



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:50 PM UTC

PDB ID : 4QY0 / pdb_00004qy0
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

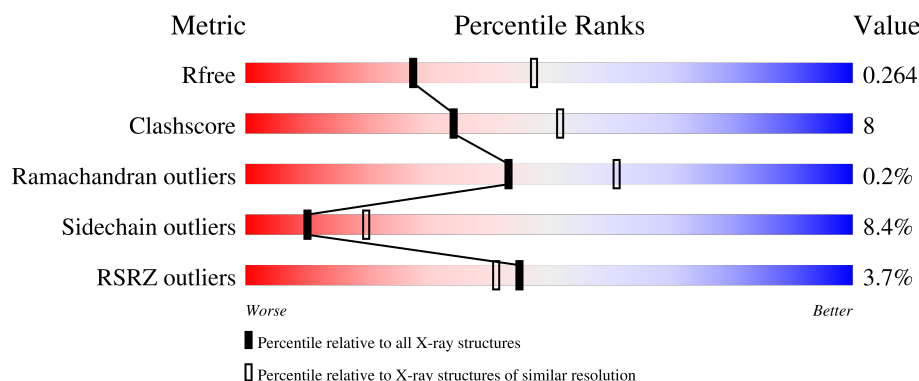
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	0% 76% 22% .
1	C	318	3% 80% 19% .
1	E	318	2% 80% 18% .
1	G	318	2% 79% 19% .
1	I	318	3% 75% 22% .

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Mol	Chain	Length	Quality of chain
1	K	318	3% 77% 22%
2	B	174	% 74% 23%
2	D	174	6% 79% 18%
2	F	174	2% 82% 17%
2	H	174	7% 78% 18%
2	J	174	11% 72% 22% 6%
2	L	174	10% 75% 21%

2 Entry composition [i](#)

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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

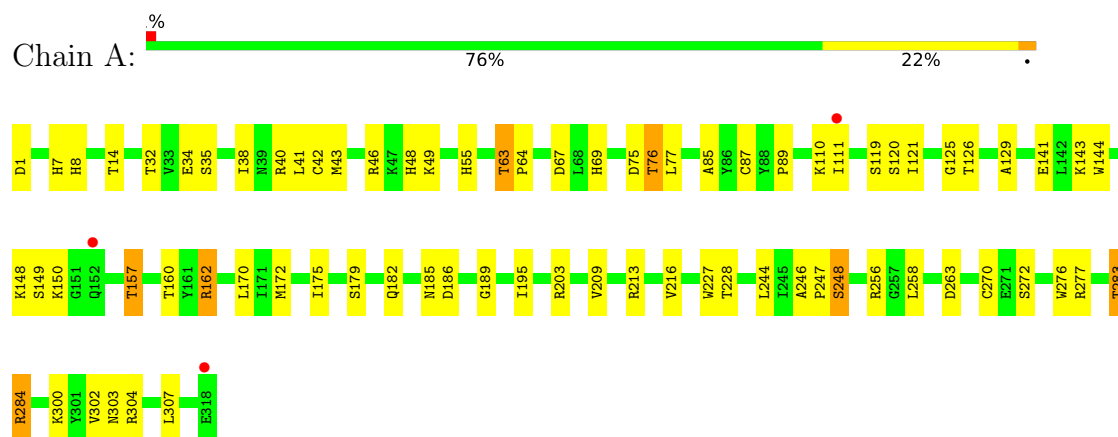
- Molecule 4 is water.

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

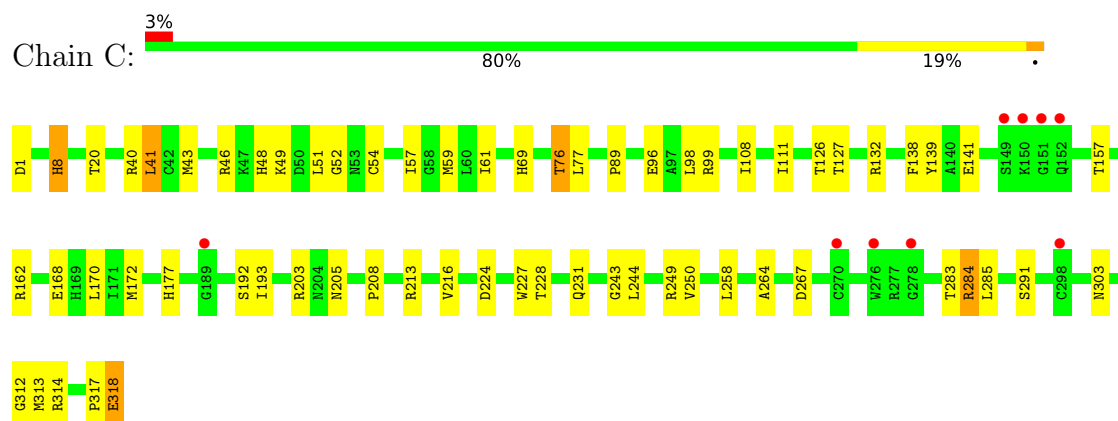
3 Residue-property plots [i](#)

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.

