Full wwPDB X-ray Structure Validation Report

Oct 13, 2020 – 10:14 AM BST

PDB ID	:	6TWH
Title	:	Crystal structure of the haemagglutinin mutant (Gln226Leu, Gly228Ser) from an H10N7 seal influenza virus isolated in Germany
Authors	:	Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on	:	2020-01-13
Resolution	:	2.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

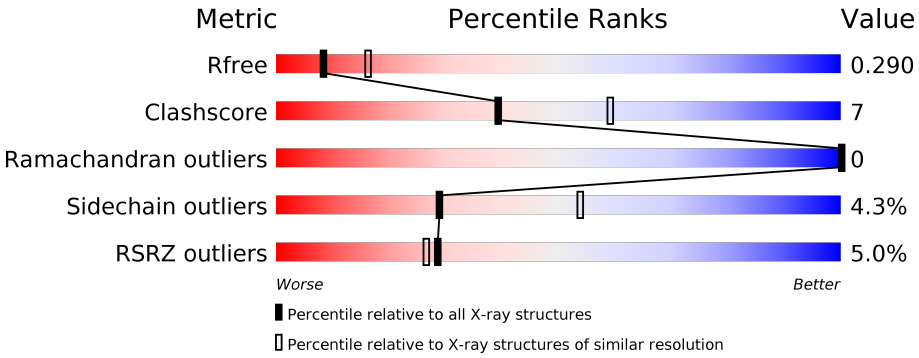
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.68 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 respectively. 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	325	7% 75% 21%
1	C	325	5% 76% 19%
1	E	325	2% 81% 17%
1	L	325	4% 81% 15%
1	N	325	7% 81% 16%
1	P	325	2% 83% 16%

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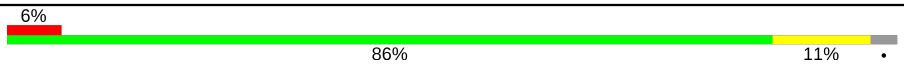
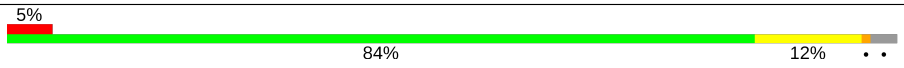
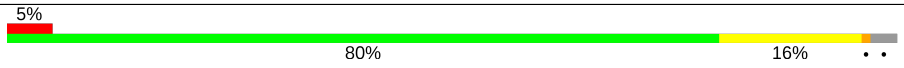
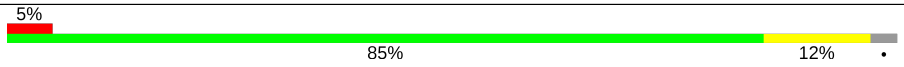
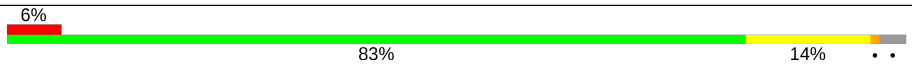
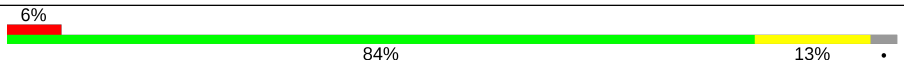
Mol	Chain	Length	Quality of chain
2	B	177	
2	D	177	
2	F	177	
2	M	177	
2	O	177	
2	Q	177	
3	G	2	
3	H	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23138 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2414	1496	436	466	16			
1	C	315	Total	C	N	O	S	0	0	0
			2402	1488	434	464	16			
1	E	322	Total	C	N	O	S	0	0	0
			2462	1529	445	472	16			
1	L	316	Total	C	N	O	S	0	0	0
			2412	1497	434	465	16			
1	N	320	Total	C	N	O	S	0	0	0
			2424	1502	438	468	16			
1	P	322	Total	C	N	O	S	0	0	0
			2462	1529	445	472	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
A	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
C	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
E	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
L	-1	ASP	-	expression tag	UNP A0A0A7HR51
L	0	PRO	-	expression tag	UNP A0A0A7HR51
L	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
N	-1	ASP	-	expression tag	UNP A0A0A7HR51
N	0	PRO	-	expression tag	UNP A0A0A7HR51
N	221	SER	GLY	engineered mutation	UNP A0A0A7HR51
P	-1	ASP	-	expression tag	UNP A0A0A7HR51
P	0	PRO	-	expression tag	UNP A0A0A7HR51

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Chain	Residue	Modelled	Actual	Comment	Reference
P	221	SER	GLY	engineered mutation	UNP A0A0A7HR51

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	D	172	Total	C	N	O	S	0	0	0
			1380	854	238	280	8			
2	F	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	M	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	O	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			
2	Q	172	Total	C	N	O	S	0	0	0
			1386	857	241	280	8			

There are 6 discrepancies between the modelled and reference sequences:

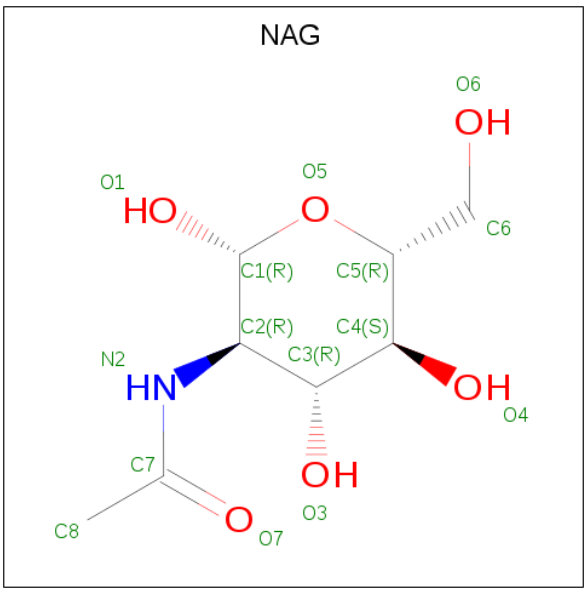
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LYS	-	expression tag	UNP A0A0A7HR51
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
M	177	LYS	-	expression tag	UNP A0A0A7HR51
O	177	LYS	-	expression tag	UNP A0A0A7HR51
Q	177	LYS	-	expression tag	UNP A0A0A7HR51

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	M	1	Total C N O 14 8 1 5	0	0
4	N	1	Total C N O 14 8 1 5	0	0
4	O	1	Total C N O 14 8 1 5	0	0
4	P	1	Total C N O 14 8 1 5	0	0
4	Q	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total Ca 1 1	0	0
5	N	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0

- Molecule 6 is water.

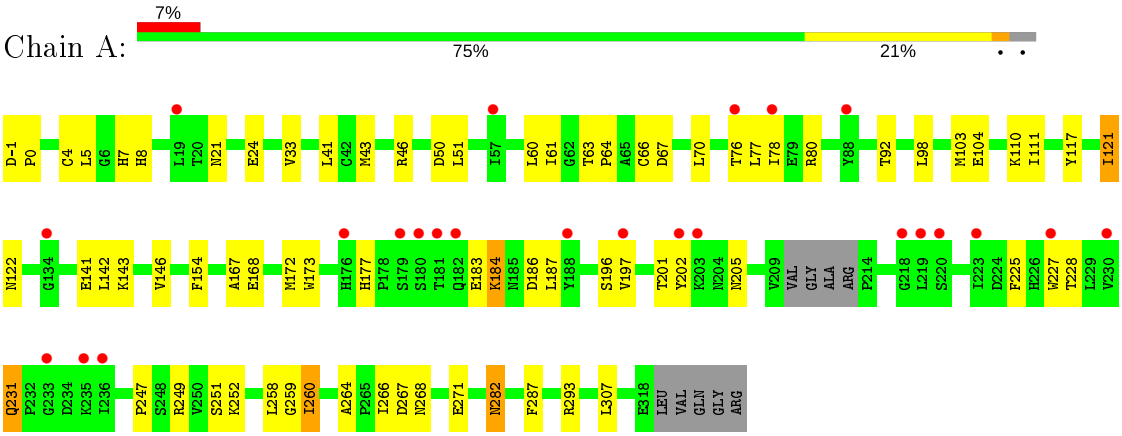
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	6	Total O 6 6	0	0
6	C	2	Total O 2 2	0	0
6	D	7	Total O 7 7	0	0
6	E	8	Total O 8 8	0	0
6	F	7	Total O 7 7	0	0
6	L	9	Total O 9 9	0	0
6	M	3	Total O 3 3	0	0
6	N	2	Total O 2 2	0	0
6	O	7	Total O 7 7	0	0
6	P	17	Total O 17 17	0	0
6	Q	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

