Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 12:59 AM EDT

PDB ID	:	5KAN
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 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 (i) 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 (i)) were used in the production of this report:

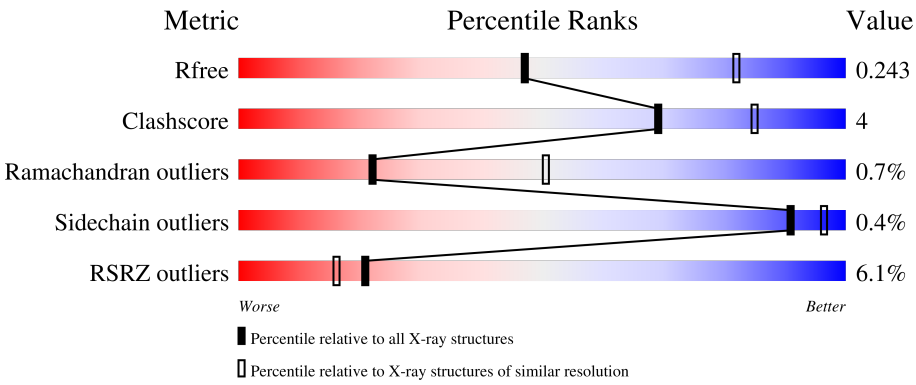
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 <=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	3% 92% 8%
1	C	319	94% 6%
1	E	319	93% 7%
2	B	173	2% 93% 7%

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Mol	Chain	Length	Quality of chain
2	D	173	2%, 92%, 6%
2	F	173	2%, 94%
3	G	231	3%, 93%, 7%
3	H	231	3%, 94%, 6%
3	J	231	26%, 94%, 5%
4	I	214	2%, 83%, 16%
4	K	214	30%, 78%, 21%
4	L	214	2%, 86%, 14%

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
5	NAG	A	401	-	-	-	X
5	NAG	A	404	-	-	-	X
5	NAG	E	401	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	319	2467	1544	433	477	13	0	0	0
1	C	319	2467	1544	433	477	13	0	0	0
1	E	319	2467	1544	433	477	13	0	0	0

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
			Total	C	N	O	S			
2	B	173	1403	869	248	280	6	0	0	0
2	D	171	1392	862	246	278	6	0	0	0
2	F	170	1383	856	244	277	6	3	0	0

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

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

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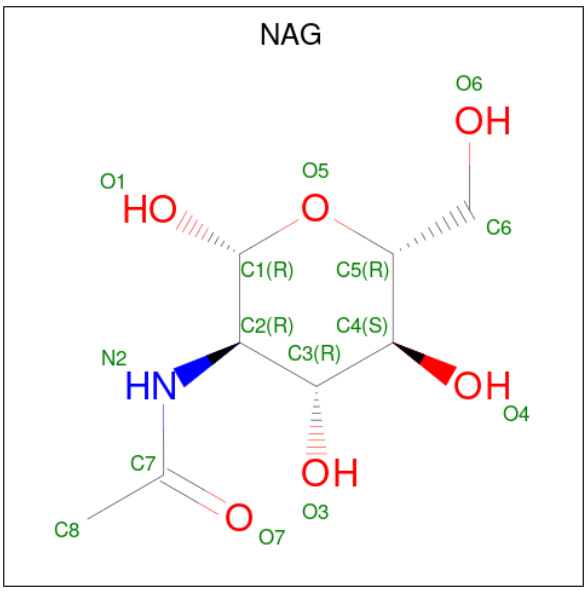
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	231	1751	1099	297	345	10	0	0	0

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

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

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



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

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

- Molecule 6 is water.

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

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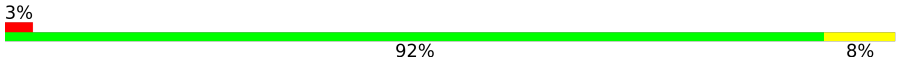
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	H	11	11	11	0	0
			Total	O		
6	I	16	16	16	0	0
			Total	O		
6	J	5	5	5	0	0
			Total	O		
6	K	8	8	8	0	0
			Total	O		
6	L	15	15	15	0	0

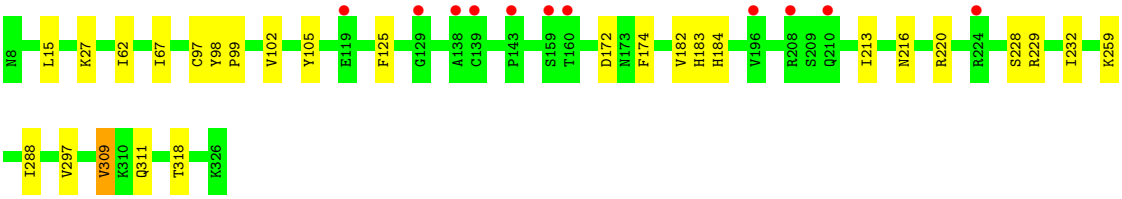
3 Residue-property plots (i)

