



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 6D7C / pdb_00006d7c
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:

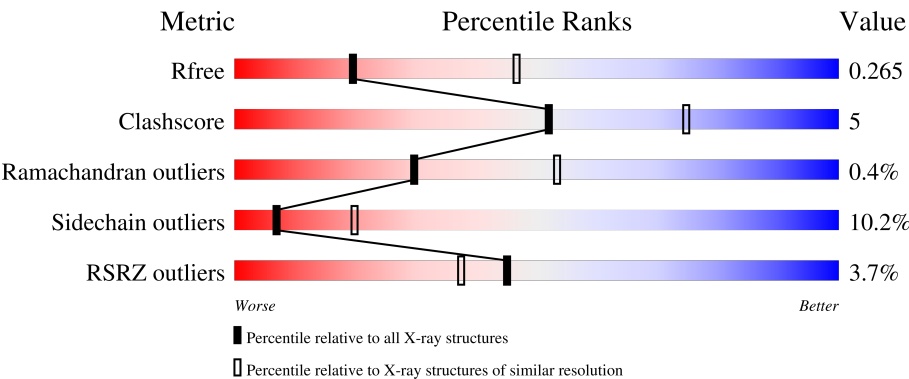
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	321	% 83% 14% ..
1	C	321	3% 83% 13% ...
1	E	321	% 83% 13% ..
1	G	321	12% 83% 13% ..
1	I	321	3% 85% 12% ...

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Mol	Chain	Length	Quality of chain
1	K	321	2% 84% 12% ••
2	B	221	4% 61% 12% •• 23%
2	D	221	2% 59% 14% •• 23%
2	F	221	3% 59% 15% •• 23%
2	H	221	3% 59% 14% •• 23%
2	J	221	3% 62% 12% •• 23%
2	L	221	2% 59% 14% •• 23%

2 Entry composition

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			

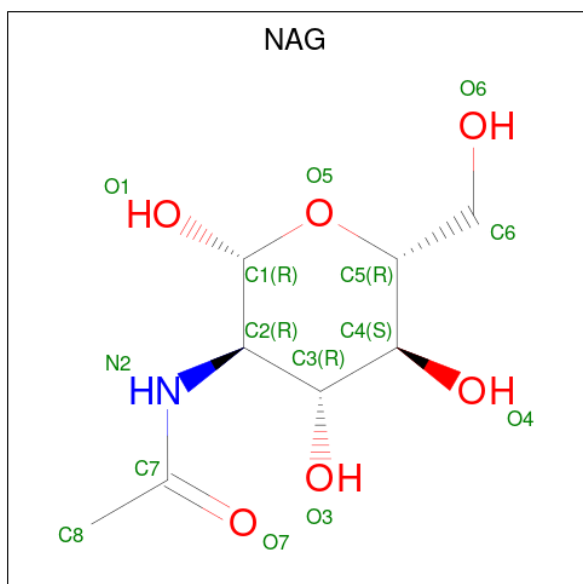
There are 12 discrepancies between the modelled and reference sequences:

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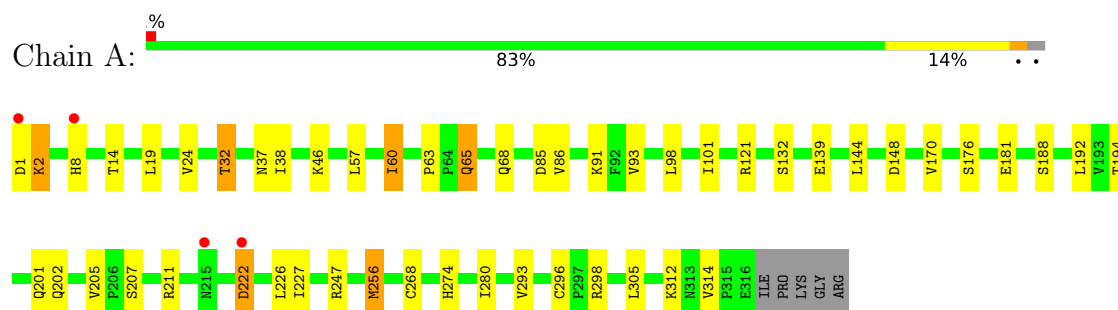
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

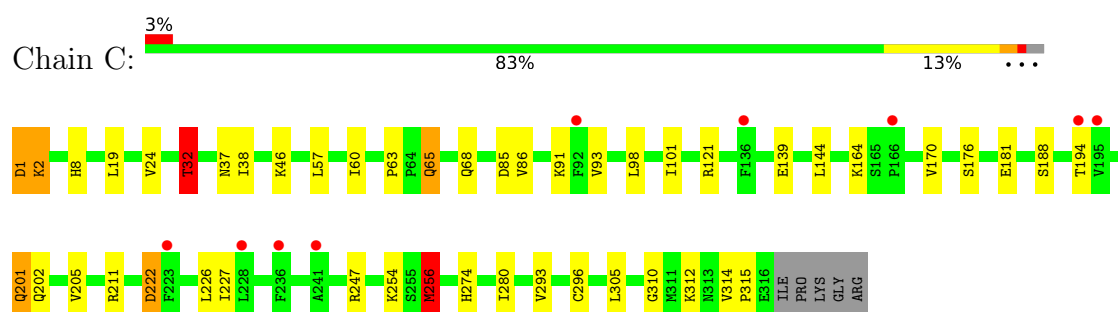
3 Residue-property plots [i](#)

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.

