



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:11 am GMT

PDB ID : 4QY1  
Title : Structure of H10 from human-infecting H10N8 in complex with avian receptor  
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 : 2.59 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

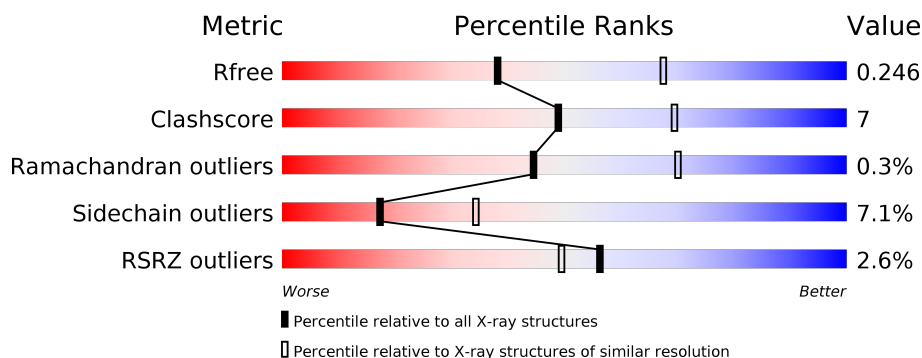
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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>20%</div> <div>.</div> </div>
1	C	318	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	E	318	<div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	G	318	<div> <div>%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	I	318	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	K	318	<div> <div>2%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	318	
1	O	318	
1	Q	318	
1	S	318	
1	U	318	
1	W	318	
2	B	174	
2	D	174	
2	F	174	
2	H	174	
2	J	174	
2	L	174	
2	N	174	
2	P	174	
2	R	174	
2	T	174	
2	V	174	
2	X	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
3	NAG	U	601	-	-	-	X
3	NAG	W	601	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48138 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			
1	M	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	O	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	Q	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	S	318	Total	C	N	O	S	0	0	0
			2436	1506	449	464	17			
1	U	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	W	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			

- Molecule 2 is a protein called hemagglutinin.

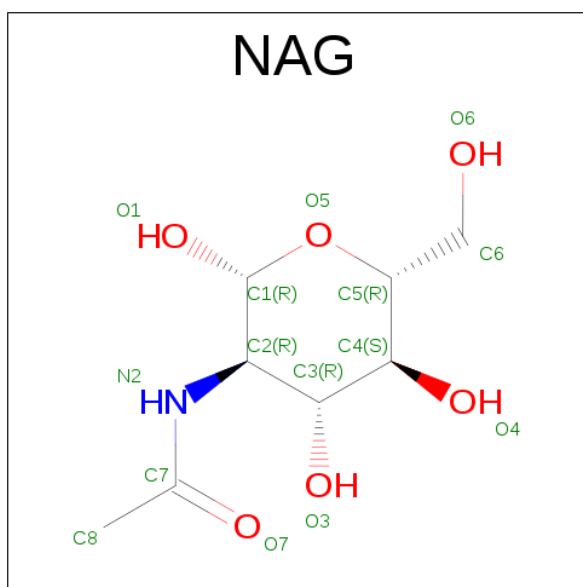
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	D	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
2	N	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	P	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	R	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	T	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	V	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	X	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		
3	O	1	Total	C	N	O	0	0
			14	8	1	5		
3	P	1	Total	C	N	O	0	0
			14	8	1	5		
3	Q	1	Total	C	N	O	0	0
			14	8	1	5		
3	R	1	Total	C	N	O	0	0
			14	8	1	5		
3	S	1	Total	C	N	O	0	0
			14	8	1	5		
3	T	1	Total	C	N	O	0	0
			14	8	1	5		
3	U	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			14	8	1	5		
3	W	1	Total	C	N	O	0	0
			14	8	1	5		
3	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	3	Total	C	N	O	0	0
			45	25	2	18		
5	G	3	Total	C	N	O	0	0
			45	25	2	18		
5	I	3	Total	C	N	O	0	0
			45	25	2	18		
5	U	3	Total	C	N	O	0	0
			45	25	2	18		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	70	Total	O	0	0
			70	70		
6	C	71	Total	O	0	0
			71	71		
6	D	87	Total	O	0	0
			87	87		
6	E	93	Total	O	0	0
			93	93		
6	F	64	Total	O	0	0
			64	64		
6	G	80	Total	O	0	0
			80	80		

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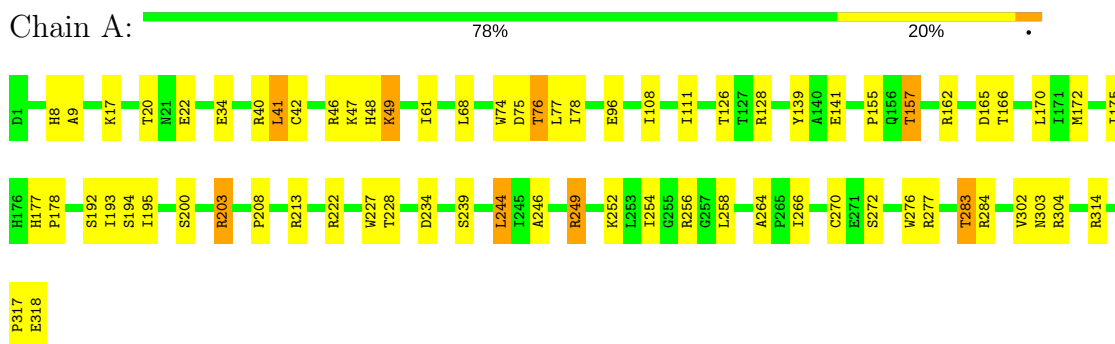
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	53	Total 53	O 53	0	0
6	I	102	Total 102	O 102	0	0
6	J	43	Total 43	O 43	0	0
6	K	93	Total 93	O 93	0	0
6	L	53	Total 53	O 53	0	0
6	M	27	Total 27	O 27	0	0
6	N	46	Total 46	O 46	0	0
6	O	40	Total 40	O 40	0	0
6	P	48	Total 48	O 48	0	0
6	Q	84	Total 84	O 84	0	0
6	R	42	Total 42	O 42	0	0
6	S	64	Total 64	O 64	0	0
6	T	49	Total 49	O 49	0	0
6	U	76	Total 76	O 76	0	0
6	V	44	Total 44	O 44	0	0
6	W	50	Total 50	O 50	0	0
6	X	28	Total 28	O 28	0	0



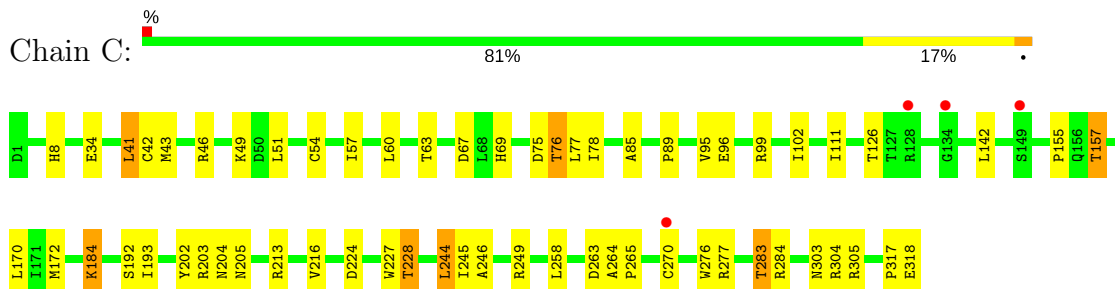
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

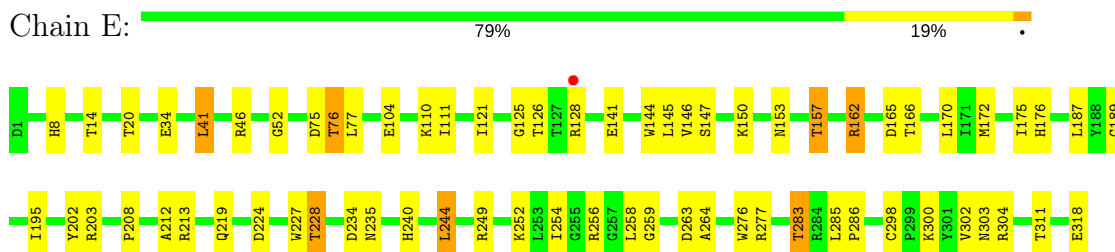
- Molecule 1: hemagglutinin



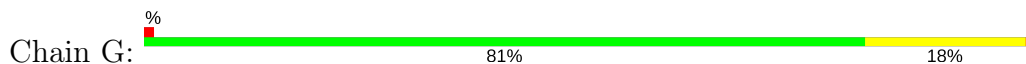
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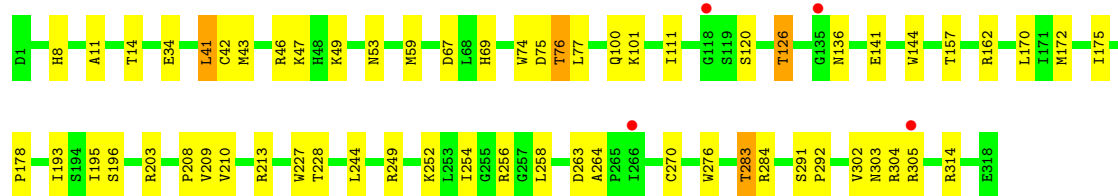


- Molecule 1: hemagglutinin

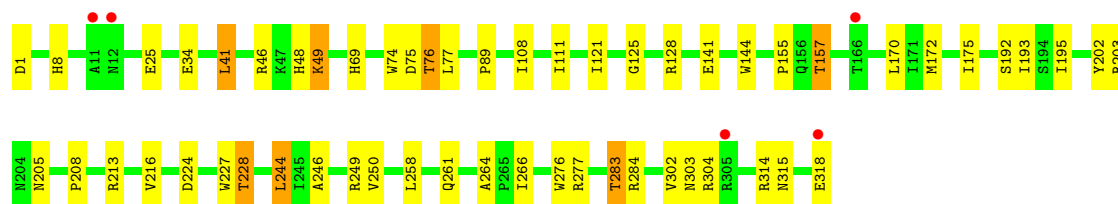
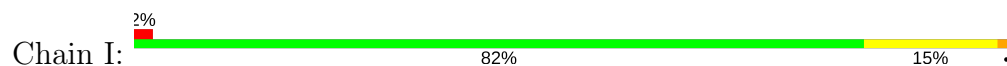


- Molecule 1: hemagglutinin

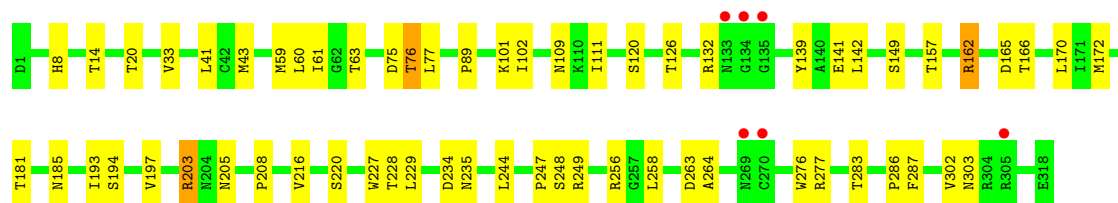
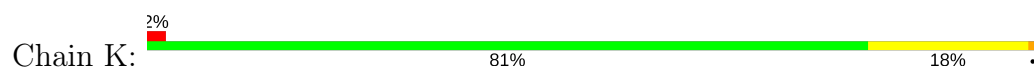




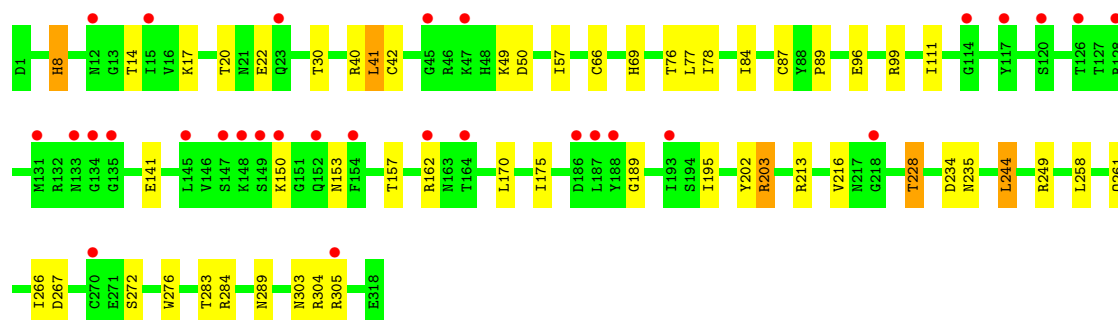
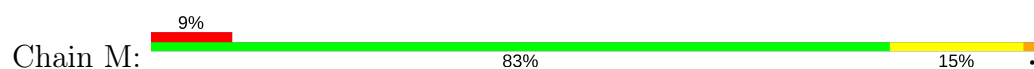
• Molecule 1: hemagglutinin



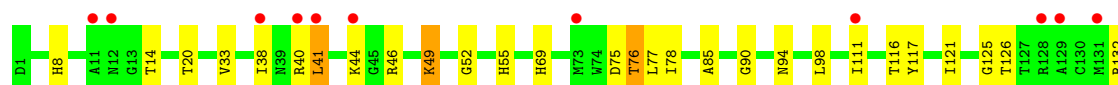
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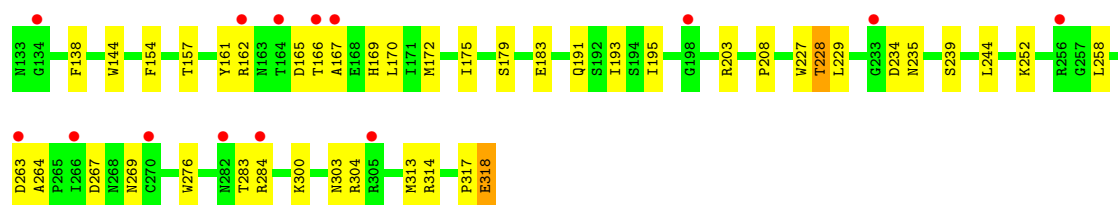