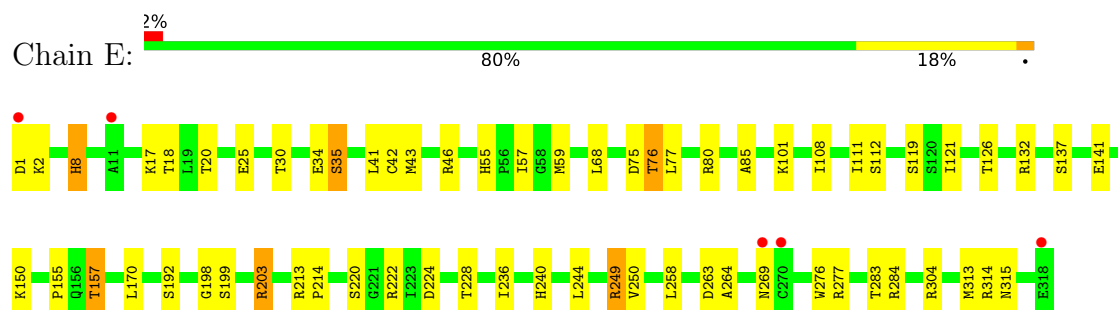
- Molecule 1: hemagglutinin



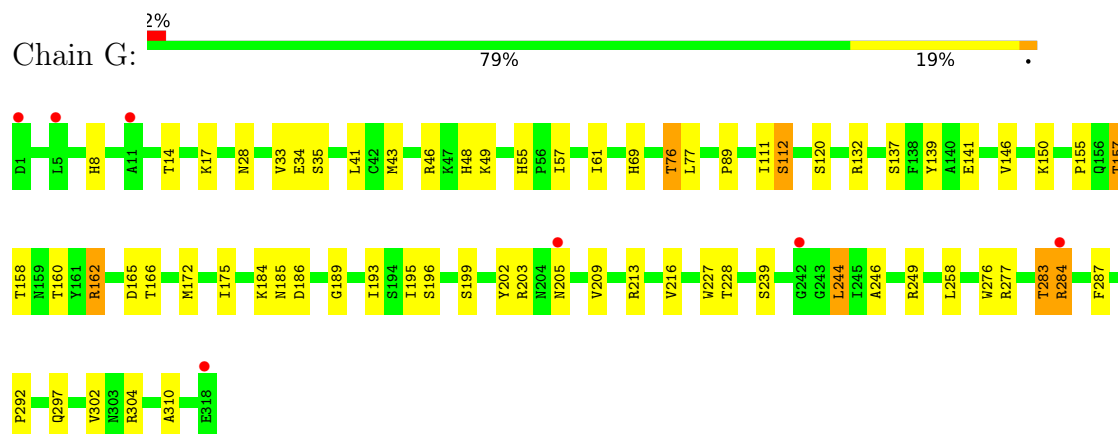
- Molecule 1: hemagglutinin



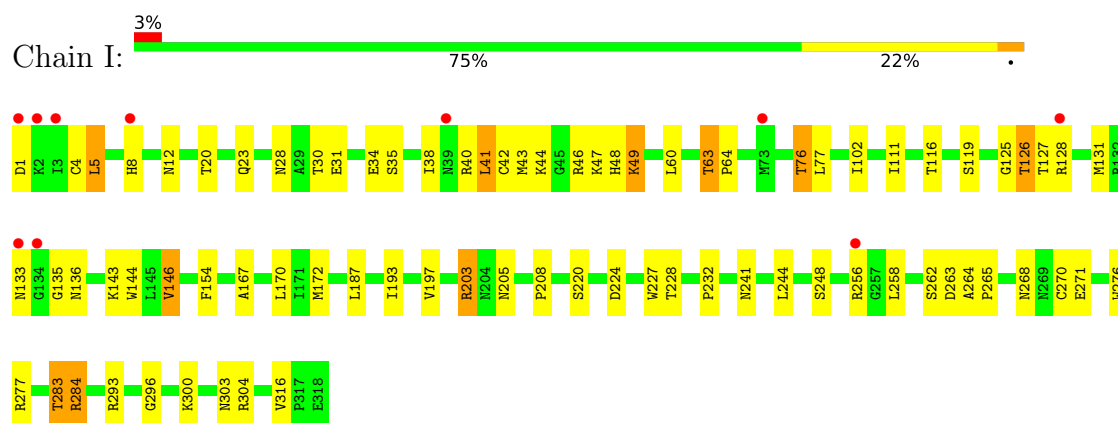
- Molecule 1: hemagglutinin



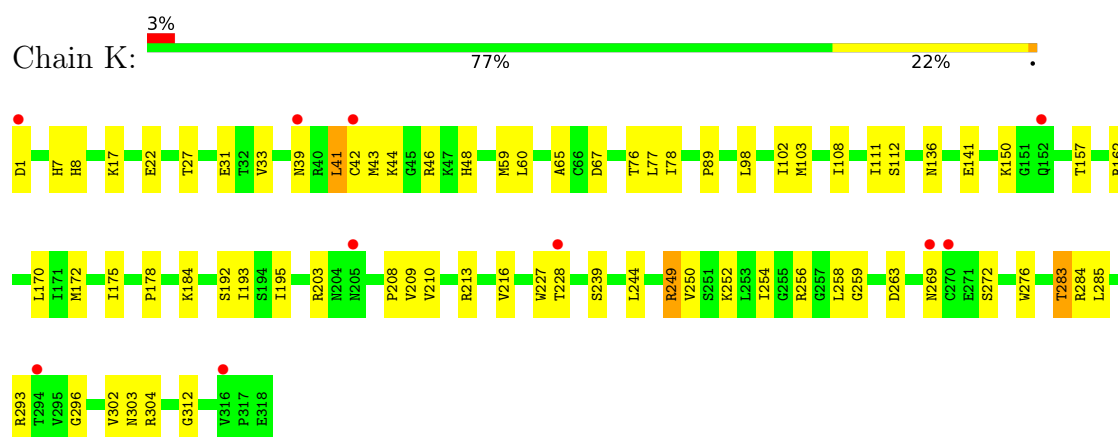
- Molecule 1: hemagglutinin



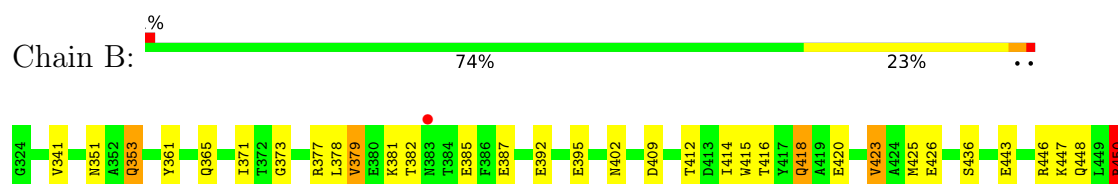
- Molecule 1: hemagglutinin

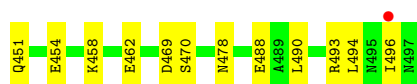


- Molecule 1: hemagglutinin

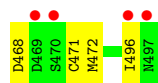
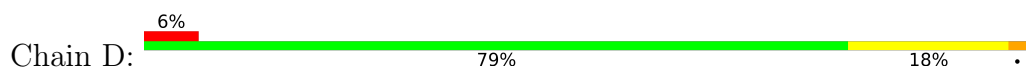


- Molecule 2: hemagglutinin

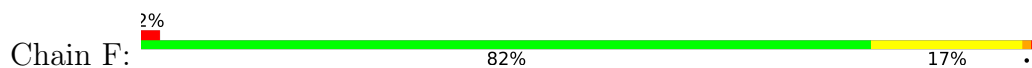




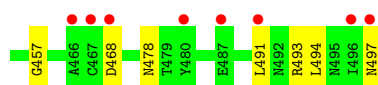
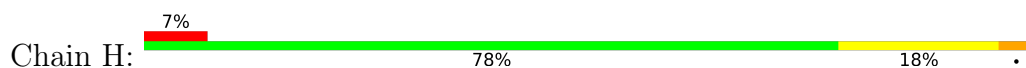
• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin



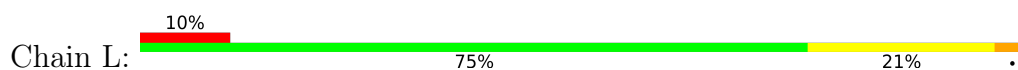
• Molecule 2: hemagglutinin

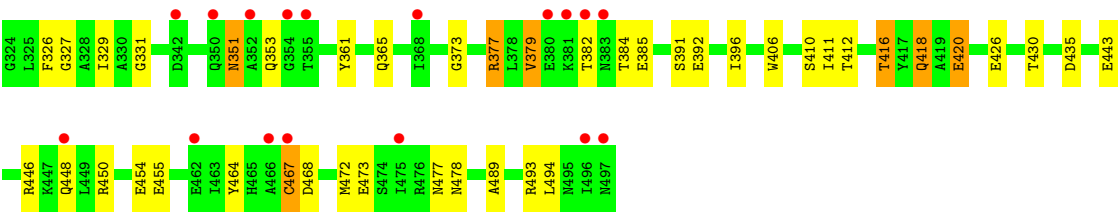


• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 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) 83.1 (39.47-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.215 , 0.264 0.216 , 0.264	Depositor DCC
