Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:47 PM GMT

PDB ID	:	5BO8
Title	:	Structure of human sialyltransferase ST8SiaIII
Authors	:	Volkers, G.; Worrall, L.; Strynadka, N.C.J.
Deposited on	:	2015-05-27
Resolution	:	2.70 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 (i) symbol.

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

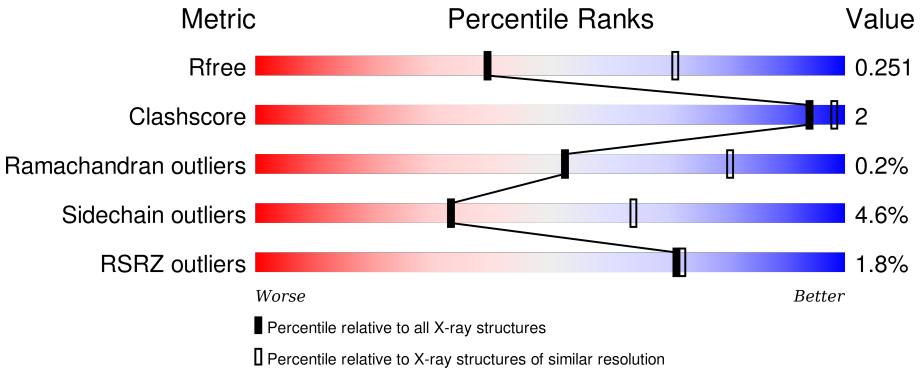
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	343	2% 73% 8% • 19%
1	B	343	% 72% 8% • 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	408	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4874 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	277	Total	C	N	O	S	0	0	0
			2270	1468	392	400	10			
1	B	276	Total	C	N	O	S	0	0	0
			2278	1474	395	399	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ALA	-	expression tag	UNP O43173
A	39	PRO	-	expression tag	UNP O43173
A	40	GLU	-	expression tag	UNP O43173
A	41	HIS	-	expression tag	UNP O43173
A	42	HIS	-	expression tag	UNP O43173
A	43	HIS	-	expression tag	UNP O43173
A	44	HIS	-	expression tag	UNP O43173
A	45	HIS	-	expression tag	UNP O43173
A	46	HIS	-	expression tag	UNP O43173
A	47	ASP	-	expression tag	UNP O43173
A	48	TYR	-	expression tag	UNP O43173
A	49	ASP	-	expression tag	UNP O43173
A	50	ILE	-	expression tag	UNP O43173
A	51	PRO	-	expression tag	UNP O43173
A	52	THR	-	expression tag	UNP O43173
A	53	THR	-	expression tag	UNP O43173
A	54	GLU	-	expression tag	UNP O43173
A	55	ASN	-	expression tag	UNP O43173
A	56	LEU	-	expression tag	UNP O43173
A	57	TYR	-	expression tag	UNP O43173
A	58	PHE	-	expression tag	UNP O43173
A	59	GLN	-	expression tag	UNP O43173
A	60	GLY	-	expression tag	UNP O43173
B	38	ALA	-	expression tag	UNP O43173

