



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:09 PM GMT

PDB ID : 4QY2
Title : Structure of H10 from human-infecting H10N8 virus in complex with human receptor analog
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 : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

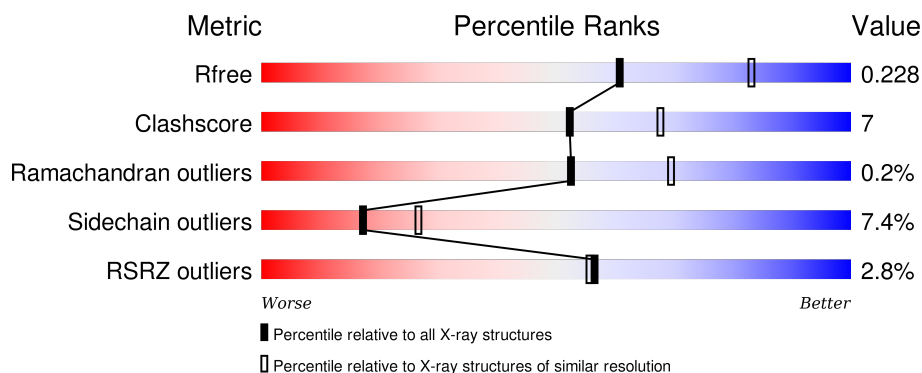
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	<div> <div>78%</div> <div>19%</div> <div>•</div> </div>
1	C	318	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	E	318	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	G	318	<div> <div>80%</div> <div>19%</div> <div>•</div> </div>
1	I	318	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	318	
2	B	174	
2	D	174	
2	F	174	
2	H	174	
2	J	174	
2	L	174	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SIA	E	602	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24413 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.

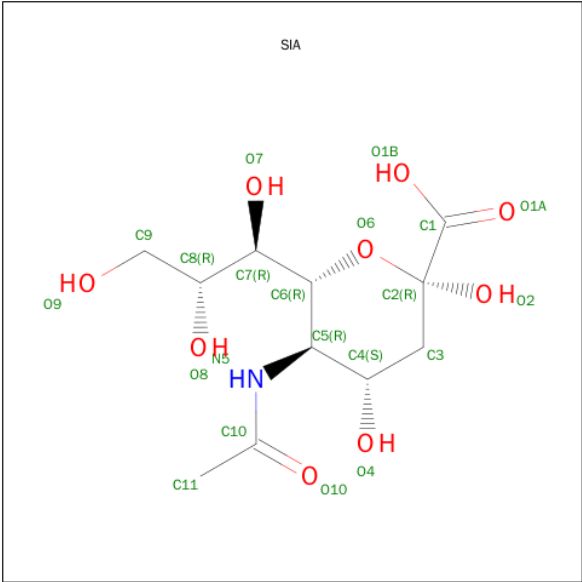
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	D	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	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: 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 SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	81	Total	O	0	0
			81	81		
5	C	124	Total	O	0	0
			124	124		
5	D	93	Total	O	0	0
			93	93		
5	E	161	Total	O	0	0
			161	161		
5	F	90	Total	O	0	0
			90	90		
5	G	126	Total	O	0	0
			126	126		
5	H	41	Total	O	0	0
			41	41		
5	I	142	Total	O	0	0
			142	142		
5	J	58	Total	O	0	0
			58	58		
5	K	90	Total	O	0	0
			90	90		

Continued on next page...

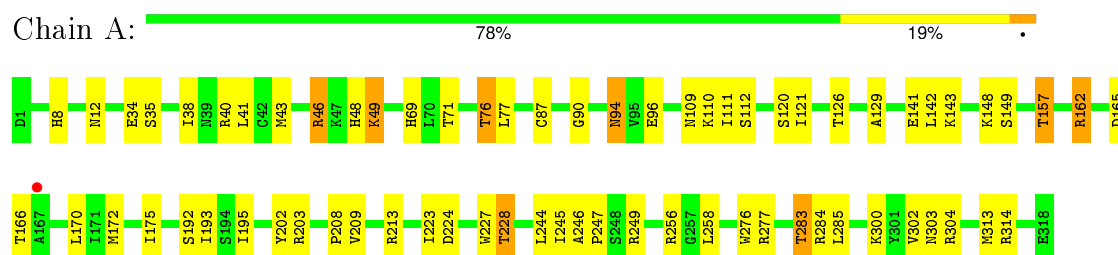
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	56	Total	O	0	0
			56	56		

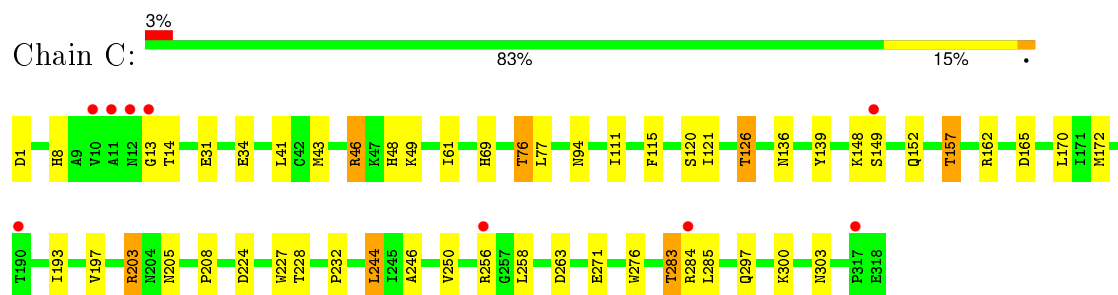
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

