Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:09 PM GMT

PDB ID	:	4QY0
Title	:	Structure of H10 from human-infecting H10N8
Authors	:	Wang, M.; Zhang, W.; Qi, J.; Wang, F.; Zhou, J.; Bi, Y.; Wu, Y.; Sun, H.; Liu, J.; Huang, C.; Li, X.; Yan, J.; Shu, Y.; Shi, Y.; Gao, G.F.
Deposited on	:	2014-07-23
Resolution	:	2.47 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

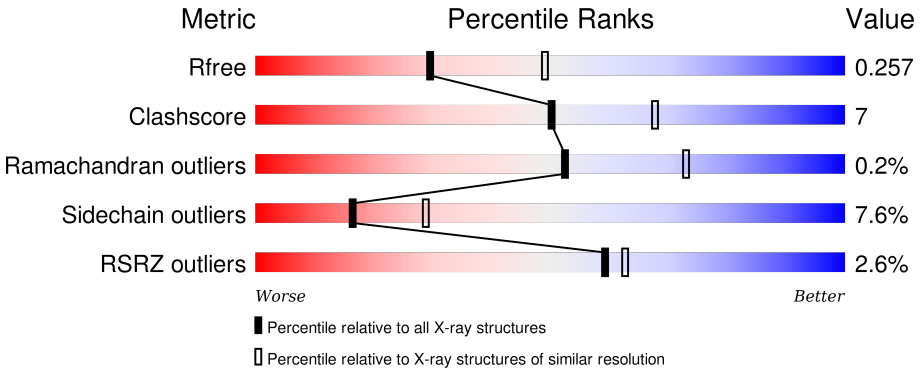
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.47 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	4309 (2.50-2.46)
Clashscore	102246	5050 (2.50-2.46)
Ramachandran outliers	100387	4961 (2.50-2.46)
Sidechain outliers	100360	4963 (2.50-2.46)
RSRZ outliers	91569	4319 (2.50-2.46)

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 <=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	318	78% 20%
1	C	318	82% 17%
1	E	318	82% 17%
1	G	318	81% 18%
1	I	318	77% 20%

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Mol	Chain	Length	Quality of chain
1	K	318	3% 79% 20%
2	B	174	2% 75% 23%
2	D	174	2% 81% 17%
2	F	174	% 83% 16%
2	H	174	6% 79% 17%
2	J	174	10% 74% 23%
2	L	174	6% 76% 24%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23653 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.

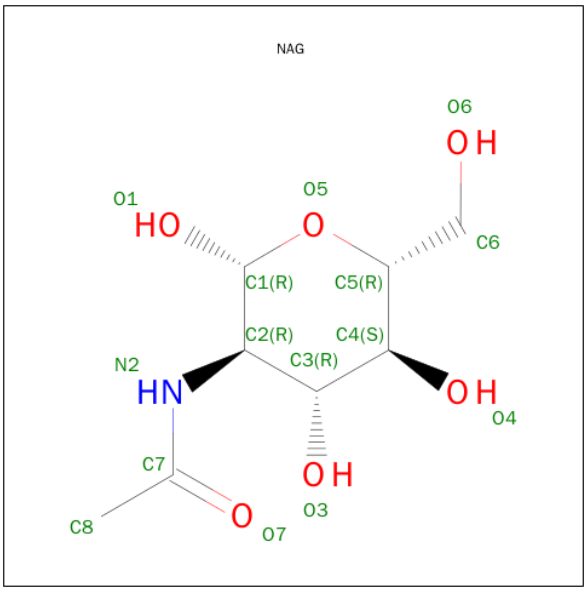
- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	C	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	G	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	I	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	K	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	D	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	L	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is water.

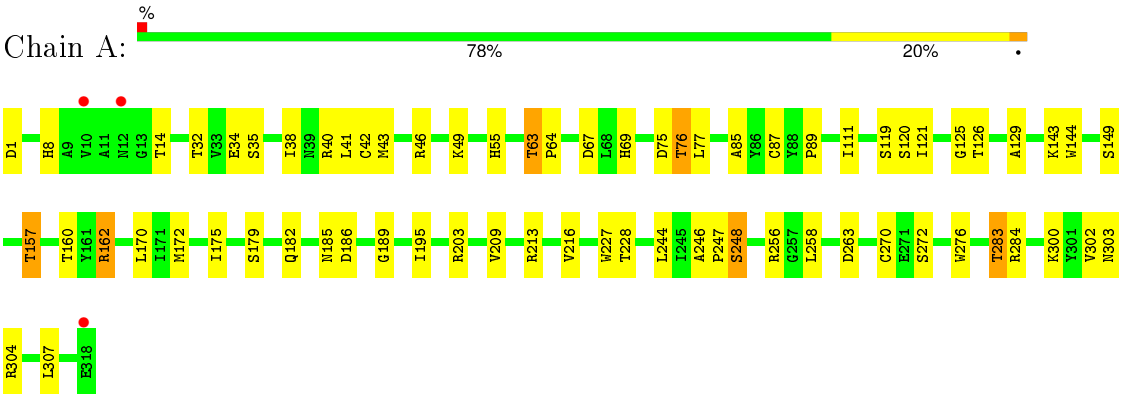
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	26	Total O 26 26	0	0
4	C	61	Total O 61 61	0	0
4	D	32	Total O 32 32	0	0
4	E	76	Total O 76 76	0	0
4	F	41	Total O 41 41	0	0
4	G	34	Total O 34 34	0	0
4	H	15	Total O 15 15	0	0
4	I	55	Total O 55 55	0	0
4	J	16	Total O 16 16	0	0
4	K	35	Total O 35 35	0	0
4	L	22	Total O 22 22	0	0

3 Residue-property plots (i)

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.

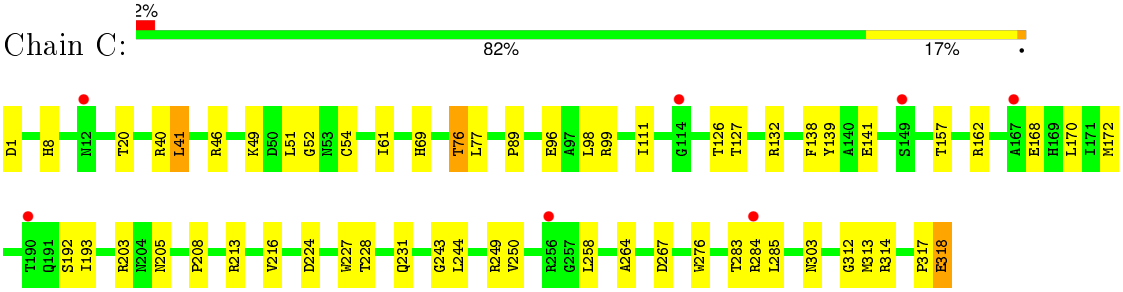
- Molecule 1: hemagglutinin

Chain A:



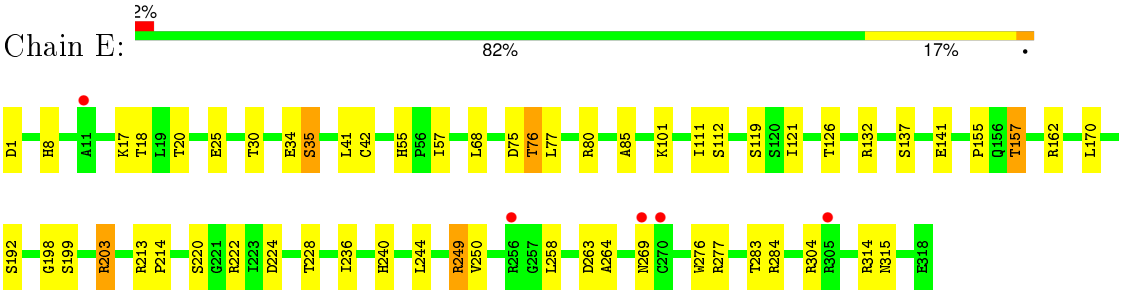
- Molecule 1: hemagglutinin

Chain C:



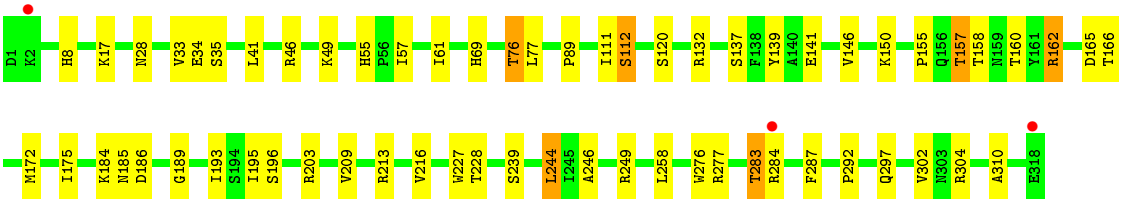
- Molecule 1: hemagglutinin

Chain E:

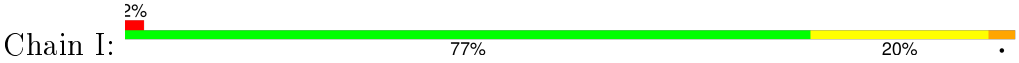


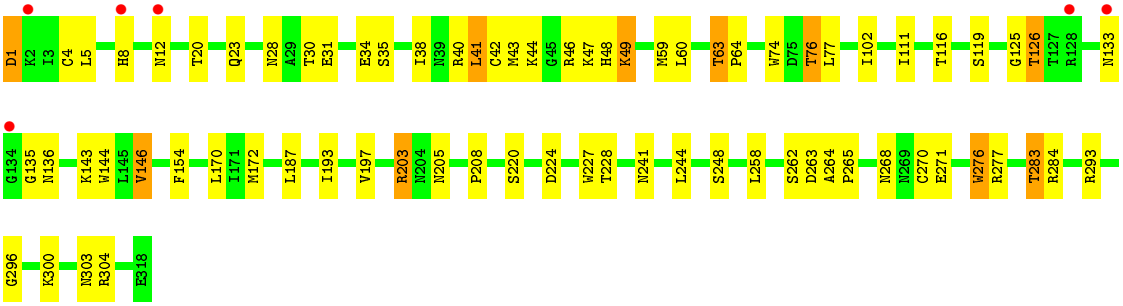
- Molecule 1: hemagglutinin

Chain G:

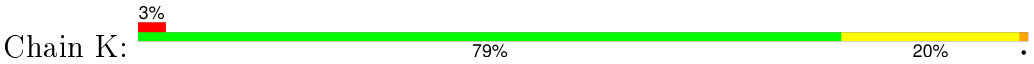


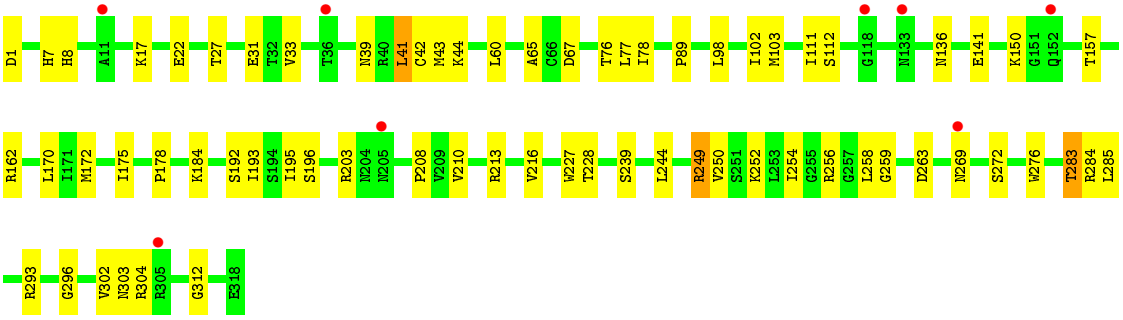
• Molecule 1: hemagglutinin



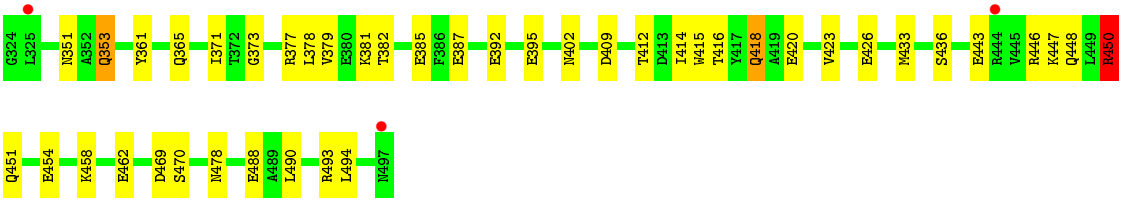


• Molecule 1: hemagglutinin

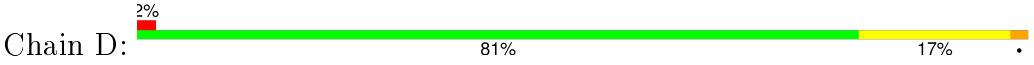


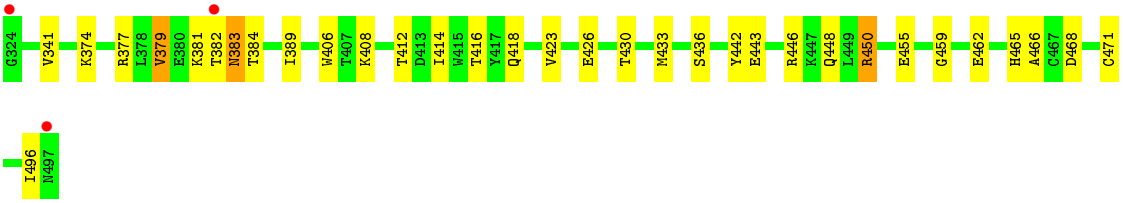


• Molecule 2: hemagglutinin



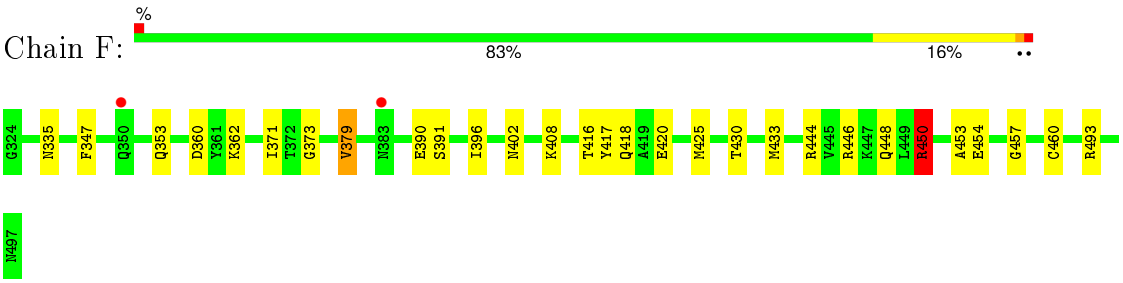
• Molecule 2: hemagglutinin





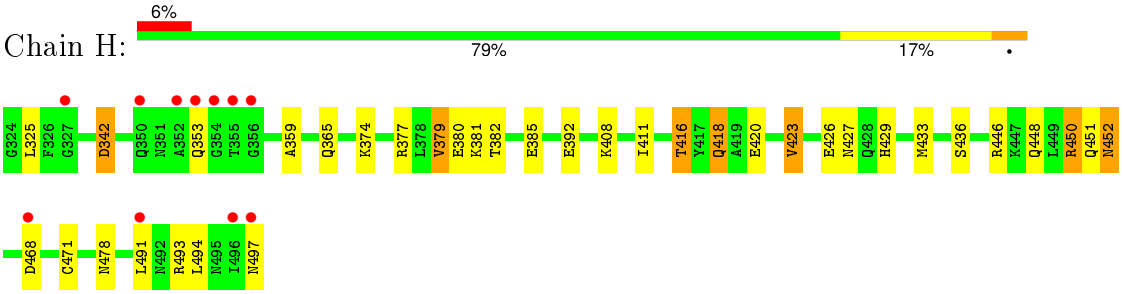
• Molecule 2: hemagglutinin

Chain F:



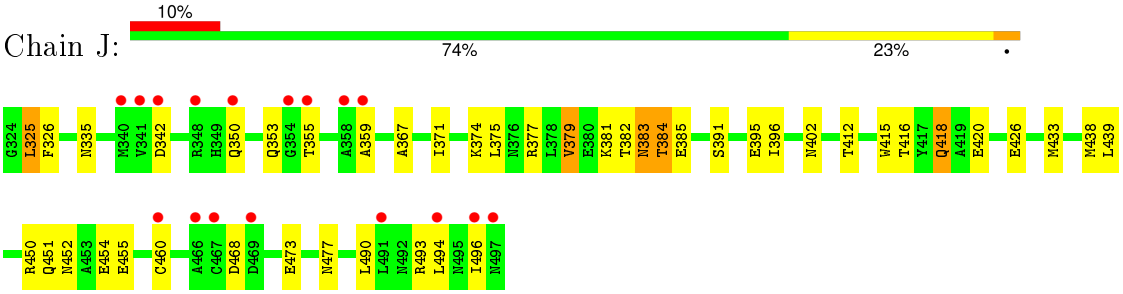
• Molecule 2: hemagglutinin

Chain H:



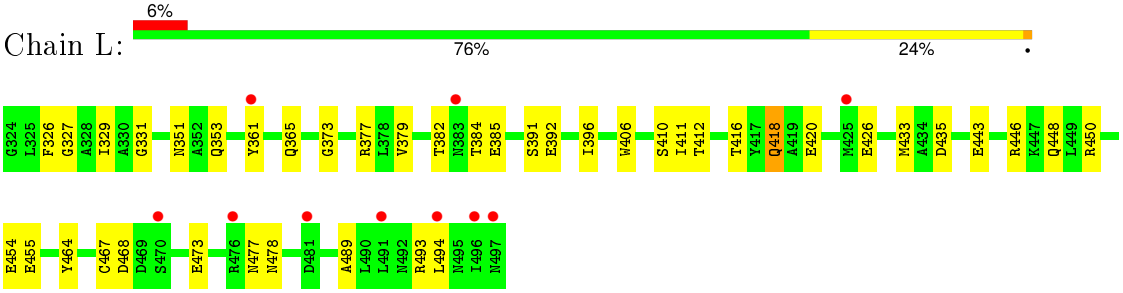
• Molecule 2: hemagglutinin

Chain J:



• Molecule 2: hemagglutinin

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.03Å 117.99Å 123.77Å 98.29° 93.37° 96.56°	Depositor
Resolution (Å)	39.47 – 2.47 39.47 – 2.47	Depositor EDS
% Data completeness (in resolution range)	93.4 (39.47-2.47) 80.4 (39.47-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.264 0.208 , 0.257	Depositor DCC
R_{free} test set	6112 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 137547 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23653	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/2486	0.50	0/3368
1	C	0.30	0/2486	0.48	0/3368
1	E	0.32	0/2486	0.49	0/3368
1	G	0.31	0/2486	0.47	0/3368
1	I	0.32	0/2486	0.50	0/3368
1	K	0.29	0/2486	0.47	0/3368
2	B	0.32	0/1427	0.46	0/1926
2	D	0.33	0/1427	0.47	0/1926
2	F	0.32	0/1427	0.47	0/1926
2	H	0.29	0/1427	0.46	0/1926
2	J	0.31	0/1427	0.45	0/1926
2	L	0.31	0/1427	0.44	0/1926
All	All	0.31	0/23478	0.48	0/31764

There are no bond length outliers.

There are no bond angle outliers.

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	2437	0	2389	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2437	0	2389	31	0
1	E	2437	0	2389	29	0
1	G	2437	0	2389	32	0
1	I	2437	0	2389	45	0
1	K	2437	0	2389	35	0
2	B	1402	0	1298	35	0
2	D	1402	0	1298	20	0
2	F	1402	0	1298	23	0
2	H	1402	0	1298	26	0
2	J	1402	0	1298	34	0
2	L	1402	0	1298	33	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
3	E	14	0	13	0	0
3	F	14	0	13	1	0
3	G	14	0	13	0	0
3	H	14	0	13	1	0
3	I	14	0	13	0	0
3	J	14	0	13	0	0
3	K	14	0	13	0	0
3	L	14	0	13	0	0
4	A	38	0	0	4	0
4	B	26	0	0	7	0
4	C	61	0	0	6	0
4	D	32	0	0	2	0
4	E	76	0	0	8	0
4	F	41	0	0	7	0
4	G	34	0	0	5	0
4	H	15	0	0	5	0
4	I	55	0	0	9	0
4	J	16	0	0	2	0
4	K	35	0	0	4	0
4	L	22	0	0	2	0
All	All	23653	0	22278	319	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 7.

