



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:55 AM BST

PDB ID : 4H32  
Title : The crystal structure of the hemagglutinin H17 derived the bat influenza A virus  
Authors : Sun, X.; Shi, Y.; Lu, X.; He, J.; Gao, F.; Yan, J.; Qi, J.; Gao, G.F.  
Deposited on : 2012-09-13  
Resolution : 2.70 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

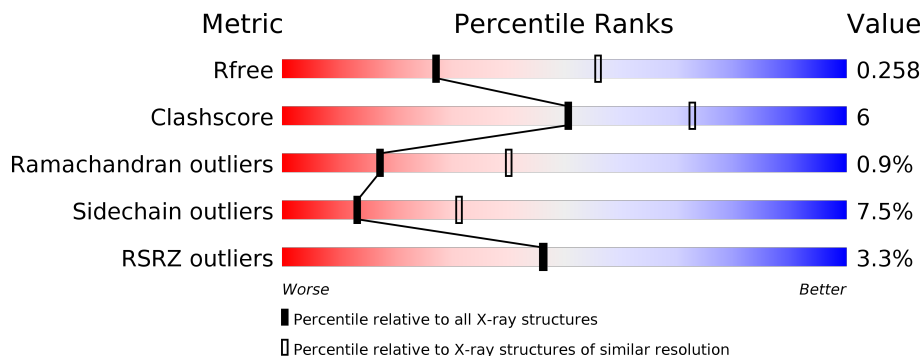
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	320	
1	C	320	
1	E	320	
1	G	320	
1	I	320	
1	K	320	

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Mol	Chain	Length	Quality of chain
2	B	171	
2	D	171	
2	F	171	
2	H	171	
2	J	171	
2	L	171	

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	A	602	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23961 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
			Total	C	N	O	S			
1	A	320	Total 2532	C 1593	N 434	O 492	S 13	0	1	0
1	C	320	Total 2532	C 1593	N 434	O 492	S 13	0	1	0
1	E	320	Total 2521	C 1584	N 433	O 491	S 13	0	0	0
1	G	320	Total 2532	C 1593	N 434	O 492	S 13	0	1	0
1	I	320	Total 2532	C 1593	N 434	O 492	S 13	0	1	0
1	K	320	Total 2521	C 1584	N 433	O 491	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP H6QM93
C	4	GLN	-	expression tag	UNP H6QM93
E	4	GLN	-	expression tag	UNP H6QM93
G	4	GLN	-	expression tag	UNP H6QM93
I	4	GLN	-	expression tag	UNP H6QM93
K	4	GLN	-	expression tag	UNP H6QM93

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	168	Total 1364	C 849	N 234	O 274	S 7	0	0	0
2	D	171	Total 1384	C 863	N 237	O 277	S 7	0	0	0
2	F	171	Total 1384	C 863	N 237	O 277	S 7	0	0	0

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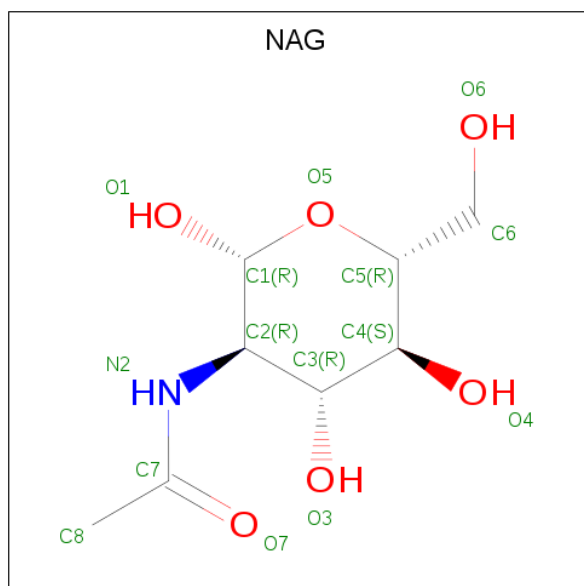
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	171	Total 1384	C 863	N 237	O 277	S 7	0	0	0
2	J	171	Total 1384	C 863	N 237	O 277	S 7	0	0	0
2	L	171	Total 1384	C 863	N 237	O 277	S 7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	505	GLU	LYS	conflict	UNP H6QM93
D	505	GLU	LYS	conflict	UNP H6QM93
F	505	GLU	LYS	conflict	UNP H6QM93
H	505	GLU	LYS	conflict	UNP H6QM93
J	505	GLU	LYS	conflict	UNP H6QM93
L	505	GLU	LYS	conflict	UNP H6QM93

- Molecule 3 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		
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	C	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	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	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	K	1	Total	C	N	O	0	0
			14	8	1	5		

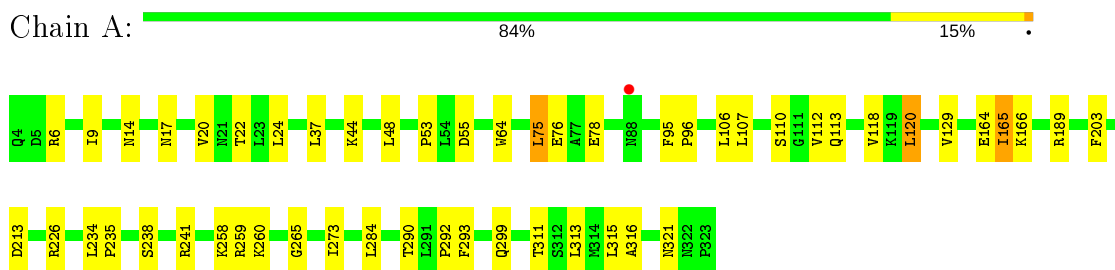
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	17	Total	O	0	0
			17	17		
4	C	63	Total	O	0	0
			63	63		
4	D	26	Total	O	0	0
			26	26		
4	E	58	Total	O	0	0
			58	58		
4	F	17	Total	O	0	0
			17	17		
4	G	21	Total	O	0	0
			21	21		
4	H	16	Total	O	0	0
			16	16		
4	I	37	Total	O	0	0
			37	37		
4	J	11	Total	O	0	0
			11	11		
4	K	43	Total	O	0	0
			43	43		
4	L	7	Total	O	0	0
			7	7		

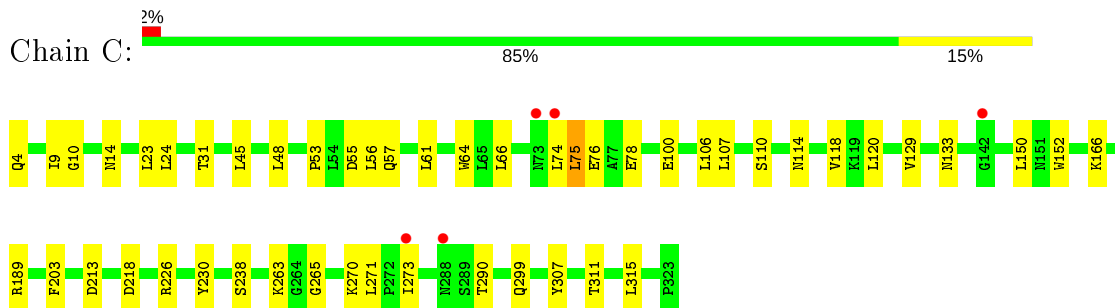
### 3 Residue-property plots [i](#)

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.

