



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2017 – 03:37 PM EST

PDB ID : 5BO6
Title : Structure of human sialyltransferase ST8SiaIII in complex with CDP
Authors : Volkers, G.; Worrall, L.; Strynadka, N.C.J.
Deposited on : unknown
Resolution : 2.07 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (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

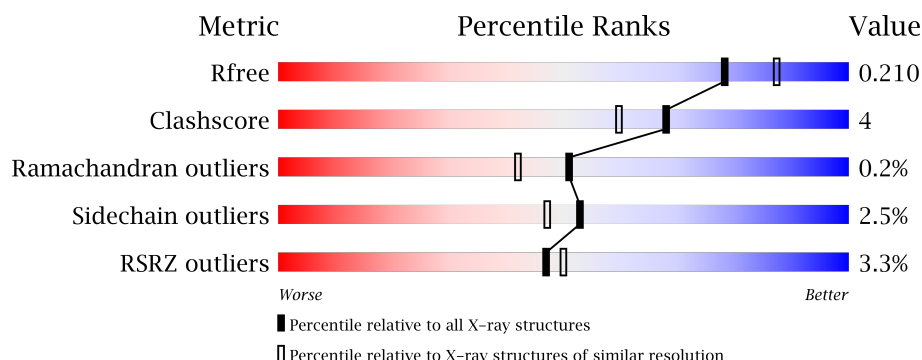
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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))
R_{free}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)

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 $\leq 5\%$. 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	323	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	323	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>14%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5388 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	291	Total	C	N	O	S	0	0	0
			2403	1553	418	422	10			
1	B	277	Total	C	N	O	S	0	0	0
			2280	1473	397	400	10			

There are 46 discrepancies between the modelled and reference sequences:

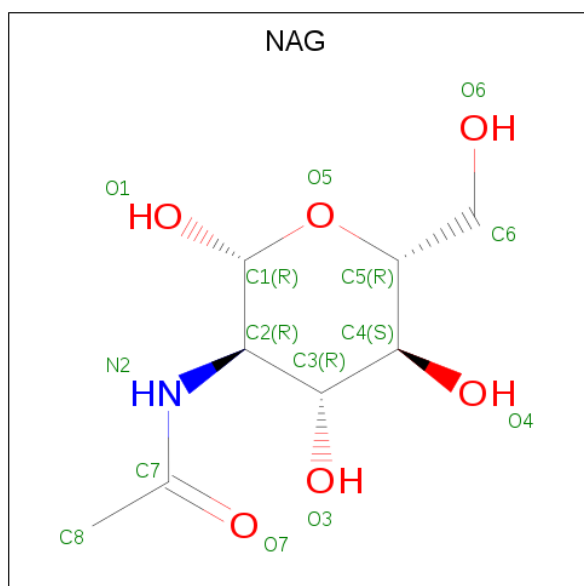
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	-	expression tag	UNP O43173
A	59	PRO	-	expression tag	UNP O43173
A	60	GLU	-	expression tag	UNP O43173
A	61	HIS	-	expression tag	UNP O43173
A	62	HIS	-	expression tag	UNP O43173
A	63	HIS	-	expression tag	UNP O43173
A	64	HIS	-	expression tag	UNP O43173
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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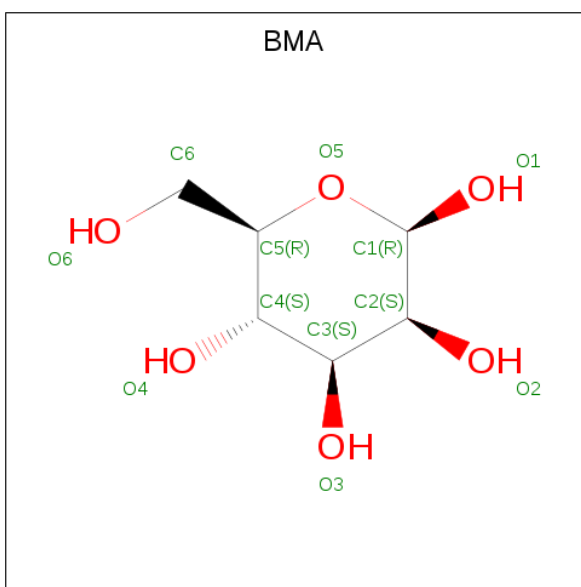
Chain	Residue	Modelled	Actual	Comment	Reference
B	59	PRO	-	expression tag	UNP O43173
B	60	GLU	-	expression tag	UNP O43173
B	61	HIS	-	expression tag	UNP O43173
B	62	HIS	-	expression tag	UNP O43173
B	63	HIS	-	expression tag	UNP O43173
B	64	HIS	-	expression tag	UNP O43173
B	65	HIS	-	expression tag	UNP O43173
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: $C_8H_{15}NO_6$).



