



Full wwPDB X-ray Structure Validation Report

Jul 25, 2014 – 02:03 AM EDT

PDB ID : 4D00
Title : Haemagglutinin of H10N8 Influenza Virus Isolated from Humans in Complex with Human Receptor Analogue 6'SLN
Authors : Xiong, X.; Haire, L.F.; Vachieri, S.G.; Collins, P.J.; Walker, P.A.; Martin, S.R.; Zhang, Y.; McCauley, J.W.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-04-23
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

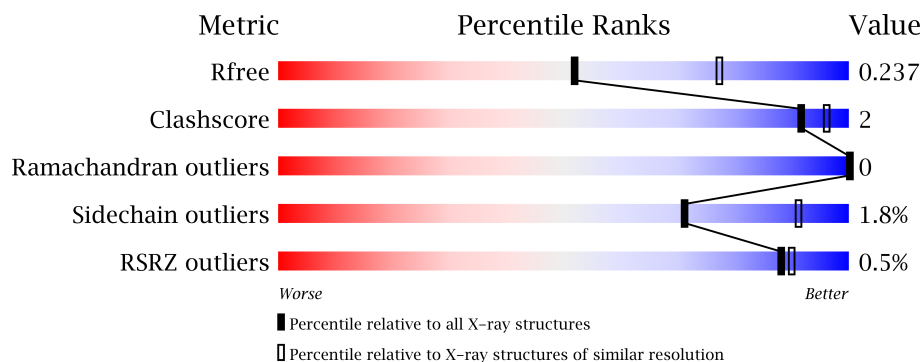
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. 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	326	
1	C	326	
1	E	326	
2	B	183	
2	D	183	
2	F	183	

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	1320	-	X
3	NAG	C	1319	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	C	1320	-	X
3	NAG	E	1319	-	X
3	NAG	E	1320	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12576 atoms, of which 0 are hydrogen 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.

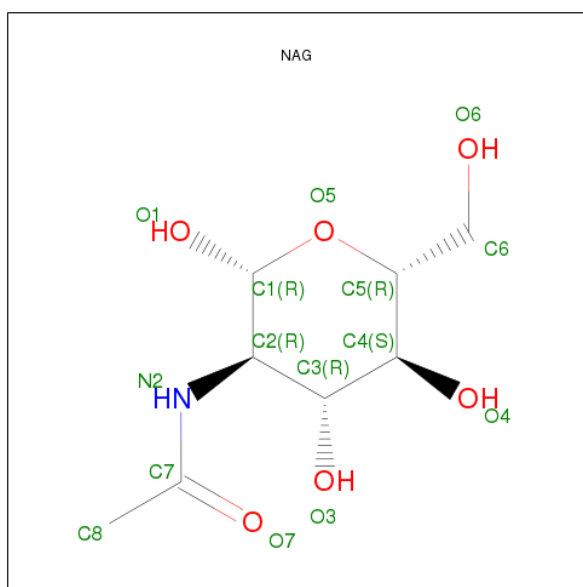
- Molecule 1 is a protein called HAEMAGGLUTININ HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2444	1511	450	466	17			
1	C	321	Total	C	N	O	S	0	0	0
			2457	1518	452	470	17			
1	E	319	Total	C	N	O	S	0	0	0
			2444	1511	450	466	17			

- Molecule 2 is a protein called HAEMAGGLUTININ HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1409	871	244	286	8			
2	D	176	Total	C	N	O	S	0	0	0
			1416	876	245	287	8			
2	F	173	Total	C	N	O	S	0	0	0
			1394	862	241	283	8			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		
4	A	1	Total	Ni	0	0
			1	1		
4	D	1	Total	Ni	0	0
			1	1		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			46	25	2	19		
5	C	3	Total	C	N	O	0	0
			46	25	2	19		
5	E	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			28	16	2	10		
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	180	Total	O	0	0
			180	180		
7	B	94	Total	O	0	0
			94	94		
7	C	151	Total	O	0	0
			151	151		
7	D	81	Total	O	0	0
			81	81		
7	E	131	Total	O	0	0
			131	131		
7	F	60	Total	O	0	0
			60	60		
7	E	4	Total	O	0	0
			4	4		
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		

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: HAEMAGGLUTININ HA1

Chain A: 



- Molecule 1: HAEMAGGLUTININ HA1

Chain C: 



- Molecule 1: HAEMAGGLUTININ HA1

Chain E: 



- Molecule 2: HAEMAGGLUTININ HA1

Chain B: 



- Molecule 2: HAEMAGGLUTININ HA1

Chain D: 