• Molecule 1: hemagglutinin

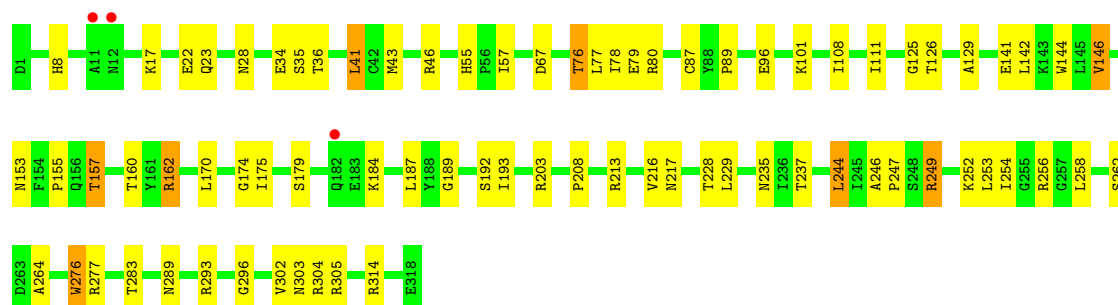
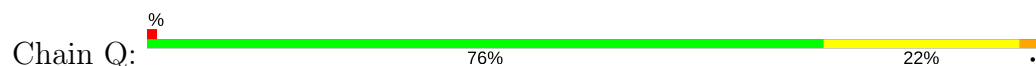


• Molecule 1: hemagglutinin

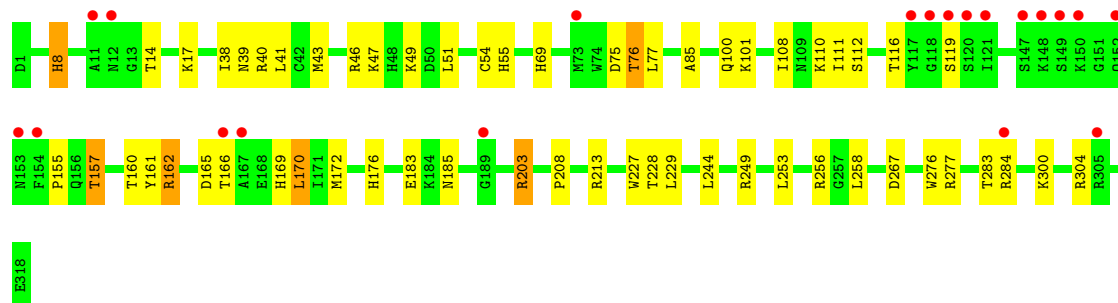
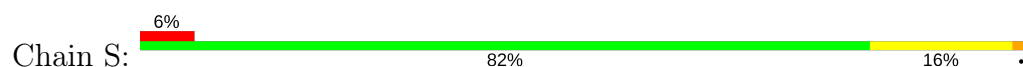




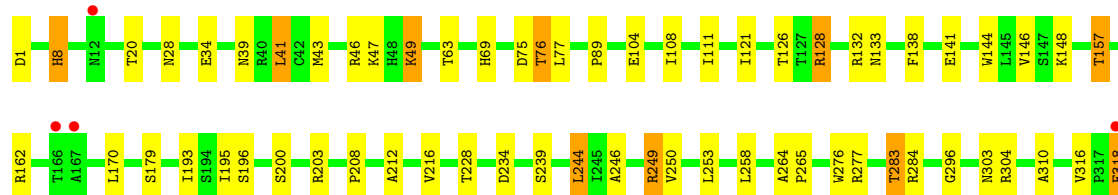
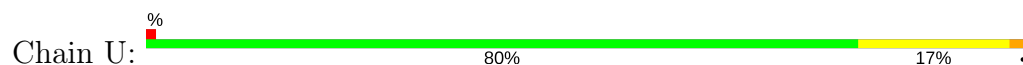
• Molecule 1: hemagglutinin



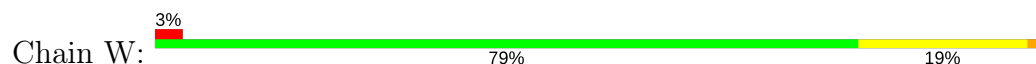
• Molecule 1: hemagglutinin

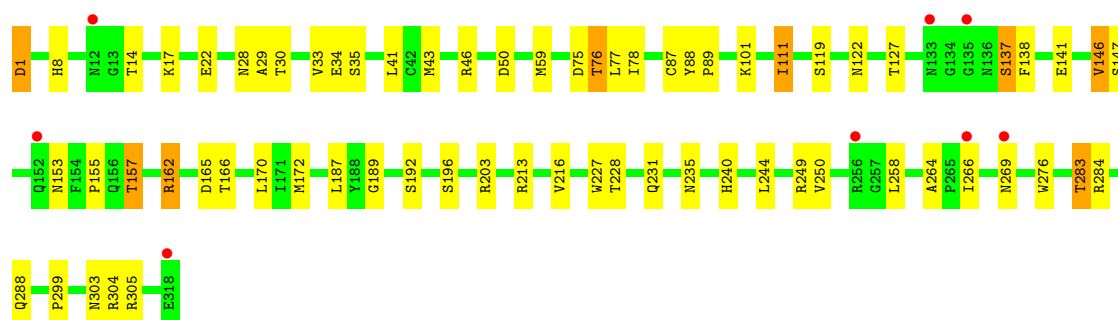


• Molecule 1: hemagglutinin

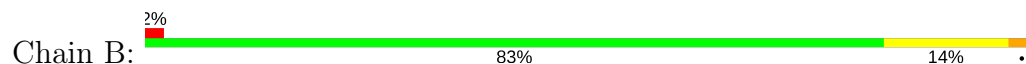


• Molecule 1: hemagglutinin

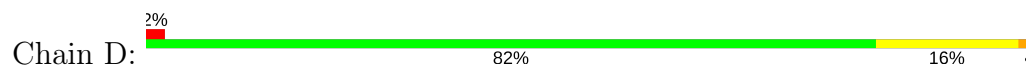




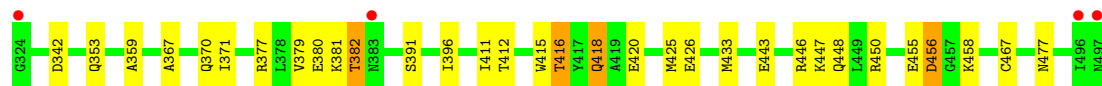
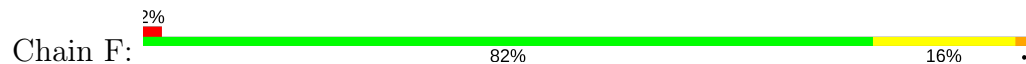
• Molecule 2: hemagglutinin



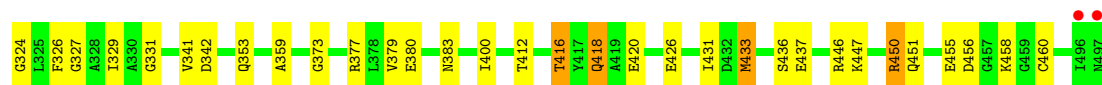
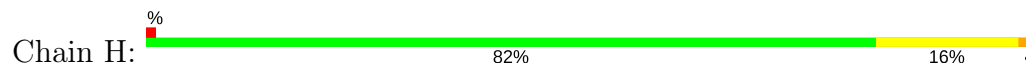
• Molecule 2: hemagglutinin



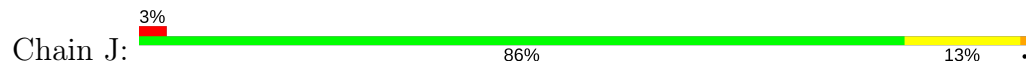
• Molecule 2: hemagglutinin



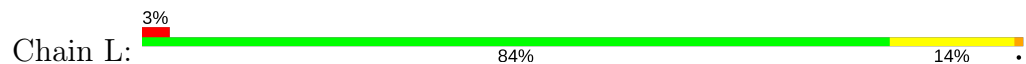
• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin

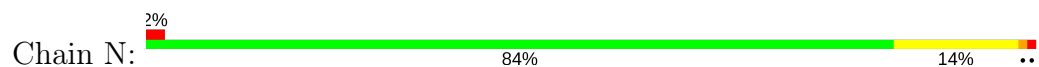


• Molecule 2: hemagglutinin

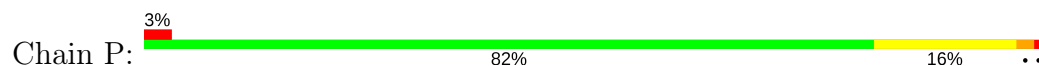




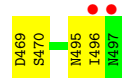
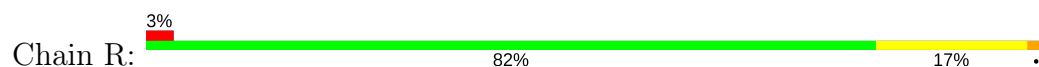
- Molecule 2: hemagglutinin



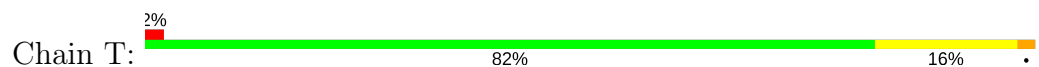
- Molecule 2: hemagglutinin



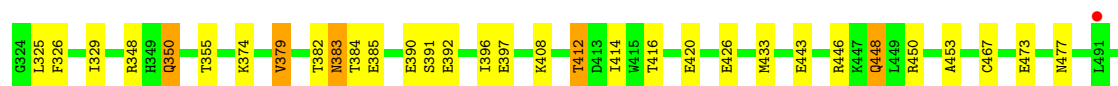
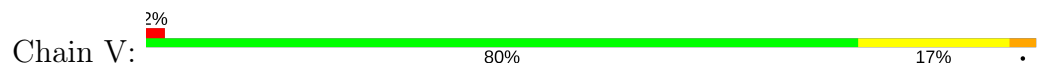
- Molecule 2: hemagglutinin



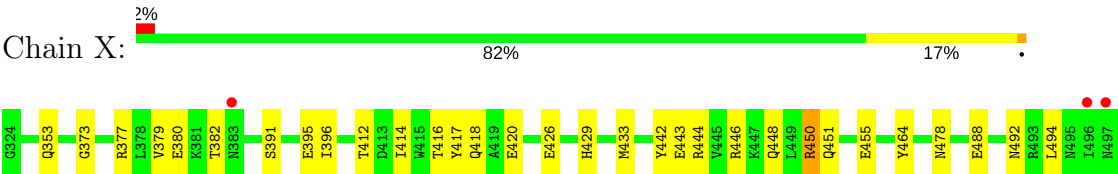
- Molecule 2: hemagglutinin



- Molecule 2: hemagglutinin



- Molecule 2: hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.26Å 111.44Å 222.35Å 94.96° 101.17° 91.90°	Depositor
Resolution (Å)	37.07 – 2.59 37.07 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.07-2.59) 86.9 (37.07-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.197 , 0.246 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	13242 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	48138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: SIA, GAL, 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	0.33	0/2486	0.50	0/3368
1	C	0.30	0/2486	0.48	0/3368
1	E	0.31	0/2486	0.49	0/3368
1	G	0.31	0/2486	0.48	0/3368
1	I	0.31	0/2486	0.49	0/3368
1	K	0.31	0/2486	0.49	0/3368
1	M	0.27	0/2486	0.45	0/3368
1	O	0.28	0/2486	0.46	0/3368
1	Q	0.31	0/2486	0.47	0/3368
1	S	0.29	0/2485	0.49	0/3366
1	U	0.30	0/2486	0.48	0/3368
1	W	0.29	0/2486	0.47	0/3368
2	B	0.33	0/1427	0.46	0/1926
2	D	0.34	0/1427	0.50	0/1926
2	F	0.34	0/1427	0.48	0/1926
2	H	0.33	0/1427	0.46	0/1926
2	J	0.31	0/1427	0.47	0/1926
2	L	0.32	0/1427	0.46	0/1926
2	N	0.31	0/1427	0.45	0/1926
2	P	0.33	0/1427	0.47	0/1926
2	R	0.31	0/1427	0.45	0/1926
2	T	0.32	0/1427	0.45	0/1926
2	V	0.31	0/1427	0.48	0/1926
2	X	0.30	0/1427	0.45	0/1926
All	All	0.31	0/46955	0.47	0/63526