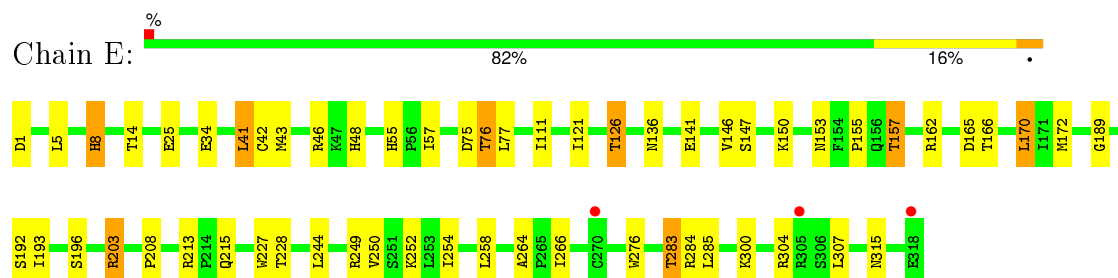
• Molecule 1: hemagglutinin



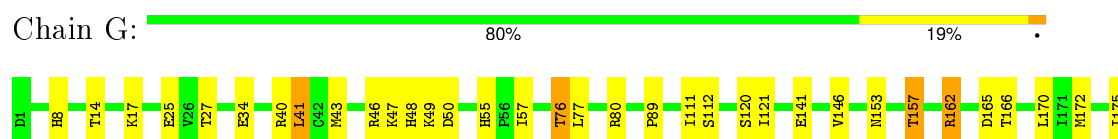
• Molecule 1: hemagglutinin



• Molecule 1: hemagglutinin

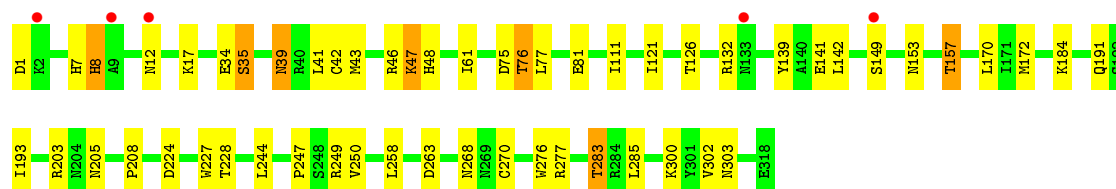
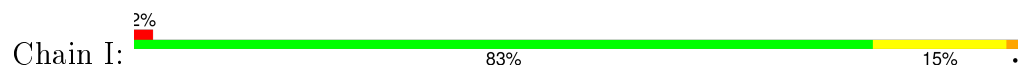


• Molecule 1: hemagglutinin

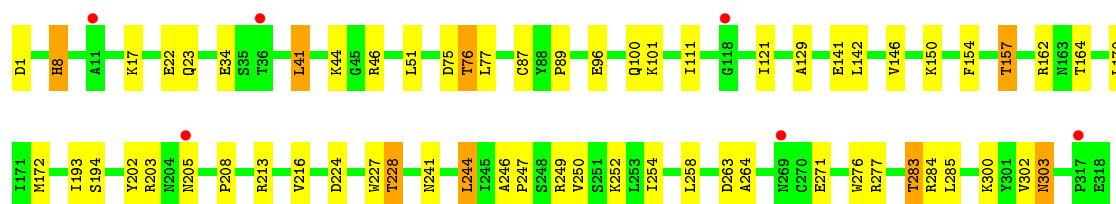
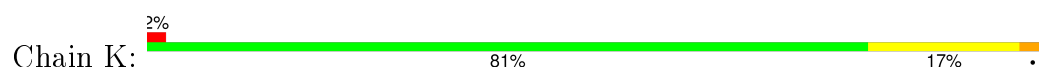




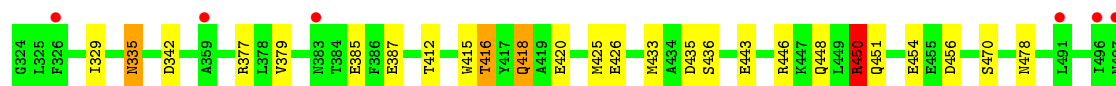
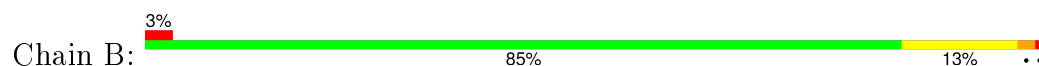
- Molecule 1: hemagglutinin



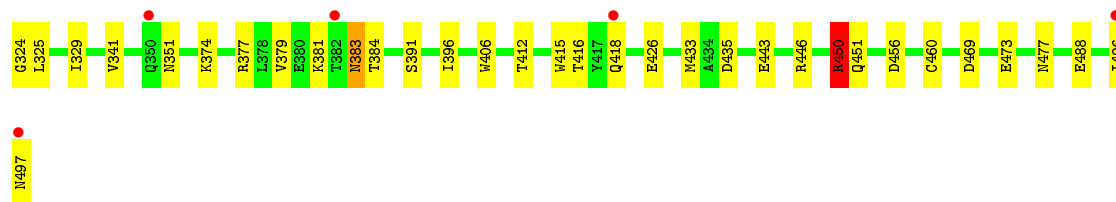
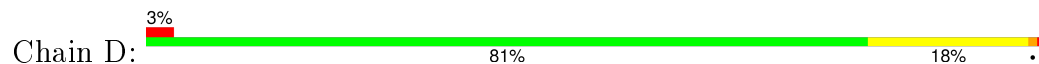
- Molecule 1: hemagglutinin



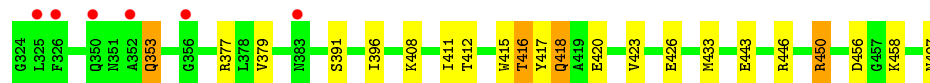
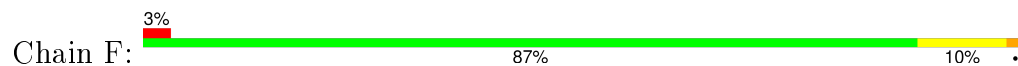
- Molecule 2: hemagglutinin



