wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 09:52 PM GMT

PDB ID	:	5BO9
Title	:	Structure of human sialyltransferase ST8SiaIII in complex with CMP-3FNeu5Ac and Sia-6S-LacNAc
Authors	:	Volkers, G.; Worrall, L.; Strynadka, N.C.J.
Deposited on	:	2015-05-27
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

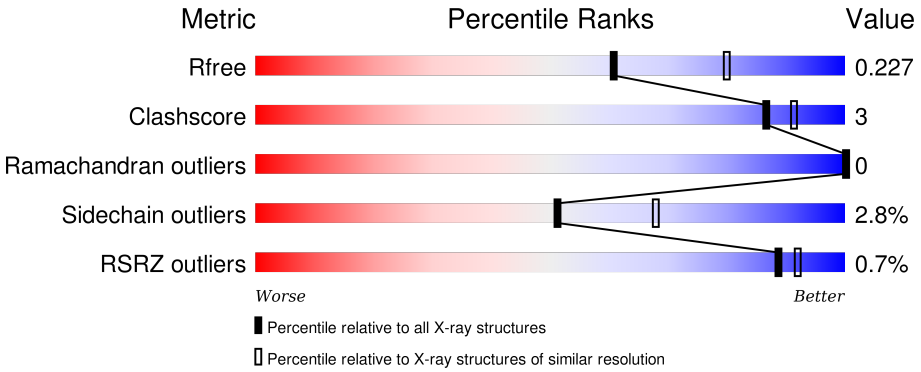
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	% 80% 7% • 11%
1	B	323	79% 7% 14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5189 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-sialyltransfera se.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2353	1521	410	412	10			
1	B	277	Total	C	N	O	S	0	0	0
			2287	1479	397	401	10			

There are 46 discrepancies between the modelled and reference sequences:

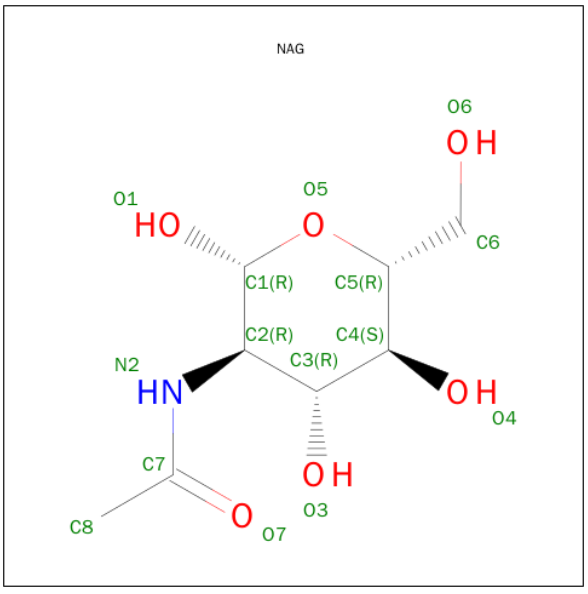
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	-	expression tag	UNP O43173
A	59	PRO	-	expression tag	UNP O43173
A	60	GLU	-	expression tag	UNP O43173
A	61	HIS	-	expression tag	UNP O43173
A	62	HIS	-	expression tag	UNP O43173
A	63	HIS	-	expression tag	UNP O43173
A	64	HIS	-	expression tag	UNP O43173
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

Continued on next page...

Continued from previous page...

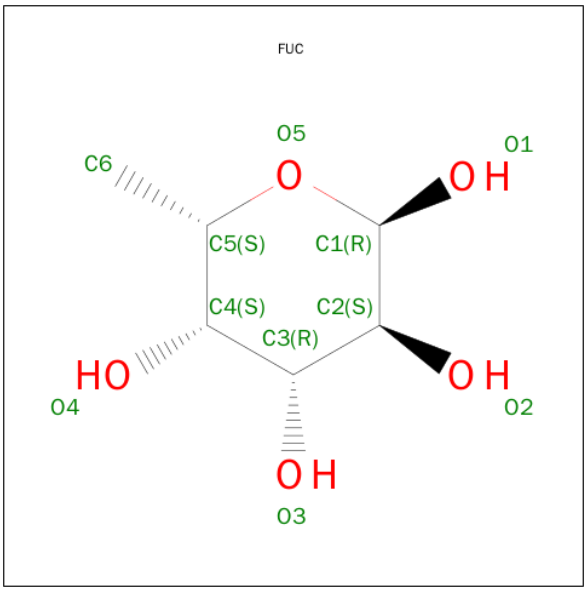
Chain	Residue	Modelled	Actual	Comment	Reference
B	59	PRO	-	expression tag	UNP O43173
B	60	GLU	-	expression tag	UNP O43173
B	61	HIS	-	expression tag	UNP O43173
B	62	HIS	-	expression tag	UNP O43173
B	63	HIS	-	expression tag	UNP O43173
B	64	HIS	-	expression tag	UNP O43173
B	65	HIS	-	expression tag	UNP O43173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



