wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 07:59 PM GMT

PDB ID	:	4WEF
Title	:	Structure of the Hemagglutinin-neuraminidase from Human parainfluenza virus type III: complex with difluorosialic acid
Authors	:	Streltsov, V.A.; Pilling, P.; Barrett, S.; McKimm-Breschkin, J.
Deposited on	:	2014-09-10
Resolution	:	2.50 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:

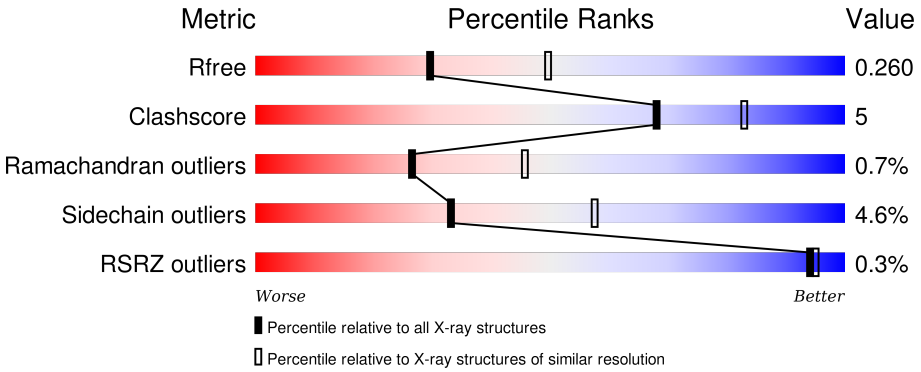
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	431	87% 12%
1	B	431	86% 14%

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	A	601	-	-	-	X
4	FUC	A	608	-	-	-	X
4	FUC	B	609	-	-	-	X
7	SFJ	A	612	-	-	-	X
7	SFJ	B	612	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7765 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.

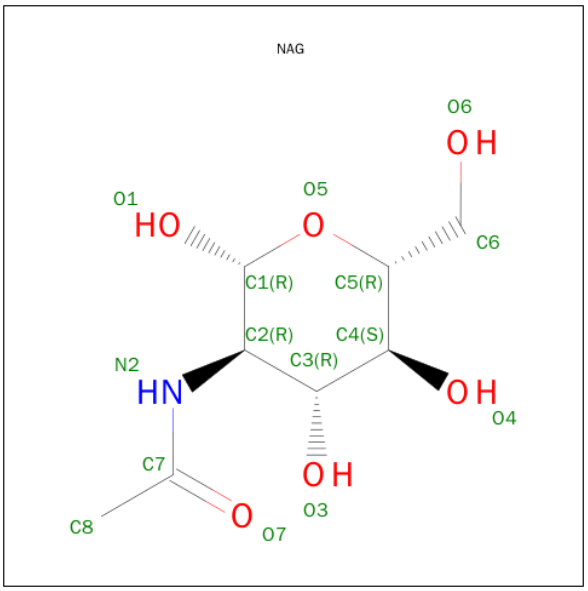
- Molecule 1 is a protein called Hemagglutinin-neuraminidase glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3378	2138	580	640	20			
1	B	431	Total	C	N	O	S	0	0	0
			3375	2137	579	639	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	SER	engineered mutation	UNP Q6WJ03
B	408	GLY	SER	engineered mutation	UNP Q6WJ03

- 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		

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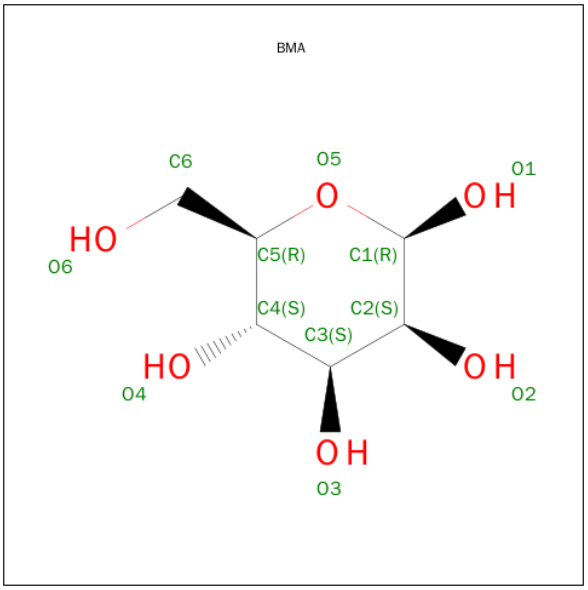
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total 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 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