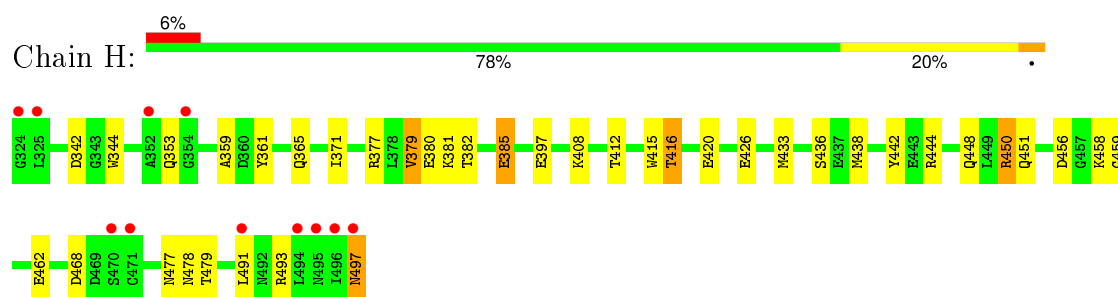
- Molecule 2: hemagglutinin



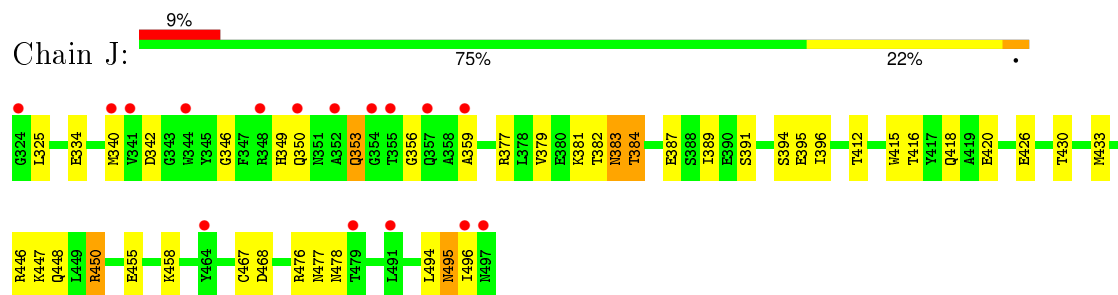
- Molecule 2: hemagglutinin



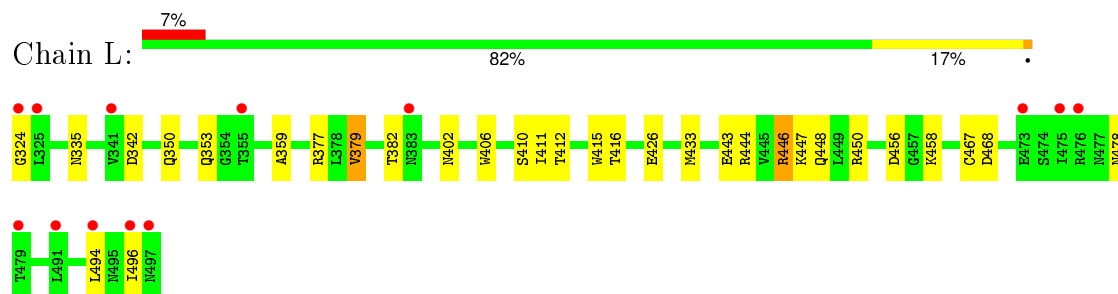
- Molecule 2: hemagglutinin



• 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	75.00Å 118.51Å 124.51Å 98.69° 93.04° 96.51°	Depositor
Resolution (Å)	39.90 – 2.40 39.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.90-2.40) 88.4 (39.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.230 0.187 , 0.228	Depositor DCC
R_{free} test set	7468 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 161413 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24413	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, 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	0.34	0/2486	0.54	0/3368
1	C	0.34	0/2486	0.54	0/3368
1	E	0.35	0/2486	0.54	1/3368 (0.0%)
1	G	0.33	0/2486	0.52	0/3368
1	I	0.35	0/2486	0.55	0/3368
1	K	0.32	0/2486	0.52	0/3368
2	B	0.36	0/1427	0.50	0/1926
2	D	0.35	0/1427	0.53	0/1926
2	F	0.37	0/1427	0.51	0/1926
2	H	0.32	0/1427	0.48	0/1926
2	J	0.32	0/1427	0.49	0/1926
2	L	0.33	0/1427	0.47	0/1926
All	All	0.34	0/23478	0.52	1/31764 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2389	40	0
1	C	2437	0	2389	34	1
1	E	2437	0	2389	31	0
1	G	2437	0	2389	34	0
1	I	2437	0	2389	31	0
1	K	2437	0	2389	32	0
2	B	1402	0	1298	19	0
2	D	1402	0	1298	27	0
2	F	1402	0	1298	16	0
2	H	1402	0	1298	26	1
2	J	1402	0	1298	29	0
2	L	1402	0	1298	27	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
3	E	14	0	13	1	0
3	F	14	0	13	0	0
3	G	14	0	13	1	0
3	H	14	0	13	0	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	E	21	0	18	1	0
5	A	128	0	0	8	0
5	B	81	0	0	4	0
5	C	124	0	0	6	0
5	D	93	0	0	7	0
5	E	161	0	0	7	0
5	F	90	0	0	3	0
5	G	126	0	0	4	0
5	H	41	0	0	4	0
5	I	142	0	0	6	0
5	J	58	0	0	9	0
5	K	90	0	0	3	0
5	L	56	0	0	9	0
All	All	24413	0	22296	306	1