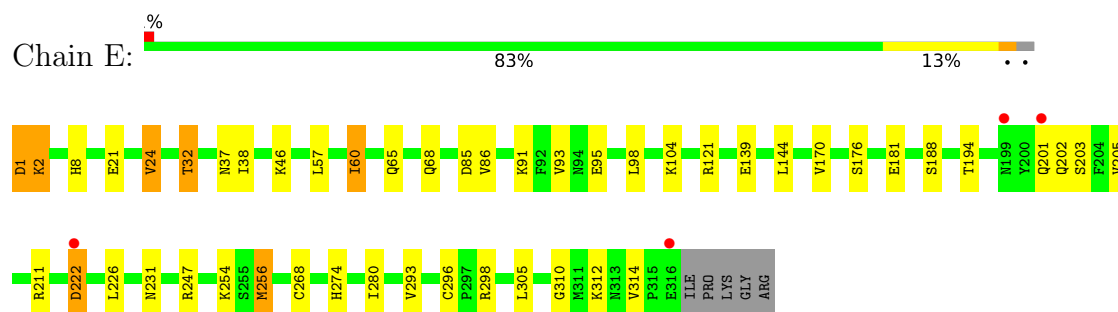
- Molecule 1: Hemagglutinin HA1 chain



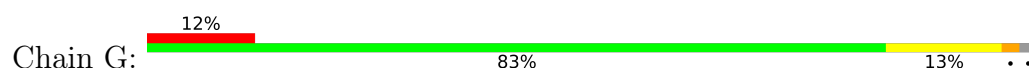
- Molecule 1: Hemagglutinin HA1 chain

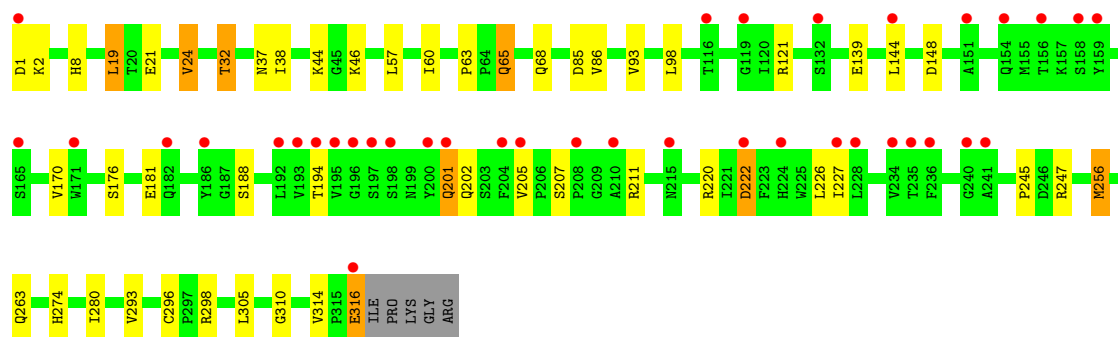


- Molecule 1: Hemagglutinin HA1 chain

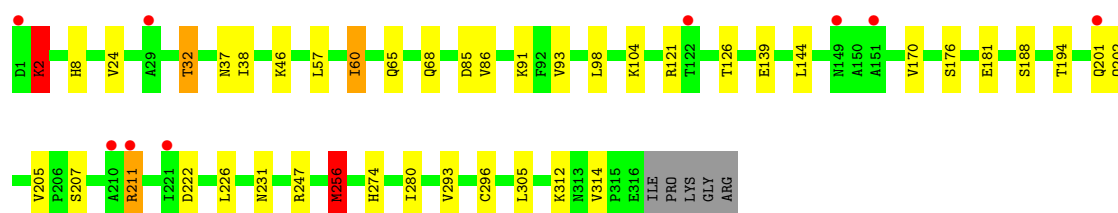
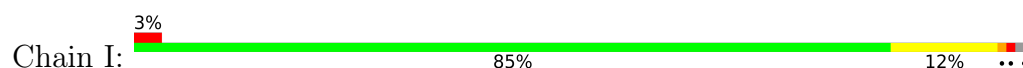


- Molecule 1: Hemagglutinin HA1 chain

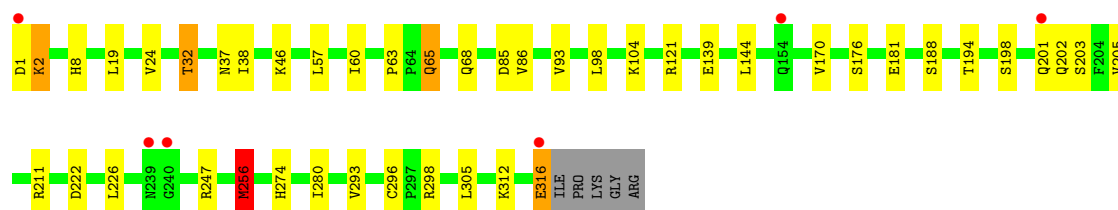
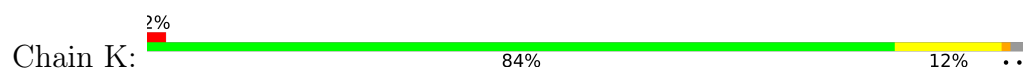