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

• Molecule 1: Hemagglutinin HA1

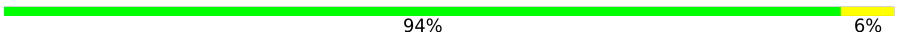
Chain A:

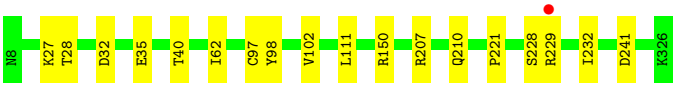




• Molecule 1: Hemagglutinin HA1

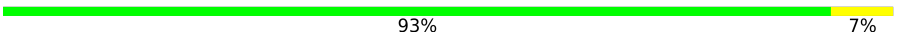
Chain C:





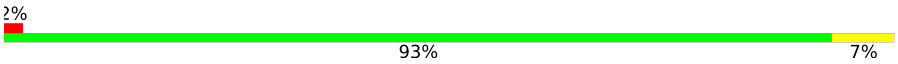
• Molecule 1: Hemagglutinin HA1

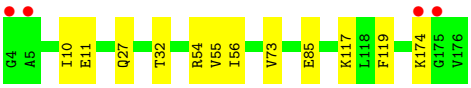
Chain E:



• Molecule 2: Hemagglutinin HA2

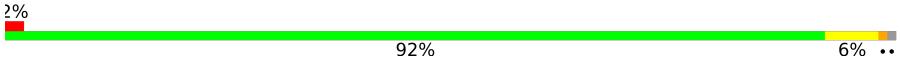
Chain B:





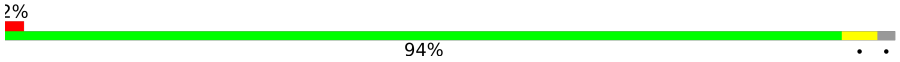
• Molecule 2: Hemagglutinin HA2

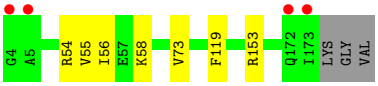
Chain D:



• Molecule 2: Hemagglutinin HA2

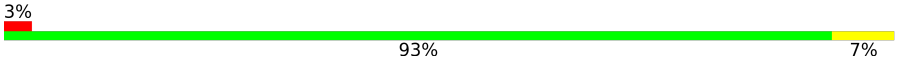
Chain F:

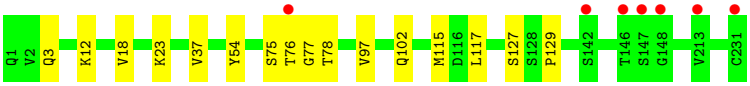




• Molecule 3: 16.g.07 Heavy chain

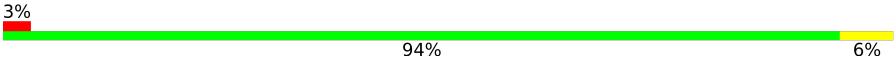
Chain G:

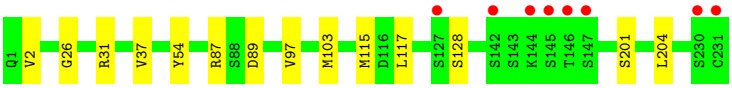




• Molecule 3: 16.g.07 Heavy chain

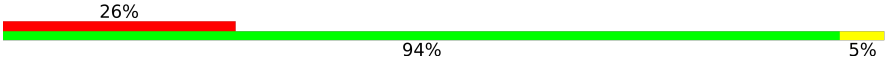
Chain H:

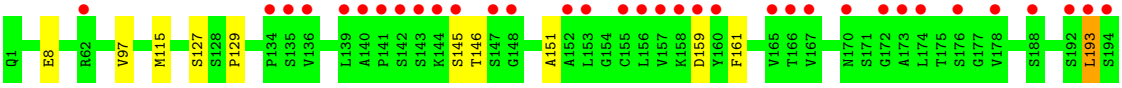


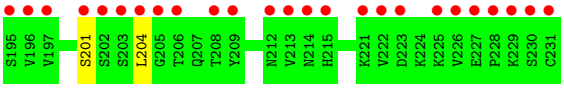


• Molecule 3: 16.g.07 Heavy chain

Chain J:

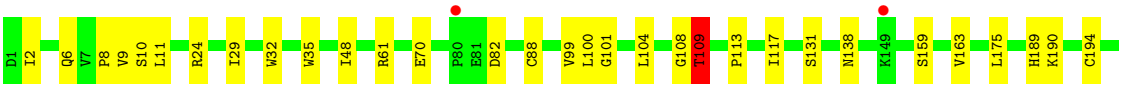


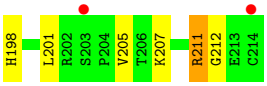




• Molecule 4: 16.g.07 Light chain

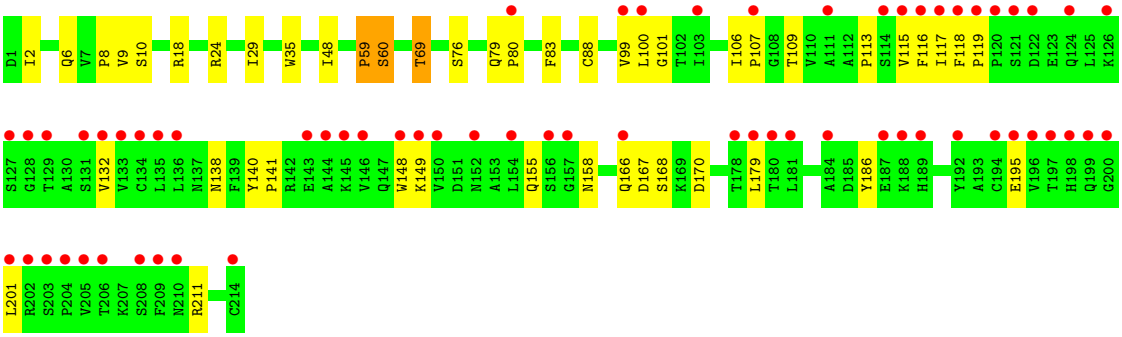
Chain I:





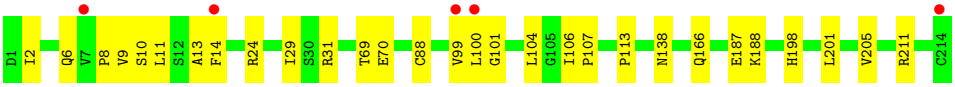
• Molecule 4: 16.g.07 Light chain

Chain K:



- Molecule 4: 16.g.07 Light chain

Chain L:



4 Data and refinement statistics (i)

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 – 2.78	Depositor EDS
% Data completeness (in resolution range)	83.2 (40.67-2.79) 83.2 (40.67-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.218 , 0.243 0.220 , 0.243	Depositor DCC
R_{free} test set	4106 reflections (4.91%)	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 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.30	1/2523 (0.0%)	0.46	0/3438
1	C	0.24	0/2523	0.44	0/3438
1	E	0.24	0/2523	0.45	0/3438
2	B	0.23	0/1426	0.45	0/1916
2	D	0.23	0/1415	0.42	0/1901
2	F	0.23	0/1406	0.44	0/1890
3	G	0.24	0/1793	0.49	0/2439
3	H	0.25	0/1793	0.49	0/2439
3	J	0.25	0/1793	0.51	1/2439 (0.0%)
4	I	0.35	1/1679 (0.1%)	0.62	1/2281 (0.0%)
4	K	0.28	0/1679	0.57	0/2281
4	L	0.26	0/1679	0.51	0/2281
All	All	0.26	2/22232 (0.0%)	0.49	2/30181 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	LYS	CE-NZ	5.74	1.63	1.49
4	I	211	ARG	CZ-NH1	5.17	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	211	ARG	NE-CZ-NH1	13.62	127.11	120.30
3	J	193	LEU	CA-CB-CG	6.04	129.19	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2467	0	2413	17	0
1	C	2467	0	2415	16	0
1	E	2467	0	2414	17	0
2	B	1403	0	1326	11	0
2	D	1392	0	1314	7	0
2	F	1383	0	1301	5	0
3	G	1751	0	1722	8	0
3	H	1751	0	1722	6	0
3	J	1751	0	1722	7	0
4	I	1642	0	1604	29	0
4	K	1642	0	1604	30	0
4	L	1642	0	1604	23	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	2	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	2	0
All	All	22144	0	21382	160	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.

