



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:25 AM BST

PDB ID : 4WSX  
Title : The crystal structure of hemagglutinin from A/Jiangxi-Donghu/346/2013 influenza virus  
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.  
Deposited on : 2014-10-28  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

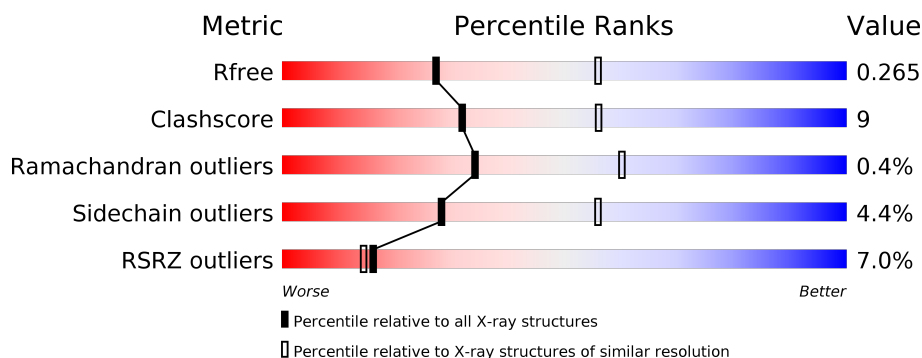
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	C	327	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	E	327	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	G	327	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	I	327	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
1	K	327	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	327	
1	O	327	
1	Q	327	
1	S	327	
1	U	327	
1	W	327	
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	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46260 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	C	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	E	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	G	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	I	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	K	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	M	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	O	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	Q	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	S	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	U	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			
1	W	319	Total	C	N	O	S	0	0	0
			2441	1508	450	466	17			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

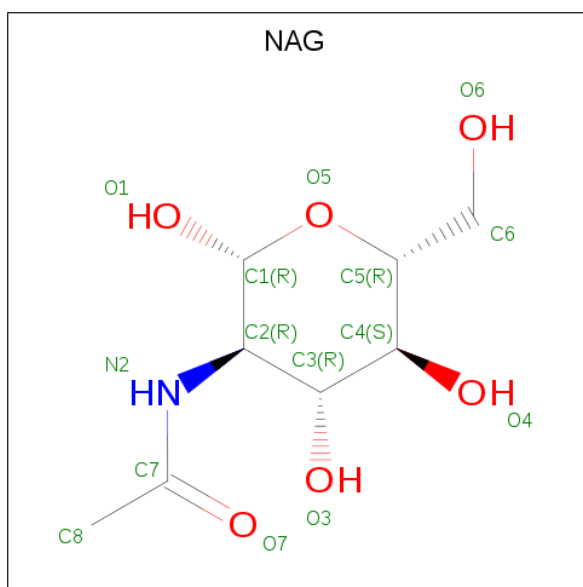
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	H	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	J	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	L	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	N	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	P	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	R	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	T	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	V	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	X	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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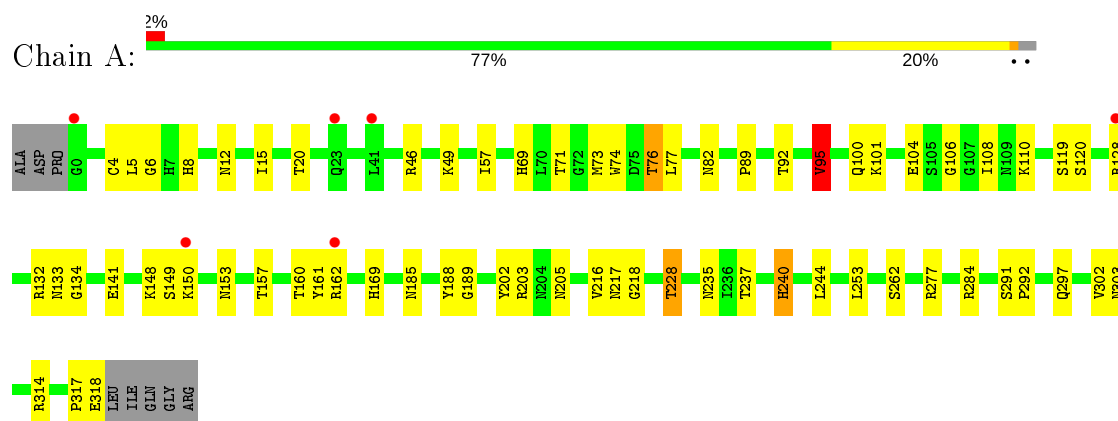
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			14	8	1	5		
3	X	1	Total	C	N	O	0	0
			14	8	1	5		

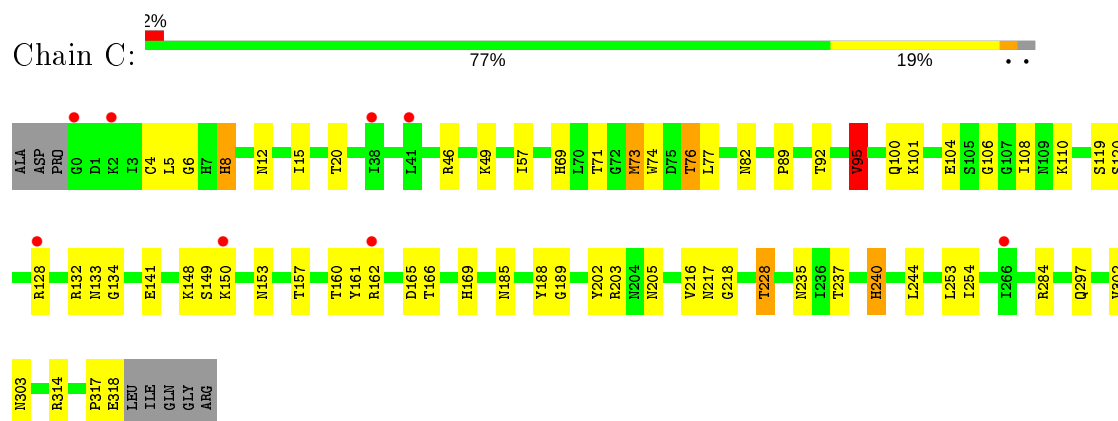
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