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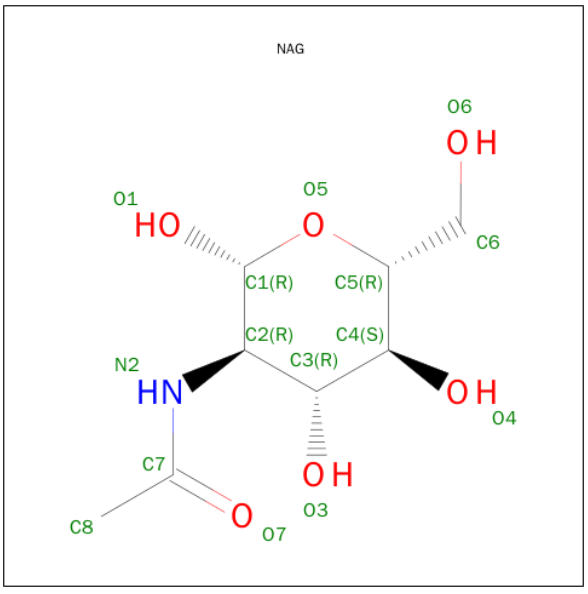
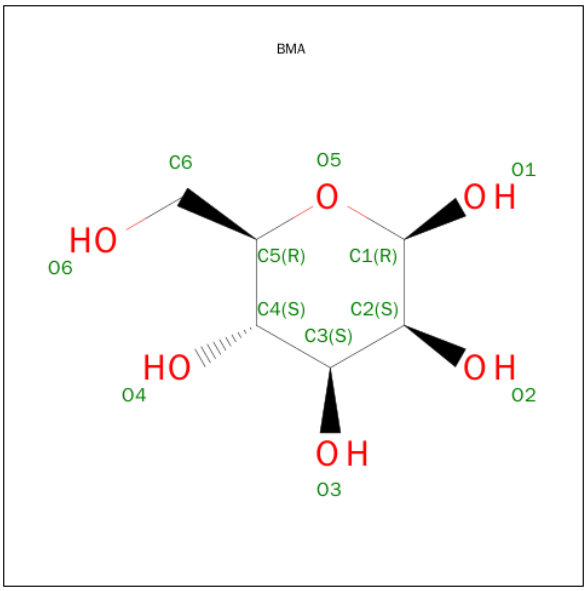
Chain	Residue	Modelled	Actual	Comment	Reference
B	39	PRO	-	expression tag	UNP O43173
B	40	GLU	-	expression tag	UNP O43173
B	41	HIS	-	expression tag	UNP O43173
B	42	HIS	-	expression tag	UNP O43173
B	43	HIS	-	expression tag	UNP O43173
B	44	HIS	-	expression tag	UNP O43173
B	45	HIS	-	expression tag	UNP O43173
B	46	HIS	-	expression tag	UNP O43173
B	47	ASP	-	expression tag	UNP O43173
B	48	TYR	-	expression tag	UNP O43173
B	49	ASP	-	expression tag	UNP O43173
B	50	ILE	-	expression tag	UNP O43173
B	51	PRO	-	expression tag	UNP O43173
B	52	THR	-	expression tag	UNP O43173
B	53	THR	-	expression tag	UNP O43173
B	54	GLU	-	expression tag	UNP O43173
B	55	ASN	-	expression tag	UNP O43173
B	56	LEU	-	expression tag	UNP O43173
B	57	TYR	-	expression tag	UNP O43173
B	58	PHE	-	expression tag	UNP O43173
B	59	GLN	-	expression tag	UNP O43173
B	60	GLY	-	expression tag	UNP O43173

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



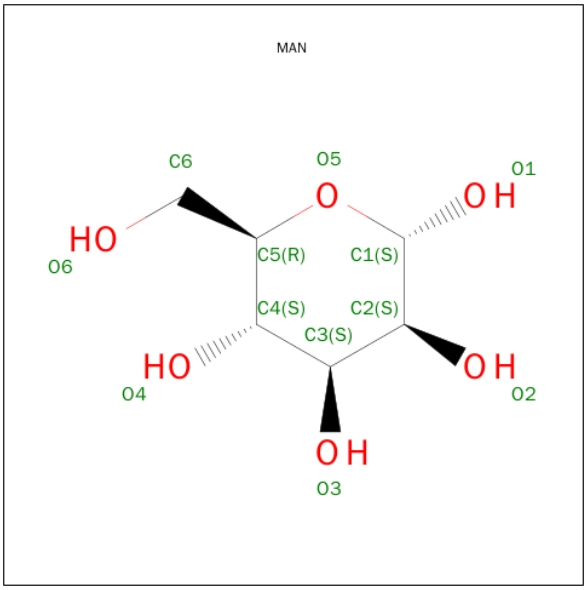
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total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

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



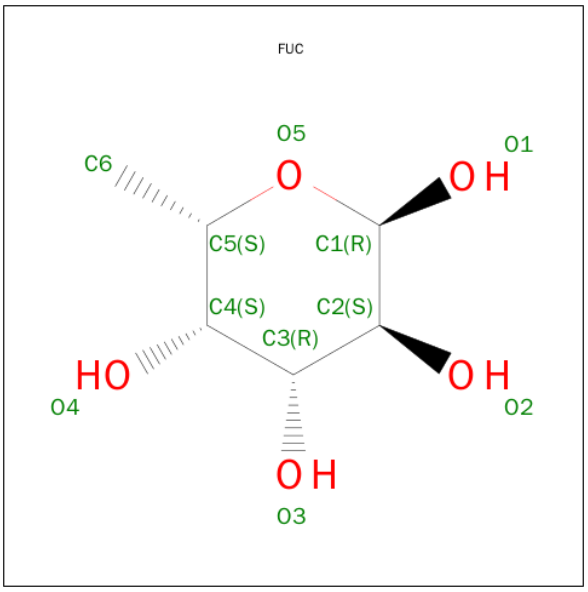
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