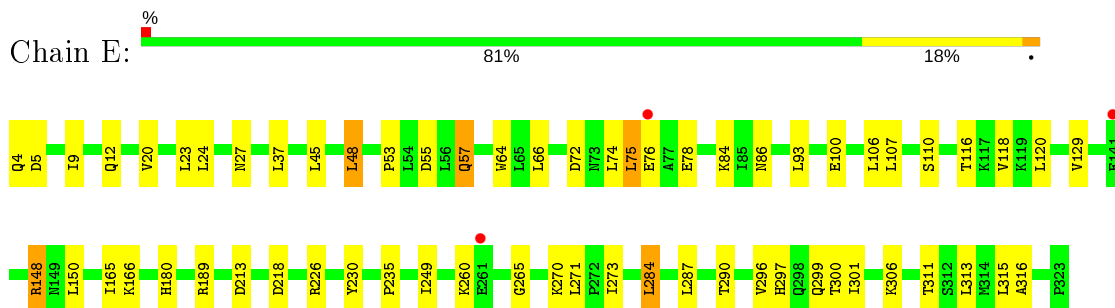
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

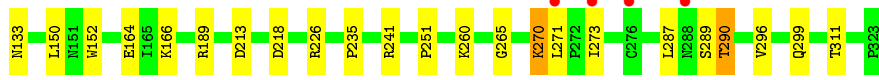
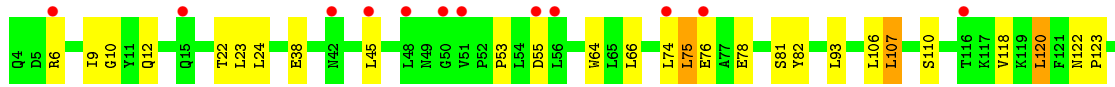


- Molecule 1: Hemagglutinin

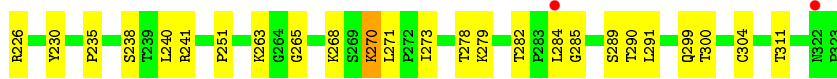
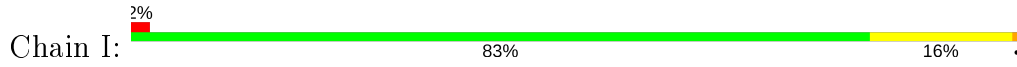


- Molecule 1: Hemagglutinin

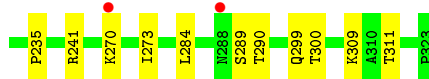
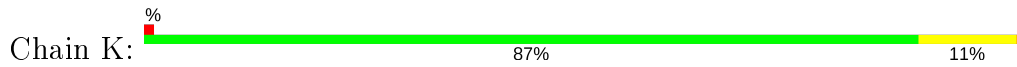




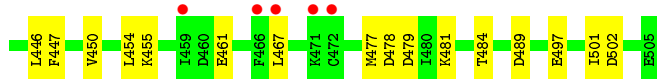
• Molecule 1: Hemagglutinin



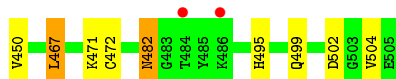
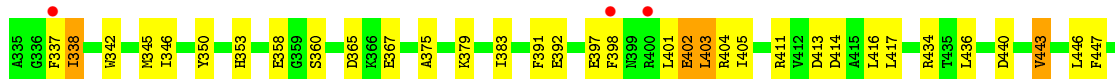
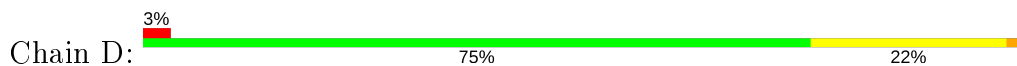
• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin