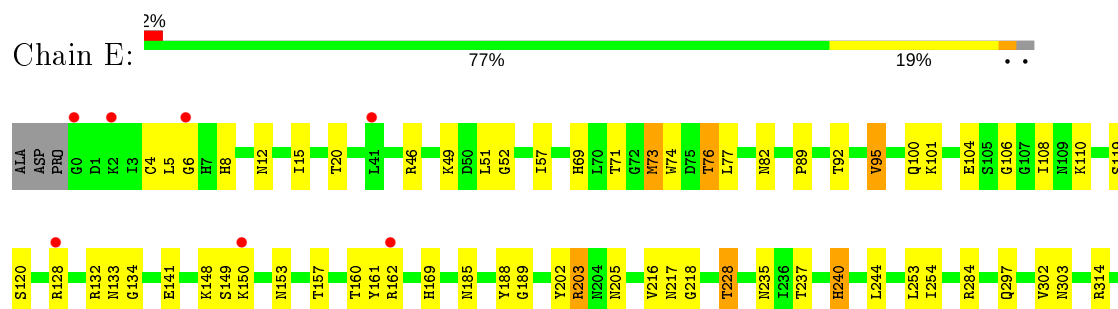
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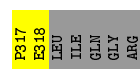
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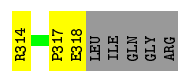
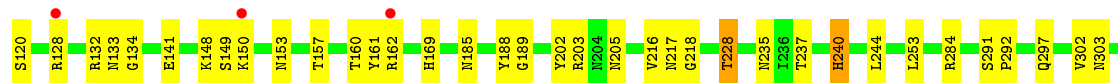
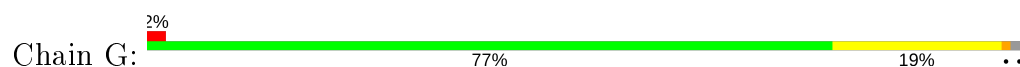
- Molecule 1: Hemagglutinin HA1 chain



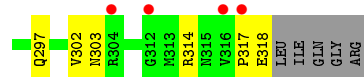
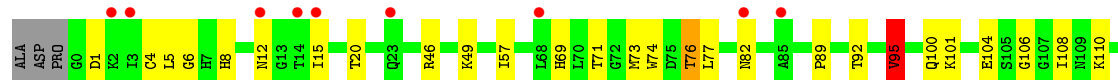
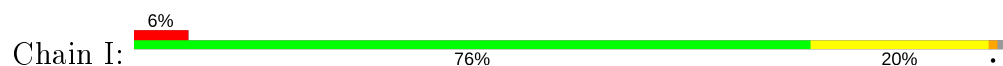




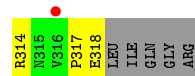
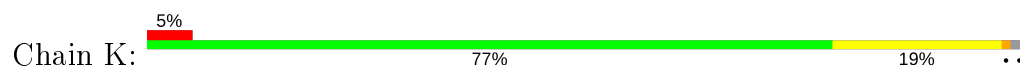
- Molecule 1: Hemagglutinin HA1 chain



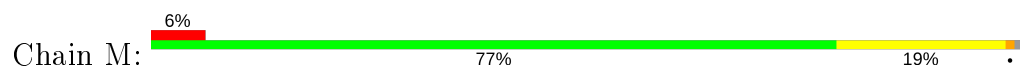
- Molecule 1: Hemagglutinin HA1 chain

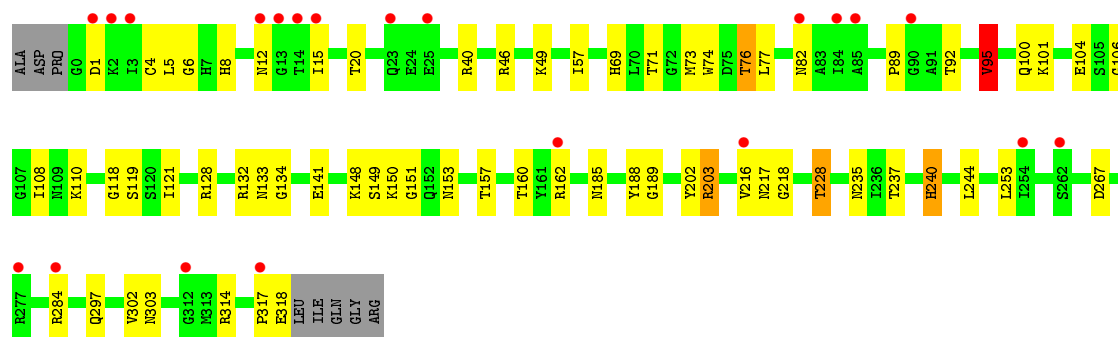


- Molecule 1: Hemagglutinin HA1 chain

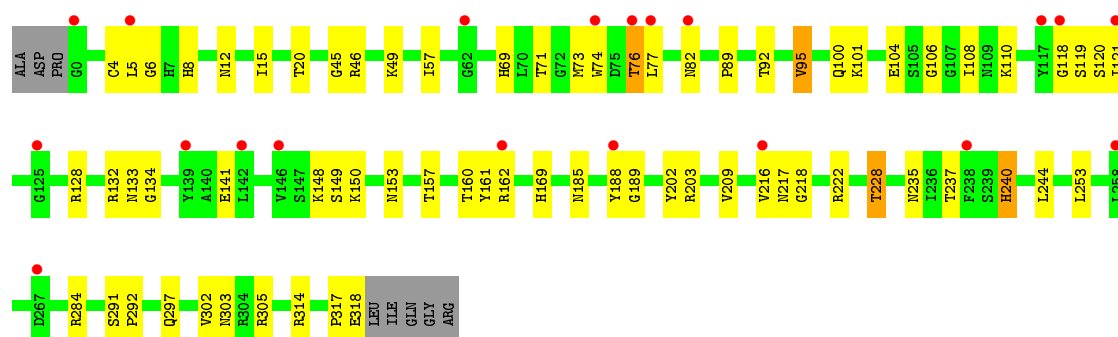
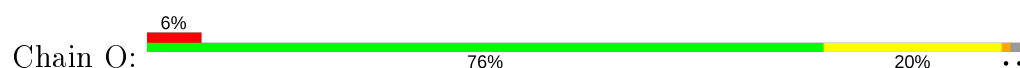