All (160) 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
1:E:287:SER:O	6:E:501:HOH:O	1.98	0.80
1:C:221:PRO:O	1:C:229:ARG:NH1	2.18	0.77
1:E:123:GLU:OE2	6:E:502:HOH:O	2.03	0.76
3:G:3:GLN:NE2	6:G:301:HOH:O	2.19	0.75
1:A:183:HIS:NE2	6:A:501:HOH:O	2.21	0.72
4:K:168:SER:OG	6:K:301:HOH:O	2.06	0.72
4:L:99:VAL:HG12	4:L:100:LEU:H	1.56	0.71
4:L:187:GLU:O	4:L:211:ARG:NH1	2.25	0.70
4:I:207:LYS:O	6:I:302:HOH:O	2.10	0.69
4:I:159:SER:OG	6:I:301:HOH:O	2.09	0.68
4:I:131:SER:N	6:I:304:HOH:O	2.25	0.68
4:K:99:VAL:HG12	4:K:100:LEU:H	1.59	0.68
4:L:106:ILE:O	4:L:166:GLN:NE2	2.28	0.66
4:L:107:PRO:O	6:L:301:HOH:O	2.13	0.65
4:K:109:THR:O	6:K:302:HOH:O	2.14	0.65
4:L:24:ARG:HH11	4:L:70:GLU:HB2	1.61	0.65
4:I:35:TRP:HD1	4:I:48:ILE:HD11	1.60	0.65
4:I:99:VAL:HG12	4:I:100:LEU:H	1.63	0.64
3:H:97:VAL:HG11	3:H:115:MET:HB3	1.80	0.62
1:C:210:GLN:HE22	1:E:218:GLU:CD	2.03	0.62
4:I:8:PRO:O	4:I:10:SER:N	2.33	0.62
2:B:54:ARG:HH12	1:C:27:LYS:HB3	1.65	0.62
4:K:8:PRO:O	4:K:10:SER:N	2.34	0.61
2:B:10:ILE:HG22	2:B:11:GLU:HG3	1.82	0.61
2:B:117:LYS:NZ	6:B:302:HOH:O	2.29	0.61
1:E:315:LYS:O	6:E:503:HOH:O	2.16	0.61
4:K:155:GLN:OE1	4:K:158:ASN:ND2	2.35	0.60
2:F:153:ARG:NH1	6:F:302:HOH:O	2.26	0.60
3:G:97:VAL:HG11	3:G:115:MET:HB3	1.84	0.60
4:I:6:GLN:HB2	4:I:99:VAL:HG11	1.83	0.59
4:L:8:PRO:O	4:L:10:SER:N	2.35	0.59
1:C:40:THR:OG1	6:C:501:HOH:O	2.09	0.58
4:K:113:PRO:HD2	4:K:201:LEU:HD11	1.85	0.58
4:I:24:ARG:NH1	4:I:70:GLU:OE2	2.37	0.58
1:A:184:HIS:ND1	1:A:216:ASN:OD1	2.37	0.58
4:I:163:VAL:HG22	4:I:175:LEU:HD12	1.86	0.57
1:A:99:PRO:HB2	1:A:229:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:60:SER:N	6:K:305:HOH:O	2.38	0.56
3:J:97:VAL:HG11	3:J:115:MET:HB3	1.86	0.56
4:K:6:GLN:HB2	4:K:99:VAL:HG11	1.88	0.56
4:L:24:ARG:NH1	4:L:70:GLU:HB2	2.21	0.55
1:E:109:ARG:NH1	6:E:504:HOH:O	2.25	0.55
1:E:255:ARG:NH2	6:E:506:HOH:O	2.39	0.55
4:L:6:GLN:HB2	4:L:99:VAL:HG11	1.88	0.54
4:L:188:LYS:NZ	6:L:305:HOH:O	2.40	0.54
4:K:83:PHE:CZ	4:K:106:ILE:HG12	2.43	0.54
4:I:207:LYS:N	6:I:302:HOH:O	2.41	0.54
2:B:55:VAL:HG13	2:B:56:ILE:HG23	1.90	0.53
1:C:228:SER:O	1:C:229:ARG:NH2	2.36	0.53
4:I:117:ILE:HG22	6:I:303:HOH:O	2.09	0.53
1:A:182:VAL:HG21	1:A:213:ILE:HG21	1.92	0.52
4:K:88:CYS:SG	4:K:99:VAL:HG21	2.50	0.52
4:K:132:VAL:HG22	4:K:179:LEU:HB3	1.91	0.52
1:C:207:ARG:HG2	1:E:221:PRO:HB2	1.92	0.52
4:I:88:CYS:SG	4:I:99:VAL:HG21	2.50	0.52
2:B:73:VAL:HG11	1:E:111:LEU:HD13	1.92	0.51
4:I:211:ARG:HG2	4:I:212:GLY:N	2.24	0.51
3:H:54:TYR:CZ	3:H:103:MET:HG3	2.46	0.51
4:K:24:ARG:NH1	4:K:69:THR:OG1	2.43	0.51
