



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:28 AM UTC

PDB ID : 5KAN / pdb_00005kan
Title : Crystal structure of multidonor HV1-18-class broadly neutralizing Influenza A antibody 16.g.07 in complex with A/Hong Kong/1-4-MA21-1/1968 (H3N2) Hemagglutinin
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-06-01
Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

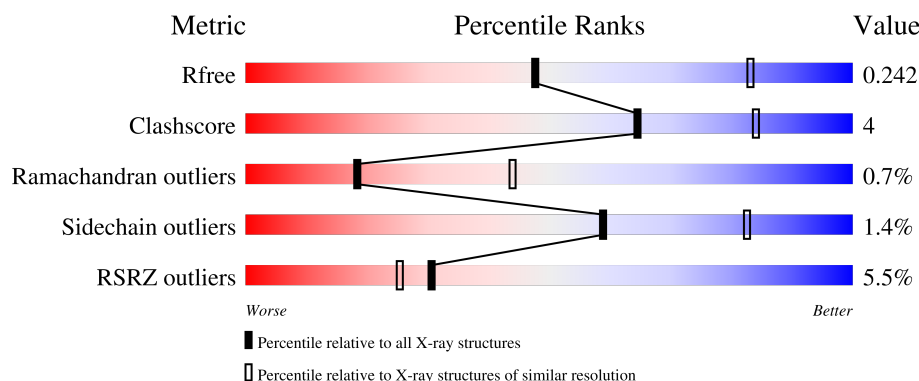
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 $\leq 5\%$. 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	319	
1	C	319	
1	E	319	
2	B	173	

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Mol	Chain	Length	Quality of chain
2	D	173	
2	F	173	
3	G	231	
3	H	231	
3	J	231	
4	I	214	
4	K	214	
4	L	214	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22144 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2467	1544	433	477	13			
1	C	319	Total	C	N	O	S	0	0	0
			2467	1544	433	477	13			
1	E	319	Total	C	N	O	S	0	0	0
			2467	1544	433	477	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLU	GLY	conflict	UNP Q91MA7
C	218	GLU	GLY	conflict	UNP Q91MA7
E	218	GLU	GLY	conflict	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1403	869	248	280	6			
2	D	171	Total	C	N	O	S	0	0	0
			1392	862	246	278	6			
2	F	170	Total	C	N	O	S	3	0	0
			1383	856	244	277	6			

- Molecule 3 is a protein called 16.g.07 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	231	Total	C	N	O	S	1	0	0
			1751	1099	297	345	10			
3	H	231	Total	C	N	O	S	0	0	0
			1751	1099	297	345	10			

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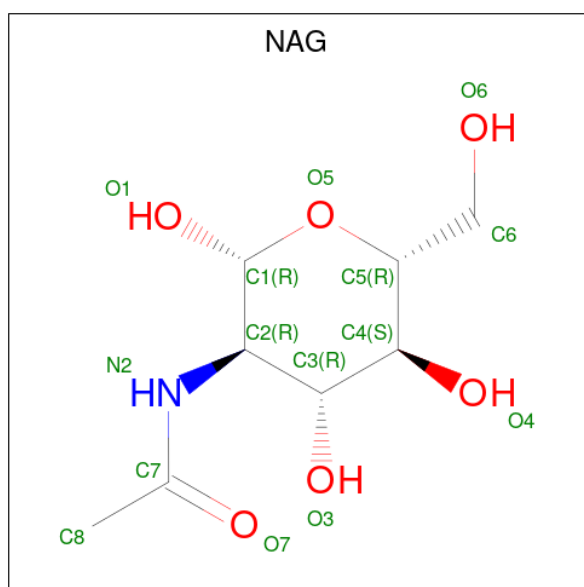
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	231	Total	C	N	O	S	0	0	0
			1751	1099	297	345	10			