All (319) 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:I:1:ASP:N	4:I:720:HOH:O	1.95	0.97
2:F:444:ARG:O	4:F:705:HOH:O	1.87	0.93
1:C:314:ARG:NH1	4:C:731:HOH:O	2.08	0.85
1:E:42:CYS:O	4:E:755:HOH:O	1.93	0.84
1:C:52:GLY:O	4:C:706:HOH:O	1.96	0.82
3:H:601:NAG:O4	4:H:712:HOH:O	1.84	0.79
2:H:418:GLN:HG3	4:H:704:HOH:O	1.85	0.77
1:A:46:ARG:HE	1:A:76:THR:HG21	1.51	0.76
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.19	0.75
2:D:455:GLU:OE1	2:F:446:ARG:NH2	2.20	0.73
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.69	0.73
2:B:402:ASN:OD1	4:B:701:HOH:O	2.06	0.73
1:K:65:ALA:O	4:K:708:HOH:O	2.07	0.72
1:C:46:ARG:HE	1:C:76:THR:HG21	1.54	0.71
2:F:402:ASN:OD1	4:F:701:HOH:O	2.09	0.70
1:E:119:SER:OG	4:E:766:HOH:O	2.09	0.69
1:C:243:GLY:N	4:C:713:HOH:O	2.10	0.69
1:A:67:ASP:O	4:A:707:HOH:O	2.11	0.68
1:K:60:LEU:O	4:K:709:HOH:O	2.10	0.68
1:I:303:ASN:H	2:J:416:THR:HG22	1.59	0.68
1:E:121:ILE:O	4:E:742:HOH:O	2.11	0.68
1:K:252:LYS:HE3	1:K:254:ILE:HD11	1.77	0.67
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.26	0.67
2:H:418:GLN:O	4:H:704:HOH:O	2.13	0.67
1:K:17:LYS:HE3	1:K:22:GLU:HG3	1.76	0.66
1:G:46:ARG:HE	1:G:76:THR:HG21	1.60	0.65
1:E:224:ASP:OD1	4:E:712:HOH:O	2.14	0.65
1:I:46:ARG:HE	1:I:76:THR:HG21	1.62	0.65
2:D:450:ARG:HB3	4:D:701:HOH:O	1.96	0.65
2:H:411:ILE:HD13	2:L:410:SER:HB3	1.77	0.65
1:G:310:ALA:O	4:G:704:HOH:O	2.15	0.65
1:C:49:LYS:NZ	4:C:711:HOH:O	2.30	0.65
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.79	0.64
2:B:409:ASP:OD2	4:B:724:HOH:O	2.15	0.64
1:A:121:ILE:HD11	1:A:157:THR:HG21	1.80	0.64
1:I:23:GLN:NE2	4:I:741:HOH:O	2.30	0.64
1:I:44:LYS:NZ	4:I:736:HOH:O	2.30	0.64
1:C:213:ARG:HG2	1:E:198:GLY:HA3	1.79	0.63
1:A:300:LYS:HG3	2:B:415:TRP:CE2	2.33	0.63
1:I:224:ASP:OD1	4:I:726:HOH:O	2.15	0.63
2:J:374:LYS:NZ	2:J:426:GLU:OE1	2.29	0.62
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:418:GLN:NE2	2:L:418:GLN:OE1	2.31	0.62
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.62
1:I:30:THR:OG1	4:I:728:HOH:O	2.07	0.62
1:K:284:ARG:HB3	2:L:379:VAL:HG13	1.83	0.61
2:H:491:LEU:HB3	2:H:497:ASN:HA	1.82	0.61
2:F:335:ASN:O	4:F:722:HOH:O	2.16	0.61
1:G:55:HIS:HE1	1:G:57:ILE:HD13	1.65	0.61
1:K:283:THR:HG22	1:K:285:LEU:H	1.65	0.60
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.82	0.60
1:E:55:HIS:CE1	1:E:57:ILE:HG12	2.37	0.59
1:I:43:MET:HE3	1:I:46:ARG:HD3	1.83	0.59
1:A:160:THR:HG22	1:A:162:ARG:HD2	1.84	0.59
2:J:383:ASN:N	2:J:383:ASN:OD1	2.35	0.59
2:L:391:SER:H	2:L:396:ILE:HD11	1.68	0.59
2:F:453:ALA:O	4:F:716:HOH:O	2.17	0.59
2:J:452:ASN:OD1	4:J:703:HOH:O	2.17	0.59
2:F:391:SER:H	2:F:396:ILE:HD11	1.68	0.59
2:J:455:GLU:OE1	2:L:446:ARG:NH2	2.36	0.58
1:K:41:LEU:HD23	1:K:78:ILE:HD13	1.84	0.58
2:B:458:LYS:NZ	4:B:709:HOH:O	2.30	0.58
2:J:353:GLN:HE22	2:J:468:ASP:HB2	1.68	0.58
1:E:284:ARG:HB3	2:F:379:VAL:HG22	1.85	0.58
1:G:184:LYS:HE2	1:G:193:ILE:HD11	1.85	0.58
1:C:285:LEU:O	2:D:381:LYS:NZ	2.36	0.58
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.36	0.58
1:I:49:LYS:NZ	4:I:706:HOH:O	2.37	0.57
2:D:389:ILE:HD11	2:D:408:LYS:HE3	1.86	0.57
3:D:601:NAG:O4	4:D:712:HOH:O	2.09	0.57
1:A:125:GLY:O	4:A:701:HOH:O	2.18	0.57
2:H:353:GLN:HE22	2:H:468:ASP:HB2	1.69	0.57
2:H:451:GLN:O	2:H:493:ARG:NH1	2.37	0.57
3:F:601:NAG:O6	4:F:726:HOH:O	2.18	0.56
2:B:443:GLU:OE2	2:B:446:ARG:NH1	2.38	0.56
2:B:377:ARG:NH2	2:B:426:GLU:OE2	2.35	0.56
1:A:42:CYS:O	4:A:712:HOH:O	2.18	0.56
1:C:49:LYS:HD2	1:C:69:HIS:ND1	2.20	0.56
2:L:455:GLU:O	4:L:719:HOH:O	2.18	0.56
1:E:1:ASP:N	4:E:754:HOH:O	2.36	0.56
1:G:28:ASN:ND2	4:G:706:HOH:O	2.24	0.55
1:I:146:VAL:HG22	1:I:187:LEU:HB3	1.89	0.55
1:C:284:ARG:HB3	2:D:379:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:381:LYS:HG3	2:J:383:ASN:OD1	2.07	0.55
1:G:302:VAL:HB	2:H:416:THR:HB	1.89	0.55
2:L:353:GLN:HE22	2:L:468:ASP:HB2	1.72	0.55
1:K:141:GLU:OE2	1:K:249:ARG:NH1	2.40	0.55
2:L:448:GLN:NE2	2:L:478:ASN:HA	2.21	0.55
2:F:493:ARG:O	4:F:708:HOH:O	2.18	0.55
1:I:48:HIS:HE1	1:I:268:ASN:HD21	1.54	0.55
2:B:450:ARG:HG3	2:B:451:GLN:H	1.71	0.55
2:B:381:LYS:NZ	2:B:382:THR:O	2.36	0.55
1:I:38:ILE:HG22	1:I:40:ARG:H	1.72	0.54
1:K:178:PRO:HG2	1:K:184:LYS:HG3	1.89	0.54
1:I:296:GLY:HA2	2:J:385:GLU:HG3	1.89	0.54
2:J:473:GLU:O	2:J:477:ASN:HB2	2.07	0.54
1:I:60:LEU:HD11	1:I:102:ILE:HD11	1.89	0.54
1:E:55:HIS:HE1	1:E:57:ILE:HG12	1.71	0.54
1:E:17:LYS:HD3	4:F:732:HOH:O	2.08	0.54
1:A:46:ARG:HB2	1:A:75:ASP:OD2	2.08	0.54
4:E:737:HOH:O	1:I:40:ARG:HD2	2.08	0.54
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.90	0.54
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.41	0.53
1:I:143:LYS:HD2	1:I:248:SER:HB3	1.91	0.53
1:C:303:ASN:H	2:D:416:THR:CG2	2.22	0.53
2:B:412:THR:O	2:B:416:THR:HG23	2.07	0.53
1:E:68:LEU:HD13	1:I:265:PRO:HA	1.89	0.53
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.39	0.53
1:A:256:ARG:NH2	2:B:387:GLU:OE1	2.41	0.53
2:J:381:LYS:HE3	2:J:383:ASN:HD21	1.73	0.52
2:L:448:GLN:HE22	2:L:478:ASN:HA	1.74	0.52
1:A:32:THR:HG22	2:B:378:LEU:HD21	1.90	0.52
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.92	0.52
3:B:601:NAG:O7	4:B:701:HOH:O	2.18	0.52
1:E:284:ARG:HH21	2:F:379:VAL:HG11	1.75	0.52
2:B:447:LYS:HD3	2:F:457:GLY:HA2	1.92	0.52
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.43	0.52
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.34	0.51
1:G:17:LYS:NZ	2:H:420:GLU:OE2	2.35	0.51
2:D:465:HIS:ND1	2:D:466:ALA:O	2.39	0.51
1:K:175:ILE:HD12	1:K:195:ILE:HD13	1.92	0.51
1:I:41:LEU:HD13	1:I:264:ALA:HB3	1.93	0.51
2:H:452:ASN:OD1	2:H:452:ASN:N	2.44	0.51
1:I:263:ASP:HB2	4:I:712:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:392:GLU:OE1	4:H:702:HOH:O	2.20	0.51
1:A:125:GLY:HA3	1:A:144:TRP:HB3	1.93	0.50
2:H:365:GLN:NE2	4:H:714:HOH:O	2.33	0.50
1:E:25:GLU:HG2	1:E:315:ASN:HB3	1.92	0.50
2:J:350:GLN:HG2	2:J:355:THR:HG22	1.93	0.50
1:K:304:ARG:NH1	2:L:420:GLU:OE1	2.44	0.50
1:A:182:GLN:NE2	1:A:186:ASP:OD1	2.45	0.50
1:G:89:PRO:HB3	1:G:216:VAL:HB	1.94	0.50
1:E:55:HIS:HB3	1:E:85:ALA:HB2	1.94	0.49
1:I:34:GLU:OE2	1:I:35:SER:N	2.45	0.49
2:B:488:GLU:OE1	4:B:726:HOH:O	2.20	0.49
1:C:317:PRO:O	1:C:318:GLU:HB2	2.12	0.49
1:G:172:MET:HG2	1:G:227:TRP:HB3	1.94	0.49
1:E:199:SER:HB3	1:E:236:ILE:HD12	1.94	0.49
1:A:143:LYS:HE3	1:A:248:SER:HB3	1.94	0.49
1:E:18:THR:O	4:E:740:HOH:O	2.20	0.49
1:A:209:VAL:HG11	1:C:205:ASN:HB2	1.94	0.49
1:E:34:GLU:OE2	1:E:35:SER:N	2.44	0.49
2:B:418:GLN:HG2	2:F:417:TYR:CE1	2.46	0.49
1:K:60:LEU:HD11	1:K:102:ILE:HD11	1.95	0.49
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.45	0.49
1:A:89:PRO:HB3	1:A:216:VAL:HB	1.95	0.49
1:C:313:MET:N	4:C:701:HOH:O	2.09	0.48
1:I:20:THR:O	2:L:373:GLY:HA3	2.13	0.48
2:H:381:LYS:NZ	2:H:382:THR:O	2.42	0.48
1:K:1:ASP:OD2	2:L:351:ASN:HA	2.14	0.48
1:C:132:ARG:NH1	1:C:138:PHE:O	2.41	0.48
2:J:494:LEU:HD22	2:L:494:LEU:HD11	1.95	0.48
1:K:263:ASP:HB2	4:K:731:HOH:O	2.14	0.48
2:B:450:ARG:NH1	2:F:454:GLU:OE1	2.37	0.48
2:F:390:GLU:OE1	2:F:408:LYS:NZ	2.37	0.48
1:I:300:LYS:HG3	2:J:415:TRP:CE2	2.48	0.48
1:G:112:SER:OG	4:G:720:HOH:O	2.19	0.48
1:I:125:GLY:HA3	1:I:144:TRP:HB3	1.96	0.48
2:H:448:GLN:NE2	2:H:478:ASN:HA	2.28	0.48
1:K:296:GLY:HA2	2:L:385:GLU:HG3	1.95	0.48
1:A:185:ASN:ND2	1:A:189:GLY:O	2.41	0.48
1:A:38:ILE:HG22	1:A:40:ARG:H	1.79	0.48
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.14	0.48
2:D:381:LYS:HG3	2:D:383:ASN:HD21	1.78	0.48
1:C:224:ASP:OD2	1:E:203:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:GLN:H	2:B:353:GLN:HE21	1.62	0.47
1:I:303:ASN:H	2:J:416:THR:CG2	2.26	0.47