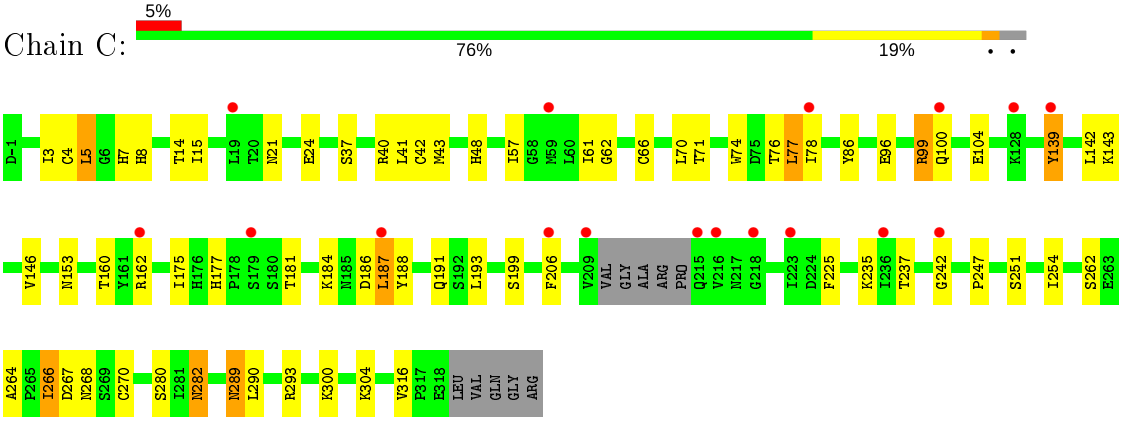
- Molecule 1: Hemagglutinin

Chain A:



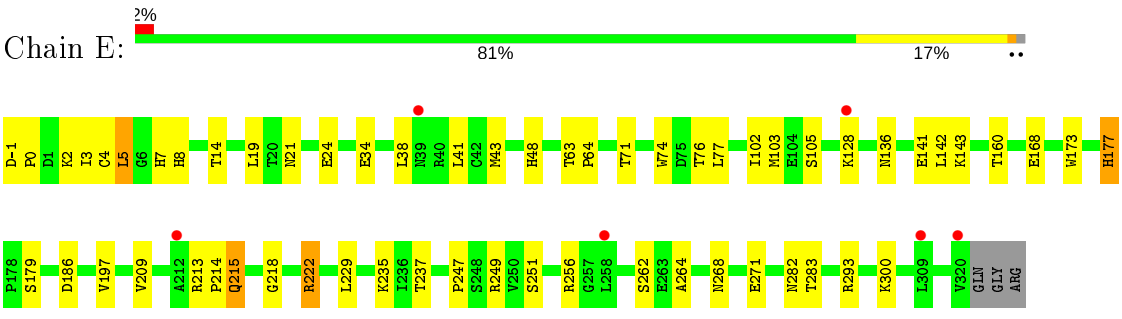
- Molecule 1: Hemagglutinin

Chain C:



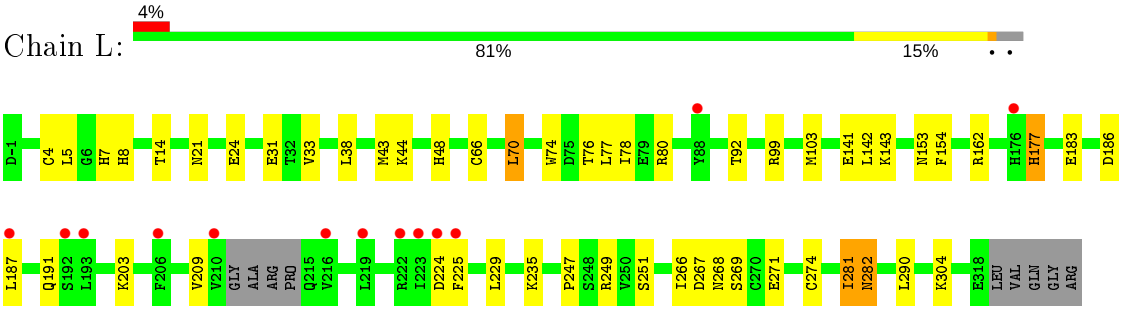
- Molecule 1: Hemagglutinin

Chain E:



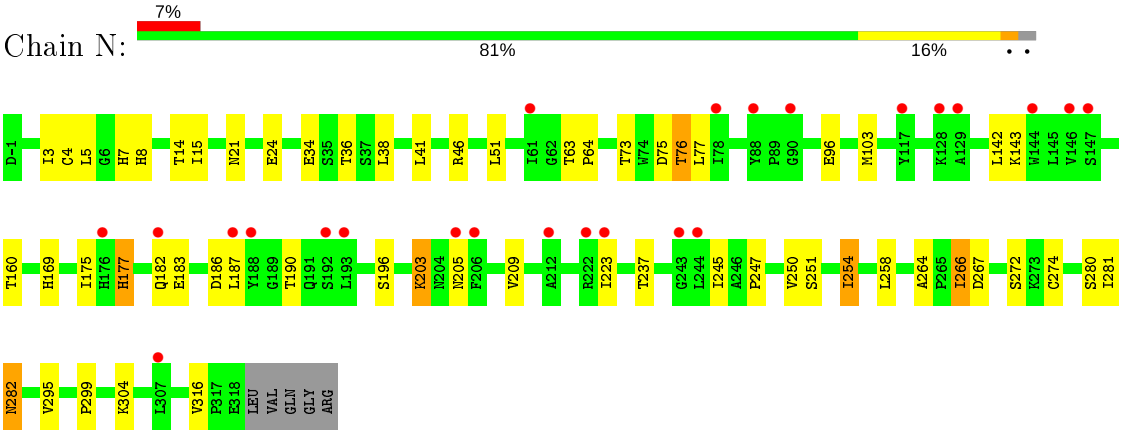
• Molecule 1: Hemagglutinin

Chain L:



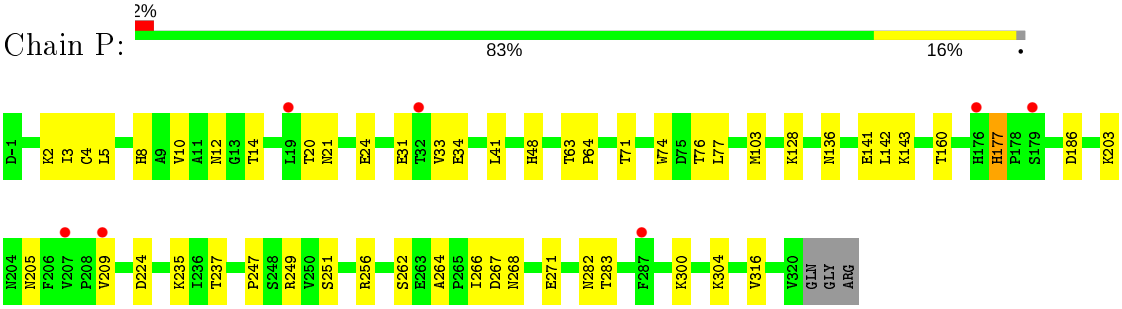
• Molecule 1: Hemagglutinin

Chain N:



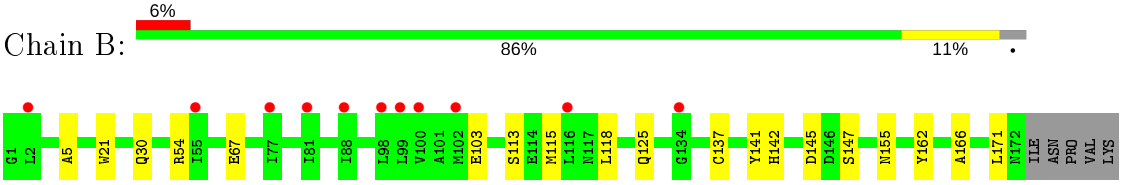
• Molecule 1: Hemagglutinin

Chain P:



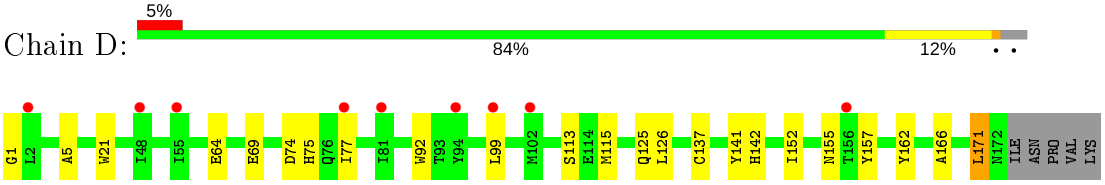
• Molecule 2: Hemagglutinin HA2

Chain B:



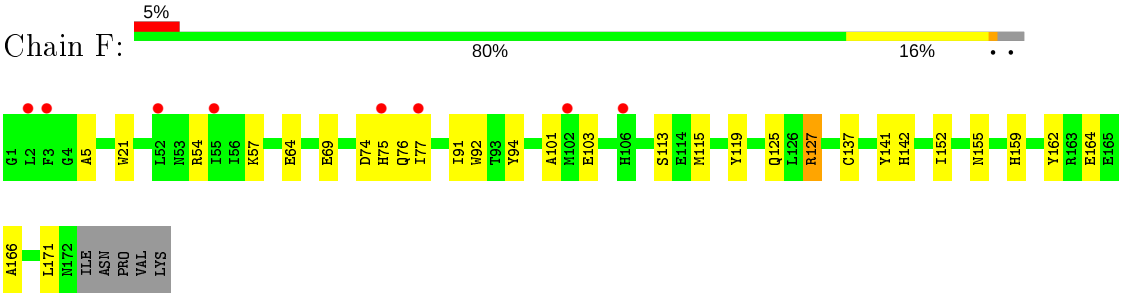
• Molecule 2: Hemagglutinin HA2

Chain D:



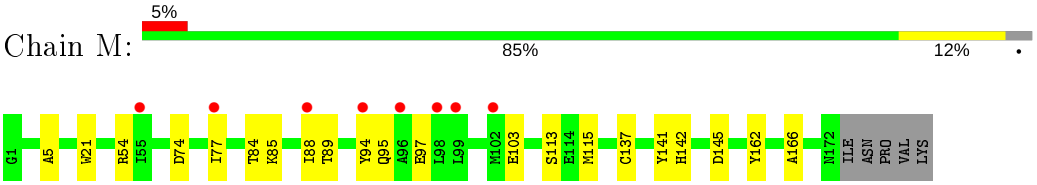
• Molecule 2: Hemagglutinin HA2

Chain F:



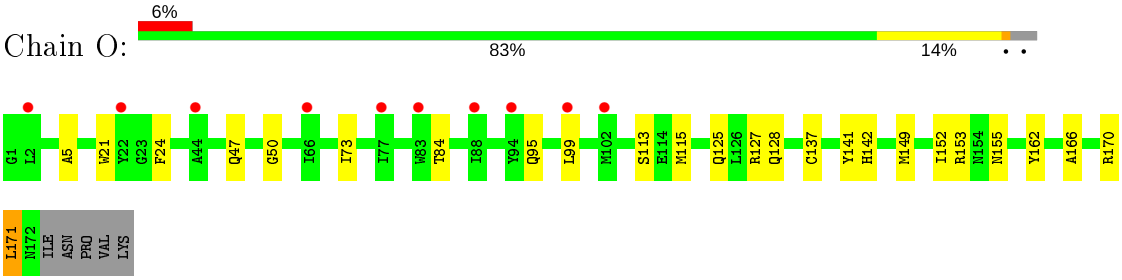
• Molecule 2: Hemagglutinin HA2

Chain M:



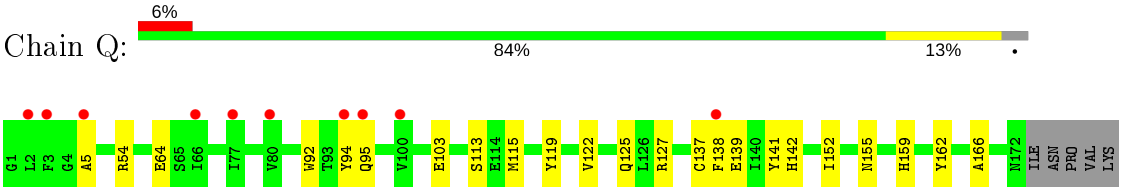
• Molecule 2: Hemagglutinin HA2

Chain O:



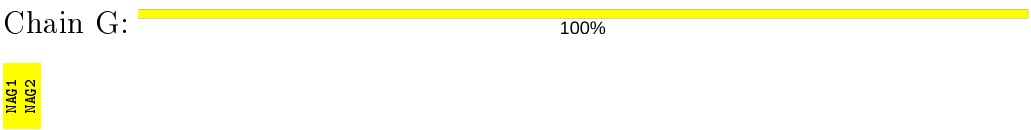
• Molecule 2: Hemagglutinin HA2

Chain Q:



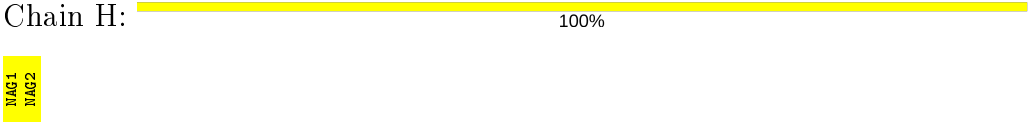
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.31Å 213.61Å 156.80Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	72.11 – 2.68 72.11 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.11-2.68) 99.9 (72.11-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.269 , 0.302 0.260 , 0.290	Depositor DCC
R_{free} test set	6188 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23138	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3055e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, 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	0.70	0/2462	0.85	0/3334
1	C	0.69	0/2449	0.79	0/3317
1	E	0.66	0/2512	0.79	0/3404
1	L	0.66	0/2460	0.79	0/3333
1	N	0.68	0/2473	0.79	0/3353
1	P	0.66	0/2512	0.79	0/3404
2	B	0.64	0/1411	0.74	0/1903
2	D	0.65	0/1405	0.74	0/1896
2	F	0.66	0/1411	0.75	0/1903
2	M	0.65	0/1411	0.75	0/1903
2	O	0.65	0/1411	0.76	0/1903
2	Q	0.66	0/1411	0.77	0/1903
All	All	0.67	0/23328	0.78	0/31556

There are no bond length outliers.

There are no bond angle outliers.

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	2414	0	2373	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2402	0	2355	58	0
1	E	2462	0	2430	33	0
1	L	2412	0	2364	38	0
1	N	2424	0	2370	49	0
1	P	2462	0	2429	35	0
2	B	1386	0	1291	12	0
2	D	1380	0	1280	26	0
2	F	1386	0	1290	23	0
2	M	1386	0	1291	15	0
2	O	1386	0	1291	29	0
2	Q	1386	0	1291	20	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	C	14	0	13	0	0
4	F	28	0	26	0	0
4	M	14	0	13	0	0
4	N	14	0	13	0	0
4	O	14	0	13	0	0
4	P	14	0	13	0	0
4	Q	14	0	13	0	0
5	E	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
6	A	8	0	0	0	0
6	B	6	0	0	0	0
6	C	2	0	0	0	0
6	D	7	0	0	2	0
6	E	8	0	0	0	0
6	F	7	0	0	0	0
6	L	9	0	0	0	0
6	M	3	0	0	0	0
6	N	2	0	0	0	0
6	O	7	0	0	0	0
6	P	17	0	0	1	0
6	Q	5	0	0	0	0
All	All	23138	0	22209	337	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 7.