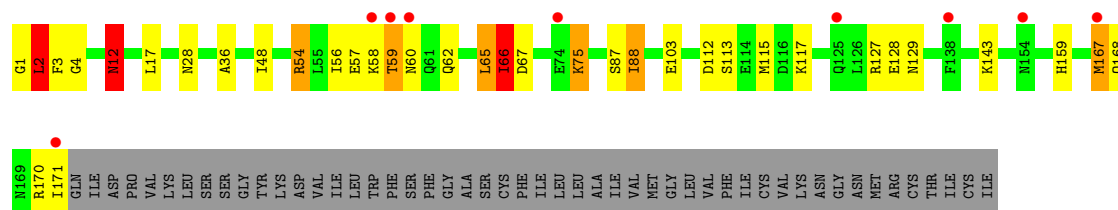
• Molecule 1: Hemagglutinin HA1 chain



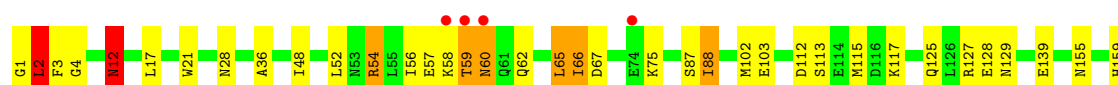
• Molecule 1: Hemagglutinin HA1 chain

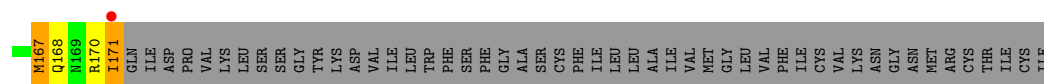


• Molecule 2: Hemagglutinin HA2 chain

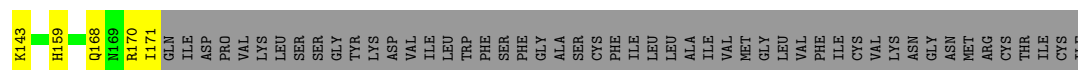


• Molecule 2: Hemagglutinin HA2 chain

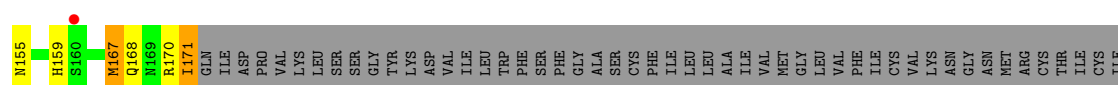
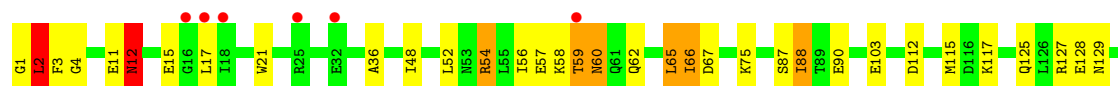




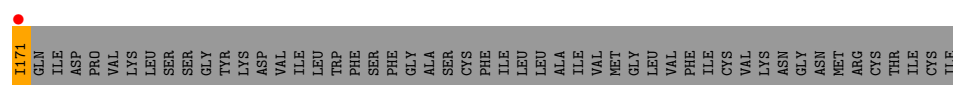
• Molecule 2: Hemagglutinin HA2 chain



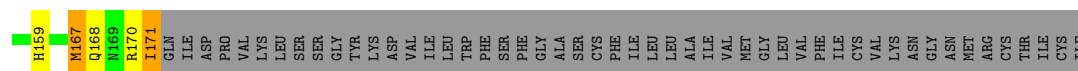
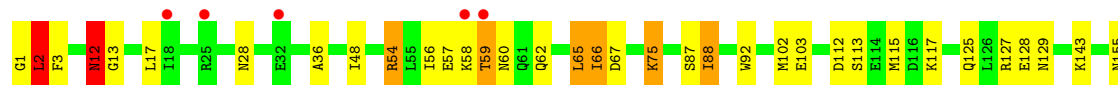
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

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 50.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.95) 93.1 (50.00-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.71%)	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)	0.29 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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	1.05	0/2459	1.09	4/3322 (0.1%)
1	C	0.94	2/2459 (0.1%)	1.05	4/3322 (0.1%)
1	E	0.97	1/2459 (0.0%)	1.06	5/3322 (0.2%)
1	G	0.93	2/2459 (0.1%)	1.04	3/3322 (0.1%)
1	I	0.98	1/2459 (0.0%)	1.07	3/3322 (0.1%)
1	K	0.93	0/2459	1.05	2/3322 (0.1%)
2	B	1.04	2/1411 (0.1%)	1.12	2/1901 (0.1%)
2	D	1.05	1/1411 (0.1%)	1.17	2/1901 (0.1%)
2	F	1.07	2/1411 (0.1%)	1.14	2/1901 (0.1%)
2	H	1.06	0/1411	1.18	3/1901 (0.2%)
2	J	1.02	3/1411 (0.2%)	1.12	2/1901 (0.1%)
2	L	1.05	0/1411	1.16	2/1901 (0.1%)
All	All	1.00	14/23220 (0.1%)	1.09	34/31338 (0.1%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	ILE	N-CA	6.88	1.53	1.46
1	C	1	ASP	CB-CG	6.15	1.67	1.52
2	B	12	ASN	CA-C	6.13	1.60	1.52
1	I	211	ARG	N-CA	6.06	1.51	1.45
1	G	1	ASP	CB-CG	5.99	1.67	1.52
2	J	74	GLU	CD-OE1	5.94	1.36	1.25
2	F	66	ILE	N-CA	5.86	1.52	1.46
2	J	66	ILE	N-CA	5.74	1.52	1.46
2	D	12	ASN	CA-C	5.49	1.60	1.52
1	G	1	ASP	N-CA	5.49	1.56	1.46
2	J	12	ASN	CA-C	5.46	1.60	1.52
2	F	12	ASN	CA-C	5.22	1.59	1.52
1	E	1	ASP	N-CA	5.13	1.55	1.46
1	C	315	PRO	C-O	-5.11	1.17	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	2	LYS	N-CA-C	7.60	120.77	108.76
1	A	2	LYS	N-CA-C	7.08	120.11	108.99
1	E	2	LYS	N-CA-C	6.83	119.71	108.99
1	I	2	LYS	N-CA-C	6.72	119.39	108.76
2	L	12	ASN	N-CA-C	6.54	124.73	110.80
1	K	256	MET	N-CA-C	-6.46	97.83	108.76
1	A	222	ASP	CB-CA-C	6.44	120.42	109.53
1	K	2	LYS	N-CA-C	6.26	118.65	108.76
2	H	12	ASN	N-CA-C	6.25	124.11	110.80
2	F	12	ASN	N-CA-C	6.24	124.09	110.80
2	D	12	ASN	N-CA-C	6.24	124.08	110.80
2	D	67	ASP	N-CA-C	-6.18	99.94	109.14
1	C	2	LYS	N-CA-C	6.03	118.46	108.99
1	A	268	CYS	CA-CB-SG	-5.93	100.76	114.40
1	E	268	CYS	CA-CB-SG	5.88	127.93	114.40
2	J	67	ASP	N-CA-C	-5.82	100.46	109.14
2	B	12	ASN	N-CA-C	5.80	123.16	110.80
2	J	12	ASN	N-CA-C	5.76	123.07	110.80
1	E	222	ASP	CB-CA-C	5.70	119.17	109.53
1	E	256	MET	N-CA-C	-5.67	99.18	108.76
2	F	67	ASP	N-CA-C	-5.56	100.67	108.96
1	G	222	ASP	CB-CA-C	5.54	118.90	109.53
1	G	263	GLN	N-CA-C	5.47	117.79	110.35
2	H	67	ASP	N-CA-C	-5.43	101.05	109.14
2	L	67	ASP	N-CA-C	-5.41	101.08	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	256	MET	N-CA-C	-5.39	99.64	108.76
2	B	67	ASP	N-CA-C	-5.34	101.18	109.14
1	C	222	ASP	CB-CA-C	5.28	118.46	109.53
1	C	256	MET	N-CA-C	-5.24	99.90	108.76
2	H	11	GLU	N-CA-C	-5.16	102.27	109.96
1	I	60	ILE	CB-CA-C	-5.11	105.39	112.24
1	E	60	ILE	CB-CA-C	-5.08	105.44	112.24
1	C	32	THR	N-CA-CB	-5.06	103.90	110.88
1	A	60	ILE	CB-CA-C	-5.02	105.52	112.24