- Molecule 4 is a protein called 16.g.07 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	214	Total	C	N	O	S	0	0	0
			1642	1033	278	325	6			
4	K	214	Total	C	N	O	S	0	0	0
			1642	1033	278	325	6			
4	L	214	Total	C	N	O	S	0	0	0
			1642	1033	278	325	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	8	Total	O	0	0
			8	8		
6	C	16	Total	O	0	0
			16	16		
6	D	10	Total	O	0	0
			10	10		
6	E	23	Total	O	0	0
			23	23		
6	F	10	Total	O	0	0
			10	10		
6	G	10	Total	O	0	0
			10	10		

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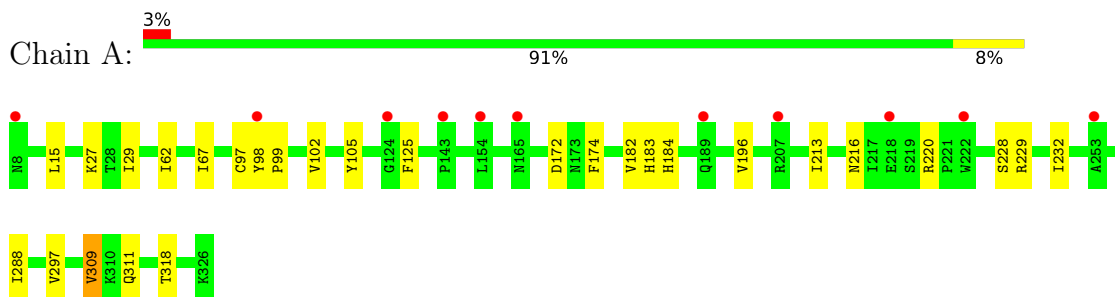
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	11	Total 11	O 11	0	0
6	I	16	Total 16	O 16	0	0
6	J	5	Total 5	O 5	0	0
6	K	8	Total 8	O 8	0	0
6	L	15	Total 15	O 15	0	0

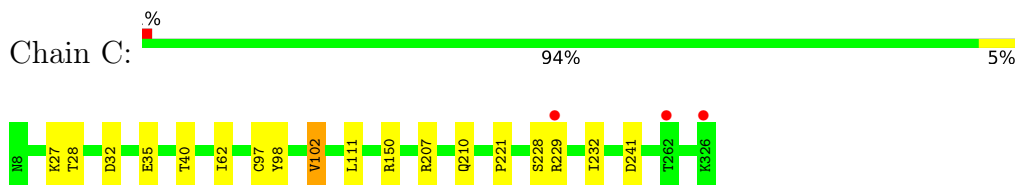
3 Residue-property plots

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.