2:J:494:LEU:HB3	2:J:496:ILE:HG13	1.95	0.47
1:G:175:ILE:HD12	1:G:195:ILE:HD13	1.95	0.47
1:K:136:ASN:ND2	4:K:724:HOH:O	2.42	0.47
1:G:284:ARG:HB3	2:H:379:VAL:HG22	1.95	0.47
1:K:302:VAL:HA	2:L:416:THR:HG22	1.96	0.47
1:G:185:ASN:HA	1:G:189:GLY:O	2.15	0.47
2:B:392:GLU:OE2	4:B:712:HOH:O	2.19	0.47
1:G:292:PRO:O	4:G:727:HOH:O	2.20	0.47
2:J:383:ASN:HA	2:J:384:THR:CB	2.45	0.47
1:C:303:ASN:H	2:D:416:THR:HG22	1.80	0.47
1:C:89:PRO:HB3	1:C:216:VAL:HB	1.97	0.47
2:L:329:ILE:N	2:L:435:ASP:OD1	2.42	0.47
2:B:351:ASN:ND2	2:B:469:ASP:OD1	2.37	0.47
2:B:490:LEU:O	2:B:494:LEU:HG	2.14	0.47
1:I:31:GLU:O	4:I:728:HOH:O	2.20	0.47
1:C:141:GLU:OE1	1:C:249:ARG:HD3	2.15	0.47
1:I:44:LYS:HD3	1:I:271:GLU:HG3	1.97	0.46
1:G:155:PRO:O	1:G:157:THR:HG22	2.15	0.46
2:B:373:GLY:HA3	1:E:20:THR:O	2.16	0.46
1:I:4:CYS:HA	2:J:460:CYS:HA	1.96	0.46
1:A:46:ARG:NH1	1:A:272:SER:O	2.48	0.46
1:A:307:LEU:HB3	2:B:423:VAL:HG21	1.97	0.46
1:A:43:MET:HE2	1:A:43:MET:HB3	1.81	0.46
2:B:454:GLU:OE2	2:B:493:ARG:NE	2.42	0.46
1:I:284:ARG:HH21	2:J:379:VAL:HG11	1.81	0.46
1:G:165:ASP:OD1	1:G:166:THR:N	2.45	0.45
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.17	0.45
1:I:28:ASN:ND2	4:I:753:HOH:O	2.48	0.45
2:F:371:ILE:HD11	2:F:430:THR:HG23	1.97	0.45
1:G:297:GLN:HG2	2:H:385:GLU:HG2	1.97	0.45
1:C:96:GLU:OE2	1:C:99:ARG:NH2	2.38	0.45
1:I:193:ILE:HG22	1:I:208:PRO:HD2	1.99	0.45
2:J:451:GLN:HB3	2:J:490:LEU:HD21	1.99	0.45
2:J:402:ASN:O	4:J:707:HOH:O	2.21	0.45
1:G:132:ARG:NH1	1:G:137:SER:OG	2.50	0.45
2:L:454:GLU:OE2	2:L:493:ARG:NE	2.48	0.45
1:A:49:LYS:HD2	1:A:69:HIS:ND1	2.31	0.45
1:A:42:CYS:HB3	1:A:270:CYS:O	2.17	0.45
2:J:391:SER:H	2:J:396:ILE:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:THR:O	2:D:416:THR:HG23	2.16	0.45
2:F:347:PHE:CE1	2:F:360:ASP:HB2	2.51	0.45
2:H:423:VAL:HG13	2:H:427:ASN:HD21	1.81	0.45
1:A:303:ASN:H	2:B:416:THR:CG2	2.30	0.45
2:D:406:TRP:CH2	2:F:408:LYS:HG2	2.51	0.45
1:A:185:ASN:HA	1:A:189:GLY:O	2.17	0.45
2:J:326:PHE:HB3	2:J:439:LEU:HD22	1.99	0.45
2:H:408:LYS:HG2	2:L:406:TRP:CH2	2.51	0.45
1:G:160:THR:HG22	1:G:162:ARG:HD2	1.99	0.44
1:A:63:THR:HG22	1:A:64:PRO:HD2	1.99	0.44
2:J:382:THR:OG1	2:J:382:THR:O	2.28	0.44
1:I:43:MET:HB3	1:I:43:MET:HE2	1.69	0.44
1:A:1:ASP:OD2	2:B:351:ASN:HA	2.17	0.44
1:G:209:VAL:HG11	1:I:205:ASN:HB2	1.99	0.44
1:C:98:LEU:HB2	1:C:227:TRP:CE2	2.52	0.44
1:G:244:LEU:HD13	1:G:246:ALA:HB2	1.98	0.44
2:B:387:GLU:HB2	4:B:714:HOH:O	2.16	0.44
2:H:448:GLN:HE22	2:H:478:ASN:HA	1.82	0.44
1:C:168:GLU:OE2	1:C:231:GLN:NE2	2.44	0.44
2:J:454:GLU:OE2	2:J:493:ARG:NE	2.45	0.44
1:I:59:MET:HE1	1:I:74:TRP:CH2	2.53	0.44
1:K:27:THR:OG1	1:K:312:GLY:HA3	2.17	0.44
2:B:462:GLU:CD	2:D:450:ARG:HH22	2.20	0.44
1:A:246:ALA:HA	1:A:247:PRO:HD3	1.81	0.44
1:K:42:CYS:HB2	1:K:272:SER:HB2	2.00	0.44
2:H:374:LYS:HZ1	2:H:429:HIS:HB3	1.82	0.44
2:D:462:GLU:OE1	2:F:450:ARG:NH2	2.38	0.43
1:G:55:HIS:CE1	1:G:57:ILE:HD13	2.49	0.43
1:A:284:ARG:HH21	2:B:379:VAL:HG11	1.83	0.43
1:I:47:LYS:HE2	1:I:47:LYS:HB3	1.68	0.43
1:I:5:LEU:HA	1:I:5:LEU:HD13	1.82	0.43
1:G:162:ARG:NE	4:G:729:HOH:O	2.29	0.43
2:L:361:TYR:CE2	2:L:365:GLN:HG3	2.53	0.43
1:I:154:PHE:HB3	1:I:241:ASN:O	2.18	0.43
2:B:361:TYR:CZ	2:B:365:GLN:HG3	2.53	0.43
1:A:55:HIS:HB3	1:A:85:ALA:HB2	2.01	0.43
1:G:196:SER:HB3	1:G:239:SER:HB3	1.99	0.43
1:E:155:PRO:O	1:E:157:THR:HG22	2.19	0.43
2:B:414:ILE:HD13	2:D:414:ILE:HG21	1.99	0.43
1:A:87:CYS:HB2	1:A:129:ALA:O	2.18	0.43
1:G:49:LYS:HD2	1:G:69:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.19	0.43
1:A:172:MET:HG2	1:A:227:TRP:HB3	2.00	0.43
2:J:342:ASP:HB3	2:J:359:ALA:HB2	1.99	0.43
1:K:303:ASN:H	2:L:416:THR:HG21	1.84	0.43
1:I:133:ASN:C	1:I:135:GLY:H	2.22	0.43
2:H:446:ARG:NH2	2:L:455:GLU:OE1	2.52	0.43
2:L:361:TYR:CZ	2:L:365:GLN:HG3	2.54	0.43
1:G:61:ILE:O	1:G:139:TYR:HB3	2.19	0.43
1:A:302:VAL:HA	2:B:416:THR:HG22	2.00	0.43
1:E:157:THR:HG23	1:E:240:HIS:CE1	2.54	0.43
1:E:220:SER:HA	1:E:222:ARG:HH12	1.84	0.43
1:K:193:ILE:HG22	1:K:208:PRO:HD2	2.00	0.43
2:B:448:GLN:NE2	2:B:478:ASN:HA	2.34	0.42
1:I:276:TRP:HB2	1:I:293:ARG:O	2.20	0.42
2:L:327:GLY:O	2:L:331:GLY:HA3	2.19	0.42
2:J:383:ASN:HA	2:J:384:THR:HB	2.01	0.42
2:L:477:ASN:ND2	4:L:710:HOH:O	2.52	0.42
1:G:33:VAL:HG22	1:G:287:PHE:HB2	2.01	0.42
1:E:41:LEU:HD13	1:E:264:ALA:HB3	2.01	0.42
1:C:193:ILE:HG21	1:C:208:PRO:HG2	2.00	0.42
1:C:40:ARG:NE	1:C:267:ASP:OD2	2.53	0.42
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.53	0.42
1:K:89:PRO:HB3	1:K:216:VAL:HB	2.01	0.42
1:I:63:THR:HG22	1:I:64:PRO:HD2	2.01	0.42
1:K:98:LEU:HD13	1:K:227:TRP:CD2	2.55	0.42
1:I:126:THR:HG23	1:I:136:ASN:HB3	2.02	0.42
1:C:20:THR:O	2:F:373:GLY:HA3	2.20	0.42
1:C:41:LEU:HD13	1:C:264:ALA:HB3	2.02	0.42
1:K:7:HIS:CD2	2:L:329:ILE:HG12	2.55	0.42
1:K:41:LEU:HD12	1:K:41:LEU:HA	1.90	0.42
1:K:178:PRO:HB2	1:K:210:VAL:HG22	2.02	0.42
2:F:347:PHE:HE1	2:F:360:ASP:HB2	1.85	0.42
2:L:473:GLU:O	2:L:477:ASN:HB2	2.20	0.42
1:E:132:ARG:NH1	1:E:137:SER:OG	2.53	0.42
1:E:80:ARG:HH11	1:E:263:ASP:HA	1.85	0.41
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.19	0.41
1:I:304:ARG:NH1	2:J:420:GLU:OE1	2.53	0.41
2:H:342:ASP:HB3	2:H:359:ALA:CB	2.51	0.41
2:H:377:ARG:O	2:H:380:GLU:HG2	2.20	0.41
2:J:375:LEU:HD23	2:J:375:LEU:HA	1.91	0.41
2:B:418:GLN:HG2	2:F:417:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:GLU:HB2	1:G:283:THR:HG21	2.03	0.41
2:D:442:TYR:CE1	2:D:459:GLY:HA2	2.56	0.41
1:G:157:THR:OG1	1:G:158:THR:N	2.53	0.41
2:L:464:TYR:O	2:L:489:ALA:HA	2.20	0.41
1:C:162:ARG:NH2	3:C:601:NAG:O6	2.53	0.41
1:C:51:LEU:O	1:C:54:CYS:HB3	2.20	0.41
2:D:374:LYS:HE3	2:D:430:THR:OG1	2.21	0.41
1:K:31:GLU:HG3	1:K:33:VAL:H	1.85	0.41
1:C:312:GLY:CA	4:C:701:HOH:O	2.68	0.41
2:J:325:LEU:HD13	2:L:326:PHE:HZ	1.85	0.41
2:D:468:ASP:O	2:D:471:CYS:N	2.48	0.41
2:J:412:THR:O	2:J:416:THR:HG23	2.20	0.41
2:H:494:LEU:HD22	2:J:494:LEU:HD11	2.01	0.41
4:A:705:HOH:O	1:E:214:PRO:HB3	2.20	0.41
1:C:61:ILE:O	1:C:139:TYR:HB3	2.20	0.41
2:H:374:LYS:NZ	2:H:426:GLU:O	2.54	0.41
2:H:342:ASP:HB3	2:H:359:ALA:HB2	2.02	0.41
1:I:42:CYS:HB3	1:I:270:CYS:O	2.21	0.41
1:K:293:ARG:HD3	2:L:392:GLU:OE1	2.21	0.41
4:E:721:HOH:O	2:F:460:CYS:SG	2.63	0.40
1:K:44:LYS:HD3	1:K:269:ASN:O	2.20	0.40
1:C:41:LEU:HA	1:C:41:LEU:HD12	1.91	0.40
2:F:444:ARG:O	2:F:448:GLN:HG3	2.21	0.40
1:K:303:ASN:H	2:L:416:THR:CG2	2.34	0.40
1:G:150:LYS:HE3	1:G:186:ASP:CG	2.41	0.40
2:J:367:ALA:O	2:J:371:ILE:HG12	2.22	0.40
1:K:41:LEU:O	1:K:43:MET:HG2	2.22	0.40
1:K:43:MET:HB3	1:K:43:MET:HE3	1.95	0.40
1:A:284:ARG:NH2	2:B:379:VAL:HG11	2.37	0.40
1:K:103:MET:O	1:K:259:GLY:HA3	2.21	0.40
1:I:197:VAL:O	1:I:203:ARG:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
1	C	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	E	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
1	G	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	I	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
1	K	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
2	B	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	30	48
2	D	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	30	48
2	F	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	30	48
2	H	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	30	48
2	J	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	30	48
2	L	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	30	48
All	All	2928/2952 (99%)	2822 (96%)	100 (3%)	6 (0%)	52	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	450	ARG
2	D	450	ARG
2	F	450	ARG
2	H	450	ARG
2	J	450	ARG
2	L	450	ARG