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

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	23	0
1	C	2413	0	2387	23	0
1	E	2413	0	2387	23	0
1	G	2413	0	2387	30	0
1	I	2413	0	2387	24	0
1	K	2413	0	2388	31	0
2	B	1387	0	1293	23	0
2	D	1387	0	1294	27	0
2	F	1387	0	1293	22	0
2	H	1387	0	1293	27	0
2	J	1387	0	1293	23	0
2	L	1387	0	1293	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	228	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 (228) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:201:GLN:CD	1:I:91:LYS:HG2	2.31	0.56
1:K:296:CYS:O	2:L:59:THR:HG21	2.05	0.56
2:J:1:GLY:C	2:J:2:LEU:O	2.50	0.54
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:F:1:GLY:C	2:F:2:LEU:O	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:115:MET:HE3	2:B:115:MET:HA	1.91	0.53
2:B:1:GLY:C	2:B:2:LEU:O	2.51	0.52
1:C:60:ILE:HG21	1:C:170:VAL:CG2	2.39	0.52
2:D:1:GLY:C	2:D:2:LEU:O	2.51	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:C:256:MET:HE3	2:D:62:GLN:NE2	2.25	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
1:K:256:MET:HE3	2:L:62:GLN:NE2	2.26	0.51
2:L:1:GLY:C	2:L:2:LEU:O	2.51	0.51
2:F:115:MET:HE3	2:F:115:MET:HA	1.93	0.51
2:J:115:MET:HE3	2:J:115:MET:HA	1.93	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:1:GLY:C	2:H:2:LEU:O	2.51	0.51
2:L:115:MET:HE3	2:L:115:MET:HA	1.92	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:H:115:MET:HA	2:H:115:MET:HE3	1.93	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:HE2	3:B:301:NAG:H83	1.95	0.49
2:D:115:MET:HE3	2:D:115:MET:HA	1.94	0.49
2:D:167:MET:HE1	2:L:171:ILE:HG12	1.94	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: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:A:1:ASP:CG	2:B:28:ASN:HA	2.39	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
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
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
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
1:I:256:MET:HE3	2:J:62:GLN:NE2	2.30	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
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:F:79:ASN:OD1	3:F:301:NAG:H82	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:56:ILE:O	2:D:56:ILE:HG22	2.16	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
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:G:256:MET:HE3	2:H:62:GLN:NE2	2.32	0.45
1:C:226:LEU:HD12	1:C:226:LEU:C	2.42	0.45
1:G:226:LEU:C	1:G:226:LEU:HD12	2.42	0.45
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:E:226:LEU:C	1:E:226:LEU:HD12	2.42	0.44
1:G:32:THR:HG22	1:G:305:LEU:HB2	2.00	0.44
1:I:226:LEU:C	1:I:226:LEU:HD12	2.42	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
1:A:226:LEU:HD12	1:A:226:LEU:C	2.43	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
1:K:226:LEU:C	1:K:226:LEU:HD12	2.43	0.43
2:L:127:ARG:HG3	2:L:159:HIS:CG	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:ND2	1:A:274:HIS:NE2	2.67	0.42
1:A:256:MET:HE3	2:B:62:GLN:NE2	2.34	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
1:G:19:LEU:HD21	2:L:102:MET:HE1	2.04	0.40
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
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:K:1:ASP:OD2	2:L:28:ASN:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	10	28
2	D	169/221 (76%)	155 (92%)	12 (7%)	2 (1%)	10	28
2	F	169/221 (76%)	155 (92%)	12 (7%)	2 (1%)	10	28
2	H	169/221 (76%)	156 (92%)	11 (6%)	2 (1%)	10	28
2	J	169/221 (76%)	156 (92%)	11 (6%)	2 (1%)	10	28
2	L	169/221 (76%)	157 (93%)	10 (6%)	2 (1%)	10	28
All	All	2898/3252 (89%)	2727 (94%)	159 (6%)	12 (0%)	30	53