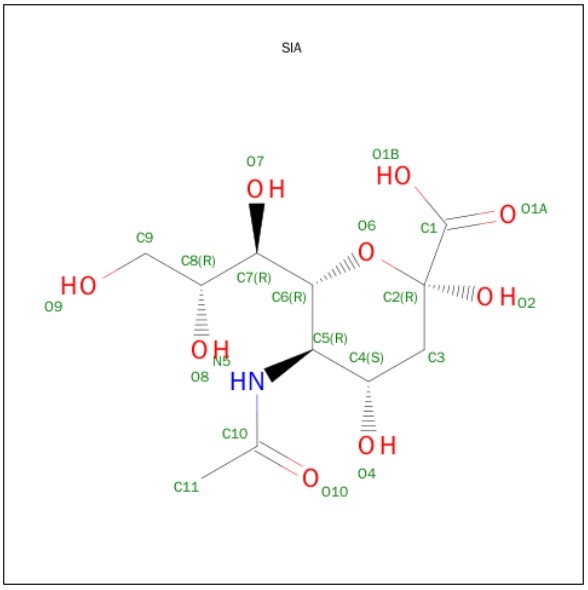
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total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

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



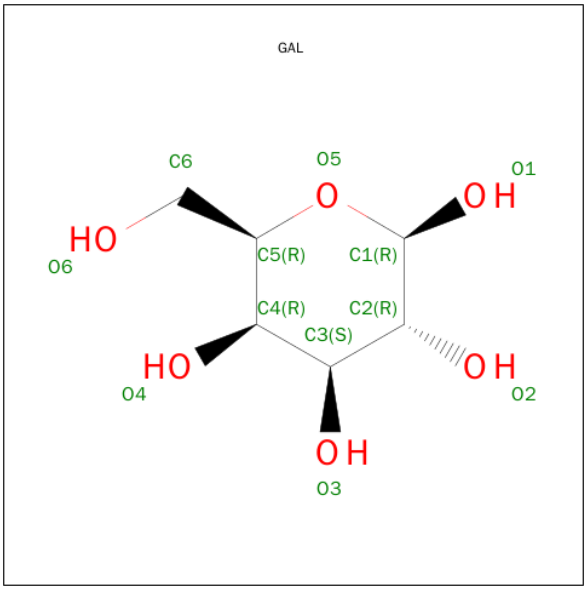
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



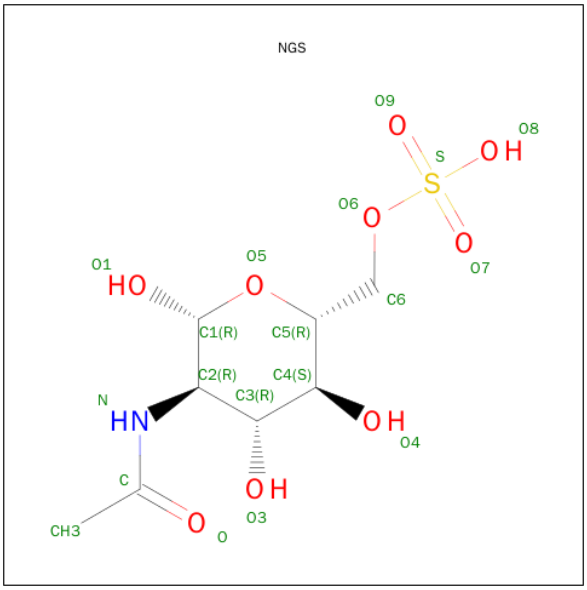
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 11 1 8	0	0
4	B	1	Total C N O 20 11 1 8	0	0