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2389	41	0
1	C	2437	0	2389	31	0
1	E	2437	0	2387	40	0
1	G	2437	0	2389	36	0
1	I	2437	0	2389	34	0
1	K	2437	0	2389	27	0
1	M	2437	0	2389	26	0
1	O	2437	0	2389	39	0
1	Q	2437	0	2389	38	0
1	S	2436	0	2389	33	0
1	U	2437	0	2389	36	0
1	W	2437	0	2389	37	0
2	B	1402	0	1298	21	0
2	D	1402	0	1298	27	0
2	F	1402	0	1298	20	0
2	H	1402	0	1298	29	0
2	J	1402	0	1298	20	0
2	L	1402	0	1298	21	0
2	N	1402	0	1298	19	0
2	P	1402	0	1298	22	0
2	R	1402	0	1298	26	0
2	T	1402	0	1298	23	0
2	V	1402	0	1298	26	0
2	X	1402	0	1298	22	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	1	0
3	E	28	0	26	1	0
3	F	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	0	0
3	J	14	0	13	1	0
3	K	14	0	13	1	0
3	L	14	0	13	0	0
3	M	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	14	0	13	1	0
3	O	14	0	13	1	0
3	P	14	0	13	0	0
3	Q	14	0	13	0	0
3	R	14	0	13	0	0
3	S	14	0	13	0	0
3	T	14	0	13	1	0
3	U	14	0	13	1	0
3	V	14	0	13	0	0
3	W	14	0	13	0	0
3	X	14	0	13	0	0
4	E	28	0	25	1	0
5	E	45	0	38	4	0
5	G	45	0	38	4	0
5	I	45	0	38	3	0
5	U	45	0	38	4	0
6	A	106	0	0	8	0
6	B	70	0	0	2	0
6	C	71	0	0	5	0
6	D	87	0	0	9	0
6	E	93	0	0	11	0
6	F	64	0	0	3	0
6	G	80	0	0	11	0
6	H	53	0	0	6	0
6	I	102	0	0	8	0
6	J	43	0	0	8	0
6	K	93	0	0	3	0
6	L	53	0	0	3	0
6	M	27	0	0	5	0
6	N	46	0	0	4	0
6	O	40	0	0	5	0
6	P	48	0	0	6	0
6	Q	84	0	0	5	0
6	R	42	0	0	8	0
6	S	64	0	0	7	0
6	T	49	0	0	3	0
6	U	76	0	0	7	0
6	V	44	0	0	9	0
6	W	50	0	0	11	0
6	X	28	0	0	4	0
All	All	48138	0	44744	619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (619) 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:409:ASP:OD2	6:L:738:HOH:O	1.81	0.98
1:A:96:GLU:OE1	6:A:712:HOH:O	1.86	0.92
2:R:444:ARG:O	6:R:723:HOH:O	1.89	0.89
2:V:390:GLU:OE2	6:V:709:HOH:O	1.90	0.89
1:G:11:ALA:O	6:G:712:HOH:O	1.91	0.88
2:B:383:ASN:ND2	6:B:757:HOH:O	2.05	0.88
2:N:324:GLY:N	6:N:733:HOH:O	2.04	0.88
1:G:67:ASP:OD1	6:G:743:HOH:O	1.91	0.87
1:A:318:GLU:OE1	6:A:759:HOH:O	1.91	0.87
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.09	0.86
1:I:202:TYR:OH	6:I:724:HOH:O	1.92	0.85
2:H:437:GLU:OE1	6:H:752:HOH:O	1.94	0.85
1:W:1:ASP:N	6:W:713:HOH:O	2.08	0.84
1:C:67:ASP:O	6:C:726:HOH:O	1.94	0.84
1:U:318:GLU:HA	6:U:736:HOH:O	1.76	0.84
2:X:391:SER:H	2:X:396:ILE:HD11	1.44	0.83
1:Q:179:SER:OG	6:Q:740:HOH:O	1.99	0.81
2:H:353:GLN:OE1	6:H:745:HOH:O	1.98	0.81
1:W:231:GLN:OE1	6:W:725:HOH:O	1.98	0.81
2:B:444:ARG:O	6:B:727:HOH:O	1.98	0.80
2:N:446:ARG:O	6:N:704:HOH:O	2.00	0.80
1:G:305:ARG:O	6:G:706:HOH:O	1.99	0.80
2:V:448:GLN:OE1	6:V:707:HOH:O	2.01	0.79
1:A:194:SER:OG	6:A:792:HOH:O	2.00	0.78
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.17	0.78
1:G:42:CYS:O	6:G:705:HOH:O	2.00	0.78
1:M:261:GLN:O	6:M:719:HOH:O	2.01	0.78
1:S:100:GLN:OE1	6:S:742:HOH:O	2.01	0.77
2:X:464:TYR:OH	6:X:711:HOH:O	2.03	0.77
1:W:240:HIS:ND1	6:W:709:HOH:O	2.16	0.77
1:E:104:GLU:OE2	6:E:725:HOH:O	2.04	0.76
2:X:442:TYR:OH	6:X:710:HOH:O	2.01	0.76
1:E:147:SER:O	6:E:712:HOH:O	2.02	0.75
2:V:391:SER:H	2:V:396:ILE:HD11	1.52	0.75
2:H:377:ARG:NH2	2:H:426:GLU:OE2	2.21	0.74
1:Q:160:THR:HG1	1:Q:237:THR:HG1	1.33	0.74
1:S:183:GLU:OE2	6:S:741:HOH:O	2.06	0.74
2:B:443:GLU:OE2	2:B:446:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:17:LYS:HE3	1:Q:22:GLU:HG3	1.69	0.74
1:Q:67:ASP:O	6:Q:713:HOH:O	2.05	0.74
2:R:437:GLU:OE1	6:R:719:HOH:O	2.06	0.74
1:S:203:ARG:NH1	6:S:750:HOH:O	2.20	0.74
1:G:252:LYS:HE3	1:G:254:ILE:HD11	1.69	0.73
1:I:41:LEU:HD13	1:I:264:ALA:HB3	1.71	0.73
1:I:314:ARG:NH1	6:I:753:HOH:O	2.21	0.73
2:J:397:GLU:OE2	6:J:738:HOH:O	2.06	0.72
1:I:304:ARG:NH1	2:J:420:GLU:OE1	2.22	0.72
1:E:252:LYS:HE3	1:E:254:ILE:HD11	1.72	0.71
1:M:84:ILE:O	6:M:721:HOH:O	2.07	0.71
2:V:374:LYS:NZ	2:V:426:GLU:OE1	2.20	0.71
3:N:601:NAG:O7	6:N:731:HOH:O	2.08	0.71
1:E:104:GLU:OE1	6:E:770:HOH:O	2.08	0.70
3:J:601:NAG:O7	6:J:726:HOH:O	2.08	0.70
1:O:121:ILE:HD11	1:O:157:THR:HG21	1.73	0.70
2:D:448:GLN:O	6:D:758:HOH:O	2.10	0.70
1:I:318:GLU:O	6:I:715:HOH:O	2.10	0.70
1:W:305:ARG:NH2	6:W:724:HOH:O	2.24	0.70
1:G:100:GLN:OE1	6:G:720:HOH:O	2.10	0.70
2:F:370:GLN:OE1	6:F:754:HOH:O	2.09	0.69
1:G:46:ARG:HE	1:G:76:THR:HG21	1.55	0.69
2:P:324:GLY:N	6:P:737:HOH:O	2.24	0.69
1:G:53:ASN:OD1	6:G:742:HOH:O	2.11	0.69
1:O:284:ARG:HB3	2:P:379:VAL:HG13	1.75	0.69
2:V:443:GLU:OE1	2:V:446:ARG:NH1	2.25	0.69
2:V:397:GLU:OE2	6:V:705:HOH:O	2.10	0.68
2:B:391:SER:H	2:B:396:ILE:HD11	1.57	0.68
5:U:602:SIA:O10	5:U:602:SIA:O7	2.05	0.68
1:C:305:ARG:O	6:C:703:HOH:O	2.11	0.68
1:M:153:ASN:HA	1:M:189:GLY:HA3	1.75	0.68
1:G:314:ARG:NH1	6:G:756:HOH:O	2.27	0.68
1:S:40:ARG:HD2	1:S:267:ASP:HB2	1.76	0.68
1:S:304:ARG:NH1	2:T:420:GLU:OE1	2.27	0.68
1:S:46:ARG:HE	1:S:76:THR:HG21	1.59	0.68
2:X:443:GLU:OE2	2:X:446:ARG:NH1	2.26	0.68
1:W:137:SER:O	6:W:733:HOH:O	2.13	0.67
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.27	0.67
1:S:185:ASN:OD1	6:S:709:HOH:O	2.13	0.67
1:G:256:ARG:O	6:G:723:HOH:O	2.12	0.67
2:N:377:ARG:NH2	2:N:426:GLU:OE2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:601:NAG:O7	6:E:770:HOH:O	2.13	0.66
1:W:33:VAL:O	6:W:740:HOH:O	2.12	0.66
1:E:298:CYS:O	6:E:722:HOH:O	2.12	0.66
2:N:443:GLU:OE2	2:N:446:ARG:NH1	2.28	0.66
2:X:377:ARG:NH2	2:X:426:GLU:OE2	2.27	0.66
1:E:286:PRO:O	6:E:767:HOH:O	2.12	0.66
2:V:392:GLU:OE1	6:V:701:HOH:O	2.14	0.66
1:E:212:ALA:O	6:E:721:HOH:O	2.13	0.65
2:P:350:GLN:HG2	2:P:355:THR:HG22	1.76	0.65
1:E:110:LYS:NZ	1:E:141:GLU:OE2	2.26	0.65
1:C:224:ASP:OD1	6:C:729:HOH:O	2.11	0.65
1:K:193:ILE:HG22	1:K:208:PRO:HD2	1.77	0.65
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.29	0.65
1:M:195:ILE:HG12	1:M:244:LEU:HB2	1.78	0.65
2:N:391:SER:H	2:N:396:ILE:HD11	1.62	0.65
1:I:261:GLN:O	6:I:770:HOH:O	2.14	0.65
2:T:350:GLN:HG3	2:T:355:THR:HG22	1.79	0.65
1:U:212:ALA:O	6:U:728:HOH:O	2.14	0.65
2:D:338:GLU:OE2	6:D:779:HOH:O	2.14	0.65
2:B:450:ARG:HG3	2:B:451:GLN:H	1.62	0.64
2:J:394:SER:OG	6:J:740:HOH:O	2.09	0.64
2:V:412:THR:O	2:V:416:THR:HG23	1.96	0.64
2:R:431:ILE:O	6:R:714:HOH:O	2.15	0.64
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.31	0.64
1:M:66:CYS:SG	6:M:721:HOH:O	2.55	0.64
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.64
2:V:348:ARG:NH1	6:V:735:HOH:O	2.29	0.64
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.31	0.64
1:A:252:LYS:HE3	1:A:254:ILE:HD11	1.80	0.63
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.80	0.63
2:V:494:LEU:HB3	2:V:496:ILE:HG12	1.78	0.63
2:N:470:SER:O	6:N:722:HOH:O	2.16	0.63
1:Q:96:GLU:OE1	6:Q:742:HOH:O	2.15	0.63
2:B:381:LYS:NZ	2:B:382:THR:O	2.32	0.63
2:D:420:GLU:HG3	6:D:728:HOH:O	1.99	0.63
1:I:1:ASP:N	6:I:729:HOH:O	2.32	0.63
1:W:101:LYS:O	6:W:735:HOH:O	2.15	0.63
1:U:41:LEU:HD13	1:U:264:ALA:HB3	1.80	0.62
1:E:283:THR:HG22	1:E:285:LEU:H	1.64	0.62
2:R:377:ARG:NH2	2:R:426:GLU:OE2	2.33	0.62
1:G:196:SER:OG	6:G:745:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:412:THR:O	2:J:416:THR:HG23	2.00	0.62
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.32	0.62
2:D:412:THR:O	2:D:416:THR:HG23	2.01	0.61
2:F:412:THR:O	2:F:416:THR:HG23	2.01	0.61
1:U:28:ASN:ND2	6:U:761:HOH:O	2.32	0.61
2:H:418:GLN:HG2	2:L:417:TYR:CE1	2.36	0.61
1:O:125:GLY:HA3	1:O:144:TRP:HB3	1.83	0.61
2:D:408:LYS:NZ	6:D:716:HOH:O	2.04	0.61
2:F:418:GLN:NE2	6:F:734:HOH:O	2.25	0.61
2:P:443:GLU:OE1	2:P:446:ARG:NH1	2.33	0.60
1:A:41:LEU:HD23	1:A:78:ILE:HD13	1.82	0.60
2:R:452:ASN:OD1	6:R:707:HOH:O	2.16	0.60
1:E:34:GLU:HB2	1:E:283:THR:HG21	1.84	0.60
2:J:387:GLU:HB2	6:J:728:HOH:O	2.01	0.60
1:U:304:ARG:NH1	2:V:420:GLU:OE1	2.34	0.60
1:O:117:TYR:HB3	1:O:121:ILE:HD12	1.84	0.60
1:A:46:ARG:HE	1:A:76:THR:HG21	1.66	0.60
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.34	0.60
1:C:41:LEU:HD23	1:C:78:ILE:HD13	1.82	0.60
1:U:8:HIS:HD2	6:V:731:HOH:O	1.84	0.60
1:O:304:ARG:NH1	2:P:420:GLU:OE1	2.34	0.59
1:S:256:ARG:NH2	2:T:387:GLU:OE1	2.36	0.59
1:A:172:MET:HG2	1:A:227:TRP:HB3	1.84	0.59
2:R:469:ASP:OD1	6:R:718:HOH:O	2.17	0.59
2:N:455:GLU:OE1	2:P:446:ARG:NH2	2.36	0.59
1:Q:41:LEU:HD13	1:Q:264:ALA:HB3	1.85	0.59
1:O:55:HIS:HB3	1:O:85:ALA:HB2	1.84	0.59
2:N:412:THR:O	2:N:416:THR:HG23	2.03	0.59
2:T:412:THR:O	2:T:416:THR:HG22	2.02	0.59
2:J:349:HIS:HE1	6:J:729:HOH:O	1.85	0.58
1:S:165:ASP:OD1	1:S:166:THR:N	2.36	0.58
1:M:303:ASN:H	2:N:416:THR:HG22	1.69	0.58
1:C:96:GLU:OE2	1:C:99:ARG:NH2	2.35	0.58
1:K:234:ASP:HA	3:K:601:NAG:H82	1.84	0.58
1:M:303:ASN:H	2:N:416:THR:CG2	2.17	0.58
1:M:304:ARG:NH2	6:M:702:HOH:O	2.37	0.58
2:R:412:THR:O	2:R:416:THR:HG23	2.04	0.58
1:U:303:ASN:H	2:V:416:THR:CG2	2.16	0.58
1:O:161:TYR:HH	1:O:169:HIS:HD1	1.52	0.58
1:W:304:ARG:NH1	2:X:420:GLU:OE1	2.37	0.58
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.03	0.57
1:S:8:HIS:HE1	6:S:701:HOH:O	1.87	0.57
1:C:304:ARG:NH1	2:D:420:GLU:OE1	2.37	0.57
2:F:377:ARG:NH2	2:F:426:GLU:OE2	2.36	0.57
1:M:304:ARG:NH1	2:N:420:GLU:OE1	2.31	0.57
1:A:141:GLU:OE1	1:A:249:ARG:HD3	2.04	0.57
2:R:353:GLN:H	2:R:353:GLN:HE21	1.52	0.57
1:W:28:ASN:ND2	6:W:708:HOH:O	2.22	0.57
2:L:456:ASP:HB3	2:L:458:LYS:H	1.70	0.57
2:D:383:ASN:OD1	2:D:383:ASN:N	2.38	0.57
1:C:303:ASN:H	2:D:416:THR:CG2	2.18	0.57
2:L:482:HIS:ND1	6:L:716:HOH:O	2.13	0.57
1:O:38:ILE:HG22	1:O:40:ARG:H	1.70	0.57
1:C:318:GLU:OE1	6:C:728:HOH:O	2.16	0.56
1:M:50:ASP:HB2	1:M:266:ILE:HD11	1.86	0.56
2:H:456:ASP:HB3	2:H:458:LYS:H	1.69	0.56
1:O:154:PHE:O	1:O:191:GLN:NE2	2.38	0.56
1:O:46:ARG:NH2	6:O:733:HOH:O	2.38	0.56
1:W:34:GLU:HB2	1:W:283:THR:HG21	1.87	0.56
1:O:41:LEU:HD23	1:O:78:ILE:HD13	1.87	0.56
2:X:412:THR:O	2:X:416:THR:HG23	2.06	0.56
2:B:412:THR:O	2:B:416:THR:HG23	2.05	0.56
2:D:455:GLU:OE1	2:F:446:ARG:NH2	2.38	0.56
1:Q:256:ARG:NH2	2:R:387:GLU:OE1	2.39	0.56
1:K:33:VAL:O	6:K:709:HOH:O	2.18	0.56
1:G:144:TRP:CH2	5:G:602:SIA:H91	2.41	0.56
1:I:49:LYS:NZ	6:I:732:HOH:O	2.38	0.55
1:E:259:GLY:O	6:E:745:HOH:O	2.18	0.55
2:J:399:GLN:OE1	6:J:732:HOH:O	2.17	0.55
1:O:165:ASP:OD1	1:O:166:THR:N	2.36	0.55
2:D:377:ARG:NH1	6:D:738:HOH:O	2.39	0.55
2:P:383:ASN:HA	2:P:384:THR:HB	1.88	0.55
2:D:387:GLU:HB2	6:D:706:HOH:O	2.05	0.55
2:P:374:LYS:NZ	2:P:426:GLU:OE1	2.39	0.55