- Molecule 1: Hemagglutinin HA1 chain

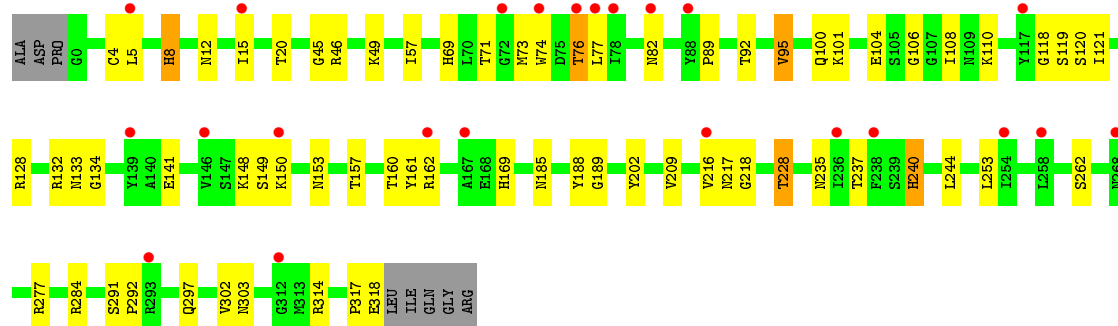
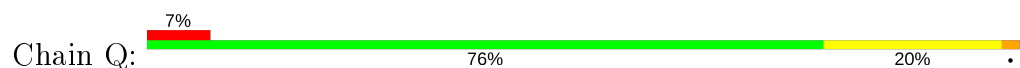




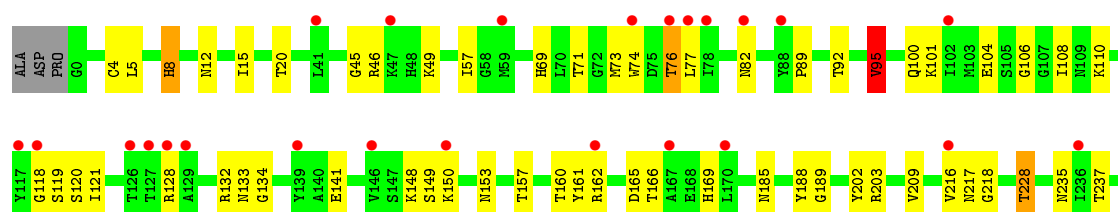
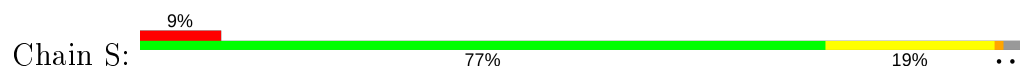
• Molecule 1: Hemagglutinin HA1 chain

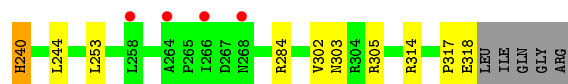


• Molecule 1: Hemagglutinin HA1 chain

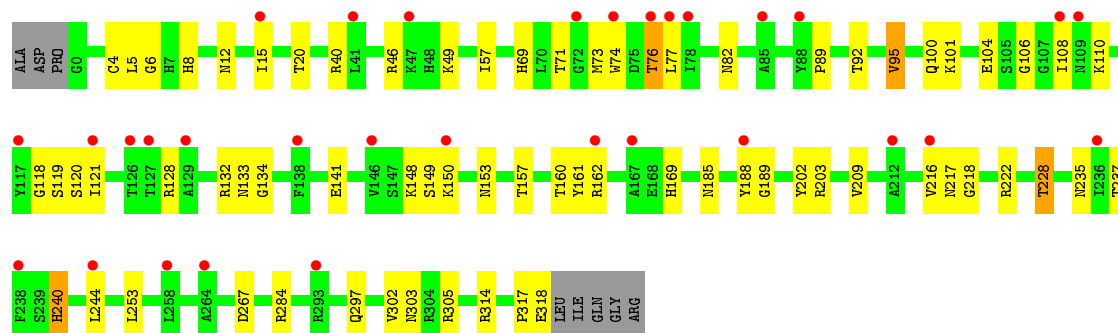
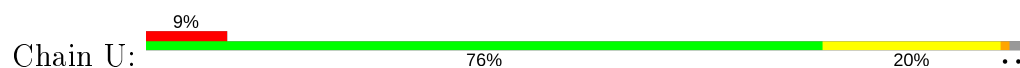


• Molecule 1: Hemagglutinin HA1 chain

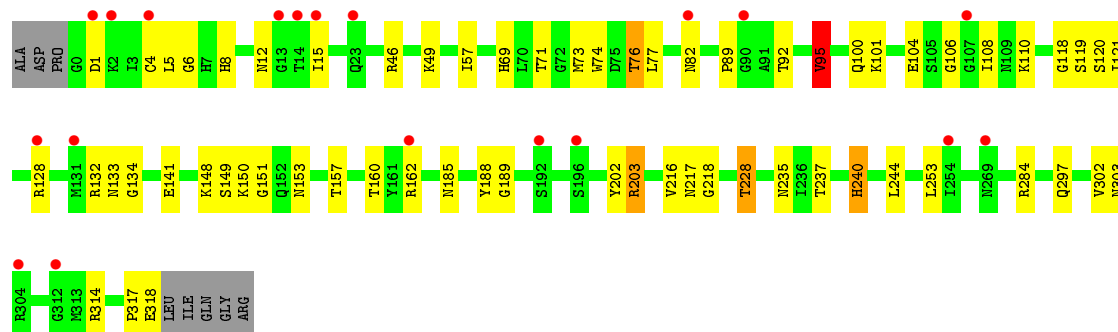
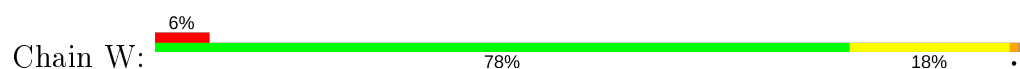