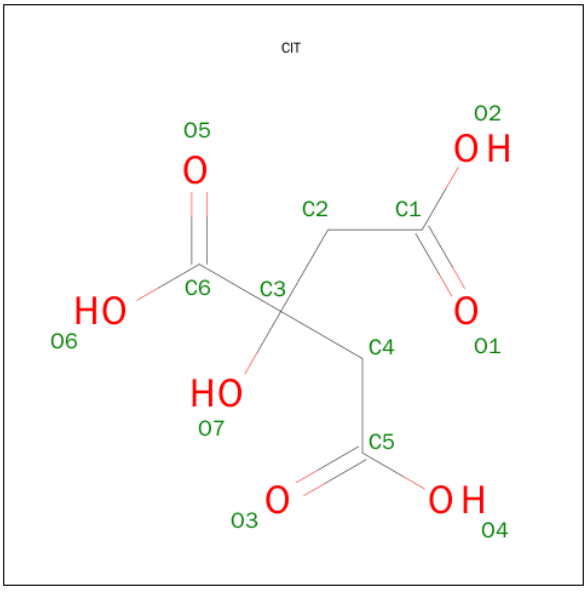
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 13 6 7	0	0

- Molecule 7 is water.

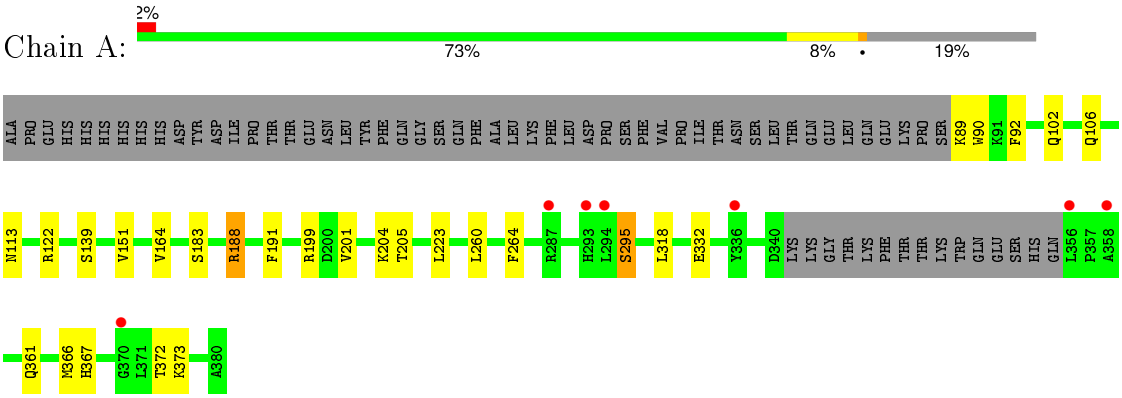
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	35	Total O 35 35	0	0
7	B	25	Total O 25 25	0	0

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.

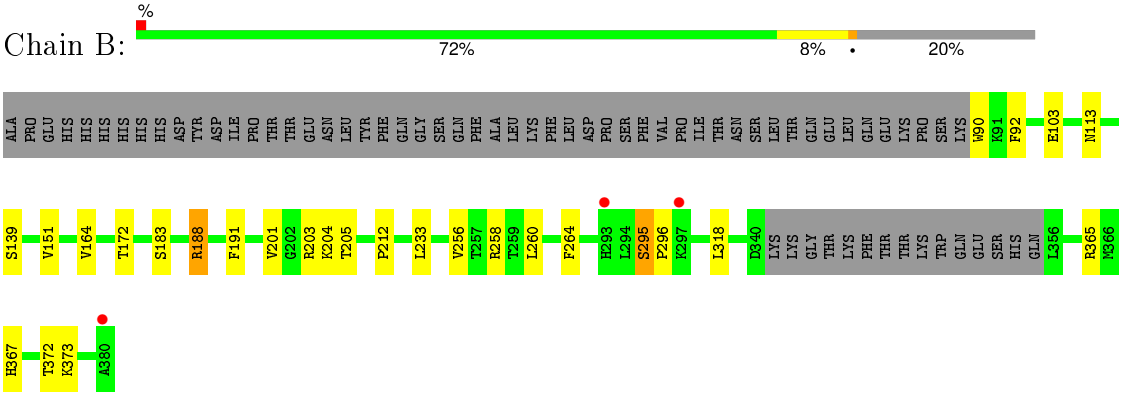
- Molecule 1: Sia-alpha-2,3-Gal-beta-1,4-GlcNAc-R:alpha 2,8-sialyltransferase

