



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LN3
Title : The crystal structure of hemagglutinin from a H7N9 influenza virus (A/Shanghai/1/2013)
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2013-07-11
Resolution : 2.65 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

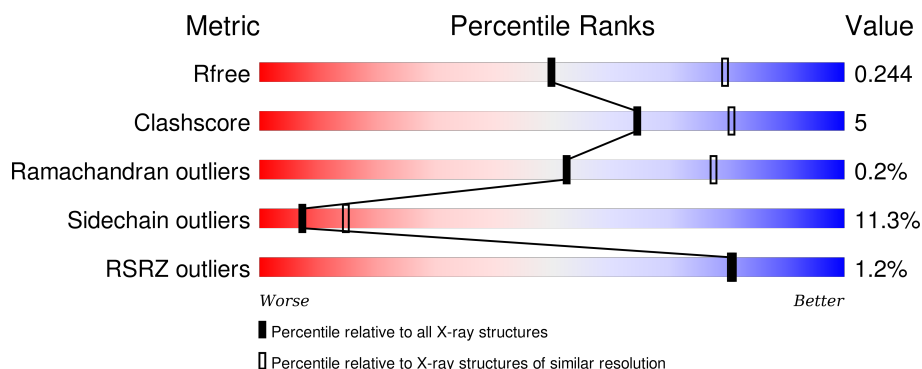
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	325	<div> <div></div> <div>78%16% . .</div> </div>
1	C	325	<div> <div></div> <div>78%16% . . .</div> </div>
1	E	325	<div> <div>%</div> <div>77%16% . .</div> </div>
1	G	325	<div> <div>%</div> <div>78%17% . .</div> </div>
1	I	325	<div> <div>%</div> <div>76%19% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	325	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	

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
4	NAG	A	404	X	-	-	-
4	NAG	D	500	-	-	-	X
4	NAG	E	404	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	C	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	E	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	G	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	I	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			
1	K	316	Total	C	N	O	S	0	0	0
			2410	1494	435	466	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	D	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	F	167	Total	C	N	O	S	0	0	0
			1359	838	237	277	7			
2	H	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			
2	J	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			
2	L	164	Total	C	N	O	S	0	0	0
			1335	823	231	274	7			

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

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	J	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

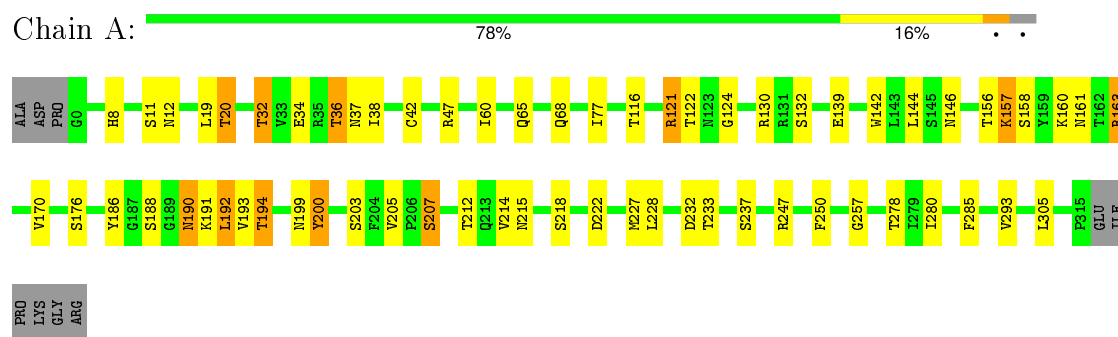
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	17	Total	O	0	0
			17	17		
5	C	38	Total	O	0	0
			38	38		
5	D	24	Total	O	0	0
			24	24		
5	E	40	Total	O	0	0
			40	40		
5	F	20	Total	O	0	0
			20	20		
5	G	22	Total	O	0	0
			22	22		
5	H	13	Total	O	0	0
			13	13		
5	I	21	Total	O	0	0
			21	21		
5	J	8	Total	O	0	0
			8	8		
5	K	17	Total	O	0	0
			17	17		
5	L	6	Total	O	0	0
			6	6		

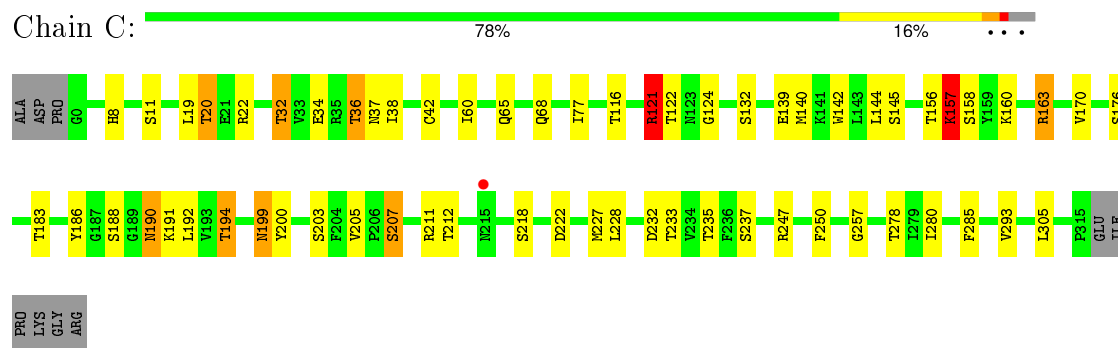
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