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

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Mol	Chain	Res	Type
2	H	2	LEU
2	J	2	LEU
2	L	2	LEU

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	265/269 (98%)	237 (89%)	28 (11%)	6	19
1	C	265/269 (98%)	238 (90%)	27 (10%)	7	20
1	E	265/269 (98%)	241 (91%)	24 (9%)	9	23
1	G	265/269 (98%)	239 (90%)	26 (10%)	7	21
1	I	265/269 (98%)	242 (91%)	23 (9%)	9	25
1	K	265/269 (98%)	243 (92%)	22 (8%)	10	27
2	B	146/190 (77%)	128 (88%)	18 (12%)	4	14
2	D	146/190 (77%)	129 (88%)	17 (12%)	5	16
2	F	146/190 (77%)	128 (88%)	18 (12%)	4	14
2	H	146/190 (77%)	130 (89%)	16 (11%)	6	17
2	J	146/190 (77%)	131 (90%)	15 (10%)	7	19
2	L	146/190 (77%)	128 (88%)	18 (12%)	4	14
All	All	2466/2754 (90%)	2214 (90%)	252 (10%)	7	20

All (252) 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	24	VAL
1	A	32	THR
1	A	46	LYS

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Mol	Chain	Res	Type
1	A	65	GLN
1	A	68	GLN
1	A	86	VAL
1	A	91	LYS
1	A	93	VAL
1	A	121	ARG
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	202	GLN
1	A	205	VAL
1	A	211	ARG
1	A	227	ILE
1	A	256	MET
1	A	298	ARG
1	A	312	LYS
1	A	314	VAL
2	B	2	LEU
2	B	12	ASN
2	B	48	ILE
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	75	LYS
2	B	88	ILE
2	B	117	LYS
2	B	129	ASN
2	B	143	LYS
2	B	167	MET
2	B	168	GLN
2	B	171	ILE
1	C	2	LYS
1	C	8	HIS
1	C	19	LEU

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Mol	Chain	Res	Type
1	C	24	VAL
1	C	32	THR
1	C	46	LYS
1	C	65	GLN
1	C	68	GLN
1	C	86	VAL
1	C	91	LYS
1	C	93	VAL
1	C	121	ARG
1	C	144	LEU
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	205	VAL
1	C	211	ARG
1	C	227	ILE
1	C	254	LYS
1	C	256	MET
1	C	312	LYS
1	C	314	VAL
2	D	2	LEU
2	D	12	ASN
2	D	48	ILE
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	75	LYS
2	D	88	ILE
2	D	117	LYS
2	D	129	ASN
2	D	139	GLU
2	D	167	MET
2	D	168	GLN
2	D	171	ILE
1	E	2	LYS

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Mol	Chain	Res	Type
1	E	8	HIS
1	E	24	VAL
1	E	32	THR
1	E	46	LYS
1	E	65	GLN
1	E	68	GLN
1	E	86	VAL
1	E	91	LYS
1	E	93	VAL
1	E	104	LYS
1	E	121	ARG
1	E	144	LEU
1	E	176	SER
1	E	181	GLU
1	E	188	SER
1	E	194	THR
1	E	202	GLN
1	E	205	VAL
1	E	211	ARG
1	E	254	LYS
1	E	256	MET
1	E	312	LYS
1	E	314	VAL
2	F	2	LEU
2	F	12	ASN
2	F	48	ILE
2	F	54	ARG
2	F	57	GLU
2	F	58	LYS
2	F	59	THR
2	F	60	ASN
2	F	65	LEU
2	F	66	ILE
2	F	75	LYS
2	F	88	ILE
2	F	117	LYS
2	F	129	ASN
2	F	139	GLU
2	F	143	LYS
2	F	168	GLN
2	F	171	ILE
1	G	8	HIS

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Mol	Chain	Res	Type
1	G	19	LEU
1	G	24	VAL
1	G	32	THR
1	G	44	LYS
1	G	46	LYS
1	G	65	GLN
1	G	68	GLN
1	G	86	VAL
1	G	93	VAL
1	G	121	ARG
1	G	144	LEU
1	G	148	ASP
1	G	176	SER
1	G	181	GLU
1	G	188	SER
1	G	194	THR
1	G	201	GLN
1	G	202	GLN
1	G	205	VAL
1	G	211	ARG
1	G	227	ILE
1	G	256	MET
1	G	298	ARG
1	G	314	VAL
1	G	316	GLU
2	H	2	LEU
2	H	12	ASN
2	H	48	ILE
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	75	LYS
2	H	88	ILE
2	H	117	LYS
2	H	129	ASN
2	H	167	MET
2	H	168	GLN
2	H	171	ILE
1	I	2	LYS

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Mol	Chain	Res	Type
1	I	8	HIS
1	I	24	VAL
1	I	32	THR
1	I	46	LYS
1	I	65	GLN
1	I	68	GLN
1	I	86	VAL
1	I	93	VAL
1	I	104	LYS
1	I	121	ARG
1	I	126	THR
1	I	144	LEU
1	I	176	SER
1	I	181	GLU
1	I	188	SER
1	I	194	THR
1	I	202	GLN
1	I	205	VAL
1	I	211	ARG
1	I	256	MET
1	I	312	LYS
1	I	314	VAL
2	J	2	LEU
2	J	12	ASN
2	J	48	ILE
2	J	54	ARG
2	J	57	GLU
2	J	60	ASN
2	J	65	LEU
2	J	66	ILE
2	J	75	LYS
2	J	88	ILE
2	J	117	LYS
2	J	129	ASN
2	J	167	MET
2	J	168	GLN
2	J	171	ILE
1	K	2	LYS
1	K	8	HIS
1	K	24	VAL
1	K	32	THR
1	K	46	LYS