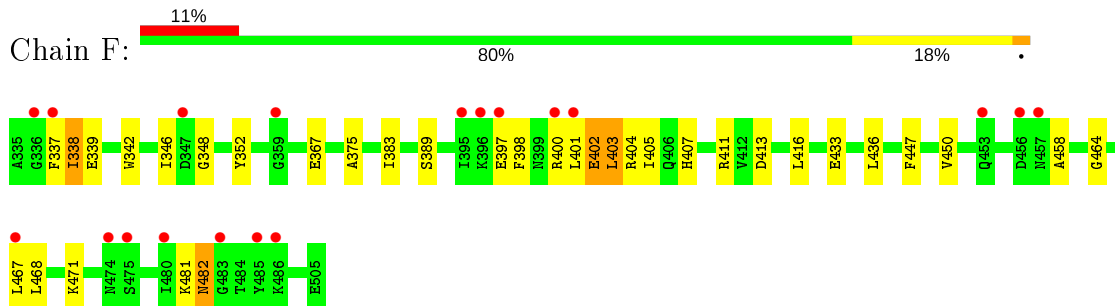


• Molecule 2: Hemagglutinin

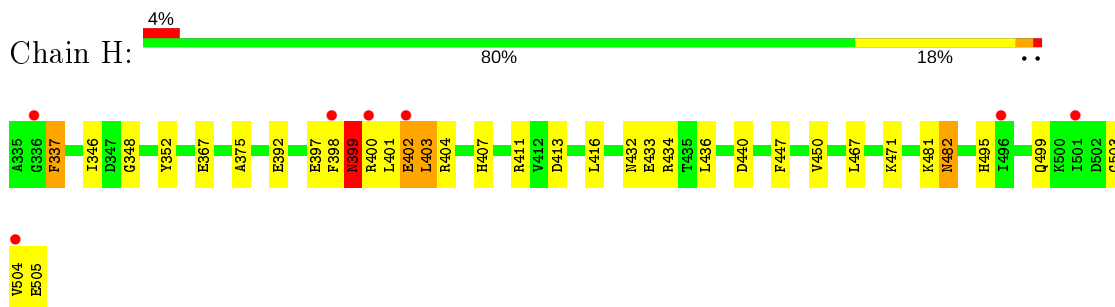




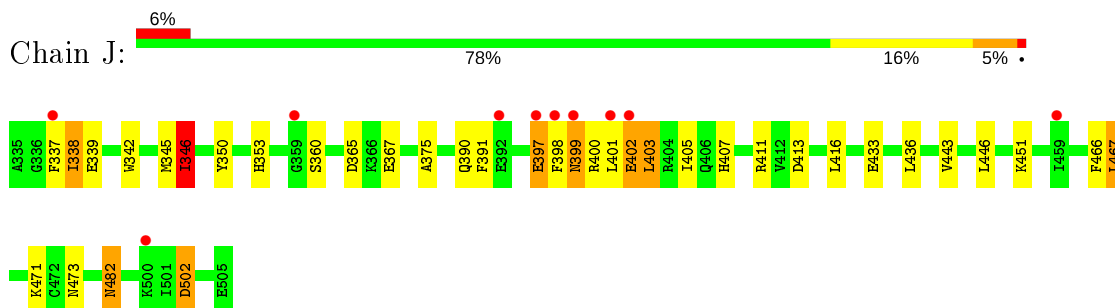
• Molecule 2: Hemagglutinin



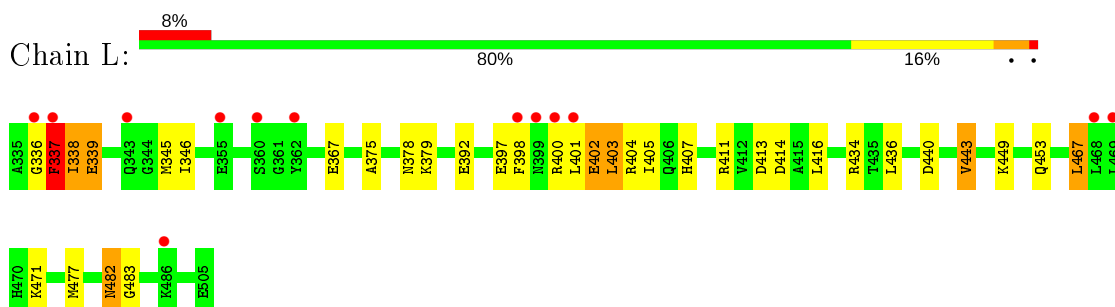
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.15Å 101.84Å 497.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.70 49.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.8 (49.88-2.70) 90.1 (49.88-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.217 , 0.263 0.210 , 0.258	Depositor DCC
$R_{free}$ test set	4892 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.26	0/2590	0.46	0/3521
1	C	0.26	0/2590	0.49	1/3521 (0.0%)
1	E	0.25	0/2578	0.46	0/3505
1	G	0.25	0/2590	0.46	0/3521
1	I	0.25	0/2590	0.47	0/3521
1	K	0.25	0/2578	0.45	0/3505
2	B	0.28	0/1387	0.48	1/1866 (0.1%)
2	D	0.25	0/1408	0.46	0/1894
2	F	0.26	0/1408	0.44	0/1894
2	H	0.24	0/1408	0.42	0/1894
2	J	0.25	0/1408	0.44	0/1894
2	L	0.25	0/1408	0.49	1/1894 (0.1%)
All	All	0.25	0/23943	0.46	3/32430 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	354	HIS	N-CA-CB	-9.27	93.91	110.60
2	L	337	PHE	CB-CA-C	8.58	127.57	110.40
1	C	57	GLN	N-CA-CB	-8.30	95.66	110.60

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	2532	0	2440	31	0
1	C	2532	0	2442	30	0
1	E	2521	0	2434	30	0
1	G	2532	0	2439	28	0
1	I	2532	0	2441	26	0
1	K	2521	0	2434	20	0
2	B	1364	0	1293	29	0
2	D	1384	0	1310	27	0
2	F	1384	0	1310	20	0
2	H	1384	0	1308	21	0
2	J	1384	0	1310	26	0
2	L	1384	0	1310	27	0
3	A	28	0	26	11	0
3	C	14	0	13	1	0
3	E	14	0	13	0	0
3	G	28	0	26	0	0
3	H	14	0	13	0	2
3	I	14	0	13	1	0
3	K	14	0	13	0	0
4	A	65	0	0	7	0
4	B	17	0	0	1	0
4	C	63	0	0	1	0
4	D	26	0	0	2	0
4	E	58	0	0	2	0
4	F	17	0	0	0	0
4	G	21	0	0	2	0
4	H	16	0	0	0	0
4	I	37	0	0	0	0
4	J	11	0	0	2	2
4	K	43	0	0	1	0
4	L	7	0	0	2	0
All	All	23961	0	22588	262	2

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 6.

