W O R L D W I D E
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wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 10:23 AM GMT

PDB ID   :   1HGF
Title   :   BINDING OF INFLUENZA VIRUS HEMAGGLUTININ TO ANALOGS OF
              ITS CELL-SURFACE RECEPTOR, SIALIC ACID: ANALYSIS BY PRO-
              TON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND X-
              RAY CRYSTALLOGRAPHY
Authors   :   Sauter, N.K.; Hanson, J.E.; Glick, G.D.; Brown, J.H.; Crowther, R.L.; Park,
              S.-J.; Skehel, J.J.; Wiley, D.C.
Deposited on :   1991-11-01
Resolution :   3.00 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance (i)

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		1.5%
Sidechain outliers		5.8%
RSRZ outliers		0.6%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
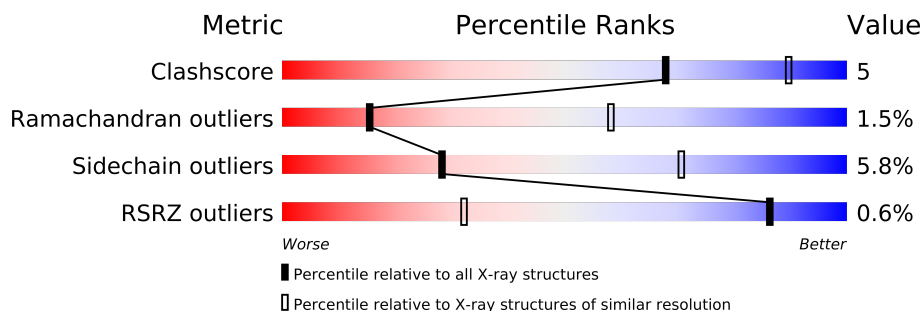
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	329	-	X
3	NAG	A	334	-	X
3	NAG	A	348	-	X
3	NAG	B	401	-	X
3	NAG	C	329	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	C	334	-	X
3	NAG	C	348	-	X
3	NAG	E	329	-	X
3	NAG	E	348	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15192 atoms, of which 3048 are hydrogens and 0 are deuterium.

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, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3122	1581	590	445	493	13			

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1754	882	333	250	283	6			

- 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	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	F	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

• Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
4	C	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
4	E	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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.
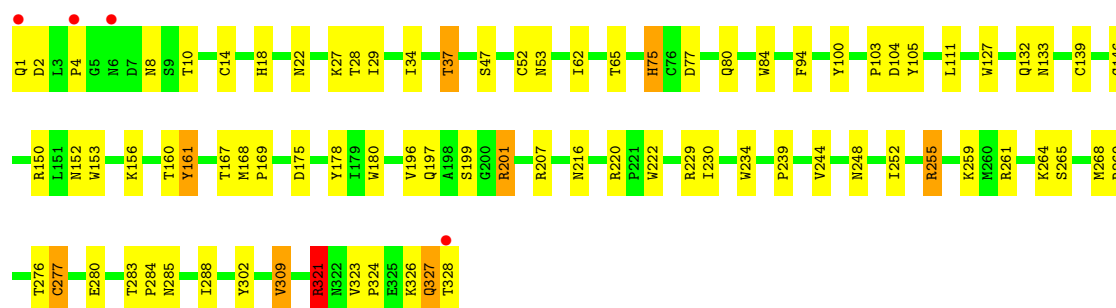
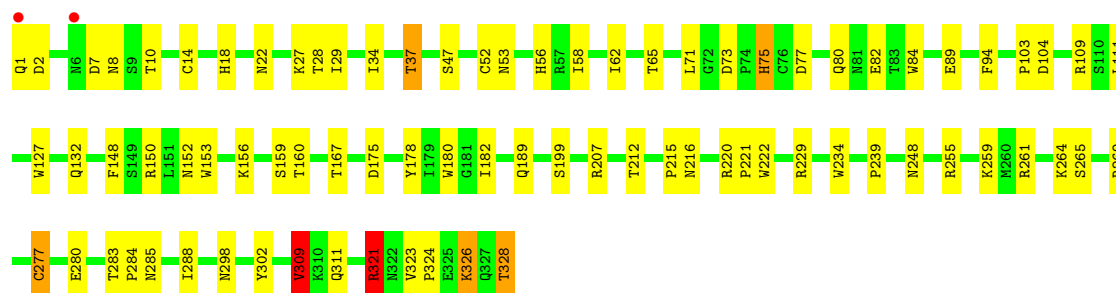- Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain A:
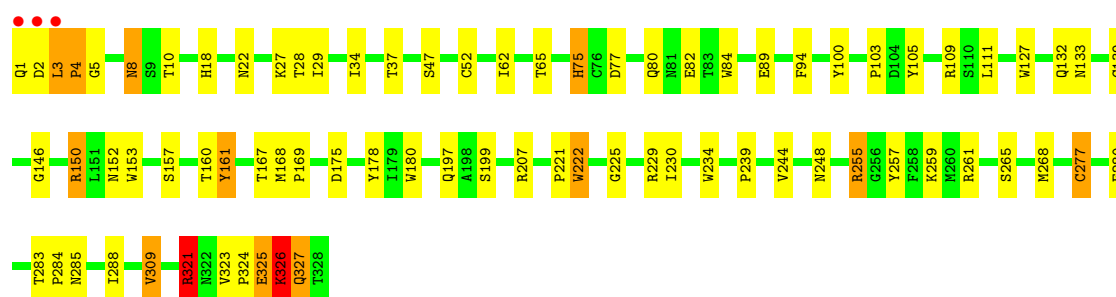
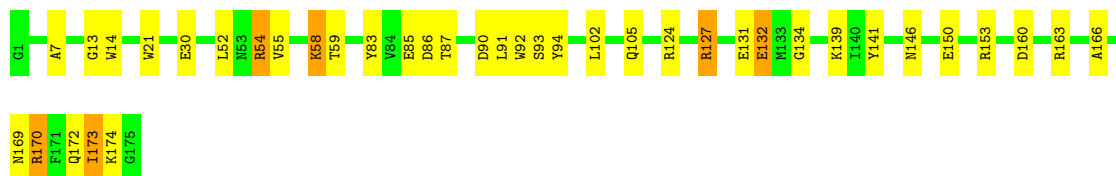- Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain C:
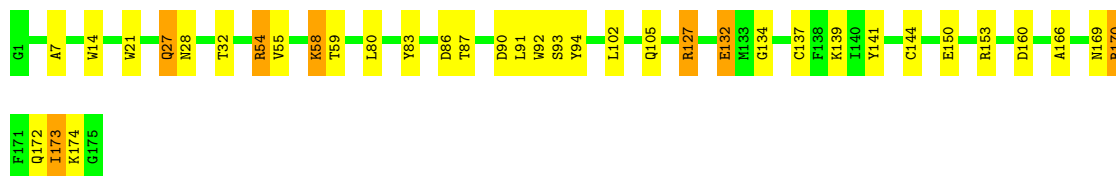

- Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain E:

- Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain B:

G1 A7 G13 W14 W21 E30 L52 N53 R54 V55 K58 T59 Y83 V84 E85 D86 T87 D90 L91 W92 S93 Y94 L102 Q105 R124 R127 E131 E132 M133 G134 K139 I140 Y141 N146 E150 R153 D160 R163 A166

N169 R170 F171 Q172 I173 K174 G175

● Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain D:

G1 A7 W14 W21 Q27 N28 T32 R54 V55 K58 T59 L80 Y83 D86 T87 D90 L91 W92 S93 Y94 L102 Q105 R127 E132 M133 G134 C137 F138 K139 I140 Y141 C144 E150 R153 D160 A166 N169 R170

F171 Q172 I173 K174 G175

● Molecule 2: HEMAGGLUTININ, CHAIN HA1

Chain F:

G1 A7 W14 W21 R54 V55 K58 T59 Y83 D86 T87 D90 L91 W92 S93 Y94 E97 L102 Q105 R123 R124 R127 E131 E132 M133 G134 C137 F138 K139 I140 Y141 E150 D160 A166 N169 R170 F171 Q172 I173 K174 G175

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants	163.20Å 163.20Å 177.40Å	Depositor
a, b, c, α, β, γ	90.00° 90.00° 90.00°	
Resolution (Å)	7.00 – 3.00	Depositor
	10.00 – 3.00	EDS
% Data completeness	(Not available) (7.00-3.00)	Depositor
(in resolution range)	76.9 (10.00-3.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.99Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
	0.232 , (Not available)	DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 18.4	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 69392 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	15192	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: BMA, NAG

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	0.94	1/2589 (0.0%)	1.55	41/3527 (1.2%)
1	C	0.91	0/2589	1.53	42/3527 (1.2%)
1	E	0.96	1/2589 (0.0%)	1.53	42/3527 (1.2%)
2	B	0.97	1/1445 (0.1%)	1.48	19/1939 (1.0%)
2	D	0.99	0/1445	1.49	19/1939 (1.0%)
2	F	0.99	1/1445 (0.1%)	1.49	20/1939 (1.0%)
All	All	0.96	4/12102 (0.0%)	1.52	183/16398 (1.1%)

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	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	150	GLU	CA-CB	-6.01	1.40	1.53
1	E	234	TRP	CG-CD2	-5.58	1.34	1.43
1	A	234	TRP	CG-CD2	-5.32	1.34	1.43
2	B	85	GLU	CD-OE1	-5.25	1.19	1.25

