



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:44 AM GMT

PDB ID : 4N60
Title : Crystal structure of hemagglutinin from an H7N9 influenza virus in complex with LSTc
Authors : Xu, R.; Wilson, I.A.
Deposited on : 2013-10-11
Resolution : 2.90 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>

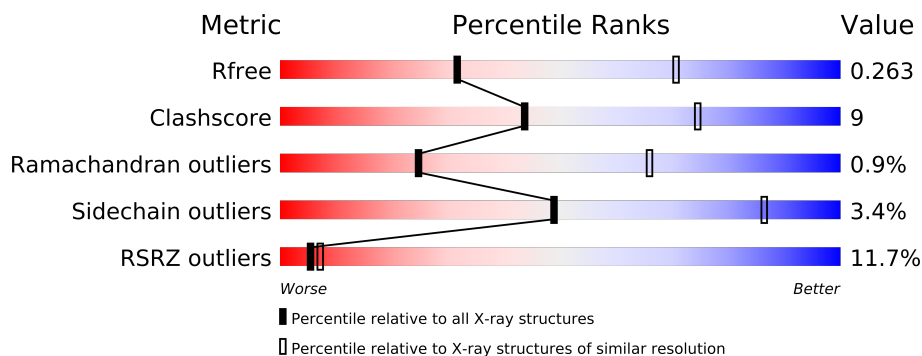
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 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





The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	321	
1	C	321	
2	B	179	
2	D	179	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7770 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2427	1509	438	465	15			
1	C	318	Total	C	N	O	S	0	0	0
			2427	1509	438	465	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1373	845	241	280	7			
2	D	169	Total	C	N	O	S	0	0	0
			1373	845	241	280	7			

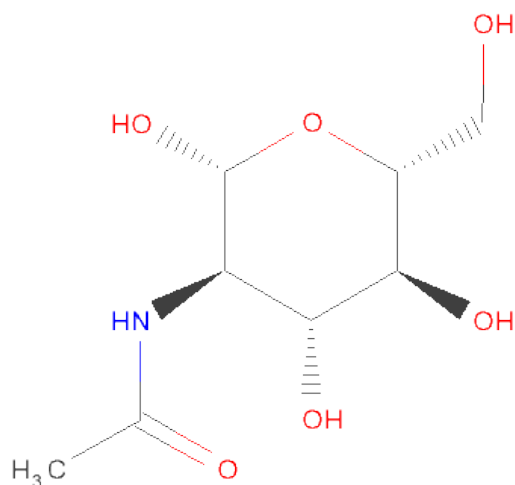
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	SER	-	EXPRESSION TAG	UNP R4NN21
B	174	GLY	-	EXPRESSION TAG	UNP R4NN21
B	175	ARG	-	EXPRESSION TAG	UNP R4NN21
B	176	LEU	-	EXPRESSION TAG	UNP R4NN21
B	177	VAL	-	EXPRESSION TAG	UNP R4NN21
B	178	PRO	-	EXPRESSION TAG	UNP R4NN21
B	179	ARG	-	EXPRESSION TAG	UNP R4NN21
D	173	SER	-	EXPRESSION TAG	UNP R4NN21
D	174	GLY	-	EXPRESSION TAG	UNP R4NN21
D	175	ARG	-	EXPRESSION TAG	UNP R4NN21
D	176	LEU	-	EXPRESSION TAG	UNP R4NN21
D	177	VAL	-	EXPRESSION TAG	UNP R4NN21
D	178	PRO	-	EXPRESSION TAG	UNP R4NN21
D	179	ARG	-	EXPRESSION TAG	UNP R4NN21

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			31	17	1	13		
5	C	2	Total	C	N	O	0	0
			31	17	1	13		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	18	Total	O	0	0
			18	18		

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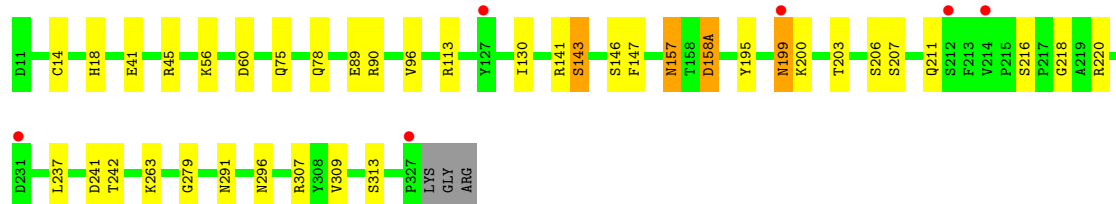
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total	O	0	0
			3	3		

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.