All (262) 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)
2:L:337:PHE:CD1	2:L:339:GLU:O	1.77	1.37
3:A:601:NAG:H62	4:A:730:HOH:O	1.52	1.07
2:L:338:ILE:HG22	2:L:339:GLU:OE2	1.52	1.07
2:L:338:ILE:CG2	2:L:339:GLU:OE2	2.02	1.06
2:L:337:PHE:CE1	2:L:339:GLU:O	2.13	1.01
2:L:337:PHE:HD1	2:L:339:GLU:O	1.38	0.98
3:A:601:NAG:C6	4:A:730:HOH:O	2.18	0.80
1:A:17:ASN:ND2	3:A:602:NAG:H82	1.98	0.79
2:D:471:LYS:NZ	4:D:621:HOH:O	2.17	0.76
2:H:400:ARG:HH22	1:K:235:PRO:HG3	1.51	0.75
2:D:413:ASP:OD1	2:F:411:ARG:NH2	2.21	0.73
2:B:390:GLN:HG3	2:D:414:ASP:HB3	1.70	0.73
2:D:495:HIS:HE1	2:D:499:GLN:HE21	1.35	0.72
2:H:413:ASP:OD1	2:J:411:ARG:NH2	2.23	0.71
1:A:17:ASN:CG	3:A:602:NAG:H82	2.11	0.70
1:C:53:PRO:HG2	1:C:273:ILE:HD13	1.74	0.70
1:I:53:PRO:HG2	1:I:273:ILE:HD13	1.74	0.70
1:K:189:ARG:NH1	1:K:195:ASP:OD1	2.25	0.70
2:B:413:ASP:OD1	2:D:411:ARG:NH2	2.25	0.70
1:A:226:ARG:NH1	4:A:729:HOH:O	2.29	0.66
2:B:338:ILE:N	4:B:617:HOH:O	2.28	0.66
1:C:55:ASP:HB2	1:C:273:ILE:HD12	1.76	0.66
2:D:375:ALA:HB1	1:E:24:LEU:HG	1.79	0.65
2:J:337:PHE:HB3	2:J:338:ILE:HA	1.77	0.65
1:G:9:ILE:HG13	2:H:447:PHE:HA	1.77	0.65
1:E:53:PRO:HG2	1:E:273:ILE:HD13	1.79	0.64
1:A:14:ASN:OD1	4:A:741:HOH:O	2.15	0.64
2:J:413:ASP:OD1	2:L:411:ARG:NH2	2.31	0.64
1:I:55:ASP:HB2	1:I:273:ILE:HD12	1.80	0.63
1:I:235:PRO:HG3	2:L:400:ARG:HH22	1.61	0.63
1:A:120:LEU:HB3	1:A:165:ILE:HD13	1.81	0.62
1:K:53:PRO:HG2	1:K:273:ILE:HD13	1.81	0.62
1:G:45:LEU:HD13	1:G:271:LEU:HB2	1.81	0.61
1:G:64:TRP:HE1	1:G:75:LEU:HD23	1.64	0.61
2:B:342:TRP:CH2	2:B:353:HIS:HB3	2.35	0.61
2:L:337:PHE:HD1	2:L:339:GLU:C	2.04	0.61
1:A:9:ILE:HG13	2:B:447:PHE:HA	1.82	0.61
2:D:337:PHE:HB3	2:D:338:ILE:HA	1.83	0.61
1:C:10:GLY:HA2	2:D:338:ILE:HG23	1.82	0.60
1:C:64:TRP:HE1	1:C:75:LEU:HD23	1.67	0.60
1:I:110:SER:HB2	1:I:265:GLY:H	1.67	0.59
1:K:9:ILE:O	2:L:337:PHE:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:375:ALA:HB1	1:K:24:LEU:HG	1.84	0.59
3:A:601:NAG:H82	4:A:720:HOH:O	2.01	0.59
1:C:114:ASN:N	4:C:752:HOH:O	2.37	0.58
2:H:411:ARG:NH2	2:L:413:ASP:OD1	2.36	0.58
1:I:4:GLN:HB3	2:J:467:LEU:HD21	1.83	0.58
1:E:84:LYS:NZ	4:E:751:HOH:O	2.36	0.58
1:A:17:ASN:OD1	3:A:602:NAG:C7	2.52	0.58
2:D:379:LYS:HG3	1:E:23:LEU:HG	1.86	0.57
2:J:473:ASN:ND2	4:J:601:HOH:O	2.38	0.57
1:G:53:PRO:HG2	1:G:273:ILE:HD13	1.84	0.57
1:G:12:GLN:NE2	2:H:348:GLY:O	2.37	0.57
1:G:235:PRO:HG3	2:J:400:ARG:HH22	1.69	0.57
2:H:504:VAL:HG13	2:H:505:GLU:HG2	1.86	0.57
1:A:24:LEU:HG	2:F:375:ALA:HB1	1.87	0.57
1:A:17:ASN:CG	3:A:602:NAG:C8	2.73	0.56
1:G:287:LEU:HD11	1:G:296:VAL:HG21	1.87	0.56
1:A:17:ASN:ND2	3:A:602:NAG:C8	2.68	0.56
1:A:17:ASN:ND2	3:A:602:NAG:C7	2.69	0.56
1:C:66:LEU:HD22	1:C:150:LEU:HD11	1.88	0.56
1:E:218:ASP:O	1:E:226:ARG:NH2	2.39	0.55
1:E:64:TRP:HE1	1:E:75:LEU:HD23	1.71	0.55
1:E:27:ASN:ND2	4:E:757:HOH:O	2.39	0.55
1:K:55:ASP:HB2	1:K:273:ILE:HD12	1.88	0.55
1:E:12:GLN:NE2	2:F:348:GLY:O	2.38	0.55
1:K:164:GLU:OE2	1:K:241:ARG:NH1	2.39	0.54
1:K:64:TRP:HE1	1:K:75:LEU:HD23	1.71	0.54
1:E:75:LEU:HD22	1:E:76:GLU:H	1.72	0.54
1:A:321:ASN:ND2	4:A:741:HOH:O	2.40	0.54
1:A:164:GLU:OE2	1:A:241:ARG:NH1	2.41	0.53
1:E:55:ASP:HB2	1:E:273:ILE:HD12	1.89	0.53
2:J:390:GLN:HG3	2:L:414:ASP:HB3	1.89	0.53
1:G:66:LEU:HD22	1:G:150:LEU:HD11	1.90	0.53
2:B:348:GLY:HA3	2:B:364:ALA:HB1	1.89	0.53
2:B:353:HIS:HB2	2:B:362:TYR:CD1	2.43	0.53
1:E:287:LEU:HD11	1:E:296:VAL:HG21	1.89	0.53
1:E:37:LEU:HB2	1:E:313:LEU:HD12	1.90	0.53
2:F:337:PHE:C	2:F:339:GLU:H	2.12	0.53
1:E:57:GLN:O	1:E:86:ASN:ND2	2.42	0.53
1:C:56:LEU:HD23	1:C:74:LEU:HD23	1.91	0.53
1:I:45:LEU:HD13	1:I:271:LEU:HB2	1.90	0.53
2:L:482:ASN:O	2:L:482:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:HB2	1:A:273:ILE:HD12	1.90	0.52
1:A:75:LEU:HD22	1:A:76:GLU:H	1.74	0.52
1:K:66:LEU:HD22	1:K:150:LEU:HD11	1.89	0.52
2:D:405:ILE:HG21	2:F:404:ARG:HG3	1.91	0.52
2:H:375:ALA:HB1	1:I:24:LEU:HG	1.90	0.52
1:A:53:PRO:HG2	1:A:273:ILE:HD13	1.90	0.52
1:E:9:ILE:HG13	2:F:447:PHE:HA	1.92	0.52
2:B:380:VAL:O	2:B:384:ILE:HG12	2.09	0.52
1:I:64:TRP:HE1	1:I:75:LEU:HD23	1.75	0.52
1:I:66:LEU:HD22	1:I:150:LEU:HD11	1.92	0.51
2:B:411:ARG:NH2	2:F:413:ASP:OD1	2.43	0.51
1:A:203[B]:PHE:HE1	1:A:238:SER:HB3	1.75	0.51
1:I:164:GLU:OE2	1:I:241:ARG:NH1	2.44	0.50
1:A:64:TRP:HE1	1:A:75:LEU:HD23	1.76	0.50
2:J:400:ARG:O	2:J:402:GLU:N	2.44	0.50
1:K:218:ASP:O	1:K:226:ARG:NH2	2.42	0.50
2:B:400:ARG:HH12	1:E:235:PRO:HG3	1.76	0.50
1:C:203[B]:PHE:HE1	1:C:238:SER:HB3	1.76	0.50
1:G:55:ASP:HB2	1:G:273:ILE:HD12	1.93	0.50
1:E:64:TRP:CD1	1:E:74:LEU:HD22	2.47	0.50
1:I:75:LEU:HD22	1:I:76:GLU:H	1.76	0.50
2:J:345:MET:O	2:J:346:ILE:HG12	2.12	0.49
2:J:482:ASN:O	2:J:482:ASN:ND2	2.43	0.49
1:K:133:ASN:HB2	1:K:152:TRP:HB3	1.94	0.49
1:C:75:LEU:HD22	1:C:76:GLU:H	1.77	0.49
1:I:300:THR:OG1	1:I:304:CYS:SG	2.65	0.49
1:C:9:ILE:HG13	2:D:447:PHE:HA	1.95	0.49
1:I:10:GLY:HA2	2:J:338:ILE:HG23	1.95	0.48
1:C:4:GLN:HB3	2:D:467:LEU:HD21	1.94	0.48
2:F:482:ASN:ND2	2:F:482:ASN:O	2.40	0.48
2:H:482:ASN:O	2:H:482:ASN:ND2	2.46	0.48
2:H:495:HIS:HE1	2:H:499:GLN:HE21	1.61	0.48
1:G:164:GLU:OE2	1:G:241:ARG:NH1	2.44	0.48
2:B:375:ALA:HB1	1:C:24:LEU:HG	1.95	0.48
1:I:189:ARG:HD2	1:I:194:ASN:C	2.34	0.48
1:G:110:SER:HB2	1:G:265:GLY:H	1.78	0.48
2:F:402:GLU:O	2:F:405:ILE:N	2.47	0.47
2:D:482:ASN:O	2:D:482:ASN:ND2	2.45	0.47
1:A:6:ARG:NH2	2:B:461:GLU:OE2	2.38	0.47
1:G:75:LEU:HD22	1:G:76:GLU:H	1.78	0.47
1:K:148:ARG:NH1	4:K:737:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:HD13	1:C:271:LEU:HB2	1.96	0.47
1:I:38:GLU:HG2	1:I:289:SER:HB2	1.97	0.47
3:A:601:NAG:C7	4:A:720:HOH:O	2.62	0.47
1:G:64:TRP:CD1	1:G:74:LEU:HD22	2.50	0.47
1:A:9:ILE:HD11	2:B:450:VAL:HG21	1.96	0.47
2:H:399:ASN:HD22	2:H:400:ARG:N	2.13	0.47
1:C:56:LEU:HD13	1:C:61:LEU:HA	1.96	0.47
2:B:418:ASP:OD2	1:E:306:LYS:NZ	2.34	0.47