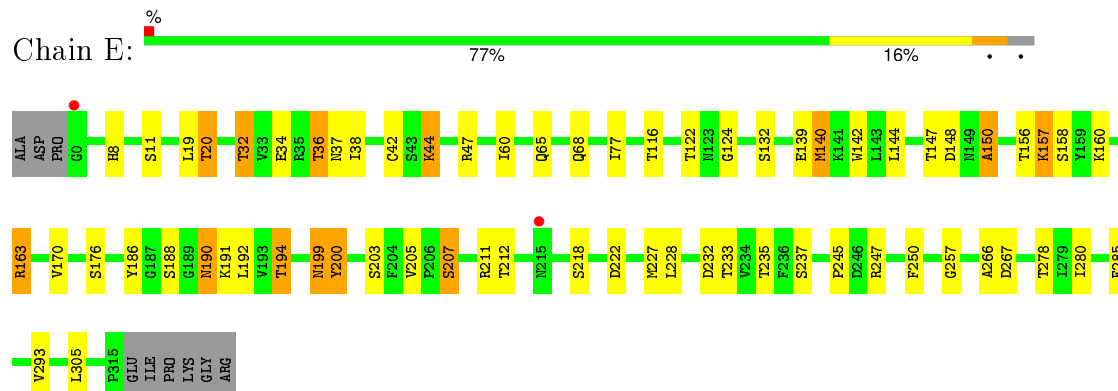
• Molecule 1: Hemagglutinin



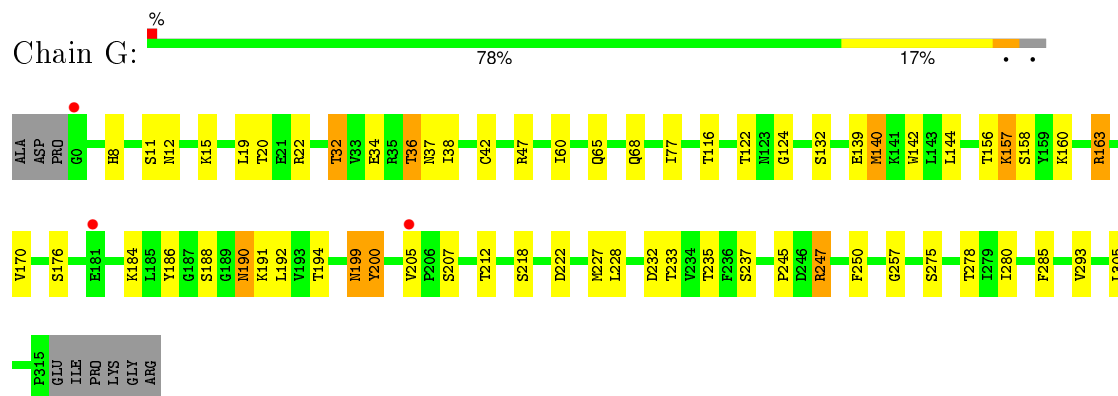
• Molecule 1: Hemagglutinin



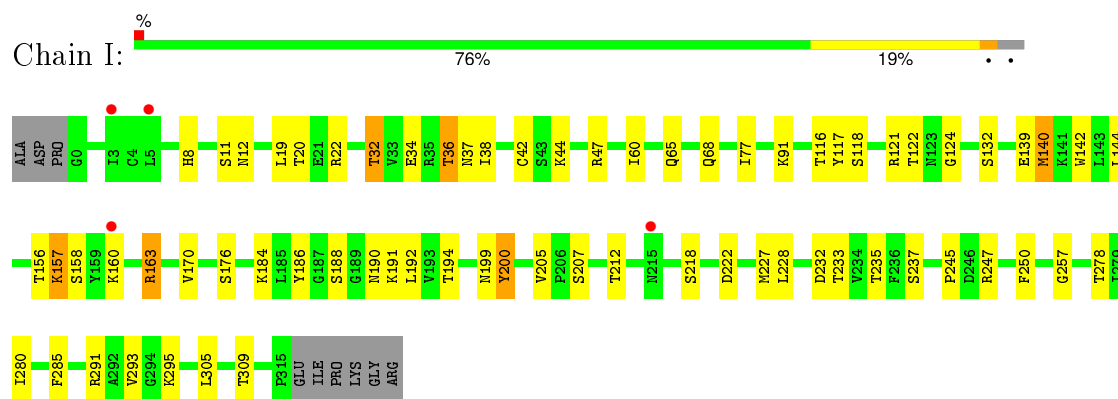
• Molecule 1: Hemagglutinin



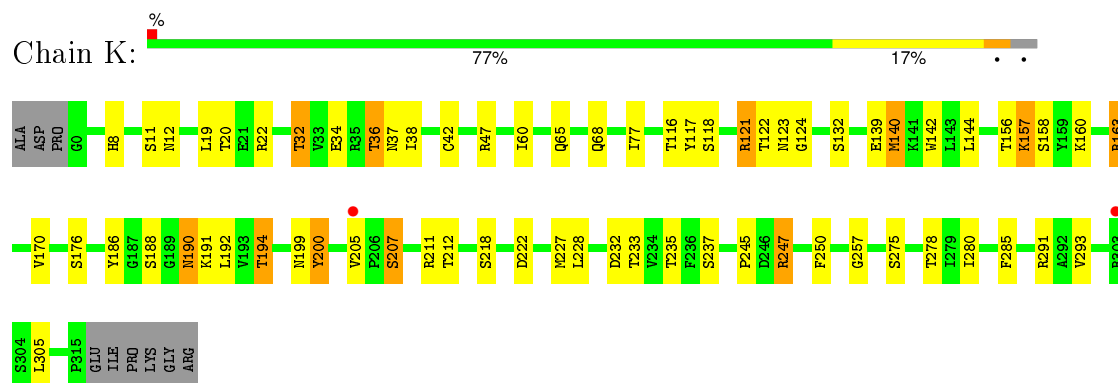
• Molecule 1: Hemagglutinin



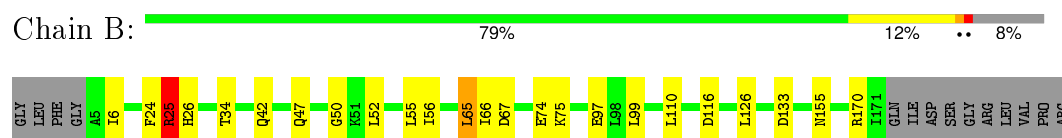
• Molecule 1: Hemagglutinin



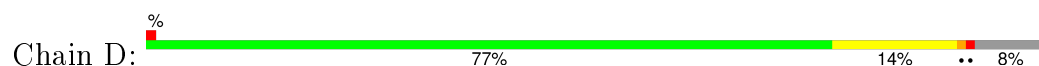
• Molecule 1: Hemagglutinin

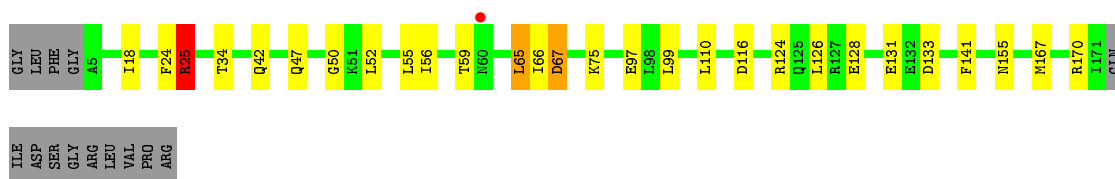


• Molecule 2: Hemagglutinin

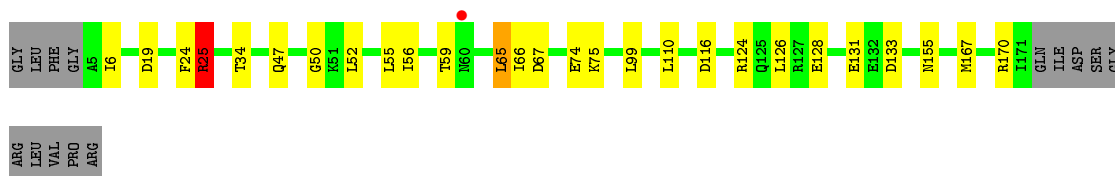
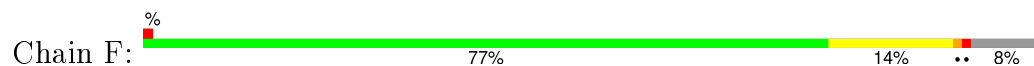


• Molecule 2: Hemagglutinin

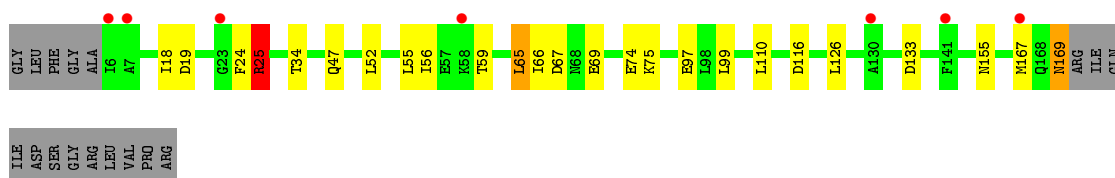
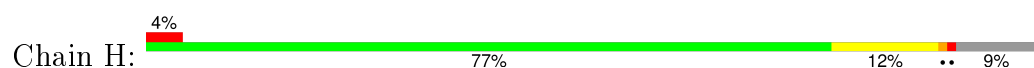