R_{free} test set	6866 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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 11.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.37	0/2486	0.77	1/3368 (0.0%)
1	C	0.36	0/2486	0.78	5/3368 (0.1%)
1	E	0.38	0/2486	0.79	0/3368
1	G	0.36	0/2486	0.75	1/3368 (0.0%)
1	I	0.37	0/2486	0.77	2/3368 (0.1%)
1	K	0.34	0/2486	0.76	0/3368
2	B	0.36	0/1427	0.74	0/1926
2	D	0.37	0/1427	0.75	0/1926
2	F	0.36	0/1427	0.76	0/1926
2	H	0.35	0/1427	0.79	1/1926 (0.1%)
2	J	0.35	0/1427	0.76	0/1926
2	L	0.35	0/1427	0.75	1/1926 (0.1%)
All	All	0.36	0/23478	0.77	11/31764 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	351	ASN	N-CA-C	6.59	117.17	108.07
1	I	284	ARG	N-CA-C	-6.45	105.45	113.38
1	G	284	ARG	N-CA-C	-6.29	105.64	113.38
1	C	284	ARG	N-CA-C	-5.59	106.51	113.38
1	A	284	ARG	N-CA-C	-5.38	106.76	113.38
1	C	177	HIS	CA-C-N	5.33	125.31	120.03
1	C	177	HIS	C-N-CA	5.33	125.31	120.03
2	H	457	GLY	N-CA-C	-5.25	107.29	114.64
1	I	127	THR	N-CA-C	5.16	117.09	108.99
1	C	291	SER	CA-C-N	5.14	124.75	119.56
1	C	291	SER	C-N-CA	5.14	124.75	119.56