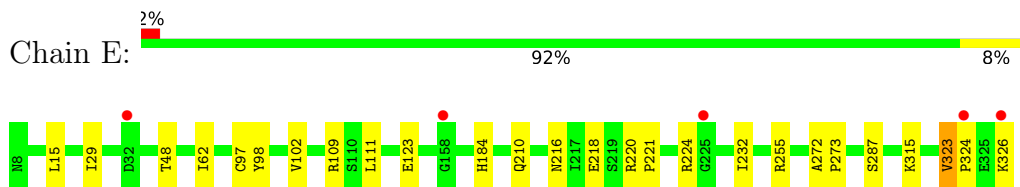
- Molecule 1: Hemagglutinin HA1



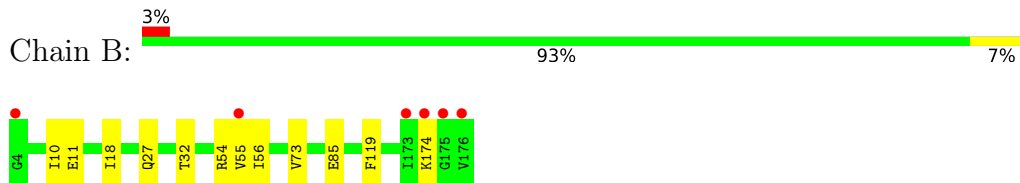
- Molecule 1: Hemagglutinin HA1



- Molecule 1: Hemagglutinin HA1

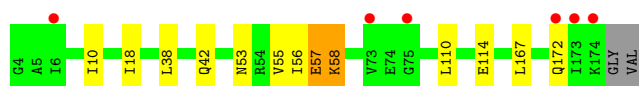


- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2





• Molecule 2: Hemagglutinin HA2



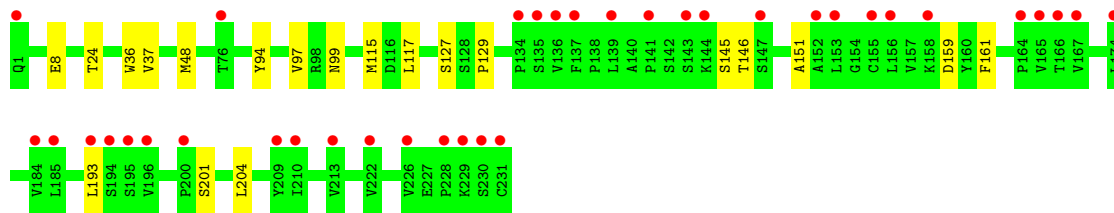
• Molecule 3: 16.g.07 Heavy chain



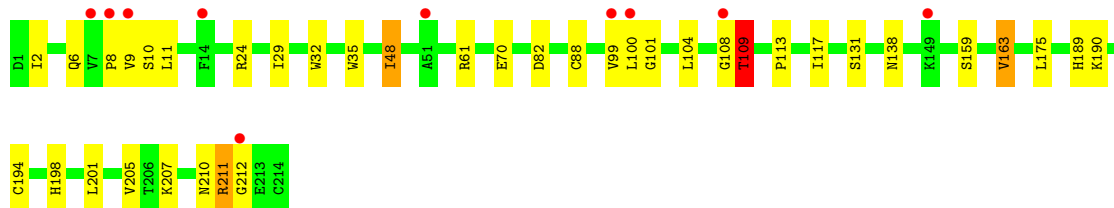
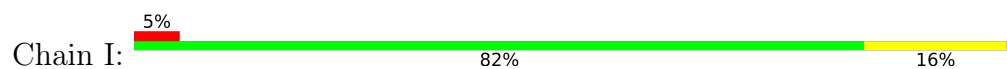
• Molecule 3: 16.g.07 Heavy chain



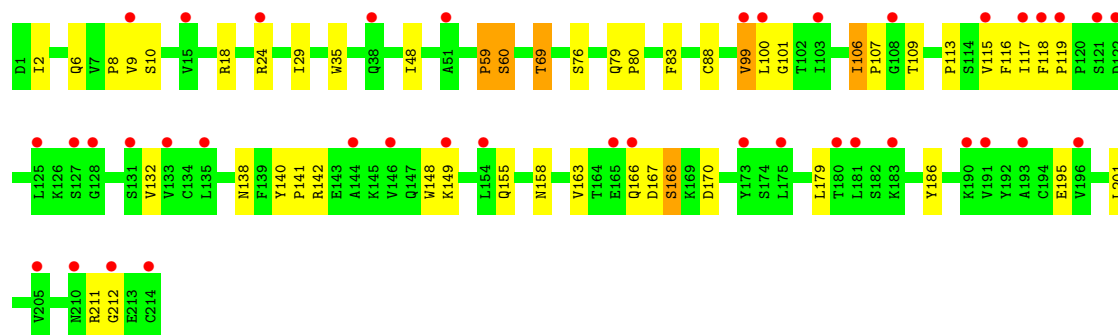
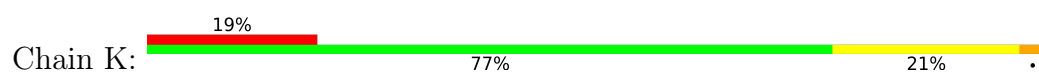
• Molecule 3: 16.g.07 Heavy chain