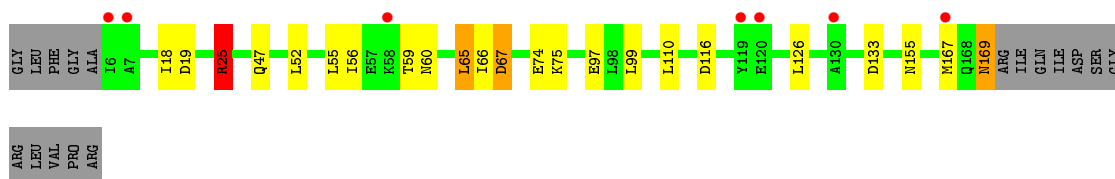
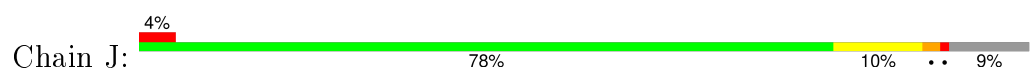
• Molecule 2: Hemagglutinin



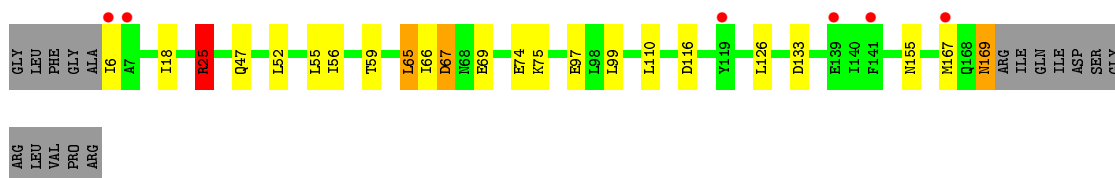
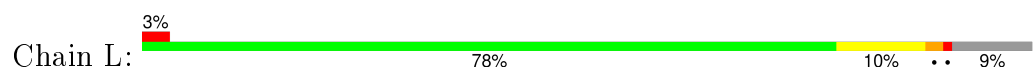
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.30Å 154.29Å 154.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.65 48.97 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.02-2.65) 98.7 (48.97-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.244 0.213 , 0.244	Depositor DCC
R_{free} test set	5391 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.1	EDS
Estimated twinning fraction	0.019 for l,-k,h 0.020 for -h,-l,-k 0.019 for k,h,-l 0.459 for l,h,k 0.459 for k,l,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 107646 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23076	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.71	0/2455	0.84	3/3316 (0.1%)
1	C	0.72	0/2455	0.85	3/3316 (0.1%)
1	E	0.71	0/2455	0.83	2/3316 (0.1%)
1	G	0.62	0/2455	0.80	2/3316 (0.1%)
1	I	0.63	0/2455	0.81	2/3316 (0.1%)
1	K	0.63	0/2455	0.81	3/3316 (0.1%)
2	B	0.71	0/1382	0.89	4/1863 (0.2%)
2	D	0.69	0/1382	0.87	3/1863 (0.2%)
2	F	0.70	0/1382	0.87	3/1863 (0.2%)
2	H	0.59	0/1358	0.80	2/1831 (0.1%)
2	J	0.59	0/1358	0.81	2/1831 (0.1%)
2	L	0.60	0/1358	0.81	2/1831 (0.1%)
All	All	0.66	0/22950	0.83	31/30978 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ARG	CG-CD-NE	7.16	126.84	111.80
2	D	25	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	E	222	ASP	CB-CG-OD1	6.35	124.02	118.30
2	B	25	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	I	295	LYS	CD-CE-NZ	6.25	126.08	111.70
2	L	25	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	J	25	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	F	25	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	C	222	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	222	ASP	CB-CG-OD1	6.07	123.77	118.30
1	G	222	ASP	CB-CG-OD1	6.04	123.73	118.30
1	K	222	ASP	CB-CG-OD1	6.03	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	25	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	I	222	ASP	CB-CG-OD1	5.85	123.56	118.30
2	H	25	ARG	CG-CD-NE	5.83	124.05	111.80
2	J	25	ARG	CG-CD-NE	5.81	123.99	111.80
2	L	25	ARG	CG-CD-NE	5.80	123.98	111.80
2	B	25	ARG	CG-CD-NE	5.78	123.94	111.80
2	D	25	ARG	CG-CD-NE	5.78	123.93	111.80
2	F	25	ARG	CG-CD-NE	5.71	123.80	111.80
1	K	121	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	121	ARG	CG-CD-NE	5.59	123.54	111.80
2	B	170	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	157	LYS	CG-CD-CE	5.43	128.18	111.90
2	B	170	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	47	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	47	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	G	247	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	D	124	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	K	247	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	F	124	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	2410	0	2361	29	0
1	C	2410	0	2362	27	0
1	E	2410	0	2361	34	0
1	G	2410	0	2362	25	0
1	I	2410	0	2362	25	0
1	K	2410	0	2362	30	0
2	B	1359	0	1263	12	0
2	D	1359	0	1263	15	0
2	F	1359	0	1263	15	0
2	H	1335	0	1234	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1335	0	1234	10	0
2	L	1335	0	1234	10	0
3	A	39	0	34	0	0
3	C	39	0	34	0	0
3	E	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
4	G	14	0	13	0	0
4	H	14	0	13	0	0
4	I	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	0	0
4	L	14	0	13	0	0
5	A	37	0	0	1	0
5	B	17	0	0	1	0
5	C	38	0	0	1	0
5	D	24	0	0	1	0
5	E	40	0	0	2	0
5	F	20	0	0	0	0
5	G	22	0	0	3	0
5	H	13	0	0	0	0
5	I	21	0	0	3	0
5	J	8	0	0	1	0
5	K	17	0	0	4	0
5	L	6	0	0	0	0
All	All	23076	0	21906	226	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 (226) 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:121:ARG:NH1	1:C:145:SER:O	1.99	0.96
2:D:131:GLU:OE1	2:D:170:ARG:HD2	1.66	0.95
2:F:131:GLU:OE1	2:F:170:ARG:HD2	1.67	0.94
1:K:47:ARG:NH1	5:K:906:HOH:O	1.89	0.86
1:I:117:TYR:HA	5:I:902:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:ARG:HG3	2:H:25:ARG:HH11	1.47	0.80
1:K:117:TYR:HA	5:K:903:HOH:O	1.80	0.80
2:J:25:ARG:HH11	2:J:25:ARG:HG3	1.48	0.79
2:F:25:ARG:HG3	2:F:25:ARG:HH11	1.48	0.78
2:D:25:ARG:HG3	2:D:25:ARG:HH11	1.48	0.77
2:L:25:ARG:HH11	2:L:25:ARG:HG3	1.48	0.77
2:B:25:ARG:HH11	2:B:25:ARG:HG3	1.48	0.76
1:I:139:GLU:OE1	1:I:247:ARG:HD3	1.86	0.74
1:K:139:GLU:OE1	1:K:247:ARG:HD3	1.87	0.74
1:E:139:GLU:OE1	1:E:247:ARG:HD3	1.87	0.74
1:G:139:GLU:OE1	1:G:247:ARG:HD3	1.88	0.74
1:C:139:GLU:OE1	1:C:247:ARG:HD3	1.88	0.74
1:A:139:GLU:OE1	1:A:247:ARG:HD3	1.88	0.73
2:F:128:GLU:HG3	2:F:170:ARG:HH21	1.59	0.68
1:C:42:CYS:SG	1:C:278:THR:HG21	2.34	0.68
2:F:128:GLU:HG3	2:F:170:ARG:NH2	2.10	0.67