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



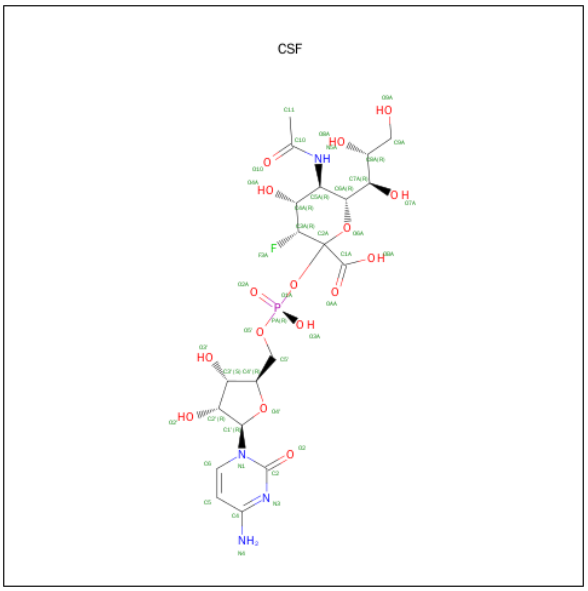
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 6 5	0	0
5	B	1	Total C O 11 6 5	0	0

- Molecule 6 is 2-(acetylamino)-2-deoxy-6-O-sulfo-beta-D-glucopyranose (three-letter code: NGS) (formula: $C_8H_{15}NO_9S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 19 8 1 9 1	0	0
6	B	1	Total C N O S 19 8 1 9 1	0	0

- Molecule 7 is CYTIDINE-5'-MONOPHOSPHATE-3-FLUORO-N-ACETYL-NEURAMINIC ACID (three-letter code: CSF) (formula: $C_{20}H_{30}FN_4O_{16}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	P	17	0
			42	20	1	4	16	1		
7	B	1	Total	C	F	N	O	P	17	0
			42	20	1	4	16	1		

- Molecule 8 is water.

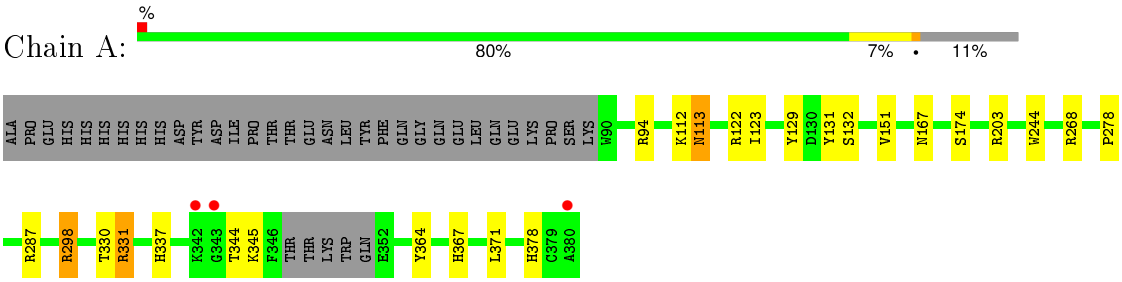
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	90	Total	O	0	0
			90	90		
8	B	83	Total	O	0	0
			83	83		

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 errors 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.

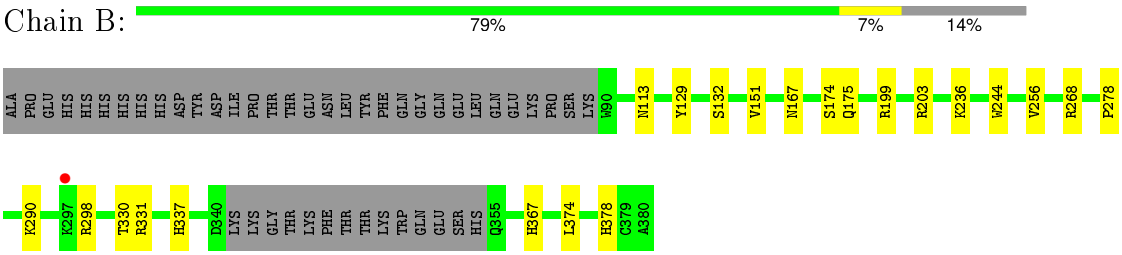
- Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase

Chain A:



- Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.35Å 94.87Å 126.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.89 – 2.30 75.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.89-2.30) 99.9 (75.89-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.230 0.190 , 0.227	Depositor DCC
R_{free} test set	1744 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 34586 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5189	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAG, CSF, SIA, GAL, FUC, NGS