1:E:284:LEU:HD22	1:E:297:HIS:HD2	1.80	0.46
1:E:72:ASP:OD2	1:E:148:ARG:NH2	2.45	0.46
1:G:23:LEU:HG	2:L:379:LYS:HG3	1.97	0.46
2:F:471:LYS:HA	2:F:471:LYS:HD3	1.70	0.46
1:G:22:THR:HG22	2:H:432:ASN:HB3	1.97	0.46
1:C:9:ILE:HD11	2:D:450:VAL:HG21	1.97	0.46
1:C:56:LEU:CD2	1:C:74:LEU:HD23	2.45	0.46
2:F:352:TYR:HB2	2:F:481:LYS:HE2	1.98	0.46
1:G:38:GLU:HG2	1:G:289:SER:HB2	1.98	0.46
2:B:399:ASN:HD22	2:B:401:LEU:H	1.62	0.46
2:B:404:ARG:HG3	2:F:405:ILE:HG21	1.96	0.46
1:A:44:LYS:HE2	1:K:118:VAL:HG13	1.96	0.46
1:K:72:ASP:OD2	1:K:148:ARG:NH2	2.48	0.46
2:D:353:HIS:HE1	2:D:360:SER:HB3	1.81	0.45
1:G:9:ILE:HD11	2:H:450:VAL:HG21	1.98	0.45
1:C:218:ASP:O	1:C:226:ARG:NH2	2.48	0.45
1:C:14:ASN:HD21	1:C:31:THR:HB	1.80	0.45
1:E:9:ILE:HD11	2:F:450:VAL:HG21	1.98	0.45
1:I:268:LYS:HD3	2:J:397:GLU:HB2	1.97	0.45
2:L:378:ASN:OD1	4:L:607:HOH:O	2.21	0.45
1:E:100:GLU:HG3	1:E:230:TYR:CE1	2.51	0.45
2:J:337:PHE:HB2	2:J:342:TRP:NE1	2.32	0.45
1:G:24:LEU:HG	2:L:375:ALA:HB1	1.99	0.45
1:G:10:GLY:HA2	2:H:337:PHE:HB3	1.99	0.45
1:I:203[A]:PHE:CE1	1:I:240:LEU:HD13	2.51	0.45
2:J:353:HIS:HE1	2:J:360:SER:HB3	1.82	0.45
2:F:400:ARG:O	2:F:403:LEU:N	2.45	0.45
1:K:107:LEU:HD13	1:K:107:LEU:HA	1.82	0.45
2:H:402:GLU:O	2:H:404:ARG:N	2.50	0.45
1:A:17:ASN:CG	3:A:602:NAG:C7	2.85	0.45
1:E:45:LEU:HD13	1:E:271:LEU:HB2	1.98	0.45
1:I:270:LYS:H	1:I:270:LYS:HG2	1.62	0.45
2:L:449:LYS:HE2	2:L:449:LYS:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:ILE:O	2:H:337:PHE:HB3	2.17	0.44
2:B:398:PHE:CD1	2:B:402:GLU:HG3	2.52	0.44
2:B:402:GLU:N	2:B:402:GLU:OE2	2.50	0.44
2:D:404:ARG:NH1	4:D:606:HOH:O	2.50	0.44
2:B:479:ASP:OD2	2:B:484:THR:OG1	2.32	0.44
1:A:37:LEU:HB2	1:A:313:LEU:HD12	2.00	0.44
2:H:352:TYR:HB2	2:H:481:LYS:HE2	1.99	0.44
1:K:38:GLU:HG2	1:K:289:SER:HB2	1.99	0.44
1:I:120:LEU:HD23	1:I:251:PRO:HB2	2.00	0.44
2:L:338:ILE:CG2	2:L:339:GLU:N	2.80	0.43
2:D:337:PHE:H	2:D:342:TRP:HE1	1.65	0.43
2:D:365:ASP:OD2	2:D:446:LEU:HD11	2.18	0.43
2:J:471:LYS:HD3	2:J:471:LYS:HA	1.79	0.43
2:L:336:GLY:O	2:L:337:PHE:CB	2.66	0.43
1:G:290:THR:O	4:G:711:HOH:O	2.21	0.43
1:G:81:SER:HG	1:G:82:TYR:HD2	1.64	0.43
1:I:278:THR:OG1	1:I:279:LYS:N	2.52	0.43
1:E:20:VAL:HG21	1:E:316:ALA:HB2	2.01	0.43
1:E:110:SER:HB2	1:E:265:GLY:H	1.82	0.43
2:L:338:ILE:HD11	2:L:443:VAL:HG23	2.01	0.43
2:B:497:GLU:O	2:B:501:ILE:HG13	2.19	0.43
2:D:434:ARG:HH22	2:F:433:GLU:CD	2.21	0.43
1:G:218:ASP:O	1:G:226:ARG:NH2	2.49	0.43
2:B:365:ASP:OD2	2:B:446:LEU:HD11	2.19	0.43
1:E:180:HIS:HB2	1:E:249:ILE:HD11	2.00	0.43
1:G:107:LEU:HA	1:G:107:LEU:HD13	1.86	0.42
2:D:358:GLU:OE1	2:D:358:GLU:N	2.52	0.42
1:A:95:PHE:HA	1:A:96:PRO:HD3	1.90	0.42
1:C:315:LEU:HD21	2:D:383:ILE:HD12	2.02	0.42
1:C:133:ASN:HB2	1:C:152:TRP:HB3	2.01	0.42
2:J:471:LYS:NZ	4:J:609:HOH:O	2.47	0.42
2:L:471:LYS:HA	2:L:471:LYS:HD3	1.86	0.42
2:B:379:LYS:HG3	1:C:23:LEU:HG	2.01	0.42
2:B:477:MET:O	2:B:481:LYS:HG3	2.20	0.42
2:F:337:PHE:HB2	2:F:342:TRP:NE1	2.35	0.42
1:I:36:ILE:HA	1:I:291:LEU:HD22	2.02	0.42
2:L:402:GLU:O	2:L:404:ARG:N	2.52	0.42
1:G:120:LEU:HD23	1:G:251:PRO:HB2	2.00	0.42
2:H:433:GLU:CD	2:L:434:ARG:HH22	2.22	0.42
1:I:100:GLU:HG3	1:I:230:TYR:CE1	2.55	0.42
1:A:234:LEU:HA	1:A:235:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PRO:HG2	1:A:293:PHE:CD2	2.55	0.42
1:E:23:LEU:HD12	1:E:23:LEU:HA	1.94	0.42
1:E:315:LEU:HD21	2:F:383:ILE:HD12	2.01	0.42
1:I:263:LYS:HG3	2:J:391:PHE:CE2	2.55	0.42
1:K:75:LEU:HD13	1:K:76:GLU:OE2	2.20	0.42
2:B:405:ILE:HG21	2:D:404:ARG:HG3	2.00	0.41
1:A:22:THR:HG22	2:B:432:ASN:HB3	2.02	0.41
1:C:56:LEU:CD1	1:C:61:LEU:HA	2.51	0.41
1:G:122:ASN:HA	1:G:123:PRO:HD3	1.87	0.41
1:G:133:ASN:HB2	1:G:152:TRP:HB3	2.02	0.41
2:J:502:ASP:OD1	2:J:502:ASP:N	2.52	0.41
2:B:489:ASP:N	2:B:489:ASP:OD1	2.54	0.41
1:C:14:ASN:ND2	1:C:31:THR:HB	2.36	0.41
2:D:350:TYR:CD1	2:D:443:VAL:HG12	2.55	0.41
2:D:471:LYS:HA	2:D:471:LYS:HD3	1.74	0.41
4:G:709:HOH:O	1:I:226:ARG:NH1	2.53	0.41
2:H:434:ARG:HH22	2:J:433:GLU:CD	2.23	0.41
1:C:307:TYR:CD2	2:D:417:LEU:HD13	2.56	0.41
2:F:447:PHE:CE1	2:F:464:GLY:HA2	2.55	0.41
2:F:458:ALA:HB2	2:F:468:LEU:HD23	2.02	0.41
1:A:113:GLN:N	1:A:258:LYS:O	2.49	0.41
3:I:601:NAG:HO3	3:I:601:NAG:C7	2.34	0.41
2:J:337:PHE:HA	2:J:338:ILE:O	2.20	0.41
2:J:402:GLU:O	2:J:405:ILE:N	2.52	0.41
1:C:100:GLU:HG3	1:C:230:TYR:CE1	2.56	0.41
1:E:48:LEU:HD21	1:E:301:ILE:HG22	2.03	0.41
2:H:400:ARG:O	2:H:402:GLU:N	2.54	0.41
1:K:4:GLN:HB3	2:L:467:LEU:HD21	2.03	0.41
1:E:4:GLN:HB3	1:E:5:ASP:H	1.62	0.41
2:J:451:LYS:HB2	2:J:466:PHE:HZ	1.86	0.41
2:J:338:ILE:HB	2:J:339:GLU:H	1.57	0.41
2:L:477:MET:N	4:L:602:HOH:O	2.54	0.41
1:I:282:THR:OG1	1:I:285:GLY:O	2.35	0.41
1:K:309:LYS:HA	1:K:309:LYS:HD2	1.95	0.41
2:L:453:GLN:NE2	2:L:483:GLY:HA2	2.36	0.41
1:A:20:VAL:HG21	1:A:316:ALA:HB2	2.03	0.41
1:C:263:LYS:HE3	1:C:263:LYS:HB2	1.83	0.41
1:C:263:LYS:HG3	2:D:391:PHE:CE2	2.56	0.41
2:D:402:GLU:O	2:D:404:ARG:N	2.54	0.41
2:J:350:TYR:CD1	2:J:443:VAL:HG12	2.55	0.41
2:B:376:ILE:HA	2:B:376:ILE:HD12	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:PHE:HB2	2:B:406:GLN:OE1	2.22	0.40
1:C:23:LEU:HD12	1:C:23:LEU:HA	1.92	0.40
1:C:114:ASN:OD1	3:C:601:NAG:O5	2.37	0.40
1:G:270:LYS:HG2	1:G:270:LYS:H	1.64	0.40
2:H:471:LYS:HD3	2:H:471:LYS:HA	1.72	0.40
2:J:365:ASP:OD2	2:J:446:LEU:HD11	2.21	0.40
1:C:110:SER:HB2	1:C:265:GLY:H	1.86	0.40
2:F:400:ARG:O	2:F:402:GLU:N	2.53	0.40
2:H:404:ARG:HG3	2:L:405:ILE:HG21	2.02	0.40
1:I:203[B]:PHE:HE1	1:I:238:SER:HB3	1.86	0.40
1:A:110:SER:HB2	1:A:265:GLY:H	1.87	0.40
1:E:66:LEU:HD22	1:E:150:LEU:HD11	2.02	0.40
2:L:336:GLY:O	2:L:337:PHE:CD2	2.74	0.40
1:A:315:LEU:HD23	2:B:380:VAL:HG22	2.02	0.40
1:K:64:TRP:CD1	1:K:74:LEU:HD22	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:601:NAG:O5	4:J:606:HOH:O[3_545]	2.00	0.20
3:H:601:NAG:C5	4:J:606:HOH:O[3_545]	2.14	0.06