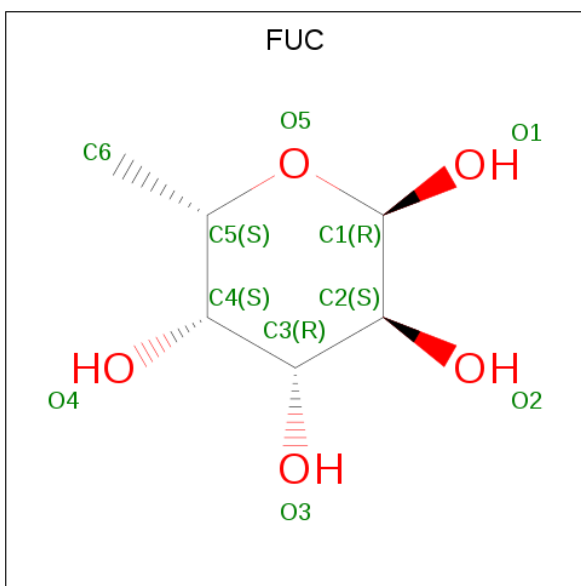
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



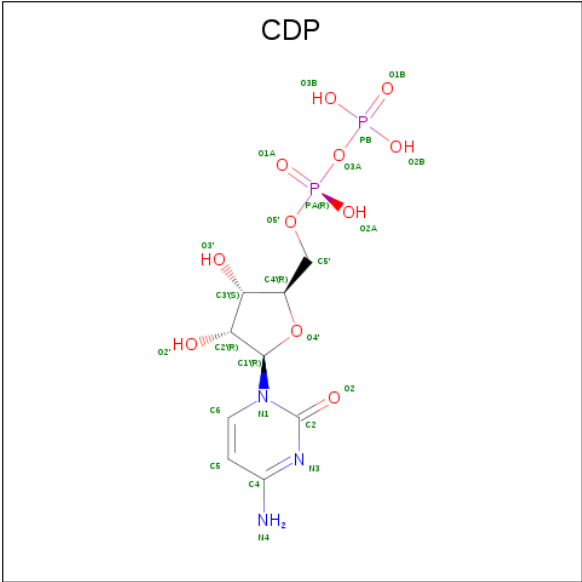
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

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



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

- Molecule 5 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
5	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

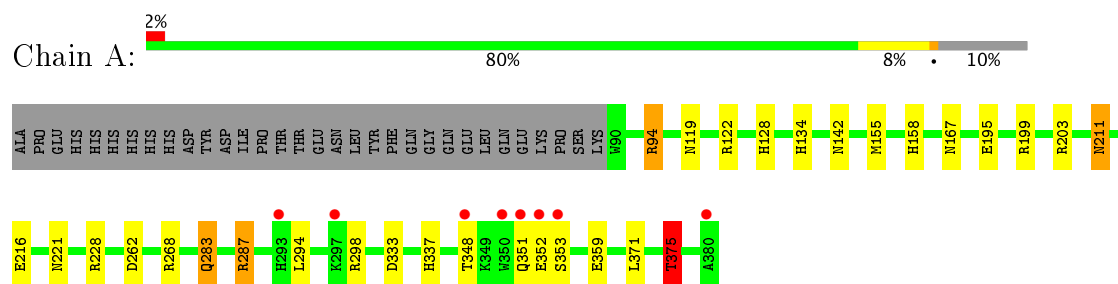
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	264	Total	O	0	0
			264	264		
6	B	174	Total	O	0	0
			174	174		