All (337) 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:146:VAL:HG12	1:C:187:LEU:HD11	1.36	1.07
1:A:121:ILE:HD11	1:A:154:PHE:CZ	1.91	1.05
2:O:149:MET:O	2:O:152:ILE:HG13	1.62	0.99
1:C:146:VAL:CG1	1:C:187:LEU:HD11	1.96	0.96
1:C:289:ASN:HD22	1:C:289:ASN:C	1.68	0.94
1:C:61:ILE:HD13	1:C:139:TYR:CD1	2.02	0.94
1:N:205:ASN:HD22	1:P:209:VAL:HG13	1.31	0.91
1:A:92:THR:HG22	1:A:225:PHE:HB2	1.51	0.91
1:C:187:LEU:HD12	1:C:188:TYR:CZ	2.06	0.91
1:L:92:THR:HG22	1:L:225:PHE:HB2	1.52	0.90
2:O:152:ILE:HD12	2:O:153:ARG:N	1.86	0.90
1:N:274:CYS:SG	1:N:281:ILE:HD11	2.14	0.88
1:N:34:GLU:OE2	1:N:36:THR:HG22	1.75	0.86
1:C:146:VAL:HG12	1:C:187:LEU:CD1	2.05	0.86
2:M:84:THR:HG21	2:O:84:THR:HG22	1.58	0.83
1:C:187:LEU:HD12	1:C:188:TYR:CE2	2.15	0.81
1:A:43:MET:HE1	1:A:46:ARG:HD3	1.66	0.78
1:L:274:CYS:SG	1:L:281:ILE:HD11	2.23	0.78
1:N:205:ASN:ND2	1:P:209:VAL:HG13	1.99	0.78
1:A:33:VAL:HG23	1:A:307:LEU:CD2	2.14	0.77
2:D:126:LEU:HD21	2:D:152:ILE:HD12	1.66	0.77
1:A:117:TYR:HB3	1:A:121:ILE:HG21	1.68	0.76
1:P:128:LYS:HG3	1:P:136:ASN:HD21	1.51	0.76
1:C:175:ILE:CD1	1:C:206:PHE:CG	2.71	0.74
2:D:126:LEU:HD21	2:D:152:ILE:CD1	2.18	0.73
2:Q:127:ARG:HD2	2:Q:159:HIS:CD2	2.23	0.73
1:C:61:ILE:HD13	1:C:139:TYR:HD1	1.53	0.73
1:N:258:LEU:HD11	1:N:295:VAL:HG22	1.73	0.71
2:F:127:ARG:HD2	2:F:159:HIS:CD2	2.26	0.70
1:A:117:TYR:CB	1:A:121:ILE:HG21	2.22	0.69
1:C:48:HIS:NE2	1:C:266:ILE:HD12	2.06	0.69
2:D:99:LEU:HD22	2:F:94:TYR:OH	1.93	0.68
1:C:153:ASN:HD21	1:C:191:GLN:HG2	1.59	0.67
1:A:43:MET:HA	1:A:46:ARG:HD2	1.77	0.67
2:O:128:GLN:HE21	2:O:128:GLN:HA	1.59	0.67
2:M:95:GLN:OE1	2:O:95:GLN:NE2	2.27	0.67
2:M:54:ARG:NH2	2:M:103:GLU:OE1	2.24	0.67
1:C:175:ILE:HD13	1:C:206:PHE:CB	2.25	0.66
1:N:274:CYS:HB3	1:N:281:ILE:HG13	1.77	0.66
1:C:96:GLU:OE2	1:C:99:ARG:NH1	2.30	0.65
1:C:289:ASN:ND2	1:C:289:ASN:C	2.43	0.64
1:A:98:LEU:HD21	1:A:172:MET:HE1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:NH1	2:D:69:GLU:OE1	2.31	0.64
1:N:3:ILE:CD1	2:O:152:ILE:CD1	2.77	0.63
1:A:196:SER:OG	1:A:205:ASN:HB3	1.99	0.63
1:A:66:CYS:O	1:A:70:LEU:HD23	1.98	0.63
2:Q:119:TYR:O	2:Q:122:VAL:HG22	1.99	0.63
1:C:42:CYS:SG	1:C:270:CYS:HB2	2.38	0.62
2:F:54:ARG:NH2	2:F:103:GLU:OE1	2.28	0.62
1:A:50:ASP:HB2	1:A:266:ILE:HD11	1.82	0.62
1:E:256:ARG:NH2	2:F:64:GLU:OE2	2.33	0.62
2:Q:122:VAL:HG23	2:Q:138:PHE:CE2	2.35	0.62
2:O:128:GLN:NE2	2:O:128:GLN:HA	2.15	0.61
1:A:78:ILE:HG22	1:A:80:ARG:NH1	2.15	0.61
1:A:260:ILE:N	1:A:260:ILE:HD12	2.15	0.61
1:P:271:GLU:O	1:P:282:ASN:ND2	2.34	0.61
1:A:258:LEU:HG	1:A:260:ILE:HD11	1.82	0.60
1:L:78:ILE:HG22	1:L:80:ARG:NH1	2.16	0.60
2:M:94:TYR:HE2	2:Q:95:GLN:OE1	1.83	0.60
2:B:54:ARG:NH2	2:B:103:GLU:OE1	2.24	0.60
1:A:60:LEU:HD12	1:A:172:MET:HE1	1.82	0.60
1:C:289:ASN:ND2	1:C:289:ASN:O	2.35	0.59
1:E:213:ARG:HD2	1:E:222:ARG:HD3	1.84	0.59
1:N:169:HIS:HB3	1:N:250:VAL:HG11	1.83	0.59
2:M:94:TYR:CE2	2:Q:95:GLN:OE1	2.56	0.59
1:A:271:GLU:O	1:A:282:ASN:ND2	2.36	0.59
1:C:146:VAL:CG1	1:C:187:LEU:CD1	2.72	0.59
2:Q:54:ARG:NH2	2:Q:103:GLU:OE1	2.30	0.58
1:C:175:ILE:HD13	1:C:206:PHE:HB3	1.85	0.58
1:A:168:GLU:HG2	1:A:231:GLN:NE2	2.19	0.57
1:N:175:ILE:CD1	1:N:177:HIS:CE1	2.88	0.57
1:P:48:HIS:CE1	1:P:268:ASN:HD21	2.23	0.57
1:L:66:CYS:O	1:L:70:LEU:HD23	2.05	0.57
1:N:175:ILE:HD12	1:N:177:HIS:NE2	2.19	0.56
1:A:43:MET:HE1	1:A:46:ARG:CD	2.34	0.56
1:C:153:ASN:ND2	1:C:191:GLN:HG2	2.19	0.56
1:C:175:ILE:HD11	1:C:206:PHE:CG	2.39	0.56
1:N:96:GLU:HG2	2:O:73:ILE:HG22	1.87	0.56
1:A:43:MET:CE	1:A:46:ARG:HD3	2.35	0.56
1:E:48:HIS:CE1	1:E:268:ASN:HD21	2.24	0.56
1:L:141:GLU:OE1	1:L:249:ARG:HD3	2.06	0.56
1:A:78:ILE:CG2	1:A:80:ARG:HH12	2.19	0.56
1:C:57:ILE:CD1	1:C:86:TYR:OH	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:10:VAL:HA	6:P:506:HOH:O	2.04	0.56
1:P:141:GLU:OE1	1:P:249:ARG:HD3	2.06	0.55
1:A:141:GLU:OE1	1:A:249:ARG:HD3	2.06	0.55
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.07	0.55
1:L:281:ILE:HG21	1:L:290:LEU:CD1	2.36	0.55
1:A:33:VAL:HG23	1:A:307:LEU:HD23	1.87	0.55
1:A:5:LEU:HD23	2:B:118:LEU:HD23	1.89	0.55
1:L:78:ILE:CG2	1:L:80:ARG:HH12	2.20	0.55
1:C:187:LEU:CD1	1:C:188:TYR:CE2	2.88	0.54
1:C:139:TYR:H	1:C:139:TYR:HD2	1.56	0.54
1:A:110:LYS:O	1:A:111:ILE:HD13	2.06	0.54
1:A:201:THR:O	1:A:202:TYR:CD1	2.61	0.54
1:A:227:TRP:O	1:A:228:THR:HG23	2.07	0.54
2:O:128:GLN:NE2	2:O:170:ARG:HH12	2.06	0.54
2:D:126:LEU:CD2	2:D:152:ILE:CD1	2.86	0.54
1:E:293:ARG:NH2	2:F:69:GLU:OE1	2.41	0.54
1:A:167:ALA:HB3	1:A:252:LYS:HE2	1.90	0.53
1:C:175:ILE:HD11	1:C:206:PHE:CD2	2.43	0.53
1:C:61:ILE:HD12	1:C:62:GLY:N	2.23	0.53
1:N:274:CYS:SG	1:N:281:ILE:CD1	2.94	0.53
1:A:43:MET:CE	1:A:46:ARG:CD	2.86	0.53
1:A:146:VAL:HG21	1:A:187:LEU:HD22	1.90	0.53
1:P:128:LYS:HG3	1:P:136:ASN:ND2	2.20	0.53
1:N:282:ASN:OD1	1:N:282:ASN:N	2.42	0.53
2:B:30:GLN:NE2	2:B:145:ASP:HB2	2.24	0.53
1:L:282:ASN:N	1:L:282:ASN:OD1	2.42	0.53
1:A:98:LEU:HD21	1:A:172:MET:CE	2.39	0.53
1:A:260:ILE:CD1	1:A:260:ILE:N	2.72	0.53
2:O:47:GLN:HA	1:P:20:THR:HB	1.91	0.52
1:P:31:GLU:OE2	1:P:33:VAL:HG12	2.09	0.52
1:C:104:GLU:OE2	2:F:75:HIS:NE2	2.37	0.52
1:N:3:ILE:HD11	2:O:152:ILE:HD11	1.90	0.52
1:A:33:VAL:CG2	1:A:307:LEU:CD2	2.88	0.52
1:A:33:VAL:HG22	1:A:287:PHE:HB2	1.92	0.52
1:C:282:ASN:OD1	1:C:282:ASN:N	2.43	0.52
1:E:3:ILE:HD13	2:F:152:ILE:HG21	1.92	0.52
1:C:48:HIS:NE2	1:C:266:ILE:CD1	2.72	0.52
1:C:57:ILE:HD12	1:C:86:TYR:OH	2.09	0.52
2:D:92:TRP:NE1	2:F:91:ILE:HD11	2.25	0.52
1:A:258:LEU:HG	1:A:260:ILE:CD1	2.40	0.51
2:Q:122:VAL:CG2	2:Q:138:PHE:CE2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:51:LEU:HD11	1:N:77:LEU:HD21	1.93	0.51
1:C:139:TYR:CE1	1:C:225:PHE:CZ	2.99	0.51
1:A:121:ILE:HD11	1:A:154:PHE:CE1	2.44	0.50
1:N:175:ILE:HD13	1:N:177:HIS:CE1	2.47	0.50
1:N:3:ILE:CD1	2:O:152:ILE:HD13	2.42	0.50
1:E:271:GLU:O	1:E:282:ASN:ND2	2.33	0.50
1:N:73:THR:HG22	1:N:254:ILE:HD11	1.94	0.50
1:A:167:ALA:HB3	1:A:252:LYS:CE	2.42	0.50
2:B:171:LEU:HD22	2:F:171:LEU:HD11	1.93	0.50
2:Q:119:TYR:O	2:Q:122:VAL:CG2	2.60	0.49
1:A:78:ILE:CG2	1:A:80:ARG:NH1	2.75	0.49
1:L:70:LEU:HD12	1:L:141:GLU:OE2	2.12	0.49
1:E:19:LEU:HD12	2:F:101:ALA:HB1	1.94	0.49
1:C:199:SER:HA	1:E:214:PRO:HG3	1.94	0.49
1:C:300:LYS:HG3	2:D:92:TRP:CE2	2.48	0.49
1:E:38:LEU:N	1:E:38:LEU:HD12	2.28	0.49
1:N:75:ASP:OD1	1:N:76:THR:CG2	2.60	0.49
1:L:78:ILE:CG2	1:L:80:ARG:NH1	2.75	0.49
1:C:66:CYS:O	1:C:70:LEU:HD13	2.13	0.49
1:L:4:CYS:HA	2:M:137:CYS:HA	1.95	0.49
1:A:4:CYS:HA	2:B:137:CYS:HA	1.95	0.48
1:C:3:ILE:HD13	2:D:152:ILE:HG21	1.94	0.48
1:L:209:VAL:HG21	1:P:205:ASN:HD22	1.78	0.48
1:P:177:HIS:HB3	1:P:209:VAL:O	2.12	0.48
1:P:256:ARG:NH2	2:Q:64:GLU:OE2	2.42	0.48
1:N:169:HIS:HB3	1:N:250:VAL:CG1	2.44	0.48
1:N:203:LYS:NZ	1:P:224:ASP:OD1	2.30	0.48
1:P:48:HIS:HE1	1:P:268:ASN:HD21	1.61	0.48
1:C:181:THR:HG23	1:C:184:LYS:HE2	1.96	0.48
2:D:92:TRP:CE2	2:F:91:ILE:CD1	2.96	0.48
2:M:88:ILE:HD12	2:M:89:THR:N	2.29	0.48
1:C:40:ARG:NH1	1:C:267:ASP:OD2	2.47	0.48
1:E:177:HIS:HB3	1:E:209:VAL:O	2.13	0.48
2:O:152:ILE:HD12	2:O:152:ILE:C	2.33	0.48
2:B:30:GLN:HE22	2:B:145:ASP:HB2	1.78	0.48
1:L:183:GLU:O	1:L:187:LEU:HD23	2.14	0.48
1:L:177:HIS:HB3	1:L:209:VAL:O	2.14	0.47
1:C:37:SER:HB2	1:C:290:LEU:HD13	1.94	0.47
2:D:126:LEU:CD2	2:D:152:ILE:HD12	2.39	0.47
1:C:74:TRP:NE1	1:C:77:LEU:HG	2.30	0.47
1:E:43:MET:HE3	1:E:48:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:267:ASP:OD1	1:L:269:SER:OG	2.26	0.47