1:A:42:CYS:SG	1:A:278:THR:HG21	2.34	0.67
1:E:42:CYS:SG	1:E:278:THR:HG21	2.34	0.67
1:K:42:CYS:SG	1:K:278:THR:HG21	2.35	0.67
1:E:147:THR:O	1:E:150:ALA:CB	2.43	0.66
2:D:128:GLU:HG3	2:D:170:ARG:NH2	2.09	0.66
1:I:42:CYS:SG	1:I:278:THR:HG21	2.36	0.66
1:E:293:VAL:HG11	2:F:65:LEU:HD13	1.77	0.66
1:G:42:CYS:SG	1:G:278:THR:HG21	2.36	0.65
2:D:128:GLU:HG3	2:D:170:ARG:HH21	1.59	0.65
1:E:147:THR:O	1:E:150:ALA:HB3	1.97	0.65
1:C:293:VAL:HG11	2:D:65:LEU:HD13	1.79	0.65
1:C:207:SER:CB	1:E:203:SER:OG	2.47	0.63
1:A:293:VAL:HG11	2:B:65:LEU:HD13	1.80	0.63
1:A:121:ARG:HD2	1:A:146:ASN:O	2.00	0.61
1:K:163:ARG:HG3	1:K:250:PHE:CZ	2.36	0.61
1:C:116:THR:O	1:C:157:LYS:HE3	2.00	0.61
1:A:163:ARG:HG3	1:A:250:PHE:CZ	2.36	0.61
1:I:118:SER:N	5:I:902:HOH:O	2.33	0.61
1:G:163:ARG:HG3	1:G:250:PHE:CZ	2.36	0.61
1:I:163:ARG:HG3	1:I:250:PHE:CZ	2.36	0.60
2:D:67:ASP:HB2	5:D:603:HOH:O	2.00	0.60
1:A:203:SER:OG	1:E:207:SER:CB	2.50	0.59
1:C:163:ARG:HG3	1:C:250:PHE:CZ	2.37	0.59
1:E:163:ARG:HG3	1:E:250:PHE:CZ	2.37	0.58
1:I:156:THR:O	1:I:157:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:ARG:HG2	1:K:123:ASN:OD1	2.05	0.56
1:K:156:THR:O	1:K:157:LYS:HG2	2.06	0.56
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.71	0.56
1:C:156:THR:O	1:C:157:LYS:HG2	2.06	0.56
1:I:293:VAL:HG11	2:J:65:LEU:HD13	1.88	0.56
1:I:116:THR:O	1:I:157:LYS:NZ	2.36	0.56
1:K:293:VAL:HG11	2:L:65:LEU:HD13	1.88	0.55
2:B:55:LEU:HD22	2:B:99:LEU:HD21	1.88	0.55
1:A:207:SER:CB	1:C:203:SER:OG	2.55	0.55
1:G:116:THR:O	1:G:157:LYS:NZ	2.36	0.55
1:E:116:THR:O	1:E:157:LYS:NZ	2.35	0.55
1:E:148:ASP:C	1:E:150:ALA:H	2.10	0.55
1:G:156:THR:O	1:G:157:LYS:HG2	2.06	0.55
1:E:44:LYS:HG3	1:E:266:ALA:O	2.07	0.55
1:A:194:THR:HG23	1:A:237:SER:HB3	1.90	0.54
1:E:194:THR:HG23	1:E:237:SER:HB3	1.90	0.54
2:F:55:LEU:HD22	2:F:99:LEU:HD21	1.89	0.54
1:E:156:THR:O	1:E:157:LYS:HG2	2.08	0.54
2:J:55:LEU:HD22	2:J:99:LEU:HD21	1.90	0.54
1:A:156:THR:O	1:A:157:LYS:HG2	2.08	0.54
2:D:55:LEU:HD22	2:D:99:LEU:HD21	1.90	0.53
1:K:140:MET:CE	1:K:245:PRO:HA	2.39	0.53
1:C:194:THR:HG23	1:C:237:SER:HB3	1.90	0.53
1:A:116:THR:O	1:A:157:LYS:NZ	2.35	0.53
2:H:55:LEU:HD22	2:H:99:LEU:HD21	1.90	0.53
1:K:194:THR:HG23	1:K:237:SER:HB3	1.89	0.53
1:E:267:ASP:HB2	5:E:513:HOH:O	2.09	0.52
1:K:140:MET:HE2	1:K:245:PRO:HA	1.91	0.52
1:G:293:VAL:HG11	2:H:65:LEU:HD13	1.91	0.52
1:E:140:MET:CE	1:E:245:PRO:HA	2.40	0.52
1:I:140:MET:CE	1:I:245:PRO:HA	2.39	0.52
1:I:32:THR:HB	1:I:305:LEU:O	2.10	0.52
1:G:140:MET:CE	1:G:245:PRO:HA	2.39	0.52
1:G:32:THR:HB	1:G:305:LEU:O	2.10	0.52
1:E:186:TYR:O	1:E:191:LYS:NZ	2.31	0.52
2:J:60:ASN:HB3	5:J:601:HOH:O	2.10	0.52
2:F:47:GLN:CD	2:F:110:LEU:HD11	2.30	0.52
2:L:55:LEU:HD22	2:L:99:LEU:HD21	1.91	0.51
1:K:32:THR:HB	1:K:305:LEU:O	2.10	0.51
1:C:32:THR:HB	1:C:305:LEU:O	2.10	0.51
1:C:34:GLU:OE2	1:C:36:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:THR:HB	1:E:305:LEU:O	2.10	0.51
1:G:186:TYR:O	1:G:191:LYS:NZ	2.32	0.51
1:A:32:THR:HB	1:A:305:LEU:O	2.10	0.51
1:E:199:ASN:N	5:E:507:HOH:O	2.43	0.51
1:I:34:GLU:OE2	1:I:36:THR:HB	2.11	0.50
1:E:34:GLU:OE2	1:E:36:THR:HB	2.11	0.50
1:G:34:GLU:OE2	1:G:36:THR:HB	2.11	0.50
1:K:34:GLU:OE2	1:K:36:THR:HB	2.11	0.50
1:C:199:ASN:N	5:C:917:HOH:O	2.43	0.50
1:K:116:THR:O	1:K:157:LYS:NZ	2.36	0.50
1:K:186:TYR:O	1:K:191:LYS:NZ	2.32	0.50
1:I:47:ARG:HD2	5:I:904:HOH:O	2.11	0.50
1:A:34:GLU:OE2	1:A:36:THR:HB	2.11	0.50
2:B:47:GLN:CD	2:B:110:LEU:HD11	2.33	0.49
2:D:47:GLN:CD	2:D:110:LEU:HD11	2.32	0.49
1:G:228:LEU:HD11	1:G:232:ASP:O	2.12	0.49
2:B:47:GLN:NE2	2:B:110:LEU:HD11	2.28	0.49
2:D:47:GLN:NE2	2:D:110:LEU:HD11	2.28	0.49
1:E:228:LEU:HD11	1:E:232:ASP:O	2.13	0.49
1:G:124:GLY:HA3	1:G:142:TRP:HB3	1.95	0.49
1:C:160:LYS:HG2	1:C:233:THR:OG1	2.13	0.48
1:E:160:LYS:HG2	1:E:233:THR:OG1	2.13	0.48
1:A:160:LYS:HG2	1:A:233:THR:OG1	2.13	0.48
1:G:47:ARG:HD2	5:G:903:HOH:O	2.11	0.48
2:D:56:ILE:CG2	2:D:56:ILE:O	2.61	0.48
1:G:190:ASN:N	1:G:190:ASN:OD1	2.45	0.48
1:I:160:LYS:HG2	1:I:233:THR:OG1	2.14	0.48
1:I:228:LEU:HD11	1:I:232:ASP:O	2.13	0.48
1:K:228:LEU:HD11	1:K:232:ASP:O	2.12	0.48
1:G:160:LYS:HG2	1:G:233:THR:OG1	2.14	0.48
1:C:228:LEU:HD11	1:C:232:ASP:O	2.13	0.48
1:K:160:LYS:HG2	1:K:233:THR:OG1	2.14	0.48
1:K:124:GLY:HA3	1:K:142:TRP:HB3	1.96	0.48
2:D:131:GLU:OE1	2:D:170:ARG:CD	2.52	0.48
2:F:56:ILE:CG2	2:F:56:ILE:O	2.62	0.48
1:A:228:LEU:HD11	1:A:232:ASP:O	2.13	0.48
1:A:186:TYR:O	1:A:191:LYS:NZ	2.32	0.48
1:I:124:GLY:HA3	1:I:142:TRP:HB3	1.95	0.47
2:B:56:ILE:CG2	2:B:56:ILE:O	2.62	0.47
1:I:140:MET:HE2	1:I:245:PRO:HA	1.96	0.47
1:K:118:SER:N	5:K:903:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:NH2	5:A:537:HOH:O	2.47	0.47
1:E:32:THR:HG23	1:E:285:PHE:HD1	1.80	0.47
2:B:26:HIS:HE1	5:B:601:HOH:O	1.97	0.47
1:A:32:THR:HG23	1:A:285:PHE:HD1	1.81	0.46
1:G:156:THR:C	1:G:157:LYS:HG2	2.35	0.46
1:A:156:THR:C	1:A:157:LYS:HG2	2.35	0.46