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	269/269 (100%)	244 (91%)	25 (9%)	11	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	269/269 (100%)	250 (93%)	19 (7%)	18 32
1	E	269/269 (100%)	244 (91%)	25 (9%)	11 19
1	G	269/269 (100%)	250 (93%)	19 (7%)	18 32
1	I	269/269 (100%)	246 (91%)	23 (9%)	13 23
1	K	269/269 (100%)	244 (91%)	25 (9%)	11 19
2	B	148/148 (100%)	139 (94%)	9 (6%)	23 40
2	D	148/148 (100%)	138 (93%)	10 (7%)	20 34
2	F	148/148 (100%)	140 (95%)	8 (5%)	27 47
2	H	148/148 (100%)	137 (93%)	11 (7%)	17 30
2	J	148/148 (100%)	139 (94%)	9 (6%)	23 40
2	L	148/148 (100%)	142 (96%)	6 (4%)	37 62
All	All	2502/2502 (100%)	2313 (92%)	189 (8%)	16 29

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	14	THR
1	A	35	SER
1	A	41	LEU
1	A	63	THR
1	A	76	THR
1	A	77	LEU
1	A	111	ILE
1	A	119	SER
1	A	120	SER
1	A	126	THR
1	A	149	SER
1	A	157	THR
1	A	162	ARG
1	A	170	LEU
1	A	179	SER
1	A	203	ARG
1	A	213	ARG
1	A	228	THR
1	A	244	LEU
1	A	248	SER
1	A	258	LEU

