Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 11:30 AM EDT

PDB ID	:	6D7C
Title	:	The crystal structure of hemagglutinin from A/Hong Kong/61/2016 H7N9 influenza virus
Authors	:	Yang, H.; Stevens, J.
Deposited on	:	2018-04-24
Resolution	:	2.95 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

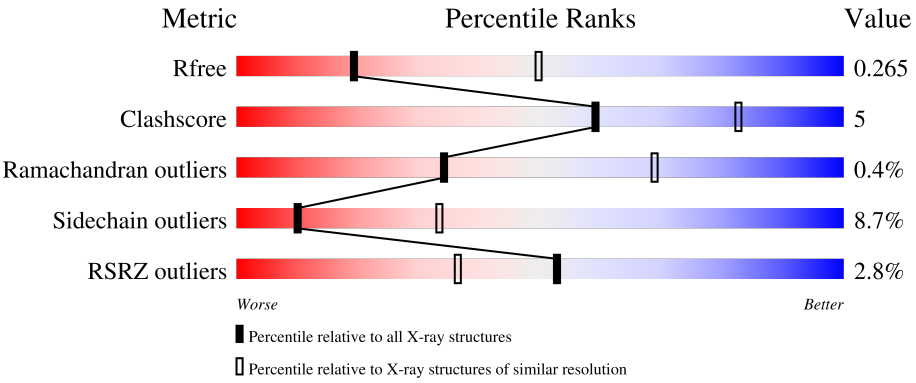
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 of 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	321	84% 13%
1	C	321	3% 84% 13%
1	E	321	83% 14%
1	G	321	10% 84% 13%
1	I	321	3% 85% 12%

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Mol	Chain	Length	Quality of chain
1	K	321	86% 11%
2	B	221	5% 60% 13% 23%
2	D	221	57% 15% 23%
2	F	221	59% 15% 23%
2	H	221	58% 15% 23%
2	J	221	61% 13% 23%
2	L	221	57% 15% 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	401	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			
1	C	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			
1	E	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			
1	G	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			
1	I	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			
1	K	316	Total	C	N	O	S	1	0	0
			2413	1502	436	461	14			

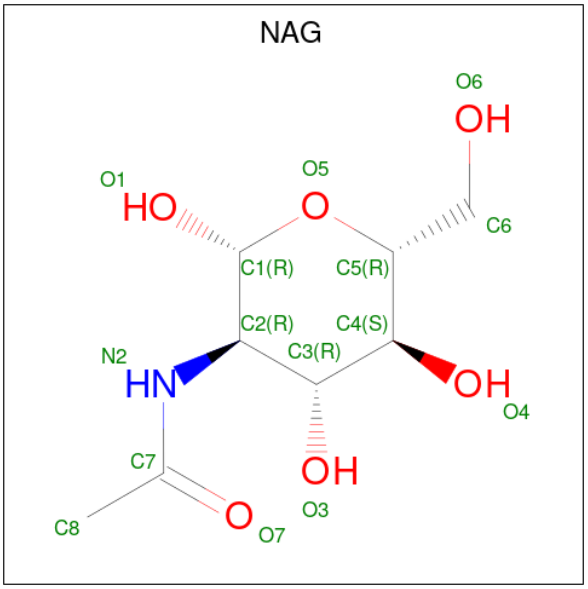
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
A	227	ILE	MET	conflict	UNP A0A0C4ZYE2
C	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
C	227	ILE	MET	conflict	UNP A0A0C4ZYE2
E	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
E	227	ILE	MET	conflict	UNP A0A0C4ZYE2
G	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
G	227	ILE	MET	conflict	UNP A0A0C4ZYE2
I	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
I	227	ILE	MET	conflict	UNP A0A0C4ZYE2
K	47	ARG	LYS	conflict	UNP A0A0C4ZYE2
K	227	ILE	MET	conflict	UNP A0A0C4ZYE2

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			
2	D	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			
2	F	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			
2	H	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			
2	J	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			
2	L	171	Total	C	N	O	S	0	0	0
			1387	857	243	280	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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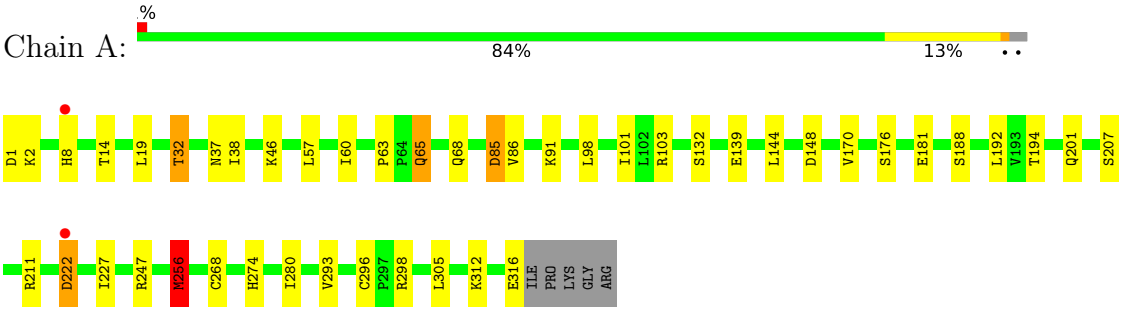
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

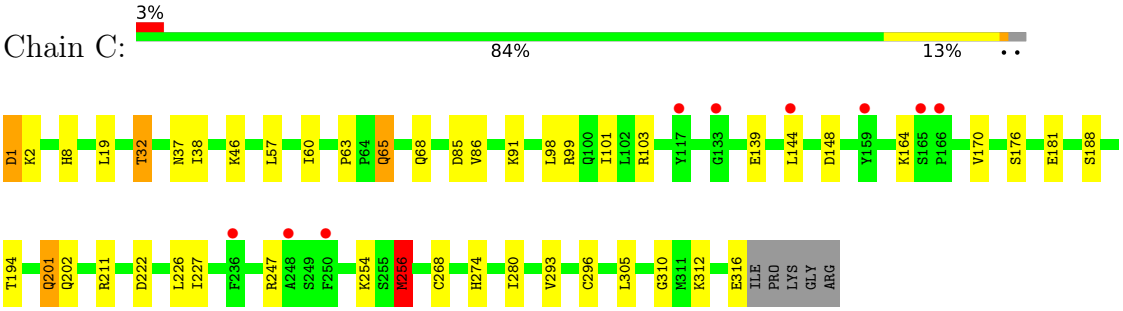
3 Residue-property plots

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.