1:E:184:HIS:HB3	1:E:220:ARG:NH1	2.25	0.51
4:L:11:LEU:HB3	4:L:104:LEU:HD12	1.92	0.51
2:B:54:ARG:NH1	1:C:27:LYS:HB3	2.26	0.51
4:L:88:CYS:SG	4:L:99:VAL:HG21	2.51	0.51
4:I:198:HIS:HB3	4:I:201:LEU:HD13	1.93	0.50
4:L:99:VAL:HG12	4:L:100:LEU:N	2.24	0.50
1:A:297:VAL:HA	5:A:405:NAG:H82	1.94	0.50
4:L:201:LEU:HD23	4:L:205:VAL:HG23	1.92	0.50
4:I:99:VAL:HG12	4:I:100:LEU:N	2.26	0.50
4:L:24:ARG:NH1	4:L:69:THR:HG23	2.27	0.50
4:I:201:LEU:HD23	4:I:205:VAL:HG23	1.94	0.49
4:K:106:ILE:HD12	4:K:166:GLN:HE22	1.78	0.48
4:K:115:VAL:O	4:K:116:PHE:HD1	1.97	0.48
1:A:220:ARG:HD3	1:E:210:GLN:OE1	2.13	0.48
2:D:110:LEU:O	2:D:114:GLU:HG2	2.14	0.48
4:K:35:TRP:CD1	4:K:48:ILE:HD11	2.49	0.48
4:K:18:ARG:NE	4:K:76:SER:OG	2.44	0.47
4:I:35:TRP:CD1	4:I:48:ILE:HD11	2.46	0.47
4:I:11:LEU:HB3	4:I:104:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ASP:OD2	6:C:502:HOH:O	2.20	0.47
2:D:42:GLN:NE2	3:G:102:GLN:O	2.31	0.47
4:I:2:ILE:HG21	4:I:29:ILE:HD11	1.96	0.47
4:K:59:PRO:HB2	4:K:60:SER:H	1.57	0.47
4:K:99:VAL:HG12	4:K:100:LEU:N	2.28	0.47
4:L:113:PRO:HD2	4:L:201:LEU:HD11	1.96	0.47
1:A:67:ILE:HG13	1:A:105:TYR:CE2	2.50	0.47
4:K:83:PHE:CE2	4:K:106:ILE:HG12	2.50	0.47
4:K:117:ILE:HD11	4:K:148:TRP:HH2	1.79	0.47
4:L:113:PRO:HD2	4:L:201:LEU:CD1	2.44	0.46
4:I:61:ARG:NH1	4:I:82:ASP:OD2	2.48	0.46
2:D:55:VAL:HG13	2:D:56:ILE:HG23	1.98	0.46
3:G:23:LYS:HA	3:G:78:THR:HG22	1.98	0.46
4:I:113:PRO:HD2	4:I:201:LEU:CD1	2.46	0.46
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.97	0.46
2:F:55:VAL:HG13	2:F:56:ILE:HG23	1.97	0.46
4:K:140:TYR:CD1	4:K:141:PRO:HA	2.51	0.45
1:E:97:CYS:O	1:E:224:ARG:NH1	2.50	0.45
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.98	0.45
4:I:108:GLY:O	4:I:109:THR:HG22	2.15	0.45
1:A:97:CYS:SG	1:A:98:TYR:N	2.87	0.45
1:A:228:SER:O	1:A:229:ARG:NH2	2.37	0.45
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.17	0.45
2:D:53:ASN:HB3	4:I:32:TRP:CH2	2.52	0.45
4:I:113:PRO:HD2	4:I:201:LEU:HD11	1.99	0.45
1:C:32:ASP:OD2	6:C:503:HOH:O	2.21	0.45
1:C:102:VAL:HB	1:C:232:ILE:HB	1.98	0.45
1:C:210:GLN:NE2	1:E:218:GLU:OE1	2.50	0.45
3:J:127:SER:OG	3:J:129:PRO:HD2	2.16	0.45
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.99	0.44
4:I:190:LYS:O	4:I:211:ARG:N	2.49	0.44
1:A:318:THR:HG22	1:A:318:THR:O	2.17	0.44
4:I:194:CYS:N	6:I:302:HOH:O	2.49	0.44
4:K:2:ILE:HG21	4:K:29:ILE:HD11	2.00	0.44
3:J:159:ASP:C	6:J:302:HOH:O	2.56	0.44
4:L:198:HIS:HB3	4:L:201:LEU:HD13	2.00	0.44
4:K:107:PRO:HA	4:K:140:TYR:CZ	2.53	0.43
4:L:100:LEU:HD12	4:L:101:GLY:O	2.18	0.43