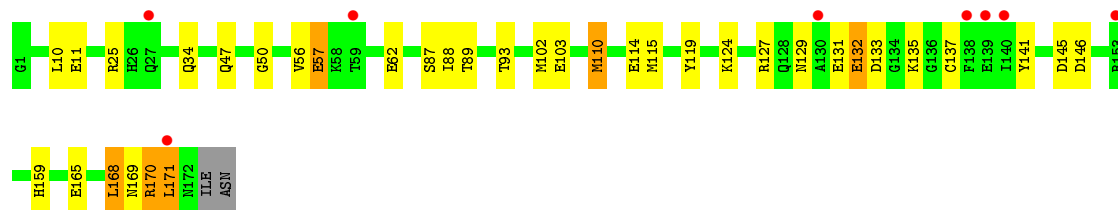
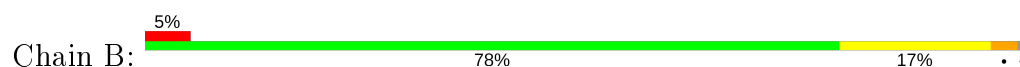
• Molecule 1: Hemagglutinin HA1 chain



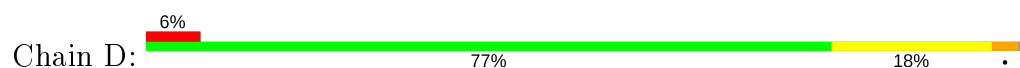
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 2: Hemagglutinin HA2 chain

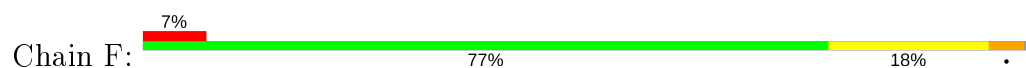


• Molecule 2: Hemagglutinin HA2 chain

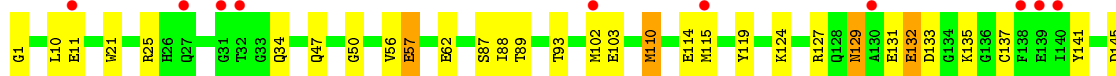
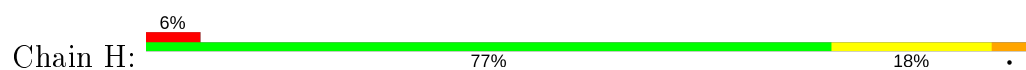




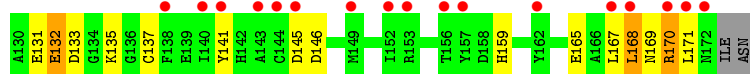
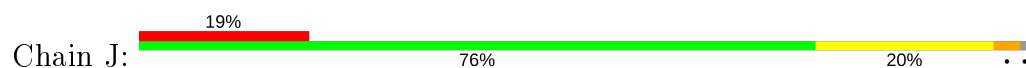
- Molecule 2: Hemagglutinin HA2 chain



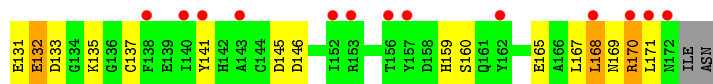
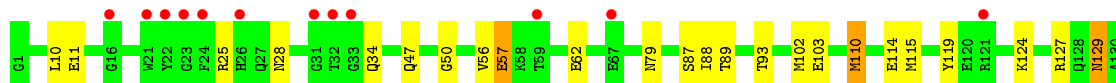
- Molecule 2: Hemagglutinin HA2 chain



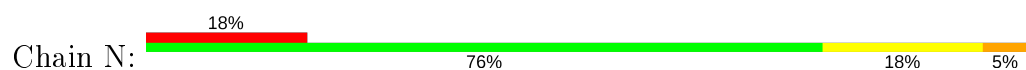
- Molecule 2: Hemagglutinin HA2 chain

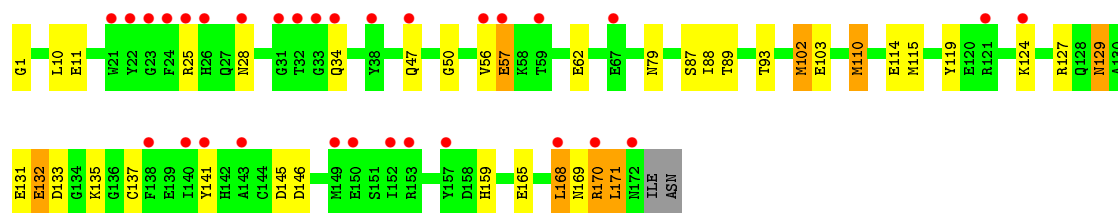


- Molecule 2: Hemagglutinin HA2 chain

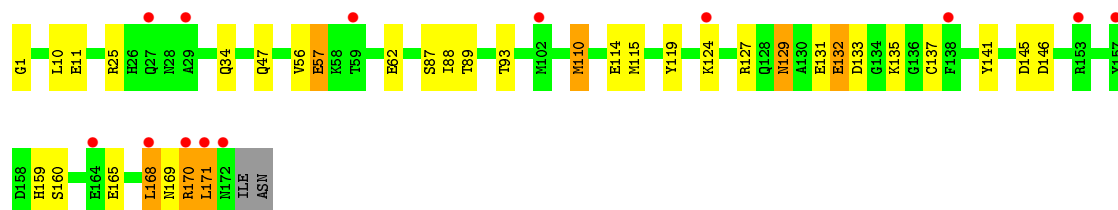
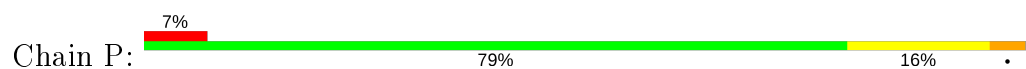