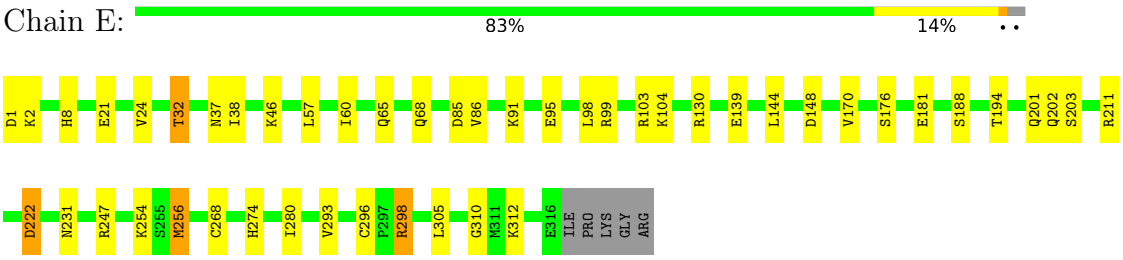
• Molecule 1: Hemagglutinin HA1 chain



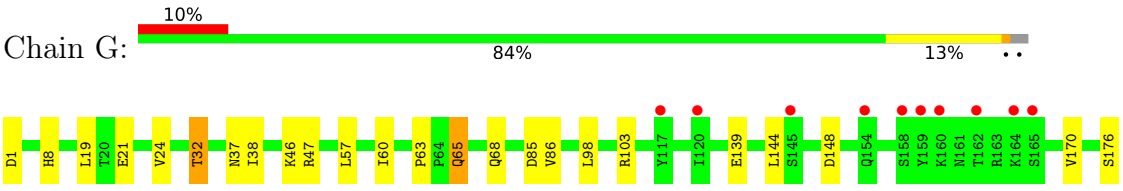
• Molecule 1: Hemagglutinin HA1 chain

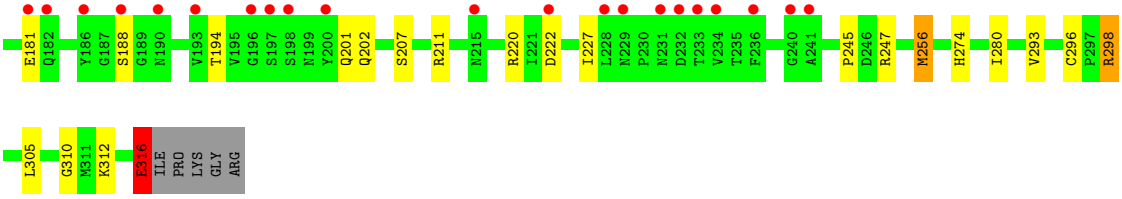


• Molecule 1: Hemagglutinin HA1 chain

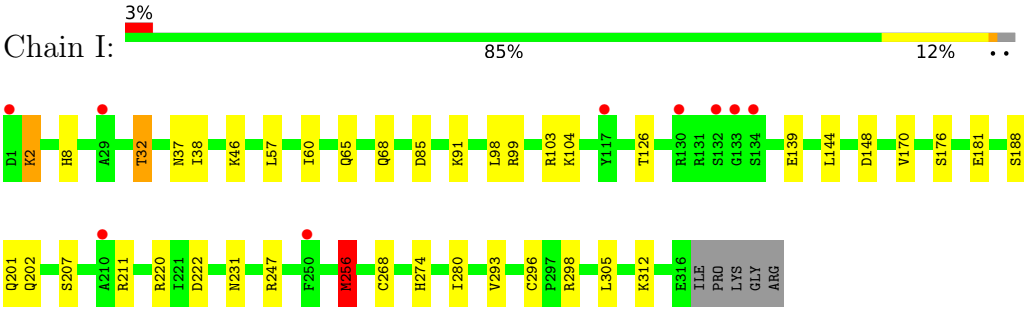


• Molecule 1: Hemagglutinin HA1 chain

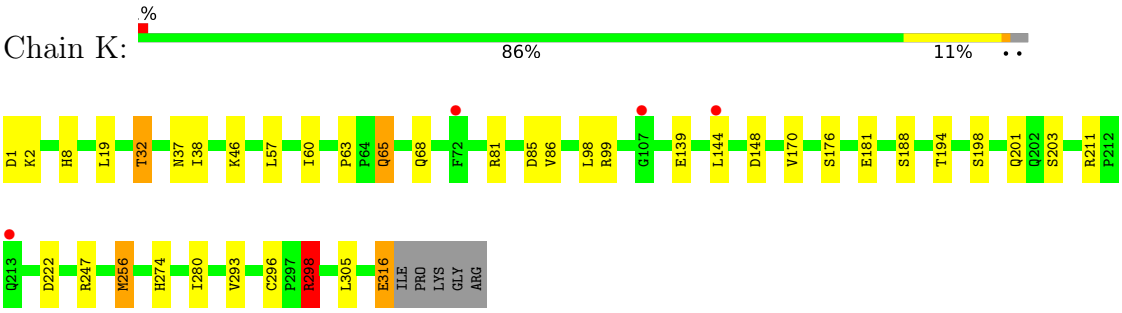




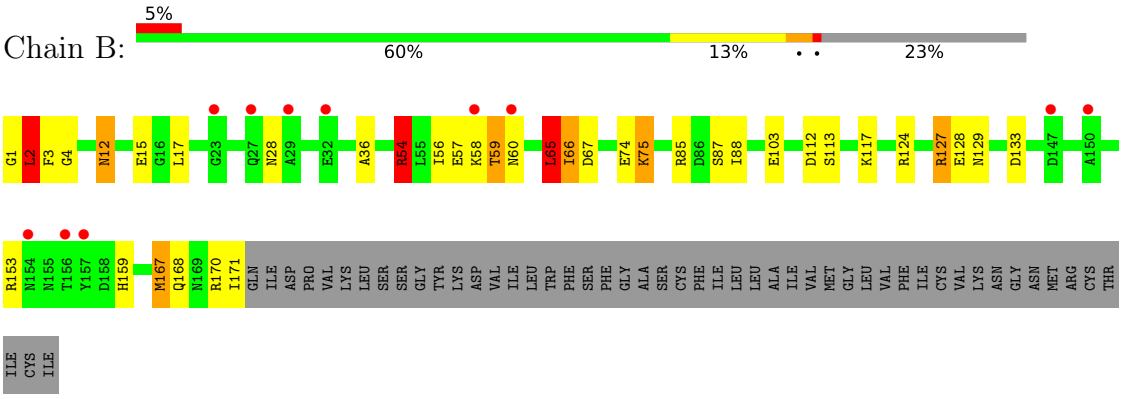
• Molecule 1: Hemagglutinin HA1 chain



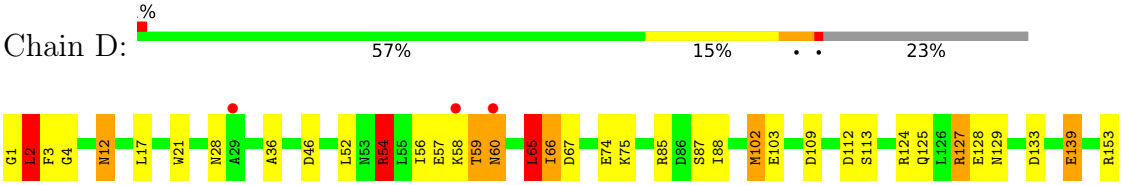
• Molecule 1: Hemagglutinin HA1 chain

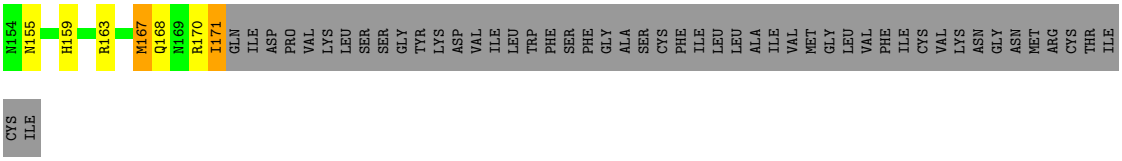


• Molecule 2: Hemagglutinin HA2 chain

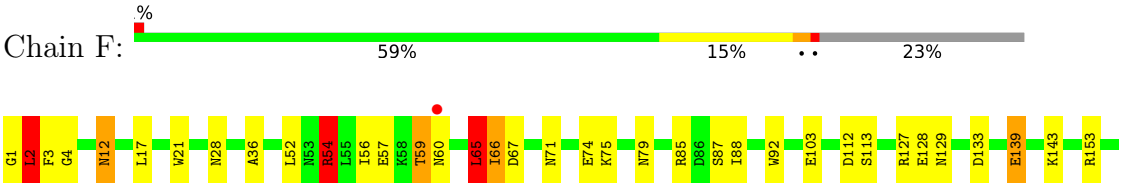


• Molecule 2: Hemagglutinin HA2 chain

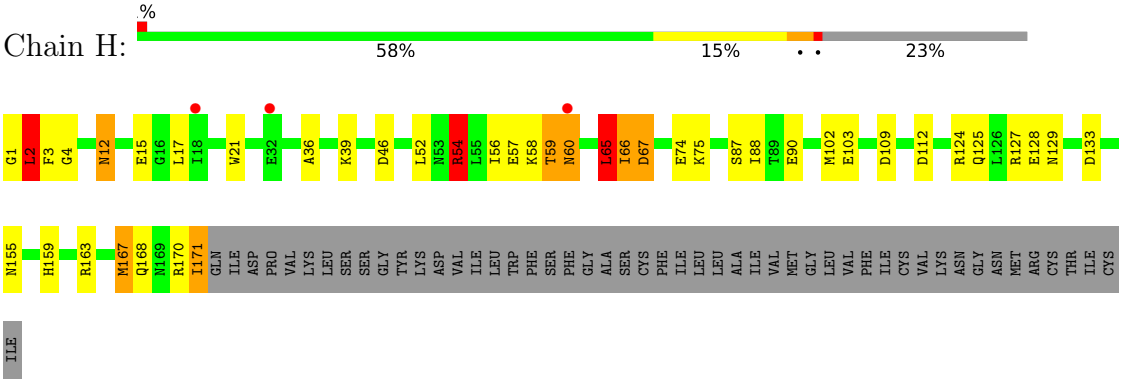




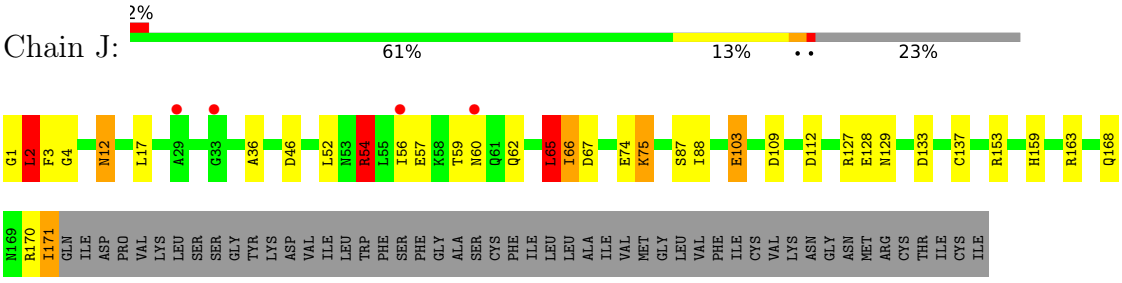
• Molecule 2: Hemagglutinin HA2 chain



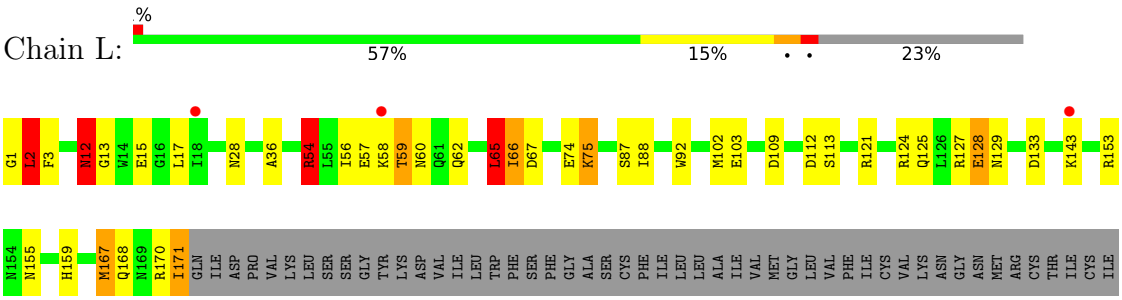
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.01Å 97.53Å 191.81Å 90.00° 108.58° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 47.35 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.95) 93.2 (47.35-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.236 , 0.267 0.235 , 0.265	Depositor DCC
R_{free} test set	3659 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 11.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22940	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: 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	0.83	2/2459 (0.1%)	0.97	8/3322 (0.2%)
1	C	0.73	2/2459 (0.1%)	0.93	5/3322 (0.2%)
1	E	0.74	0/2459	0.96	7/3322 (0.2%)
1	G	0.74	4/2459 (0.2%)	0.94	7/3322 (0.2%)
1	I	0.77	1/2459 (0.0%)	0.97	6/3322 (0.2%)
1	K	0.70	0/2459	0.94	4/3322 (0.1%)
2	B	0.84	3/1411 (0.2%)	1.00	7/1901 (0.4%)
2	D	0.84	2/1411 (0.1%)	1.07	10/1901 (0.5%)
2	F	0.87	4/1411 (0.3%)	1.01	4/1901 (0.2%)
2	H	0.84	1/1411 (0.1%)	1.06	8/1901 (0.4%)
2	J	0.85	3/1411 (0.2%)	1.01	7/1901 (0.4%)
2	L	0.88	4/1411 (0.3%)	1.06	8/1901 (0.4%)
All	All	0.79	26/23220 (0.1%)	0.98	81/31338 (0.3%)

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
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
All	All	0	6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	74	GLU	CD-OE1	9.98	1.36	1.25
1	A	268	CYS	CB-SG	8.50	1.96	1.82
1	C	1	ASP	CB-CG	7.47	1.67	1.51
1	I	268	CYS	CB-SG	-7.30	1.69	1.82
1	G	1	ASP	CB-CG	7.27	1.67	1.51
2	D	74	GLU	CG-CD	6.96	1.62	1.51
1	G	316	GLU	CG-CD	6.94	1.62	1.51
2	F	74	GLU	CD-OE1	6.80	1.33	1.25
2	F	74	GLU	CG-CD	6.54	1.61	1.51
2	H	74	GLU	CG-CD	6.52	1.61	1.51
2	J	74	GLU	CG-CD	6.41	1.61	1.51
2	L	74	GLU	CD-OE1	6.39	1.32	1.25
2	L	74	GLU	CG-CD	6.25	1.61	1.51
2	B	74	GLU	CG-CD	6.04	1.61	1.51
2	B	15	GLU	CD-OE2	6.01	1.32	1.25
1	G	316	GLU	CD-OE2	-5.93	1.19	1.25
1	C	316	GLU	CG-CD	5.64	1.60	1.51
2	B	15	GLU	CG-CD	5.63	1.60	1.51
1	A	316	GLU	CG-CD	5.54	1.60	1.51
2	L	15	GLU	CG-CD	5.34	1.59	1.51
2	L	128	GLU	CD-OE1	5.33	1.31	1.25
2	D	139	GLU	CD-OE1	-5.28	1.19	1.25
2	J	103	GLU	CD-OE1	-5.21	1.20	1.25
1	G	1	ASP	N-CA	5.17	1.56	1.46
2	F	139	GLU	CD-OE1	-5.14	1.20	1.25
2	F	139	GLU	CG-CD	5.01	1.59	1.51