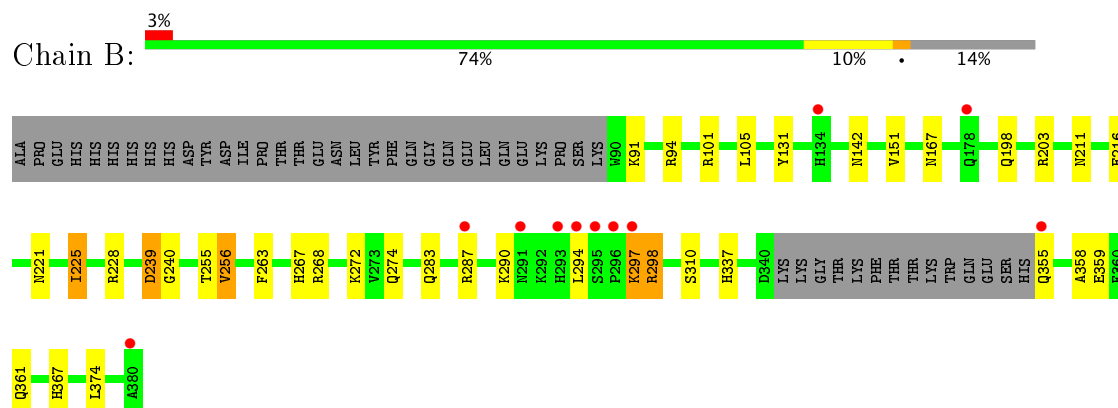
3 Residue-property plots [i](#)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.93 Å 96.87 Å 124.98 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.26 – 2.07 47.45 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.26-2.07) 98.4 (47.45-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.07 Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.168 , 0.202 0.177 , 0.210	Depositor DCC
R_{free} test set	2670 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CDP, 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	1.12	4/2474 (0.2%)	1.01	11/3352 (0.3%)
1	B	1.03	1/2345 (0.0%)	1.03	11/3177 (0.3%)
All	All	1.08	5/4819 (0.1%)	1.02	22/6529 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	THR	CB-CG2	-6.35	1.31	1.52
1	B	142	ASN	CB-CG	6.33	1.65	1.51
1	A	94	ARG	CZ-NH1	6.22	1.41	1.33
1	A	211	ASN	CB-CG	6.12	1.65	1.51
1	A	142	ASN	CB-CG	5.75	1.64	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	B	268	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	A	268	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	B	268	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	94	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	B	272	LYS	CD-CE-NZ	6.63	126.94	111.70
1	A	287	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	94	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	203	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	122	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	94	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	228	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	225	ILE	CG1-CB-CG2	5.90	124.39	111.40
1	B	256	VAL	CB-CA-C	-5.76	100.46	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	94	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	333	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	262	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	268	ARG	CD-NE-CZ	5.19	130.86	123.60
1	A	203	ARG	N-CA-CB	-5.09	101.44	110.60
1	B	268	ARG	CG-CD-NE	-5.05	101.19	111.80
1	B	198	GLN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2403	0	2341	18	0
1	B	2280	0	2223	23	0
2	A	112	0	98	2	0