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Mol	Chain	Res	Type
1	A	263	ASP
1	A	276	TRP
1	A	283	THR
2	B	353	GLN
2	B	371	ILE
2	B	385	GLU
2	B	395	GLU
2	B	418	GLN
2	B	433	MET
2	B	436	SER
2	B	450	ARG
2	B	470	SER
1	C	1	ASP
1	C	8	HIS
1	C	41	LEU
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	126	THR
1	C	127	THR
1	C	157	THR
1	C	170	LEU
1	C	192	SER
1	C	203	ARG
1	C	228	THR
1	C	244	LEU
1	C	250	VAL
1	C	258	LEU
1	C	276	TRP
1	C	283	THR
1	C	318	GLU
2	D	341	VAL
2	D	379	VAL
2	D	382	THR
2	D	383	ASN
2	D	384	THR
2	D	423	VAL
2	D	433	MET
2	D	436	SER
2	D	448	GLN
2	D	496	ILE
1	E	8	HIS

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Mol	Chain	Res	Type
1	E	30	THR
1	E	35	SER
1	E	76	THR
1	E	77	LEU
1	E	101	LYS
1	E	111	ILE
1	E	112	SER
1	E	126	THR
1	E	157	THR
1	E	162	ARG
1	E	170	LEU
1	E	192	SER
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	249	ARG
1	E	250	VAL
1	E	258	LEU
1	E	269	ASN
1	E	276	TRP
1	E	277	ARG
1	E	283	THR
1	E	314	ARG
2	F	353	GLN
2	F	362	LYS
2	F	379	VAL
2	F	416	THR
2	F	418	GLN
2	F	425	MET
2	F	433	MET
2	F	450	ARG
1	G	8	HIS
1	G	35	SER
1	G	41	LEU
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	112	SER
1	G	120	SER
1	G	146	VAL
1	G	157	THR

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Mol	Chain	Res	Type
1	G	162	ARG
1	G	203	ARG
1	G	213	ARG
1	G	228	THR
1	G	244	LEU
1	G	258	LEU
1	G	276	TRP
1	G	277	ARG
1	G	283	THR
2	H	325	LEU
2	H	342	ASP
2	H	379	VAL
2	H	416	THR
2	H	418	GLN
2	H	423	VAL
2	H	433	MET
2	H	436	SER
2	H	450	ARG
2	H	452	ASN
2	H	471	CYS
1	I	1	ASP
1	I	8	HIS
1	I	12	ASN
1	I	41	LEU
1	I	49	LYS
1	I	63	THR
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	116	THR
1	I	119	SER
1	I	126	THR
1	I	146	VAL
1	I	170	LEU
1	I	203	ARG
1	I	220	SER
1	I	228	THR
1	I	244	LEU
1	I	258	LEU
1	I	262	SER
1	I	276	TRP
1	I	277	ARG