1:N:183:GLU:O	1:N:187:LEU:HD23	2.14	0.47
1:N:3:ILE:HD11	2:O:152:ILE:CD1	2.44	0.47
1:A:122:ASN:HB3	1:A:146:VAL:HG13	1.95	0.47
2:O:127:ARG:NH2	2:Q:139:GLU:OE1	2.37	0.47
1:A:77:LEU:HD22	1:A:103:MET:SD	2.55	0.47
1:L:38:LEU:HD12	1:L:38:LEU:N	2.30	0.47
2:Q:125:GLN:OE1	2:Q:155:ASN:HA	2.14	0.47
1:C:139:TYR:CE1	1:C:225:PHE:HZ	2.33	0.47
1:C:199:SER:HA	1:E:214:PRO:CG	2.45	0.47
1:N:281:ILE:CD1	1:N:299:PRO:HD2	2.44	0.47
1:A:51:LEU:HD11	1:A:77:LEU:HD21	1.96	0.47
2:M:85:LYS:O	2:M:88:ILE:HG13	2.14	0.47
1:N:3:ILE:CD1	2:O:152:ILE:HD11	2.45	0.47
2:B:125:GLN:OE1	2:B:155:ASN:HA	2.15	0.47
1:P:160:THR:HG23	1:P:237:THR:HG22	1.96	0.47
1:P:5:LEU:HD22	2:Q:119:TYR:HA	1.96	0.47
2:B:142:HIS:CE1	2:B:162:TYR:CD1	3.03	0.47
1:C:78:ILE:N	1:C:78:ILE:HD12	2.29	0.47
1:N:177:HIS:HB3	1:N:209:VAL:O	2.14	0.47
2:O:125:GLN:OE1	2:O:155:ASN:HA	2.15	0.47
1:N:160:THR:HG23	1:N:237:THR:HG22	1.97	0.46
1:C:15:ILE:HD12	1:C:15:ILE:H	1.79	0.46
1:E:128:LYS:HG3	1:E:136:ASN:HD21	1.80	0.46
1:N:41:LEU:HD11	1:N:264:ALA:HB3	1.97	0.46
2:D:125:GLN:OE1	2:D:155:ASN:HA	2.16	0.46
1:E:215:GLN:HG3	1:E:218:GLY:HA2	1.97	0.46
1:E:160:THR:HG23	1:E:237:THR:HG22	1.96	0.46
1:N:223:ILE:HG23	1:N:245:ILE:HD13	1.96	0.46
1:P:33:VAL:HG13	1:P:33:VAL:O	2.15	0.46
1:A:259:GLY:C	1:A:260:ILE:HD12	2.36	0.46
2:B:141:TYR:O	2:B:166:ALA:HA	2.15	0.46
2:D:1:GLY:HA2	6:D:302:HOH:O	2.15	0.46
2:D:92:TRP:NE1	2:F:91:ILE:CD1	2.79	0.46
1:L:31:GLU:OE2	1:L:33:VAL:HG22	2.15	0.46
2:Q:142:HIS:CE1	2:Q:162:TYR:CD1	3.04	0.46
1:E:168:GLU:OE1	1:E:229:LEU:HD23	2.16	0.46
2:D:64:GLU:OE1	6:D:301:HOH:O	2.20	0.46
2:F:125:GLN:OE1	2:F:155:ASN:HA	2.15	0.46
2:O:141:TYR:O	2:O:166:ALA:HA	2.15	0.46
2:O:142:HIS:CE1	2:O:162:TYR:CD1	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:141:TYR:O	2:Q:166:ALA:HA	2.16	0.46
1:P:300:LYS:HG3	2:Q:92:TRP:CE2	2.50	0.46
1:C:146:VAL:HG11	1:C:187:LEU:HD11	1.93	0.45
1:C:193:LEU:HD23	1:C:242:GLY:O	2.16	0.45
2:F:141:TYR:O	2:F:166:ALA:HA	2.15	0.45
1:N:205:ASN:HB2	1:P:209:VAL:CG1	2.46	0.45
1:A:33:VAL:HG23	1:A:307:LEU:HD21	1.95	0.45
1:C:160:THR:HG23	1:C:237:THR:HG22	1.96	0.45
1:L:304:LYS:HE2	2:M:97:GLU:OE2	2.16	0.45
2:D:141:TYR:O	2:D:166:ALA:HA	2.16	0.45
2:M:142:HIS:CE1	2:M:162:TYR:CD1	3.04	0.45
2:F:142:HIS:CE1	2:F:162:TYR:CD1	3.04	0.45
1:N:142:LEU:HD23	1:N:247:PRO:HA	1.99	0.45
1:L:224:ASP:OD2	1:P:203:LYS:HE3	2.17	0.45
1:L:80:ARG:HH22	1:L:266:ILE:CD1	2.29	0.45
2:M:141:TYR:O	2:M:166:ALA:HA	2.16	0.45
1:A:142:LEU:HD23	1:A:247:PRO:HA	1.99	0.45
1:A:266:ILE:HG22	1:A:267:ASP:N	2.32	0.45
2:D:126:LEU:HD21	2:D:152:ILE:HD11	1.96	0.45
2:D:152:ILE:HD11	2:D:157:TYR:CD1	2.52	0.45
1:E:7:HIS:HA	2:F:21:TRP:O	2.17	0.45
2:D:92:TRP:CZ2	2:F:91:ILE:HD13	2.52	0.45
1:C:42:CYS:SG	1:C:270:CYS:CB	3.04	0.45
1:N:41:LEU:CD1	1:N:264:ALA:HB3	2.47	0.45
1:N:77:LEU:HD22	1:N:103:MET:SD	2.57	0.45
1:A:121:ILE:HD11	1:A:154:PHE:CE2	2.48	0.44
1:E:142:LEU:HD23	1:E:247:PRO:HA	1.99	0.44
2:O:128:GLN:CA	2:O:128:GLN:HE21	2.25	0.44
1:N:75:ASP:OD1	1:N:76:THR:HG22	2.16	0.44
1:E:48:HIS:HE1	1:E:268:ASN:HD21	1.62	0.44
1:L:224:ASP:OD2	1:P:203:LYS:CE	2.66	0.44
2:D:142:HIS:CE1	2:D:162:TYR:CD1	3.05	0.44
1:P:142:LEU:HD23	1:P:247:PRO:HA	1.99	0.44
1:C:43:MET:HE3	1:C:48:HIS:HB3	1.99	0.44
1:E:173:TRP:CZ2	1:E:197:VAL:HG11	2.53	0.44
2:O:50:GLY:HA3	1:P:20:THR:O	2.18	0.44
1:N:63:THR:HG22	1:N:64:PRO:HD2	2.00	0.44
1:A:61:ILE:HG23	1:A:172:MET:SD	2.58	0.44
1:E:41:LEU:CD1	1:E:264:ALA:HB3	2.48	0.44
1:L:162:ARG:HB2	1:L:235:LYS:HG2	2.00	0.44
1:L:142:LEU:HD23	1:L:247:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:274:CYS:SG	1:L:281:ILE:CD1	2.99	0.44
1:C:61:ILE:HD13	1:C:139:TYR:CE1	2.50	0.43
1:P:41:LEU:CD1	1:P:264:ALA:HB3	2.48	0.43
1:P:77:LEU:HD23	1:P:103:MET:SD	2.58	0.43
2:O:99:LEU:HD22	2:Q:94:TYR:OH	2.18	0.43
1:C:142:LEU:HD23	1:C:247:PRO:HA	2.00	0.43
1:L:66:CYS:O	1:L:70:LEU:CD2	2.66	0.43
1:E:77:LEU:HD23	1:E:103:MET:SD	2.59	0.43
1:L:21:ASN:HD22	1:L:24:GLU:CD	2.22	0.43
1:C:153:ASN:ND2	1:C:191:GLN:CG	2.82	0.43
1:L:44:LYS:HB3	1:L:271:GLU:CG	2.48	0.43
1:L:7:HIS:HA	2:M:21:TRP:O	2.19	0.43
1:A:41:LEU:CD1	1:A:264:ALA:HB3	2.49	0.43
1:N:15:ILE:HD12	1:N:15:ILE:H	1.82	0.43
1:L:274:CYS:SG	1:L:281:ILE:CG1	3.07	0.43
1:A:21:ASN:HD22	1:A:24:GLU:CD	2.22	0.43
1:C:5:LEU:CD2	1:C:5:LEU:N	2.82	0.43
2:D:126:LEU:CD2	2:D:152:ILE:HD11	2.49	0.43
1:N:175:ILE:CD1	1:N:177:HIS:NE2	2.82	0.43
1:A:266:ILE:CG2	1:A:267:ASP:N	2.82	0.42
1:E:102:ILE:O	1:E:105:SER:OG	2.32	0.42
2:M:5:ALA:HB1	2:M:115:MET:HG2	2.00	0.42
1:N:266:ILE:HG22	1:N:267:ASP:N	2.33	0.42
2:O:5:ALA:HB1	2:O:115:MET:HG2	2.00	0.42
2:B:5:ALA:HB1	2:B:115:MET:HG2	2.01	0.42
2:D:5:ALA:HB1	2:D:115:MET:HG2	2.01	0.42
1:E:5:LEU:HD12	2:F:119:TYR:HA	2.02	0.42
1:L:304:LYS:CE	2:M:97:GLU:OE2	2.68	0.42
1:N:46:ARG:NH1	1:N:272:SER:O	2.52	0.42
1:C:4:CYS:HA	2:D:137:CYS:HA	2.02	0.42
1:N:3:ILE:HD13	2:O:152:ILE:HD13	2.02	0.42
1:E:74:TRP:CE2	1:E:77:LEU:HD13	2.54	0.42
1:A:-1:ASP:HB3	1:A:0:PRO:HD3	2.02	0.42
1:A:293:ARG:HG2	2:B:67:GLU:OE1	2.20	0.42
1:C:7:HIS:HA	2:D:21:TRP:O	2.19	0.42
1:L:33:VAL:O	1:L:33:VAL:HG23	2.18	0.42
1:L:5:LEU:N	1:L:5:LEU:CD2	2.82	0.42
1:N:182:GLN:O	1:N:186:ASP:HB2	2.20	0.42
1:P:74:TRP:CE2	1:P:77:LEU:HD13	2.54	0.42
1:C:21:ASN:HD22	1:C:24:GLU:CD	2.22	0.42
1:L:77:LEU:HD23	1:L:103:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:ASN:HD22	1:N:24:GLU:CD	2.23	0.42
1:A:67:ASP:O	1:A:70:LEU:HG	2.20	0.42
1:E:63:THR:HG22	1:E:64:PRO:HD2	2.02	0.42
1:P:4:CYS:HA	2:Q:137:CYS:HA	2.02	0.42
2:O:152:ILE:HD12	2:O:153:ARG:CA	2.50	0.42
2:O:24:PHE:CD2	2:O:153:ARG:HD3	2.55	0.42
1:L:266:ILE:CG2	1:L:267:ASP:N	2.83	0.41
2:O:171:LEU:CD1	2:O:171:LEU:N	2.82	0.41
1:E:21:ASN:HD22	1:E:24:GLU:CD	2.22	0.41
1:N:266:ILE:CG2	1:N:267:ASP:N	2.83	0.41
1:P:63:THR:HG22	1:P:64:PRO:HD2	2.03	0.41
1:P:41:LEU:HD11	1:P:262:SER:OG	2.21	0.41
1:E:41:LEU:HD11	1:E:262:SER:OG	2.20	0.41
1:L:74:TRP:CE2	1:L:77:LEU:HD13	2.55	0.41
1:A:173:TRP:CZ2	1:A:197:VAL:HG11	2.55	0.41
2:D:171:LEU:N	2:D:171:LEU:CD1	2.83	0.41
1:C:41:LEU:CD1	1:C:264:ALA:HB3	2.50	0.41
1:N:4:CYS:HA	2:O:137:CYS:HA	2.02	0.41
1:P:21:ASN:HD22	1:P:24:GLU:CD	2.23	0.41
1:A:104:GLU:CD	2:D:75:HIS:HE2	2.24	0.41
1:E:-1:ASP:HB3	1:E:0:PRO:HD3	2.03	0.41
1:E:4:CYS:HA	2:F:137:CYS:HA	2.02	0.41
1:N:274:CYS:SG	1:N:281:ILE:CG1	3.09	0.41
1:N:63:THR:CG2	1:N:64:PRO:HD2	2.50	0.41
2:Q:122:VAL:HG23	2:Q:138:PHE:CZ	2.56	0.41
1:A:43:MET:HA	1:A:46:ARG:CD	2.48	0.41
1:N:38:LEU:HD12	1:N:38:LEU:N	2.36	0.41
1:P:266:ILE:HD12	1:P:266:ILE:N	2.35	0.41
1:E:34:GLU:HG2	1:E:283:THR:HB	2.02	0.41
1:L:281:ILE:HG21	1:L:290:LEU:HD12	2.03	0.41
1:N:7:HIS:HA	2:O:21:TRP:O	2.21	0.41
1:P:3:ILE:HD13	2:Q:152:ILE:HG21	2.03	0.41
1:L:154:PHE:H	1:L:191:GLN:HE22	1.69	0.41
1:A:7:HIS:HA	2:B:21:TRP:O	2.21	0.41
1:N:41:LEU:N	1:N:41:LEU:HD12	2.36	0.41
1:A:184:LYS:HE3	1:A:184:LYS:HB3	1.88	0.40
1:C:100:GLN:NE2	2:F:76:GLN:OE1	2.54	0.40
2:D:74:ASP:HB3	2:D:77:ILE:HG22	2.03	0.40
2:F:5:ALA:HB1	2:F:115:MET:HG2	2.02	0.40
2:F:74:ASP:HB3	2:F:77:ILE:HG22	2.03	0.40
1:P:266:ILE:CG2	1:P:267:ASP:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:HD11	1:C:262:SER:OG	2.21	0.40
1:E:300:LYS:HG3	2:F:92:TRP:CE2	2.56	0.40
1:A:63:THR:CG2	1:A:64:PRO:HD2	2.52	0.40
1:L:43:MET:HE3	1:L:48:HIS:HB3	2.03	0.40
2:M:74:ASP:HB3	2:M:77:ILE:HG22	2.04	0.40
1:A:66:CYS:O	1:A:70:LEU:CD2	2.68	0.40
1:P:34:GLU:HG2	1:P:283:THR:HB	2.03	0.40
2:Q:5:ALA:HB1	2:Q:115:MET:HG2	2.02	0.40