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Mol	Chain	Res	Type
1	K	65	GLN
1	K	68	GLN
1	K	86	VAL
1	K	93	VAL
1	K	104	LYS
1	K	121	ARG
1	K	144	LEU
1	K	176	SER
1	K	181	GLU
1	K	188	SER
1	K	194	THR
1	K	202	GLN
1	K	205	VAL
1	K	211	ARG
1	K	256	MET
1	K	312	LYS
1	K	316	GLU
2	L	2	LEU
2	L	12	ASN
2	L	48	ILE
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	75	LYS
2	L	88	ILE
2	L	117	LYS
2	L	129	ASN
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 (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	37	ASN
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	154	GLN
2	B	60	ASN
2	B	62	GLN
2	B	105	GLN
2	B	159	HIS
2	B	169	ASN
1	C	8	HIS
1	C	37	ASN
1	C	94	ASN
1	C	154	GLN
1	C	201	GLN
2	D	60	ASN
2	D	62	GLN
2	D	159	HIS
2	D	169	ASN
1	E	8	HIS
1	E	37	ASN
1	E	94	ASN
1	E	154	GLN
2	F	60	ASN
2	F	62	GLN
2	F	159	HIS
2	F	169	ASN
1	G	8	HIS
1	G	37	ASN
1	G	94	ASN
1	G	154	GLN
1	G	201	GLN
2	H	60	ASN
2	H	62	GLN
2	H	159	HIS
2	H	169	ASN
1	I	8	HIS
1	I	37	ASN
1	I	94	ASN
1	I	149	ASN
1	I	154	GLN
2	J	60	ASN
2	J	62	GLN
2	J	105	GLN
2	J	159	HIS
2	J	169	ASN

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Mol	Chain	Res	Type
1	K	8	HIS
1	K	37	ASN
1	K	94	ASN
1	K	149	ASN
1	K	154	GLN
1	K	231	ASN
2	L	60	ASN
2	L	62	GLN
2	L	159	HIS
2	L	169	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	301	2	14,14,15	1.53	3 (21%)	17,19,21	2.72	8 (47%)
3	NAG	J	301	2	14,14,15	1.55	3 (21%)	17,19,21	2.23	7 (41%)
3	NAG	I	401	1	14,14,15	1.23	1 (7%)	17,19,21	3.10	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	401	1	14,14,15	0.83	0	17,19,21	2.06	5 (29%)
3	NAG	E	401	1	14,14,15	2.63	5 (35%)	17,19,21	4.10	9 (52%)
3	NAG	A	401	1	14,14,15	1.76	4 (28%)	17,19,21	3.68	8 (47%)
3	NAG	H	301	2	14,14,15	1.53	2 (14%)	17,19,21	3.01	8 (47%)
3	NAG	F	301	2	14,14,15	2.26	5 (35%)	17,19,21	3.41	9 (52%)
3	NAG	C	401	1	14,14,15	1.42	2 (14%)	17,19,21	2.91	6 (35%)
3	NAG	L	301	2	14,14,15	1.42	2 (14%)	17,19,21	1.74	2 (11%)

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	B	301	2	-	0/6/23/26	0/1/1/1
3	NAG	J	301	2	-	2/6/23/26	0/1/1/1
3	NAG	I	401	1	-	3/6/23/26	0/1/1/1
3	NAG	G	401	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	3/6/23/26	0/1/1/1
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	H	301	2	-	0/6/23/26	0/1/1/1
3	NAG	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1
3	NAG	L	301	2	-	2/6/23/26	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	5.38	1.52	1.43
3	E	401	NAG	O5-C5	4.30	1.51	1.43
3	E	401	NAG	C4-C5	4.10	1.61	1.53
3	F	301	NAG	C3-C2	4.10	1.61	1.52
3	F	301	NAG	C1-C2	4.05	1.57	1.52
3	F	301	NAG	C4-C3	3.85	1.62	1.52
3	L	301	NAG	C1-C2	3.73	1.57	1.52
3	E	401	NAG	C2-N2	3.34	1.51	1.46
3	J	301	NAG	O5-C1	3.24	1.49	1.43
3	C	401	NAG	C1-C2	3.21	1.56	1.52
3	H	301	NAG	C3-C2	3.20	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	NAG	O4-C4	3.16	1.50	1.43
3	A	401	NAG	C4-C5	3.09	1.59	1.53
3	F	301	NAG	O5-C1	3.06	1.48	1.43
3	A	401	NAG	O5-C5	2.93	1.49	1.43
3	C	401	NAG	C2-N2	2.78	1.50	1.46
3	A	401	NAG	C1-C2	2.77	1.56	1.52
3	I	401	NAG	C1-C2	2.66	1.56	1.52
3	A	401	NAG	O5-C1	2.59	1.48	1.43
3	B	301	NAG	O5-C1	2.55	1.48	1.43
3	J	301	NAG	C2-N2	2.43	1.50	1.46
3	H	301	NAG	O4-C4	2.41	1.48	1.43
3	E	401	NAG	C6-C5	2.35	1.59	1.51
3	B	301	NAG	O3-C3	2.31	1.48	1.43
3	B	301	NAG	C4-C5	2.19	1.57	1.53
3	J	301	NAG	C4-C3	2.17	1.58	1.52
3	L	301	NAG	O5-C1	2.00	1.47	1.43