- Molecule 2: Hemagglutinin HA2 chain

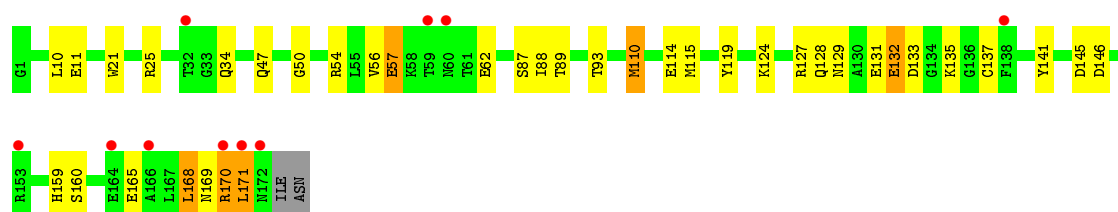
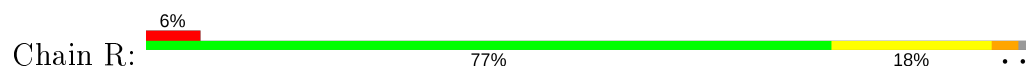




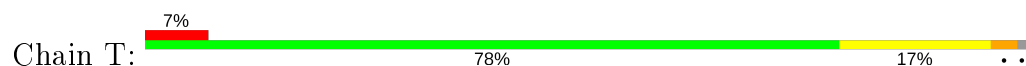
• Molecule 2: Hemagglutinin HA2 chain



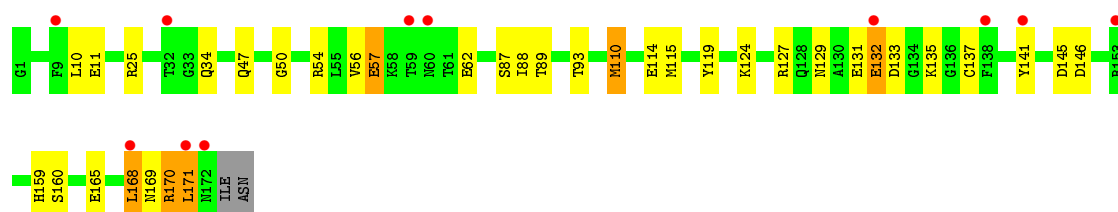
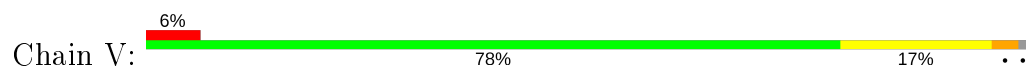
• Molecule 2: Hemagglutinin HA2 chain



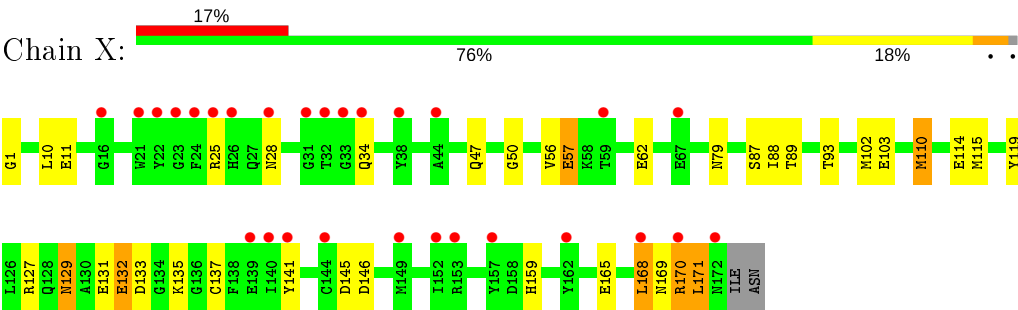
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



● Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.40Å 217.61Å 146.27Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	48.76 – 2.70 48.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-2.70) 99.6 (48.62-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.243 , 0.266 0.243 , 0.265	Depositor DCC
$R_{free}$ test set	9317 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.466 for k,h,-l 0.460 for -k,-h,-l 0.001 for -1/2*h-1/2*k+l,1/2*h+1/2*k+l,-1/2*h+1/2*k 0.002 for -1/2*h-1/2*k-l,1/2*h+1/2*k-l,1/2*h-1/2*k 0.001 for -1/2*h+1/2*k-l,-1/2*h+1/2*k+l,1/2*h+1/2*k 0.002 for -1/2*h+1/2*k+l,-1/2*h+1/2*k-l,-1/2*h-1/2*k 0.003 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.003 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.002 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/2*h+1/2*k 0.004 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2*h-1/2*k 0.466 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	46260	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

<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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.66	0/2490	0.80	1/3373 (0.0%)
1	C	0.66	0/2490	0.80	1/3373 (0.0%)
1	E	0.66	0/2490	0.80	1/3373 (0.0%)
1	G	0.66	0/2490	0.80	1/3373 (0.0%)
1	I	0.58	0/2490	0.79	3/3373 (0.1%)
1	K	0.59	0/2490	0.78	3/3373 (0.1%)
1	M	0.58	0/2490	0.78	3/3373 (0.1%)
1	O	0.57	0/2490	0.78	0/3373
1	Q	0.56	0/2490	0.77	0/3373
1	S	0.57	0/2490	0.77	1/3373 (0.0%)
1	U	0.57	0/2490	0.77	0/3373
1	W	0.59	0/2490	0.78	3/3373 (0.1%)
2	B	0.65	0/1411	0.75	0/1904
2	D	0.65	1/1411 (0.1%)	0.75	0/1904
2	F	0.66	1/1411 (0.1%)	0.76	0/1904
2	H	0.66	1/1411 (0.1%)	0.75	0/1904
2	J	0.64	1/1411 (0.1%)	0.73	0/1904
2	L	0.63	0/1411	0.73	0/1904
2	N	0.64	1/1411 (0.1%)	0.73	1/1904 (0.1%)
2	P	0.64	1/1411 (0.1%)	0.76	0/1904
2	R	0.63	0/1411	0.76	1/1904 (0.1%)
2	T	0.64	1/1411 (0.1%)	0.77	1/1904 (0.1%)
2	V	0.64	0/1411	0.76	1/1904 (0.1%)
2	X	0.63	1/1411 (0.1%)	0.73	0/1904
All	All	0.62	8/46812 (0.0%)	0.77	21/63324 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
1	G	0	2
1	I	0	2
1	K	0	2
1	M	0	2
1	O	0	2
1	Q	0	2
1	S	0	2
1	U	0	2
1	W	0	2
All	All	0	24