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	312/325 (96%)	309 (99%)	3 (1%)	0	100	100
1	C	311/325 (96%)	308 (99%)	3 (1%)	0	100	100
1	E	320/325 (98%)	316 (99%)	4 (1%)	0	100	100
1	L	312/325 (96%)	308 (99%)	4 (1%)	0	100	100
1	N	318/325 (98%)	314 (99%)	4 (1%)	0	100	100
1	P	320/325 (98%)	316 (99%)	4 (1%)	0	100	100
2	B	170/177 (96%)	161 (95%)	9 (5%)	0	100	100
2	D	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
2	F	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
2	M	170/177 (96%)	161 (95%)	9 (5%)	0	100	100
2	O	170/177 (96%)	161 (95%)	9 (5%)	0	100	100
2	Q	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
All	All	2913/3012 (97%)	2838 (97%)	75 (3%)	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	269/276 (98%)	256 (95%)	13 (5%)	25	49
1	C	267/276 (97%)	244 (91%)	23 (9%)	10	22
1	E	274/276 (99%)	260 (95%)	14 (5%)	24	46
1	L	268/276 (97%)	253 (94%)	15 (6%)	21	42
1	N	267/276 (97%)	251 (94%)	16 (6%)	19	39
1	P	274/276 (99%)	261 (95%)	13 (5%)	26	50
2	B	146/151 (97%)	144 (99%)	2 (1%)	67	85
2	D	145/151 (96%)	143 (99%)	2 (1%)	67	85
2	F	146/151 (97%)	142 (97%)	4 (3%)	44	71
2	M	146/151 (97%)	144 (99%)	2 (1%)	67	85
2	O	146/151 (97%)	144 (99%)	2 (1%)	67	85
2	Q	146/151 (97%)	145 (99%)	1 (1%)	84	93
All	All	2494/2562 (97%)	2387 (96%)	107 (4%)	29	54