## 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	319/320 (100%)	302 (95%)	17 (5%)	0	100	100
1	C	319/320 (100%)	302 (95%)	17 (5%)	0	100	100
1	E	318/320 (99%)	303 (95%)	14 (4%)	1 (0%)	41	66
1	G	319/320 (100%)	301 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	319/320 (100%)	302 (95%)	16 (5%)	1 (0%)	41	66
1	K	318/320 (99%)	300 (94%)	17 (5%)	1 (0%)	41	66
2	B	166/171 (97%)	150 (90%)	15 (9%)	1 (1%)	25	50
2	D	169/171 (99%)	156 (92%)	9 (5%)	4 (2%)	6	15
2	F	169/171 (99%)	156 (92%)	8 (5%)	5 (3%)	4	10
2	H	169/171 (99%)	159 (94%)	4 (2%)	6 (4%)	3	7
2	J	169/171 (99%)	154 (91%)	10 (6%)	5 (3%)	4	10
2	L	169/171 (99%)	154 (91%)	12 (7%)	3 (2%)	8	21
All	All	2923/2946 (99%)	2739 (94%)	157 (5%)	27 (1%)	17	40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	346	ILE
2	D	403	LEU
2	F	338	ILE
2	F	346	ILE
2	H	346	ILE
2	H	403	LEU
2	J	346	ILE
2	J	401	LEU
2	J	403	LEU
1	K	76	GLU
2	L	346	ILE
2	L	403	LEU
2	D	338	ILE
2	D	401	LEU
2	F	403	LEU
2	J	338	ILE
1	E	57	GLN
2	F	389	SER
2	F	401	LEU
2	H	401	LEU
1	I	76	GLU
2	L	401	LEU
2	H	503	GLY
2	H	399	ASN
2	J	399	ASN
2	H	337	PHE

