W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:46 PM GMT

|		
PDB ID	:	3S11
Title	:	Crystal structure of H5N1 influenza virus hemagglutinin, strain 437-10
Authors	:	DuBois, R.M.; Zaraket, H.; Reddivari, M.; Heath, R.J.; White, S.W.; Russell, C.J.
Deposited on	:	2011-05-14
Resolution	:	2.50 Å(reported)

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.
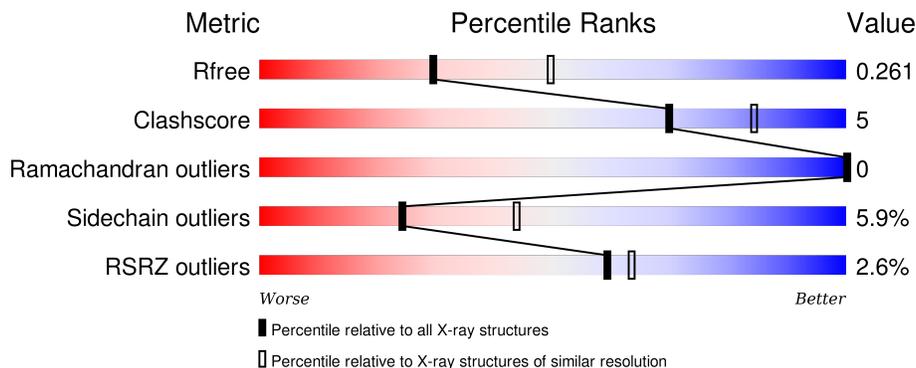
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	331	
1	C	331	
1	E	331	
2	B	182	
2	D	182	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	182	

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
5	GOL	A	328	-	-	-	X
7	BMA	C	330	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12093 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total 2542	C 1604	N 439	O 484	S 15	0	0	0
1	C	321	Total 2535	C 1599	N 438	O 483	S 15	0	0	0
1	E	322	Total 2542	C 1604	N 439	O 484	S 15	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASP	-	EXPRESSION TAG	UNP Q9EA62
A	4	LEU	-	EXPRESSION TAG	UNP Q9EA62
A	5	GLY	-	EXPRESSION TAG	UNP Q9EA62
A	6	SER	-	EXPRESSION TAG	UNP Q9EA62
A	7	ALA	-	EXPRESSION TAG	UNP Q9EA62
A	8	ASP	-	EXPRESSION TAG	UNP Q9EA62
A	9	PRO	-	EXPRESSION TAG	UNP Q9EA62
A	10	GLY	-	EXPRESSION TAG	UNP Q9EA62
C	3	ASP	-	EXPRESSION TAG	UNP Q9EA62
C	4	LEU	-	EXPRESSION TAG	UNP Q9EA62
C	5	GLY	-	EXPRESSION TAG	UNP Q9EA62
C	6	SER	-	EXPRESSION TAG	UNP Q9EA62
C	7	ALA	-	EXPRESSION TAG	UNP Q9EA62
C	8	ASP	-	EXPRESSION TAG	UNP Q9EA62
C	9	PRO	-	EXPRESSION TAG	UNP Q9EA62
C	10	GLY	-	EXPRESSION TAG	UNP Q9EA62
E	3	ASP	-	EXPRESSION TAG	UNP Q9EA62
E	4	LEU	-	EXPRESSION TAG	UNP Q9EA62
E	5	GLY	-	EXPRESSION TAG	UNP Q9EA62
E	6	SER	-	EXPRESSION TAG	UNP Q9EA62
E	7	ALA	-	EXPRESSION TAG	UNP Q9EA62
E	8	ASP	-	EXPRESSION TAG	UNP Q9EA62
E	9	PRO	-	EXPRESSION TAG	UNP Q9EA62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	EXPRESSION TAG	UNP Q9EA62