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Mol	Chain	Res	Type
1	I	283	THR
2	J	325	LEU
2	J	335	ASN
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	395	GLU
2	J	418	GLN
2	J	433	MET
2	J	438	MET
1	K	8	HIS
1	K	39	ASN
1	K	41	LEU
1	K	67	ASP
1	K	76	THR
1	K	77	LEU
1	K	111	ILE
1	K	112	SER
1	K	150	LYS
1	K	157	THR
1	K	162	ARG
1	K	170	LEU
1	K	192	SER
1	K	196	SER
1	K	203	ARG
1	K	213	ARG
1	K	228	THR
1	K	239	SER
1	K	244	LEU
1	K	249	ARG
1	K	250	VAL
1	K	256	ARG
1	K	258	LEU
1	K	276	TRP
1	K	283	THR
2	L	382	THR
2	L	384	THR
2	L	411	ILE
2	L	418	GLN
2	L	433	MET
2	L	467	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
2	D	484	GLN
2	H	353	GLN
2	H	418	GLN
1	I	268	ASN
2	J	418	GLN
2	L	370	GLN
2	L	418	GLN
2	L	448	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

12 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	A	601	1	14,14,15	0.42	0	15,19,21	0.49	0
3	NAG	B	601	2	14,14,15	0.46	0	15,19,21	0.27	0
3	NAG	C	601	1	14,14,15	0.38	0	15,19,21	0.51	0
3	NAG	D	601	2	14,14,15	0.32	0	15,19,21	0.44	0
3	NAG	E	601	1	14,14,15	0.26	0	15,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	601	2	14,14,15	0.53	0	15,19,21	0.52	0
3	NAG	G	601	1	14,14,15	0.27	0	15,19,21	0.61	0
3	NAG	H	601	2	14,14,15	0.47	0	15,19,21	0.44	0
3	NAG	I	601	1	14,14,15	0.45	0	15,19,21	0.63	0
3	NAG	J	601	2	14,14,15	0.35	0	15,19,21	0.42	0
3	NAG	K	601	1	14,14,15	0.27	0	15,19,21	0.40	0
3	NAG	L	601	2	14,14,15	0.20	0	15,19,21	0.36	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
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1
3	NAG	F	601	2	-	0/6/23/26	0/1/1/1
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1
3	NAG	H	601	2	-	0/6/23/26	0/1/1/1
3	NAG	I	601	1	-	0/6/23/26	0/1/1/1
3	NAG	J	601	2	-	0/6/23/26	0/1/1/1
3	NAG	K	601	1	-	0/6/23/26	0/1/1/1
3	NAG	L	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
3	C	601	NAG	1	0
3	D	601	NAG	1	0
3	F	601	NAG	1	0
3	H	601	NAG	1	0

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	318/318 (100%)	-0.01	3 (0%)	85	88	20, 41, 65, 106	0
1	C	318/318 (100%)	0.06	7 (2%)	65	69	21, 44, 65, 92	0
1	E	318/318 (100%)	-0.01	5 (1%)	74	77	23, 37, 61, 91	0
1	G	318/318 (100%)	0.01	3 (0%)	85	88	28, 45, 68, 104	0
1	I	318/318 (100%)	0.11	6 (1%)	70	73	22, 40, 67, 106	0
1	K	318/318 (100%)	0.10	8 (2%)	61	64	32, 49, 77, 105	0
2	B	174/174 (100%)	0.34	3 (1%)	73	76	23, 43, 68, 118	0
2	D	174/174 (100%)	0.41	3 (1%)	73	76	24, 46, 80, 136	0
2	F	174/174 (100%)	0.24	2 (1%)	82	84	22, 43, 66, 95	0
2	H	174/174 (100%)	0.61	11 (6%)	23	26	27, 62, 103, 147	0
2	J	174/174 (100%)	0.82	17 (9%)	10	10	29, 61, 98, 174	0
2	L	174/174 (100%)	0.58	10 (5%)	27	31	26, 59, 98, 129	0
All	All	2952/2952 (100%)	0.21	78 (2%)	59	63	20, 45, 80, 174	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	497	ASN	14.2
2	J	497	ASN	14.0
2	J	496	ILE	12.1
2	H	496	ILE	10.5
2	D	497	ASN	8.4
2	B	497	ASN	6.4
1	I	134	GLY	5.8
2	L	497	ASN	5.5
2	D	382	THR	3.8
2	J	341	VAL	3.7
2	H	352	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	350	GLN	3.6
2	J	354	GLY	3.6
2	J	359	ALA	3.5
2	L	383	ASN	3.4
1	K	11	ALA	3.3
2	F	350	GLN	3.3
1	K	133	ASN	3.2
2	L	496	ILE	3.2
2	H	491	LEU	3.1
2	J	460	CYS	3.0
2	H	468	ASP	3.0
1	G	284	ARG	3.0
1	E	269	ASN	2.9
2	J	491	LEU	2.9
1	A	12	ASN	2.9
2	J	355	THR	2.9
1	I	133	ASN	2.8
1	E	11	ALA	2.8
1	C	12	ASN	2.7
2	D	324	GLY	2.7
1	G	2	LYS	2.7
2	B	325	LEU	2.6
1	C	149	SER	2.6
1	K	152	GLN	2.6
2	J	358	ALA	2.6
2	F	383	ASN	2.6
1	I	2	LYS	2.6
2	H	350	GLN	2.6
1	E	270	CYS	2.6
2	L	481	ASP	2.5
2	J	494	LEU	2.5
2	J	469	ASP	2.5
1	C	284	ARG	2.5
1	K	205	ASN	2.5
2	H	327	GLY	2.4
1	E	305	ARG	2.4
2	L	476	ARG	2.4
2	J	466	ALA	2.4
1	I	12	ASN	2.3
1	C	114	GLY	2.3
2	H	353	GLN	2.3
1	I	128	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	2.3
1	G	318	GLU	2.3
2	J	340	MET	2.2
2	L	425	MET	2.2
2	L	494	LEU	2.2
2	H	355	THR	2.2
1	I	8	HIS	2.2
2	J	348	ARG	2.2
2	J	342	ASP	2.2
2	J	467	CYS	2.2
1	K	118	GLY	2.2
2	L	361	TYR	2.2
1	C	167	ALA	2.1
1	K	269	ASN	2.1
2	L	470	SER	2.1
1	E	256	ARG	2.1
1	K	305	ARG	2.1
1	A	318	GLU	2.1
2	L	491	LEU	2.1
1	K	36	THR	2.1
2	H	354	GLY	2.1
1	C	190	THR	2.1
2	B	444	ARG	2.0
2	H	356	GLY	2.0
1	C	256	ARG	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 carbohydrates 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. 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, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	F	601	14/15	0.88	0.19	2.39	41,53,63,66	0
3	NAG	I	601	14/15	0.84	0.20	1.31	56,68,76,84	0
3	NAG	C	601	14/15	0.80	0.17	0.82	56,69,73,81	0
3	NAG	G	601	14/15	0.81	0.20	0.73	74,92,96,97	0
3	NAG	H	601	14/15	0.85	0.17	0.35	41,56,60,62	0
3	NAG	E	601	14/15	0.89	0.14	-0.20	56,63,74,74	0
3	NAG	K	601	14/15	0.88	0.14	-0.27	56,63,70,79	0
3	NAG	A	601	14/15	0.91	0.15	-0.29	51,62,71,77	0
3	NAG	B	601	14/15	0.89	0.14	-0.33	52,58,66,68	0
3	NAG	J	601	14/15	0.95	0.13	-0.79	46,48,53,55	0
3	NAG	L	601	14/15	0.90	0.12	-0.93	49,63,67,72	0
3	NAG	D	601	14/15	0.91	0.12	-0.97	37,49,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.