1:U:303:ASN:H	2:V:416:THR:HG22	1.72	0.55
2:D:324:GLY:N	6:D:709:HOH:O	2.40	0.55
1:S:119:SER:N	6:S:720:HOH:O	2.40	0.55
1:A:41:LEU:HD13	1:A:264:ALA:HB3	1.87	0.55
2:D:381:LYS:HG3	2:D:383:ASN:OD1	2.07	0.55
2:D:448:GLN:OE1	6:D:739:HOH:O	2.18	0.55
2:H:450:ARG:HG3	2:H:451:GLN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:455:GLU:O	6:H:705:HOH:O	2.17	0.55
2:V:414:ILE:HD13	2:X:414:ILE:HG21	1.89	0.55
1:I:244:LEU:HD13	1:I:246:ALA:HB2	1.89	0.55
2:X:488:GLU:O	2:X:492:ASN:ND2	2.40	0.55
1:O:162:ARG:NH2	3:O:601:NAG:O6	2.40	0.54
2:P:412:THR:O	2:P:416:THR:HG23	2.05	0.54
1:I:284:ARG:HB3	2:J:379:VAL:HG22	1.89	0.54
1:O:132:ARG:NH1	1:O:138:PHE:O	2.39	0.54
2:P:496:ILE:HD12	2:P:497:ASN:HB2	1.89	0.54
2:T:377:ARG:NH2	2:T:426:GLU:OE2	2.41	0.54
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.40	0.54
1:I:89:PRO:HB3	1:I:216:VAL:HB	1.89	0.54
1:O:161:TYR:OH	1:O:169:HIS:ND1	2.37	0.54
2:J:473:GLU:O	2:J:477:ASN:HB2	2.08	0.54
1:Q:193:ILE:HG22	1:Q:208:PRO:HD2	1.87	0.54
2:R:450:ARG:HG3	2:R:451:GLN:H	1.73	0.54
1:U:89:PRO:HB3	1:U:216:VAL:HB	1.89	0.54
1:A:47:LYS:NZ	6:A:804:HOH:O	2.41	0.54
1:S:161:TYR:OH	1:S:169:HIS:ND1	2.41	0.54
1:U:162:ARG:NH2	3:U:601:NAG:O6	2.41	0.54
1:A:74:TRP:HH2	1:A:108:ILE:HG13	1.73	0.54
1:A:155:PRO:O	1:A:157:THR:HG22	2.08	0.54
1:Q:41:LEU:HD23	1:Q:78:ILE:HD13	1.90	0.54
2:V:329:ILE:O	6:V:714:HOH:O	2.17	0.54
1:A:284:ARG:HB3	2:B:379:VAL:HG22	1.91	0.53
1:E:121:ILE:HD11	1:E:157:THR:HG21	1.90	0.53
1:E:165:ASP:OD1	1:E:166:THR:N	2.37	0.53
1:Q:79:GLU:OE2	6:Q:730:HOH:O	2.17	0.53
1:U:193:ILE:HG22	1:U:208:PRO:HD2	1.90	0.53
1:M:141:GLU:OE1	1:M:249:ARG:HD3	2.08	0.53
1:I:202:TYR:CD2	1:I:228:THR:HG21	2.43	0.53
1:I:303:ASN:H	2:J:416:THR:HG21	1.73	0.53
1:C:204:ASN:OD1	1:C:205:ASN:N	2.38	0.53
1:E:302:VAL:HA	2:F:416:THR:HG22	1.91	0.53
1:K:303:ASN:H	2:L:416:THR:HG22	1.73	0.53
1:O:90:GLY:O	6:O:709:HOH:O	2.18	0.53
1:U:195:ILE:HG12	1:U:244:LEU:HB2	1.91	0.53
2:J:420:GLU:HG3	6:J:720:HOH:O	2.08	0.53
2:J:494:LEU:HD22	2:L:494:LEU:HD11	1.90	0.53
1:U:49:LYS:HD2	1:U:69:HIS:ND1	2.24	0.53
1:O:52:GLY:O	6:O:712:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:473:GLU:O	2:V:477:ASN:HB2	2.09	0.53
1:C:49:LYS:HD2	1:C:69:HIS:ND1	2.25	0.52
1:S:161:TYR:HH	1:S:169:HIS:HD1	1.58	0.52
1:U:20:THR:O	2:X:373:GLY:HA3	2.09	0.52
1:C:75:ASP:OD2	1:C:76:THR:HG22	2.09	0.52
1:E:234:ASP:HA	3:E:601:NAG:H82	1.92	0.52
1:S:38:ILE:O	1:S:40:ARG:N	2.43	0.52
2:T:324:GLY:N	6:T:701:HOH:O	2.42	0.52
1:W:41:LEU:HD13	1:W:264:ALA:HB3	1.92	0.52
1:S:49:LYS:HD2	1:S:69:HIS:ND1	2.25	0.52
1:C:249:ARG:O	6:C:757:HOH:O	2.19	0.52
1:O:20:THR:HG22	2:R:374:LYS:HG3	1.92	0.52
5:I:602:SIA:O10	5:I:602:SIA:O7	2.17	0.51
1:W:111:ILE:HG23	1:W:250:VAL:HG12	1.91	0.51
1:W:141:GLU:OE1	1:W:249:ARG:HD3	2.10	0.51
2:F:443:GLU:OE2	2:F:446:ARG:NH1	2.44	0.51
1:I:25:GLU:HG2	1:I:315:ASN:HB3	1.91	0.51
1:O:317:PRO:O	1:O:318:GLU:HB2	2.10	0.51
1:C:303:ASN:H	2:D:416:THR:HG22	1.75	0.51
1:Q:87:CYS:O	1:Q:217:ASN:ND2	2.38	0.51
1:C:184:LYS:HE3	1:C:193:ILE:HD11	1.93	0.51
1:G:49:LYS:HD2	1:G:69:HIS:ND1	2.26	0.51
1:E:128:ARG:HG2	5:E:605:SIA:O1A	2.10	0.51
1:G:144:TRP:HH2	5:G:602:SIA:H91	1.76	0.51
2:N:381:LYS:NZ	2:N:382:THR:O	2.44	0.51
1:K:75:ASP:OD2	1:K:76:THR:HG22	2.11	0.50
2:N:450:ARG:HB3	6:R:704:HOH:O	2.11	0.50
2:R:329:ILE:O	6:R:701:HOH:O	2.19	0.50
2:V:355:THR:O	6:V:722:HOH:O	2.19	0.50
1:I:46:ARG:NH2	6:I:739:HOH:O	2.45	0.50
1:M:41:LEU:HD23	1:M:78:ILE:HD13	1.94	0.50
2:X:377:ARG:NH1	6:X:707:HOH:O	2.41	0.50
1:G:178:PRO:HB2	1:G:210:VAL:HG22	1.94	0.50
1:G:144:TRP:CH2	5:G:602:SIA:H7	2.46	0.50
1:K:303:ASN:H	2:L:416:THR:CG2	2.24	0.50
1:M:89:PRO:HB3	1:M:216:VAL:HB	1.92	0.50
1:Q:244:LEU:HD13	1:Q:246:ALA:HB2	1.92	0.50
1:W:46:ARG:NH2	6:W:739:HOH:O	2.44	0.50
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.93	0.50
1:A:203:ARG:NH2	1:E:224:ASP:OD2	2.43	0.50
2:H:446:ARG:HH12	2:H:447:LYS:HE3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:602:SIA:O1B	5:I:602:SIA:H6	2.12	0.50
2:R:391:SER:H	2:R:396:ILE:HD11	1.76	0.50
1:I:224:ASP:HB2	6:I:718:HOH:O	2.11	0.50
1:U:284:ARG:HB3	2:V:379:VAL:HG22	1.94	0.50
1:U:200:SER:OG	1:U:234:ASP:OD1	2.25	0.50
1:W:75:ASP:OD2	1:W:76:THR:HG22	2.12	0.50
1:W:284:ARG:HB3	2:X:379:VAL:HG22	1.94	0.49
1:W:138:PHE:HA	6:W:733:HOH:O	2.12	0.49
2:D:418:GLN:HB3	6:D:764:HOH:O	2.12	0.49
2:R:342:ASP:N	2:R:342:ASP:OD1	2.44	0.49
1:A:303:ASN:H	2:B:416:THR:CG2	2.26	0.49
2:L:451:GLN:O	2:L:493:ARG:NH1	2.40	0.49
2:T:325:LEU:HD13	2:V:326:PHE:HZ	1.78	0.49
1:O:303:ASN:H	2:P:416:THR:CG2	2.26	0.49
2:H:324:GLY:N	6:H:701:HOH:O	2.46	0.49
2:V:494:LEU:HD22	2:X:494:LEU:HD11	1.95	0.49
1:K:126:THR:HG23	6:K:712:HOH:O	2.11	0.49
1:W:88:TYR:HD1	1:W:127:THR:HG21	1.78	0.49
1:K:89:PRO:HB3	1:K:216:VAL:HB	1.93	0.49
2:T:377:ARG:NH1	6:T:730:HOH:O	2.32	0.49
2:T:383:ASN:ND2	2:T:383:ASN:O	2.45	0.49
1:I:46:ARG:HE	1:I:76:THR:HG21	1.77	0.48
1:I:302:VAL:HA	2:J:416:THR:HG22	1.93	0.48
2:L:456:ASP:HB2	2:L:460:CYS:O	2.12	0.48
1:Q:303:ASN:H	2:R:416:THR:CG2	2.25	0.48
1:S:108:ILE:HG12	1:S:253:LEU:HD23	1.94	0.48
1:U:108:ILE:HG12	1:U:253:LEU:HD23	1.95	0.48
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.14	0.48
1:M:175:ILE:HD12	1:M:195:ILE:HD13	1.96	0.48
1:U:244:LEU:HD13	1:U:246:ALA:HB2	1.95	0.48
2:F:381:LYS:NZ	2:F:382:THR:O	2.35	0.48
1:M:17:LYS:HE2	1:M:22:GLU:HG3	1.96	0.48
1:C:34:GLU:HB2	1:C:283:THR:HG21	1.95	0.48
5:E:605:SIA:H6	5:E:605:SIA:O1B	2.13	0.48
2:L:442:TYR:OH	2:L:455:GLU:OE2	2.18	0.48
1:O:314:ARG:NH1	6:O:716:HOH:O	2.22	0.48
2:R:495:ASN:ND2	2:R:495:ASN:O	2.47	0.48
1:U:128:ARG:HE	1:U:128:ARG:HB2	1.43	0.48
2:T:418:GLN:HG2	2:X:417:TYR:CE1	2.49	0.48
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.95	0.48
1:U:310:ALA:O	6:U:714:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:469:ASP:O	2:J:473:GLU:HB2	2.13	0.48
1:Q:28:ASN:ND2	6:Q:708:HOH:O	2.47	0.48
2:V:453:ALA:O	6:V:730:HOH:O	2.20	0.48
1:W:17:LYS:HE3	1:W:22:GLU:HG3	1.96	0.48
2:H:326:PHE:HZ	2:L:325:LEU:HD13	1.79	0.47
2:P:387:GLU:N	6:P:713:HOH:O	2.15	0.47
1:Q:141:GLU:OE1	1:Q:249:ARG:HD3	2.13	0.47
1:U:141:GLU:OE1	1:U:249:ARG:HD3	2.13	0.47
1:U:1:ASP:HA	2:V:350:GLN:O	2.14	0.47
1:W:41:LEU:HD23	1:W:78:ILE:HD13	1.95	0.47
2:X:450:ARG:HG3	2:X:451:GLN:H	1.79	0.47
2:B:344:TRP:HH2	2:B:371:ILE:HD12	1.78	0.47
2:H:418:GLN:HG2	2:L:417:TYR:HE1	1.77	0.47
1:W:172:MET:HG2	1:W:227:TRP:HB3	1.96	0.47
1:A:244:LEU:HD13	1:A:246:ALA:HB2	1.97	0.47
1:K:101:LYS:HE3	1:K:229:LEU:HD11	1.96	0.47
1:O:98:LEU:HD13	1:O:227:TRP:CD2	2.50	0.47
2:R:374:LYS:NZ	2:R:426:GLU:O	2.48	0.47
1:S:155:PRO:O	1:S:157:THR:HG22	2.13	0.47
1:W:14:THR:HG21	1:W:29:ALA:HB3	1.96	0.47
1:A:303:ASN:H	2:B:416:THR:HG21	1.80	0.47
1:E:41:LEU:HD13	1:E:264:ALA:HB3	1.97	0.47
1:G:43:MET:HE2	1:G:43:MET:HB3	1.83	0.47
1:I:303:ASN:H	2:J:416:THR:CG2	2.27	0.47
1:U:318:GLU:OE2	6:U:736:HOH:O	2.21	0.47
1:E:234:ASP:OD1	1:E:235:ASN:N	2.47	0.47
1:E:153:ASN:HA	1:E:189:GLY:HA3	1.97	0.47
2:F:446:ARG:HH12	2:F:447:LYS:HE3	1.79	0.47
1:G:193:ILE:HG22	1:G:208:PRO:HD2	1.97	0.47
1:O:41:LEU:HD13	1:O:264:ALA:HB3	1.96	0.47
1:S:17:LYS:NZ	2:T:420:GLU:OE2	2.39	0.47
2:B:446:ARG:NH2	2:F:455:GLU:OE1	2.48	0.47
1:E:125:GLY:HA3	1:E:144:TRP:HB3	1.96	0.47
2:L:377:ARG:O	2:L:380:GLU:HG2	2.15	0.47
1:I:49:LYS:HD2	1:I:69:HIS:ND1	2.30	0.47
1:O:40:ARG:NE	1:O:267:ASP:OD2	2.48	0.47
1:W:122:ASN:HB3	1:W:146:VAL:HG12	1.95	0.47
1:G:284:ARG:HB3	2:H:379:VAL:HG13	1.97	0.47
2:R:391:SER:O	6:R:737:HOH:O	2.20	0.47
2:F:342:ASP:HB3	2:F:359:ALA:HB2	1.97	0.46
1:Q:146:VAL:HG22	1:Q:187:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:408:LYS:HG2	2:R:406:TRP:CH2	2.50	0.46
2:L:446:ARG:HD2	2:L:455:GLU:OE1	2.14	0.46
1:M:40:ARG:NE	1:M:267:ASP:OD2	2.45	0.46
2:V:408:LYS:O	2:V:412:THR:HG23	2.15	0.46
2:F:391:SER:H	2:F:396:ILE:HD11	1.81	0.46
1:E:303:ASN:H	2:F:416:THR:HG21	1.80	0.46
2:H:329:ILE:O	6:H:701:HOH:O	2.21	0.46
2:H:412:THR:O	2:H:416:THR:HG23	2.15	0.46
2:B:406:TRP:CZ2	2:D:408:LYS:HE2	2.51	0.46
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.16	0.46
1:A:193:ILE:HG21	1:A:208:PRO:HG2	1.95	0.46
1:K:162:ARG:HG3	1:K:235:ASN:OD1	2.15	0.46
1:Q:34:GLU:OE2	1:Q:36:THR:N	2.33	0.46
1:W:146:VAL:HG22	1:W:187:LEU:HB3	1.96	0.46
1:W:153:ASN:HA	1:W:189:GLY:HA3	1.98	0.46
1:I:175:ILE:HD12	1:I:195:ILE:HD13	1.97	0.46
1:Q:108:ILE:HG12	1:Q:253:LEU:HD23	1.97	0.46
1:Q:296:GLY:HA2	2:R:385:GLU:HG3	1.97	0.46
1:A:128:ARG:NH1	1:U:133:ASN:O	2.49	0.46
1:E:303:ASN:H	2:F:416:THR:CG2	2.29	0.46
1:G:41:LEU:HD13	1:G:264:ALA:HB3	1.97	0.46
1:K:194:SER:OG	1:K:205:ASN:ND2	2.46	0.46
2:T:456:ASP:HB2	2:T:460:CYS:O	2.15	0.46
2:D:383:ASN:HA	2:D:384:THR:HB	1.98	0.46
1:M:202:TYR:CD2	1:M:228:THR:HG21	2.51	0.46
2:X:448:GLN:NE2	2:X:478:ASN:HA	2.30	0.46
2:T:400:ILE:HD12	2:T:400:ILE:HA	1.87	0.46
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.98	0.45
1:C:317:PRO:O	1:C:318:GLU:HB2	2.16	0.45
1:C:60:LEU:HD11	1:C:102:ILE:HD11	1.97	0.45
2:N:448:GLN:OE1	2:N:478:ASN:HA	2.15	0.45
2:N:478:ASN:O	2:N:478:ASN:ND2	2.49	0.45
1:W:59:MET:HE2	1:W:59:MET:HB3	1.87	0.45
1:E:162:ARG:HE	1:E:162:ARG:HB2	1.59	0.45
1:G:303:ASN:H	2:H:416:THR:HG21	1.81	0.45
1:O:303:ASN:H	2:P:416:THR:HG21	1.81	0.45
2:T:446:ARG:NH2	2:X:455:GLU:OE1	2.49	0.45
1:M:289:ASN:HD22	1:M:305:ARG:HA	1.81	0.45
2:P:446:ARG:HH12	2:P:447:LYS:HE3	1.80	0.45
1:Q:155:PRO:O	1:Q:157:THR:HG22	2.17	0.45
2:T:456:ASP:HB3	2:T:458:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:CH2	1:A:108:ILE:HG13	2.50	0.45
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.99	0.45
2:P:450:ARG:HB3	6:P:710:HOH:O	2.15	0.45
1:S:55:HIS:HB3	1:S:85:ALA:HB2	1.98	0.45
1:C:202:TYR:CD2	1:C:228:THR:HG21	2.52	0.45
1:Q:302:VAL:HA	2:R:416:THR:HG22	1.98	0.45
1:S:8:HIS:CE1	6:S:701:HOH:O	2.67	0.45
1:W:288:GLN:HG3	1:W:299:PRO:HB2	1.99	0.45
2:D:383:ASN:HA	2:D:384:THR:CB	2.46	0.45
2:H:342:ASP:HB3	2:H:359:ALA:HB2	1.98	0.45
1:Q:34:GLU:OE2	1:Q:35:SER:N	2.49	0.45
1:E:219:GLN:NE2	5:E:605:SIA:C1	2.79	0.45
1:U:104:GLU:OE1	6:U:757:HOH:O	2.21	0.45
1:W:89:PRO:HB3	1:W:216:VAL:HB	1.99	0.45
1:A:165:ASP:OD1	1:A:166:THR:N	2.44	0.45
1:G:209:VAL:HG21	1:I:205:ASN:ND2	2.32	0.45