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 (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:ND2	5:C:792:HOH:O	1.81	0.99
1:G:46:ARG:HE	1:G:76:THR:HG21	1.33	0.93
2:J:381:LYS:O	5:J:734:HOH:O	1.90	0.90
1:I:7:HIS:NE2	5:I:746:HOH:O	2.07	0.87
1:I:224:ASP:OD1	5:I:748:HOH:O	1.92	0.85
2:F:497:ASN:O	5:F:754:HOH:O	1.94	0.85
2:D:488:GLU:OE1	5:D:761:HOH:O	1.94	0.84
1:A:46:ARG:HE	1:A:76:THR:HG21	1.41	0.83
3:E:601:NAG:O4	5:E:854:HOH:O	1.95	0.83
3:G:601:NAG:O4	5:G:767:HOH:O	1.96	0.83
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.11	0.82
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.15	0.80
1:A:71:THR:OG1	5:A:826:HOH:O	1.99	0.79
1:I:46:ARG:HE	1:I:76:THR:HG21	1.46	0.78
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.16	0.78
2:J:478:ASN:O	5:J:745:HOH:O	2.02	0.77
1:A:96:GLU:OE2	5:A:786:HOH:O	2.02	0.77
1:A:94:ASN:OD1	5:A:789:HOH:O	2.02	0.77
1:E:42:CYS:O	5:E:743:HOH:O	2.02	0.76
1:E:1:ASP:N	5:E:717:HOH:O	2.19	0.76
2:B:335:ASN:O	5:B:766:HOH:O	2.02	0.75
2:F:377:ARG:NH2	2:F:426:GLU:OE2	2.18	0.75
3:D:601:NAG:O7	5:D:702:HOH:O	2.04	0.75
2:L:478:ASN:OD1	5:L:715:HOH:O	2.04	0.75
1:G:27:THR:O	5:G:798:HOH:O	2.04	0.73
1:K:224:ASP:OD1	5:K:706:HOH:O	2.06	0.73
1:K:164:THR:OG1	5:K:741:HOH:O	2.06	0.73
2:B:377:ARG:NH2	2:B:426:GLU:OE2	2.21	0.73
1:E:215:GLN:O	5:E:806:HOH:O	2.06	0.72
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.24	0.71
2:J:334:GLU:HG3	5:J:724:HOH:O	1.90	0.70
2:J:389:ILE:O	5:J:749:HOH:O	2.08	0.70
1:G:17:LYS:NZ	2:H:420:GLU:OE2	2.25	0.70
1:K:41:LEU:HD13	1:K:264:ALA:HB3	1.75	0.69
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.25	0.69
2:L:448:GLN:NE2	5:L:715:HOH:O	2.26	0.69
1:C:31:GLU:O	5:C:721:HOH:O	2.10	0.68
2:J:387:GLU:OE1	5:J:708:HOH:O	2.11	0.68
1:A:12:ASN:O	5:A:765:HOH:O	2.10	0.68
1:C:46:ARG:HE	1:C:76:THR:HG21	1.58	0.67
1:K:17:LYS:HE3	1:K:22:GLU:HG3	1.76	0.67
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.28	0.67
2:L:377:ARG:HD2	5:L:736:HOH:O	1.96	0.66
1:I:8:HIS:O	5:I:771:HOH:O	2.12	0.66
2:F:456:ASP:HB3	2:F:458:LYS:H	1.62	0.65
2:B:456:ASP:OD2	5:B:781:HOH:O	2.13	0.65
2:B:412:THR:O	2:B:416:THR:HG23	1.96	0.65
2:F:353:GLN:H	2:F:353:GLN:HE21	1.44	0.65
1:A:224:ASP:OD1	5:A:734:HOH:O	2.14	0.65
1:C:13:GLY:O	5:C:807:HOH:O	2.15	0.64
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.64
2:D:412:THR:O	2:D:416:THR:HG23	1.98	0.63
1:E:283:THR:HG22	1:E:285:LEU:H	1.63	0.63
1:I:121:ILE:HD11	1:I:157:THR:HG21	1.80	0.63
1:A:141:GLU:OE1	1:A:249:ARG:HD3	1.99	0.63
1:I:141:GLU:OE1	1:I:249:ARG:HD3	1.99	0.62
1:A:162:ARG:NH2	5:A:808:HOH:O	2.31	0.62
1:K:284:ARG:HB3	2:L:379:VAL:HG22	1.83	0.61
2:F:391:SER:H	2:F:396:ILE:HD11	1.65	0.61
2:D:477:ASN:ND2	5:D:786:HOH:O	2.33	0.61
1:A:165:ASP:OD1	1:A:166:THR:N	2.32	0.61
1:I:48:HIS:HE1	1:I:268:ASN:HD21	1.49	0.60
1:I:81:GLU:OE1	5:I:758:HOH:O	2.16	0.60
1:E:41:LEU:HD13	1:E:264:ALA:HB3	1.84	0.60
1:E:193:ILE:HG21	1:E:208:PRO:HG2	1.84	0.59
1:E:147:SER:O	5:E:708:HOH:O	2.17	0.59
1:C:49:LYS:HD2	1:C:69:HIS:ND1	2.17	0.59
1:I:17:LYS:NZ	2:J:420:GLU:OE2	2.26	0.59
1:A:172:MET:HG2	1:A:227:TRP:HB3	1.83	0.59
1:A:110:LYS:NZ	1:A:141:GLU:OE2	2.32	0.59
2:F:443:GLU:OE2	2:F:446:ARG:NH1	2.36	0.59
1:K:193:ILE:HG21	1:K:208:PRO:HG2	1.85	0.59
2:J:391:SER:H	2:J:396:ILE:HD11	1.68	0.59
1:C:303:ASN:H	2:D:416:THR:CG2	2.16	0.59
2:H:456:ASP:HB3	2:H:458:LYS:H	1.68	0.58
2:D:391:SER:H	2:D:396:ILE:HD11	1.68	0.58
2:H:458:LYS:O	5:H:732:HOH:O	2.17	0.58
1:G:297:GLN:HG2	2:H:385:GLU:HG2	1.84	0.58
2:L:324:GLY:N	5:L:704:HOH:O	2.36	0.57
1:C:121:ILE:HD11	1:C:157:THR:HG21	1.86	0.57
1:C:303:ASN:H	2:D:416:THR:HG22	1.70	0.57
2:B:443:GLU:OE2	2:B:446:ARG:NH1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:468:ASP:OD1	5:L:739:HOH:O	2.17	0.57
2:D:469:ASP:OD1	5:D:748:HOH:O	2.17	0.56
2:B:454:GLU:OE1	2:D:450:ARG:NH1	2.35	0.56
2:J:455:GLU:OE1	2:L:446:ARG:NH2	2.38	0.56
2:L:410:SER:O	5:L:702:HOH:O	2.17	0.56
1:G:121:ILE:HD11	1:G:157:THR:HG21	1.88	0.56
1:C:126:THR:HG23	1:C:136:ASN:HB3	1.87	0.56
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.87	0.56
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.39	0.55
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.89	0.55
1:C:224:ASP:OD2	1:E:203:ARG:NH2	2.36	0.55
2:J:412:THR:O	2:J:416:THR:HG23	2.07	0.55
2:J:394:SER:OG	5:J:725:HOH:O	2.18	0.55
2:J:458:LYS:NZ	5:J:724:HOH:O	2.38	0.54
1:I:43:MET:HE3	1:I:46:ARG:HD3	1.89	0.54
2:J:446:ARG:HH12	2:J:447:LYS:HE3	1.72	0.54
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.90	0.54
1:K:46:ARG:HE	1:K:76:THR:HG21	1.73	0.54
1:E:126:THR:HG23	1:E:136:ASN:HB3	1.90	0.54
1:C:284:ARG:HB3	2:D:379:VAL:HG22	1.90	0.54
2:H:444:ARG:O	5:H:719:HOH:O	2.19	0.53
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.08	0.53
2:H:397:GLU:OE2	5:H:727:HOH:O	2.19	0.53
2:H:353:GLN:HE22	2:H:468:ASP:HB2	1.72	0.53
1:K:121:ILE:HD11	1:K:157:THR:HG21	1.90	0.53
1:G:284:ARG:HB3	2:H:379:VAL:HG22	1.90	0.53
2:L:448:GLN:NE2	2:L:478:ASN:HA	2.23	0.52
1:A:256:ARG:NH2	2:B:387:GLU:OE1	2.43	0.52
1:E:34:GLU:HB2	1:E:283:THR:HG21	1.91	0.52
2:L:448:GLN:HE22	2:L:478:ASN:HA	1.75	0.52
2:H:344:TRP:HH2	2:H:371:ILE:HD12	1.75	0.52
1:G:252:LYS:NZ	5:G:802:HOH:O	2.43	0.51
1:E:8:HIS:HE1	5:E:724:HOH:O	1.92	0.51
1:G:43:MET:CE	1:G:48:HIS:HB3	2.40	0.51
1:C:224:ASP:OD1	5:C:714:HOH:O	2.19	0.51
1:K:283:THR:HG22	1:K:285:LEU:H	1.75	0.51
1:K:34:GLU:HB2	1:K:283:THR:HG21	1.92	0.51
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.92	0.51
2:D:473:GLU:O	2:D:477:ASN:HB2	2.11	0.51
1:E:155:PRO:O	1:E:157:THR:HG22	2.11	0.51
1:G:172:MET:HG2	1:G:227:TRP:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:494:LEU:HB3	2:J:496:ILE:HG13	1.94	0.50
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.11	0.50
1:C:34:GLU:HB2	1:C:283:THR:HG21	1.93	0.50
1:G:89:PRO:HB3	1:G:216:VAL:HB	1.94	0.50
1:K:303:ASN:H	2:L:416:THR:CG2	2.25	0.50
1:I:39:ASN:O	5:I:765:HOH:O	2.19	0.50
1:I:302:VAL:HB	2:J:416:THR:HG22	1.93	0.50
1:G:209:VAL:HG11	1:I:205:ASN:HB2	1.94	0.50
1:G:193:ILE:HG21	1:G:208:PRO:HG2	1.94	0.49
2:D:456:ASP:OD1	2:D:460:CYS:HB2	2.12	0.49
1:A:300:LYS:HG3	2:B:415:TRP:CE2	2.47	0.49
1:G:41:LEU:HD13	1:G:264:ALA:HB3	1.94	0.49
2:H:381:LYS:NZ	2:H:382:THR:O	2.38	0.49
2:L:377:ARG:NH1	5:L:736:HOH:O	2.20	0.49
1:C:244:LEU:HD13	1:C:246:ALA:HB2	1.94	0.49
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.93	0.49
2:D:324:GLY:N	5:D:703:HOH:O	2.45	0.49
1:K:89:PRO:HB3	1:K:216:VAL:HB	1.95	0.48
2:H:342:ASP:HB3	2:H:359:ALA:HB2	1.95	0.48
2:H:377:ARG:NH2	2:H:426:GLU:OE2	2.46	0.48
2:D:374:LYS:NZ	2:D:426:GLU:OE1	2.43	0.48
2:L:444:ARG:O	2:L:448:GLN:HG3	2.13	0.48
1:A:193:ILE:HG21	1:A:208:PRO:HG2	1.94	0.48
2:H:448:GLN:NE2	2:H:478:ASN:HA	2.28	0.48
2:J:353:GLN:HE22	2:J:468:ASP:HA	1.78	0.48
2:H:436:SER:OG	5:H:733:HOH:O	2.20	0.48
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.14	0.48