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	0.74	0/2421	0.88	8/3278 (0.2%)
1	B	0.73	0/2353	0.85	3/3188 (0.1%)
All	All	0.74	0/4774	0.87	11/6466 (0.2%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	ARG	NE-CZ-NH2	11.07	125.83	120.30
1	A	298	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	B	298	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	B	298	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	A	94	ARG	NE-CZ-NH2	-7.11	116.75	120.30

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	2353	0	2291	13	0
1	B	2287	0	2230	9	0
2	A	98	0	87	6	0
2	B	84	0	76	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	10	0	0
4	A	20	0	17	1	0
4	B	20	0	17	2	0
5	A	11	0	9	0	0
5	B	11	0	9	0	0
6	A	19	0	13	0	0
6	B	19	0	13	0	0
7	A	42	0	29	0	0
7	B	42	0	29	0	0
8	A	90	0	0	2	0
8	B	83	0	0	1	0
All	All	5189	0	4830	26	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 3.

The worst 5 of 26 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)
4:B:407:SIA:H111	8:B:501:HOH:O	1.72	0.88
1:B:367:HIS:HD2	1:B:374:LEU:H	1.20	0.86
2:A:401:NAG:H81	8:A:562:HOH:O	1.79	0.82
1:A:113:ASN:HD22	2:A:401:NAG:H83	1.59	0.67
1:A:131:TYR:CE2	1:A:298:ARG:HG2	2.34	0.62

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	282/323 (87%)	270 (96%)	12 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	273/323 (84%)	265 (97%)	8 (3%)	0	100	100
All	All	555/646 (86%)	535 (96%)	20 (4%)	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	257/294 (87%)	249 (97%)	8 (3%)	47	64
1	B	251/294 (85%)	245 (98%)	6 (2%)	57	74
All	All	508/588 (86%)	494 (97%)	14 (3%)	51	68

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	LYS
1	A	371	LEU
1	B	236	LYS
1	A	344	THR
1	B	203	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	378	HIS
1	B	291	ASN
1	A	291	ASN
1	B	229	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 carbohydrates in this entry.

5.6 Ligand geometry

22 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	14,14,15	1.29	1 (7%)	15,19,21	3.75	11 (73%)
2	NAG	A	402	1,2	14,14,15	0.67	0	15,19,21	1.94	5 (33%)
2	NAG	A	403	2	14,14,15	0.63	0	15,19,21	1.75	3 (20%)
2	NAG	A	404	1,3,2	14,14,15	1.18	1 (7%)	15,19,21	1.05	0
2	NAG	A	405	2	14,14,15	0.70	0	15,19,21	1.21	2 (13%)
3	FUC	A	406	2	10,10,11	0.97	1 (10%)	13,14,16	1.32	1 (7%)
2	NAG	A	407	1,2	14,14,15	1.00	1 (7%)	15,19,21	1.59	3 (20%)
2	NAG	A	408	2	14,14,15	0.78	0	15,19,21	0.82	0
4	SIA	A	409	5	17,20,21	1.05	2 (11%)	18,28,31	1.68	6 (33%)
5	GAL	A	410	4,6	11,11,12	0.39	0	15,15,17	1.29	2 (13%)
6	NGS	A	411	5	19,19,19	0.66	1 (5%)	22,28,28	1.29	2 (9%)
7	CSF	A	412	-	36,44,44	0.75	0	42,67,67	0.98	1 (2%)
2	NAG	B	401	1,2	14,14,15	0.92	0	15,19,21	2.50	6 (40%)
2	NAG	B	402	2	14,14,15	0.84	1 (7%)	15,19,21	1.49	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	403	1,2	14,14,15	0.96	0	15,19,21	1.26	2 (13%)
2	NAG	B	404	2	14,14,15	0.87	0	15,19,21	1.57	4 (26%)
2	NAG	B	405	1	14,14,15	0.59	0	15,19,21	2.44	4 (26%)
2	NAG	B	406	1	14,14,15	0.76	0	15,19,21	2.35	6 (40%)
4	SIA	B	407	5	17,20,21	1.14	2 (11%)	18,28,31	2.02	5 (27%)
5	GAL	B	408	4,6	11,11,12	0.53	0	15,15,17	1.82	3 (20%)
6	NGS	B	409	5	19,19,19	0.62	0	22,28,28	1.29	2 (9%)
7	CSF	B	410	-	36,44,44	0.73	0	42,67,67	1.11	4 (9%)