1:M:8:HIS:HE1	6:M:707:HOH:O	2.00	0.45
1:A:256:ARG:NE	6:A:776:HOH:O	2.47	0.45
1:E:300:LYS:HG3	2:F:415:TRP:CE2	2.51	0.45
2:H:383:ASN:ND2	2:H:383:ASN:O	2.50	0.45
1:I:193:ILE:HG21	1:I:208:PRO:HG2	1.98	0.45
1:Q:80:ARG:NH1	1:Q:262:SER:O	2.43	0.45
1:A:61:ILE:O	1:A:139:TYR:HB3	2.18	0.44
1:E:202:TYR:CD2	1:E:228:THR:HG21	2.52	0.44
1:I:144:TRP:CH2	5:I:602:SIA:H7	2.52	0.44
1:W:17:LYS:NZ	2:X:420:GLU:OE2	2.39	0.44
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.17	0.44
1:Q:162:ARG:HG3	1:Q:235:ASN:OD1	2.17	0.44
1:C:142:LEU:HB3	1:C:245:ILE:HG22	2.00	0.44
2:B:373:GLY:HA3	1:E:20:THR:O	2.18	0.44
1:O:49:LYS:HD2	1:O:69:HIS:ND1	2.32	0.44
1:O:20:THR:O	2:R:373:GLY:HA3	2.17	0.44
1:U:121:ILE:HD11	1:U:157:THR:HG21	1.99	0.44
2:R:361:TYR:CZ	2:R:365:GLN:HG3	2.53	0.44
2:F:367:ALA:O	2:F:371:ILE:HG12	2.18	0.44
2:H:377:ARG:O	2:H:380:GLU:HG2	2.18	0.44
2:T:391:SER:H	2:T:396:ILE:HD11	1.82	0.44
2:B:473:GLU:O	2:B:477:ASN:HB2	2.18	0.44
1:G:175:ILE:HD12	1:G:195:ILE:HD13	1.98	0.44
1:C:155:PRO:O	1:C:157:THR:HG22	2.16	0.44
1:E:52:GLY:O	6:E:704:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:448:GLN:NE2	6:F:730:HOH:O	2.47	0.44
1:W:155:PRO:O	1:W:157:THR:HG22	2.18	0.44
1:I:121:ILE:HD11	1:I:157:THR:HG21	2.00	0.43
1:K:142:LEU:HD23	1:K:247:PRO:HA	2.00	0.43
2:P:432:ASP:OD1	6:P:729:HOH:O	2.21	0.43
1:U:46:ARG:HE	1:U:76:THR:HG21	1.83	0.43
1:S:170:LEU:HD22	1:S:229:LEU:HD21	2.01	0.43
1:A:9:ALA:HB2	2:B:336:GLY:HA3	2.00	0.43
1:A:20:THR:O	2:D:373:GLY:HA3	2.18	0.43
1:E:176:HIS:O	1:E:208:PRO:HB3	2.18	0.43
2:H:327:GLY:O	2:H:331:GLY:HA3	2.18	0.43
1:M:203:ARG:O	1:M:203:ARG:HG3	2.18	0.43
1:O:167:ALA:HB3	1:O:252:LYS:HE3	2.00	0.43
1:S:46:ARG:HB2	1:S:75:ASP:OD2	2.19	0.43
1:A:49:LYS:NZ	6:A:740:HOH:O	2.40	0.43
1:S:300:LYS:HG3	2:T:415:TRP:CE2	2.53	0.43
1:A:213:ARG:HD2	1:A:222:ARG:HG2	2.00	0.43
2:D:342:ASP:HB3	2:D:359:ALA:HB2	2.00	0.43
1:G:314:ARG:HG3	2:H:431:ILE:HG23	2.01	0.43
2:H:450:ARG:HB3	6:H:721:HOH:O	2.18	0.43
1:M:49:LYS:HD2	1:M:69:HIS:ND1	2.34	0.43
1:A:317:PRO:O	1:A:318:GLU:HB2	2.18	0.43
1:U:264:ALA:HA	1:U:265:PRO:HD3	1.91	0.43
1:W:165:ASP:OD1	1:W:166:THR:N	2.43	0.43
1:O:44:LYS:HD2	1:O:269:ASN:O	2.18	0.43
1:Q:252:LYS:HE3	1:Q:254:ILE:HD11	1.99	0.43
5:G:602:SIA:O10	5:G:602:SIA:O7	2.24	0.43
2:L:456:ASP:CG	2:L:460:CYS:HB2	2.39	0.43
1:Q:174:GLY:O	1:Q:175:ILE:HD13	2.18	0.43
1:Q:46:ARG:HE	1:Q:76:THR:HG21	1.84	0.43
1:A:42:CYS:HB3	1:A:270:CYS:O	2.19	0.43
1:S:101:LYS:HE3	1:S:229:LEU:HD11	2.01	0.43
1:U:34:GLU:HB2	1:U:283:THR:HG21	2.01	0.43
2:D:414:ILE:O	2:D:418:GLN:HG3	2.19	0.43
1:S:110:LYS:HB2	1:S:249:ARG:HH21	1.83	0.43
1:S:160:THR:HG22	1:S:162:ARG:HD2	2.00	0.42
1:W:41:LEU:O	1:W:43:MET:HG2	2.19	0.42
1:G:302:VAL:HA	2:H:416:THR:HG22	2.01	0.42
1:K:197:VAL:O	1:K:203:ARG:HA	2.19	0.42
1:S:47:LYS:HB3	1:S:47:LYS:HE2	1.86	0.42
1:U:144:TRP:HH2	5:U:602:SIA:H91	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:GLU:HB2	1:G:283:THR:HG21	2.00	0.42
1:G:67:ASP:CG	6:G:743:HOH:O	2.50	0.42
2:T:457:GLY:N	6:T:725:HOH:O	2.38	0.42
1:O:300:LYS:HD3	1:O:300:LYS:HA	1.83	0.42
3:T:601:NAG:O7	6:U:757:HOH:O	2.21	0.42
2:X:429:HIS:NE2	6:X:721:HOH:O	2.05	0.42
1:A:200:SER:OG	1:A:234:ASP:OD1	2.29	0.42
1:G:101:LYS:O	6:G:764:HOH:O	2.21	0.42
1:G:126:THR:HG23	1:G:136:ASN:HB3	2.01	0.42
2:T:361:TYR:CZ	2:T:365:GLN:HG3	2.54	0.42
1:U:144:TRP:CH2	5:U:602:SIA:H7	2.55	0.42
1:W:303:ASN:H	2:X:416:THR:CG2	2.32	0.42
1:A:48:HIS:CD2	1:A:266:ILE:HD13	2.55	0.42
1:G:193:ILE:HG21	1:G:208:PRO:HG2	2.00	0.42
1:I:74:TRP:CH2	1:I:108:ILE:HG13	2.55	0.42
2:J:381:LYS:HA	2:J:381:LYS:HD2	1.83	0.42
1:K:165:ASP:OD1	1:K:166:THR:N	2.42	0.42
1:O:313:MET:HG3	1:O:314:ARG:O	2.20	0.42
1:C:284:ARG:HB3	2:D:379:VAL:HG22	2.02	0.42
1:O:175:ILE:HD12	1:O:195:ILE:HD13	2.01	0.42
1:C:51:LEU:HB3	1:C:54:CYS:O	2.20	0.42
1:G:46:ARG:HB2	1:G:75:ASP:OD2	2.19	0.42
2:H:400:ILE:HD12	2:H:400:ILE:HA	1.89	0.42
1:K:41:LEU:HD13	1:K:264:ALA:HB3	2.02	0.42
1:M:96:GLU:OE2	1:M:99:ARG:NH2	2.37	0.42
1:O:75:ASP:OD2	1:O:76:THR:HG22	2.20	0.42
1:Q:276:TRP:HB2	1:Q:293:ARG:O	2.19	0.42
2:B:422:LEU:O	2:B:426:GLU:HG2	2.18	0.42
1:I:75:ASP:OD2	1:I:76:THR:HG22	2.19	0.42
1:Q:101:LYS:HE3	1:Q:229:LEU:HD11	2.02	0.42
1:Q:43:MET:HB3	1:Q:43:MET:HE2	1.96	0.42
1:A:40:ARG:NH2	6:A:800:HOH:O	2.30	0.42
1:O:33:VAL:O	6:O:706:HOH:O	2.21	0.42
1:Q:55:HIS:CE1	1:Q:57:ILE:HG12	2.55	0.42
1:C:89:PRO:HB3	1:C:216:VAL:HB	2.02	0.41
1:C:244:LEU:HD13	1:C:246:ALA:HB2	2.02	0.41
1:C:42:CYS:HB3	1:C:270:CYS:O	2.20	0.41
1:I:48:HIS:CD2	1:I:266:ILE:HD13	2.55	0.41
1:M:284:ARG:HB3	2:N:379:VAL:HG13	2.02	0.41
2:R:367:ALA:O	2:R:371:ILE:HG12	2.19	0.41
1:U:296:GLY:HA2	2:V:385:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:127:THR:HG22	6:W:733:HOH:O	2.19	0.41
1:K:172:MET:O	1:K:247:PRO:HB3	2.19	0.41
1:A:17:LYS:HE2	1:A:22:GLU:HG3	2.02	0.41
1:E:240:HIS:CE1	1:E:244:LEU:HD12	2.55	0.41
2:F:377:ARG:O	2:F:380:GLU:HG2	2.20	0.41
1:K:61:ILE:HD12	1:K:139:TYR:CE1	2.55	0.41
2:H:446:ARG:NH2	2:L:455:GLU:OE1	2.53	0.41
1:O:193:ILE:HG21	1:O:208:PRO:HG2	2.01	0.41
2:P:386:PHE:HA	6:P:713:HOH:O	2.19	0.41
1:A:302:VAL:HA	2:B:416:THR:HG22	2.03	0.41
1:A:42:CYS:HB2	1:A:272:SER:HB3	2.02	0.41
1:A:68:LEU:HB2	6:A:739:HOH:O	2.20	0.41
1:C:57:ILE:HD12	1:C:95:VAL:HG23	2.02	0.41
2:L:324:GLY:HA3	6:L:740:HOH:O	2.20	0.41
1:M:42:CYS:HB2	1:M:272:SER:HB2	2.02	0.41
2:N:451:GLN:O	2:N:493:ARG:NH1	2.48	0.41
2:X:444:ARG:HD3	2:X:478:ASN:OD1	2.20	0.41
2:J:377:ARG:NH2	6:J:714:HOH:O	2.52	0.41
1:K:302:VAL:HA	2:L:416:THR:HG22	2.02	0.41
6:P:708:HOH:O	2:R:450:ARG:HB3	2.20	0.41
1:A:177:HIS:HA	1:A:178:PRO:HD3	1.84	0.41
1:A:46:ARG:HB2	1:A:75:ASP:OD2	2.21	0.41
1:C:303:ASN:HB2	2:D:416:THR:HG21	2.02	0.41
1:E:175:ILE:HD12	1:E:195:ILE:HD13	2.01	0.41
1:E:172:MET:HG2	1:E:227:TRP:HB3	2.03	0.41
1:E:311:THR:HG21	4:E:603:NAG:O6	2.21	0.41
1:I:141:GLU:OE1	1:I:249:ARG:HD3	2.20	0.41
1:Q:89:PRO:HB3	1:Q:216:VAL:HB	2.03	0.41
2:T:444:ARG:HD3	2:T:478:ASN:OD1	2.21	0.41
2:X:377:ARG:O	2:X:380:GLU:HG2	2.20	0.41
1:E:318:GLU:O	6:E:708:HOH:O	2.22	0.41
2:H:433:MET:O	2:H:436:SER:HB3	2.21	0.41
2:H:455:GLU:OE1	2:J:446:ARG:NH2	2.54	0.41
1:O:234:ASP:OD1	1:O:235:ASN:N	2.54	0.41
1:I:125:GLY:HA3	1:I:144:TRP:HB3	2.03	0.41
1:K:181:THR:HG22	1:K:185:ASN:ND2	2.36	0.41
1:Q:289:ASN:ND2	1:Q:305:ARG:HA	2.36	0.41
1:U:75:ASP:OD2	1:U:76:THR:HG22	2.21	0.41
1:C:43:MET:HE2	1:C:43:MET:HB3	1.94	0.41
1:G:59:MET:HE1	1:G:74:TRP:CH2	2.55	0.41
2:J:400:ILE:HA	2:J:400:ILE:HD12	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:153:ASN:HA	1:Q:189:GLY:HA3	2.01	0.41
1:Q:142:LEU:HD23	1:Q:247:PRO:HA	2.03	0.41
1:E:145:LEU:HB2	6:E:715:HOH:O	2.20	0.41
2:H:456:ASP:HB2	2:H:460:CYS:HB2	2.02	0.41
1:I:74:TRP:HH2	1:I:108:ILE:HG13	1.85	0.41
1:I:155:PRO:O	1:I:157:THR:HG22	2.21	0.41
1:K:286:PRO:HG2	1:K:287:PHE:CD2	2.56	0.41
1:S:176:HIS:O	1:S:208:PRO:HB3	2.20	0.41
1:S:43:MET:O	1:S:46:ARG:HG2	2.21	0.41
1:K:109:ASN:OD1	6:K:779:HOH:O	2.22	0.41
1:K:43:MET:HE2	1:K:43:MET:HB3	1.94	0.41
1:M:20:THR:O	2:P:373:GLY:HA3	2.21	0.41
1:C:63:THR:OG1	1:C:85:ALA:O	2.33	0.40
5:E:605:SIA:O7	5:E:605:SIA:O10	2.32	0.40
1:G:291:SER:HA	1:G:292:PRO:HD3	1.87	0.40
1:O:179:SER:OG	1:O:183:GLU:OE1	2.38	0.40
2:P:381:LYS:HD2	2:P:381:LYS:HA	1.91	0.40
1:Q:87:CYS:HB2	1:Q:129:ALA:O	2.20	0.40
1:O:228:THR:HG22	1:O:229:LEU:H	1.86	0.40
2:P:377:ARG:O	2:P:380:GLU:HG2	2.21	0.40
2:N:410:SER:HB3	2:P:411:ILE:HD13	2.03	0.40
1:Q:125:GLY:HA3	1:Q:144:TRP:HB3	2.03	0.40
2:T:375:LEU:HD23	2:T:375:LEU:HA	1.89	0.40
2:B:344:TRP:CH2	2:B:371:ILE:HD12	2.56	0.40
2:F:456:ASP:HB3	2:F:458:LYS:H	1.86	0.40
1:M:234:ASP:OD1	1:M:235:ASN:N	2.54	0.40
1:O:172:MET:HG2	1:O:227:TRP:HB3	2.03	0.40
1:S:110:LYS:HB3	1:S:249:ARG:HE	1.86	0.40
1:S:284:ARG:HB3	2:T:379:VAL:HG13	2.03	0.40
1:U:132:ARG:NH1	1:U:138:PHE:O	2.54	0.40
1:U:43:MET:HE2	1:U:43:MET:HB3	1.94	0.40
1:U:46:ARG:HB2	1:U:75:ASP:OD2	2.21	0.40
2:V:383:ASN:HA	2:V:384:THR:HB	2.04	0.40
1:W:87:CYS:SG	1:W:88:TYR:N	2.93	0.40
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.93	0.40
1:G:172:MET:HG2	1:G:227:TRP:HB3	2.03	0.40
1:K:59:MET:HE2	1:K:59:MET:HB3	1.98	0.40
2:P:455:GLU:OE1	2:R:446:ARG:NH2	2.53	0.40
1:Q:303:ASN:O	1:Q:304:ARG:NE	2.52	0.40
1:S:172:MET:HG2	1:S:227:TRP:HB3	2.04	0.40
5:U:602:SIA:O10	5:U:602:SIA:C7	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:50:ASP:HB2	1:W:266:ILE:HD11	2.03	0.40
1:E:146:VAL:HG21	1:E:187:LEU:HD22	2.04	0.40
1:K:60:LEU:HD11	1:K:102:ILE:HD11	2.03	0.40
2:H:373:GLY:HA3	1:K:20:THR:O	2.21	0.40
1:S:51:LEU:HB3	1:S:54:CYS:O	2.21	0.40
2:T:406:TRP:CH2	2:V:408:LYS:HG2	2.56	0.40
1:W:162:ARG:HG3	1:W:235:ASN:CG	2.41	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%)	309 (98%)	7 (2%)	0	100	100
1	C	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	E	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	G	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
1	I	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	K	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	M	316/318 (99%)	302 (96%)	13 (4%)	1 (0%)	44	70
1	O	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
1	Q	316/318 (99%)	304 (96%)	12 (4%)	0	100	100
1	S	316/318 (99%)	305 (96%)	10 (3%)	1 (0%)	44	70
1	U	316/318 (99%)	307 (97%)	8 (2%)	1 (0%)	44	70
1	W	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
2	B	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	28	53
2	D	172/174 (99%)	166 (96%)	4 (2%)	2 (1%)	15	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	28	53
2	H	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	28	53
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	28	53
2	L	172/174 (99%)	169 (98%)	2 (1%)	1 (1%)	28	53
2	N	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	28	53
2	P	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	28	53
2	R	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	28	53
2	T	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	28	53
2	V	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	28	53
2	X	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	28	53
All	All	5856/5904 (99%)	5662 (97%)	178 (3%)	16 (0%)	44	70