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	42	0
1	C	2437	0	2389	35	0
1	E	2437	0	2389	33	0
1	G	2437	0	2389	36	0
1	I	2437	0	2389	47	0
1	K	2437	0	2389	39	0
2	B	1402	0	1298	36	0
2	D	1402	0	1298	21	0
2	F	1402	0	1298	24	0
2	H	1402	0	1298	27	0
2	J	1402	0	1298	36	0
2	L	1402	0	1298	34	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	6	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	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	347	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 8.

All (347) 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
3:H:601:NAG:O4	4:H:712:HOH:O	1.84	0.94
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
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:A:7:HIS:NE2	4:A:717:HOH:O	2.20	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:I:43:MET:HE2	1:I:48:HIS:HB3	1.75	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:C:43:MET:HE3	1:C:46:ARG:HG3	1.74	0.68
3:D:601:NAG:O4	4:D:712:HOH:O	2.09	0.68
1:E:2:LYS:NZ	4:E:721:HOH:O	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:MET:HE3	1:G:46:ARG:HG3	1.77	0.66
2:D:349:HIS:HB2	2:D:472:MET:HE3	1.77	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
2:B:409:ASP:OD2	4:B:724:HOH:O	2.15	0.64
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.79	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:C:213:ARG:HG2	1:E:198:GLY:HA3	1.79	0.63
1:K:43:MET:HE3	1:K:46:ARG:HG3	1.80	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
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
2:H:491:LEU:HB3	2:H:497:ASN:HA	1.82	0.61
1:K:284:ARG:HB3	2:L:379:VAL:HG13	1.83	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:A:1:ASP:N	4:A:719:HOH:O	2.34	0.60
1:K:283:THR:HG22	1:K:285:LEU:H	1.65	0.60
1:A:43:MET:HE2	1:A:48:HIS:HB3	1.83	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:A:160:THR:HG22	1:A:162:ARG:HD2	1.84	0.59
2:J:383:ASN:OD1	2:J:383:ASN:N	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
1:C:59:MET:HE2	1:C:108:ILE:HD12	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:O	2:D:381:LYS:NZ	2.36	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:G:304:ARG:NH1	2:H:420:GLU:OE1	2.36	0.58
2:B:381:LYS:NZ	2:B:382:THR:O	2.36	0.58
1:C:49:LYS:NZ	4:C:711:HOH:O	2.30	0.57
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
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
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
1:K:141:GLU:OE2	1:K:249:ARG:NH1	2.40	0.55
2:L:353:GLN:HE22	2:L:468:ASP:HB2	1.72	0.55
2:B:425:MET:HE1	2:F:421:LEU:HD11	1.88	0.55
2:F:493:ARG:O	4:F:708:HOH:O	2.18	0.55
2:L:448:GLN:NE2	2:L:478:ASN:HA	2.21	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
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
1:C:43:MET:HE2	1:C:48:HIS:HB3	1.90	0.54
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.90	0.54
4:E:737:HOH:O	1:I:40:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:LYS:HD2	1:I:248:SER:HB3	1.91	0.53
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.41	0.53
2:B:412:THR:O	2:B:416:THR:HG23	2.07	0.53
1:C:303:ASN:H	2:D:416:THR:CG2	2.22	0.53
1:A:43:MET:HE3	1:A:46:ARG:HG3	1.91	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
1:I:44:LYS:NZ	4:I:736:HOH:O	2.30	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:H:421:LEU:HD11	2:J:425:MET:HE1	1.92	0.52
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.34	0.51
2:D:465:HIS:ND1	2:D:466:ALA:O	2.39	0.51
1:G:17:LYS:NZ	2:H:420:GLU:OE2	2.35	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:N	2:H:452:ASN:OD1	2.44	0.51
1:K:43:MET:HE2	1:K:48:HIS:HB3	1.93	0.51