1:I:300:LYS:HG3	2:J:415:TRP:CE2	2.48	0.48
1:K:303:ASN:H	2:L:416:THR:HG22	1.77	0.48
2:B:448:GLN:NE2	2:B:478:ASN:HA	2.28	0.48
1:A:43:MET:CE	1:A:46:ARG:HG3	2.44	0.47
1:I:193:ILE:HG22	1:I:208:PRO:HD2	1.96	0.47
1:G:283:THR:HG22	1:G:285:LEU:H	1.79	0.47
1:E:172:MET:HG2	1:E:227:TRP:HB3	1.95	0.47
2:H:412:THR:O	2:H:416:THR:HG23	2.15	0.47
1:C:43:MET:CE	1:C:48:HIS:HB3	2.44	0.47
1:C:162:ARG:NH2	3:C:601:NAG:O6	2.47	0.47
2:L:402:ASN:OD1	5:L:701:HOH:O	2.20	0.47
1:G:34:GLU:HB2	1:G:283:THR:HG21	1.96	0.47
2:D:496:ILE:HD12	2:D:497:ASN:HB2	1.95	0.47
2:J:495:ASN:ND2	2:J:495:ASN:O	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:TYR:CD2	1:A:228:THR:HG21	2.49	0.47
1:C:43:MET:HE1	1:C:48:HIS:HB3	1.97	0.47
2:B:329:ILE:HD12	2:B:435:ASP:HA	1.97	0.47
2:L:342:ASP:HB3	2:L:359:ALA:HB2	1.97	0.47
2:J:349:HIS:HD2	2:J:476:ARG:HH12	1.62	0.47
1:I:285:LEU:O	2:J:381:LYS:NZ	2.48	0.47
1:A:302:VAL:HA	2:B:416:THR:HG22	1.97	0.47
1:I:193:ILE:HG21	1:I:208:PRO:HG2	1.96	0.47
1:I:75:ASP:OD2	1:I:76:THR:HG22	2.14	0.47
1:I:142:LEU:HD23	1:I:247:PRO:HA	1.97	0.46
2:B:377:ARG:NH1	5:B:774:HOH:O	2.39	0.46
1:G:165:ASP:OD1	1:G:166:THR:N	2.44	0.46
1:A:284:ARG:HB3	2:B:379:VAL:HG22	1.97	0.46
1:K:8:HIS:O	5:K:722:HOH:O	2.20	0.46
2:H:442:TYR:CE1	2:H:459:GLY:HA2	2.50	0.46
1:C:263:ASP:HB2	5:C:748:HOH:O	2.15	0.46
1:G:55:HIS:HE1	1:G:57:ILE:HD13	1.80	0.46
2:L:353:GLN:HE22	2:L:468:ASP:HB2	1.80	0.46
1:I:303:ASN:H	2:J:416:THR:CG2	2.27	0.46
2:H:377:ARG:O	2:H:380:GLU:HG2	2.16	0.46
1:E:284:ARG:HB3	2:F:379:VAL:HG22	1.98	0.46
1:I:43:MET:CE	1:I:48:HIS:HB3	2.46	0.46
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.49	0.46
1:K:244:LEU:HD13	1:K:246:ALA:HB2	1.97	0.46
1:A:223:ILE:HD13	1:A:245:ILE:HG13	1.97	0.46
2:F:377:ARG:HD2	5:F:722:HOH:O	2.16	0.45
1:E:55:HIS:CE1	1:E:57:ILE:HG12	2.52	0.45
2:B:450:ARG:HG3	2:B:451:GLN:H	1.81	0.45
2:D:329:ILE:HD12	2:D:435:ASP:HA	1.97	0.45
1:C:61:ILE:O	1:C:139:TYR:HB3	2.16	0.45
2:B:387:GLU:HB2	5:B:705:HOH:O	2.16	0.45
1:A:109:ASN:ND2	5:A:813:HOH:O	2.49	0.45
2:J:382:THR:OG1	2:J:382:THR:O	2.33	0.45
2:F:353:GLN:N	2:F:353:GLN:HE21	2.10	0.45
1:E:146:VAL:HG21	4:E:602:SIA:H111	1.97	0.45
1:I:34:GLU:OE2	1:I:35:SER:N	2.49	0.45
1:E:252:LYS:HE3	1:E:254:ILE:HD11	1.98	0.45
1:E:284:ARG:NH2	5:E:853:HOH:O	2.49	0.45
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.99	0.45
1:I:42:CYS:HB3	1:I:270:CYS:O	2.17	0.45
1:A:209:VAL:HG11	1:C:205:ASN:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:456:ASP:HB3	2:L:458:LYS:H	1.82	0.45
1:K:194:SER:HG	1:K:205:ASN:HD21	1.64	0.44
2:H:450:ARG:HG3	2:H:451:GLN:H	1.82	0.44
1:A:49:LYS:HD2	1:A:69:HIS:ND1	2.32	0.44
1:A:303:ASN:H	2:B:416:THR:HG21	1.83	0.44
1:K:302:VAL:HA	2:L:416:THR:HG22	2.00	0.44
1:A:46:ARG:HD3	5:A:708:HOH:O	2.17	0.44
2:J:349:HIS:NE2	2:J:356:GLY:HA3	2.32	0.44
2:B:418:GLN:HG2	2:F:417:TYR:CE1	2.53	0.44
1:G:43:MET:CE	1:G:46:ARG:HG3	2.48	0.44
2:D:451:GLN:HB2	5:D:768:HOH:O	2.18	0.44
1:G:185:ASN:HA	1:G:189:GLY:O	2.16	0.44
2:J:430:THR:OG1	5:J:706:HOH:O	2.21	0.44
1:G:162:ARG:HG3	1:G:235:ASN:OD1	2.16	0.44
2:H:408:LYS:HG2	2:L:406:TRP:CH2	2.52	0.44
1:A:142:LEU:HD23	1:A:247:PRO:HA	2.00	0.44
1:I:48:HIS:CE1	1:I:268:ASN:HD21	2.33	0.44
1:A:283:THR:HG22	1:A:285:LEU:H	1.83	0.44
2:J:342:ASP:HB3	2:J:359:ALA:HB2	2.00	0.43
2:D:406:TRP:CH2	2:F:408:LYS:HG2	2.53	0.43
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.17	0.43
1:A:121:ILE:HD11	1:A:157:THR:HG21	2.00	0.43
1:I:153:ASN:ND2	1:I:191:GLN:HB3	2.34	0.43
1:K:193:ILE:HG22	1:K:208:PRO:HD2	2.00	0.43
1:G:50:ASP:CG	1:G:80:ARG:HH21	2.22	0.43
1:E:307:LEU:HB3	2:F:423:VAL:HG21	2.00	0.43
1:K:300:LYS:HG3	2:L:415:TRP:CE2	2.53	0.43
1:I:43:MET:HE2	1:I:48:HIS:HB3	2.00	0.43
2:H:451:GLN:O	2:H:493:ARG:NH1	2.49	0.43
1:G:256:ARG:NE	5:G:733:HOH:O	2.51	0.43
2:H:497:ASN:N	2:H:497:ASN:OD1	2.52	0.43
1:G:40:ARG:NE	1:G:267:ASP:OD2	2.48	0.43
1:E:25:GLU:HG2	1:E:315:ASN:HB3	2.01	0.43
1:G:41:LEU:HD22	1:G:264:ALA:O	2.18	0.43
1:K:202:TYR:CD2	1:K:228:THR:HG21	2.54	0.43
1:C:148:LYS:HE3	1:C:148:LYS:HB2	1.86	0.43
1:G:300:LYS:HG3	2:H:415:TRP:CE2	2.54	0.43
1:G:43:MET:HE3	1:G:48:HIS:HB3	2.01	0.43
1:E:43:MET:O	1:E:46:ARG:HG2	2.19	0.43
1:K:142:LEU:HD23	1:K:247:PRO:HA	2.01	0.43
1:C:193:ILE:HG22	1:C:208:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:VAL:HG21	1:G:187:LEU:HD22	2.01	0.42
2:L:494:LEU:HB2	2:L:496:ILE:HG12	2.02	0.42
1:A:38:ILE:HG22	1:A:40:ARG:H	1.84	0.42
2:F:418:GLN:NE2	5:F:705:HOH:O	2.40	0.42
1:K:154:PHE:HB3	1:K:241:ASN:O	2.18	0.42
1:A:87:CYS:HB2	1:A:129:ALA:O	2.20	0.42
1:K:96:GLU:O	1:K:100:GLN:HG3	2.19	0.42
1:G:175:ILE:HD12	1:G:195:ILE:HD13	2.01	0.42
1:K:252:LYS:HE3	1:K:254:ILE:HD11	2.00	0.42
1:A:43:MET:HE1	1:A:46:ARG:HG3	2.01	0.42
2:L:468:ASP:CG	5:L:739:HOH:O	2.58	0.42
1:G:25:GLU:HG2	1:G:315:ASN:HB3	2.02	0.42
1:A:43:MET:HE2	1:A:48:HIS:HB3	2.02	0.42
1:K:75:ASP:OD2	1:K:76:THR:HG22	2.20	0.42
1:C:149:SER:O	1:C:152:GLN:HB2	2.20	0.42
1:A:148:LYS:HB2	1:A:148:LYS:HE3	1.87	0.42
2:H:462:GLU:CD	2:J:450:ARG:HH22	2.23	0.42
1:K:87:CYS:HB2	1:K:129:ALA:O	2.20	0.42
1:A:143:LYS:N	1:A:246:ALA:O	2.49	0.42
2:J:340:MET:SD	2:J:346:GLY:HA3	2.60	0.41
1:C:43:MET:CE	1:C:46:ARG:HG3	2.50	0.41
1:A:110:LYS:HB2	1:A:249:ARG:NH2	2.35	0.41
1:C:165:ASP:O	1:C:232:PRO:HB3	2.20	0.41
1:E:300:LYS:HG3	2:F:415:TRP:CE2	2.55	0.41
2:D:381:LYS:HG3	2:D:383:ASN:OD1	2.19	0.41
2:D:450:ARG:HG3	2:D:451:GLN:H	1.86	0.41
1:A:49:LYS:HB2	1:A:49:LYS:HE2	1.84	0.41
2:F:412:THR:O	2:F:416:THR:HG23	2.20	0.41
1:E:48:HIS:CD2	1:E:266:ILE:HD13	2.55	0.41
1:E:121:ILE:HD11	1:E:157:THR:HG21	2.02	0.41
1:I:61:ILE:O	1:I:139:TYR:HB3	2.20	0.41
1:A:90:GLY:HA3	1:A:223:ILE:O	2.20	0.41
1:I:47:LYS:HE2	1:I:47:LYS:HB3	1.53	0.41
1:E:165:ASP:OD1	1:E:166:THR:N	2.42	0.41
1:C:1:ASP:N	5:D:701:HOH:O	2.52	0.41
1:C:1:ASP:OD2	2:D:351:ASN:HA	2.21	0.41
1:C:303:ASN:HB2	2:D:416:THR:HG21	2.03	0.41
1:K:34:GLU:HG2	1:K:283:THR:OG1	2.21	0.41
2:H:491:LEU:HD13	2:H:497:ASN:HA	2.02	0.41
1:C:285:LEU:O	2:D:381:LYS:NZ	2.54	0.41
1:I:12:ASN:HA	5:I:774:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:383:ASN:HA	2:J:384:THR:CB	2.50	0.41
1:G:153:ASN:OD1	1:G:191:GLN:HG2	2.21	0.41
1:C:115:PHE:HA	5:C:752:HOH:O	2.20	0.41
2:L:446:ARG:HH12	2:L:447:LYS:HE3	1.85	0.41
1:E:46:ARG:HE	1:E:76:THR:HG21	1.85	0.41
1:G:55:HIS:CE1	1:G:57:ILE:HD13	2.55	0.40
1:G:43:MET:HE2	1:G:48:HIS:HB3	2.02	0.40
1:K:51:LEU:HA	1:K:51:LEU:HD23	1.91	0.40
1:K:44:LYS:O	1:K:271:GLU:HG3	2.22	0.40
2:J:477:ASN:ND2	5:J:737:HOH:O	2.30	0.40
1:C:300:LYS:HG3	2:D:415:TRP:CE2	2.57	0.40
1:C:297:GLN:HB3	2:D:383:ASN:HB2	2.04	0.40
1:E:153:ASN:HA	1:E:189:GLY:HA3	2.02	0.40
2:H:361:TYR:CZ	2:H:365:GLN:HG3	2.56	0.40
1:C:197:VAL:O	1:C:203:ARG:HA	2.22	0.40
1:E:5:LEU:HA	1:E:5:LEU:HD13	1.97	0.40
1:K:193:ILE:HG21	1:K:193:ILE:HD13	1.83	0.40
1:A:313:MET:HG3	1:A:314:ARG:O	2.21	0.40