2:L:47:GLN:CD	2:L:110:LEU:HD11	2.36	0.46
1:C:190:ASN:OD1	1:C:190:ASN:N	2.46	0.46
2:F:131:GLU:OE1	2:F:170:ARG:CD	2.52	0.46
1:C:32:THR:HG23	1:C:285:PHE:HD1	1.80	0.46
1:G:15:LYS:HG3	5:G:910:HOH:O	2.14	0.46
2:J:47:GLN:CD	2:J:110:LEU:HD11	2.35	0.46
2:F:47:GLN:OE1	2:F:110:LEU:HD11	2.16	0.46
1:I:32:THR:HG23	1:I:285:PHE:HD1	1.81	0.46
1:A:192:LEU:HG	1:A:193:VAL:N	2.31	0.45
2:J:56:ILE:O	2:J:56:ILE:CG2	2.64	0.45
1:E:156:THR:C	1:E:157:LYS:HG2	2.36	0.45
2:L:47:GLN:NE2	2:L:110:LEU:HD11	2.31	0.45
1:K:156:THR:C	1:K:157:LYS:HG2	2.36	0.45
2:J:47:GLN:NE2	2:J:110:LEU:HD11	2.31	0.45
1:C:186:TYR:O	1:C:191:LYS:NZ	2.32	0.45
2:L:169:ASN:OD1	2:L:169:ASN:N	2.49	0.45
1:K:190:ASN:OD1	1:K:190:ASN:N	2.45	0.45
2:L:56:ILE:CG2	2:L:56:ILE:O	2.64	0.45
1:C:77:ILE:O	1:C:257:GLY:HA2	2.17	0.45
2:H:47:GLN:CD	2:H:110:LEU:HD11	2.35	0.45
2:H:47:GLN:OE1	2:H:110:LEU:HD11	2.17	0.45
1:A:77:ILE:O	1:A:257:GLY:HA2	2.16	0.45
2:H:169:ASN:OD1	2:H:169:ASN:N	2.49	0.45
1:I:156:THR:C	1:I:157:LYS:HG2	2.35	0.45
1:I:186:TYR:O	1:I:191:LYS:NZ	2.32	0.45
1:K:32:THR:HG23	1:K:285:PHE:HD1	1.82	0.45
2:H:56:ILE:O	2:H:56:ILE:CG2	2.64	0.44
1:K:47:ARG:HD2	5:K:906:HOH:O	2.16	0.44
2:B:56:ILE:HG23	2:B:56:ILE:O	2.18	0.44
1:K:38:ILE:CD1	1:K:280:ILE:HD12	2.48	0.44
1:C:124:GLY:HA3	1:C:142:TRP:HB3	1.99	0.44
1:I:60:ILE:HG21	1:I:170:VAL:HG21	1.99	0.44
1:E:60:ILE:HG21	1:E:170:VAL:HG21	1.98	0.44
1:K:60:ILE:HG21	1:K:170:VAL:HG21	2.00	0.44
1:G:32:THR:HG23	1:G:285:PHE:HD1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ILE:CD1	1:C:280:ILE:HD12	2.48	0.44
2:J:169:ASN:OD1	2:J:169:ASN:N	2.49	0.44
1:A:38:ILE:CD1	1:A:280:ILE:HD12	2.47	0.44
1:E:38:ILE:CD1	1:E:280:ILE:HD12	2.48	0.44
2:F:56:ILE:HG23	2:F:56:ILE:O	2.18	0.44
1:I:200:TYR:C	1:I:200:TYR:CD2	2.91	0.44
1:E:77:ILE:O	1:E:257:GLY:HA2	2.18	0.44
2:D:56:ILE:O	2:D:56:ILE:HG23	2.18	0.43
1:C:60:ILE:HG21	1:C:170:VAL:HG21	1.99	0.43
1:A:60:ILE:HG21	1:A:170:VAL:HG21	1.99	0.43
2:F:47:GLN:NE2	2:F:110:LEU:HD11	2.34	0.43
1:A:20:THR:O	2:D:50:GLY:HA3	2.18	0.43
1:E:148:ASP:O	1:E:150:ALA:N	2.51	0.43
1:I:38:ILE:CD1	1:I:280:ILE:HD12	2.48	0.43
1:G:60:ILE:HG21	1:G:170:VAL:HG21	2.00	0.43
1:I:77:ILE:O	1:I:257:GLY:HA2	2.18	0.43
1:G:77:ILE:O	1:G:257:GLY:HA2	2.18	0.43
1:K:77:ILE:O	1:K:257:GLY:HA2	2.19	0.43
1:E:190:ASN:N	1:E:190:ASN:OD1	2.47	0.43
1:C:156:THR:C	1:C:157:LYS:HG2	2.39	0.42
1:A:124:GLY:HA3	1:A:142:TRP:HB3	2.01	0.42
1:C:20:THR:O	2:F:50:GLY:HA3	2.19	0.42
1:G:38:ILE:CD1	1:G:280:ILE:HD12	2.48	0.42
1:C:207:SER:O	1:C:211:ARG:NH2	2.48	0.42
2:F:6:ILE:O	2:F:6:ILE:HG23	2.19	0.42
1:G:200:TYR:C	1:G:200:TYR:CD2	2.92	0.42
1:A:214:VAL:O	1:A:215:ASN:HB2	2.18	0.42
1:E:200:TYR:CD2	1:E:200:TYR:C	2.93	0.42
1:C:121:ARG:HH11	1:C:121:ARG:CG	2.33	0.42
2:J:56:ILE:O	2:J:56:ILE:HG23	2.20	0.42
1:A:12:ASN:N	1:A:12:ASN:OD1	2.49	0.42
1:K:291:ARG:HH21	2:L:67:ASP:HB3	1.85	0.42
2:F:24:PHE:O	2:F:34:THR:HA	2.20	0.42
2:H:56:ILE:O	2:H:56:ILE:HG23	2.19	0.41
1:E:147:THR:HG22	1:E:148:ASP:N	2.35	0.41
1:I:309:THR:HG21	4:I:800:NAG:O6	2.19	0.41
2:B:50:GLY:HA3	1:E:20:THR:O	2.18	0.41
1:G:275:SER:HB3	2:H:69:GLU:OE2	2.19	0.41
1:G:199:ASN:HB3	5:G:901:HOH:O	2.20	0.41
1:A:190:ASN:OD1	1:A:190:ASN:N	2.46	0.41
2:D:141:PHE:CG	2:D:170:ARG:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:MET:HE2	1:E:245:PRO:HA	2.01	0.41
1:K:200:TYR:C	1:K:200:TYR:CD2	2.93	0.41
2:B:6:ILE:HG23	2:B:6:ILE:O	2.20	0.41
2:B:24:PHE:O	2:B:34:THR:HA	2.21	0.41
1:A:200:TYR:CD2	1:A:200:TYR:C	2.94	0.41
1:E:124:GLY:HA3	1:E:142:TRP:HB3	2.02	0.41
2:H:24:PHE:O	2:H:34:THR:HA	2.21	0.41
2:L:6:ILE:O	2:L:6:ILE:HG23	2.21	0.41
2:D:24:PHE:O	2:D:34:THR:HA	2.21	0.41
2:B:25:ARG:NH1	2:B:25:ARG:HG3	2.26	0.40
1:G:140:MET:HE2	1:G:245:PRO:HA	2.03	0.40
1:I:291:ARG:HH21	2:J:67:ASP:HB3	1.87	0.40
1:E:207:SER:O	1:E:211:ARG:NH2	2.47	0.40
1:A:161:ASN:HB2	1:A:228:LEU:HD12	2.04	0.40
1:K:275:SER:HB3	2:L:69:GLU:OE2	2.21	0.40
1:K:207:SER:O	1:K:211:ARG:NH2	2.49	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	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	46	72
1	C	314/325 (97%)	295 (94%)	18 (6%)	1 (0%)	46	72
1	E	314/325 (97%)	296 (94%)	16 (5%)	2 (1%)	30	54
1	G	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	46	72
1	I	314/325 (97%)	298 (95%)	15 (5%)	1 (0%)	46	72
1	K	314/325 (97%)	297 (95%)	16 (5%)	1 (0%)	46	72
2	B	165/181 (91%)	159 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	165/181 (91%)	159 (96%)	6 (4%)	0	100	100
2	F	165/181 (91%)	159 (96%)	6 (4%)	0	100	100
2	H	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
2	J	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
2	L	162/181 (90%)	156 (96%)	6 (4%)	0	100	100
All	All	2865/3036 (94%)	2727 (95%)	131 (5%)	7 (0%)	52	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	C	199	ASN
1	E	199	ASN
1	G	199	ASN
1	I	199	ASN
1	K	199	ASN
1	E	150	ALA