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Mol	Chain	Res	Type
2	B	346	ILE

### 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	283/282 (100%)	264 (93%)	19 (7%)	16	37
1	C	283/282 (100%)	268 (95%)	15 (5%)	22	48
1	E	282/282 (100%)	260 (92%)	22 (8%)	12	29
1	G	283/282 (100%)	267 (94%)	16 (6%)	20	44
1	I	283/282 (100%)	266 (94%)	17 (6%)	19	42
1	K	282/282 (100%)	262 (93%)	20 (7%)	14	34
2	B	148/149 (99%)	131 (88%)	17 (12%)	5	13
2	D	149/149 (100%)	133 (89%)	16 (11%)	6	15
2	F	149/149 (100%)	139 (93%)	10 (7%)	16	37
2	H	149/149 (100%)	136 (91%)	13 (9%)	10	23
2	J	149/149 (100%)	136 (91%)	13 (9%)	10	23
2	L	149/149 (100%)	132 (89%)	17 (11%)	5	13
All	All	2589/2586 (100%)	2394 (92%)	195 (8%)	13	31

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	75	LEU
1	A	78	GLU
1	A	106	LEU
1	A	107	LEU
1	A	112	VAL
1	A	118	VAL
1	A	120	LEU
1	A	129	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	165	ILE
1	A	166	LYS
1	A	189	ARG
1	A	213	ASP
1	A	259	ARG
1	A	260	LYS
1	A	284	LEU
1	A	290	THR
1	A	299	GLN
1	A	311	THR
2	B	338	ILE
2	B	346	ILE
2	B	350	TYR
2	B	353	HIS
2	B	358	GLU
2	B	367	GLU
2	B	376	ILE
2	B	390	GLN
2	B	397	GLU
2	B	399	ASN
2	B	416	LEU
2	B	436	LEU
2	B	454	LEU
2	B	455	LYS
2	B	467	LEU
2	B	478	ASP
2	B	502	ASP
1	C	48	LEU
1	C	75	LEU
1	C	78	GLU
1	C	106	LEU
1	C	107	LEU
1	C	118	VAL
1	C	120	LEU
1	C	129	VAL
1	C	166	LYS
1	C	189	ARG
1	C	213	ASP
1	C	270	LYS
1	C	290	THR
1	C	299	GLN
1	C	311	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	345	MET
2	D	367	GLU
2	D	392	GLU
2	D	397	GLU
2	D	398	PHE
2	D	402	GLU
2	D	403	LEU
2	D	416	LEU
2	D	436	LEU
2	D	440	ASP
2	D	443	VAL
2	D	467	LEU
2	D	472	CYS
2	D	482	ASN
2	D	502	ASP
2	D	504	VAL
1	E	48	LEU
1	E	75	LEU
1	E	78	GLU
1	E	93	LEU
1	E	106	LEU
1	E	107	LEU
1	E	116	THR
1	E	118	VAL
1	E	120	LEU
1	E	129	VAL
1	E	148	ARG
1	E	165	ILE
1	E	166	LYS
1	E	189	ARG
1	E	213	ASP
1	E	260	LYS
1	E	270	LYS
1	E	284	LEU
1	E	290	THR
1	E	299	GLN
1	E	300	THR
1	E	311	THR
2	F	338	ILE
2	F	367	GLU
2	F	397	GLU
2	F	398	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	402	GLU
2	F	407	HIS
2	F	416	LEU
2	F	436	LEU
2	F	467	LEU
2	F	482	ASN
1	G	6	ARG
1	G	75	LEU
1	G	78	GLU
1	G	93	LEU
1	G	106	LEU
1	G	107	LEU
1	G	118	VAL
1	G	120	LEU
1	G	166	LYS
1	G	189	ARG
1	G	213	ASP
1	G	260	LYS
1	G	270	LYS
1	G	290	THR
1	G	299	GLN
1	G	311	THR
2	H	367	GLU
2	H	392	GLU
2	H	397	GLU
2	H	398	PHE
2	H	399	ASN
2	H	402	GLU
2	H	403	LEU
2	H	407	HIS
2	H	416	LEU
2	H	436	LEU
2	H	440	ASP
2	H	467	LEU
2	H	482	ASN
1	I	75	LEU
1	I	78	GLU
1	I	87	GLU
1	I	93	LEU
1	I	106	LEU
1	I	107	LEU
1	I	116	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	118	VAL
1	I	120	LEU
1	I	129	VAL
1	I	213	ASP
1	I	220	ILE
1	I	270	LYS
1	I	284	LEU
1	I	290	THR
1	I	299	GLN
1	I	311	THR
2	J	346	ILE
2	J	367	GLU
2	J	397	GLU
2	J	398	PHE
2	J	399	ASN
2	J	402	GLU
2	J	403	LEU
2	J	407	HIS
2	J	416	LEU
2	J	436	LEU
2	J	467	LEU
2	J	482	ASN
2	J	502	ASP
1	K	24	LEU
1	K	45	LEU
1	K	75	LEU
1	K	78	GLU
1	K	106	LEU
1	K	107	LEU
1	K	118	VAL
1	K	120	LEU
1	K	129	VAL
1	K	148	ARG
1	K	166	LYS
1	K	189	ARG
1	K	213	ASP
1	K	220	ILE
1	K	270	LYS
1	K	284	LEU
1	K	290	THR
1	K	299	GLN
1	K	300	THR

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Mol	Chain	Res	Type
1	K	311	THR
2	L	337	PHE
2	L	338	ILE
2	L	339	GLU
2	L	345	MET
2	L	367	GLU
2	L	392	GLU
2	L	397	GLU
2	L	398	PHE
2	L	402	GLU
2	L	403	LEU
2	L	407	HIS
2	L	416	LEU
2	L	436	LEU
2	L	440	ASP
2	L	443	VAL
2	L	467	LEU
2	L	482	ASN

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

Mol	Chain	Res	Type
2	B	390	GLN
2	B	399	ASN
1	C	190	ASN
2	D	499	GLN
2	F	399	ASN
2	F	499	GLN
2	H	399	ASN
2	H	499	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](#)

9 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	E	601	1	14,14,15	0.46	0	17,19,21	1.23	3 (17%)
3	NAG	C	601	1	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	G	602	1	14,14,15	0.62	0	17,19,21	1.11	2 (11%)
3	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	H	601	2	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	K	601	1	14,14,15	0.61	0	17,19,21	0.72	0
3	NAG	I	601	1	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	A	602	1	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	G	601	1	14,14,15	0.59	0	17,19,21	0.99	1 (5%)

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	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	4/6/23/26	0/1/1/1
3	NAG	G	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	H	601	2	-	6/6/23/26	0/1/1/1
3	NAG	K	601	1	-	2/6/23/26	0/1/1/1
3	NAG	I	601	1	-	6/6/23/26	0/1/1/1
3	NAG	A	602	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	NAG	C1-O5-C5	2.89	116.11	112.19
3	G	602	NAG	O5-C5-C6	2.29	110.79	107.20
3	G	602	NAG	O5-C1-C2	2.27	114.88	111.29
3	E	601	NAG	O5-C5-C6	2.21	110.66	107.20
3	E	601	NAG	C2-N2-C7	-2.07	119.96	122.90
3	G	601	NAG	O5-C1-C2	2.03	114.49	111.29