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	450	ARG
2	F	450	ARG
2	H	450	ARG
2	J	450	ARG
2	L	450	ARG
1	M	150	LYS
2	N	450	ARG
2	P	450	ARG
2	R	450	ARG
1	S	39	ASN
2	T	450	ARG
2	V	450	ARG
2	X	450	ARG
2	B	450	ARG
1	U	39	ASN
2	D	496	ILE

### 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%)	248 (92%)	21 (8%)	15	29
1	C	269/269 (100%)	249 (93%)	20 (7%)	16	32
1	E	269/269 (100%)	247 (92%)	22 (8%)	13	26
1	G	269/269 (100%)	248 (92%)	21 (8%)	15	29
1	I	269/269 (100%)	250 (93%)	19 (7%)	17	34
1	K	269/269 (100%)	246 (91%)	23 (9%)	12	23
1	M	269/269 (100%)	250 (93%)	19 (7%)	17	34
1	O	269/269 (100%)	249 (93%)	20 (7%)	16	32
1	Q	269/269 (100%)	246 (91%)	23 (9%)	12	23
1	S	269/269 (100%)	250 (93%)	19 (7%)	17	34
1	U	269/269 (100%)	241 (90%)	28 (10%)	8	15
1	W	269/269 (100%)	245 (91%)	24 (9%)	11	22
2	B	148/148 (100%)	139 (94%)	9 (6%)	22	43
2	D	148/148 (100%)	138 (93%)	10 (7%)	18	37
2	F	148/148 (100%)	137 (93%)	11 (7%)	16	32
2	H	148/148 (100%)	144 (97%)	4 (3%)	50	77
2	J	148/148 (100%)	140 (95%)	8 (5%)	26	49
2	L	148/148 (100%)	140 (95%)	8 (5%)	26	49
2	N	148/148 (100%)	141 (95%)	7 (5%)	30	57
2	P	148/148 (100%)	137 (93%)	11 (7%)	16	32
2	R	148/148 (100%)	141 (95%)	7 (5%)	30	57
2	T	148/148 (100%)	141 (95%)	7 (5%)	30	57
2	V	148/148 (100%)	139 (94%)	9 (6%)	22	43
2	X	148/148 (100%)	143 (97%)	5 (3%)	42	69
All	All	5004/5004 (100%)	4649 (93%)	355 (7%)	17	34