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	76	THR
1	A	121	ILE
1	A	143	LYS
1	A	177	HIS
1	A	183	GLU
1	A	184	LYS
1	A	186	ASP
1	A	231	GLN
1	A	251	SER
1	A	260	ILE

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Mol	Chain	Res	Type
1	A	268	ASN
1	A	282	ASN
2	B	113	SER
2	B	147	SER
1	C	5	LEU
1	C	8	HIS
1	C	14	THR
1	C	71	THR
1	C	76	THR
1	C	77	LEU
1	C	99	ARG
1	C	139	TYR
1	C	143	LYS
1	C	162	ARG
1	C	177	HIS
1	C	186	ASP
1	C	187	LEU
1	C	235	LYS
1	C	251	SER
1	C	254	ILE
1	C	266	ILE
1	C	268	ASN
1	C	280	SER
1	C	282	ASN
1	C	289	ASN
1	C	304	LYS
1	C	316	VAL
2	D	113	SER
2	D	171	LEU
1	E	2	LYS
1	E	5	LEU
1	E	8	HIS
1	E	14	THR
1	E	71	THR
1	E	76	THR
1	E	143	LYS
1	E	177	HIS
1	E	179	SER
1	E	186	ASP
1	E	215	GLN
1	E	222	ARG
1	E	235	LYS

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Mol	Chain	Res	Type
1	E	251	SER
2	F	57	LYS
2	F	113	SER
2	F	127	ARG
2	F	164	GLU
1	L	8	HIS
1	L	14	THR
1	L	70	LEU
1	L	76	THR
1	L	99	ARG
1	L	143	LYS
1	L	153	ASN
1	L	177	HIS
1	L	186	ASP
1	L	203	LYS
1	L	229	LEU
1	L	251	SER
1	L	268	ASN
1	L	281	ILE
1	L	282	ASN
2	M	113	SER
2	M	145	ASP
1	N	5	LEU
1	N	8	HIS
1	N	14	THR
1	N	76	THR
1	N	143	LYS
1	N	177	HIS
1	N	190	THR
1	N	196	SER
1	N	203	LYS
1	N	251	SER
1	N	254	ILE
1	N	266	ILE
1	N	280	SER
1	N	282	ASN
1	N	304	LYS
1	N	316	VAL
2	O	113	SER
2	O	171	LEU
1	P	2	LYS
1	P	8	HIS

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Mol	Chain	Res	Type
1	P	12	ASN
1	P	14	THR
1	P	71	THR
1	P	76	THR
1	P	143	LYS
1	P	177	HIS
1	P	186	ASP
1	P	235	LYS
1	P	251	SER
1	P	304	LYS
1	P	316	VAL
2	Q	113	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	149	ASN
1	A	159	ASN
1	A	176	HIS
1	A	185	ASN
1	A	215	GLN
1	A	231	GLN
1	A	268	ASN
2	B	30	GLN
2	B	95	GLN
1	C	215	GLN
1	C	268	ASN
1	C	289	ASN
1	E	48	HIS
1	E	240	HIS
2	F	12	ASN
2	F	155	ASN
1	L	215	GLN
1	L	261	GLN
1	L	268	ASN
2	M	161	GLN
1	N	205	ASN
2	O	12	ASN
2	O	128	GLN
1	P	48	HIS
1	P	176	HIS

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Mol	Chain	Res	Type
1	P	240	HIS
2	Q	12	ASN
2	Q	159	HIS
2	Q	161	GLN

5.3.3 RNA

There are no RNA molecules 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

4 monosaccharides 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	G	1	3,2,5	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
3	NAG	G	2	3	14,14,15	0.46	0	17,19,21	1.49	2 (11%)
3	NAG	H	1	3,2	14,14,15	0.43	0	17,19,21	0.95	1 (5%)
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	1.41	3 (17%)

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	G	1	3,2,5	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C1-O5-C5	3.61	117.08	112.19
3	H	2	NAG	O5-C5-C6	3.60	112.84	107.20
3	G	2	NAG	O5-C1-C2	-3.38	105.95	111.29
3	G	1	NAG	C1-O5-C5	2.94	116.17	112.19
3	H	2	NAG	O5-C5-C4	-2.76	104.10	110.83
3	H	1	NAG	C4-C3-C2	2.27	114.35	111.02
3	H	2	NAG	C3-C4-C5	-2.03	106.63	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\#\|Z\|>2$
4	NAG	C	401	1	14,14,15	0.64	0	17,19,21	0.91	1 (5%)
4	NAG	F	201	2	14,14,15	0.56	0	17,19,21	1.36	3 (17%)
4	NAG	O	201	2	14,14,15	0.62	0	17,19,21	1.44	2 (11%)
4	NAG	F	202	2	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
4	NAG	Q	201	2,5	14,14,15	0.46	0	17,19,21	1.31	2 (11%)
4	NAG	M	201	2,5	14,14,15	0.95	0	17,19,21	1.70	1 (5%)
4	NAG	N	401	1	14,14,15	0.71	0	17,19,21	1.23	1 (5%)
4	NAG	P	401	1	14,14,15	1.04	1 (7%)	17,19,21	1.16	1 (5%)