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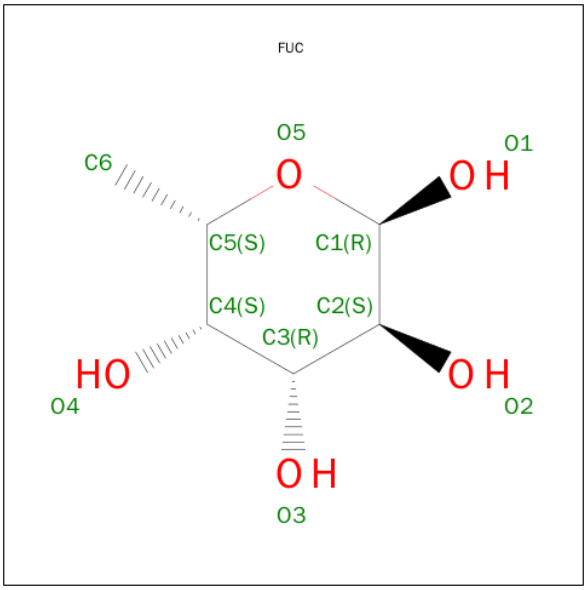
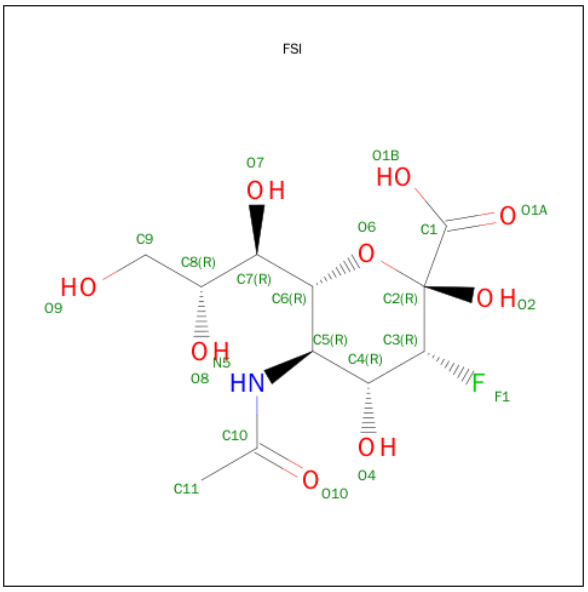
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0

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



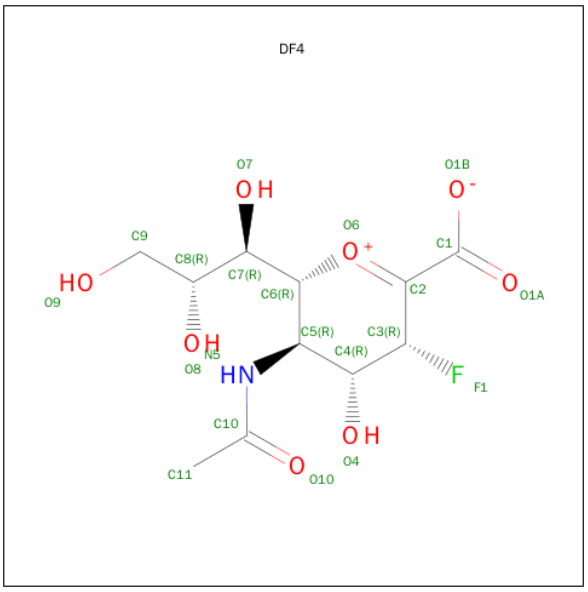
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is 5-(acetylamino)-3,5-dideoxy-3-fluoro-D-erythro-alpha-L-manno-non-2-ulopyranosonic acid (three-letter code: FSI) (formula: $C_{11}H_{18}FNO_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	1
			21	11	1	1	8		
5	B	1	Total	C	F	N	O	0	1
			21	11	1	1	8		