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	321	ARG	NE-CZ-NH2	-15.10	112.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH2	-14.08	113.26	120.30
1	C	321	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	E	321	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	E	180	TRP	CD1-CG-CD2	10.14	114.41	106.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain
1	C	161	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	590	1887	31	0
1	C	2532	590	1887	33	0
1	E	2532	590	1887	30	0
2	B	1421	333	1013	20	0
2	D	1421	333	1013	18	0
2	F	1421	333	1013	19	0
3	A	42	42	0	0	0
3	B	14	14	0	0	0
3	C	42	42	0	0	0
3	D	14	14	0	0	0
3	E	42	42	0	0	0
3	F	14	14	0	0	0
4	A	39	37	0	1	0
4	C	39	37	0	2	0
4	E	39	37	0	1	0
All	All	12144	3048	8700	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:83:TYR:O	2:B:87:THR:HG23	1.85	0.77
2:F:83:TYR:O	2:F:87:THR:HG23	1.86	0.75
2:D:83:TYR:O	2:D:87:THR:HG23	1.87	0.74
2:F:132:GLU:HG2	2:F:134:GLY:H	1.54	0.73
2:D:27:GLN:HG3	2:D:32:THR:HG22	1.69	0.71

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	326/328 (99%)	303 (93%)	15 (5%)	8 (2%)	9	40
1	C	326/328 (99%)	303 (93%)	19 (6%)	4 (1%)	19	64
1	E	326/328 (99%)	306 (94%)	18 (6%)	2 (1%)	33	81
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	54
2	D	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	14	54
2	F	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	54
All	All	1497/1509 (99%)	1393 (93%)	81 (5%)	23 (2%)	15	58

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LEU
2	B	58	LYS
2	B	173	ILE
2	D	58	LYS

5.3.2 Protein sidechains ⓘ

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	289/289 (100%)	269 (93%)	20 (7%)	22	62
1	C	289/289 (100%)	269 (93%)	20 (7%)	22	62
1	E	289/289 (100%)	267 (92%)	22 (8%)	19	57
2	B	149/149 (100%)	145 (97%)	4 (3%)	57	91
2	D	149/149 (100%)	144 (97%)	5 (3%)	49	88
2	F	149/149 (100%)	144 (97%)	5 (3%)	49	88
All	All	1314/1314 (100%)	1238 (94%)	76 (6%)	28	71

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	199	SER
1	C	324	PRO
1	E	328	THR
1	C	259	LYS
1	C	277	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
1	C	327	GLN
1	E	38	ASN
1	C	81	ASN
1	E	81	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 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	339	1,4	12,14,15	0.53	0	15,19,21	1.10	1 (6%)
4	NAG	A	340	4	12,14,15	0.82	1 (8%)	15,19,21	1.23	1 (6%)
4	BMA	A	341	4	10,11,12	0.76	0	11,15,17	1.16	0
4	NAG	C	339	1,4	12,14,15	0.55	0	15,19,21	1.19	1 (6%)
4	NAG	C	340	4	12,14,15	0.45	0	15,19,21	1.30	1 (6%)
4	BMA	C	341	4	10,11,12	0.66	0	11,15,17	1.42	2 (18%)
4	NAG	E	339	1,4	12,14,15	0.70	0	15,19,21	1.06	1 (6%)
4	NAG	E	340	4	12,14,15	0.61	0	15,19,21	1.23	1 (6%)
4	BMA	E	341	4	10,11,12	0.73	0	11,15,17	1.40	2 (18%)

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	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	340	4	-	0/6/23/26	0/1/1/1
4	BMA	A	341	4	-	0/2/19/22	0/1/1/1
4	NAG	C	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	340	4	-	0/6/23/26	0/1/1/1
4	BMA	C	341	4	-	0/2/19/22	0/1/1/1
4	NAG	E	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	340	4	-	0/6/23/26	0/1/1/1
4	BMA	E	341	4	-	0/2/19/22	0/1/1/1

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All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	340	NAG	O5-C5	-2.10	1.41	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	339	NAG	C3-C2-N2	-4.12	105.49	111.76
4	A	339	NAG	C3-C2-N2	-3.67	106.17	111.76
4	C	340	NAG	C3-C2-N2	-3.64	106.21	111.76
4	E	339	NAG	C3-C2-N2	-3.49	106.44	111.76
4	E	340	NAG	C3-C2-N2	-3.36	106.65	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