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	99	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	I	99	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	E	99	ARG	NE-CZ-NH1	9.45	125.02	120.30
2	D	54	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	1	ASP	CB-CG-OD1	8.39	125.85	118.30
2	H	109	ASP	CB-CG-OD2	8.04	125.54	118.30
2	L	109	ASP	CB-CG-OD2	7.76	125.29	118.30
1	E	268	CYS	CA-CB-SG	7.74	127.93	114.00
2	D	124	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	I	298	ARG	NE-CZ-NH2	-7.66	116.47	120.30
2	F	85	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	D	109	ASP	CB-CG-OD2	7.46	125.01	118.30
2	J	109	ASP	CB-CG-OD2	7.39	124.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	CYS	CA-CB-SG	-7.36	100.76	114.00
1	I	99	ARG	NE-CZ-NH2	-7.31	116.64	120.30
2	L	54	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	G	316	GLU	OE1-CD-OE2	-7.18	114.68	123.30
1	A	85	ASP	CB-CG-OD2	-6.82	112.17	118.30
2	B	127	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	I	220	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	B	54	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	103	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	D	85	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	L	124	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	L	121	ARG	NE-CZ-NH2	-6.37	117.11	120.30
2	F	54	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	L	153	ARG	NE-CZ-NH2	-6.27	117.17	120.30
2	H	102	MET	CG-SD-CE	-6.15	90.36	100.20
1	G	103	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	K	99	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	B	153	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	B	65	LEU	CA-CB-CG	5.89	128.85	115.30
1	G	1	ASP	CB-CG-OD1	5.87	123.59	118.30
2	F	65	LEU	CA-CB-CG	5.82	128.70	115.30
2	J	153	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	G	312	LYS	CD-CE-NZ	-5.76	98.46	111.70
2	D	102	MET	CG-SD-CE	-5.75	90.99	100.20
2	B	54	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	F	153	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	J	65	LEU	CA-CB-CG	5.75	128.51	115.30
1	I	103	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	I	256	MET	CA-CB-CG	5.68	122.95	113.30
1	A	316	GLU	OE1-CD-OE2	-5.62	116.56	123.30
2	L	54	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	103	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	K	298	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	256	MET	CA-CB-CG	5.57	122.77	113.30
1	A	103	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	G	298	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	H	65	LEU	CB-CG-CD1	5.56	120.45	111.00
1	G	256	MET	CA-CB-CG	5.53	122.70	113.30
2	D	127	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	268	CYS	CA-CB-SG	-5.51	104.09	114.00
1	A	256	MET	CA-CB-CG	5.51	122.66	113.30
2	H	54	ARG	NE-CZ-NH2	-5.48	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	163	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	D	46	ASP	CB-CG-OD1	-5.44	113.41	118.30
2	B	124	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	E	222	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	256	MET	CA-CB-CG	5.39	122.47	113.30
2	H	46	ASP	CB-CG-OD2	5.37	123.14	118.30
1	K	81	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	J	74	GLU	CG-CD-OE2	-5.32	107.66	118.30
2	L	65	LEU	CB-CG-CD1	5.29	119.99	111.00
2	H	163	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	J	46	ASP	CB-CG-OD2	5.28	123.06	118.30
1	C	99	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	103	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	85	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	99	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	H	67	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	G	47	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	J	54	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	E	130	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	J	163	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	222	ASP	CB-CG-OD2	5.10	122.89	118.30
2	L	12	ASN	N-CA-C	5.09	124.73	111.00
2	D	65	LEU	CA-CB-CG	5.03	126.86	115.30
2	D	153	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	222	ASP	CB-CA-C	5.01	120.42	110.40
2	H	124	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ASP	Peptide
1	C	85	ASP	Peptide
1	E	85	ASP	Peptide
1	G	85	ASP	Peptide
1	I	85	ASP	Peptide
1	K	85	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2413	0	2387	22	0
1	C	2413	0	2387	23	0
1	E	2413	0	2387	22	0
1	G	2413	0	2387	27	0
1	I	2413	0	2387	23	0
1	K	2413	0	2388	30	0
2	B	1387	0	1293	21	0
2	D	1387	0	1294	24	0
2	F	1387	0	1293	21	0
2	H	1387	0	1293	25	0
2	J	1387	0	1293	22	0
2	L	1387	0	1293	24	0
3	A	14	0	13	0	0
3	B	14	0	13	2	0
3	C	14	0	13	0	0
3	E	14	0	13	2	0
3	F	14	0	13	1	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	1	0
3	J	14	0	13	0	0
3	L	14	0	13	0	0
All	All	22940	0	22212	214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (214) 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:201:GLN:NE2	1:K:222:ASP:HB3	1.70	1.06
1:A:201:GLN:HE21	1:I:222:ASP:HB3	1.15	1.04
1:C:201:GLN:HE21	1:K:222:ASP:HB3	1.14	1.04
1:E:222:ASP:HB3	1:I:201:GLN:NE2	1.87	0.89
1:A:201:GLN:NE2	1:I:222:ASP:HB3	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HD12	1:A:280:ILE:HD12	1.58	0.85
2:D:167:MET:SD	2:L:171:ILE:HG23	2.17	0.83
1:C:222:ASP:HB3	1:G:201:GLN:NE2	1.94	0.83
1:A:101:ILE:HD11	2:J:75:LYS:HD2	1.62	0.81
2:H:171:ILE:HG23	2:L:167:MET:SD	2.22	0.80
1:I:293:VAL:HG11	2:J:65:LEU:HD13	1.65	0.78
1:C:38:ILE:HD12	1:C:280:ILE:HD12	1.65	0.78
1:E:38:ILE:HD12	1:E:280:ILE:HD12	1.63	0.78
1:K:38:ILE:HD12	1:K:280:ILE:HD12	1.65	0.76
1:I:38:ILE:HD12	1:I:280:ILE:HD12	1.66	0.75
1:C:222:ASP:HB3	1:G:201:GLN:HE21	1.50	0.74
1:G:38:ILE:HD12	1:G:280:ILE:HD12	1.67	0.74
2:D:171:ILE:HG23	2:H:167:MET:SD	2.28	0.72
1:K:293:VAL:HG11	2:L:65:LEU:HD13	1.72	0.72
1:E:1:ASP:OD2	2:F:28:ASN:HA	1.91	0.71
1:G:293:VAL:HG11	2:H:65:LEU:HD13	1.72	0.70
1:E:293:VAL:HG11	2:F:65:LEU:HD13	1.74	0.69
2:D:54:ARG:NH2	2:D:103:GLU:OE2	2.26	0.68
1:E:222:ASP:HB3	1:I:201:GLN:HE22	1.56	0.68
1:G:207:SER:HB2	1:K:203:SER:HB2	1.76	0.68
2:L:54:ARG:NH2	2:L:103:GLU:OE2	2.26	0.68
2:J:54:ARG:NH2	2:J:103:GLU:OE2	2.27	0.67
2:F:54:ARG:NH2	2:F:103:GLU:OE2	2.27	0.67
2:H:54:ARG:NH2	2:H:103:GLU:OE2	2.28	0.67
1:G:60:ILE:HG21	1:G:170:VAL:HG21	1.77	0.66
1:G:207:SER:CB	1:K:203:SER:HB2	2.25	0.66
1:E:95:GLU:OE1	2:F:71:ASN:ND2	2.29	0.66
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.29	0.66
1:I:60:ILE:HG21	1:I:170:VAL:HG21	1.77	0.65
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.78	0.65
1:E:60:ILE:HG21	1:E:170:VAL:HG21	1.77	0.65
1:A:57:LEU:HD22	1:A:98:LEU:HD23	1.78	0.65
1:C:101:ILE:HD11	2:L:75:LYS:HD2	1.78	0.65
1:E:296:CYS:O	2:F:59:THR:HG21	1.97	0.65
1:C:60:ILE:HG21	1:C:170:VAL:HG21	1.79	0.64
1:G:296:CYS:O	2:H:59:THR:HG21	1.99	0.63
1:K:60:ILE:HG21	1:K:170:VAL:HG21	1.79	0.62
1:G:57:LEU:HD22	1:G:98:LEU:HD23	1.82	0.61
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.82	0.61
2:B:167:MET:SD	2:J:171:ILE:HG23	2.40	0.60
1:G:316:GLU:OE1	2:H:15:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLN:HE21	1:K:222:ASP:CB	2.02	0.60
1:G:220:ARG:HH21	1:K:198:SER:HA	1.66	0.60
1:A:222:ASP:OD1	1:E:201:GLN:NE2	2.35	0.60
1:C:293:VAL:HG11	2:D:65:LEU:HD13	1.84	0.60
1:C:57:LEU:HD22	1:C:98:LEU:HD23	1.84	0.59
1:E:57:LEU:HD22	1:E:98:LEU:HD23	1.85	0.56
1:K:57:LEU:HD22	1:K:98:LEU:HD23	1.87	0.56
1:K:296:CYS:O	2:L:59:THR:HG21	2.05	0.56