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	41	LEU
1	A	49	LYS
1	A	76	THR

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Mol	Chain	Res	Type
1	A	77	LEU
1	A	111	ILE
1	A	126	THR
1	A	157	THR
1	A	162	ARG
1	A	170	LEU
1	A	192	SER
1	A	203	ARG
1	A	228	THR
1	A	239	SER
1	A	244	LEU
1	A	249	ARG
1	A	258	LEU
1	A	276	TRP
1	A	277	ARG
1	A	283	THR
1	A	314	ARG
2	B	341	VAL
2	B	382	THR
2	B	416	THR
2	B	420	GLU
2	B	433	MET
2	B	456	ASP
2	B	470	SER
2	B	477	ASN
2	B	492	ASN
1	C	8	HIS
1	C	41	LEU
1	C	46	ARG
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	126	THR
1	C	157	THR
1	C	170	LEU
1	C	184	LYS
1	C	192	SER
1	C	203	ARG
1	C	213	ARG
1	C	228	THR
1	C	244	LEU
1	C	258	LEU

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Mol	Chain	Res	Type
1	C	263	ASP
1	C	276	TRP
1	C	277	ARG
1	C	283	THR
2	D	341	VAL
2	D	353	GLN
2	D	377	ARG
2	D	383	ASN
2	D	433	MET
2	D	444	ARG
2	D	450	ARG
2	D	470	SER
2	D	491	LEU
2	D	495	ASN
1	E	8	HIS
1	E	14	THR
1	E	41	LEU
1	E	46	ARG
1	E	76	THR
1	E	77	LEU
1	E	111	ILE
1	E	126	THR
1	E	150	LYS
1	E	157	THR
1	E	162	ARG
1	E	170	LEU
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	256	ARG
1	E	258	LEU
1	E	263	ASP
1	E	276	TRP
1	E	277	ARG
1	E	283	THR
2	F	353	GLN
2	F	379	VAL
2	F	382	THR
2	F	411	ILE
2	F	416	THR
2	F	418	GLN

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Mol	Chain	Res	Type
2	F	425	MET
2	F	433	MET
2	F	456	ASP
2	F	467	CYS
2	F	477	ASN
1	G	8	HIS
1	G	14	THR
1	G	41	LEU
1	G	47	LYS
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	120	SER
1	G	126	THR
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	263	ASP
1	G	270	CYS
1	G	276	TRP
1	G	283	THR
2	H	341	VAL
2	H	416	THR
2	H	418	GLN
2	H	433	MET
1	I	8	HIS
1	I	41	LEU
1	I	49	LYS
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	128	ARG
1	I	157	THR
1	I	170	LEU
1	I	192	SER
1	I	203	ARG
1	I	213	ARG

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Mol	Chain	Res	Type
1	I	228	THR
1	I	244	LEU
1	I	250	VAL
1	I	258	LEU
1	I	276	TRP
1	I	277	ARG
1	I	283	THR
2	J	341	VAL
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	416	THR
2	J	433	MET
2	J	467	CYS
2	J	495	ASN
1	K	8	HIS
1	K	14	THR
1	K	63	THR
1	K	76	THR
1	K	77	LEU
1	K	111	ILE
1	K	120	SER
1	K	132	ARG
1	K	149	SER
1	K	157	THR
1	K	162	ARG
1	K	170	LEU
1	K	203	ARG
1	K	220	SER
1	K	228	THR
1	K	244	LEU
1	K	248	SER
1	K	256	ARG
1	K	258	LEU
1	K	263	ASP
1	K	276	TRP
1	K	277	ARG
1	K	283	THR
2	L	325	LEU
2	L	335	ASN
2	L	418	GLN
2	L	423	VAL

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Mol	Chain	Res	Type
2	L	433	MET
2	L	436	SER
2	L	456	ASP
2	L	484	GLN
1	M	8	HIS
1	M	14	THR
1	M	30	THR
1	M	41	LEU
1	M	57	ILE
1	M	76	THR
1	M	77	LEU
1	M	87	CYS
1	M	111	ILE
1	M	157	THR
1	M	162	ARG
1	M	170	LEU
1	M	203	ARG
1	M	213	ARG
1	M	228	THR
1	M	244	LEU
1	M	258	LEU
1	M	276	TRP
1	M	283	THR
2	N	335	ASN
2	N	371	ILE
2	N	418	GLN
2	N	433	MET
2	N	446	ARG
2	N	450	ARG
2	N	484	GLN
1	O	8	HIS
1	O	14	THR
1	O	41	LEU
1	O	49	LYS
1	O	76	THR
1	O	77	LEU
1	O	94	ASN
1	O	111	ILE
1	O	116	THR
1	O	126	THR
1	O	170	LEU
1	O	203	ARG

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Mol	Chain	Res	Type
1	O	228	THR
1	O	239	SER
1	O	244	LEU
1	O	258	LEU
1	O	263	ASP
1	O	276	TRP
1	O	283	THR
1	O	318	GLU
2	P	335	ASN
2	P	341	VAL
2	P	342	ASP
2	P	372	THR
2	P	377	ARG
2	P	383	ASN
2	P	395	GLU
2	P	416	THR
2	P	420	GLU
2	P	433	MET
2	P	450	ARG
1	Q	8	HIS
1	Q	23	GLN
1	Q	41	LEU
1	Q	76	THR
1	Q	77	LEU
1	Q	111	ILE
1	Q	126	THR
1	Q	146	VAL
1	Q	157	THR
1	Q	162	ARG
1	Q	170	LEU
1	Q	184	LYS
1	Q	192	SER
1	Q	203	ARG
1	Q	213	ARG
1	Q	228	THR
1	Q	244	LEU
1	Q	249	ARG
1	Q	258	LEU
1	Q	276	TRP
1	Q	277	ARG
1	Q	283	THR
1	Q	314	ARG

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Mol	Chain	Res	Type
2	R	341	VAL
2	R	342	ASP
2	R	353	GLN
2	R	433	MET
2	R	467	CYS
2	R	470	SER
2	R	496	ILE
1	S	8	HIS
1	S	14	THR
1	S	41	LEU
1	S	76	THR
1	S	77	LEU
1	S	111	ILE
1	S	112	SER
1	S	116	THR
1	S	157	THR
1	S	162	ARG
1	S	170	LEU
1	S	203	ARG
1	S	213	ARG
1	S	228	THR
1	S	244	LEU
1	S	258	LEU
1	S	276	TRP
1	S	277	ARG
1	S	283	THR
2	T	325	LEU
2	T	383	ASN
2	T	416	THR
2	T	418	GLN
2	T	433	MET
2	T	436	SER
2	T	467	CYS
1	U	8	HIS
1	U	41	LEU
1	U	47	LYS
1	U	49	LYS
1	U	63	THR
1	U	76	THR
1	U	77	LEU
1	U	111	ILE
1	U	126	THR

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Mol	Chain	Res	Type
1	U	128	ARG
1	U	146	VAL
1	U	148	LYS
1	U	157	THR
1	U	170	LEU
1	U	179	SER
1	U	196	SER
1	U	203	ARG
1	U	228	THR
1	U	239	SER
1	U	244	LEU
1	U	249	ARG
1	U	250	VAL
1	U	258	LEU
1	U	276	TRP
1	U	277	ARG
1	U	283	THR
1	U	316	VAL
1	U	318	GLU
2	V	325	LEU
2	V	350	GLN
2	V	379	VAL
2	V	382	THR
2	V	383	ASN
2	V	412	THR
2	V	433	MET
2	V	448	GLN
2	V	467	CYS
1	W	1	ASP
1	W	8	HIS
1	W	30	THR
1	W	35	SER
1	W	76	THR
1	W	77	LEU
1	W	111	ILE
1	W	119	SER
1	W	137	SER
1	W	146	VAL
1	W	147	SER
1	W	157	THR
1	W	162	ARG
1	W	170	LEU

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Mol	Chain	Res	Type
1	W	192	SER
1	W	196	SER
1	W	203	ARG
1	W	213	ARG
1	W	228	THR
1	W	244	LEU
1	W	258	LEU
1	W	269	ASN
1	W	276	TRP
1	W	283	THR
2	X	353	GLN
2	X	382	THR
2	X	395	GLU
2	X	418	GLN
2	X	433	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	418	GLN
2	D	448	GLN
1	E	268	ASN
2	F	370	GLN
1	I	226	HIS
2	J	399	GLN
1	S	8	HIS
1	S	163	ASN
2	T	418	GLN
1	U	303	ASN
2	V	418	GLN
2	V	448	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

14 carbohydrates 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$
4	NAG	E	603	1,4	14,14,15	0.23	0	15,19,21	0.52	0
4	NAG	E	604	4	14,14,15	0.82	0	15,19,21	0.72	0
5	SIA	E	605	5	17,20,21	0.25	0	19,28,31	0.50	0
5	GAL	E	606	5	11,11,12	0.76	0	13,15,17	1.09	0
5	NAG	E	607	5	14,14,15	0.30	0	15,19,21	0.44	0
5	SIA	G	602	5	17,20,21	0.25	0	19,28,31	0.51	0
5	GAL	G	603	5	11,11,12	0.28	0	13,15,17	0.72	0
5	NAG	G	604	5	14,14,15	0.26	0	15,19,21	0.40	0
5	SIA	I	602	5	17,20,21	0.24	0	19,28,31	0.50	0
5	GAL	I	603	5	11,11,12	0.89	0	13,15,17	1.37	2 (15%)
5	NAG	I	604	5	14,14,15	0.37	0	15,19,21	0.52	0
5	SIA	U	602	5	17,20,21	2.03	8 (47%)	19,28,31	2.70	9 (47%)
5	GAL	U	603	5	11,11,12	0.75	0	13,15,17	1.19	1 (7%)
5	NAG	U	604	5	14,14,15	0.23	0	15,19,21	0.53	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
4	NAG	E	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	604	4	-	0/6/23/26	0/1/1/1
5	SIA	E	605	5	-	0/14/34/38	0/1/1/1
5	GAL	E	606	5	-	0/2/19/22	0/1/1/1
5	NAG	E	607	5	-	0/6/23/26	0/1/1/1
5	SIA	G	602	5	-	0/14/34/38	0/1/1/1
5	GAL	G	603	5	-	0/2/19/22	0/1/1/1
5	NAG	G	604	5	-	0/6/23/26	0/1/1/1
5	SIA	I	602	5	-	0/14/34/38	0/1/1/1
5	GAL	I	603	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	604	5	-	0/6/23/26	0/1/1/1
5	SIA	U	602	5	-	0/14/34/38	0/1/1/1
5	GAL	U	603	5	-	0/2/19/22	0/1/1/1
5	NAG	U	604	5	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	602	SIA	C8-C7	-3.32	1.46	1.53
5	U	602	SIA	O10-C10	-2.93	1.16	1.23
5	U	602	SIA	C4-C5	-2.72	1.50	1.53
5	U	602	SIA	C7-C6	-2.71	1.49	1.52
5	U	602	SIA	C11-C10	-2.06	1.46	1.50
5	U	602	SIA	O8-C8	-2.02	1.38	1.43
5	U	602	SIA	C3-C2	2.31	1.56	1.52
5	U	602	SIA	C3-C4	2.84	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	602	SIA	O6-C2-C3	-6.60	97.95	109.82
5	U	602	SIA	O9-C9-C8	-5.29	99.45	111.11
5	U	602	SIA	O10-C10-C11	-4.09	114.62	122.06
5	U	602	SIA	O8-C8-C9	-2.41	103.62	109.21
5	U	602	SIA	C9-C8-C7	-2.08	107.77	112.41
5	U	602	SIA	C6-C5-N5	2.11	114.71	111.00
5	U	602	SIA	O4-C4-C3	2.24	115.45	110.02
5	I	603	GAL	C1-O5-C5	2.26	115.28	112.17
5	U	602	SIA	C3-C4-C5	2.58	114.58	111.46
5	U	603	GAL	C1-C2-C3	2.90	113.32	109.65
5	I	603	GAL	C1-C2-C3	3.10	113.59	109.65
5	U	602	SIA	C11-C10-N5	3.61	122.63	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	603	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	605	SIA	4	0
5	G	602	SIA	4	0
5	I	602	SIA	3	0
5	U	602	SIA	4	0