2	B	84	0	76	0	0
3	A	11	0	10	0	0
4	A	10	0	10	0	0
5	A	25	0	12	0	0
5	B	25	0	12	0	0
6	A	264	0	0	14	1
6	B	174	0	0	7	1
All	All	5388	0	4782	43	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 (43) 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:155:MET:HE2	6:A:763:HOH:O	1.70	0.92
1:A:119:ASN:HB2	6:A:657:HOH:O	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLN:HG3	1:B:358:ALA:HB3	1.59	0.82
1:B:367:HIS:HD2	1:B:374:LEU:H	1.28	0.79
1:B:239:ASP:CG	1:B:240:GLY:H	1.90	0.74
1:A:199:ARG:HD3	6:A:671:HOH:O	1.89	0.73
1:A:94:ARG:NH2	6:A:501:HOH:O	2.20	0.70
1:B:287:ARG:NH1	6:B:502:HOH:O	2.27	0.68
1:B:255:THR:HG22	6:B:553:HOH:O	1.95	0.66
1:A:375:THR:HG23	6:A:637:HOH:O	1.95	0.66
1:A:158:HIS:CE1	6:A:535:HOH:O	2.51	0.64
2:A:409:NAG:H83	6:A:658:HOH:O	1.98	0.64
1:B:355:GLN:HG3	1:B:358:ALA:CB	2.28	0.64
1:A:211:ASN:HB2	6:A:712:HOH:O	1.98	0.62
1:A:94:ARG:NE	6:A:501:HOH:O	2.06	0.61
1:B:297:LYS:HG3	1:B:298:ARG:HB2	1.82	0.61
1:B:101:ARG:HD3	1:B:310:SER:O	2.00	0.61
1:B:367:HIS:CD2	1:B:374:LEU:H	2.14	0.59
1:B:283:GLN:HG3	6:B:638:HOH:O	2.02	0.58
1:A:216:GLU:HG3	1:A:221:ASN:HD21	1.67	0.58
1:B:239:ASP:CG	1:B:240:GLY:N	2.52	0.57
1:A:375:THR:CG2	6:A:637:HOH:O	2.54	0.56
1:B:105:LEU:HD22	6:B:634:HOH:O	2.07	0.53
1:B:274:GLN:HG3	6:B:630:HOH:O	2.08	0.52
1:B:297:LYS:HG3	1:B:298:ARG:HD3	1.93	0.50
2:A:409:NAG:O6	6:A:502:HOH:O	2.20	0.48
1:B:216:GLU:HG3	1:B:221:ASN:HD21	1.78	0.48
1:A:294:LEU:HD21	1:A:359:GLU:HG2	1.95	0.47
1:A:211:ASN:ND2	6:A:510:HOH:O	2.48	0.46
1:B:225:ILE:HD12	1:B:225:ILE:H	1.81	0.46
1:A:283:GLN:HG2	6:A:506:HOH:O	2.15	0.45
1:A:348:THR:OG1	1:A:351:GLN:NE2	2.50	0.44
1:A:351:GLN:O	1:A:353:SER:N	2.49	0.44
1:B:263:PHE:O	1:B:267:HIS:HD2	2.00	0.44
1:B:105:LEU:HG	6:B:601:HOH:O	2.17	0.43
1:B:239:ASP:OD2	1:B:240:GLY:N	2.28	0.43
1:A:128:HIS:CE1	1:A:134:HIS:CE1	3.07	0.42
1:B:294:LEU:HD21	1:B:359:GLU:HG2	2.02	0.42
1:A:167:ASN:O	1:A:337:HIS:HA	2.20	0.42
1:B:167:ASN:O	1:B:337:HIS:HA	2.20	0.41
1:B:211:ASN:OD1	6:B:501:HOH:O	2.21	0.41
1:A:195:GLU:HB2	6:A:693:HOH:O	2.20	0.40
1:B:131:TYR:CE1	1:B:298:ARG:HG3	2.56	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:A:561:HOH:O	6:B:565:HOH:O[4_455]	2.11	0.09