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	NAG	C1-O5-C5	9.26	124.60	112.19
3	E	401	NAG	C1-C2-N2	8.95	124.53	110.43
3	A	401	NAG	C1-O5-C5	8.74	123.89	112.19
3	A	401	NAG	C1-C2-N2	8.46	123.77	110.43
3	E	401	NAG	C2-N2-C7	7.79	133.34	122.90
3	I	401	NAG	C1-C2-N2	7.79	122.70	110.43
3	H	301	NAG	C1-O5-C5	6.99	121.55	112.19
3	F	301	NAG	O4-C4-C3	6.77	126.33	110.38
3	F	301	NAG	C2-N2-C7	6.33	131.38	122.90
3	I	401	NAG	C2-N2-C7	5.85	130.74	122.90
3	B	301	NAG	C1-O5-C5	5.75	119.90	112.19
3	A	401	NAG	C2-N2-C7	5.66	130.49	122.90
3	H	301	NAG	O5-C1-C2	-5.62	102.59	111.29
3	C	401	NAG	C2-N2-C7	5.61	130.42	122.90
3	G	401	NAG	C1-O5-C5	5.52	119.58	112.19
3	C	401	NAG	C1-O5-C5	5.48	119.53	112.19
3	I	401	NAG	C1-O5-C5	5.43	119.46	112.19
3	C	401	NAG	C1-C2-N2	5.42	118.97	110.43
3	C	401	NAG	C3-C4-C5	5.15	119.58	110.23
3	F	301	NAG	C1-C2-N2	-5.03	102.51	110.43
3	B	301	NAG	O3-C3-C2	4.77	119.31	109.40
3	F	301	NAG	C3-C4-C5	-4.74	101.65	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	NAG	C1-O5-C5	4.64	118.40	112.19
3	J	301	NAG	C2-N2-C7	4.59	129.05	122.90
3	F	301	NAG	O7-C7-N2	4.18	129.38	121.98
3	E	401	NAG	O4-C4-C5	4.16	119.57	109.32
3	B	301	NAG	C4-C3-C2	-4.01	105.13	111.02
3	A	401	NAG	O4-C4-C5	4.00	119.19	109.32
3	H	301	NAG	C3-C4-C5	-3.93	103.11	110.23
3	F	301	NAG	O7-C7-C8	-3.85	115.19	122.05
3	H	301	NAG	C2-N2-C7	3.83	128.03	122.90
3	J	301	NAG	C1-O5-C5	3.54	116.94	112.19
3	H	301	NAG	C1-C2-N2	-3.43	105.03	110.43
3	B	301	NAG	O7-C7-N2	3.26	127.74	121.98
3	J	301	NAG	O5-C5-C6	3.18	113.86	107.66
3	B	301	NAG	O5-C1-C2	3.16	116.17	111.29
3	B	301	NAG	C2-N2-C7	3.15	127.13	122.90
3	E	401	NAG	O6-C6-C5	3.05	121.72	111.33
3	H	301	NAG	O4-C4-C3	3.03	117.52	110.38
3	I	401	NAG	C4-C3-C2	-3.01	106.61	111.02
3	L	301	NAG	C2-N2-C7	2.96	126.86	122.90
3	F	301	NAG	O6-C6-C5	-2.95	101.29	111.33
3	J	301	NAG	O4-C4-C3	2.92	117.26	110.38
3	G	401	NAG	C1-C2-N2	-2.92	105.83	110.43
3	G	401	NAG	C4-C3-C2	-2.88	106.80	111.02
3	J	301	NAG	O5-C1-C2	2.84	115.69	111.29
3	G	401	NAG	O3-C3-C2	2.84	115.30	109.40
3	J	301	NAG	O3-C3-C4	2.76	116.88	110.38
3	B	301	NAG	O7-C7-C8	-2.64	117.36	122.05
3	B	301	NAG	O5-C5-C4	2.61	117.17	110.83
3	F	301	NAG	O3-C3-C2	2.51	114.62	109.40
3	I	401	NAG	C6-C5-C4	-2.51	106.86	113.02
3	C	401	NAG	O5-C1-C2	-2.50	107.42	111.29
3	F	301	NAG	O5-C5-C6	-2.47	102.86	107.66
3	H	301	NAG	O3-C3-C2	2.39	114.38	109.40
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	E	401	NAG	O5-C5-C6	2.38	112.30	107.66
3	J	301	NAG	O7-C7-C8	-2.30	117.95	122.05
3	A	401	NAG	C4-C3-C2	-2.30	107.65	111.02
3	E	401	NAG	O3-C3-C4	-2.29	104.98	110.38
3	C	401	NAG	O7-C7-C8	-2.23	118.08	122.05
3	E	401	NAG	C8-C7-N2	2.21	119.78	116.12
3	A	401	NAG	O6-C6-C5	2.19	118.80	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	401	NAG	O3-C3-C2	2.17	113.91	109.40
3	A	401	NAG	O5-C5-C4	2.14	116.04	110.83
3	I	401	NAG	O4-C4-C3	2.10	115.33	110.38
3	G	401	NAG	O4-C4-C5	2.07	114.42	109.32
3	E	401	NAG	O7-C7-C8	-2.06	118.38	122.05
3	A	401	NAG	C6-C5-C4	-2.03	108.04	113.02

There are no chirality outliers.