- Molecule 6 is (3R,4R,5R,6R)-5-(acetylamino)-3-fluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-3,4,5,6-tetrahydropyranium-2-carboxylate (three-letter code: DF4) (formula: $C_{11}H_{16}FNO_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	1
			21	11	1	1	8		

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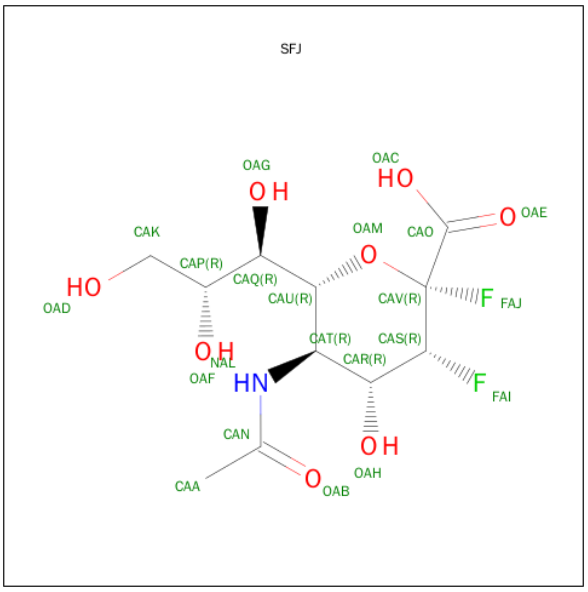
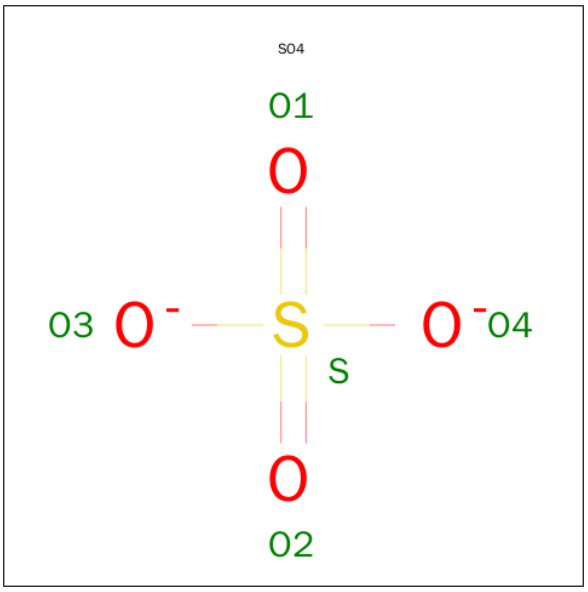
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	F	N	O	0	1
			21	11	1	1	8		

- Molecule 7 is (2R,3R,4R,5R,6R)-5-(acetylamino)-2,3-difluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]tetrahydro-2H-pyran-2-carboxylic acid (three-letter code: SFJ) (formula: $C_{11}H_{17}F_2NO_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			22	11	2	1	8		
7	A	1	Total	C	F	N	O	0	0
			22	11	2	1	8		
7	B	1	Total	C	F	N	O	0	0
			22	11	2	1	8		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Ca 1 1	0	0
9	A	1	Total Ca 1 1	0	0

- Molecule 10 is water.

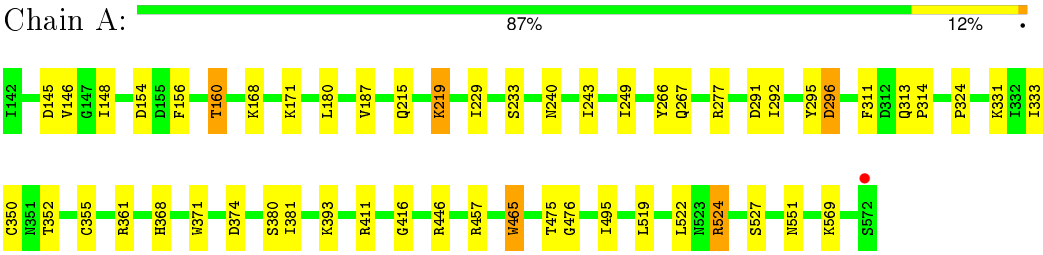
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	293	Total O 293 293	0	0
10	B	298	Total O 298 298	0	0

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.