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	289/323 (90%)	284 (98%)	4 (1%)	1 (0%)	44	35
1	B	273/323 (84%)	269 (98%)	4 (2%)	0	100	100
All	All	562/646 (87%)	553 (98%)	8 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	GLU

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	263/294 (90%)	258 (98%)	5 (2%)	62	58
1	B	250/294 (85%)	242 (97%)	8 (3%)	44	37
All	All	513/588 (87%)	500 (98%)	13 (2%)	53	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	287	ARG
1	A	298	ARG
1	A	371	LEU
1	A	375	THR
1	B	91	LYS
1	B	151	VAL
1	B	239	ASP
1	B	256	VAL
1	B	290	LYS
1	B	297	LYS
1	B	298	ARG
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	128	HIS
1	A	134	HIS
1	A	156	ASN
1	A	221	ASN
1	A	351	GLN
1	A	378	HIS
1	B	221	ASN
1	B	229	ASN
1	B	251	HIS
1	B	267	HIS
1	B	274	GLN
1	B	367	HIS
1	B	378	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	0.50	0	15,19,21	1.31	2 (13%)
2	NAG	A	402	3,2	14,14,15	0.61	0	15,19,21	1.21	1 (6%)
3	BMA	A	403	2	11,11,12	0.50	0	13,15,17	0.89	0
2	NAG	A	404	1,2	14,14,15	0.61	0	15,19,21	0.94	0
2	NAG	A	405	2	14,14,15	0.41	0	15,19,21	1.43	3 (20%)
2	NAG	A	406	1,2,4	14,14,15	0.85	1 (7%)	15,19,21	1.04	2 (13%)
2	NAG	A	407	2	14,14,15	0.67	0	15,19,21	1.18	1 (6%)
4	FUC	A	408	2	9,10,11	0.59	0	13,14,16	0.95	0
2	NAG	A	409	1,2	14,14,15	1.04	1 (7%)	15,19,21	1.97	4 (26%)
2	NAG	A	410	2	14,14,15	0.63	0	15,19,21	1.32	1 (6%)
5	CDP	A	411	-	22,26,26	1.04	2 (9%)	23,40,40	1.34	6 (26%)
2	NAG	B	401	1,2	14,14,15	0.52	0	15,19,21	1.07	0
2	NAG	B	402	2	14,14,15	0.53	0	15,19,21	1.01	0
2	NAG	B	403	1,2	14,14,15	0.82	1 (7%)	15,19,21	1.68	3 (20%)
2	NAG	B	404	2	14,14,15	0.67	0	15,19,21	0.97	1 (6%)
2	NAG	B	405	1	14,14,15	0.56	0	15,19,21	2.69	5 (33%)
2	NAG	B	406	1	14,14,15	1.18	1 (7%)	15,19,21	1.35	2 (13%)
5	CDP	B	407	-	22,26,26	0.84	0	23,40,40	1.26	4 (17%)