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	C8-C7-N2-C2
3	E	601	NAG	O7-C7-N2-C2
3	H	601	NAG	O7-C7-N2-C2
3	K	601	NAG	C8-C7-N2-C2
3	K	601	NAG	O7-C7-N2-C2
3	I	601	NAG	C8-C7-N2-C2
3	I	601	NAG	O7-C7-N2-C2
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
3	G	602	NAG	C8-C7-N2-C2
3	G	602	NAG	O7-C7-N2-C2
3	H	601	NAG	C8-C7-N2-C2
3	C	601	NAG	O5-C5-C6-O6
3	H	601	NAG	O5-C5-C6-O6
3	I	601	NAG	O5-C5-C6-O6
3	I	601	NAG	C1-C2-N2-C7
3	H	601	NAG	C4-C5-C6-O6
3	I	601	NAG	C4-C5-C6-O6
3	C	601	NAG	C8-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	C	601	NAG	O7-C7-N2-C2
3	C	601	NAG	C4-C5-C6-O6
3	H	601	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	G	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	G	601	NAG	C8-C7-N2-C2
3	A	601	NAG	C4-C5-C6-O6
3	G	601	NAG	O7-C7-N2-C2
3	H	601	NAG	C3-C2-N2-C7
3	I	601	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAG	1	0
3	A	601	NAG	4	0
3	H	601	NAG	0	2
3	I	601	NAG	1	0
3	A	602	NAG	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	320/320 (100%)	-0.28	1 (0%) 94 95	20, 37, 78, 122	0
1	C	320/320 (100%)	-0.18	5 (1%) 72 74	20, 40, 82, 148	0
1	E	320/320 (100%)	-0.21	3 (0%) 84 85	22, 37, 75, 125	0
1	G	320/320 (100%)	0.20	16 (5%) 28 27	32, 54, 97, 137	0
1	I	320/320 (100%)	-0.06	6 (1%) 66 69	25, 49, 89, 134	0
1	K	320/320 (100%)	-0.16	3 (0%) 84 85	24, 44, 85, 133	0
2	B	168/171 (98%)	0.22	9 (5%) 25 24	27, 64, 109, 156	0
2	D	171/171 (100%)	0.06	5 (2%) 51 52	29, 54, 97, 148	0
2	F	171/171 (100%)	0.52	19 (11%) 5 4	27, 62, 112, 153	0
2	H	171/171 (100%)	0.27	7 (4%) 37 36	36, 64, 114, 171	0
2	J	171/171 (100%)	0.39	10 (5%) 23 22	36, 64, 117, 158	0
2	L	171/171 (100%)	0.35	13 (7%) 13 12	38, 62, 107, 172	0
All	All	2943/2946 (99%)	0.03	97 (3%) 46 46	20, 50, 97, 172	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	337	PHE	4.8
2	F	480	ILE	4.7
2	J	398	PHE	3.9
1	G	74	LEU	3.8
2	L	398	PHE	3.8
2	B	400	ARG	3.7
2	F	401	LEU	3.6
1	I	15	GLN	3.6
1	G	56	LEU	3.5
2	F	337	PHE	3.4
2	F	486	LYS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	L	337	PHE	3.4
2	H	504	VAL	3.4
2	B	459	ILE	3.3
1	K	87	GLU	3.3
2	L	400	ARG	3.2
1	G	50	GLY	3.2
2	F	396	LYS	3.1
2	F	395	ILE	3.0
2	F	485	TYR	3.0
1	K	270	LYS	3.0
1	I	76	GLU	3.0
2	H	400	ARG	2.9
1	G	288	ASN	2.9
2	L	401	LEU	2.8
1	E	76	GLU	2.8
2	D	486	LYS	2.8
1	G	42	ASN	2.8
1	G	76	GLU	2.8
1	C	74	LEU	2.8
2	F	359	GLY	2.8
1	G	276	CYS	2.8
2	J	397	GLU	2.8
1	G	48	LEU	2.7
2	L	336	GLY	2.7
1	G	273	ILE	2.7
2	F	397	GLU	2.7
2	H	496	ILE	2.7
2	H	402	GLU	2.7
1	I	75	LEU	2.6
2	J	500	LYS	2.6
2	D	337	PHE	2.6
2	B	357	GLN	2.6
2	J	399	ASN	2.5
2	L	355	GLU	2.5
1	I	10	GLY	2.5
2	D	400	ARG	2.5
2	D	398	PHE	2.5
2	F	474	ASN	2.5
2	F	467	LEU	2.4
2	B	360	SER	2.4
1	C	288	ASN	2.4
1	G	271	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	142	GLY	2.4
2	J	402	GLU	2.4
2	B	466	PHE	2.4
1	G	6	ARG	2.3
2	J	459	ILE	2.3
2	B	471	LYS	2.3
2	L	486	LYS	2.3
2	F	456	ASP	2.3
2	B	467	LEU	2.3
1	A	88	ASN	2.3
2	L	399	ASN	2.3
2	H	398	PHE	2.3
2	F	347	ASP	2.3
2	F	457	ASN	2.3
1	K	288	ASN	2.3
2	L	362	TYR	2.2
2	L	343	GLN	2.2
1	I	284	LEU	2.2
1	G	55	ASP	2.2
2	F	453	GLN	2.2
2	L	468	LEU	2.2
1	G	116	THR	2.2
2	D	484	THR	2.2
2	H	501	ILE	2.2
2	B	472	CYS	2.2
1	C	73	ASN	2.2
2	L	469	LEU	2.2
2	F	475	SER	2.2
2	H	336	GLY	2.2
2	J	359	GLY	2.1
1	C	273	ILE	2.1
2	F	400	ARG	2.1
1	G	15	GLN	2.1
1	G	45	LEU	2.1
1	E	141	GLU	2.1
1	E	261	GLU	2.1
2	L	360	SER	2.1
2	F	483	GLY	2.1
2	F	336	GLY	2.1
1	G	51	VAL	2.0
1	I	322	ASN	2.0
2	J	392	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	359	GLY	2.0
2	J	401	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	602	14/15	0.45	0.31	98,120,130,134	0
3	NAG	G	602	14/15	0.49	0.35	89,124,138,141	0
3	NAG	G	601	14/15	0.67	0.19	86,112,124,128	0
3	NAG	C	601	14/15	0.71	0.24	52,97,121,128	0
3	NAG	A	601	14/15	0.74	0.25	47,70,85,86	0
3	NAG	H	601	14/15	0.74	0.22	57,81,105,113	0
3	NAG	I	601	14/15	0.75	0.20	66,88,107,110	0
3	NAG	K	601	14/15	0.80	0.26	71,97,106,109	0
3	NAG	E	601	14/15	0.87	0.19	80,93,107,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.