2:H:392:GLU:OE1	4:H:702:HOH:O	2.20	0.51
1:I:263:ASP:HB2	4:I:712:HOH:O	2.10	0.51
1:A:125:GLY:HA3	1:A:144:TRP:HB3	1.93	0.50
1:E:25:GLU:HG2	1:E:315:ASN:HB3	1.92	0.50
2:H:365:GLN:NE2	4:H:714:HOH:O	2.33	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
2:B:488:GLU:OE1	4:B:726:HOH:O	2.20	0.49
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
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:43:MET:HE3	1:E:46:ARG:HG3	1.95	0.49
1:A:143:LYS:HE3	1:A:248:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:SER:HB3	1:E:236:ILE:HD12	1.94	0.49
1:A:209:VAL:HG11	1:C:205:ASN:HB2	1.94	0.49
1:E:18:THR:O	4:E:740:HOH:O	2.20	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
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.45	0.49
1:K:60:LEU:HD11	1:K:102:ILE:HD11	1.95	0.49
1:A:89:PRO:HB3	1:A:216:VAL:HB	1.95	0.49
2:B:462:GLU:CD	2:D:450:ARG:HH22	2.20	0.48
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
1:A:110:LYS:NZ	1:A:141:GLU:OE2	2.41	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:1:ASP:OD2	2:L:351:ASN:HA	2.14	0.48
1:K:263:ASP:HB2	4:K:731:HOH:O	2.14	0.48
1:A:43:MET:HE2	1:A:48:HIS:CB	2.44	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:43:MET:HE2	1:I:48:HIS:CB	2.43	0.48
1:I:43:MET:HE1	1:I:76:THR:HG21	1.95	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:A:38:ILE:HG22	1:A:40:ARG:H	1.79	0.48
1:A:185:ASN:ND2	1:A:189:GLY:O	2.41	0.48
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.14	0.48
1:K:296:GLY:HA2	2:L:385:GLU:HG3	1.95	0.48
1:C:224:ASP:OD2	1:E:203:ARG:NH2	2.47	0.48
2:D:381:LYS:HG3	2:D:383:ASN:HD21	1.78	0.48
2:B:353:GLN:H	2:B:353:GLN:HE21	1.62	0.47
1:I:133:ASN:C	1:I:135:GLY:H	2.22	0.47
1:G:175:ILE:HD12	1:G:195:ILE:HD13	1.95	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: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
2:B:392:GLU:OE2	4:B:712:HOH:O	2.19	0.47
1:G:185:ASN:HA	1:G:189:GLY:O	2.15	0.47
1:G:292:PRO:O	4:G:727:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:VAL:HA	2:L:416:THR:HG22	1.96	0.47
1:C:89:PRO:HB3	1:C:216:VAL:HB	1.97	0.47
1:C:303:ASN:H	2:D:416:THR:HG22	1.80	0.47
1:I:128:ARG:HD3	1:I:131:MET:HE2	1.97	0.47
2:J:383:ASN:HA	2:J:384:THR:CB	2.45	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:C:8:HIS:CE1	1:C:313:MET:HE3	2.51	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:G:199:SER:HG	1:G:202:TYR:H	1.64	0.46
2:B:454:GLU:OE2	2:B:493:ARG:NE	2.42	0.46
2:H:381:LYS:NZ	2:H:382:THR:O	2.42	0.46
1:I:284:ARG:HH21	2:J:379:VAL:HG11	1.81	0.46
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.17	0.45
1:G:43:MET:HE2	1:G:48:HIS:HB3	1.97	0.45
1:G:165:ASP:OD1	1:G:166:THR:N	2.45	0.45
1:I:28:ASN:ND2	4:I:753:HOH:O	2.48	0.45
1:E:8:HIS:CE1	1:E:313:MET:HE3	2.52	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:E:59:MET:HE2	1:E:108:ILE:HD12	1.98	0.45
1:I:193:ILE:HG22	1:I:208:PRO:HD2	1.99	0.45
1:G:132:ARG:NH1	1:G:137:SER:OG	2.50	0.45
2:J:402:ASN:O	4:J:707:HOH:O	2.21	0.45
2:J:451:GLN:HB3	2:J:490:LEU:HD21	1.99	0.45
1:A:49:LYS:HD2	1:A:69:HIS:ND1	2.31	0.45
2:L:454:GLU:OE2	2:L:493:ARG:NE	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:LYS:HE3	1:G:186:ASP:CG	2.41	0.45
1:K:59:MET:HE2	1:K:108:ILE:HD12	1.99	0.45
1:A:185:ASN:HA	1:A:189:GLY:O	2.17	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
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
2:J:382:THR:O	2:J:382:THR:OG1	2.28	0.44
1:A:63:THR:HG22	1:A:64:PRO:HD2	1.99	0.44
1:A:1:ASP:OD2	2:B:351:ASN:HA	2.17	0.44
1:G:205:ASN:CG	1:K:209:VAL:HG11	2.43	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
1:C:168:GLU:OE2	1:C:231:GLN:NE2	2.44	0.44