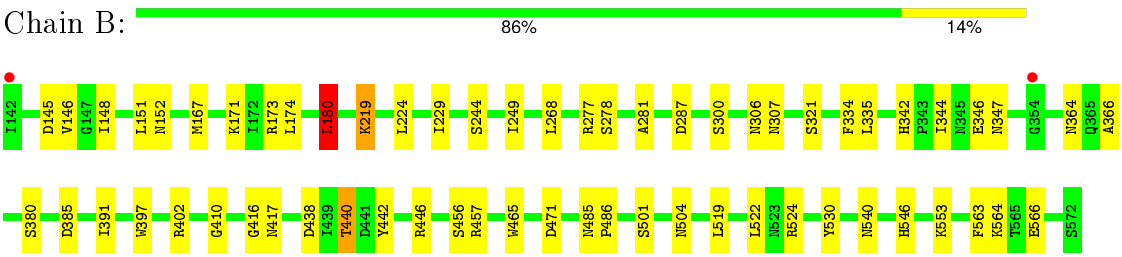
- Molecule 1: Hemagglutinin-neuraminidase glycoprotein

Chain A:



- Molecule 1: Hemagglutinin-neuraminidase glycoprotein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	218.67Å 218.67Å 109.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.46 – 2.50 77.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (77.46-2.50) 99.9 (77.46-2.50)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.189 , 0.258 0.196 , 0.260	Depositor DCC
R_{free} test set	2666 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53542 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7765	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: BMA, NAG, FSI, CA, SFJ, FUC, DF4, SO4

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	0.73	1/3464 (0.0%)	0.84	1/4723 (0.0%)
1	B	0.69	0/3456	0.84	1/4712 (0.0%)
All	All	0.71	1/6920 (0.0%)	0.84	2/9435 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	TRP	CB-CG	-5.07	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	361	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	180	LEU	CB-CG-CD2	5.29	120.00	111.00

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	3378	0	3344	24	0
1	B	3375	0	3342	36	0
2	A	70	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	70	0	61	3	0
3	A	22	0	19	0	0
3	B	22	0	19	0	0
4	A	10	0	10	0	0
4	B	10	0	10	1	0
5	A	21	0	16	0	0
5	B	21	0	16	0	0
6	A	21	0	16	1	0
6	B	21	0	16	1	0
7	A	44	0	32	2	0
7	B	22	0	16	4	0
8	A	30	0	0	0	0
8	B	35	0	0	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	293	0	0	3	0
10	B	298	0	0	15	0
All	All	7765	0	6978	66	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 5.

The worst 5 of 66 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:540:ASN:HB2	10:B:843:HOH:O	1.85	0.77
1:B:416:GLY:HA3	10:B:716:HOH:O	1.92	0.69
1:B:277:ARG:HD2	10:B:703:HOH:O	1.94	0.68
1:B:530:TYR:OH	6:B:611[B]:DF4:C2	2.45	0.64
1:B:540:ASN:CB	10:B:843:HOH:O	2.41	0.64

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	430/431 (100%)	401 (93%)	25 (6%)	4 (1%)	21 37
1	B	429/431 (100%)	399 (93%)	28 (6%)	2 (0%)	34 55
All	All	859/862 (100%)	800 (93%)	53 (6%)	6 (1%)	26 46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	SER
1	A	160	THR
1	A	416	GLY
1	B	287	ASP
1	A	350	CYS

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	390/389 (100%)	373 (96%)	17 (4%)	35 60
1	B	389/389 (100%)	370 (95%)	19 (5%)	31 55
All	All	779/778 (100%)	743 (95%)	36 (5%)	33 57

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	ARG
1	B	180	LEU
1	B	553	LYS
1	B	167	MET
1	B	219	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	B	294	ASN
1	B	504	ASN
1	A	347	ASN
1	B	417	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	601	1	14,14,15	0.50	0	15,19,21	1.82	3 (20%)
2	NAG	A	602	1,2	14,14,15	0.86	0	15,19,21	1.98	4 (26%)
2	NAG	A	603	3,2	14,14,15	0.49	0	15,19,21	1.76	4 (26%)
2	NAG	A	606	1,2,4	14,14,15	0.97	1 (7%)	15,19,21	1.42	2 (13%)
2	NAG	A	607	2	14,14,15	0.55	0	15,19,21	1.47	3 (20%)
2	NAG	B	603	1,2	14,14,15	0.60	0	15,19,21	1.80	4 (26%)
2	NAG	B	604	3,2	14,14,15	0.39	0	15,19,21	1.42	2 (13%)
2	NAG	B	608	2	14,14,15	0.85	1 (7%)	15,19,21	2.08	3 (20%)