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1377	857	239	273	8			
2	D	172	Total	C	N	O	S	0	0	0
			1395	867	241	279	8			
2	F	173	Total	C	N	O	S	0	0	0
			1403	873	242	280	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	EXPRESSION TAG	UNP Q9EA62
B	178	SER	-	EXPRESSION TAG	UNP Q9EA62
B	179	LEU	-	EXPRESSION TAG	UNP Q9EA62
B	180	VAL	-	EXPRESSION TAG	UNP Q9EA62
B	181	PRO	-	EXPRESSION TAG	UNP Q9EA62
B	182	ARG	-	EXPRESSION TAG	UNP Q9EA62
D	177	ARG	-	EXPRESSION TAG	UNP Q9EA62
D	178	SER	-	EXPRESSION TAG	UNP Q9EA62
D	179	LEU	-	EXPRESSION TAG	UNP Q9EA62
D	180	VAL	-	EXPRESSION TAG	UNP Q9EA62
D	181	PRO	-	EXPRESSION TAG	UNP Q9EA62
D	182	ARG	-	EXPRESSION TAG	UNP Q9EA62
F	177	ARG	-	EXPRESSION TAG	UNP Q9EA62
F	178	SER	-	EXPRESSION TAG	UNP Q9EA62
F	179	LEU	-	EXPRESSION TAG	UNP Q9EA62
F	180	VAL	-	EXPRESSION TAG	UNP Q9EA62
F	181	PRO	-	EXPRESSION TAG	UNP Q9EA62
F	182	ARG	-	EXPRESSION TAG	UNP Q9EA62

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
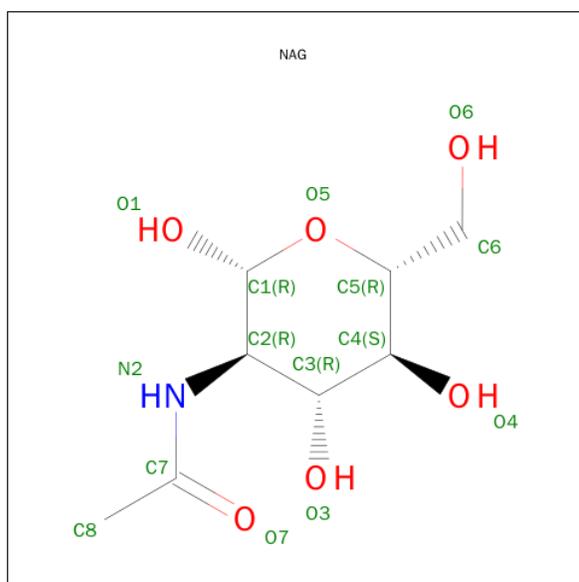
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0
3	E	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total 28	C 16	N 2	O 10	0	0
4	E	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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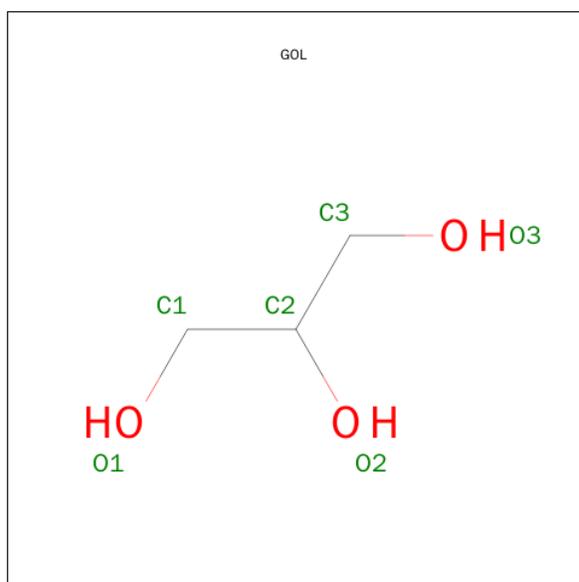
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	E	1	Total 6	C 3	O 3	0	0

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).