2:H:448:GLN:HE22	2:H:478:ASN:HA	1.82	0.44
2:J:454:GLU:OE2	2:J:493:ARG:NE	2.45	0.44
2:J:349:HIS:HB2	2:J:472:MET:HE3	1.98	0.44
1:K:27:THR:OG1	1:K:312:GLY:HA3	2.17	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:D:462:GLU:OE1	2:F:450:ARG:NH2	2.38	0.43
1:A:284:ARG:HH21	2:B:379:VAL:HG11	1.83	0.43
1:G:55:HIS:CE1	1:G:57:ILE:HD13	2.49	0.43
1:I:5:LEU:HD13	1:I:5:LEU:HA	1.82	0.43
1:I:47:LYS:HB3	1:I:47:LYS:HE2	1.68	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:A:55:HIS:HB3	1:A:85:ALA:HB2	2.01	0.43
2:B:361:TYR:CZ	2:B:365:GLN:HG3	2.53	0.43
1:G:196:SER:HB3	1:G:239:SER:HB3	1.99	0.43
1:I:154:PHE:HB3	1:I:241:ASN:O	2.18	0.43
1:A:87:CYS:HB2	1:A:129:ALA:O	2.18	0.43
2:B:414:ILE:HD13	2:D:414:ILE:HG21	1.99	0.43
1:E:155:PRO:O	1:E:157:THR:HG22	2.19	0.43
1:G:49:LYS:HD2	1:G:69:HIS:ND1	2.34	0.43
1:A:172:MET:HG2	1:A:227:TRP:HB3	2.00	0.43
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.19	0.43
2:J:342:ASP:HB3	2:J:359:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:303:ASN:H	2:L:416:THR:HG21	1.84	0.43
1:G:61:ILE:O	1:G:139:TYR:HB3	2.19	0.43
2:H:446:ARG:NH2	2:L:455:GLU:OE1	2.52	0.43
1:K:141:GLU:CD	1:K:249:ARG:HH11	2.27	0.43
2:L:361:TYR:CZ	2:L:365:GLN:HG3	2.54	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
1:A:42:CYS:HB3	1:A:270:CYS:C	2.44	0.42
1:C:193:ILE:HG21	1:C:208:PRO:HG2	2.00	0.42
1:E:41:LEU:HD13	1:E:264:ALA:HB3	2.01	0.42
1:G:33:VAL:HG22	1:G:287:PHE:HB2	2.01	0.42
2:L:477:ASN:ND2	4:L:710:HOH:O	2.52	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:I:63:THR:HG22	1:I:64:PRO:HD2	2.01	0.42
1:K:89:PRO:HB3	1:K:216:VAL:HB	2.01	0.42
1:K:98:LEU:HD13	1:K:227:TRP:CD2	2.55	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:I:126:THR:HG23	1:I:136:ASN:HB3	2.02	0.42
1:K:7:HIS:CD2	2:L:329:ILE:HG12	2.55	0.42
2:L:467:CYS:HB3	2:L:472:MET:HE2	2.02	0.42
1:E:132:ARG:NH1	1:E:137:SER:OG	2.53	0.42
2:F:347:PHE:HE1	2:F:360:ASP:HB2	1.85	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:L:473:GLU:O	2:L:477:ASN:HB2	2.20	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
2:D:442:TYR:CE1	2:D:459:GLY:HA2	2.56	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
1:C:51:LEU:O	1:C:54:CYS:HB3	2.20	0.41
1:C:162:ARG:NH2	3:C:601:NAG:O6	2.53	0.41
2:D:374:LYS:HE3	2:D:430:THR:OG1	2.21	0.41
1:G:157:THR:OG1	1:G:158:THR:N	2.53	0.41
1:I:167:ALA:C	1:I:232:PRO:HG3	2.46	0.41
1:K:31:GLU:HG3	1:K:33:VAL:H	1.85	0.41
2:L:464:TYR:O	2:L:489:ALA:HA	2.20	0.41
1:C:312:GLY:CA	4:C:701:HOH:O	2.68	0.41
2:D:468:ASP:O	2:D:471:CYS:N	2.48	0.41
2:H:374:LYS:HZ2	2:H:430:THR:HG1	1.64	0.41
2:J:325:LEU:HD13	2:L:326:PHE:HZ	1.85	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:494:LEU:HD22	2:J:494:LEU:HD11	2.01	0.41
2:J:412:THR:O	2:J:416:THR:HG23	2.20	0.41
2:H:342:ASP:HB3	2:H:359:ALA:HB2	2.02	0.41
2:H:374:LYS:NZ	2:H:426:GLU:O	2.54	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:HD12	1:C:41:LEU:HA	1.91	0.40
2:F:444:ARG:O	2:F:448:GLN:HG3	2.21	0.40
2:J:367:ALA:O	2:J:371:ILE:HG12	2.22	0.40
1:K:303:ASN:H	2:L:416:THR:CG2	2.34	0.40
1:A:284:ARG:NH2	2:B:379:VAL:HG11	2.37	0.40
1:I:197:VAL:O	1:I:203:ARG:HA	2.22	0.40
1:K:41:LEU:O	1:K:43:MET:HG2	2.22	0.40
1:K:103:MET:O	1:K:259:GLY:HA3	2.21	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%)	21	35
2	D	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	35
2	F	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	21	35
2	H	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	21	35
2	J	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	21	35
2	L	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	21	35
All	All	2928/2952 (99%)	2822 (96%)	100 (3%)	6 (0%)	43	61