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	GLY	N-CA	5.82	1.54	1.46
2	H	1	GLY	N-CA	5.37	1.54	1.46
2	N	1	GLY	N-CA	5.31	1.54	1.46
2	J	1	GLY	N-CA	5.28	1.53	1.46
2	P	1	GLY	N-CA	5.12	1.53	1.46
2	D	1	GLY	N-CA	5.06	1.53	1.46
2	T	1	GLY	N-CA	5.04	1.53	1.46
2	X	1	GLY	N-CA	5.03	1.53	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	102	MET	CG-SD-CE	-5.41	91.54	100.20
1	I	95	VAL	CB-CA-C	-5.38	101.17	111.40
1	W	95	VAL	CB-CA-C	-5.37	101.20	111.40
1	I	203	ARG	CG-CD-NE	-5.36	100.54	111.80
2	R	54	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	T	54	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	M	203	ARG	CG-CD-NE	-5.21	100.87	111.80
1	W	151	GLY	N-CA-C	-5.20	100.10	113.10
1	K	203	ARG	CG-CD-NE	-5.18	100.91	111.80
1	A	95	VAL	CB-CA-C	-5.18	101.56	111.40
1	M	151	GLY	N-CA-C	-5.16	100.20	113.10
1	W	203	ARG	CG-CD-NE	-5.12	101.04	111.80
1	K	95	VAL	CB-CA-C	-5.12	101.67	111.40
1	K	151	GLY	N-CA-C	-5.10	100.35	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	95	VAL	CB-CA-C	-5.08	101.75	111.40
1	G	95	VAL	CB-CA-C	-5.07	101.78	111.40
1	S	95	VAL	CB-CA-C	-5.07	101.77	111.40
2	V	54	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	203	ARG	CG-CD-NE	-5.06	101.18	111.80
1	C	95	VAL	CB-CA-C	-5.03	101.84	111.40
1	I	151	GLY	N-CA-C	-5.02	100.56	113.10

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	SER	Peptide
1	A	82	ASN	Peptide
1	C	149	SER	Peptide
1	C	82	ASN	Peptide
1	E	149	SER	Peptide
1	E	82	ASN	Peptide
1	G	149	SER	Peptide
1	G	82	ASN	Peptide
1	I	149	SER	Peptide
1	I	82	ASN	Peptide
1	K	149	SER	Peptide
1	K	82	ASN	Peptide
1	M	149	SER	Peptide
1	M	82	ASN	Peptide
1	O	149	SER	Peptide
1	O	82	ASN	Peptide
1	Q	149	SER	Peptide
1	Q	82	ASN	Peptide
1	S	149	SER	Peptide
1	S	82	ASN	Peptide
1	U	149	SER	Peptide
1	U	82	ASN	Peptide
1	W	149	SER	Peptide
1	W	82	ASN	Peptide

## 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	2441	0	2392	42	0
1	C	2441	0	2392	44	0
1	E	2441	0	2392	41	0
1	G	2441	0	2392	42	0
1	I	2441	0	2392	40	0
1	K	2441	0	2392	39	0
1	M	2441	0	2392	38	0
1	O	2441	0	2392	46	0
1	Q	2441	0	2392	44	0
1	S	2441	0	2392	46	0
1	U	2441	0	2392	43	0
1	W	2441	0	2392	37	0
2	B	1386	0	1284	37	0
2	D	1386	0	1284	38	0
2	F	1386	0	1284	41	0
2	H	1386	0	1284	41	0
2	J	1386	0	1284	45	0
2	L	1386	0	1284	44	0
2	N	1386	0	1284	41	1
2	P	1386	0	1284	37	0
2	R	1386	0	1284	36	0
2	T	1386	0	1284	34	0
2	V	1386	0	1284	36	0
2	X	1386	0	1284	41	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	0	0
3	E	14	0	13	0	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	1	0
3	J	14	0	13	1	0
3	K	14	0	13	0	0
3	L	14	0	13	1	0
3	M	14	0	13	0	0
3	N	14	0	13	1	0
3	O	14	0	13	0	0
3	P	14	0	13	0	0
3	Q	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	14	0	13	0	0
3	S	14	0	13	0	0
3	T	14	0	13	0	0
3	U	14	0	13	0	0
3	V	14	0	13	0	0
3	W	14	0	13	0	0
3	X	14	0	13	1	0
All	All	46260	0	44424	806	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 9.