2:B:113:SER:OG	2:J:2:LEU:HA	2.07	0.54
1:G:139:GLU:OE1	1:G:247:ARG:HD3	2.08	0.54
1:K:19:LEU:CD1	2:L:102:MET:HA	2.37	0.54
2:D:88:ILE:HD13	2:L:87:SER:HB3	1.90	0.54
1:I:57:LEU:HD22	1:I:98:LEU:HD23	1.89	0.54
1:A:139:GLU:OE1	1:A:247:ARG:HD3	2.08	0.53
1:K:139:GLU:OE1	1:K:247:ARG:HD3	2.08	0.53
2:J:128:GLU:HG3	2:J:170:ARG:HH12	1.74	0.53
1:I:139:GLU:OE1	1:I:247:ARG:HD3	2.08	0.53
1:C:60:ILE:HG21	1:C:170:VAL:CG2	2.39	0.52
1:C:139:GLU:OE1	1:C:247:ARG:HD3	2.09	0.52
1:I:293:VAL:CG1	2:J:65:LEU:HD13	2.37	0.52
1:E:222:ASP:HB3	1:I:201:GLN:HE21	1.71	0.52
1:C:296:CYS:O	2:D:59:THR:HG21	2.10	0.52
2:L:128:GLU:HG3	2:L:170:ARG:HH12	1.75	0.52
2:D:2:LEU:O	2:D:112:ASP:OD2	2.28	0.52
2:F:2:LEU:O	2:F:112:ASP:OD2	2.28	0.52
1:E:139:GLU:OE1	1:E:247:ARG:HD3	2.09	0.52
1:I:296:CYS:O	2:J:59:THR:HG21	2.10	0.51
1:A:201:GLN:CD	1:I:91:LYS:HG2	2.31	0.51
1:G:60:ILE:HG21	1:G:170:VAL:CG2	2.39	0.51
1:A:60:ILE:HG21	1:A:170:VAL:CG2	2.40	0.51
2:B:2:LEU:O	2:B:112:ASP:OD2	2.28	0.51
1:E:60:ILE:HG21	1:E:170:VAL:CG2	2.40	0.51
2:H:2:LEU:O	2:H:112:ASP:OD2	2.29	0.51
1:A:207:SER:HB2	1:E:203:SER:HB2	1.93	0.50
2:J:2:LEU:O	2:J:112:ASP:OD2	2.29	0.50
2:L:17:LEU:HD11	2:L:36:ALA:HB2	1.93	0.50
2:B:17:LEU:HD11	2:B:36:ALA:HB2	1.94	0.50
1:A:296:CYS:O	2:B:59:THR:HG21	2.11	0.50
2:F:128:GLU:HG3	2:F:170:ARG:HH12	1.76	0.50
2:H:128:GLU:HG3	2:H:170:ARG:HH12	1.77	0.50
2:B:128:GLU:HG3	2:B:170:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:GLY:C	2:J:2:LEU:O	2.50	0.49
1:K:60:ILE:HG21	1:K:170:VAL:CG2	2.42	0.49
1:I:60:ILE:HG21	1:I:170:VAL:CG2	2.43	0.49
1:G:60:ILE:CG2	1:G:170:VAL:HG21	2.42	0.49
2:L:1:GLY:C	2:L:2:LEU:O	2.51	0.49
2:L:2:LEU:O	2:L:112:ASP:OD2	2.29	0.49
1:I:231:ASN:ND2	3:I:401:NAG:O7	2.45	0.49
2:B:75:LYS:HE2	3:B:301:NAG:H83	1.95	0.49
2:H:1:GLY:C	2:H:2:LEU:O	2.51	0.49
2:J:17:LEU:HD11	2:J:36:ALA:HB2	1.94	0.49
1:K:316:GLU:OE1	2:L:13:GLY:O	2.31	0.49
2:D:66:ILE:HD13	2:D:66:ILE:H	1.78	0.48
2:B:88:ILE:HD13	2:J:87:SER:HB3	1.94	0.48
2:F:1:GLY:C	2:F:2:LEU:O	2.51	0.48
2:H:17:LEU:HD11	2:H:36:ALA:HB2	1.95	0.48
2:B:2:LEU:HA	2:F:113:SER:OG	2.14	0.48
2:J:66:ILE:HD13	2:J:66:ILE:H	1.77	0.48
2:D:113:SER:OG	2:L:2:LEU:HA	2.13	0.48
1:E:231:ASN:ND2	3:E:401:NAG:O7	2.47	0.48
1:E:310:GLY:HA2	2:F:21:TRP:CH2	2.49	0.48
2:H:66:ILE:HD13	2:H:66:ILE:H	1.78	0.48
1:A:256:MET:HB2	1:A:256:MET:HE2	1.67	0.48
2:D:58:LYS:HE3	2:D:60:ASN:ND2	2.29	0.48
2:D:102:MET:CE	1:K:19:LEU:HD21	2.44	0.48
1:E:60:ILE:CG2	1:E:170:VAL:HG21	2.44	0.48
1:I:60:ILE:CG2	1:I:170:VAL:HG21	2.42	0.48
2:B:1:GLY:C	2:B:2:LEU:O	2.51	0.47
1:I:2:LYS:HE3	2:J:137:CYS:HB3	1.95	0.47
2:D:17:LEU:HD11	2:D:36:ALA:HB2	1.96	0.47
1:E:21:GLU:OE1	1:E:24:VAL:HG12	2.15	0.47
2:L:66:ILE:HD13	2:L:66:ILE:H	1.80	0.47
2:D:1:GLY:C	2:D:2:LEU:O	2.51	0.47
1:G:310:GLY:HA2	2:H:21:TRP:CH2	2.50	0.47
2:F:87:SER:HB3	2:J:88:ILE:HD13	1.97	0.47
2:F:66:ILE:HD13	2:F:66:ILE:H	1.80	0.47
2:D:87:SER:HB3	2:H:88:ILE:HD13	1.98	0.46
1:K:60:ILE:CG2	1:K:170:VAL:HG21	2.43	0.46
2:B:66:ILE:HD13	2:B:66:ILE:H	1.80	0.46
2:L:3:PHE:HB2	2:L:112:ASP:OD2	2.16	0.46
1:A:60:ILE:CG2	1:A:170:VAL:HG21	2.46	0.46
1:G:222:ASP:HB3	1:K:201:GLN:HE22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:PHE:HB2	2:H:112:ASP:OD2	2.16	0.46
1:E:298:ARG:HG2	2:F:92:TRP:CE2	2.50	0.46
2:H:87:SER:HB3	2:L:88:ILE:HD13	1.98	0.46
1:C:60:ILE:CG2	1:C:170:VAL:HG21	2.44	0.46
2:D:128:GLU:HG3	2:D:170:ARG:HH12	1.80	0.46
2:J:3:PHE:HB2	2:J:112:ASP:OD2	2.16	0.46
2:L:56:ILE:HG22	2:L:56:ILE:O	2.17	0.45
2:D:56:ILE:O	2:D:56:ILE:HG22	2.16	0.45
2:F:79:ASN:OD1	3:F:301:NAG:H82	2.16	0.45
2:J:56:ILE:HG22	2:J:56:ILE:O	2.17	0.45
2:B:3:PHE:HB2	2:B:112:ASP:OD2	2.16	0.45
1:G:222:ASP:HB3	1:K:201:GLN:NE2	2.31	0.45
2:H:56:ILE:HG22	2:H:56:ILE:O	2.17	0.45
1:K:256:MET:HE3	2:L:62:GLN:NE2	2.32	0.45
1:C:1:ASP:OD2	2:D:28:ASN:HA	2.16	0.45
2:F:17:LEU:HD11	2:F:36:ALA:HB2	1.97	0.45
2:F:56:ILE:O	2:F:56:ILE:HG22	2.17	0.45
1:I:256:MET:HE3	2:J:62:GLN:NE2	2.32	0.45
2:F:3:PHE:HB2	2:F:112:ASP:OD2	2.16	0.45
2:B:56:ILE:HG22	2:B:56:ILE:O	2.17	0.45
2:D:3:PHE:HB2	2:D:112:ASP:OD2	2.16	0.45
1:C:256:MET:HB2	1:C:256:MET:HE2	1.67	0.44
2:J:2:LEU:O	2:J:4:GLY:N	2.49	0.44
1:E:231:ASN:HD22	3:E:401:NAG:C7	2.30	0.44
1:G:32:THR:HG22	1:G:305:LEU:HB2	2.00	0.44
1:G:21:GLU:OE1	1:G:24:VAL:HG12	2.17	0.44
1:G:207:SER:HB3	1:K:203:SER:HB2	1.99	0.44
2:H:58:LYS:HE3	2:H:60:ASN:ND2	2.33	0.44
2:D:2:LEU:O	2:D:4:GLY:N	2.49	0.44
1:A:192:LEU:HD11	1:I:207:SER:HB2	1.99	0.43
2:H:52:LEU:HD12	2:H:52:LEU:HA	1.89	0.43
2:L:127:ARG:HG3	2:L:159:HIS:CG	2.53	0.43
1:A:1:ASP:CG	2:B:28:ASN:HA	2.39	0.43
2:F:52:LEU:HD12	2:F:52:LEU:HA	1.90	0.43
1:G:222:ASP:OD1	1:K:201:GLN:NE2	2.48	0.43
2:D:127:ARG:HG3	2:D:159:HIS:CG	2.54	0.43
2:H:2:LEU:O	2:H:4:GLY:N	2.50	0.43
2:F:127:ARG:HG3	2:F:159:HIS:CG	2.53	0.43
1:G:293:VAL:CG1	2:H:65:LEU:HD13	2.44	0.43
2:B:127:ARG:HG3	2:B:159:HIS:CG	2.54	0.43
1:G:38:ILE:CD1	1:G:280:ILE:HD12	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:SER:HB3	2:F:88:ILE:HD13	2.00	0.42
1:E:32:THR:HG22	1:E:305:LEU:HB2	2.01	0.42
1:I:32:THR:HG22	1:I:305:LEU:HB2	2.01	0.42
1:C:37:ASN:ND2	1:C:274:HIS:NE2	2.67	0.42
2:F:2:LEU:O	2:F:4:GLY:N	2.49	0.42
1:A:37:ASN:ND2	1:A:274:HIS:NE2	2.67	0.42
1:G:37:ASN:ND2	1:G:274:HIS:NE2	2.68	0.42
2:H:90:GLU:OE1	1:K:298:ARG:NH2	2.53	0.42
1:I:37:ASN:ND2	1:I:274:HIS:NE2	2.67	0.42
2:J:52:LEU:HD12	2:J:52:LEU:HA	1.90	0.42
1:G:32:THR:HB	1:G:305:LEU:O	2.20	0.42
1:K:37:ASN:ND2	1:K:274:HIS:NE2	2.68	0.42
2:J:127:ARG:HG3	2:J:159:HIS:CG	2.54	0.42
2:D:52:LEU:HD12	2:D:52:LEU:HA	1.91	0.42
1:E:37:ASN:ND2	1:E:274:HIS:NE2	2.67	0.42
1:C:32:THR:HB	1:C:305:LEU:O	2.19	0.42
2:H:127:ARG:HG3	2:H:159:HIS:CG	2.55	0.42
1:C:32:THR:HG22	1:C:305:LEU:HB2	2.02	0.41
1:K:298:ARG:HG2	2:L:92:TRP:CE2	2.55	0.41
1:A:201:GLN:HG2	1:I:91:LYS:HD3	2.02	0.41
1:C:63:PRO:HB2	1:C:65:GLN:OE1	2.21	0.41
1:C:310:GLY:HA2	2:D:21:TRP:CH2	2.55	0.41
1:K:38:ILE:CD1	1:K:280:ILE:HD12	2.43	0.41
1:A:32:THR:HG22	1:A:305:LEU:HB2	2.02	0.41
2:H:2:LEU:HA	2:L:113:SER:OG	2.21	0.41
1:C:38:ILE:CD1	1:C:280:ILE:HD12	2.43	0.41
2:B:128:GLU:O	2:B:170:ARG:NH1	2.53	0.41
1:K:32:THR:HG22	1:K:305:LEU:HB2	2.01	0.41
2:L:125:GLN:NE2	2:L:155:ASN:HA	2.36	0.41
1:I:32:THR:HB	1:I:305:LEU:O	2.21	0.41
1:K:32:THR:HB	1:K:305:LEU:O	2.20	0.41
1:A:32:THR:HB	1:A:305:LEU:O	2.21	0.41
2:B:2:LEU:O	2:B:4:GLY:N	2.49	0.41
2:D:125:GLN:NE2	2:D:155:ASN:HA	2.36	0.41
1:G:63:PRO:HB2	1:G:65:GLN:OE1	2.21	0.41
2:H:128:GLU:O	2:H:170:ARG:NH1	2.52	0.40
1:K:63:PRO:HB2	1:K:65:GLN:OE1	2.22	0.40
2:H:125:GLN:NE2	2:H:155:ASN:HA	2.36	0.40
2:J:66:ILE:HD13	2:J:66:ILE:N	2.36	0.40
1:A:63:PRO:HB2	1:A:65:GLN:OE1	2.22	0.40
2:B:75:LYS:HE2	3:B:301:NAG:C8	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ILE:HD13	2:D:66:ILE:N	2.37	0.40
1:G:170:VAL:O	1:G:245:PRO:HB3	2.22	0.40
1:C:226:LEU:C	1:C:226:LEU:HD12	2.42	0.40
1:K:1:ASP:OD2	2:L:28:ASN:HA	2.22	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	314/321 (98%)	298 (95%)	16 (5%)	0	100	100
1	C	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	E	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	G	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	I	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
1	K	314/321 (98%)	299 (95%)	15 (5%)	0	100	100
2	B	169/221 (76%)	155 (92%)	12 (7%)	2 (1%)	13	43
2	D	169/221 (76%)	155 (92%)	12 (7%)	2 (1%)	13	43
2	F	169/221 (76%)	155 (92%)	12 (7%)	2 (1%)	13	43
2	H	169/221 (76%)	156 (92%)	11 (6%)	2 (1%)	13	43
2	J	169/221 (76%)	156 (92%)	11 (6%)	2 (1%)	13	43
2	L	169/221 (76%)	157 (93%)	10 (6%)	2 (1%)	13	43
All	All	2898/3252 (89%)	2727 (94%)	159 (6%)	12 (0%)	34	69