12 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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
3	NAG	A	329	1	12,14,15	0.54	0	15,19,21	0.79	0
3	NAG	A	334	1	12,14,15	0.72	0	15,19,21	1.25	2 (13%)
3	NAG	A	348	1	12,14,15	0.55	0	15,19,21	1.32	3 (20%)
3	NAG	B	401	2	12,14,15	0.70	0	15,19,21	1.02	0
3	NAG	C	329	1	12,14,15	0.72	0	15,19,21	0.78	0
3	NAG	C	334	1	12,14,15	0.75	1 (8%)	15,19,21	1.27	2 (13%)
3	NAG	C	348	1	12,14,15	0.70	0	15,19,21	1.46	2 (13%)
3	NAG	D	401	2	12,14,15	0.75	0	15,19,21	0.95	0
3	NAG	E	329	1	12,14,15	0.68	0	15,19,21	0.76	0
3	NAG	E	334	1	12,14,15	0.60	0	15,19,21	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	E	348	1	12,14,15	0.76	0	15,19,21	1.38	2 (13%)
3	NAG	F	401	2	12,14,15	0.77	0	15,19,21	0.99	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	329	1	-	0/6/23/26	0/1/1/1
3	NAG	A	334	1	-	0/6/23/26	0/1/1/1
3	NAG	A	348	1	-	0/6/23/26	0/1/1/1
3	NAG	B	401	2	-	0/6/23/26	0/1/1/1
3	NAG	C	329	1	-	0/6/23/26	0/1/1/1
3	NAG	C	334	1	-	0/6/23/26	0/1/1/1
3	NAG	C	348	1	-	0/6/23/26	0/1/1/1
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1
3	NAG	E	329	1	-	0/6/23/26	0/1/1/1
3	NAG	E	334	1	-	0/6/23/26	0/1/1/1
3	NAG	E	348	1	-	0/6/23/26	0/1/1/1
3	NAG	F	401	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	334	NAG	C6-C5	2.02	1.59	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	334	NAG	O5-C5-C6	3.25	110.39	106.98
3	C	334	NAG	O5-C5-C6	3.01	110.14	106.98
3	C	348	NAG	C8-C7-N2	2.59	121.17	116.11
3	E	334	NAG	O5-C5-C6	2.56	109.67	106.98
3	C	334	NAG	O5-C5-C4	-2.52	107.45	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7　Other polymers (i)

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, 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	328/328 (100%)	-0.44	3 (0%)	81	24	5, 24, 51, 151	0
1	C	328/328 (100%)	-0.42	4 (1%)	75	20	5, 24, 51, 148	0
1	E	328/328 (100%)	-0.45	2 (0%)	86	32	5, 24, 51, 148	0
2	B	175/175 (100%)	-0.48	0	100	100	3, 18, 50, 105	0
2	D	175/175 (100%)	-0.50	0	100	100	2, 18, 47, 105	0
2	F	175/175 (100%)	-0.50	0	100	100	3, 18, 48, 105	0
All	All	1509/1509 (100%)	-0.46	9 (0%)	86	32	2, 23, 51, 151	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	6	ASN	3.3
1	E	1	GLN	2.9
1	A	3	LEU	2.6
1	A	1	GLN	2.3
1	C	328	THR	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 ⓘ

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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	NAG	E	340	14/15	0.23	1.36	0,0,60,64	0
4	NAG	C	340	14/15	0.22	1.01	0,0,60,64	0
4	NAG	A	340	14/15	0.22	0.81	0,0,60,63	0
4	NAG	C	339	14/15	0.18	0.45	0,0,49,51	0
4	NAG	E	339	14/15	0.16	0.18	0,0,47,51	0
4	NAG	A	339	14/15	0.15	0.14	0,0,48,52	0
4	BMA	C	341	11/12	0.38	-	0,0,71,72	0
4	BMA	E	341	11/12	0.37	-	0,0,73,75	0
4	BMA	A	341	11/12	0.33	-	0,0,69,70	0

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, 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	NAG	E	348	14/15	0.30	13.50	0,0,45,47	0
3	NAG	C	348	14/15	0.31	7.78	0,0,45,48	0
3	NAG	A	348	14/15	0.22	5.66	0,0,45,46	0
3	NAG	C	329	14/15	0.30	4.98	0,0,45,47	0
3	NAG	C	334	14/15	0.27	4.98	0,0,45,46	0
3	NAG	A	329	14/15	0.28	4.86	0,0,45,47	0
3	NAG	E	329	14/15	0.29	4.52	0,0,45,47	0
3	NAG	A	334	14/15	0.22	2.59	0,0,44,46	0
3	NAG	B	401	14/15	0.29	2.31	0,0,59,60	0
3	NAG	F	401	14/15	0.30	1.76	0,0,60,60	0
3	NAG	E	334	14/15	0.20	1.32	0,0,44,46	0
3	NAG	D	401	14/15	0.27	1.07	0,0,59,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.