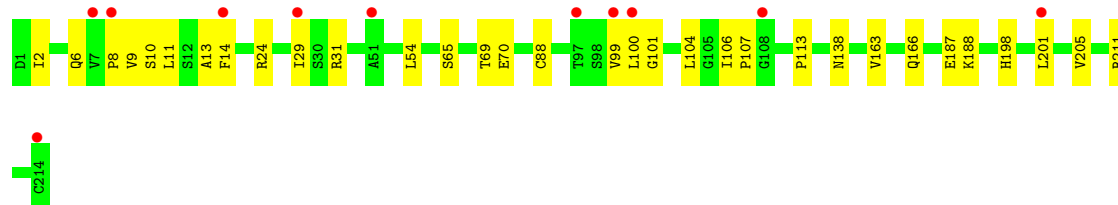
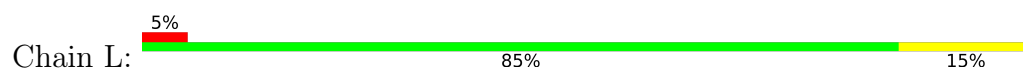
• Molecule 4: 16.g.07 Light chain



• Molecule 4: 16.g.07 Light chain



• Molecule 4: 16.g.07 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.85Å 147.56Å 209.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.67 – 2.79 40.67 – 2.79	Depositor EDS
% Data completeness (in resolution range)	83.2 (40.67-2.79) 83.2 (40.67-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.243 0.219 , 0.242	Depositor DCC
R_{free} test set	4107 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22144	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/2523	0.73	0/3438
1	C	0.33	0/2523	0.71	0/3438
1	E	0.33	0/2523	0.74	3/3438 (0.1%)
2	B	0.32	0/1426	0.75	0/1916
2	D	0.30	0/1415	0.71	1/1901 (0.1%)
2	F	0.31	0/1406	0.74	1/1890 (0.1%)
3	G	0.33	0/1793	0.76	2/2439 (0.1%)
3	H	0.33	0/1793	0.76	3/2439 (0.1%)
3	J	0.36	0/1793	0.78	1/2439 (0.0%)
4	I	0.45	1/1679 (0.1%)	0.83	3/2281 (0.1%)
4	K	0.42	0/1679	0.89	5/2281 (0.2%)
4	L	0.37	0/1679	0.77	0/2281
All	All	0.36	1/22232 (0.0%)	0.76	19/30181 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	211	ARG	CZ-NH1	5.02	1.39	1.32

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	324	PRO	N-CA-C	7.92	124.02	113.40
4	K	168	SER	N-CA-C	7.75	119.51	111.14
3	G	102	GLN	N-CA-C	6.89	121.35	112.12
3	H	128	SER	CA-C-N	-6.63	112.83	119.92
3	H	128	SER	C-N-CA	-6.63	112.83	119.92

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	2467	0	2413	17	0
1	C	2467	0	2415	16	0
1	E	2467	0	2414	17	0
2	B	1403	0	1326	10	0
2	D	1392	0	1314	7	0
2	F	1383	0	1301	6	0
3	G	1751	0	1722	10	0
3	H	1751	0	1722	8	0
3	J	1751	0	1722	9	0
4	I	1642	0	1604	29	0
4	K	1642	0	1604	32	0
4	L	1642	0	1604	25	0
5	A	70	0	65	1	0
5	B	14	0	13	0	0
5	C	56	0	52	1	0
5	D	14	0	13	0	0
5	E	70	0	65	0	0
5	F	14	0	13	0	0
6	A	16	0	0	1	0
6	B	8	0	0	1	0
6	C	16	0	0	4	0
6	D	10	0	0	1	0
6	E	23	0	0	6	0
6	F	10	0	0	1	0
6	G	10	0	0	1	0
6	H	11	0	0	0	0
6	I	16	0	0	6	0
6	J	5	0	0	2	0
6	K	8	0	0	3	0
6	L	15	0	0	3	0
All	All	22144	0	21382	170	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 4.