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	ASN
2	D	12	ASN
2	F	12	ASN
2	H	12	ASN
2	J	12	ASN
2	L	12	ASN
2	B	2	LEU
2	D	2	LEU
2	F	2	LEU
2	H	2	LEU
2	J	2	LEU
2	L	2	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/269 (98%)	243 (92%)	22 (8%)	11	35
1	C	265/269 (98%)	242 (91%)	23 (9%)	10	33
1	E	265/269 (98%)	244 (92%)	21 (8%)	12	37
1	G	265/269 (98%)	246 (93%)	19 (7%)	14	42
1	I	265/269 (98%)	247 (93%)	18 (7%)	16	45
1	K	265/269 (98%)	248 (94%)	17 (6%)	17	47
2	B	146/190 (77%)	129 (88%)	17 (12%)	5	20
2	D	146/190 (77%)	130 (89%)	16 (11%)	6	22
2	F	146/190 (77%)	130 (89%)	16 (11%)	6	22
2	H	146/190 (77%)	130 (89%)	16 (11%)	6	22
2	J	146/190 (77%)	133 (91%)	13 (9%)	9	32
2	L	146/190 (77%)	129 (88%)	17 (12%)	5	20
All	All	2466/2754 (90%)	2251 (91%)	215 (9%)	10	33