- Molecule 2: HAEMAGGLUTININ HA1

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 183.17Å 192.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.58 – 2.50 39.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (132.58-2.50) 92.7 (39.99-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.209 , 0.235 0.211 , 0.237	Depositor DCC
R_{free} test set	5013 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.1	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 103031 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, SIA, GAL, 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	0.33	0/2494	0.57	0/3379
1	C	0.33	0/2507	0.57	0/3398
1	E	0.33	0/2494	0.56	0/3379
2	B	0.36	0/1435	0.54	0/1938
2	D	0.35	0/1442	0.56	0/1948
2	F	0.36	0/1419	0.55	0/1915
All	All	0.34	0/11791	0.56	0/15957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2444	0	2395	13	0
1	C	2457	0	2404	11	0
1	E	2444	0	2395	9	0
2	B	1409	0	1308	5	0
2	D	1416	0	1317	7	0
2	F	1394	0	1295	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	26	1	0
3	C	28	0	26	0	0
3	E	28	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	46	0	40	0	0
5	C	46	0	40	0	0
5	E	46	0	40	1	0
6	B	28	0	25	0	0
6	D	28	0	25	0	0
6	F	28	0	25	0	0
7	A	181	0	0	5	0
7	B	94	0	0	0	0
7	C	152	0	0	2	1
7	D	81	0	0	0	0
7	E	135	0	0	2	0
7	F	60	0	0	0	0
All	All	12576	0	11387	43	1

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 2.

All (43) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:162:ARG:HD2	1:C:235:ASN:OD1	1.59	1.00
1:C:158:THR:N	7:C:2090:HOH:O	2.00	0.94
2:D:173:ILE:HG22	2:D:173:ILE:O	1.79	0.80
1:C:162:ARG:CD	1:C:235:ASN:OD1	2.34	0.74
1:C:104:GLU:HG3	1:C:256:ARG:HH21	1.60	0.67
1:C:205:ASN:HB3	7:C:2111:HOH:O	1.98	0.62
2:D:169:ASN:OD1	2:D:174:ASN:ND2	2.35	0.59
2:D:173:ILE:O	2:D:173:ILE:CG2	2.50	0.57
1:E:5:LEU:HD22	2:F:119:TYR:HA	1.88	0.55
1:A:162:ARG:NH1	3:A:1319:NAG:O5	2.40	0.55
1:E:128:ARG:NH1	1:E:136:ASN:OD1	2.40	0.55
1:A:226:HIS:HD2	7:A:2022:HOH:O	1.90	0.54
1:E:268:ASN:ND2	7:E:2026:HOH:O	2.42	0.52
1:A:109:ASN:CG	7:A:2088:HOH:O	2.48	0.51
1:C:256:ARG:NH2	2:D:64:GLU:OE2	2.43	0.50
1:A:57:ILE:CD1	1:A:95:VAL:HG23	2.43	0.49
1:E:57:ILE:CD1	1:E:95:VAL:HG23	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:ILE:CD1	1:C:95:VAL:HG23	2.43	0.48
1:A:268:ASN:ND2	7:A:2031:HOH:O	2.42	0.48
1:A:205:ASN:HB2	7:A:2123:HOH:O	2.14	0.48
1:A:67:ASP:OD1	1:A:132:ARG:NH1	2.46	0.48
1:C:-1:ASP:HB2	1:C:0:PRO:CD	2.44	0.48
2:B:75:HIS:CE1	1:C:101:LYS:HG2	2.49	0.48
2:D:30:GLN:HE22	2:D:146:ASP:H	1.62	0.47
2:F:30:GLN:HE22	2:F:146:ASP:H	1.63	0.47
2:F:9:PHE:CD1	2:F:10:LEU:HD13	2.51	0.46
2:B:30:GLN:HE22	2:B:146:ASP:H	1.62	0.46
1:A:177:HIS:O	1:A:213:ARG:NH2	2.49	0.46
1:A:5:LEU:HD22	2:B:119:TYR:HA	1.99	0.44
2:B:48:ILE:CD1	2:B:107:THR:HG23	2.48	0.44
2:B:173:ILE:HG12	2:D:164:GLU:HG3	2.00	0.44
2:F:9:PHE:CE1	2:F:10:LEU:HD13	2.52	0.44
1:E:136:ASN:ND2	5:E:1323:NAG:H82	2.34	0.43
2:F:48:ILE:CD1	2:F:107:THR:HG23	2.49	0.43
2:D:48:ILE:CD1	2:D:107:THR:HG23	2.48	0.43
1:E:93:VAL:HB	7:E:2055:HOH:O	2.18	0.42
1:A:178:PRO:O	1:A:213:ARG:NH2	2.53	0.42
1:A:198:GLY:HA3	1:E:213:ARG:HG2	2.02	0.41
1:A:109:ASN:CB	7:A:2088:HOH:O	2.69	0.41
1:E:57:ILE:CD1	1:E:95:VAL:CG2	2.98	0.41
1:A:57:ILE:CD1	1:A:95:VAL:CG2	2.99	0.41
1:C:-1:ASP:HB2	1:C:0:PRO:HD3	2.02	0.41
1:C:209:VAL:HG11	1:E:205:ASN:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:32:THR:N	7:C:2090:HOH:O[3.545]	1.94	0.26