The worst 5 of 170 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)
4:K:186:TYR:O	4:K:211:ARG:NH1	1.84	1.11
2:B:54:ARG:NH1	1:C:28:THR:O	1.99	0.94
3:J:145:SER:OG	6:J:301:HOH:O	1.88	0.90
4:K:149:LYS:NZ	4:K:195:GLU:OE1	2.08	0.87
2:D:10:ILE:O	6:D:301:HOH:O	1.94	0.86

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	317/319 (99%)	304 (96%)	11 (4%)	2 (1%)	21	47
1	C	317/319 (99%)	306 (96%)	10 (3%)	1 (0%)	36	63
1	E	317/319 (99%)	307 (97%)	9 (3%)	1 (0%)	36	63
2	B	171/173 (99%)	164 (96%)	6 (4%)	1 (1%)	21	47
2	D	169/173 (98%)	160 (95%)	7 (4%)	2 (1%)	10	30
2	F	168/173 (97%)	161 (96%)	6 (4%)	1 (1%)	21	47
3	G	229/231 (99%)	215 (94%)	13 (6%)	1 (0%)	30	57
3	H	229/231 (99%)	214 (93%)	14 (6%)	1 (0%)	30	57
3	J	229/231 (99%)	217 (95%)	12 (5%)	0	100	100
4	I	212/214 (99%)	197 (93%)	12 (6%)	3 (1%)	9	26
4	K	212/214 (99%)	197 (93%)	11 (5%)	4 (2%)	6	19
4	L	212/214 (99%)	197 (93%)	13 (6%)	2 (1%)	14	37
All	All	2782/2811 (99%)	2639 (95%)	124 (4%)	19 (1%)	18	44

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PHE

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Mol	Chain	Res	Type
2	F	58	LYS
3	H	128	SER
4	K	59	PRO
4	I	9	VAL

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	282/282 (100%)	279 (99%)	3 (1%)	65	85
1	C	282/282 (100%)	281 (100%)	1 (0%)	84	93
1	E	282/282 (100%)	278 (99%)	4 (1%)	59	82
2	B	148/148 (100%)	147 (99%)	1 (1%)	76	90
2	D	147/148 (99%)	145 (99%)	2 (1%)	59	82
2	F	146/148 (99%)	145 (99%)	1 (1%)	76	90
3	G	199/199 (100%)	195 (98%)	4 (2%)	48	77
3	H	199/199 (100%)	195 (98%)	4 (2%)	48	77
3	J	199/199 (100%)	194 (98%)	5 (2%)	42	73
4	I	184/184 (100%)	181 (98%)	3 (2%)	55	81
4	K	184/184 (100%)	181 (98%)	3 (2%)	55	81
4	L	184/184 (100%)	182 (99%)	2 (1%)	65	85
All	All	2436/2439 (100%)	2403 (99%)	33 (1%)	59	82