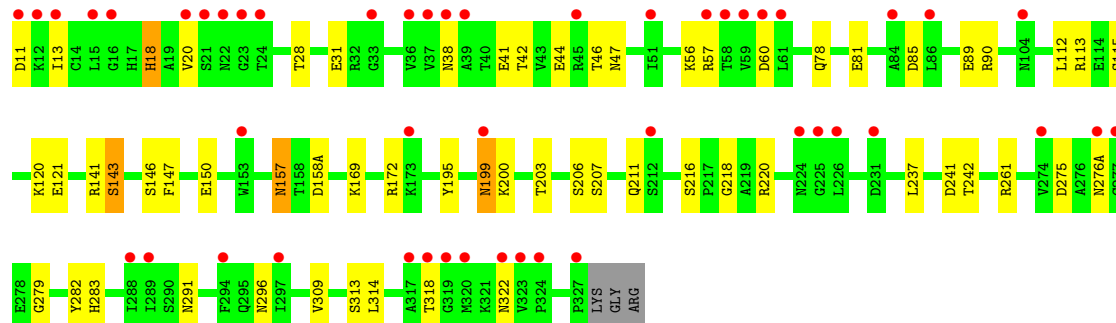
• Molecule 1: Hemagglutinin HA1

Chain A: 



• Molecule 1: Hemagglutinin HA1

Chain C: 



• Molecule 2: Hemagglutinin HA2

Chain B: 



• Molecule 2: Hemagglutinin HA2

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	154.77 Å 154.77 Å 154.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 2.90 46.67 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.67-2.90) 99.6 (46.67-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.91 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.223 , 0.262 0.225 , 0.263	Depositor DCC
R_{free} test set	1375 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.4	EDS
Estimated twinning fraction	0.030 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27536 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7770	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: SIA, GAL, 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	0.25	0/2474	0.44	0/3345
1	C	0.24	0/2474	0.41	0/3345
2	B	0.26	0/1396	0.41	0/1881
2	D	0.22	0/1396	0.39	0/1881
All	All	0.24	0/7740	0.41	0/10452

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	2427	0	0	18	0
1	C	2427	0	0	32	0
2	B	1373	0	0	8	0
2	D	1373	0	0	16	0
3	A	39	0	34	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	31	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	31	0	26	0	0
6	A	20	0	0	1	0
6	B	18	0	0	0	0
6	C	3	0	0	1	0
All	All	7770	0	112	68	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 9.