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	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	603	3,2	-	0/6/23/26	0/1/1/1
2	NAG	A	606	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	607	2	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	604	3,2	-	0/6/23/26	0/1/1/1
2	NAG	B	608	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	NAG	O5-C1	-2.06	1.40	1.43
2	B	608	NAG	C1-C2	2.43	1.55	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	608	NAG	O7-C7-C8	-3.46	115.71	122.07
2	A	602	NAG	O5-C5-C4	-3.03	105.12	110.13
2	A	607	NAG	O7-C7-C8	-2.97	116.60	122.07
2	A	606	NAG	O4-C4-C3	-2.64	104.42	110.36
2	B	608	NAG	C6-C5-C4	-2.32	107.17	112.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
2	A	606	NAG	1	0
2	B	604	NAG	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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	601	1	14,14,15	0.50	0	15,19,21	1.82	3 (20%)
2	NAG	A	602	1,2	14,14,15	0.86	0	15,19,21	1.98	4 (26%)
2	NAG	A	603	3,2	14,14,15	0.49	0	15,19,21	1.76	4 (26%)
3	BMA	A	604	3,2	11,11,12	0.56	0	15,15,17	1.27	2 (13%)
3	BMA	A	605	3	11,11,12	0.78	0	15,15,17	1.52	4 (26%)
2	NAG	A	606	1,2,4	14,14,15	0.97	1 (7%)	15,19,21	1.42	2 (13%)
2	NAG	A	607	2	14,14,15	0.55	0	15,19,21	1.47	3 (20%)
4	FUC	A	608	2	10,10,11	0.65	0	13,14,16	2.88	5 (38%)
5	FSI	A	609[A]	1	18,21,22	0.61	0	21,30,33	1.69	5 (23%)
6	DF4	A	610[B]	-	15,21,21	0.57	0	18,30,30	2.08	3 (16%)
7	SFJ	A	611	-	16,22,22	0.87	1 (6%)	19,33,33	1.50	4 (21%)
7	SFJ	A	612	-	16,22,22	0.96	1 (6%)	19,33,33	1.73	5 (26%)
8	SO4	A	613	-	4,4,4	0.58	0	6,6,6	0.23	0
8	SO4	A	614	-	4,4,4	0.82	0	6,6,6	0.71	0
8	SO4	A	615	-	4,4,4	0.60	0	6,6,6	0.62	0
8	SO4	A	616	-	4,4,4	0.58	0	6,6,6	1.12	1 (16%)
8	SO4	A	617	-	4,4,4	0.44	0	6,6,6	0.22	0
8	SO4	A	618	-	4,4,4	0.59	0	6,6,6	0.38	0
8	SO4	B	601	-	4,4,4	0.46	0	6,6,6	0.19	0
2	NAG	B	602	1	14,14,15	0.47	0	15,19,21	1.34	2 (13%)
2	NAG	B	603	1,2	14,14,15	0.60	0	15,19,21	1.80	4 (26%)
2	NAG	B	604	3,2	14,14,15	0.39	0	15,19,21	1.42	2 (13%)
3	BMA	B	605	3,2	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
3	BMA	B	606	3	11,11,12	0.88	1 (9%)	15,15,17	2.62	6 (40%)
2	NAG	B	607	1,2,4	14,14,15	1.07	1 (7%)	15,19,21	1.94	4 (26%)
2	NAG	B	608	2	14,14,15	0.85	1 (7%)	15,19,21	2.08	3 (20%)
4	FUC	B	609	2	10,10,11	1.05	1 (10%)	13,14,16	2.53	6 (46%)
5	FSI	B	610[A]	1	18,21,22	0.88	1 (5%)	21,30,33	1.20	2 (9%)
6	DF4	B	611[B]	-	15,21,21	0.39	0	18,30,30	0.90	0
7	SFJ	B	612	-	16,22,22	1.71	2 (12%)	19,33,33	3.11	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	B	613	-	4,4,4	0.58	0	6,6,6	0.30	0