All (1) 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)
1:C:149:SER:OG	2:H:497:ASN:OD1[1_456]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	C	316/318 (99%)	310 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	316/318 (99%)	308 (98%)	8 (2%)	0	100	100
1	G	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	I	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	K	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
2	B	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	30	43
2	D	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	30	43
2	F	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	30	43
2	H	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	30	43
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	30	43
2	L	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	30	43
All	All	2928/2952 (99%)	2835 (97%)	87 (3%)	6 (0%)	52	69

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%)	244 (91%)	25 (9%)	11	16
1	C	269/269 (100%)	249 (93%)	20 (7%)	17	26
1	E	269/269 (100%)	248 (92%)	21 (8%)	16	24
1	G	269/269 (100%)	248 (92%)	21 (8%)	16	24
1	I	269/269 (100%)	245 (91%)	24 (9%)	12	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	269/269 (100%)	245 (91%)	24 (9%)	12	18
2	B	148/148 (100%)	138 (93%)	10 (7%)	20	31
2	D	148/148 (100%)	142 (96%)	6 (4%)	37	57
2	F	148/148 (100%)	142 (96%)	6 (4%)	37	57
2	H	148/148 (100%)	140 (95%)	8 (5%)	27	43
2	J	148/148 (100%)	136 (92%)	12 (8%)	15	22
2	L	148/148 (100%)	140 (95%)	8 (5%)	27	43
All	All	2502/2502 (100%)	2317 (93%)	185 (7%)	17	26