All (68) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:291:ASN:OD1	2:D:58:LYS:NZ	2.13	0.81
1:C:216:SER:O	1:C:220:ARG:NH2	2.17	0.77
1:A:216:SER:O	1:A:220:ARG:NH2	2.20	0.74
2:B:128:GLU:O	2:B:170:ARG:NH1	2.21	0.73
1:A:56:LYS:NZ	1:A:279:GLY:O	2.21	0.73
1:C:296:ASN:ND2	1:C:309:VAL:O	2.24	0.71
1:C:121:GLU:OE2	1:C:172:ARG:NH1	2.25	0.69
1:C:11:ASP:OD2	2:D:144:CYS:N	2.26	0.68
2:D:51:LYS:NZ	2:D:107:THR:OG1	2.30	0.64
3:A:401:NAG:H61	3:A:402:NAG:HN2	1.62	0.64
1:A:45:ARG:NH1	1:A:296:ASN:OD1	2.31	0.63
1:C:41:GLU:OE1	1:C:313:SER:OG	2.17	0.63
2:D:141:PHE:O	2:D:169:ASN:ND2	2.32	0.63
1:C:81:GLU:O	1:C:261:ARG:NH2	2.32	0.63
1:C:199:ASN:N	1:C:199:ASN:OD1	2.32	0.62
1:C:206:SER:OG	1:C:207:SER:N	2.32	0.62
2:D:67:ASP:OD2	2:D:85:ARG:NH2	2.35	0.59
1:C:18:HIS:N	2:D:21:TRP:O	2.36	0.59
2:D:24:PHE:N	2:D:35:ALA:O	2.36	0.59
1:C:275:ASP:OD1	1:C:276(A):ASN:N	2.35	0.58
1:A:206:SER:OG	1:A:207:SER:N	2.37	0.57
1:C:218:GLY:O	1:C:220:ARG:NH1	2.37	0.57
1:A:89:GLU:OE2	1:A:113:ARG:NE	2.39	0.55
2:D:145:ASP:OD1	2:D:148:CYS:N	2.40	0.54
1:C:20:VAL:O	1:C:322:ASN:ND2	2.40	0.54
1:C:89:GLU:OE2	1:C:113:ARG:NH2	2.40	0.54
1:C:146:SER:OG	1:C:147:PHE:N	2.40	0.53
1:C:60:ASP:OD1	1:C:90:ARG:NE	2.40	0.53
2:D:148:CYS:O	2:D:151:SER:OG	2.27	0.53
1:A:60:ASP:OD1	1:A:90:ARG:NE	2.43	0.52
1:A:141:ARG:O	1:A:143:SER:OG	2.28	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:241:ASP:OD1	1:C:242:THR:N	2.43	0.52
1:A:291:ASN:OD1	2:B:58:LYS:NZ	2.42	0.52
1:A:263:LYS:NZ	2:B:62:GLN:OE1	2.43	0.51
2:B:24:PHE:N	2:B:35:ALA:O	2.44	0.50
1:C:169:LYS:N	6:C:503:HOH:O	2.44	0.50
1:C:38:ASN:O	1:C:318:THR:N	2.45	0.50
1:C:42:THR:OG1	1:C:314:LEU:O	2.30	0.50
1:C:195:TYR:O	1:C:200:LYS:NZ	2.45	0.50
1:C:141:ARG:O	1:C:143:SER:OG	2.29	0.50
1:A:146:SER:OG	1:A:147:PHE:N	2.45	0.49
1:C:44:GLU:OE2	1:C:46:THR:N	2.45	0.49
2:B:148:CYS:O	2:B:151:SER:OG	2.31	0.48
1:C:56:LYS:NZ	1:C:279:GLY:O	2.47	0.48
1:C:13:ILE:O	2:D:138:PHE:N	2.47	0.48
1:A:307:ARG:NE	6:A:510:HOH:O	2.46	0.48
1:C:20:VAL:N	1:C:322:ASN:OD1	2.47	0.47
2:D:154:ASN:OD1	2:D:156:THR:OG1	2.33	0.47
1:A:41:GLU:OE1	1:A:313:SER:OG	2.33	0.46
1:A:218:GLY:O	1:A:220:ARG:NH1	2.49	0.46
2:D:103:GLU:O	2:D:107:THR:N	2.49	0.46
1:A:199:ASN:OD1	1:A:199:ASN:N	2.47	0.46
2:B:145:ASP:OD1	2:B:148:CYS:N	2.49	0.45
1:C:56:LYS:NZ	1:C:282:TYR:OH	2.50	0.45
1:C:57:ARG:O	1:C:85:ASP:N	2.51	0.44
1:A:241:ASP:OD1	1:A:242:THR:N	2.50	0.44
1:A:296:ASN:ND2	1:A:309:VAL:O	2.51	0.43
1:A:195:TYR:O	1:A:200:LYS:NZ	2.52	0.43
2:D:128:GLU:O	2:D:170:ARG:NH1	2.52	0.43
2:B:19:ASP:N	2:B:19:ASP:OD1	2.52	0.43
1:C:112:LEU:O	1:C:115:SER:OG	2.36	0.43
2:D:68:ASN:OD1	2:D:70:PHE:N	2.51	0.43
2:D:19:ASP:N	2:D:19:ASP:OD1	2.51	0.43
1:C:47:ASN:OD1	1:C:283:HIS:NE2	2.51	0.42
1:A:14:CYS:N	2:B:25:ARG:O	2.53	0.42
1:C:120:LYS:NZ	1:C:150:GLU:OE2	2.53	0.41
1:C:28:THR:OG1	1:C:31:GLU:N	2.54	0.41
2:D:22:TYR:OH	2:D:111:ALA:O	2.39	0.40