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	C	401	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	NAG	O	201	2	-	2/6/23/26	0/1/1/1
4	NAG	F	202	2	-	1/6/23/26	0/1/1/1
4	NAG	Q	201	2,5	-	0/6/23/26	0/1/1/1
4	NAG	M	201	2,5	-	1/6/23/26	0/1/1/1
4	NAG	N	401	1	-	3/6/23/26	0/1/1/1
4	NAG	P	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	401	NAG	C1-C2	2.94	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	201	NAG	C1-O5-C5	5.49	119.63	112.19
4	O	201	NAG	C1-O5-C5	4.15	117.81	112.19
4	N	401	NAG	C2-N2-C7	3.26	127.55	122.90
4	Q	201	NAG	C1-O5-C5	3.07	116.35	112.19
4	F	202	NAG	C1-O5-C5	2.83	116.03	112.19
4	P	401	NAG	C2-N2-C7	2.83	126.93	122.90
4	F	201	NAG	C1-O5-C5	2.72	115.88	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	201	NAG	O5-C1-C2	-2.66	107.08	111.29
4	C	401	NAG	O5-C5-C6	2.35	110.89	107.20
4	O	201	NAG	O5-C1-C2	-2.29	107.68	111.29
4	F	201	NAG	C3-C4-C5	-2.27	106.19	110.24
4	Q	201	NAG	C3-C4-C5	-2.22	106.28	110.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	401	NAG	C3-C2-N2-C7
4	N	401	NAG	C4-C5-C6-O6
4	N	401	NAG	O5-C5-C6-O6
4	O	201	NAG	C4-C5-C6-O6
4	F	202	NAG	O5-C5-C6-O6
4	O	201	NAG	O5-C5-C6-O6
4	P	401	NAG	C4-C5-C6-O6
4	P	401	NAG	O5-C5-C6-O6
4	M	201	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

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	316/325 (97%)	0.54	24 (7%)	13	11	54, 105, 163, 213	0
1	C	315/325 (96%)	0.47	17 (5%)	25	24	64, 102, 153, 198	0
1	E	322/325 (99%)	0.32	6 (1%)	66	67	55, 79, 113, 152	0
1	L	316/325 (97%)	0.41	13 (4%)	37	35	52, 93, 142, 175	0
1	N	320/325 (98%)	0.57	24 (7%)	14	12	63, 112, 174, 241	0
1	P	322/325 (99%)	0.33	7 (2%)	62	61	54, 75, 110, 156	0
2	B	172/177 (97%)	0.51	11 (6%)	19	17	48, 75, 98, 117	0
2	D	172/177 (97%)	0.54	9 (5%)	27	25	60, 84, 109, 119	0
2	F	172/177 (97%)	0.45	8 (4%)	31	29	53, 78, 107, 132	0
2	M	172/177 (97%)	0.48	8 (4%)	31	29	48, 73, 97, 121	0
2	O	172/177 (97%)	0.54	10 (5%)	23	21	63, 86, 114, 137	0
2	Q	172/177 (97%)	0.48	10 (5%)	23	21	50, 75, 104, 114	0
All	All	2943/3012 (97%)	0.46	147 (4%)	28	26	48, 87, 146, 241	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	146	VAL	7.3
1	N	182	GLN	7.2
1	N	188	TYR	4.8
1	N	129	ALA	4.6
1	A	134	GLY	4.5
1	N	223	ILE	4.4
2	O	94	TYR	4.2
1	N	128	LYS	4.0
2	D	77	ILE	3.9
1	N	222	ARG	3.8
1	A	180	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	176	HIS	3.7
2	O	99	LEU	3.7
1	A	236	ILE	3.6
1	N	147	SER	3.6
1	N	243	GLY	3.6
1	L	176	HIS	3.5
1	A	176	HIS	3.5
1	C	139	TYR	3.5
1	C	162	ARG	3.5
1	L	216	VAL	3.4
1	A	181	THR	3.4
2	F	2	LEU	3.4
1	N	205	ASN	3.3
2	M	94	TYR	3.3
1	N	212	ALA	3.3
2	B	2	LEU	3.3
1	A	218	GLY	3.2
2	O	77	ILE	3.2
1	E	309	LEU	3.2
1	C	179	SER	3.2
2	B	55	ILE	3.1
1	A	220	SER	3.1
1	N	88	TYR	3.1
1	A	219	LEU	3.0
1	C	216	VAL	3.0
1	A	223	ILE	3.0
1	A	188	TYR	3.0
2	Q	100	VAL	3.0
1	C	223	ILE	2.9
1	A	197	VAL	2.9
1	L	225	PHE	2.9
1	C	78	ILE	2.9
1	A	179	SER	2.8
1	A	203	LYS	2.8
2	B	102	MET	2.8
2	O	102	MET	2.8
1	L	219	LEU	2.8
2	B	116	LEU	2.8
1	A	182	GLN	2.8
2	M	99	LEU	2.7
2	B	99	LEU	2.7
1	P	209	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	81	ILE	2.7
1	N	144	TRP	2.6
1	A	76	THR	2.6
1	L	222	ARG	2.6
2	Q	95	GLN	2.6
2	F	102	MET	2.6
1	P	32	THR	2.5
1	N	206	PHE	2.5
1	L	206	PHE	2.5
2	O	66	ILE	2.5
2	B	134	GLY	2.5
2	Q	138	PHE	2.5
2	D	99	LEU	2.5
2	Q	5	ALA	2.5
1	C	215	GLN	2.5
1	A	235	LYS	2.5
1	A	233	GLY	2.5
1	N	90	GLY	2.5
1	A	57	ILE	2.5
1	L	224	ASP	2.5
1	E	258	LEU	2.4
1	N	187	LEU	2.4
1	E	320	VAL	2.4
1	N	193	LEU	2.4
1	C	218	GLY	2.4
2	D	102	MET	2.4
2	Q	77	ILE	2.4
2	O	83	TRP	2.4
1	L	193	LEU	2.4
2	M	98	LEU	2.4
2	Q	80	VAL	2.4
1	L	88	TYR	2.4
2	F	3	PHE	2.4
1	L	187	LEU	2.4
2	B	88	ILE	2.4
1	C	128	LYS	2.3
2	B	98	LEU	2.3
2	D	2	LEU	2.3
1	A	78	ILE	2.3
1	A	230	VAL	2.3
1	P	287	PHE	2.3
2	F	106	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	88	TYR	2.3
2	D	94	TYR	2.3
1	N	244	LEU	2.3
1	N	117	TYR	2.3
1	N	307	LEU	2.2
2	F	55	ILE	2.2
2	M	77	ILE	2.2
2	O	44	ALA	2.2
2	M	88	ILE	2.2
2	O	88	ILE	2.2
1	E	39	ASN	2.2
1	P	176	HIS	2.2
1	E	212	ALA	2.2
2	D	55	ILE	2.2
1	N	192	SER	2.2
1	C	187	LEU	2.2
1	C	100	GLN	2.2
2	M	96	ALA	2.2
2	Q	94	TYR	2.2
1	P	179	SER	2.2
2	B	100	VAL	2.2
2	Q	66	ILE	2.2
1	C	59	MET	2.2
2	B	81	ILE	2.2
1	N	61	ILE	2.1
1	N	78	ILE	2.1
1	A	227	TRP	2.1
1	A	202	TYR	2.1
1	P	207	VAL	2.1
2	B	77	ILE	2.1
1	C	206	PHE	2.1
1	C	242	GLY	2.1
2	O	2	LEU	2.1
1	L	210	VAL	2.1
2	M	55	ILE	2.1
2	O	22	TYR	2.1
2	D	156	THR	2.1
1	L	223	ILE	2.1
2	D	48	ILE	2.1
2	Q	2	LEU	2.1
1	L	192	SER	2.1
1	P	19	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	M	102	MET	2.0
1	E	128	LYS	2.0
2	Q	3	PHE	2.0
1	C	19	LEU	2.0
1	C	209	VAL	2.0
2	F	75	HIS	2.0
2	F	52	LEU	2.0
1	C	236	ILE	2.0
2	F	77	ILE	2.0
1	A	19	LEU	2.0

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. 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	B-factors(Å^2)	Q<0.9
3	NAG	H	2	14/15	0.83	0.24	120,145,154,155	0
3	NAG	G	2	14/15	0.84	0.29	98,125,136,137	0
3	NAG	H	1	14/15	0.88	0.13	107,118,126,130	0
3	NAG	G	1	14/15	0.95	0.15	84,90,98,102	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. 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	B-factors(Å^2)	Q<0.9
4	NAG	O	201	14/15	0.72	0.17	110,127,130,132	0
4	NAG	C	401	14/15	0.78	0.18	113,139,147,149	0
4	NAG	P	401	14/15	0.80	0.17	88,117,136,141	0
4	NAG	N	401	14/15	0.81	0.13	122,140,152,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	Q	201	14/15	0.82	0.17	103,108,113,114	0
4	NAG	F	201	14/15	0.86	0.19	97,106,114,119	0
4	NAG	F	202	14/15	0.87	0.13	119,145,153,154	0
4	NAG	M	201	14/15	0.91	0.14	70,78,84,86	0
5	CA	P	402	1/1	0.96	0.15	67,67,67,67	0
5	CA	E	401	1/1	0.97	0.12	69,69,69,69	0
5	CA	N	402	1/1	0.97	0.04	106,106,106,106	0

6.5 Other polymers

There are no such residues in this entry.