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 ⓘ

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%)	241 (90%)	28 (10%)	7	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	269/269 (100%)	250 (93%)	19 (7%)	13	26
1	E	269/269 (100%)	244 (91%)	25 (9%)	8	16
1	G	269/269 (100%)	249 (93%)	20 (7%)	13	24
1	I	269/269 (100%)	245 (91%)	24 (9%)	9	18
1	K	269/269 (100%)	245 (91%)	24 (9%)	9	18
2	B	148/148 (100%)	136 (92%)	12 (8%)	11	21
2	D	148/148 (100%)	135 (91%)	13 (9%)	9	18
2	F	148/148 (100%)	138 (93%)	10 (7%)	14	28
2	H	148/148 (100%)	136 (92%)	12 (8%)	11	21
2	J	148/148 (100%)	134 (90%)	14 (10%)	8	15
2	L	148/148 (100%)	138 (93%)	10 (7%)	14	28
All	All	2502/2502 (100%)	2291 (92%)	211 (8%)	10	20

All (211) 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	148	LYS
1	A	149	SER
1	A	150	LYS
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

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Mol	Chain	Res	Type
1	A	248	SER
1	A	258	LEU
1	A	263	ASP
1	A	276	TRP
1	A	277	ARG
1	A	283	THR
2	B	341	VAL
2	B	353	GLN
2	B	371	ILE
2	B	379	VAL
2	B	385	GLU
2	B	395	GLU
2	B	418	GLN
2	B	423	VAL
2	B	436	SER
2	B	450	ARG
2	B	470	SER
2	B	496	ILE
1	C	1	ASP
1	C	8	HIS
1	C	41	LEU
1	C	57	ILE
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	283	THR
1	C	318	GLU
2	D	325	LEU
2	D	341	VAL
2	D	364	THR
2	D	377	ARG
2	D	379	VAL

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Mol	Chain	Res	Type
2	D	382	THR
2	D	383	ASN
2	D	384	THR
2	D	423	VAL
2	D	425	MET
2	D	448	GLN
2	D	450	ARG
2	D	496	ILE
1	E	8	HIS
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	150	LYS
1	E	157	THR
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	341	VAL
2	F	353	GLN
2	F	362	LYS
2	F	377	ARG
2	F	379	VAL
2	F	411	ILE
2	F	416	THR
2	F	418	GLN
2	F	425	MET

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Mol	Chain	Res	Type
2	F	450	ARG
1	G	8	HIS
1	G	14	THR
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
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	371	ILE
2	H	379	VAL
2	H	383	ASN
2	H	395	GLU
2	H	416	THR
2	H	418	GLN
2	H	423	VAL
2	H	436	SER
2	H	450	ARG
2	H	452	ASN
1	I	5	LEU
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

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Mol	Chain	Res	Type
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	256	ARG
1	I	258	LEU
1	I	262	SER
1	I	277	ARG
1	I	283	THR
1	I	316	VAL
2	J	325	LEU
2	J	335	ASN
2	J	377	ARG
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	385	GLU
2	J	395	GLU
2	J	418	GLN
2	J	423	VAL
2	J	425	MET
2	J	438	MET
2	J	450	ARG
2	J	496	ILE
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

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Mol	Chain	Res	Type
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	377	ARG
2	L	379	VAL
2	L	382	THR
2	L	384	THR
2	L	411	ILE
2	L	416	THR
2	L	418	GLN
2	L	420	GLU
2	L	430	THR
2	L	467	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	269	ASN
1	C	205	ASN
2	D	398	HIS
2	D	484	GLN
1	E	55	HIS
1	E	231	GLN
2	F	448	GLN
2	F	478	ASN
1	G	205	ASN
2	H	353	GLN
2	H	365	GLN
2	H	418	GLN
1	I	8	HIS
1	I	268	ASN
2	J	418	GLN
1	K	94	ASN