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	316/321 (98%)	294 (93%)	19 (6%)	3 (1%)	25	66
1	C	316/321 (98%)	294 (93%)	20 (6%)	2 (1%)	33	76
2	B	167/179 (93%)	156 (93%)	9 (5%)	2 (1%)	19	57
2	D	167/179 (93%)	155 (93%)	10 (6%)	2 (1%)	19	57
All	All	966/1000 (97%)	899 (93%)	58 (6%)	9 (1%)	25	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	ASN
2	D	12	ASN
1	A	157	ASN
1	C	157	ASN
1	A	143	SER
1	C	143	SER
1	A	158(A)	ASP
2	B	10	ILE
2	D	10	ILE

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	267/269 (99%)	256 (96%)	11 (4%)	41	80
1	C	267/269 (99%)	259 (97%)	8 (3%)	53	89
2	B	145/153 (95%)	141 (97%)	4 (3%)	56	90
2	D	145/153 (95%)	140 (97%)	5 (3%)	49	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	824/844 (98%)	796 (97%)	28 (3%)	49 86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	75	GLN
1	A	78	GLN
1	A	96	VAL
1	A	130	ILE
1	A	157	ASN
1	A	158(A)	ASP
1	A	199	ASN
1	A	203	THR
1	A	211	GLN
1	A	237	LEU
2	B	11	GLU
2	B	52	LEU
2	B	56	ILE
2	B	65	LEU
1	C	18	HIS
1	C	78	GLN
1	C	157	ASN
1	C	158(A)	ASP
1	C	199	ASN
1	C	203	THR
1	C	211	GLN
1	C	237	LEU
2	D	11	GLU
2	D	52	LEU
2	D	56	ILE
2	D	65	LEU
2	D	124	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	$\# Z > 2$
3	NAG	A	401	1,3	12,14,15	0.28	0	15,19,21	0.59	0
3	NAG	A	402	3	12,14,15	0.24	0	15,19,21	0.30	0
3	BMA	A	403	3	10,11,12	0.55	0	11,15,17	0.95	0
5	SIA	A	405	5	20,20,21	3.89	1 (5%)	23,28,31	2.47	3 (13%)
5	GAL	A	406	5	10,11,12	0.38	0	11,15,17	0.88	0
5	SIA	C	401	5	20,20,21	3.88	1 (5%)	23,28,31	2.46	3 (13%)
5	GAL	C	402	5	10,11,12	0.43	0	11,15,17	0.95	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	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
5	SIA	A	405	5	-	0/15/34/38	1/1/1/1
5	GAL	A	406	5	-	0/2/19/22	0/1/1/1
5	SIA	C	401	5	-	0/15/34/38	1/1/1/1
5	GAL	C	402	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	SIA	O6-C2	17.15	1.44	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	401	SIA	O6-C2	17.09	1.43	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	SIA	O6-C2-C3	-10.70	110.93	124.91
5	A	405	SIA	O6-C2-C3	-10.70	110.94	124.91
5	A	405	SIA	O6-C6-C7	3.74	112.66	105.73
5	C	401	SIA	O6-C6-C7	3.43	112.10	105.73
5	C	401	SIA	C3-C2-C1	-2.58	106.63	121.08
5	A	405	SIA	C3-C2-C1	-2.52	107.01	121.08

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	SIA	C2-C3-C4-C5-C6-O6
5	C	401	SIA	C2-C3-C4-C5-C6-O6