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	88.17Å 94.22Å 126.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.43 – 2.70 51.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (52.43-2.70) 96.5 (51.31-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.246 0.201 , 0.251	Depositor DCC
R_{free} test set	1450 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 28521 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4874	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: MAN, BMA, CIT, 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	0.71	0/2336	0.86	5/3168 (0.2%)
1	B	0.68	0/2344	0.82	3/3176 (0.1%)
All	All	0.69	0/4680	0.84	8/6344 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	188	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	122	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	199	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	366	MET	CG-SD-CE	-5.26	91.78	100.20
1	B	258	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	365	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	223	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	SER	Peptide
1	B	295	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	2270	0	2193	7	0
1	B	2278	0	2222	8	0
2	A	112	0	99	0	0
2	B	98	0	86	0	0
3	A	11	0	9	1	0
3	B	11	0	10	0	0
4	A	11	0	10	2	0
5	B	10	0	10	0	0
6	B	13	0	5	0	0
7	A	35	0	0	0	0
7	B	25	0	0	0	0
All	All	4874	0	4644	17	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 2.

All (17) 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:212:PRO:O	1:B:256:VAL:HG11	1.89	0.73
1:B:188:ARG:NH1	1:B:204:LYS:O	2.36	0.59
1:A:188:ARG:NH1	1:A:204:LYS:O	2.37	0.58
4:A:410:MAN:H62	4:A:410:MAN:O3	2.04	0.57
1:A:188:ARG:NH2	1:A:201:VAL:O	2.40	0.54
1:A:188:ARG:HD2	1:A:205:THR:OG1	2.08	0.53
1:B:188:ARG:NH2	1:B:201:VAL:O	2.40	0.53
1:B:188:ARG:HD2	1:B:205:THR:OG1	2.10	0.52
1:A:260:LEU:HD22	1:A:264:PHE:CE2	2.45	0.51
1:B:260:LEU:HD22	1:B:264:PHE:CE2	2.46	0.51
1:B:367:HIS:HD2	1:B:373:LYS:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:HIS:HD2	1:A:373:LYS:HA	1.82	0.45
3:A:409:BMA:H61	4:A:410:MAN:O2	2.19	0.43
1:B:90:TRP:CH2	1:B:92:PHE:HB2	2.55	0.41
1:A:90:TRP:CH2	1:A:92:PHE:HB2	2.56	0.41
1:A:164:VAL:HB	1:A:318:LEU:HD23	2.02	0.40
1:B:164:VAL:HB	1:B:318:LEU:HD23	2.02	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	273/343 (80%)	264 (97%)	9 (3%)	0	100 100
1	B	272/343 (79%)	261 (96%)	10 (4%)	1 (0%)	39 69
All	All	545/686 (79%)	525 (96%)	19 (4%)	1 (0%)	52 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	PRO

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	247/313 (79%)	235 (95%)	12 (5%)	31	61
1	B	250/313 (80%)	239 (96%)	11 (4%)	35	65
All	All	497/626 (79%)	474 (95%)	23 (5%)	33	64

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

Mol	Chain	Res	Type
1	A	89	LYS
1	A	102	GLN
1	A	106	GLN
1	A	113	ASN
1	A	139	SER
1	A	151	VAL
1	A	183	SER
1	A	191	PHE
1	A	295	SER
1	A	332	GLU
1	A	361	GLN
1	A	372	THR
1	B	103	GLU
1	B	113	ASN
1	B	139	SER
1	B	151	VAL
1	B	172	THR
1	B	183	SER
1	B	191	PHE
1	B	203	ARG
1	B	233	LEU
1	B	295	SER
1	B	372	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	102	GLN
1	A	156	ASN
1	A	291	ASN
1	A	367	HIS
1	B	100	GLN
1	B	291	ASN

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Mol	Chain	Res	Type
1	B	317	HIS
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