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Mol	Chain	Res	Type
1	K	152	GLN
1	K	205	ASN
1	K	303	ASN
2	L	335	ASN
2	L	370	GLN
2	L	418	GLN
2	L	448	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.44	0	17,19,21	0.61	0
3	NAG	E	601	1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	F	601	2	14,14,15	0.54	0	17,19,21	0.58	0
3	NAG	G	601	1	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	H	601	2	14,14,15	0.49	0	17,19,21	0.52	0
3	NAG	J	601	2	14,14,15	0.37	0	17,19,21	0.53	0
3	NAG	K	601	1	14,14,15	0.28	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	601	1	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	I	601	1	14,14,15	0.47	0	17,19,21	0.68	0
3	NAG	L	601	2	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	B	601	2	14,14,15	0.49	0	17,19,21	0.39	0
3	NAG	D	601	2	14,14,15	0.34	0	17,19,21	0.48	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	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	F	601	2	-	2/6/23/26	0/1/1/1
3	NAG	G	601	1	-	2/6/23/26	0/1/1/1
3	NAG	H	601	2	-	1/6/23/26	0/1/1/1
3	NAG	J	601	2	-	0/6/23/26	0/1/1/1
3	NAG	K	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1
3	NAG	I	601	1	-	2/6/23/26	0/1/1/1
3	NAG	L	601	2	-	2/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	0/1/1/1
3	NAG	D	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.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	601	NAG	C4-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	K	601	NAG	O5-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	L	601	NAG	O5-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	G	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	601	NAG	O5-C5-C6-O6
3	I	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	K	601	NAG	C4-C5-C6-O6
3	L	601	NAG	C4-C5-C6-O6
3	C	601	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	NAG	1	0
3	H	601	NAG	1	0
3	C	601	NAG	1	0
3	B	601	NAG	1	0
3	D	601	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	318/318 (100%)	0.26	3 (0%) 81 79	20, 41, 65, 106	0
1	C	318/318 (100%)	0.37	9 (2%) 55 51	21, 44, 65, 92	0
1	E	318/318 (100%)	0.25	5 (1%) 70 68	23, 37, 61, 91	0
1	G	318/318 (100%)	0.40	7 (2%) 62 59	28, 45, 68, 104	0
1	I	318/318 (100%)	0.40	10 (3%) 51 48	22, 40, 67, 106	0
1	K	318/318 (100%)	0.55	10 (3%) 51 48	32, 49, 77, 105	0
2	B	174/174 (100%)	0.38	2 (1%) 78 76	23, 43, 68, 118	0
2	D	174/174 (100%)	0.57	10 (5%) 29 26	24, 46, 80, 136	0
2	F	174/174 (100%)	0.38	4 (2%) 61 58	22, 43, 66, 95	0
2	H	174/174 (100%)	0.91	13 (7%) 20 18	27, 62, 103, 147	0
2	J	174/174 (100%)	0.92	20 (11%) 9 8	29, 61, 98, 174	0
2	L	174/174 (100%)	0.85	17 (9%) 13 11	26, 59, 98, 129	0
All	All	2952/2952 (100%)	0.48	110 (3%) 45 41	20, 45, 80, 174	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	496	ILE	7.1
1	I	134	GLY	6.9
2	D	382	THR	6.1
2	H	497	ASN	5.8
2	J	496	ILE	5.4
1	K	1	ASP	4.6
2	H	358	ALA	4.2
2	B	496	ILE	4.0
2	H	467	CYS	3.9
1	C	149	SER	3.7
2	J	382	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	381	LYS	3.6
2	J	497	ASN	3.6
2	L	466	ALA	3.6
1	G	11	ALA	3.4
2	D	383	ASN	3.4
2	L	355	THR	3.4
1	I	133	ASN	3.3
2	L	352	ALA	3.3
2	D	497	ASN	3.3
2	D	496	ILE	3.3
2	H	382	THR	3.3
2	D	341	VAL	3.2
1	A	318	GLU	3.2
1	G	242	GLY	3.1
2	L	382	THR	3.1
2	D	350	GLN	3.1
2	J	350	GLN	3.0
1	E	318	GLU	3.0
1	C	270	CYS	3.0
1	G	318	GLU	2.9
1	A	152	GLN	2.9
2	L	496	ILE	2.9
2	L	467	CYS	2.9
2	J	324	GLY	2.8
2	L	497	ASN	2.8
2	F	382	THR	2.8
2	L	381	LYS	2.8
2	J	480	TYR	2.7
1	I	256	ARG	2.7
2	J	358	ALA	2.7
2	J	466	ALA	2.7
2	F	341	VAL	2.7
2	F	350	GLN	2.7
1	K	270	CYS	2.6
2	J	461	PHE	2.6
1	G	5	LEU	2.6
1	G	1	ASP	2.6
1	K	205	ASN	2.6
1	C	278	GLY	2.5
2	J	460	CYS	2.5
1	A	111	ILE	2.5
2	H	354	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	448	GLN	2.5
1	C	150	LYS	2.4
2	H	480	TYR	2.4
2	L	342	ASP	2.4
2	J	491	LEU	2.4
2	H	359	ALA	2.4
2	J	359	ALA	2.4
1	I	1	ASP	2.4
1	G	205	ASN	2.4
2	H	466	ALA	2.4
1	C	151	GLY	2.4
1	C	189	GLY	2.4
1	K	152	GLN	2.4
2	D	324	GLY	2.4
1	K	316	VAL	2.4
2	J	385	GLU	2.4
2	L	354	GLY	2.3
2	L	350	GLN	2.3
2	J	485	TYR	2.3
1	I	39	ASN	2.3
2	J	383	ASN	2.3
2	H	487	GLU	2.3
2	D	448	GLN	2.3
2	L	475	ILE	2.3
2	L	383	ASN	2.3
1	E	269	ASN	2.2
2	D	470	SER	2.2
2	H	491	LEU	2.2
1	I	2	LYS	2.2
2	L	380	GLU	2.2
1	E	11	ALA	2.2
1	K	42	CYS	2.2
2	D	469	ASP	2.2
1	G	284	ARG	2.2
1	K	269	ASN	2.2
1	I	128	ARG	2.1
2	H	350	GLN	2.1
1	K	39	ASN	2.1
1	E	1	ASP	2.1
1	I	8	HIS	2.1
1	C	276	TRP	2.1
2	J	489	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	368	ILE	2.1
2	J	345	TYR	2.1
1	C	298	CYS	2.1
1	E	270	CYS	2.1
2	F	324	GLY	2.1
2	J	384	THR	2.1
1	I	3	ILE	2.1
1	I	73	MET	2.1
2	J	352	ALA	2.0
2	B	383	ASN	2.0
2	L	462	GLU	2.0
1	K	228	THR	2.0
2	H	468	ASP	2.0
1	C	152	GLN	2.0
1	K	294	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	601	14/15	0.76	0.16	56,69,73,81	0
3	NAG	G	601	14/15	0.77	0.17	74,92,96,97	0
3	NAG	H	601	14/15	0.77	0.12	41,56,60,62	0
3	NAG	I	601	14/15	0.77	0.14	56,68,76,84	0
3	NAG	L	601	14/15	0.78	0.13	49,63,67,72	0
3	NAG	K	601	14/15	0.80	0.14	56,63,70,79	0
3	NAG	E	601	14/15	0.81	0.12	56,63,74,74	0
3	NAG	B	601	14/15	0.81	0.12	52,58,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	601	14/15	0.84	0.11	41,53,63,66	0
3	NAG	A	601	14/15	0.86	0.11	51,62,71,77	0
3	NAG	D	601	14/15	0.89	0.09	37,49,52,52	0
3	NAG	J	601	14/15	0.90	0.08	46,48,53,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.