5.6 Ligand geometry

2 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	$\# Z > 2$
4	NAG	A	404	1	12,14,15	0.25	0	15,19,21	0.35	0
4	NAG	B	201	2	12,14,15	0.29	0	15,19,21	0.42	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
4	NAG	A	404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	318/321 (99%)	-0.07	6 (1%) 64 72	45, 75, 119, 178	0
1	C	318/321 (99%)	0.83	48 (15%) 3 4	87, 135, 232, 299	0
2	B	169/179 (94%)	-0.09	1 (0%) 86 91	41, 71, 117, 160	0
2	D	169/179 (94%)	1.82	60 (35%) 1 1	99, 213, 283, 337	0
All	All	974/1000 (97%)	0.55	115 (11%) 5 7	41, 106, 250, 337	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	21.1
2	D	7	ALA	11.0
2	D	23	GLY	10.3
2	D	130	ALA	9.5
1	C	13	ILE	9.3
2	D	138	PHE	8.8
2	D	36	ALA	8.8
2	D	126	LEU	8.4
2	D	6	ILE	8.0
2	D	122	VAL	7.7
1	C	289	ILE	7.7
2	D	140	ILE	7.3
2	D	35	ALA	7.1
2	D	131	GLU	6.8
2	D	24	PHE	6.6
2	D	171	ILE	6.6
2	D	172	GLN	6.4
1	A	327	PRO	6.2
2	D	170	ARG	5.9
1	C	12	LYS	5.9
1	C	58	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	11	ASP	5.5
1	C	37	VAL	5.3
1	C	15	LEU	5.3
2	D	33	GLY	5.2
2	D	129	ASN	5.0
1	C	323	VAL	5.0
2	D	141	PHE	4.6
1	C	318	THR	4.3
2	D	143	LYS	4.2
2	D	51	LYS	4.1
1	C	33	GLY	4.1
2	D	119	TYR	4.0
1	C	297	ILE	4.0
2	D	48	ILE	3.9
2	D	157	TYR	3.9
2	D	25	ARG	3.9
1	C	16	GLY	3.8
2	D	5	ALA	3.7
1	C	224	ASN	3.7
2	D	32	GLU	3.6
1	A	199	ASN	3.5
2	D	166	ALA	3.4
1	C	226	LEU	3.4
1	C	288	ILE	3.4
1	C	45	ARG	3.4
1	C	86	LEU	3.3
2	D	99	LEU	3.3
2	D	26	HIS	3.3
2	D	153	ARG	3.2
2	D	55	LEU	3.2
1	C	22	ASN	3.1
2	D	19	ASP	3.1
1	C	322	ASN	3.1
2	D	118	LEU	3.1
1	C	320	MET	3.1
1	C	59	VAL	3.0
1	C	39	ALA	3.0
2	D	18	ILE	3.0
1	C	104	ASN	2.9
1	C	277	CYS	2.9
1	C	38	ASN	2.9
2	D	152	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	100	VAL	2.8
2	D	16	GLY	2.8
2	D	44	ALA	2.8
2	D	8	GLY	2.8
2	D	132	GLU	2.8
1	C	324	PRO	2.7
2	D	168	GLN	2.7
1	C	20	VAL	2.7
1	C	231	ASP	2.7
1	A	212	SER	2.7
2	D	121	ARG	2.6
2	D	59	THR	2.6
2	D	102	MET	2.6
2	D	125	GLN	2.5
1	C	84	ALA	2.5
2	D	21	TRP	2.5
2	D	52	LEU	2.5
1	A	127	TYR	2.5
2	D	22	TYR	2.5
1	C	51	ILE	2.5
1	C	57	ARG	2.5
1	C	317	ALA	2.5
2	D	167	MET	2.5
1	C	274	VAL	2.4
2	D	103	GLU	2.4
1	A	231	ASP	2.4
1	C	276(A)	ASN	2.3
1	C	21	SER	2.3
1	C	173	LYS	2.3
2	D	69	GLU	2.3
2	D	74	GLU	2.3
1	C	294	PHE	2.3
1	C	327	PRO	2.3
1	C	199	ASN	2.2
2	D	27	GLN	2.2
2	D	142	HIS	2.2
1	A	214	VAL	2.2
1	C	24	THR	2.2
2	D	150	ALA	2.2
2	D	34	THR	2.2
1	C	36	VAL	2.1
2	B	55	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	23	GLY	2.1
1	C	212	SER	2.1
1	C	153	TRP	2.1
1	C	60	ASP	2.1
2	D	60	ASN	2.1
1	C	61	LEU	2.1
2	D	45	ILE	2.1
2	D	139	GLU	2.0
2	D	37	ASP	2.0
1	C	225	GLY	2.0

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
5	SIA	A	405	20/21	0.25	-	89,105,117,117	0
5	GAL	C	402	11/12	0.39	-	199,205,206,206	0
3	NAG	A	402	14/15	0.27	-	144,151,160,167	0
5	GAL	A	406	11/12	0.22	-	156,167,171,171	0
5	SIA	C	401	20/21	0.37	-	131,141,161,161	0
3	NAG	A	401	14/15	0.19	-	97,111,119,132	0
3	BMA	A	403	11/12	0.21	-	171,173,174,175	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(\AA^2)	Q<0.9
4	NAG	A	404	14/15	0.18	-	146,158,174,177	0
4	NAG	B	201	14/15	0.25	-	103,114,119,119	0

6.5 Other polymers ⓘ

There are no such residues in this entry.