20 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	0.72	0	15,19,21	1.84	7 (46%)
2	NAG	A	402	2	14,14,15	0.55	0	15,19,21	1.07	2 (13%)
2	NAG	A	403	1,2	14,14,15	0.61	0	15,19,21	1.80	5 (33%)
2	NAG	A	404	2	14,14,15	0.70	0	15,19,21	1.15	2 (13%)
2	NAG	A	405	1,2	14,14,15	0.78	0	15,19,21	1.03	0
2	NAG	A	406	2	14,14,15	0.44	0	15,19,21	1.05	1 (6%)
2	NAG	A	407	1,2	14,14,15	0.67	0	15,19,21	1.45	3 (20%)
2	NAG	A	408	3,2	14,14,15	0.37	0	15,19,21	0.90	1 (6%)
3	BMA	A	409	2,4	11,11,12	0.61	0	15,15,17	1.26	1 (6%)
4	MAN	A	410	3	11,11,12	0.23	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	401	1,2,5	14,14,15	0.43	0	15,19,21	1.33	1 (6%)
2	NAG	B	402	3,2	14,14,15	0.51	0	15,19,21	1.25	2 (13%)
3	BMA	B	403	2	11,11,12	0.57	0	15,15,17	1.02	1 (6%)
5	FUC	B	404	2	10,10,11	0.47	0	13,14,16	1.40	1 (7%)
2	NAG	B	405	1	14,14,15	1.26	2 (14%)	15,19,21	2.35	7 (46%)
2	NAG	B	406	1,2	14,14,15	0.70	0	15,19,21	1.54	3 (20%)
2	NAG	B	407	2	14,14,15	0.36	0	15,19,21	1.31	2 (13%)
2	NAG	B	408	1,2	14,14,15	0.67	0	15,19,21	1.84	2 (13%)
2	NAG	B	409	2	14,14,15	0.61	0	15,19,21	1.70	3 (20%)
6	CIT	B	410	-	3,12,12	1.52	0	3,17,17	3.32	1 (33%)

