	2.25	1.44	1.41
5	B	407	55T	C18-C17	2.34	1.43	1.39
2	B	405	NAG	C1-C2	2.37	1.55	1.52
2	B	406	NAG	C1-C2	2.37	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	411	55T	O4'-C1'	2.54	1.44	1.41
5	B	407	55T	P9-O12	2.62	1.54	1.49
2	A	407	NAG	C1-C2	3.09	1.56	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	405	NAG	O5-C1-C2	-6.32	102.69	111.47
2	B	406	NAG	O5-C1-C2	-3.75	106.25	111.47
2	A	407	NAG	C3-C4-C5	-3.60	103.88	110.22
5	B	407	55T	C16-C17-C18	-3.38	115.69	119.66
2	B	401	NAG	O5-C1-C2	-3.33	106.85	111.47
2	B	403	NAG	O5-C1-C2	-3.23	106.98	111.47
5	B	407	55T	C4'-O4'-C1'	-3.19	106.37	109.77
2	B	401	NAG	O4-C4-C3	-2.76	104.35	110.36
5	B	407	55T	O33-C32-C34	-2.75	117.05	122.06
5	A	411	55T	O10-P9-O12	-2.74	106.46	113.41
2	B	405	NAG	O3-C3-C4	-2.68	104.52	110.36
2	A	409	NAG	O5-C1-C2	-2.66	107.78	111.47
2	A	401	NAG	O3-C3-C2	-2.53	103.97	109.39
2	A	410	NAG	C1-O5-C5	-2.38	108.89	112.17
2	A	409	NAG	C1-C2-N2	-2.36	106.46	110.49
2	A	405	NAG	O4-C4-C3	-2.34	105.26	110.36
2	A	402	NAG	O3-C3-C2	-2.33	104.39	109.39
2	A	404	NAG	C8-C7-N2	-2.31	111.94	116.11
2	B	405	NAG	O7-C7-C8	-2.29	117.89	122.06
2	B	402	NAG	O5-C1-C2	-2.23	108.38	111.47
2	B	401	NAG	O7-C7-C8	-2.22	118.02	122.06
2	A	410	NAG	C3-C4-C5	-2.21	106.32	110.22
5	A	411	55T	C16-C17-C18	-2.21	117.06	119.66
2	A	409	NAG	O4-C4-C3	-2.19	105.59	110.36
5	B	407	55T	O11-P9-O12	-2.18	107.88	113.41
2	B	404	NAG	C3-C4-C5	-2.15	106.43	110.22
2	A	401	NAG	C8-C7-N2	-2.08	112.34	116.11
5	A	411	55T	C6-N1-C2	-2.07	117.93	121.28
2	A	410	NAG	C1-C2-N2	-2.05	106.98	110.49
2	B	402	NAG	C4-C3-C2	-2.02	108.06	111.02
2	B	405	NAG	O4-C4-C3	-2.01	105.98	110.36
2	A	405	NAG	C2-N2-C7	2.01	125.88	122.94
2	A	410	NAG	O4-C4-C5	2.02	114.38	109.28
5	A	411	55T	C15-C16-C17	2.04	122.19	119.72
2	A	407	NAG	C6-C5-C4	2.12	117.97	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	NAG	C2-N2-C7	2.13	126.06	122.94
5	A	411	55T	C18-C17-N19	2.15	127.09	120.16
5	A	411	55T	N4-C4-N3	2.16	120.27	116.64
2	B	404	NAG	C2-N2-C7	2.25	126.22	122.94
2	A	404	NAG	O6-C6-C5	2.27	119.00	111.34
2	B	402	NAG	C1-O5-C5	2.29	115.32	112.17
2	B	405	NAG	C6-C5-C4	2.33	118.44	113.00
2	B	406	NAG	C2-N2-C7	2.35	126.37	122.94
2	A	404	NAG	O7-C7-N2	2.50	126.73	121.92
2	B	405	NAG	C2-N2-C7	2.52	126.62	122.94
2	A	407	NAG	O4-C4-C5	2.55	115.72	109.28
5	B	407	55T	C18-C17-N19	2.55	128.37	120.16
5	A	411	55T	C34-C32-N19	2.60	118.83	115.02
2	B	405	NAG	O6-C6-C5	2.71	120.45	111.34
5	B	407	55T	C34-C32-N19	2.72	119.02	115.02
2	B	402	NAG	O4-C4-C5	2.73	116.15	109.28
2	B	401	NAG	C1-C2-N2	2.77	115.22	110.49
5	B	407	55T	N4-C4-N3	2.86	121.45	116.64
2	B	401	NAG	C4-C3-C2	2.89	115.25	111.02
5	B	407	55T	C15-C16-C17	2.89	123.21	119.72
2	B	406	NAG	C8-C7-N2	3.04	121.60	116.11
2	B	404	NAG	O4-C4-C5	3.14	117.20	109.28
2	B	405	NAG	O4-C4-C5	3.19	117.32	109.28
2	A	409	NAG	C1-O5-C5	3.34	116.77	112.17
2	B	405	NAG	C8-C7-N2	3.48	122.40	116.11
2	A	404	NAG	C2-N2-C7	3.73	128.39	122.94
2	B	403	NAG	C1-O5-C5	4.80	118.79	112.17
2	A	409	NAG	C2-N2-C7	4.92	130.12	122.94
2	A	406	NAG	C1-C2-N2	5.00	119.02	110.49
2	B	406	NAG	C1-O5-C5	5.07	119.15	112.17
2	B	405	NAG	C1-O5-C5	5.69	120.01	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	411	55T	2	0
5	B	407	55T	1	0