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	8	HIS
1	A	14	THR
1	A	19	LEU
1	A	32	THR
1	A	46	LYS
1	A	65	GLN
1	A	68	GLN
1	A	86	VAL
1	A	91	LYS
1	A	132	SER
1	A	144	LEU
1	A	148	ASP
1	A	176	SER
1	A	181	GLU
1	A	188	SER
1	A	194	THR
1	A	211	ARG
1	A	227	ILE
1	A	256	MET
1	A	298	ARG
1	A	312	LYS
2	B	2	LEU
2	B	12	ASN
2	B	54	ARG
2	B	57	GLU
2	B	58	LYS
2	B	59	THR
2	B	60	ASN
2	B	65	LEU
2	B	66	ILE
2	B	67	ASP
2	B	75	LYS
2	B	117	LYS
2	B	129	ASN
2	B	133	ASP
2	B	167	MET
2	B	168	GLN
2	B	171	ILE
1	C	2	LYS
1	C	8	HIS
1	C	19	LEU
1	C	32	THR

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Mol	Chain	Res	Type
1	C	46	LYS
1	C	65	GLN
1	C	68	GLN
1	C	86	VAL
1	C	91	LYS
1	C	144	LEU
1	C	148	ASP
1	C	164	LYS
1	C	176	SER
1	C	181	GLU
1	C	188	SER
1	C	194	THR
1	C	201	GLN
1	C	202	GLN
1	C	211	ARG
1	C	227	ILE
1	C	254	LYS
1	C	256	MET
1	C	312	LYS
2	D	2	LEU
2	D	12	ASN
2	D	54	ARG
2	D	57	GLU
2	D	59	THR
2	D	60	ASN
2	D	65	LEU
2	D	66	ILE
2	D	67	ASP
2	D	75	LYS
2	D	129	ASN
2	D	133	ASP
2	D	139	GLU
2	D	167	MET
2	D	168	GLN
2	D	171	ILE
1	E	2	LYS
1	E	8	HIS
1	E	32	THR
1	E	46	LYS
1	E	65	GLN
1	E	68	GLN
1	E	86	VAL

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Mol	Chain	Res	Type
1	E	91	LYS
1	E	104	LYS
1	E	144	LEU
1	E	148	ASP
1	E	176	SER
1	E	181	GLU
1	E	188	SER
1	E	194	THR
1	E	202	GLN
1	E	211	ARG
1	E	254	LYS
1	E	256	MET
1	E	298	ARG
1	E	312	LYS
2	F	2	LEU
2	F	12	ASN
2	F	54	ARG
2	F	57	GLU
2	F	59	THR
2	F	60	ASN
2	F	65	LEU
2	F	66	ILE
2	F	67	ASP
2	F	75	LYS
2	F	129	ASN
2	F	133	ASP
2	F	139	GLU
2	F	143	LYS
2	F	168	GLN
2	F	171	ILE
1	G	8	HIS
1	G	19	LEU
1	G	32	THR
1	G	46	LYS
1	G	65	GLN
1	G	68	GLN
1	G	86	VAL
1	G	144	LEU
1	G	148	ASP
1	G	176	SER
1	G	181	GLU
1	G	188	SER

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Mol	Chain	Res	Type
1	G	194	THR
1	G	202	GLN
1	G	211	ARG
1	G	227	ILE
1	G	256	MET
1	G	298	ARG
1	G	316	GLU
2	H	2	LEU
2	H	12	ASN
2	H	39	LYS
2	H	54	ARG
2	H	57	GLU
2	H	59	THR
2	H	60	ASN
2	H	65	LEU
2	H	66	ILE
2	H	67	ASP
2	H	75	LYS
2	H	129	ASN
2	H	133	ASP
2	H	167	MET
2	H	168	GLN
2	H	171	ILE
1	I	2	LYS
1	I	8	HIS
1	I	32	THR
1	I	46	LYS
1	I	65	GLN
1	I	68	GLN
1	I	104	LYS
1	I	126	THR
1	I	144	LEU
1	I	148	ASP
1	I	176	SER
1	I	181	GLU
1	I	188	SER
1	I	194	THR
1	I	202	GLN
1	I	211	ARG
1	I	256	MET
1	I	312	LYS
2	J	2	LEU