All (806) 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:T:89:THR:O	2:T:93:THR:HG23	1.65	0.97
2:V:89:THR:O	2:V:93:THR:HG23	1.66	0.96
2:L:89:THR:O	2:L:93:THR:HG23	1.66	0.96
2:P:89:THR:O	2:P:93:THR:HG23	1.66	0.95
2:X:89:THR:O	2:X:93:THR:HG23	1.66	0.95
2:D:89:THR:O	2:D:93:THR:HG23	1.67	0.94
2:N:89:THR:O	2:N:93:THR:HG23	1.67	0.94
2:B:89:THR:O	2:B:93:THR:HG23	1.67	0.94
2:H:89:THR:O	2:H:93:THR:HG23	1.68	0.94
2:R:89:THR:O	2:R:93:THR:HG23	1.66	0.94
2:J:89:THR:O	2:J:93:THR:HG23	1.67	0.93
2:F:89:THR:O	2:F:93:THR:HG23	1.67	0.93
2:H:131:GLU:HG3	2:J:127:ARG:HH21	1.44	0.81
2:L:170:ARG:HH21	2:L:171:LEU:HD22	1.48	0.79
2:J:170:ARG:HH21	2:J:171:LEU:HD22	1.49	0.76
2:H:131:GLU:HG3	2:J:127:ARG:NH2	2.00	0.76
2:L:170:ARG:NH2	2:L:171:LEU:HD22	2.01	0.75
2:J:170:ARG:NH2	2:J:171:LEU:HD22	2.01	0.74
2:F:131:GLU:HG3	2:L:127:ARG:HH21	1.52	0.73
2:D:131:GLU:HG3	2:N:127:ARG:HH21	1.52	0.73
2:N:131:GLU:HG3	2:V:127:ARG:HH21	1.54	0.73
1:A:74:TRP:CD1	1:A:106:GLY:HA2	2.23	0.72
1:C:74:TRP:CD1	1:C:106:GLY:HA2	2.23	0.72
2:B:131:GLU:HG3	2:X:127:ARG:HH21	1.55	0.72
1:S:46:ARG:HE	1:S:76:THR:HG21	1.55	0.72
1:E:74:TRP:CD1	1:E:106:GLY:HA2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:131:GLU:HG3	2:R:127:ARG:HH21	1.55	0.71
2:F:132:GLU:CD	2:L:124:LYS:HE2	2.11	0.71
2:F:131:GLU:HG3	2:L:127:ARG:NH2	2.06	0.71
1:U:46:ARG:HE	1:U:76:THR:HG21	1.56	0.71
1:G:74:TRP:CD1	1:G:106:GLY:HA2	2.25	0.70
2:D:132:GLU:CD	2:N:124:LYS:HE2	2.12	0.70
2:B:132:GLU:CD	2:X:124:LYS:HE2	2.12	0.70
1:I:127:THR:OG1	1:I:219:GLN:NE2	2.25	0.69
2:D:131:GLU:HG3	2:N:127:ARG:NH2	2.06	0.69
1:Q:46:ARG:HE	1:Q:76:THR:HG21	1.57	0.69
1:I:74:TRP:CD1	1:I:106:GLY:HA2	2.27	0.69
2:L:131:GLU:HG3	2:T:127:ARG:HH21	1.55	0.69
2:H:132:GLU:CD	2:J:124:LYS:HE2	2.12	0.69
1:U:74:TRP:CD1	1:U:106:GLY:HA2	2.27	0.69
1:U:108:ILE:HG22	1:U:253:LEU:HD23	1.73	0.69
1:O:74:TRP:CD1	1:O:106:GLY:HA2	2.27	0.69
2:B:131:GLU:HG3	2:X:127:ARG:NH2	2.07	0.69
1:S:74:TRP:CD1	1:S:106:GLY:HA2	2.28	0.69
1:E:108:ILE:HG22	1:E:253:LEU:HD23	1.75	0.69
1:Q:74:TRP:CD1	1:Q:106:GLY:HA2	2.28	0.68
1:Q:108:ILE:HG22	1:Q:253:LEU:HD23	1.74	0.68
1:W:74:TRP:CD1	1:W:106:GLY:HA2	2.28	0.68
1:C:108:ILE:HG22	1:C:253:LEU:HD23	1.75	0.68
1:K:74:TRP:CD1	1:K:106:GLY:HA2	2.27	0.68
1:M:74:TRP:CD1	1:M:106:GLY:HA2	2.28	0.68
1:I:108:ILE:HG22	1:I:253:LEU:HD23	1.76	0.68
1:S:108:ILE:HG22	1:S:253:LEU:HD23	1.74	0.68
1:O:108:ILE:HG22	1:O:253:LEU:HD23	1.73	0.68
1:A:108:ILE:HG22	1:A:253:LEU:HD23	1.76	0.68
2:P:127:ARG:HH21	2:X:131:GLU:HG3	1.57	0.67
1:O:46:ARG:HE	1:O:76:THR:HG21	1.58	0.67
1:K:108:ILE:HG22	1:K:253:LEU:HD23	1.77	0.67
1:W:108:ILE:HG22	1:W:253:LEU:HD23	1.76	0.67
1:G:108:ILE:HG22	1:G:253:LEU:HD23	1.77	0.67
1:S:46:ARG:HE	1:S:76:THR:CG2	2.07	0.66
2:R:10:LEU:CD1	2:R:115:MET:HE3	2.25	0.66
2:T:10:LEU:CD1	2:T:115:MET:HE3	2.26	0.66
1:M:108:ILE:HG22	1:M:253:LEU:HD23	1.77	0.66
1:U:46:ARG:HE	1:U:76:THR:CG2	2.09	0.65
1:G:46:ARG:HE	1:G:76:THR:HG21	1.62	0.65
1:M:157:THR:HB	1:M:240:HIS:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:46:ARG:HE	1:Q:76:THR:CG2	2.09	0.65
1:M:240:HIS:CD2	1:M:244:LEU:HD23	2.32	0.65
1:M:46:ARG:HE	1:M:76:THR:HG21	1.61	0.65
1:O:46:ARG:HE	1:O:76:THR:CG2	2.10	0.64
1:K:46:ARG:HE	1:K:76:THR:HG21	1.62	0.64
2:B:10:LEU:CD1	2:B:115:MET:HE3	2.28	0.64
1:K:240:HIS:CD2	1:K:244:LEU:HD23	2.33	0.64
1:I:46:ARG:HE	1:I:76:THR:HG21	1.62	0.64
1:C:157:THR:HB	1:C:240:HIS:CE1	2.33	0.63