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	264/271 (97%)	238 (90%)	26 (10%)	10	20
1	C	264/271 (97%)	233 (88%)	31 (12%)	7	13
1	E	264/271 (97%)	235 (89%)	29 (11%)	8	16
1	G	264/271 (97%)	232 (88%)	32 (12%)	6	12
1	I	264/271 (97%)	229 (87%)	35 (13%)	5	10
1	K	264/271 (97%)	234 (89%)	30 (11%)	7	14
2	B	144/155 (93%)	131 (91%)	13 (9%)	12	24
2	D	144/155 (93%)	129 (90%)	15 (10%)	9	18
2	F	144/155 (93%)	130 (90%)	14 (10%)	10	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	142/155 (92%)	125 (88%)	17 (12%)	6	13
2	J	142/155 (92%)	125 (88%)	17 (12%)	6	13
2	L	142/155 (92%)	126 (89%)	16 (11%)	7	15
All	All	2442/2556 (96%)	2167 (89%)	275 (11%)	7	15

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	SER
1	A	19	LEU
1	A	20	THR
1	A	32	THR
1	A	36	THR
1	A	37	ASN
1	A	65	GLN
1	A	68	GLN
1	A	122	THR
1	A	132	SER
1	A	144	LEU
1	A	157	LYS
1	A	158	SER
1	A	163	ARG
1	A	176	SER
1	A	188	SER
1	A	190	ASN
1	A	192	LEU
1	A	194	THR
1	A	200	TYR
1	A	205	VAL
1	A	207	SER
1	A	212	THR
1	A	218	SER
1	A	227	MET
2	B	25	ARG
2	B	42	GLN
2	B	52	LEU
2	B	65	LEU
2	B	66	ILE
2	B	67	ASP
2	B	74	GLU

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Mol	Chain	Res	Type
2	B	75	LYS
2	B	97	GLU
2	B	116	ASP
2	B	126	LEU
2	B	133	ASP
2	B	155	ASN
1	C	8	HIS
1	C	11	SER
1	C	19	LEU
1	C	20	THR
1	C	22	ARG
1	C	32	THR
1	C	36	THR
1	C	37	ASN
1	C	65	GLN
1	C	68	GLN
1	C	121	ARG
1	C	122	THR
1	C	132	SER
1	C	140	MET
1	C	144	LEU
1	C	157	LYS
1	C	158	SER
1	C	163	ARG
1	C	176	SER
1	C	183	THR
1	C	188	SER
1	C	190	ASN
1	C	192	LEU
1	C	194	THR
1	C	200	TYR
1	C	205	VAL
1	C	207	SER
1	C	212	THR
1	C	218	SER
1	C	227	MET
1	C	235	THR
2	D	18	ILE
2	D	25	ARG
2	D	42	GLN
2	D	52	LEU
2	D	59	THR

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Mol	Chain	Res	Type
2	D	65	LEU
2	D	66	ILE
2	D	67	ASP
2	D	75	LYS
2	D	97	GLU
2	D	116	ASP
2	D	126	LEU
2	D	133	ASP
2	D	155	ASN
2	D	167	MET
1	E	8	HIS
1	E	11	SER
1	E	19	LEU
1	E	20	THR
1	E	32	THR
1	E	36	THR
1	E	37	ASN
1	E	44	LYS
1	E	65	GLN
1	E	68	GLN
1	E	122	THR
1	E	132	SER
1	E	140	MET
1	E	144	LEU
1	E	157	LYS
1	E	158	SER
1	E	163	ARG
1	E	176	SER
1	E	188	SER
1	E	190	ASN
1	E	192	LEU
1	E	194	THR
1	E	200	TYR
1	E	205	VAL
1	E	207	SER
1	E	212	THR
1	E	218	SER
1	E	227	MET
1	E	235	THR
2	F	19	ASP
2	F	25	ARG
2	F	52	LEU