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	292/323 (90%)	-0.02	5 (1%)	70	76	18, 28, 61, 97	0
1	B	292/323 (90%)	0.14	14 (4%)	31	39	20, 36, 83, 140	0
All	All	584/646 (90%)	0.06	19 (3%)	47	54	18, 32, 73, 140	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	THR	17.6
1	B	342	LYS	6.2
1	B	346	PHE	5.9
1	B	343	GLY	4.1
1	B	341	LYS	4.0
1	B	350	TRP	3.9
1	B	380	ALA	3.2
1	B	291	ASN	2.9
1	B	347	THR	2.8
1	B	348	THR	2.6
1	A	380	ALA	2.5
1	B	351	GLN	2.5
1	B	195	GLU	2.4
1	A	297	LYS	2.4
1	B	354	HIS	2.4
1	A	295	SER	2.2
1	A	293	HIS	2.2
1	A	296	PRO	2.1
1	B	352	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	406	14/15	0.93	0.11	0.20	27,33,39,45	0
5	55T	B	407	36/36	0.95	0.14	0.05	33,44,69,80	0
2	NAG	B	401	14/15	0.97	0.11	-0.22	24,29,33,41	0
5	55T	A	411	36/36	0.97	0.12	-0.37	21,25,62,68	0
2	NAG	A	409	14/15	0.96	0.10	-0.62	22,28,36,36	0
2	NAG	B	403	14/15	0.95	0.10	-0.66	33,39,41,41	0
2	NAG	A	401	14/15	0.96	0.10	-1.31	27,30,33,43	0
2	NAG	A	404	14/15	0.83	0.17	-	50,60,70,86	0
3	BMA	A	403	11/12	0.73	0.16	-	71,80,85,87	0
2	NAG	B	404	14/15	0.85	0.21	-	46,55,64,65	0
2	NAG	A	407	14/15	0.78	0.33	-	63,71,78,80	0
4	FUC	A	408	10/11	0.96	0.09	-	41,42,45,46	0
2	NAG	B	406	14/15	0.45	0.36	-	81,93,104,105	0
2	NAG	A	402	14/15	0.91	0.12	-	36,51,71,73	0
2	NAG	A	405	14/15	0.87	0.32	-	79,97,105,108	0
2	NAG	B	405	14/15	0.77	0.15	-	50,56,61,64	0
2	NAG	B	402	14/15	0.89	0.12	-	41,52,69,71	0
2	NAG	A	410	14/15	0.92	0.13	-	43,51,66,75	0

6.5 Other polymers (i)

There are no such residues in this entry.