4:L:2:ILE:HG21	4:L:29:ILE:HD11	2.00	0.43
2:B:27:GLN:HG3	2:B:32:THR:HG22	1.99	0.43
2:B:85:GLU:OE2	6:B:301:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASP:HB3	1:A:174:PHE:CE2	2.54	0.43
1:E:48:THR:N	6:E:501:HOH:O	2.20	0.43
3:G:75:SER:HA	3:G:76:THR:HA	1.87	0.43
4:K:118:PHE:HA	4:K:119:PRO:HD3	1.87	0.43
4:K:132:VAL:CG2	4:K:179:LEU:HB3	2.49	0.43
3:J:201:SER:HA	3:J:204:LEU:HD13	2.01	0.43
1:E:97:CYS:SG	1:E:98:TYR:N	2.90	0.43
3:G:127:SER:OG	3:G:129:PRO:HD2	2.19	0.43
3:H:87:ARG:HB2	3:H:89:ASP:OD1	2.18	0.43
4:L:14:PHE:HD1	4:L:107:PRO:O	2.02	0.43
1:C:97:CYS:SG	1:C:98:TYR:N	2.91	0.42
2:D:57:GLU:O	2:D:58:LYS:HB2	2.18	0.42
4:I:100:LEU:HD12	4:I:101:GLY:O	2.19	0.42
4:I:189:HIS:O	4:I:211:ARG:NH1	2.51	0.42
4:I:88:CYS:O	4:I:99:VAL:HG23	2.18	0.42
3:J:146:THR:HG21	3:J:151:ALA:HA	2.02	0.42
1:E:272:ALA:HA	1:E:273:PRO:HD3	1.93	0.42
1:C:150:ARG:HH12	5:C:402:NAG:H5	1.84	0.42
3:J:127:SER:HB3	3:J:161:PHE:CZ	2.55	0.42
4:L:24:ARG:HD3	4:L:70:GLU:OE1	2.20	0.42
1:C:111:LEU:HD13	2:F:73:VAL:HG11	2.02	0.41
2:D:38:LEU:HD22	3:G:54:TYR:CE1	2.55	0.41
1:A:27:LYS:HB3	2:F:54:ARG:NH1	2.34	0.41
4:K:79:GLN:HB3	4:K:80:PRO:HD2	2.02	0.41
3:H:201:SER:HA	3:H:204:LEU:HD13	2.03	0.41
1:A:288:ILE:HG21	1:A:297:VAL:HG11	2.02	0.41
1:C:35:GLU:OE2	6:C:504:HOH:O	2.22	0.41
2:B:56:ILE:O	4:L:31:ARG:NH1	2.54	0.41
1:A:182:VAL:HG21	1:A:213:ILE:CG2	2.50	0.41
4:L:13:ALA:O	4:L:107:PRO:HD2	2.21	0.40
1:A:102:VAL:HG22	1:A:232:ILE:HB	2.03	0.40
3:H:31:ARG:HG2	3:H:103:MET:HE3	2.03	0.40
4:K:167:ASP:OD1	4:K:170:ASP:OD1	2.39	0.40
1:E:102:VAL:HG22	1:E:232:ILE:HB	2.03	0.40
4:K:100:LEU:HD12	4:K:101:GLY:O	2.22	0.40
3:G:12:LYS:HG3	3:G:18:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/319 (99%)	304 (96%)	11 (4%)	2 (1%)	25	54
1	C	317/319 (99%)	306 (96%)	10 (3%)	1 (0%)	41	70
1	E	317/319 (99%)	307 (97%)	9 (3%)	1 (0%)	41	70
2	B	171/173 (99%)	164 (96%)	6 (4%)	1 (1%)	25	54
2	D	169/173 (98%)	160 (95%)	7 (4%)	2 (1%)	13	36
2	F	168/173 (97%)	161 (96%)	6 (4%)	1 (1%)	25	54
3	G	229/231 (99%)	215 (94%)	13 (6%)	1 (0%)	34	64
3	H	229/231 (99%)	214 (93%)	14 (6%)	1 (0%)	34	64
3	J	229/231 (99%)	217 (95%)	12 (5%)	0	100	100
4	I	212/214 (99%)	197 (93%)	12 (6%)	3 (1%)	11	31
4	K	212/214 (99%)	197 (93%)	11 (5%)	4 (2%)	8	23
4	L	212/214 (99%)	197 (93%)	13 (6%)	2 (1%)	17	44
All	All	2782/2811 (99%)	2639 (95%)	124 (4%)	19 (1%)	22	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PHE
2	F	58	LYS
3	H	128	SER
4	K	59	PRO
4	I	9	VAL
4	I	109	THR
4	K	9	VAL
4	K	60	SER
4	L	9	VAL
1	A	62	ILE
1	C	62	ILE
2	D	58	LYS