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	K	69	THR
4	K	99	VAL
4	L	163	VAL
3	G	24	THR
2	F	18	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	110	GLN
4	K	210	ASN
4	L	199	GLN
4	L	27	GLN
1	E	33	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
5	NAG	E	404	1	14,14,15	0.35	0	17,19,21	0.38	0
5	NAG	C	403	1	14,14,15	0.48	0	17,19,21	0.42	0
5	NAG	A	404	1	14,14,15	0.31	0	17,19,21	0.34	0
5	NAG	B	201	2	14,14,15	0.32	0	17,19,21	0.70	0
5	NAG	A	405	1	14,14,15	0.43	0	17,19,21	0.45	0
5	NAG	E	403	1	14,14,15	0.23	0	17,19,21	0.69	1 (5%)
5	NAG	A	401	1	14,14,15	1.13	1 (7%)	17,19,21	1.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	401	1	14,14,15	0.20	0	17,19,21	0.52	0
5	NAG	A	403	1	14,14,15	0.22	0	17,19,21	0.52	0
5	NAG	D	201	2	14,14,15	0.23	0	17,19,21	0.66	0
5	NAG	E	401	1	14,14,15	0.91	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	E	405	1	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	C	402	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	A	402	1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	E	402	1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	C	404	1	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	F	201	2	14,14,15	0.32	0	17,19,21	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	404	1	-	1/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	NAG	E	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	NAG	E	402	1	-	0/6/23/26	0/1/1/1
5	NAG	C	404	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	NAG	C1-C2	3.25	1.56	1.52
5	E	401	NAG	O5-C1	3.01	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NAG	C1-O5-C5	6.94	121.49	112.19
5	E	401	NAG	C1-O5-C5	3.92	117.44	112.19
5	E	403	NAG	C1-O5-C5	2.42	115.43	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	402	NAG	O5-C5-C6-O6
5	C	402	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	E	403	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	NAG	1	0
5	C	402	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	319/319 (100%)	0.46	11 (3%)	48 41	30, 80, 110, 158	6 (1%)
1	C	319/319 (100%)	0.05	3 (0%)	81 76	31, 54, 79, 138	6 (1%)
1	E	319/319 (100%)	0.03	5 (1%)	70 63	33, 49, 77, 127	8 (2%)
2	B	173/173 (100%)	0.12	6 (3%)	47 40	31, 45, 79, 132	2 (1%)
2	D	171/173 (98%)	0.18	6 (3%)	47 40	34, 53, 86, 118	3 (1%)
2	F	170/173 (98%)	0.09	3 (1%)	67 60	31, 54, 78, 128	4 (2%)
3	G	231/231 (100%)	0.51	13 (5%)	30 25	37, 63, 107, 169	5 (2%)
3	H	231/231 (100%)	0.28	10 (4%)	40 33	32, 60, 114, 181	1 (0%)
3	J	231/231 (100%)	0.98	37 (16%)	5 4	42, 101, 212, 225	2 (0%)
4	I	214/214 (100%)	0.52	10 (4%)	36 31	35, 64, 119, 142	1 (0%)
4	K	214/214 (100%)	1.20	40 (18%)	3 2	53, 124, 208, 233	1 (0%)
4	L	214/214 (100%)	0.33	11 (5%)	33 27	33, 54, 92, 121	4 (1%)
All	All	2806/2811 (99%)	0.39	155 (5%)	30 25	30, 60, 164, 233	43 (1%)

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	176	VAL	5.2
3	H	146	THR	4.7
3	J	230	SER	4.6
3	J	231	CYS	4.6
1	E	326	LYS	4.5

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	401	14/15	0.25	0.16	128,138,144,147	0
5	NAG	A	401	14/15	0.32	0.20	118,138,143,146	0
5	NAG	C	402	14/15	0.39	0.20	103,115,122,127	0
5	NAG	A	404	14/15	0.40	0.26	128,142,157,158	0
5	NAG	E	404	14/15	0.59	0.18	100,111,127,130	0
5	NAG	E	403	14/15	0.61	0.13	75,80,85,86	0
5	NAG	C	403	14/15	0.62	0.15	96,111,118,121	0
5	NAG	A	403	14/15	0.72	0.14	97,100,113,116	0
5	NAG	D	201	14/15	0.77	0.12	64,79,86,86	0
5	NAG	E	402	14/15	0.77	0.13	61,74,82,89	0
5	NAG	C	404	14/15	0.78	0.11	55,65,78,86	0
5	NAG	C	401	14/15	0.80	0.12	57,71,76,79	0
5	NAG	A	405	14/15	0.81	0.12	67,86,99,100	0
5	NAG	E	405	14/15	0.82	0.10	64,76,84,90	0
5	NAG	B	201	14/15	0.83	0.10	49,61,64,70	0
5	NAG	A	402	14/15	0.84	0.12	68,78,85,90	0
5	NAG	F	201	14/15	0.87	0.10	61,74,80,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.