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	317/326 (97%)	312 (98%)	5 (2%)	0	100	100
1	C	319/326 (98%)	314 (98%)	5 (2%)	0	100	100
1	E	317/326 (97%)	312 (98%)	5 (2%)	0	100	100
2	B	173/183 (94%)	169 (98%)	4 (2%)	0	100	100
2	D	174/183 (95%)	170 (98%)	4 (2%)	0	100	100
2	F	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
All	All	1471/1527 (96%)	1444 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	270/275 (98%)	266 (98%)	4 (2%)	76	93
1	C	271/275 (98%)	268 (99%)	3 (1%)	84	96
1	E	270/275 (98%)	263 (97%)	7 (3%)	59	84
2	B	149/156 (96%)	145 (97%)	4 (3%)	57	83
2	D	150/156 (96%)	149 (99%)	1 (1%)	91	98
2	F	147/156 (94%)	144 (98%)	3 (2%)	68	89
All	All	1257/1293 (97%)	1235 (98%)	22 (2%)	71	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	133	ASN
1	A	184	LYS
1	A	196	SER
2	B	58	LYS
2	B	60	ASN
2	B	113	SER

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Mol	Chain	Res	Type
2	B	161	GLN
1	C	8	HIS
1	C	53	ASN
1	C	196	SER
2	D	113	SER
1	E	2	LYS
1	E	8	HIS
1	E	12	ASN
1	E	128	ARG
1	E	196	SER
1	E	200	SER
1	E	305	ARG
2	F	10	LEU
2	F	60	ASN
2	F	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	177	HIS
1	A	226	HIS
1	A	268	ASN
2	B	30	GLN
1	C	7	HIS
1	C	53	ASN
1	C	226	HIS
2	D	26	HIS
2	D	30	GLN
2	D	60	ASN
2	D	174	ASN
1	E	7	HIS
1	E	8	HIS
1	E	156	GLN
1	E	226	HIS
1	E	268	ASN
2	F	30	GLN
2	F	95	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	319/326 (97%)	-0.41	1 (0%) 91 93	21, 29, 44, 57	0
1	C	321/326 (98%)	-0.39	1 (0%) 91 93	22, 32, 44, 56	0
1	E	319/326 (97%)	-0.49	2 (0%) 86 88	22, 30, 43, 54	0
2	B	175/183 (95%)	-0.33	1 (0%) 86 88	20, 28, 44, 71	0
2	D	176/183 (96%)	-0.40	1 (0%) 86 88	20, 27, 45, 79	0
2	F	173/183 (94%)	-0.40	1 (0%) 86 88	20, 27, 45, 82	0
All	All	1483/1527 (97%)	-0.41	7 (0%) 88 90	20, 29, 44, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	173	ILE	4.9
1	C	-2	ALA	3.5
2	D	176	VAL	3.0
2	B	60	ASN	2.3
1	E	11	ALA	2.2
1	E	12	ASN	2.2
1	A	12	ASN	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
6	NAG	F	1175	14/15	0.27	36.33	62,70,74,74	0
6	NAG	B	1177	14/15	0.30	34.71	61,69,74,75	0
5	GAL	C	1322	11/12	0.31	10.07	54,80,90,91	0
5	NAG	E	1323	15/15	0.35	5.38	65,74,76,78	0
5	NAG	C	1323	15/15	0.47	3.43	87,99,101,102	0
5	GAL	A	1323	11/12	0.31	1.64	50,72,81,84	0
5	GAL	E	1322	11/12	0.22	1.35	46,56,60,62	0
6	NAG	B	1176	14/15	0.14	1.06	32,37,44,51	0
5	SIA	A	1322	20/21	0.11	-0.06	34,36,40,41	0
6	NAG	F	1174	14/15	0.11	-0.07	30,36,42,51	0
5	SIA	C	1321	20/21	0.12	-0.14	35,39,45,46	0
6	NAG	D	1177	14/15	0.12	-0.24	32,36,45,52	0
5	SIA	E	1321	20/21	0.10	-0.65	35,38,40,41	0
5	NAG	A	1324	15/15	0.52	-	93,105,107,109	0
6	NAG	D	1178	14/15	0.30	-	63,71,77,81	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	A	1320	14/15	0.27	17.37	58,67,69,71	0
3	NAG	E	1320	14/15	0.22	9.93	44,51,54,54	0
3	NAG	C	1320	14/15	0.27	8.60	49,58,59,60	0
3	NAG	C	1319	14/15	0.24	2.38	52,56,65,70	0
3	NAG	E	1319	14/15	0.19	2.01	41,44,48,49	0
3	NAG	A	1319	14/15	0.23	1.48	39,43,48,51	0
4	NI	D	1179	1/1	0.04	-2.75	39,39,39,39	0
4	NI	B	1178	1/1	0.04	-3.37	38,38,38,38	0
4	NI	A	1321	1/1	0.03	-3.73	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.