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Mol	Chain	Res	Type
2	F	59	THR
2	F	65	LEU
2	F	66	ILE
2	F	67	ASP
2	F	74	GLU
2	F	75	LYS
2	F	116	ASP
2	F	126	LEU
2	F	133	ASP
2	F	155	ASN
2	F	167	MET
1	G	8	HIS
1	G	11	SER
1	G	12	ASN
1	G	19	LEU
1	G	20	THR
1	G	22	ARG
1	G	32	THR
1	G	36	THR
1	G	37	ASN
1	G	65	GLN
1	G	68	GLN
1	G	122	THR
1	G	132	SER
1	G	140	MET
1	G	144	LEU
1	G	157	LYS
1	G	158	SER
1	G	163	ARG
1	G	176	SER
1	G	184	LYS
1	G	188	SER
1	G	190	ASN
1	G	192	LEU
1	G	194	THR
1	G	200	TYR
1	G	205	VAL
1	G	207	SER
1	G	212	THR
1	G	218	SER
1	G	227	MET
1	G	235	THR

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Mol	Chain	Res	Type
1	G	237	SER
2	H	18	ILE
2	H	19	ASP
2	H	25	ARG
2	H	52	LEU
2	H	59	THR
2	H	65	LEU
2	H	66	ILE
2	H	67	ASP
2	H	74	GLU
2	H	75	LYS
2	H	97	GLU
2	H	116	ASP
2	H	126	LEU
2	H	133	ASP
2	H	155	ASN
2	H	167	MET
2	H	169	ASN
1	I	8	HIS
1	I	11	SER
1	I	12	ASN
1	I	19	LEU
1	I	20	THR
1	I	22	ARG
1	I	32	THR
1	I	36	THR
1	I	37	ASN
1	I	44	LYS
1	I	65	GLN
1	I	68	GLN
1	I	91	LYS
1	I	121	ARG
1	I	122	THR
1	I	132	SER
1	I	140	MET
1	I	144	LEU
1	I	157	LYS
1	I	158	SER
1	I	163	ARG
1	I	176	SER
1	I	184	LYS
1	I	188	SER

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Mol	Chain	Res	Type
1	I	190	ASN
1	I	192	LEU
1	I	194	THR
1	I	200	TYR
1	I	205	VAL
1	I	207	SER
1	I	212	THR
1	I	218	SER
1	I	227	MET
1	I	235	THR
1	I	237	SER
2	J	18	ILE
2	J	19	ASP
2	J	25	ARG
2	J	52	LEU
2	J	59	THR
2	J	65	LEU
2	J	66	ILE
2	J	67	ASP
2	J	74	GLU
2	J	75	LYS
2	J	97	GLU
2	J	116	ASP
2	J	126	LEU
2	J	133	ASP
2	J	155	ASN
2	J	167	MET
2	J	169	ASN
1	K	8	HIS
1	K	11	SER
1	K	12	ASN
1	K	19	LEU
1	K	20	THR
1	K	22	ARG
1	K	32	THR
1	K	36	THR
1	K	37	ASN
1	K	65	GLN
1	K	68	GLN
1	K	122	THR
1	K	132	SER
1	K	140	MET

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Mol	Chain	Res	Type
1	K	144	LEU
1	K	157	LYS
1	K	158	SER
1	K	163	ARG
1	K	176	SER
1	K	188	SER
1	K	190	ASN
1	K	192	LEU
1	K	194	THR
1	K	200	TYR
1	K	205	VAL
1	K	207	SER
1	K	212	THR
1	K	218	SER
1	K	227	MET
1	K	235	THR
2	L	18	ILE
2	L	25	ARG
2	L	52	LEU
2	L	59	THR
2	L	65	LEU
2	L	66	ILE
2	L	67	ASP
2	L	74	GLU
2	L	75	LYS
2	L	97	GLU
2	L	116	ASP
2	L	126	LEU
2	L	133	ASP
2	L	155	ASN
2	L	167	MET
2	L	169	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	C	37	ASN
1	E	37	ASN
1	E	165	ASN
1	G	37	ASN
1	I	37	ASN

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Mol	Chain	Res	Type
1	K	37	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 ⓘ

9 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	401	1,3	14,14,15	0.56	0	15,19,21	1.22	2 (13%)
3	NAG	A	402	3	14,14,15	0.76	1 (7%)	15,19,21	1.47	2 (13%)
3	BMA	A	403	3	11,11,12	0.56	0	14,15,17	0.98	0
3	NAG	C	800	1,3	14,14,15	0.81	1 (7%)	15,19,21	1.35	2 (13%)
3	NAG	C	801	3	14,14,15	0.81	1 (7%)	15,19,21	1.46	3 (20%)
3	BMA	C	802	3	11,11,12	0.56	0	14,15,17	1.54	1 (7%)
3	NAG	E	401	1,3	14,14,15	0.53	0	15,19,21	1.47	1 (6%)
3	NAG	E	402	3	14,14,15	0.67	0	15,19,21	1.32	2 (13%)
3	BMA	E	403	3	11,11,12	0.50	0	14,15,17	1.08	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
3	NAG	C	800	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	801	3	-	0/6/23/26	0/1/1/1
3	BMA	C	802	3	-	0/2/19/22	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	BMA	E	403	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAG	C1-C2	2.16	1.55	1.52
3	C	801	NAG	C1-C2	2.23	1.55	1.52
3	C	800	NAG	C1-C2	2.42	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	NAG	C3-C4-C5	-2.54	105.76	110.20
3	A	401	NAG	C3-C4-C5	-2.22	106.33	110.20
3	C	801	NAG	C3-C4-C5	-2.20	106.36	110.20
3	E	402	NAG	C3-C4-C5	-2.19	106.38	110.20
3	E	402	NAG	O7-C7-C8	-2.07	118.27	122.06
3	A	402	NAG	C1-O5-C5	2.01	114.80	112.25
3	A	402	NAG	C2-N2-C7	2.31	126.01	123.04
3	C	801	NAG	O4-C4-C5	2.42	115.66	109.24
3	E	403	BMA	O5-C5-C6	2.45	112.64	107.35
3	A	401	NAG	C1-O5-C5	3.24	116.36	112.25
3	C	801	NAG	C1-O5-C5	3.44	116.61	112.25
3	C	800	NAG	C1-O5-C5	3.75	117.01	112.25
3	E	401	NAG	C1-O5-C5	4.00	117.33	112.25
3	C	802	BMA	O5-C5-C6	4.23	116.51	107.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	404	1	14,14,15	0.61	0	15,19,21	2.02	2 (13%)
4	NAG	B	500	2	14,14,15	0.71	0	15,19,21	2.12	4 (26%)
4	NAG	D	500	2	14,14,15	0.69	0	15,19,21	2.13	4 (26%)
4	NAG	E	404	1	14,14,15	0.78	1 (7%)	15,19,21	1.29	1 (6%)
4	NAG	F	500	2	14,14,15	0.60	0	15,19,21	2.25	3 (20%)
4	NAG	G	800	1	14,14,15	0.37	0	15,19,21	1.45	3 (20%)
4	NAG	H	500	2	14,14,15	0.64	0	15,19,21	1.38	2 (13%)
4	NAG	I	800	1	14,14,15	0.37	0	15,19,21	2.27	5 (33%)
4	NAG	J	500	2	14,14,15	0.68	0	15,19,21	1.33	1 (6%)
4	NAG	K	800	1	14,14,15	0.42	0	15,19,21	1.87	2 (13%)
4	NAG	L	500	2	14,14,15	0.58	0	15,19,21	1.64	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	404	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	500	2	-	0/6/23/26	0/1/1/1
4	NAG	D	500	2	-	0/6/23/26	0/1/1/1
4	NAG	E	404	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	F	500	2	-	0/6/23/26	0/1/1/1
4	NAG	G	800	1	-	0/6/23/26	0/1/1/1
4	NAG	H	500	2	-	0/6/23/26	0/1/1/1
4	NAG	I	800	1	-	0/6/23/26	0/1/1/1
4	NAG	J	500	2	-	0/6/23/26	0/1/1/1
4	NAG	K	800	1	-	0/6/23/26	0/1/1/1
4	NAG	L	500	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	404	NAG	C1-C2	2.17	1.55	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAG	C4-C3-C2	-3.28	106.12	111.23
4	I	800	NAG	C4-C3-C2	-3.15	106.33	111.23
4	L	500	NAG	C3-C4-C5	-3.07	104.84	110.20
4	B	500	NAG	C3-C4-C5	-3.03	104.91	110.20
4	F	500	NAG	C3-C4-C5	-2.93	105.09	110.20
4	D	500	NAG	C3-C4-C5	-2.58	105.70	110.20
4	H	500	NAG	C3-C4-C5	-2.45	105.93	110.20
4	I	800	NAG	C3-C4-C5	-2.43	105.96	110.20
4	L	500	NAG	O6-C6-C5	-2.33	103.62	111.33
4	K	800	NAG	C4-C3-C2	-2.32	107.62	111.23
4	G	800	NAG	C4-C3-C2	-2.25	107.73	111.23
4	B	500	NAG	O5-C5-C6	-2.16	102.68	107.35
4	I	800	NAG	O6-C6-C5	-2.08	104.45	111.33
4	G	800	NAG	C3-C4-C5	-2.05	106.62	110.20
4	L	500	NAG	C4-C3-C2	-2.03	108.08	111.23
4	I	800	NAG	O4-C4-C3	2.02	114.88	110.34
4	B	500	NAG	C2-N2-C7	2.07	125.70	123.04
4	F	500	NAG	O3-C3-C4	2.11	115.08	110.34
4	D	500	NAG	O3-C3-C4	2.52	116.01	110.34
4	E	404	NAG	C1-O5-C5	2.59	115.53	112.25
4	H	500	NAG	C1-O5-C5	2.95	115.99	112.25
4	L	500	NAG	C1-O5-C5	3.34	116.49	112.25
4	J	500	NAG	C1-O5-C5	3.96	117.28	112.25
4	G	800	NAG	C1-O5-C5	4.00	117.32	112.25
4	D	500	NAG	C2-N2-C7	4.08	128.28	123.04
4	D	500	NAG	C1-O5-C5	5.40	119.10	112.25
4	K	800	NAG	C1-O5-C5	5.71	119.49	112.25
4	B	500	NAG	C1-O5-C5	6.18	120.09	112.25
4	A	404	NAG	C1-O5-C5	6.41	120.38	112.25
4	I	800	NAG	C1-O5-C5	6.83	120.92	112.25
4	F	500	NAG	C1-O5-C5	6.84	120.93	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	404	NAG	C1