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Mol	Chain	Res	Type
2	J	12	ASN
2	J	54	ARG
2	J	57	GLU
2	J	60	ASN
2	J	65	LEU
2	J	66	ILE
2	J	67	ASP
2	J	75	LYS
2	J	129	ASN
2	J	133	ASP
2	J	168	GLN
2	J	171	ILE
1	K	2	LYS
1	K	8	HIS
1	K	32	THR
1	K	46	LYS
1	K	65	GLN
1	K	68	GLN
1	K	86	VAL
1	K	144	LEU
1	K	148	ASP
1	K	176	SER
1	K	181	GLU
1	K	188	SER
1	K	194	THR
1	K	211	ARG
1	K	256	MET
1	K	298	ARG
1	K	316	GLU
2	L	2	LEU
2	L	12	ASN
2	L	54	ARG
2	L	57	GLU
2	L	58	LYS
2	L	59	THR
2	L	60	ASN
2	L	65	LEU
2	L	66	ILE
2	L	67	ASP
2	L	75	LYS
2	L	129	ASN
2	L	133	ASP

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Mol	Chain	Res	Type
2	L	143	LYS
2	L	167	MET
2	L	168	GLN
2	L	171	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	154	GLN
1	A	201	GLN
2	B	60	ASN
2	B	62	GLN
1	C	37	ASN
1	C	149	ASN
1	C	154	GLN
1	C	201	GLN
2	D	60	ASN
2	D	62	GLN
1	E	37	ASN
1	E	149	ASN
1	E	154	GLN
2	F	60	ASN
2	F	62	GLN
1	G	37	ASN
1	G	154	GLN
1	G	201	GLN
2	H	60	ASN
2	H	62	GLN
1	I	37	ASN
1	I	149	ASN
1	I	154	GLN
1	I	201	GLN
2	J	60	ASN
2	J	62	GLN
1	K	37	ASN
1	K	149	ASN
1	K	154	GLN
2	L	60	ASN
2	L	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	F	301	2	14,14,15	2.25	5 (35%)	17,19,21	3.35	9 (52%)
3	NAG	J	301	2	14,14,15	1.57	3 (21%)	17,19,21	2.30	7 (41%)
3	NAG	L	301	2	14,14,15	1.36	2 (14%)	17,19,21	1.73	2 (11%)
3	NAG	I	401	1	14,14,15	1.18	1 (7%)	17,19,21	2.97	8 (47%)
3	NAG	B	301	2	14,14,15	1.55	3 (21%)	17,19,21	2.69	8 (47%)
3	NAG	A	401	1	14,14,15	1.73	4 (28%)	17,19,21	3.58	10 (58%)
3	NAG	C	401	1	14,14,15	1.36	2 (14%)	17,19,21	2.85	7 (41%)
3	NAG	E	401	1	14,14,15	2.64	5 (35%)	17,19,21	3.98	8 (47%)
3	NAG	H	301	2	14,14,15	1.53	2 (14%)	17,19,21	3.00	9 (52%)
3	NAG	G	401	1	14,14,15	0.83	0	17,19,21	2.03	5 (29%)