TAM
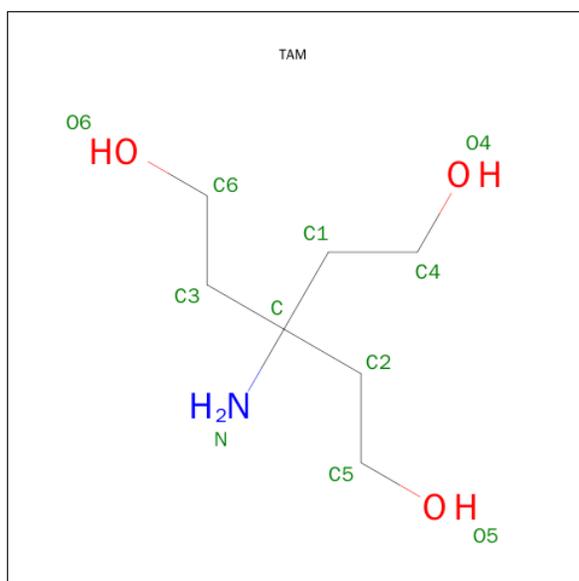
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 11	C 7	N 1	O 3	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	38	Total 38	O 38	0	0
8	B	16	Total 16	O 16	0	0
8	C	43	Total 43	O 43	0	0
8	D	9	Total 9	O 9	0	0
8	E	18	Total 18	O 18	0	0
8	F	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 HA1 chain
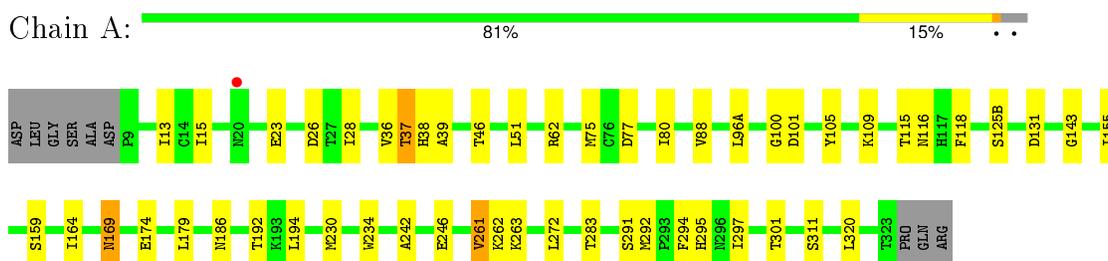
- Molecule 1: Hemagglutinin HA1 chain
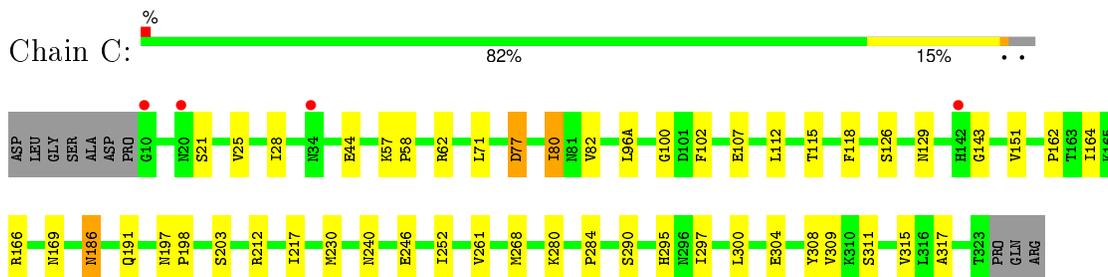
- Molecule 1: Hemagglutinin HA1 chain

- Molecule 2: Hemagglutinin HA2 chain

Y162 S163 E164 E165 A166 R167 L168 N169 R170 GLU GLU ILE SER GLY VAL ARG SER LEU VAL PRO ARG

• Molecule 2: Hemagglutinin HA2 chain

Chain D:

4%

82% 11% 5%

G1 L2 V18 D19 Y22 H26 S27 N28 E29 Q30 G31 S32 G33 A36 K43 S54 K58 Q62 L89 W92 E97 I98 L99 V100 L101 L124 N146 E150 M154 Y159 P160 L168 E172 ILE SER GLY VAL ARG SER LEU VAL PRO

ARG

• Molecule 2: Hemagglutinin HA2 chain

Chain F:

5%

74% 17% 5%

G1 Q15 D19 Y22 G23 Y24 G31 S54 M59 Q62 V66 G67 R68 R75 L80 M84 E85 L89 W92 E97 V100 L101 L108 Y119 D120 R123 L124 Q125 L126 R127 D128 N129 Y141 D145 N146 E147 C148 M149 E150 S151

V152 K153 M154 G155 T156 Y157 D158 Y159 P160 Q161 E164 R167 E171 E172 I173 SER GLY VAL ARG SER LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.36Å 241.05Å 70.06Å 90.00° 116.69° 90.00°	Depositor
Resolution (Å)	49.07 – 2.50 49.07 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.07-2.50) 95.9 (49.07-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.221 , 0.265 0.219 , 0.261	Depositor DCC
R_{free} test set	3457 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.1	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 67806 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, TAM