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	-	0/6/23/26	0/1/1/1
2	NAG	A	402	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	403	2	-	0/6/23/26	0/1/1/1
2	NAG	A	404	1,3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	405	2	-	0/6/23/26	0/1/1/1
3	FUC	A	406	2	-	0/0/17/20	0/1/1/1
2	NAG	A	407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	408	2	-	0/6/23/26	0/1/1/1
4	SIA	A	409	5	-	0/14/34/38	0/1/1/1
5	GAL	A	410	4,6	-	0/2/19/22	0/1/1/1
6	NGS	A	411	5	-	0/10/30/30	0/1/1/1
7	CSF	A	412	-	-	0/23/75/75	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
4	SIA	B	407	5	-	0/14/34/38	0/1/1/1
5	GAL	B	408	4,6	-	0/2/19/22	0/1/1/1
6	NGS	B	409	5	-	0/10/30/30	0/1/1/1
7	CSF	B	410	-	-	0/23/75/75	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	NAG	O5-C1	-3.74	1.37	1.43
2	A	407	NAG	C2-N2	-2.42	1.42	1.46
4	B	407	SIA	C4-C5	-2.24	1.50	1.53
2	B	402	NAG	C1-C2	-2.13	1.49	1.52
3	A	406	FUC	O2-C2	-2.00	1.38	1.43

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	408	GAL	O5-C1-C2	-5.14	102.67	110.89
2	B	406	NAG	C4-C3-C2	-5.03	103.53	111.34
2	A	401	NAG	O3-C3-C2	-4.84	99.02	109.37
4	B	407	SIA	O9-C9-C8	-4.43	101.25	111.07
2	A	401	NAG	O7-C7-C8	-4.28	114.18	122.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAG	6	0
4	A	409	SIA	1	0
4	B	407	SIA	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

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	286/323 (88%)	-0.22	3 (1%)	84	88	25, 39, 65, 98	0
1	B	277/323 (85%)	-0.18	1 (0%)	93	95	27, 41, 72, 93	0
All	All	563/646 (87%)	-0.20	4 (0%)	89	92	25, 40, 70, 98	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	ALA	3.5
1	A	342	LYS	3.1
1	B	297	LYS	2.6
1	A	343	GLY	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	LLDF	B-factors(Å^2)	Q<0.9
4	SIA	B	407	20/21	0.93	0.14	0.74	36,44,50,51	0
2	NAG	A	401	14/15	0.90	0.12	0.63	31,36,39,43	0
5	GAL	A	410	11/12	0.94	0.15	0.48	41,55,63,64	0
7	CSF	B	410	42/42	0.96	0.12	-0.06	35,54,128,151	17
7	CSF	A	412	42/42	0.95	0.12	-0.08	31,53,108,114	17
5	GAL	B	408	11/12	0.92	0.13	-0.14	44,53,59,60	0
4	SIA	A	409	20/21	0.95	0.12	-0.31	33,40,55,60	0
2	NAG	B	401	14/15	0.97	0.12	-0.43	31,35,42,46	0
2	NAG	A	407	14/15	0.96	0.10	-0.97	31,37,39,44	0
2	NAG	B	403	14/15	0.98	0.10	-1.27	38,42,51,55	0
2	NAG	A	404	14/15	0.95	0.10	-2.32	38,40,49,52	0
2	NAG	A	408	14/15	0.91	0.14	-	50,54,68,77	0
2	NAG	B	404	14/15	0.91	0.13	-	53,60,66,69	0
2	NAG	B	402	14/15	0.91	0.14	-	44,53,55,62	0
6	NGS	B	409	19/19	0.91	0.15	-	71,81,88,90	0
2	NAG	B	406	14/15	0.87	0.18	-	79,86,98,98	0
2	NAG	A	403	14/15	0.75	0.23	-	87,95,100,100	0
6	NGS	A	411	19/19	0.89	0.22	-	77,96,122,125	0
2	NAG	A	405	14/15	0.90	0.14	-	59,63,68,69	0
2	NAG	B	405	14/15	0.85	0.13	-	71,78,83,83	0
3	FUC	A	406	10/11	0.95	0.12	-	45,48,51,51	0
2	NAG	A	402	14/15	0.81	0.14	-	71,76,82,89	0

6.5 Other polymers (i)

There are no such residues in this entry.