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	CDP	A	411	-	-	0/12/32/32	0/2/2/2
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	CDP	B	407	-	-	0/12/32/32	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	NAG	C8-C7	-3.01	1.44	1.50
2	B	403	NAG	C1-C2	-2.18	1.49	1.52
5	A	411	CDP	O4'-C1'	2.15	1.44	1.41
2	A	406	NAG	C1-C2	2.66	1.56	1.52
5	A	411	CDP	PB-O3A	2.88	1.64	1.60
2	B	406	NAG	C1-C2	3.32	1.57	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	405	NAG	O5-C1-C2	-5.96	103.18	111.47
2	A	409	NAG	O5-C1-C2	-4.34	105.44	111.47
2	A	405	NAG	O5-C1-C2	-3.40	106.74	111.47
2	A	402	NAG	O5-C1-C2	-3.00	107.30	111.47
2	B	403	NAG	O4-C4-C3	-2.64	104.62	110.36
2	B	403	NAG	C1-C2-N2	-2.63	106.00	110.49
2	A	409	NAG	O6-C6-C5	-2.39	103.30	111.34
2	A	401	NAG	O5-C1-C2	-2.38	108.16	111.47
2	B	405	NAG	C3-C4-C5	-2.20	106.35	110.22
5	A	411	CDP	C6-N1-C2	-2.20	117.72	121.28
5	A	411	CDP	O4'-C1'-N1	-2.18	103.71	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	411	CDP	O3A-PB-O1B	-2.13	98.36	111.44
2	B	405	NAG	O7-C7-N2	-2.12	117.83	121.92
2	A	407	NAG	C1-C2-N2	-2.08	106.93	110.49
2	A	406	NAG	O5-C1-C2	-2.06	108.60	111.47
2	A	405	NAG	C1-O5-C5	2.01	114.94	112.17
5	B	407	CDP	O3'-C3'-C4'	2.03	117.03	111.09
5	B	407	CDP	O3B-PB-O1B	2.05	118.51	110.50
2	B	404	NAG	O4-C4-C5	2.13	114.66	109.28
5	A	411	CDP	N4-C4-N3	2.15	120.26	116.64
5	B	407	CDP	O2A-PA-O1A	2.20	123.65	112.28
2	B	406	NAG	C2-N2-C7	2.23	126.20	122.94
5	B	407	CDP	N4-C4-N3	2.31	120.53	116.64
5	A	411	CDP	O2B-PB-O3B	2.32	116.99	107.61
2	A	410	NAG	C2-N2-C7	2.33	126.34	122.94
2	A	406	NAG	C1-C2-N2	2.55	114.84	110.49
2	A	405	NAG	C1-C2-N2	2.71	115.11	110.49
5	A	411	CDP	O3B-PB-O1B	3.05	122.42	110.50
2	B	406	NAG	C1-C2-N2	3.11	115.81	110.49
2	A	401	NAG	C1-C2-N2	3.13	115.84	110.49
2	A	409	NAG	C2-N2-C7	3.20	127.61	122.94
2	A	409	NAG	C1-O5-C5	3.26	116.66	112.17
2	B	405	NAG	C8-C7-N2	3.63	122.66	116.11
2	B	403	NAG	C1-O5-C5	4.15	117.89	112.17
2	B	405	NAG	C1-O5-C5	5.70	120.02	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	409	NAG	2	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	291/323 (90%)	-0.11	8 (2%) 55 58	21, 32, 54, 91	0
1	B	277/323 (85%)	0.09	11 (3%) 39 41	24, 40, 66, 100	0
All	All	568/646 (87%)	-0.01	19 (3%) 47 50	21, 36, 61, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	TRP	4.8
1	B	380	ALA	4.8
1	B	355	GLN	4.0
1	A	352	GLU	3.9
1	A	353	SER	3.8
1	B	291	ASN	3.6
1	B	293	HIS	3.5
1	A	351	GLN	3.5
1	B	297	LYS	3.4
1	A	348	THR	3.3
1	B	287	ARG	3.1
1	B	295	SER	2.5
1	B	294	LEU	2.4
1	A	297	LYS	2.4
1	A	293	HIS	2.3
1	B	296	PRO	2.3
1	B	134	HIS	2.2
1	A	380	ALA	2.1
1	B	178	GLN	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
5	CDP	B	407	25/25	0.96	0.09	-0.35	37,44,50,52	0
2	NAG	B	403	14/15	0.95	0.08	-0.52	34,41,44,56	0
5	CDP	A	411	25/25	0.98	0.09	-0.57	25,27,35,38	0
2	NAG	B	401	14/15	0.95	0.09	-0.75	28,33,37,44	0
2	NAG	A	409	14/15	0.94	0.12	-0.76	25,30,39,40	0
2	NAG	A	401	14/15	0.96	0.09	-1.08	31,35,41,47	0
2	NAG	A	406	14/15	0.94	0.10	-1.58	27,31,36,40	0
2	NAG	A	404	14/15	0.83	0.29	-	57,71,78,87	0
2	NAG	A	410	14/15	0.92	0.14	-	44,51,64,70	0
2	NAG	B	405	14/15	0.79	0.29	-	58,68,76,79	0
2	NAG	A	405	14/15	0.84	0.39	-	72,92,98,99	0
2	NAG	B	402	14/15	0.90	0.17	-	44,51,65,69	0
2	NAG	A	402	14/15	0.92	0.12	-	40,47,67,72	0
3	BMA	A	403	11/12	0.74	0.20	-	69,76,81,86	0
2	NAG	B	406	14/15	0.69	0.40	-	71,89,100,105	0
4	FUC	A	408	10/11	0.95	0.10	-	38,42,45,47	0
2	NAG	B	404	14/15	0.89	0.34	-	57,63,73,77	0
2	NAG	A	407	14/15	0.93	0.15	-	47,52,64,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.