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	0.38	0/2606	0.52	0/3542
1	C	0.38	0/2598	0.55	1/3531 (0.0%)
1	E	0.35	0/2606	0.51	0/3542
2	B	0.36	0/1404	0.49	1/1888 (0.1%)
2	D	0.38	0/1422	0.49	0/1912
2	F	0.39	0/1430	0.53	1/1923 (0.1%)
All	All	0.37	0/12066	0.52	3/16338 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	80	LEU	CA-CB-CG	5.49	127.93	115.30
2	B	80	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	143	GLY	N-CA-C	-5.25	99.96	113.10

There are no chirality outliers.

There are no planarity outliers.

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	2542	0	2470	27	0
1	C	2535	0	2462	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2542	0	2470	17	0
2	B	1377	0	1284	18	0
2	D	1395	0	1296	13	0
2	F	1403	0	1307	25	0
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
4	A	28	0	25	1	0
4	E	28	0	25	0	0
5	A	6	0	8	1	0
5	C	6	0	8	1	0
5	E	6	0	8	0	0
6	A	11	0	17	1	0
7	C	39	0	34	0	0
8	A	38	0	0	0	0
8	B	16	0	0	0	0
8	C	43	0	0	1	0
8	D	9	0	0	0	0
8	E	18	0	0	0	0
8	F	9	0	0	0	0
All	All	12093	0	11453	106	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 106 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:C:151:VAL:HG13	1:C:252:ILE:HG22	1.50	0.94
2:F:123:ARG:HH11	2:F:123:ARG:HG3	1.35	0.90
1:E:116:ASN:HB2	1:E:262:LYS:HG2	1.61	0.80
1:A:28:ILE:HD13	2:B:101:LEU:HD23	1.63	0.79
1:C:311:SER:HB3	2:D:97:GLU:OE2	1.86	0.76

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	320/331 (97%)	311 (97%)	9 (3%)	0	100	100
1	C	319/331 (96%)	307 (96%)	12 (4%)	0	100	100
1	E	320/331 (97%)	307 (96%)	13 (4%)	0	100	100
2	B	168/182 (92%)	162 (96%)	6 (4%)	0	100	100
2	D	170/182 (93%)	166 (98%)	4 (2%)	0	100	100
2	F	171/182 (94%)	164 (96%)	7 (4%)	0	100	100
All	All	1468/1539 (95%)	1417 (96%)	51 (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	286/293 (98%)	267 (93%)	19 (7%)	21	38
1	C	285/293 (97%)	269 (94%)	16 (6%)	26	47
1	E	286/293 (98%)	279 (98%)	7 (2%)	57	82
2	B	145/156 (93%)	132 (91%)	13 (9%)	12	22
2	D	147/156 (94%)	139 (95%)	8 (5%)	27	49
2	F	148/156 (95%)	134 (90%)	14 (10%)	11	20
All	All	1297/1347 (96%)	1220 (94%)	77 (6%)	24	44

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	62	ARG
1	C	186	ASN
2	F	123	ARG
1	C	71	LEU
1	C	96(A)	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	211	GLN
2	D	95	ASN
2	F	114	ASN
1	C	289	ASN
1	C	295	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

7 carbohydrates 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	$\#|Z| > 2$
4	NAG	A	2	1,4	14,14,15	0.49	0	15,19,21	0.96	0
4	NAG	A	327	4	14,14,15	0.46	0	15,19,21	0.69	0
7	NAG	C	328	1,7	14,14,15	0.47	0	15,19,21	1.23	2 (13%)
7	NAG	C	329	7	14,14,15	0.52	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	BMA	C	330	7	11,11,12	0.40	0	14,15,17	1.19	1 (7%)
4	NAG	E	328	1,4	14,14,15	0.49	0	15,19,21	0.78	0
4	NAG	E	329	4	14,14,15	0.48	0	15,19,21	1.17	1 (6%)