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Mol	Chain	Res	Type
2	D	172	GLN
1	E	62	ILE
4	I	138	ASN
2	B	174	LYS
4	L	138	ASN
4	K	138	ASN
3	G	77	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/282 (100%)	281 (100%)	1 (0%)	91	96
1	C	282/282 (100%)	282 (100%)	0	100	100
1	E	282/282 (100%)	282 (100%)	0	100	100
2	B	148/148 (100%)	148 (100%)	0	100	100
2	D	147/148 (99%)	146 (99%)	1 (1%)	84	94
2	F	146/148 (99%)	146 (100%)	0	100	100
3	G	199/199 (100%)	197 (99%)	2 (1%)	76	91
3	H	199/199 (100%)	197 (99%)	2 (1%)	76	91
3	J	199/199 (100%)	197 (99%)	2 (1%)	76	91
4	I	184/184 (100%)	183 (100%)	1 (0%)	88	95
4	K	184/184 (100%)	183 (100%)	1 (0%)	88	95
4	L	184/184 (100%)	184 (100%)	0	100	100
All	All	2436/2439 (100%)	2426 (100%)	10 (0%)	91	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	VAL
2	D	167	LEU
3	G	37	VAL

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Mol	Chain	Res	Type
3	G	117	LEU
3	H	37	VAL
3	H	117	LEU
4	I	109	THR
3	J	8	GLU
3	J	193	LEU
4	K	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	248	ASN
4	K	166	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	401	1	14,14,15	1.07	1 (7%)	17,19,21	1.84	1 (5%)
5	NAG	B	201	2	14,14,15	0.32	0	17,19,21	0.68	0
5	NAG	E	404	1	14,14,15	0.33	0	17,19,21	0.36	0
5	NAG	C	404	1	14,14,15	0.35	0	17,19,21	0.45	0
5	NAG	C	401	1	14,14,15	0.20	0	17,19,21	0.50	0
5	NAG	C	402	1	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	E	403	1	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
5	NAG	A	404	1	14,14,15	0.29	0	17,19,21	0.32	0
5	NAG	C	403	1	14,14,15	0.45	0	17,19,21	0.41	0
5	NAG	A	402	1	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	E	402	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	A	405	1	14,14,15	0.41	0	17,19,21	0.43	0
5	NAG	F	201	2	14,14,15	0.31	0	17,19,21	0.73	0
5	NAG	E	401	1	14,14,15	0.93	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	A	403	1	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	E	405	1	14,14,15	0.34	0	17,19,21	0.44	0
5	NAG	D	201	2	14,14,15	0.22	0	17,19,21	0.64	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	A	401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	403	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	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	F	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	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	E	405	1	-	0/6/23/26	0/1/1/1
5	NAG	D	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	E	401	NAG	O5-C1	3.15	1.48	1.43
5	A	401	NAG	C1-C2	2.97	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	C1-O5-C5	6.86	121.49	112.19
5	E	401	NAG	C1-O5-C5	3.87	117.44	112.19
5	E	403	NAG	C1-O5-C5	2.39	115.43	112.19