8	SO4	B	614	-	4,4,4	0.57	0	6,6,6	0.42	0
8	SO4	B	615	-	4,4,4	0.57	0	6,6,6	0.26	0
8	SO4	B	616	-	4,4,4	0.68	0	6,6,6	0.38	0
8	SO4	B	617	-	4,4,4	0.48	0	6,6,6	0.29	0
8	SO4	B	618	-	4,4,4	0.34	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	604	3,2	-	0/2/19/22	0/1/1/1
3	BMA	A	605	3	-	0/2/19/22	0/1/1/1
2	NAG	A	606	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	A	607	2	-	0/6/23/26	0/1/1/1
4	FUC	A	608	2	-	0/0/17/20	0/1/1/1
5	FSI	A	609[A]	1	-	0/14/38/43	0/1/1/1
6	DF4	A	610[B]	-	-	0/14/38/38	0/0/1/1
7	SFJ	A	611	-	-	0/14/43/43	0/1/1/1
7	SFJ	A	612	-	-	0/14/43/43	0/1/1/1
8	SO4	A	613	-	-	0/0/0/0	0/0/0/0
8	SO4	A	614	-	-	0/0/0/0	0/0/0/0
8	SO4	A	615	-	-	0/0/0/0	0/0/0/0
8	SO4	A	616	-	-	0/0/0/0	0/0/0/0
8	SO4	A	617	-	-	0/0/0/0	0/0/0/0
8	SO4	A	618	-	-	0/0/0/0	0/0/0/0
8	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	NAG	B	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	604	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	605	3,2	-	0/2/19/22	0/1/1/1
3	BMA	B	606	3	-	0/2/19/22	0/1/1/1
2	NAG	B	607	1,2,4	-	0/6/23/26	0/1/1/1
2	NAG	B	608	2	-	0/6/23/26	0/1/1/1
4	FUC	B	609	2	-	0/0/17/20	0/1/1/1
5	FSI	B	610[A]	1	-	0/14/38/43	0/1/1/1
6	DF4	B	611[B]	-	-	0/14/38/38	0/0/1/1
7	SFJ	B	612	-	-	0/14/43/43	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	B	613	-	-	0/0/0/0	0/0/0/0
8	SO4	B	614	-	-	0/0/0/0	0/0/0/0
8	SO4	B	615	-	-	0/0/0/0	0/0/0/0
8	SO4	B	616	-	-	0/0/0/0	0/0/0/0
8	SO4	B	617	-	-	0/0/0/0	0/0/0/0
8	SO4	B	618	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	NAG	O5-C1	-3.30	1.38	1.43
2	A	606	NAG	O5-C1	-2.06	1.40	1.43
5	B	610[A]	FSI	O6-C2	-2.03	1.41	1.44
3	B	606	BMA	C2-C3	2.16	1.55	1.52
7	A	611	SFJ	CAQ-CAU	2.43	1.56	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	607	NAG	O5-C5-C6	-4.50	97.71	107.34
3	B	606	BMA	C3-C4-C5	-4.22	102.70	110.23
2	B	607	NAG	C2-N2-C7	-3.97	117.95	123.11
5	A	609[A]	FSI	F1-C3-C2	-3.93	103.38	108.17
7	A	612	SFJ	OAM-CAU-CAQ	-3.88	101.36	107.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
2	A	606	NAG	1	0
6	A	610[B]	DF4	1	0
7	A	612	SFJ	2	0
2	B	604	NAG	1	0
2	B	607	NAG	2	0
4	B	609	FUC	1	0
6	B	611[B]	DF4	1	0
7	B	612	SFJ	4	0
8	B	618	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	431/431 (100%)	-0.20	1 (0%)	95	96	17, 32, 55, 86	0
1	B	431/431 (100%)	-0.18	2 (0%)	91	92	19, 32, 58, 90	0
All	All	862/862 (100%)	-0.19	3 (0%)	94	95	17, 32, 56, 90	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	SER	3.8
1	B	142	ILE	2.8
1	B	354	GLY	2.1