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	F	301	2	-	2/6/23/26	0/1/1/1
3	NAG	J	301	2	-	2/6/23/26	0/1/1/1
3	NAG	L	301	2	-	3/6/23/26	0/1/1/1
3	NAG	I	401	1	-	3/6/23/26	0/1/1/1
3	NAG	B	301	2	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1
3	NAG	E	401	1	-	3/6/23/26	0/1/1/1
3	NAG	H	301	2	-	0/6/23/26	0/1/1/1
3	NAG	G	401	1	-	0/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	NAG	O5-C1	5.64	1.52	1.43
3	E	401	NAG	C4-C5	4.15	1.61	1.53
3	E	401	NAG	O5-C5	4.13	1.51	1.43
3	F	301	NAG	C3-C2	4.04	1.61	1.52
3	F	301	NAG	C4-C3	3.93	1.62	1.52
3	F	301	NAG	C1-C2	3.70	1.57	1.52
3	L	301	NAG	C1-C2	3.41	1.57	1.52
3	J	301	NAG	O5-C1	3.40	1.49	1.43
3	F	301	NAG	O4-C4	3.32	1.50	1.43
3	E	401	NAG	C2-N2	3.22	1.51	1.46
3	F	301	NAG	O5-C1	3.20	1.48	1.43
3	H	301	NAG	C3-C2	3.16	1.59	1.52
3	A	401	NAG	C4-C5	3.13	1.59	1.53
3	C	401	NAG	C1-C2	2.93	1.56	1.52
3	A	401	NAG	O5-C5	2.81	1.49	1.43
3	A	401	NAG	O5-C1	2.71	1.48	1.43
3	C	401	NAG	C2-N2	2.67	1.50	1.46
3	B	301	NAG	O5-C1	2.67	1.48	1.43
3	H	301	NAG	O4-C4	2.53	1.48	1.43
3	A	401	NAG	C1-C2	2.53	1.56	1.52
3	I	401	NAG	C1-C2	2.43	1.56	1.52
3	B	301	NAG	O3-C3	2.42	1.48	1.43
3	E	401	NAG	C6-C5	2.34	1.59	1.51
3	J	301	NAG	C2-N2	2.33	1.50	1.46
3	J	301	NAG	C4-C3	2.21	1.58	1.52
3	B	301	NAG	C4-C5	2.21	1.57	1.53
3	L	301	NAG	O5-C1	2.09	1.47	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	NAG	C1-O5-C5	9.15	124.60	112.19
3	A	401	NAG	C1-O5-C5	8.64	123.89	112.19
3	E	401	NAG	C1-C2-N2	8.22	124.53	110.49
3	A	401	NAG	C1-C2-N2	7.78	123.77	110.49
3	E	401	NAG	C2-N2-C7	7.33	133.34	122.90
3	I	401	NAG	C1-C2-N2	7.15	122.70	110.49
3	F	301	NAG	O4-C4-C3	6.91	126.33	110.35
3	H	301	NAG	C1-O5-C5	6.91	121.55	112.19
3	F	301	NAG	C2-N2-C7	5.95	131.38	122.90
3	B	301	NAG	C1-O5-C5	5.69	119.90	112.19
3	H	301	NAG	O5-C1-C2	-5.51	102.59	111.29
3	I	401	NAG	C2-N2-C7	5.50	130.74	122.90
3	G	401	NAG	C1-O5-C5	5.45	119.58	112.19
3	C	401	NAG	C1-O5-C5	5.42	119.53	112.19
3	I	401	NAG	C1-O5-C5	5.36	119.46	112.19
3	A	401	NAG	C2-N2-C7	5.33	130.49	122.90
3	C	401	NAG	C2-N2-C7	5.28	130.42	122.90
3	C	401	NAG	C3-C4-C5	5.23	119.58	110.24
3	C	401	NAG	C1-C2-N2	4.96	118.97	110.49
3	F	301	NAG	C3-C4-C5	-4.82	101.65	110.24
3	B	301	NAG	O3-C3-C2	4.76	119.31	109.47
3	F	301	NAG	C1-C2-N2	-4.67	102.51	110.49
3	L	301	NAG	C1-O5-C5	4.58	118.40	112.19
3	J	301	NAG	C2-N2-C7	4.32	129.05	122.90
3	J	301	NAG	O5-C5-C6	4.24	113.86	107.20
3	E	401	NAG	O4-C4-C5	4.14	119.57	109.30
3	F	301	NAG	O7-C7-N2	4.04	129.38	121.95
3	B	301	NAG	C4-C3-C2	-4.01	105.13	111.02
3	H	301	NAG	C3-C4-C5	-4.00	103.11	110.24
3	A	401	NAG	O4-C4-C5	3.98	119.19	109.30
3	F	301	NAG	O7-C7-C8	-3.70	115.19	122.06
3	H	301	NAG	C2-N2-C7	3.60	128.03	122.90
3	J	301	NAG	C1-O5-C5	3.50	116.94	112.19
3	E	401	NAG	O5-C5-C6	3.25	112.30	107.20
3	H	301	NAG	C1-C2-N2	-3.19	105.03	110.49
3	B	301	NAG	O7-C7-N2	3.15	127.74	121.95
3	H	301	NAG	O4-C4-C3	3.10	117.52	110.35
3	B	301	NAG	O5-C1-C2	3.09	116.17	111.29
3	E	401	NAG	O6-C6-C5	3.04	121.72	111.29
3	I	401	NAG	C4-C3-C2	-3.01	106.61	111.02
3	J	301	NAG	O4-C4-C3	2.99	117.26	110.35
3	B	301	NAG	C2-N2-C7	2.97	127.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	NAG	O6-C6-C5	-2.91	101.29	111.29
3	G	401	NAG	C4-C3-C2	-2.88	106.80	111.02
3	J	301	NAG	O3-C3-C4	2.83	116.88	110.35
3	G	401	NAG	O3-C3-C2	2.82	115.30	109.47
3	J	301	NAG	O5-C1-C2	2.78	115.69	111.29
3	L	301	NAG	C2-N2-C7	2.78	126.86	122.90
3	F	301	NAG	O5-C5-C6	-2.77	102.86	107.20
3	A	401	NAG	O5-C5-C6	2.76	111.53	107.20
3	G	401	NAG	C1-C2-N2	-2.73	105.83	110.49
3	C	401	NAG	O5-C5-C6	2.64	111.35	107.20
3	I	401	NAG	C6-C5-C4	-2.63	106.86	113.00
3	B	301	NAG	O5-C5-C4	2.61	117.17	110.83
3	H	301	NAG	O5-C5-C6	2.59	111.26	107.20
3	B	301	NAG	O7-C7-C8	-2.53	117.36	122.06
3	F	301	NAG	O3-C3-C2	2.49	114.62	109.47
3	C	401	NAG	O5-C1-C2	-2.45	107.42	111.29
3	H	301	NAG	C4-C3-C2	2.39	114.52	111.02
3	I	401	NAG	O5-C5-C4	2.38	116.63	110.83
3	H	301	NAG	O3-C3-C2	2.37	114.38	109.47
3	E	401	NAG	O3-C3-C4	-2.32	104.98	110.35
3	A	401	NAG	C4-C3-C2	-2.30	107.65	111.02
3	J	301	NAG	O7-C7-C8	-2.21	117.95	122.06
3	A	401	NAG	O6-C6-C5	2.19	118.80	111.29
3	E	401	NAG	C8-C7-N2	2.18	119.78	116.10
3	I	401	NAG	O4-C4-C3	2.16	115.33	110.35
3	I	401	NAG	O3-C3-C2	2.15	113.91	109.47
3	A	401	NAG	O5-C5-C4	2.14	116.04	110.83
3	C	401	NAG	O7-C7-C8	-2.14	118.08	122.06
3	A	401	NAG	C6-C5-C4	-2.12	108.04	113.00
3	G	401	NAG	O4-C4-C5	2.06	114.42	109.30
3	A	401	NAG	O4-C4-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAG	C1-C2-N2-C7
3	C	401	NAG	C3-C2-N2-C7
3	E	401	NAG	C1-C2-N2-C7
3	F	301	NAG	C1-C2-N2-C7
3	I	401	NAG	C1-C2-N2-C7
3	E	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	401	NAG	C4-C5-C6-O6
3	I	401	NAG	C4-C5-C6-O6
3	J	301	NAG	O5-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6
3	I	401	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	J	301	NAG	C4-C5-C6-O6
3	F	301	NAG	C3-C2-N2-C7
3	L	301	NAG	O5-C5-C6-O6
3	L	301	NAG	C3-C2-N2-C7
3	L	301	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	NAG	1	0
3	I	401	NAG	1	0
3	B	301	NAG	2	0
3	E	401	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	316/321 (98%)	-0.11	2 (0%) 89 78	37, 51, 76, 97	1 (0%)
1	C	316/321 (98%)	0.08	9 (2%) 53 36	42, 68, 103, 112	1 (0%)
1	E	316/321 (98%)	-0.11	0 100 100	42, 55, 75, 101	1 (0%)
1	G	316/321 (98%)	0.41	31 (9%) 7 4	43, 80, 142, 160	1 (0%)
1	I	316/321 (98%)	0.17	10 (3%) 47 31	42, 66, 99, 109	1 (0%)
1	K	316/321 (98%)	0.06	4 (1%) 77 61	41, 73, 98, 116	1 (0%)
2	B	171/221 (77%)	0.45	11 (6%) 19 11	41, 75, 110, 128	0
2	D	171/221 (77%)	0.04	3 (1%) 68 51	36, 59, 81, 129	0
2	F	171/221 (77%)	0.09	2 (1%) 79 63	42, 67, 88, 124	0
2	H	171/221 (77%)	0.13	3 (1%) 68 51	39, 57, 95, 125	0
2	J	171/221 (77%)	0.29	4 (2%) 60 43	41, 76, 105, 127	0
2	L	171/221 (77%)	0.05	3 (1%) 68 51	39, 56, 86, 128	0
All	All	2922/3252 (89%)	0.11	82 (2%) 53 36	36, 63, 105, 160	6 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	228	LEU	5.8
2	J	33	GLY	5.4
2	B	60	ASN	5.4
2	D	60	ASN	4.9
1	G	117	TYR	4.9
2	B	156	THR	4.8
2	B	23	GLY	4.6
2	F	60	ASN	4.5
1	G	145	SER	4.4
2	J	60	ASN	4.4
1	G	159	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	190	ASN	4.3
1	G	215	ASN	4.2
1	G	165	SER	4.1
2	J	29	ALA	4.1
1	G	164	LYS	4.1
2	H	18	ILE	4.0
1	G	231	ASN	3.9
2	B	58	LYS	3.7
1	C	166	PRO	3.6
1	I	190	ASN	3.3
1	G	229	ASN	3.3
1	G	186	TYR	3.2
1	G	233	THR	3.2
1	G	196	GLY	3.2
1	G	241	ALA	3.1
1	G	197	SER	3.1
1	G	158	SER	3.0
1	K	107	GLY	3.0
2	H	60	ASN	2.9
2	B	29	ALA	2.9
1	C	165	SER	2.9
1	G	222	ASP	2.9
1	C	144	LEU	2.9
1	G	162	THR	2.8
1	G	236	PHE	2.7
1	I	29	ALA	2.7
2	B	32	GLU	2.7
2	B	147	ASP	2.7
2	L	143	LYS	2.6
2	B	154	ASN	2.6
1	A	8	HIS	2.6
2	B	150	ALA	2.6
2	L	58	LYS	2.6
2	B	157	TYR	2.5
2	J	56	ILE	2.5
1	C	159	TYR	2.5
1	G	154	GLN	2.5
1	G	193	VAL	2.4
1	I	117	TYR	2.4
1	G	240	GLY	2.4
1	I	130	ARG	2.4
1	G	182	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	168	GLN	2.3
1	K	144	LEU	2.3
1	I	1	ASP	2.3
1	G	198	SER	2.3
2	L	18	ILE	2.3
1	G	200	TYR	2.3
2	D	58	LYS	2.2
1	C	236	PHE	2.2
1	G	181	GLU	2.2
2	B	27	GLN	2.2
1	C	248	ALA	2.2
1	G	188	SER	2.2
2	H	32	GLU	2.2
1	G	120	ILE	2.2
1	I	134	SER	2.2
1	C	133	GLY	2.1
1	A	222	ASP	2.1
2	D	29	ALA	2.1
1	I	132	SER	2.1
1	I	210	ALA	2.1
1	G	234	VAL	2.1
1	C	250	PHE	2.1
1	G	160	LYS	2.1
1	C	117	TYR	2.1
1	G	232	ASP	2.0
1	I	250	PHE	2.0
1	K	72	PHE	2.0
1	K	213	GLN	2.0
1	I	133	GLY	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)

There are no monosaccharides in this entry.

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
3	NAG	A	401	14/15	0.67	0.35	92,102,107,107	0
3	NAG	E	401	14/15	0.78	0.17	71,74,78,78	0
3	NAG	F	301	14/15	0.78	0.21	67,68,73,76	0
3	NAG	I	401	14/15	0.78	0.24	97,107,114,115	0
3	NAG	C	401	14/15	0.79	0.46	114,118,120,120	0
3	NAG	B	301	14/15	0.84	0.20	68,70,77,77	0
3	NAG	G	401	14/15	0.85	0.25	77,85,94,95	0
3	NAG	H	301	14/15	0.86	0.19	72,78,86,87	0
3	NAG	J	301	14/15	0.87	0.19	67,71,76,79	0
3	NAG	L	301	14/15	0.87	0.21	85,93,97,100	0

6.5 Other polymers (i)

There are no such residues in this entry.