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
4	NAG	A	2	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	327	4	-	0/6/23/26	0/1/1/1
7	NAG	C	328	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	329	7	-	0/6/23/26	0/1/1/1
7	BMA	C	330	7	-	0/2/19/22	0/1/1/1
4	NAG	E	328	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	329	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	330	BMA	C1-O5-C5	-3.61	107.67	112.25
7	C	328	NAG	C3-C2-N2	-2.01	105.73	110.56
7	C	329	NAG	C1-O5-C5	2.35	115.22	112.25
7	C	328	NAG	C1-O5-C5	2.35	115.23	112.25
4	E	329	NAG	C1-O5-C5	3.85	117.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	NAG	1	0

5.6 Ligand geometry (i)

7 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	$\#|Z| > 2$
3	NAG	A	1	1	14,14,15	1.54	2 (14%)	15,19,21	1.62	4 (26%)
5	GOL	A	328	-	5,5,5	0.38	0	5,5,5	0.14	0
6	TAM	A	329	-	7,10,10	0.72	0	9,12,12	0.84	0
5	GOL	C	2	-	5,5,5	0.34	0	5,5,5	0.26	0
3	NAG	C	327	1	14,14,15	0.53	0	15,19,21	0.59	0
3	NAG	E	327	1	14,14,15	0.53	0	15,19,21	0.58	0
5	GOL	E	330	-	5,5,5	0.43	0	5,5,5	0.43	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
3	NAG	A	1	1	-	0/6/23/26	0/1/1/1
5	GOL	A	328	-	-	0/4/4/4	0/0/0/0
6	TAM	A	329	-	-	0/12/12/12	0/0/0/0
5	GOL	C	2	-	-	0/4/4/4	0/0/0/0
3	NAG	C	327	1	-	0/6/23/26	0/1/1/1
3	NAG	E	327	1	-	0/6/23/26	0/1/1/1
5	GOL	E	330	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	NAG	C1-C2	-3.65	1.47	1.52
3	A	1	NAG	O5-C1	-2.68	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	NAG	C1-O5-C5	-3.97	107.21	112.25
3	A	1	NAG	C3-C4-C5	2.10	113.86	110.20
3	A	1	NAG	O5-C5-C6	2.25	112.21	107.35

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	NAG	C2-N2-C7	2.42	126.14	123.04

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
5	A	328	GOL	1	0
6	A	329	TAM	1	0
5	C	2	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	322/331 (97%)	-0.03	1 (0%)	94	95	25, 38, 48, 63	0
1	C	321/331 (96%)	0.03	4 (1%)	81	83	27, 37, 48, 57	0
1	E	322/331 (97%)	0.03	2 (0%)	90	91	28, 40, 50, 54	0
2	B	170/182 (93%)	0.69	15 (8%)	12	13	26, 51, 83, 85	0
2	D	172/182 (94%)	0.41	7 (4%)	41	46	27, 44, 59, 63	0
2	F	173/182 (95%)	0.57	10 (5%)	26	30	26, 45, 72, 74	0
All	All	1480/1539 (96%)	0.20	39 (2%)	59	63	25, 40, 62, 85	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	PRO	4.4
2	B	160	PRO	4.3
2	D	29	GLU	3.9
2	B	168	LEU	3.4
2	F	19	ASP	3.4

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)

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(Å²)	Q<0.9
7	BMA	C	330	11/12	0.72	0.25	3.59	20,20,20,20	0
4	NAG	A	2	14/15	0.89	0.17	-0.26	50,53,55,57	0
4	NAG	E	328	14/15	0.87	0.15	-0.44	54,56,58,60	0
7	NAG	C	328	14/15	0.93	0.13	-0.76	37,40,42,45	0
4	NAG	E	329	14/15	0.85	0.28	-	62,63,64,64	0
7	NAG	C	329	14/15	0.91	0.21	-	47,49,49,51	0
4	NAG	A	327	14/15	0.80	0.30	-	59,61,62,62	0

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(Å²)	Q<0.9
5	GOL	A	328	6/6	0.89	0.25	2.27	52,54,55,56	0
5	GOL	E	330	6/6	0.94	0.23	1.39	41,41,42,43	0
6	TAM	A	329	11/11	0.80	0.20	1.27	50,50,51,51	0
5	GOL	C	2	6/6	0.94	0.19	0.47	60,60,60,61	0
3	NAG	C	327	14/15	0.84	0.36	-	65,67,68,68	0
3	NAG	A	1	14/15	0.90	0.42	-	20,20,20,20	0
3	NAG	E	327	14/15	0.82	0.28	-	58,61,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.