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

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	A	601	14/15	0.75	0.26	6.32	82,92,101,105	0
2	NAG	A	606	14/15	0.69	0.17	0.28	70,81,97,99	0
2	NAG	A	603	14/15	0.90	0.22	-	73,85,90,97	0
2	NAG	A	607	14/15	0.73	0.29	-	96,114,124,129	0
2	NAG	B	603	14/15	0.93	0.21	-	71,74,86,92	0
2	NAG	B	604	14/15	0.88	0.21	-	58,75,79,99	0
2	NAG	A	602	14/15	0.83	0.23	-	72,84,90,94	0
2	NAG	B	608	14/15	0.85	0.27	-	72,80,94,99	0

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, 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	FUC	A	608	10/11	0.79	0.34	12.94	97,105,111,111	0
7	SFJ	A	612	22/22	0.80	0.29	6.42	54,76,87,91	0
2	NAG	A	601	14/15	0.75	0.26	6.32	82,92,101,105	0
4	FUC	B	609	10/11	0.81	0.22	3.05	57,62,64,66	0
7	SFJ	B	612	22/22	0.85	0.31	2.88	51,67,74,80	0
8	SO4	B	618	5/5	0.95	0.22	1.63	85,85,89,91	0
8	SO4	A	614	5/5	0.95	0.18	1.53	52,54,62,69	0
8	SO4	B	614	5/5	0.95	0.16	1.29	70,71,73,77	0
6	DF4	A	610[B]	21/21	0.97	0.15	0.86	17,18,19,20	21
5	FSI	B	610[A]	21/22	0.98	0.14	0.30	23,25,30,31	21
6	DF4	B	611[B]	21/21	0.98	0.14	0.29	13,13,14,14	21
2	NAG	A	606	14/15	0.69	0.17	0.28	70,81,97,99	0
8	SO4	B	615	5/5	0.91	0.15	0.01	79,82,85,89	0
8	SO4	A	616	5/5	0.95	0.16	-0.01	64,65,69,70	0
7	SFJ	A	611	22/22	0.91	0.14	-0.25	36,49,55,57	0
2	NAG	B	602	14/15	0.91	0.14	-0.68	46,66,79,80	0
5	FSI	A	609[A]	21/22	0.97	0.12	-0.87	21,24,29,30	21
8	SO4	B	601	5/5	0.97	0.11	-1.84	70,71,75,75	0
9	CA	B	619	1/1	0.99	0.07	-2.88	32,32,32,32	0
9	CA	A	619	1/1	0.98	0.07	-3.95	37,37,37,37	0
2	NAG	B	607	14/15	0.90	0.15	-	52,60,71,72	0
2	NAG	A	607	14/15	0.73	0.29	-	96,114,124,129	0
3	BMA	A	604	11/12	0.74	0.28	-	94,102,106,108	0
3	BMA	A	605	11/12	0.75	0.28	-	70,93,102,104	0
8	SO4	A	618	5/5	0.98	0.13	-	61,61,64,64	0
8	SO4	A	613	5/5	0.91	0.19	-	64,80,83,84	0
8	SO4	B	617	5/5	0.92	0.24	-	72,79,82,93	0
2	NAG	B	608	14/15	0.85	0.27	-	72,80,94,99	0
3	BMA	B	606	11/12	0.73	0.29	-	84,98,102,105	0
8	SO4	A	615	5/5	0.91	0.23	-	79,79,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	B	603	14/15	0.93	0.21	-	71,74,86,92	0
2	NAG	A	603	14/15	0.90	0.22	-	73,85,90,97	0
3	BMA	B	605	11/12	0.76	0.36	-	98,111,114,115	0
8	SO4	A	617	5/5	0.96	0.18	-	77,83,83,92	0
8	SO4	B	613	5/5	0.92	0.24	-	75,77,87,88	0
2	NAG	B	604	14/15	0.88	0.21	-	58,75,79,99	0
2	NAG	A	602	14/15	0.83	0.23	-	72,84,90,94	0
8	SO4	B	616	5/5	0.90	0.26	-	77,77,84,92	0

6.5 Other polymers

There are no such residues in this entry.