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Mol	Chain	Res	Type	Atom
4	E	404	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	800	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 ⓘ

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	316/325 (97%)	-0.10	0 100 100	38, 59, 84, 103	1 (0%)
1	C	316/325 (97%)	-0.10	1 (0%) 94 95	40, 59, 84, 104	1 (0%)
1	E	316/325 (97%)	-0.09	2 (0%) 90 91	37, 58, 85, 106	1 (0%)
1	G	316/325 (97%)	-0.04	3 (0%) 85 86	50, 73, 100, 128	1 (0%)
1	I	316/325 (97%)	-0.03	4 (1%) 79 79	49, 72, 99, 124	1 (0%)
1	K	316/325 (97%)	-0.03	2 (0%) 90 91	49, 72, 99, 127	1 (0%)
2	B	167/181 (92%)	-0.13	0 100 100	33, 59, 82, 125	0
2	D	167/181 (92%)	-0.13	1 (0%) 90 91	34, 60, 83, 122	0
2	F	167/181 (92%)	-0.11	1 (0%) 90 91	32, 60, 81, 125	0
2	H	164/181 (90%)	0.24	7 (4%) 39 37	47, 83, 103, 130	0
2	J	164/181 (90%)	0.22	7 (4%) 39 37	46, 82, 105, 133	0
2	L	164/181 (90%)	0.14	6 (3%) 45 44	46, 83, 104, 120	0
All	All	2889/3036 (95%)	-0.03	34 (1%) 81 80	32, 67, 97, 133	6 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	7	ALA	5.5
2	L	7	ALA	5.4
2	H	7	ALA	5.1
2	H	58	LYS	4.3
2	L	119	TYR	3.2
2	L	141	PHE	3.2
2	H	141	PHE	3.0
2	H	130	ALA	2.8
2	F	60	ASN	2.8
2	H	6	ILE	2.8
1	G	0	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	5	LEU	2.6
2	H	167	MET	2.6
1	K	205	VAL	2.5
2	J	120	GLU	2.5
1	I	3	ILE	2.5
1	E	0	GLY	2.4
2	L	139	GLU	2.4
1	G	205	VAL	2.4
1	E	215	ASN	2.4
1	G	181	GLU	2.4
1	C	215	ASN	2.3
2	L	167	MET	2.2
1	K	303	ARG	2.2
2	H	23	GLY	2.2
1	I	215	ASN	2.1
2	J	119	TYR	2.1
1	I	160	LYS	2.1
2	J	167	MET	2.1
2	L	6	ILE	2.1
2	J	58	LYS	2.1
2	D	60	ASN	2.1
2	J	6	ILE	2.1
2	J	130	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	401	14/15	0.90	0.18	-	79,90,93,100	0
3	BMA	E	403	11/12	0.57	0.19	-	124,145,156,158	0
3	BMA	A	403	11/12	0.71	0.19	-	113,138,144,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	801	14/15	0.91	0.18	-	80,105,126,134	0
3	NAG	C	800	14/15	0.90	0.15	-	74,89,94,95	0
3	NAG	E	401	14/15	0.84	0.18	-	82,89,96,105	0
3	NAG	A	402	14/15	0.91	0.15	-	85,110,124,140	0
3	NAG	E	402	14/15	0.86	0.23	-	86,122,138,146	0
3	BMA	C	802	11/12	0.57	0.27	-	124,143,151,161	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	D	500	14/15	0.85	0.21	3.18	70,84,92,93	0
4	NAG	F	500	14/15	0.83	0.23	1.42	70,86,90,107	0
4	NAG	B	500	14/15	0.87	0.18	1.05	66,80,90,97	0
4	NAG	J	500	14/15	0.84	0.15	-0.31	82,91,98,98	0
4	NAG	H	500	14/15	0.86	0.15	-0.48	81,89,95,96	0
4	NAG	L	500	14/15	0.90	0.12	-1.38	83,92,97,99	0
4	NAG	E	404	14/15	0.74	0.30	-	123,141,151,160	0
4	NAG	A	404	14/15	0.74	0.24	-	125,139,162,165	0
4	NAG	I	800	14/15	0.90	0.14	-	95,110,114,115	0
4	NAG	K	800	14/15	0.88	0.15	-	92,107,110,111	0
4	NAG	G	800	14/15	0.88	0.14	-	98,111,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.