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	35	SER
1	A	41	LEU
1	A	46	ARG
1	A	49	LYS
1	A	76	THR
1	A	77	LEU
1	A	94	ASN
1	A	111	ILE
1	A	112	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	192	SER
1	A	203	ARG
1	A	213	ARG
1	A	228	THR
1	A	244	LEU
1	A	258	LEU
1	A	276	TRP
1	A	277	ARG
1	A	283	THR
2	B	335	ASN
2	B	342	ASP
2	B	385	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	416	THR
2	B	418	GLN
2	B	425	MET
2	B	433	MET
2	B	436	SER
2	B	450	ARG
2	B	470	SER
1	C	8	HIS
1	C	14	THR
1	C	41	LEU
1	C	46	ARG
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	120	SER
1	C	126	THR
1	C	157	THR
1	C	170	LEU
1	C	203	ARG
1	C	228	THR
1	C	244	LEU
1	C	250	VAL
1	C	256	ARG
1	C	258	LEU
1	C	271	GLU
1	C	276	TRP
1	C	283	THR
2	D	325	LEU
2	D	341	VAL
2	D	383	ASN
2	D	384	THR
2	D	433	MET
2	D	450	ARG
1	E	8	HIS
1	E	14	THR
1	E	41	LEU
1	E	76	THR
1	E	77	LEU
1	E	111	ILE
1	E	126	THR
1	E	150	LYS
1	E	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	162	ARG
1	E	170	LEU
1	E	192	SER
1	E	196	SER
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	250	VAL
1	E	258	LEU
1	E	276	TRP
1	E	283	THR
2	F	353	GLN
2	F	411	ILE
2	F	416	THR
2	F	418	GLN
2	F	433	MET
2	F	450	ARG
1	G	8	HIS
1	G	14	THR
1	G	41	LEU
1	G	47	LYS
1	G	49	LYS
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	112	SER
1	G	120	SER
1	G	157	THR
1	G	162	ARG
1	G	170	LEU
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	379	VAL
2	H	385	GLU
2	H	416	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	433	MET
2	H	438	MET
2	H	477	ASN
2	H	479	THR
2	H	497	ASN
1	I	1	ASP
1	I	8	HIS
1	I	35	SER
1	I	39	ASN
1	I	41	LEU
1	I	47	LYS
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	126	THR
1	I	132	ARG
1	I	149	SER
1	I	157	THR
1	I	170	LEU
1	I	184	LYS
1	I	203	ARG
1	I	228	THR
1	I	244	LEU
1	I	250	VAL
1	I	258	LEU
1	I	263	ASP
1	I	276	TRP
1	I	277	ARG
1	I	283	THR
2	J	325	LEU
2	J	350	GLN
2	J	353	GLN
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	448	GLN
2	J	467	CYS
2	J	495	ASN
1	K	1	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	8	HIS
1	K	23	GLN
1	K	41	LEU
1	K	76	THR
1	K	77	LEU
1	K	101	LYS
1	K	111	ILE
1	K	146	VAL
1	K	150	LYS
1	K	157	THR
1	K	162	ARG
1	K	170	LEU
1	K	203	ARG
1	K	213	ARG
1	K	228	THR
1	K	244	LEU
1	K	250	VAL
1	K	258	LEU
1	K	263	ASP
1	K	276	TRP
1	K	277	ARG
1	K	283	THR
1	K	303	ASN
2	L	335	ASN
2	L	350	GLN
2	L	379	VAL
2	L	382	THR
2	L	411	ILE
2	L	433	MET
2	L	446	ARG
2	L	467	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	E	8	HIS
2	H	484	GLN
1	I	268	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	0.28	0	15,19,21	0.46	0
3	NAG	B	601	2	14,14,15	0.52	0	15,19,21	0.39	0
3	NAG	C	601	1	14,14,15	0.43	0	15,19,21	0.47	0
3	NAG	D	601	2	14,14,15	0.62	0	15,19,21	0.56	0
3	NAG	E	601	1	14,14,15	0.37	0	15,19,21	0.49	0
4	SIA	E	602	-	17,21,21	1.09	1 (5%)	19,31,31	1.00	1 (5%)
3	NAG	F	601	2	14,14,15	0.45	0	15,19,21	0.71	1 (6%)
3	NAG	G	601	1	14,14,15	0.19	0	15,19,21	0.41	0
3	NAG	H	601	2	14,14,15	0.32	0	15,19,21	0.34	0
3	NAG	I	601	1	14,14,15	0.36	0	15,19,21	0.42	0
3	NAG	J	601	2	14,14,15	0.44	0	15,19,21	0.47	0
3	NAG	K	601	1	14,14,15	0.21	0	15,19,21	0.35	0
3	NAG	L	601	2	14,14,15	0.36	0	15,19,21	0.50	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
4	SIA	E	602	-	-	0/14/38/38	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	SIA	O2-C2	4.10	1.44	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	SIA	C8-C7-C6	-2.44	108.11	113.01
3	F	601	NAG	C1-O5-C5	2.33	115.21	112.25