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	2	-	0/6/23/26	0/1/1/1
2	NAG	A	403	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	404	2	-	0/6/23/26	0/1/1/1
2	NAG	A	405	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	406	2	-	0/6/23/26	0/1/1/1
2	NAG	A	407	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	408	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	409	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	410	3	-	0/2/19/22	0/1/1/1
2	NAG	B	401	1,2,5	-	0/6/23/26	0/1/1/1
2	NAG	B	402	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	403	2	-	0/2/19/22	0/1/1/1
5	FUC	B	404	2	-	0/0/17/20	0/1/1/1
2	NAG	B	405	1	-	0/6/23/26	0/1/1/1
2	NAG	B	406	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	407	2	-	0/6/23/26	0/1/1/1
2	NAG	B	408	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	409	2	-	0/6/23/26	0/1/1/1
6	CIT	B	410	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	NAG	C3-C2	2.23	1.57	1.52
2	B	405	NAG	C1-C2	3.49	1.57	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	408	NAG	C1-O5-C5	-5.70	103.76	112.14
2	B	409	NAG	C3-C4-C5	-4.19	102.75	110.23
2	B	405	NAG	O5-C5-C4	-3.92	103.65	110.13
2	B	401	NAG	O3-C3-C2	-3.47	101.94	109.37
2	A	407	NAG	C2-N2-C7	-2.87	119.37	123.11
2	B	408	NAG	C2-N2-C7	-2.63	119.69	123.11
2	B	405	NAG	C3-C4-C5	-2.48	105.80	110.23
2	A	401	NAG	O6-C6-C5	-2.48	103.02	111.30
2	A	401	NAG	O3-C3-C4	-2.35	105.05	110.36
2	A	401	NAG	O7-C7-N2	-2.33	117.10	121.84
2	B	407	NAG	O5-C5-C4	-2.28	106.36	110.13
2	A	402	NAG	C3-C4-C5	-2.27	106.17	110.23
2	B	406	NAG	O4-C4-C3	-2.27	105.24	110.36
2	B	405	NAG	O7-C7-C8	-2.24	117.95	122.07
2	A	403	NAG	O7-C7-N2	-2.11	117.55	121.84
2	B	409	NAG	O6-C6-C5	-2.10	104.28	111.30
2	A	408	NAG	C4-C3-C2	-2.05	108.16	111.34
2	A	407	NAG	O6-C6-C5	-2.03	104.51	111.30
2	A	402	NAG	O4-C4-C5	2.00	114.50	109.23
2	B	402	NAG	C1-O5-C5	2.03	115.13	112.14
2	A	401	NAG	C2-N2-C7	2.11	125.85	123.11
2	B	407	NAG	C2-N2-C7	2.19	125.95	123.11
2	B	406	NAG	C3-C4-C5	2.20	114.15	110.23
3	B	403	BMA	O3-C3-C4	2.21	115.34	110.36
2	B	409	NAG	O4-C4-C5	2.29	115.27	109.23
2	A	407	NAG	C8-C7-N2	2.30	120.51	116.10
2	A	403	NAG	C6-C5-C4	2.33	118.82	112.99
2	A	401	NAG	C8-C7-N2	2.35	120.61	116.10
2	B	405	NAG	C6-C5-C4	2.38	118.96	112.99
2	A	403	NAG	C2-N2-C7	2.39	126.21	123.11
2	A	404	NAG	O5-C5-C6	2.42	112.52	107.34
2	A	403	NAG	C1-O5-C5	2.44	115.72	112.14
2	A	401	NAG	C1-O5-C5	2.64	116.02	112.14
2	A	406	NAG	C1-O5-C5	2.65	116.04	112.14
2	A	404	NAG	C2-N2-C7	2.67	126.57	123.11
2	B	405	NAG	C1-O5-C5	2.82	116.29	112.14
3	A	409	BMA	C3-C4-C5	3.15	115.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	NAG	C4-C3-C2	3.21	116.32	111.34
2	A	401	NAG	O5-C5-C4	3.31	115.61	110.13
2	B	405	NAG	O3-C3-C2	3.55	116.98	109.37
5	B	404	FUC	O5-C5-C6	3.60	112.73	106.28
2	A	403	NAG	C8-C7-N2	3.61	123.01	116.10
2	B	406	NAG	C1-O5-C5	3.91	117.89	112.14
2	B	405	NAG	C2-N2-C7	4.14	128.49	123.11
6	B	410	CIT	C3-C2-C1	5.40	123.38	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	BMA	1	0
4	A	410	MAN	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	277/343 (80%)	0.03	7 (2%) 61 61	30, 52, 96, 138	0
1	B	276/343 (80%)	0.05	3 (1%) 82 83	32, 56, 101, 141	0
All	All	553/686 (80%)	0.04	10 (1%) 71 72	30, 54, 101, 141	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	LYS	4.4
1	B	293	HIS	3.7
1	A	293	HIS	3.6
1	B	380	ALA	3.5
1	A	294	LEU	2.6
1	A	287	ARG	2.6
1	A	370	GLY	2.4
1	A	358	ALA	2.3
1	A	336	TYR	2.3
1	A	356	LEU	2.2

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
2	NAG	B	408	14/15	0.96	0.32	4.21	27,32,35,36	14
2	NAG	A	407	14/15	0.97	0.16	-0.81	38,47,59,71	0
2	NAG	A	401	14/15	0.97	0.14	-0.82	44,51,57,66	0
2	NAG	B	406	14/15	0.97	0.13	-1.09	41,45,56,57	0
2	NAG	B	401	14/15	0.97	0.10	-3.42	43,52,65,73	0
2	NAG	A	402	14/15	0.93	0.16	-	66,79,89,92	0
2	NAG	A	405	14/15	0.85	0.31	-	83,99,114,122	0
3	BMA	A	409	11/12	0.90	0.12	-	107,118,120,126	0
2	NAG	B	407	14/15	0.96	0.17	-	60,68,74,75	0
6	CIT	B	410	13/13	0.65	0.30	-	83,104,110,112	0
4	MAN	A	410	11/12	0.81	0.21	-	89,109,116,126	0
2	NAG	A	408	14/15	0.92	0.17	-	67,82,99,120	0
2	NAG	A	403	14/15	0.79	0.21	-	83,103,123,135	0
2	NAG	B	402	14/15	0.94	0.17	-	72,87,100,116	0
2	NAG	A	404	14/15	0.78	0.32	-	92,129,142,146	0
5	FUC	B	404	10/11	0.96	0.13	-	63,69,73,74	0
3	BMA	B	403	11/12	0.82	0.21	-	111,120,126,128	0
2	NAG	B	409	14/15	0.90	0.23	-	34,41,48,52	14
2	NAG	B	405	14/15	0.83	0.28	-	79,93,100,111	0
2	NAG	A	406	14/15	0.85	0.43	-	106,128,138,140	0

6.5 Other polymers

There are no such residues in this entry.