## 5.6 Ligand geometry

25 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	0.59	0
3	NAG	B	601	2	14,14,15	0.35	0	15,19,21	0.55	0
3	NAG	C	601	1	14,14,15	0.20	0	15,19,21	0.46	0
3	NAG	D	601	2	14,14,15	0.30	0	15,19,21	0.48	0
3	NAG	E	601	1	14,14,15	0.38	0	15,19,21	0.54	0
3	NAG	E	602	1	14,14,15	0.87	1 (7%)	15,19,21	0.97	0
3	NAG	F	601	2	14,14,15	0.30	0	15,19,21	0.64	0
3	NAG	G	601	1	14,14,15	0.17	0	15,19,21	0.52	0
3	NAG	H	601	2	14,14,15	0.42	0	15,19,21	0.61	0
3	NAG	I	601	1	14,14,15	0.22	0	15,19,21	0.51	0
3	NAG	J	601	2	14,14,15	0.68	0	15,19,21	0.77	0
3	NAG	K	601	1	14,14,15	0.34	0	15,19,21	0.59	0
3	NAG	L	601	2	14,14,15	0.37	0	15,19,21	0.50	0
3	NAG	M	601	1	14,14,15	0.35	0	15,19,21	0.63	0
3	NAG	N	601	2	14,14,15	0.47	0	15,19,21	0.46	0
3	NAG	O	601	1	14,14,15	0.20	0	15,19,21	0.42	0
3	NAG	P	601	2	14,14,15	0.36	0	15,19,21	0.49	0
3	NAG	Q	601	1	14,14,15	0.27	0	15,19,21	0.43	0
3	NAG	R	601	2	14,14,15	0.20	0	15,19,21	0.67	0
3	NAG	S	601	1	14,14,15	0.28	0	15,19,21	0.61	0
3	NAG	T	601	2	14,14,15	0.57	0	15,19,21	0.42	0
3	NAG	U	601	1	14,14,15	0.42	0	15,19,21	0.48	0
3	NAG	V	601	2	14,14,15	0.39	0	15,19,21	0.55	0
3	NAG	W	601	1	14,14,15	0.28	0	15,19,21	0.57	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	X	601	2	14,14,15	0.52	0	15,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	601	2	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	D	601	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	602	1	-	0/6/23/26	0/1/1/1
3	NAG	F	601	2	-	0/6/23/26	0/1/1/1
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1
3	NAG	H	601	2	-	0/6/23/26	0/1/1/1
3	NAG	I	601	1	-	0/6/23/26	0/1/1/1
3	NAG	J	601	2	-	0/6/23/26	0/1/1/1
3	NAG	K	601	1	-	0/6/23/26	0/1/1/1
3	NAG	L	601	2	-	0/6/23/26	0/1/1/1
3	NAG	M	601	1	-	0/6/23/26	0/1/1/1
3	NAG	N	601	2	-	0/6/23/26	0/1/1/1
3	NAG	O	601	1	-	0/6/23/26	0/1/1/1
3	NAG	P	601	2	-	0/6/23/26	0/1/1/1
3	NAG	Q	601	1	-	0/6/23/26	0/1/1/1
3	NAG	R	601	2	-	0/6/23/26	0/1/1/1
3	NAG	S	601	1	-	0/6/23/26	0/1/1/1
3	NAG	T	601	2	-	0/6/23/26	0/1/1/1
3	NAG	U	601	1	-	0/6/23/26	0/1/1/1
3	NAG	V	601	2	-	0/6/23/26	0/1/1/1
3	NAG	W	601	1	-	0/6/23/26	0/1/1/1
3	NAG	X	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)
3	E	602	NAG	C2-N2	2.18	1.50	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	NAG	1	0
3	E	601	NAG	1	0
3	J	601	NAG	1	0
3	K	601	NAG	1	0
3	N	601	NAG	1	0
3	O	601	NAG	1	0
3	T	601	NAG	1	0
3	U	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, 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	318/318 (100%)	-0.19	0 100 100	10, 25, 42, 69	0
1	C	318/318 (100%)	0.11	4 (1%) 77 73	10, 36, 64, 95	0
1	E	318/318 (100%)	-0.05	1 (0%) 93 93	11, 30, 48, 70	0
1	G	318/318 (100%)	0.04	4 (1%) 77 73	15, 34, 54, 80	0
1	I	318/318 (100%)	-0.02	5 (1%) 72 67	11, 29, 52, 101	0
1	K	318/318 (100%)	-0.08	6 (1%) 67 61	13, 29, 52, 84	0
1	M	318/318 (100%)	0.62	30 (9%) 9 6	24, 56, 87, 123	0
1	O	318/318 (100%)	0.47	25 (7%) 13 9	22, 52, 82, 112	0
1	Q	318/318 (100%)	-0.10	3 (0%) 84 81	12, 33, 54, 92	0
1	S	318/318 (100%)	0.32	20 (6%) 21 15	17, 43, 70, 107	0
1	U	318/318 (100%)	-0.05	4 (1%) 77 73	16, 31, 53, 83	0
1	W	318/318 (100%)	0.22	8 (2%) 58 50	24, 44, 71, 94	0
2	B	174/174 (100%)	0.23	3 (1%) 70 65	12, 26, 54, 108	0
2	D	174/174 (100%)	0.24	3 (1%) 70 65	11, 25, 52, 130	0
2	F	174/174 (100%)	0.17	4 (2%) 61 54	10, 27, 56, 101	0
2	H	174/174 (100%)	0.18	2 (1%) 80 77	12, 29, 55, 125	0
2	J	174/174 (100%)	0.39	5 (2%) 52 45	12, 37, 74, 132	0
2	L	174/174 (100%)	0.31	5 (2%) 52 45	14, 35, 67, 108	0
2	N	174/174 (100%)	0.32	3 (1%) 70 65	23, 38, 71, 109	0
2	P	174/174 (100%)	0.36	5 (2%) 52 45	18, 37, 66, 125	0
2	R	174/174 (100%)	0.29	6 (3%) 46 38	16, 33, 55, 110	0
2	T	174/174 (100%)	0.19	3 (1%) 70 65	13, 37, 61, 119	0
2	V	174/174 (100%)	0.29	3 (1%) 70 65	14, 39, 71, 127	0
2	X	174/174 (100%)	0.35	3 (1%) 70 65	19, 45, 69, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5904/5904 (100%)	0.17	155 (2%)	56 49	10, 35, 69, 132	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	497	ASN	13.1
2	P	497	ASN	12.8
2	J	497	ASN	11.2
2	V	496	ILE	10.7
2	X	497	ASN	10.3
2	L	497	ASN	10.1
2	H	496	ILE	9.4
2	H	497	ASN	9.4
2	X	496	ILE	9.1
2	D	496	ILE	9.0
2	V	497	ASN	8.6
2	P	496	ILE	7.3
2	J	496	ILE	6.9
2	F	496	ILE	6.8
2	B	496	ILE	6.8
2	F	497	ASN	6.7
2	F	383	ASN	5.4
2	R	496	ILE	5.2
2	B	497	ASN	5.1
2	L	496	ILE	5.0
1	S	120	SER	4.5
1	M	131	MET	4.2
1	M	134	GLY	3.8
1	K	269	ASN	3.8
1	W	318	GLU	3.8
1	O	256	ARG	3.8
1	O	128	ARG	3.7
2	N	496	ILE	3.7
2	T	383	ASN	3.7
1	M	305	ARG	3.7
1	O	12	ASN	3.6
1	M	135	GLY	3.6
1	M	152	GLN	3.6
1	S	152	GLN	3.5
1	M	150	LYS	3.4
1	I	318	GLU	3.4
1	O	167	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	P	324	GLY	3.4
1	O	134	GLY	3.4
2	R	497	ASN	3.4
1	M	270	CYS	3.4
2	L	495	ASN	3.2
1	K	133	ASN	3.2
1	O	270	CYS	3.2
1	O	166	THR	3.2
2	T	342	ASP	3.1
2	X	383	ASN	3.1
1	M	45	GLY	3.1
1	O	129	ALA	3.1
1	M	120	SER	3.0
1	E	128	ARG	3.0
1	S	150	LYS	3.0
1	S	121	ILE	3.0
1	C	149	SER	2.9
1	G	135	GLY	2.9
1	O	233	GLY	2.9
1	G	305	ARG	2.9
1	S	305	ARG	2.9
1	M	117	TYR	2.9
1	M	187	LEU	2.8
1	M	128	ARG	2.8
1	S	149	SER	2.8
1	O	11	ALA	2.8
1	M	12	ASN	2.8
2	L	383	ASN	2.8
1	O	131	MET	2.8
1	C	128	ARG	2.8
1	S	167	ALA	2.8
1	M	15	ILE	2.7
1	O	284	ARG	2.7
1	I	166	THR	2.7
1	U	166	THR	2.7
1	M	162	ARG	2.7
1	O	198	GLY	2.7
1	M	145	LEU	2.7
1	O	38	ILE	2.7
1	K	305	ARG	2.7
1	I	12	ASN	2.6
1	M	23	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	S	153	ASN	2.6
1	M	154	PHE	2.6
1	W	256	ARG	2.6
1	O	164	THR	2.6
1	S	284	ARG	2.6
1	W	152	GLN	2.6
2	J	356	GLY	2.6
1	Q	11	ALA	2.5
2	T	491	LEU	2.5
1	M	133	ASN	2.5
1	M	188	TYR	2.5
1	O	111	ILE	2.5
1	O	41	LEU	2.4
2	N	378	LEU	2.4
1	M	114	GLY	2.4
1	W	133	ASN	2.4
2	L	352	ALA	2.4
1	M	218	GLY	2.4
1	O	44	LYS	2.4
1	S	117	TYR	2.4
1	O	40	ARG	2.4
1	S	12	ASN	2.4
2	N	361	TYR	2.4
1	I	11	ALA	2.4
1	S	148	LYS	2.4
1	M	149	SER	2.3
2	R	439	LEU	2.3
1	Q	182	GLN	2.3
1	O	73	MET	2.3
1	M	147	SER	2.3
2	P	382	THR	2.3
1	O	266	ILE	2.3
1	W	12	ASN	2.3
1	M	126	THR	2.3
1	M	186	ASP	2.3
1	S	166	THR	2.3
1	S	118	GLY	2.3
2	D	324	GLY	2.3
2	F	324	GLY	2.3
1	G	266	ILE	2.3
1	K	134	GLY	2.2
1	S	73	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	263	ASP	2.2
1	C	270	CYS	2.2
1	S	119	SER	2.2
2	R	436	SER	2.2
1	U	12	ASN	2.2
2	R	383	ASN	2.2
1	G	118	GLY	2.2
1	U	167	ALA	2.2
1	M	148	LYS	2.2
1	S	11	ALA	2.2
1	S	154	PHE	2.2
2	P	326	PHE	2.2
2	R	352	ALA	2.2
1	Q	12	ASN	2.2
1	I	305	ARG	2.2
1	S	189	GLY	2.2
1	K	135	GLY	2.1
1	C	134	GLY	2.1
1	M	193	ILE	2.1
2	J	491	LEU	2.1
1	O	162	ARG	2.1
1	W	135	GLY	2.1
1	M	47	LYS	2.1
1	O	305	ARG	2.1
2	B	383	ASN	2.1
2	J	378	LEU	2.1
2	V	491	LEU	2.1
1	O	282	ASN	2.1
1	W	269	ASN	2.1
1	U	318	GLU	2.0
1	K	270	CYS	2.0
1	W	266	ILE	2.0
1	M	164	THR	2.0
1	S	147	SER	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SIA	G	602	20/21	0.87	0.24	1.72	44,57,71,72	0
5	SIA	I	602	20/21	0.89	0.19	1.10	26,35,46,47	0
5	GAL	E	606	11/12	0.86	0.24	0.44	90,98,116,120	0
5	SIA	E	605	20/21	0.87	0.19	0.33	34,45,58,60	0
5	SIA	U	602	20/21	0.94	0.15	-0.02	24,34,46,47	0
5	GAL	U	603	11/12	0.78	0.27	-	58,69,81,85	0
5	NAG	U	604	14/15	0.76	0.58	-	99,115,125,128	0
5	NAG	G	604	14/15	0.71	0.79	-	125,140,147,147	0
5	GAL	G	603	11/12	0.74	0.24	-	72,90,112,114	0
5	NAG	E	607	14/15	0.71	0.55	-	100,109,111,112	0
5	NAG	I	604	14/15	0.77	0.49	-	97,103,110,110	0
4	NAG	E	603	14/15	0.94	0.22	-	46,54,64,68	0
4	NAG	E	604	14/15	0.89	0.26	-	48,69,77,80	0
5	GAL	I	603	11/12	0.78	0.24	-	66,76,99,100	0

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	U	601	14/15	0.84	0.31	3.17	80,98,105,113	0
3	NAG	W	601	14/15	0.73	0.30	2.02	79,87,91,92	0
3	NAG	K	601	14/15	0.88	0.26	1.21	46,71,77,79	0
3	NAG	Q	601	14/15	0.87	0.20	1.18	76,87,98,99	0
3	NAG	A	601	14/15	0.92	0.18	0.99	34,57,68,74	0
3	NAG	V	601	14/15	0.90	0.18	0.93	28,38,40,44	0
3	NAG	O	601	14/15	0.72	0.30	0.91	61,88,97,101	0
3	NAG	M	601	14/15	0.87	0.28	0.74	66,83,89,92	0
3	NAG	G	601	14/15	0.86	0.17	0.67	43,64,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	I	601	14/15	0.92	0.17	0.56	52,62,65,65	0
3	NAG	S	601	14/15	0.78	0.20	0.40	54,75,88,92	0
3	NAG	R	601	14/15	0.86	0.15	0.33	32,39,49,50	0
3	NAG	C	601	14/15	0.87	0.19	0.19	46,67,77,77	0
3	NAG	L	601	14/15	0.85	0.17	-0.08	23,32,38,38	0
3	NAG	X	601	14/15	0.87	0.16	-0.09	37,46,54,54	0
3	NAG	F	601	14/15	0.89	0.14	-0.10	25,30,33,36	0
3	NAG	P	601	14/15	0.93	0.13	-0.26	34,38,44,44	0
3	NAG	J	601	14/15	0.95	0.13	-0.55	18,28,36,38	0
3	NAG	E	601	14/15	0.91	0.14	-0.72	48,62,69,70	0
3	NAG	N	601	14/15	0.91	0.13	-1.01	40,50,51,54	0
3	NAG	D	601	14/15	0.95	0.11	-1.22	20,28,36,37	0
3	NAG	T	601	14/15	0.93	0.12	-1.28	23,34,41,43	0
3	NAG	H	601	14/15	0.91	0.13	-1.94	22,30,33,33	0
3	NAG	B	601	14/15	0.93	0.10	-2.34	29,38,43,50	0
3	NAG	E	602	14/15	0.88	0.27	-	54,58,73,77	0

## 6.5 Other polymers

There are no such residues in this entry.