There are no chirality outliers.

All (14) 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	E	403	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
5	A	403	NAG	O5-C5-C6-O6
5	A	404	NAG	O5-C5-C6-O6
5	E	404	NAG	O5-C5-C6-O6
5	E	403	NAG	C4-C5-C6-O6
5	E	404	NAG	C1-C2-N2-C7
5	E	401	NAG	C4-C5-C6-O6
5	C	403	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	402	NAG	1	0
5	A	405	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%)	0.23	11 (3%)	45	39	30, 81, 111, 158	6 (1%)
1	C	319/319 (100%)	-0.10	1 (0%)	94	94	31, 55, 79, 138	6 (1%)
1	E	319/319 (100%)	-0.16	0	100	100	33, 50, 78, 127	8 (2%)
2	B	173/173 (100%)	0.07	4 (2%)	60	55	31, 46, 83, 132	3 (1%)
2	D	171/173 (98%)	0.07	4 (2%)	60	55	34, 54, 87, 118	3 (1%)
2	F	170/173 (98%)	0.01	4 (2%)	59	54	31, 54, 79, 128	4 (2%)
3	G	231/231 (100%)	0.19	7 (3%)	50	45	37, 64, 107, 169	5 (2%)
3	H	231/231 (100%)	0.20	8 (3%)	44	38	32, 60, 114, 181	1 (0%)
3	J	231/231 (100%)	1.32	59 (25%)	0	0	42, 101, 212, 235	2 (0%)
4	I	214/214 (100%)	0.21	4 (1%)	66	63	35, 64, 119, 142	1 (0%)
4	K	214/214 (100%)	1.56	64 (29%)	0	0	53, 124, 208, 233	1 (0%)
4	L	214/214 (100%)	0.02	5 (2%)	60	55	33, 55, 92, 127	4 (1%)
All	All	2806/2811 (99%)	0.28	171 (6%)	21	16	30, 61, 164, 235	44 (1%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	231	CYS	16.8
3	H	231	CYS	16.2
3	J	230	SER	11.1
4	K	196	VAL	10.7
4	K	117	ILE	9.7
4	L	214	CYS	9.0
3	J	166	THR	9.0
3	G	231	CYS	8.2
3	J	226	VAL	8.1
3	J	229	LYS	7.8
4	K	195	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
4	K	202	ARG	7.1
3	J	214	ASN	7.1
4	K	214	CYS	6.8
4	K	157	GLY	6.7
3	J	136	VAL	6.4
4	K	144	ALA	6.2
4	K	119	PRO	6.1
3	J	213	VAL	6.0
4	K	129	THR	6.0
4	K	201	LEU	5.9
3	H	146	THR	5.8
4	K	180	THR	5.8
3	J	145	SER	5.8
4	K	194	CYS	5.7
3	H	230	SER	5.7
3	J	193	LEU	5.6
4	K	115	VAL	5.4
4	K	122	ASP	5.3
3	J	197	VAL	5.2
4	K	184	ALA	5.2
3	J	142	SER	5.0
4	K	179	LEU	5.0
3	G	146	THR	4.9
4	K	203	SER	4.9
4	K	187	GLU	4.8
4	K	206	THR	4.7
4	K	205	VAL	4.7
3	J	205	GLY	4.7
3	H	144	LYS	4.7
3	J	222	VAL	4.7
3	H	142	SER	4.6
4	K	145	LYS	4.5
3	J	225	LYS	4.5
3	J	227	GLU	4.5
4	K	121	SER	4.5
4	K	133	VAL	4.4
4	K	199	GLN	4.3
4	I	214	CYS	4.3
3	J	196	VAL	4.3
3	H	145	SER	4.3
3	J	156	LEU	4.3
4	K	154	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
4	K	204	PRO	4.2
3	J	143	SER	4.1
3	J	194	SER	4.1
3	J	208	THR	4.0
3	J	212	ASN	4.0
4	K	197	THR	3.9
4	I	149	LYS	3.9
4	K	128	GLY	3.9
4	K	156	SER	3.9
4	K	208	SER	3.9
4	K	150	VAL	3.8
2	B	175	GLY	3.8
3	J	134	PRO	3.8
3	J	172	GLY	3.8
3	J	155	CYS	3.7
4	K	189	HIS	3.7
3	J	157	VAL	3.7
4	K	146	VAL	3.7
4	K	152	ASN	3.7
4	K	127	SER	3.7
3	J	135	SER	3.6
4	K	198	HIS	3.6
3	J	223	ASP	3.5
3	J	209	TYR	3.5
4	K	107	PRO	3.5
3	G	148	GLY	3.5
2	B	4	GLY	3.5
3	J	144	LYS	3.5
3	G	147	SER	3.5
4	K	131	SER	3.5
3	J	167	VAL	3.5
4	K	209	PHE	3.5
4	K	120	PRO	3.5
3	J	170	ASN	3.4
3	J	204	LEU	3.4
4	K	148	TRP	3.4
1	A	138	ALA	3.3
4	K	134	CYS	3.3
3	J	153	LEU	3.3
4	K	80	PRO	3.3
4	K	166	GLN	3.2
1	A	129	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	160	THR	3.1
3	H	127	SER	3.1
1	A	196	VAL	3.1
4	K	188	LYS	3.1
3	J	165	VAL	3.0
1	A	159	SER	3.0
4	K	99	VAL	3.0
3	J	195	SER	2.9
1	A	143	PRO	2.9
2	B	174	LYS	2.9
3	J	174	LEU	2.9
3	J	206	THR	2.9
2	D	173	ILE	2.8
3	J	228	PRO	2.8
4	K	143	GLU	2.8
3	J	203	SER	2.8
4	K	178	THR	2.8
2	D	149	ILE	2.8
4	K	181	LEU	2.8
3	J	221	LYS	2.8
3	G	213	VAL	2.7
4	K	136	LEU	2.7
3	G	76	THR	2.7
4	K	149	LYS	2.7
4	L	14	PHE	2.7
3	J	158	LYS	2.7
3	J	147	SER	2.7
2	F	172	GLN	2.6
4	K	118	PHE	2.6
1	A	210	GLN	2.6
4	K	200	GLY	2.6
1	A	224	ARG	2.6
4	K	124	GLN	2.6
3	J	176	SER	2.6
4	I	80	PRO	2.6
3	J	192	SER	2.6
2	F	173	ILE	2.6
3	J	201	SER	2.5
2	D	6	ILE	2.5
3	J	159	ASP	2.5
4	K	135	LEU	2.5
4	K	192	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	152	ALA	2.5
3	J	202	SER	2.5
3	J	141	PRO	2.5
3	J	139	LEU	2.5
3	G	142	SER	2.4
4	K	210	ASN	2.4
2	B	5	ALA	2.4
4	K	116	PHE	2.4
3	J	173	ALA	2.4
4	K	126	LYS	2.4
4	K	111	ALA	2.4
2	F	4	GLY	2.4
3	J	62	ARG	2.4
3	J	178	VAL	2.4
3	H	147	SER	2.3
4	K	100	LEU	2.3
4	K	132	VAL	2.3
3	J	148	GLY	2.3
3	J	140	ALA	2.3
4	K	103	ILE	2.3
3	J	188	SER	2.3
1	A	208	ARG	2.3
1	A	119	GLU	2.2
4	I	203	SER	2.2
1	C	229	ARG	2.2
4	L	99	VAL	2.2
2	F	5	ALA	2.2
4	K	114	SER	2.2
2	D	174	LYS	2.1
3	J	160	TYR	2.1
4	L	100	LEU	2.1
1	A	139	CYS	2.0
3	J	215	HIS	2.0
4	L	7	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A	404	14/15	0.46	0.51	128,142,157,158	0
5	NAG	A	401	14/15	0.54	0.55	118,138,143,146	0
5	NAG	E	401	14/15	0.63	0.44	128,138,144,147	0
5	NAG	C	402	14/15	0.67	0.36	103,115,122,127	0
5	NAG	E	404	14/15	0.77	0.37	100,111,127,130	0
5	NAG	C	403	14/15	0.82	0.40	96,111,118,121	0
5	NAG	A	405	14/15	0.82	0.29	67,86,99,100	0
5	NAG	A	403	14/15	0.82	0.23	97,100,113,116	0
5	NAG	E	403	14/15	0.86	0.28	75,80,85,86	0
5	NAG	D	201	14/15	0.89	0.18	64,79,86,86	0
5	NAG	E	405	14/15	0.89	0.24	64,76,84,90	0
5	NAG	C	404	14/15	0.90	0.23	55,65,78,86	0
5	NAG	B	201	14/15	0.90	0.18	49,61,64,70	0
5	NAG	E	402	14/15	0.91	0.23	61,74,82,89	0
5	NAG	C	401	14/15	0.92	0.13	57,71,76,79	0
5	NAG	A	402	14/15	0.92	0.21	68,78,85,90	0
5	NAG	F	201	14/15	0.93	0.17	61,74,80,82	0

6.5 Other polymers (i)

There are no such residues in this entry.