All (15) 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	I	401	NAG	C1-C2-N2-C7
3	E	401	NAG	C4-C5-C6-O6
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	C3-C2-N2-C7
3	L	301	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/321 (98%)	-0.00	4 (1%) 75 69	37, 51, 76, 97	1 (0%)
1	C	316/321 (98%)	0.40	9 (2%) 55 47	42, 68, 103, 112	1 (0%)
1	E	316/321 (98%)	0.07	4 (1%) 75 69	42, 55, 75, 101	1 (0%)
1	G	316/321 (98%)	0.67	38 (12%) 9 8	43, 80, 142, 160	1 (0%)
1	I	316/321 (98%)	0.44	9 (2%) 55 47	42, 66, 99, 109	1 (0%)
1	K	316/321 (98%)	0.33	6 (1%) 66 58	41, 73, 98, 116	1 (0%)
2	B	171/221 (77%)	0.44	9 (5%) 32 27	41, 75, 110, 128	0
2	D	171/221 (77%)	0.18	5 (2%) 53 46	36, 59, 81, 129	0
2	F	171/221 (77%)	0.29	6 (3%) 47 40	42, 67, 88, 124	0
2	H	171/221 (77%)	0.20	7 (4%) 41 34	39, 57, 95, 125	0
2	J	171/221 (77%)	0.44	6 (3%) 47 40	41, 76, 105, 127	0
2	L	171/221 (77%)	0.17	5 (2%) 53 46	39, 56, 86, 128	0
All	All	2922/3252 (89%)	0.31	108 (3%) 45 37	36, 63, 105, 160	6 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	222	ASP	6.7
1	G	197	SER	4.3
1	G	192	LEU	4.0
1	A	222	ASP	3.8
2	H	18	ILE	3.8
1	G	234	VAL	3.7
2	B	60	ASN	3.7
2	B	58	LYS	3.5
2	D	59	THR	3.5
2	H	32	GLU	3.5
1	G	215	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	201	GLN	3.3
2	F	58	LYS	3.3
1	E	222	ASP	3.2
1	G	200	TYR	3.2
1	G	228	LEU	3.2
1	G	224	HIS	3.2
1	G	240	GLY	3.2
1	G	195	VAL	3.1
2	H	17	LEU	3.1
1	G	201	GLN	3.1
2	B	171	ILE	3.1
1	C	223	PHE	3.0
1	G	1	ASP	3.0
1	A	8	HIS	3.0
2	F	60	ASN	3.0
2	J	171	ILE	3.0
2	H	160	SER	2.9
2	J	9	PHE	2.9
2	B	59	THR	2.9
1	G	171	TRP	2.9
1	G	196	GLY	2.8
1	I	210	ALA	2.8
2	D	60	ASN	2.8
1	G	158	SER	2.8
2	D	58	LYS	2.8
1	G	144	LEU	2.7
2	L	18	ILE	2.7
1	K	240	GLY	2.7
2	H	25	ARG	2.7
1	I	1	ASP	2.7
1	G	236	PHE	2.6
2	B	74	GLU	2.6
1	G	186	TYR	2.6
1	G	235	THR	2.6
1	G	193	VAL	2.6
1	C	166	PRO	2.6
2	L	59	THR	2.6
1	I	149	ASN	2.6
1	K	154	GLN	2.6
2	B	167	MET	2.6
1	E	199	ASN	2.5
1	G	165	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	227	ILE	2.5
2	F	59	THR	2.5
2	J	132	GLU	2.5
1	I	151	ALA	2.5
2	L	25	ARG	2.5
1	K	316	GLU	2.4
2	D	74	GLU	2.4
1	G	210	ALA	2.4
1	G	204	PHE	2.4
2	J	167	MET	2.4
1	I	29	ALA	2.4
1	G	194	THR	2.4
1	C	194	THR	2.4
1	G	156	THR	2.4
1	G	132	SER	2.3
1	A	215	ASN	2.3
1	C	92	PHE	2.3
1	C	236	PHE	2.3
1	E	201	GLN	2.3
1	C	195	VAL	2.3
2	F	132	GLU	2.3
1	A	1	ASP	2.3
1	K	1	ASP	2.3
2	D	171	ILE	2.3
2	H	16	GLY	2.3
1	I	221	ILE	2.2
1	C	241	ALA	2.2
1	G	205	VAL	2.2
1	C	228	LEU	2.2
1	G	316	GLU	2.2
2	F	56	ILE	2.2
1	K	239	ASN	2.2
2	B	125	GLN	2.2
1	G	159	TYR	2.2
1	I	211	ARG	2.1
1	K	201	GLN	2.1
2	B	154	ASN	2.1
2	J	60	ASN	2.1
1	G	198	SER	2.1
1	G	208	PRO	2.1
1	G	119	GLY	2.1
1	I	122	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	138	PHE	2.1
1	G	182	GLN	2.1
2	L	58	LYS	2.1
2	J	35	ALA	2.1
2	F	74	GLU	2.1
1	G	154	GLN	2.0
1	C	136	PHE	2.0
1	G	116	THR	2.0
2	H	59	THR	2.0
1	G	241	ALA	2.0
2	L	32	GLU	2.0
1	G	151	ALA	2.0
1	E	316	GLU	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
3	NAG	I	401	14/15	0.58	0.13	97,107,114,115	0
3	NAG	C	401	14/15	0.62	0.12	114,118,120,120	0
3	NAG	E	401	14/15	0.63	0.14	71,74,78,78	0
3	NAG	A	401	14/15	0.63	0.15	92,102,107,107	0
3	NAG	G	401	14/15	0.74	0.13	77,85,94,95	0
3	NAG	H	301	14/15	0.75	0.12	72,78,86,87	0
3	NAG	F	301	14/15	0.75	0.13	67,68,73,76	0
3	NAG	J	301	14/15	0.76	0.14	67,71,76,79	0
3	NAG	L	301	14/15	0.81	0.12	85,93,97,100	0
3	NAG	B	301	14/15	0.83	0.11	68,70,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.