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	C	601	NAG	1	0
3	D	601	NAG	1	0
3	E	601	NAG	1	0
4	E	602	SIA	1	0
3	G	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, 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%)	-0.08	1 (0%) 94 94	21, 35, 57, 90	0
1	C	318/318 (100%)	0.02	9 (2%) 56 55	19, 37, 55, 90	0
1	E	318/318 (100%)	-0.02	3 (0%) 85 85	20, 33, 52, 97	0
1	G	318/318 (100%)	-0.08	1 (0%) 94 94	23, 38, 60, 89	0
1	I	318/318 (100%)	0.04	5 (1%) 74 74	17, 34, 58, 100	0
1	K	318/318 (100%)	0.02	6 (1%) 70 69	26, 39, 62, 105	0
2	B	174/174 (100%)	0.41	6 (3%) 49 49	22, 37, 61, 126	0
2	D	174/174 (100%)	0.34	5 (2%) 55 54	21, 37, 74, 130	0
2	F	174/174 (100%)	0.29	6 (3%) 49 49	18, 37, 61, 97	0
2	H	174/174 (100%)	0.72	11 (6%) 23 24	20, 53, 89, 177	0
2	J	174/174 (100%)	0.78	16 (9%) 11 11	22, 51, 88, 145	0
2	L	174/174 (100%)	0.58	13 (7%) 17 17	21, 49, 87, 146	0
All	All	2952/2952 (100%)	0.17	82 (2%) 56 55	17, 38, 70, 177	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	497	ASN	22.3
2	J	496	ILE	15.3
2	H	496	ILE	14.0
2	J	497	ASN	12.3
2	L	497	ASN	10.2
2	B	497	ASN	9.1
2	D	497	ASN	9.0
2	L	496	ILE	6.0
2	D	496	ILE	5.7
2	H	494	LEU	4.9
2	B	496	ILE	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	133	ASN	4.7
2	J	341	VAL	4.6
2	H	491	LEU	4.1
1	K	317	PRO	3.9
2	L	494	LEU	3.9
2	D	382	THR	3.7
2	L	383	ASN	3.6
1	C	11	ALA	3.5
2	H	495	ASN	3.4
2	H	352	ALA	3.4
2	J	479	THR	3.3
1	C	12	ASN	3.2
2	J	464	TYR	3.1
2	H	470	SER	3.1
1	C	149	SER	3.0
2	B	383	ASN	2.9
2	H	354	GLY	2.8
2	J	355	THR	2.8
2	J	354	GLY	2.8
2	L	324	GLY	2.8
2	J	348	ARG	2.7
2	F	325	LEU	2.7
2	L	491	LEU	2.7
2	J	491	LEU	2.6
1	C	10	VAL	2.6
1	C	256	ARG	2.6
1	K	269	ASN	2.6
2	J	357	GLN	2.5
2	B	326	PHE	2.5
2	J	350	GLN	2.5
2	H	471	CYS	2.5
1	K	11	ALA	2.5
1	I	149	SER	2.5
2	F	350	GLN	2.5
2	H	325	LEU	2.4
1	E	305	ARG	2.4
2	L	341	VAL	2.4
2	L	355	THR	2.4
2	J	352	ALA	2.4
1	C	317	PRO	2.4
1	E	318	GLU	2.4
2	J	340	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	356	GLY	2.4
1	I	12	ASN	2.3
2	L	475	ILE	2.3
2	F	383	ASN	2.3
2	B	491	LEU	2.3
2	L	325	LEU	2.3
2	J	324	GLY	2.3
2	L	479	THR	2.3
1	E	270	CYS	2.2
2	F	326	PHE	2.2
1	C	284	ARG	2.2
1	I	9	ALA	2.2
1	G	230	VAL	2.2
1	C	13	GLY	2.2
1	K	118	GLY	2.2
1	I	2	LYS	2.2
2	D	350	GLN	2.2
1	A	167	ALA	2.1
2	J	359	ALA	2.1
2	B	359	ALA	2.1
1	C	190	THR	2.1
1	K	36	THR	2.1
1	K	205	ASN	2.1
2	F	352	ALA	2.1
2	D	418	GLN	2.0
2	L	473	GLU	2.0
2	J	344	TRP	2.0
2	L	476	ARG	2.0
2	H	324	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SIA	E	602	21/21	0.61	0.40	10.79	73,92,103,105	0
3	NAG	H	601	14/15	0.93	0.19	1.92	32,50,53,54	0
3	NAG	F	601	14/15	0.93	0.18	1.67	33,41,50,52	0
3	NAG	C	601	14/15	0.86	0.17	1.04	50,56,64,71	0
3	NAG	I	601	14/15	0.84	0.18	0.75	39,58,63,69	0
3	NAG	G	601	14/15	0.90	0.15	0.54	69,82,86,88	0
3	NAG	K	601	14/15	0.90	0.16	0.49	51,60,67,68	0
3	NAG	E	601	14/15	0.92	0.12	-0.03	50,61,72,73	0
3	NAG	D	601	14/15	0.94	0.13	-0.05	30,41,48,51	0
3	NAG	B	601	14/15	0.90	0.13	-0.25	36,43,51,51	0
3	NAG	L	601	14/15	0.93	0.12	-0.57	32,47,54,57	0
3	NAG	A	601	14/15	0.93	0.12	-0.75	52,68,74,74	0
3	NAG	J	601	14/15	0.94	0.10	-1.55	30,38,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.