1:I:157:THR:HB	1:I:240:HIS:CE1	2.32	0.63
1:I:240:HIS:CD2	1:I:244:LEU:HD23	2.33	0.63
1:Q:157:THR:HB	1:Q:240:HIS:CE1	2.33	0.63
1:W:157:THR:HB	1:W:240:HIS:CE1	2.33	0.63
1:O:157:THR:HB	1:O:240:HIS:CE1	2.32	0.63
1:E:157:THR:HB	1:E:240:HIS:CE1	2.33	0.63
1:U:157:THR:HB	1:U:240:HIS:CE1	2.34	0.63
1:K:157:THR:HB	1:K:240:HIS:CE1	2.34	0.63
1:W:240:HIS:CD2	1:W:244:LEU:HD23	2.34	0.63
1:G:157:THR:HB	1:G:240:HIS:CE1	2.34	0.62
2:P:25:ARG:NH1	2:P:34:GLN:OE1	2.33	0.62
2:T:47:GLN:NE2	2:T:110:MET:HE3	2.13	0.62
2:V:25:ARG:NH1	2:V:34:GLN:OE1	2.33	0.62
1:W:46:ARG:HE	1:W:76:THR:HG21	1.62	0.62
1:S:157:THR:HB	1:S:240:HIS:CE1	2.35	0.62
1:A:157:THR:HB	1:A:240:HIS:CE1	2.34	0.62
2:D:10:LEU:CD1	2:D:115:MET:HE3	2.31	0.61
1:K:46:ARG:HE	1:K:76:THR:CG2	2.13	0.61
1:C:46:ARG:HE	1:C:76:THR:HG21	1.65	0.61
1:E:46:ARG:HE	1:E:76:THR:HG21	1.65	0.61
2:F:10:LEU:CD1	2:F:115:MET:HE3	2.29	0.61
1:A:46:ARG:HE	1:A:76:THR:HG21	1.65	0.61
1:M:46:ARG:HE	1:M:76:THR:CG2	2.13	0.61
2:P:47:GLN:NE2	2:P:110:MET:HE3	2.15	0.61
2:X:10:LEU:CD1	2:X:115:MET:HE3	2.30	0.61
1:I:46:ARG:HE	1:I:76:THR:CG2	2.14	0.61
2:P:10:LEU:CD1	2:P:115:MET:HE3	2.31	0.61
2:R:25:ARG:NH1	2:R:34:GLN:OE1	2.33	0.61
1:W:202:TYR:CD1	1:W:228:THR:HG21	2.36	0.61
1:G:46:ARG:HE	1:G:76:THR:CG2	2.13	0.60
1:K:202:TYR:CD1	1:K:228:THR:HG21	2.36	0.60
2:L:47:GLN:NE2	2:L:110:MET:HE3	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:46:ARG:HE	1:W:76:THR:CG2	2.13	0.60
2:D:57:GLU:O	2:D:57:GLU:OE1	2.20	0.60
2:H:10:LEU:CD1	2:H:115:MET:HE3	2.31	0.60
2:H:57:GLU:O	2:H:57:GLU:OE1	2.20	0.60
2:X:47:GLN:NE2	2:X:110:MET:HE3	2.15	0.60
1:A:240:HIS:CD2	1:A:244:LEU:HD23	2.37	0.60
2:J:25:ARG:NH1	2:J:34:GLN:OE1	2.35	0.60
2:L:25:ARG:NH1	2:L:34:GLN:OE1	2.35	0.60
1:O:240:HIS:CD2	1:O:244:LEU:HD23	2.37	0.60
1:M:202:TYR:CD1	1:M:228:THR:HG21	2.37	0.60
2:T:25:ARG:NH1	2:T:34:GLN:OE1	2.34	0.60
2:B:11:GLU:OE2	2:B:135:LYS:HE3	2.02	0.59
1:I:202:TYR:CD1	1:I:228:THR:HG21	2.37	0.59
2:N:25:ARG:NH1	2:N:34:GLN:OE1	2.35	0.59
2:X:25:ARG:NH1	2:X:34:GLN:OE1	2.35	0.59
1:C:240:HIS:CD2	1:C:244:LEU:HD23	2.37	0.59
1:E:240:HIS:CD2	1:E:244:LEU:HD23	2.37	0.59
2:B:57:GLU:O	2:B:57:GLU:OE1	2.20	0.59
2:F:11:GLU:OE2	2:F:135:LYS:HE3	2.02	0.59
2:V:57:GLU:O	2:V:57:GLU:OE1	2.21	0.59
2:F:57:GLU:OE1	2:F:57:GLU:O	2.20	0.59
1:G:240:HIS:CD2	1:G:244:LEU:HD23	2.37	0.59
2:H:11:GLU:OE2	2:H:135:LYS:HE3	2.02	0.59
2:J:11:GLU:OE2	2:J:135:LYS:HE3	2.03	0.59
2:V:11:GLU:OE2	2:V:135:LYS:HE3	2.03	0.59
1:E:46:ARG:HE	1:E:76:THR:CG2	2.16	0.59
2:N:168:LEU:HG	2:N:169:ASN:N	2.18	0.59
2:P:11:GLU:OE2	2:P:135:LYS:HE3	2.03	0.59
2:T:57:GLU:O	2:T:57:GLU:OE1	2.21	0.59
2:V:10:LEU:CD1	2:V:115:MET:HE3	2.33	0.59
1:Q:240:HIS:CD2	1:Q:244:LEU:HD23	2.38	0.59
2:N:11:GLU:OE2	2:N:135:LYS:HE3	2.03	0.59
2:R:11:GLU:OE2	2:R:135:LYS:HE3	2.02	0.59
2:T:11:GLU:OE2	2:T:135:LYS:HE3	2.03	0.59
2:X:11:GLU:OE2	2:X:135:LYS:HE3	2.03	0.59
1:C:46:ARG:HE	1:C:76:THR:CG2	2.16	0.58
2:R:127:ARG:HD3	2:R:159:HIS:CE1	2.38	0.58
2:D:11:GLU:OE2	2:D:135:LYS:HE3	2.02	0.58
2:D:25:ARG:NH1	2:D:34:GLN:OE1	2.37	0.58
2:P:57:GLU:O	2:P:57:GLU:OE1	2.21	0.58
1:C:133:ASN:N	1:C:134:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ARG:NH1	2:B:34:GLN:OE1	2.36	0.58
2:P:127:ARG:HD3	2:P:159:HIS:CE1	2.39	0.58
1:U:240:HIS:CD2	1:U:244:LEU:HD23	2.38	0.58
2:X:168:LEU:HG	2:X:169:ASN:N	2.18	0.58
2:L:11:GLU:OE2	2:L:135:LYS:HE3	2.03	0.58
2:X:57:GLU:OE1	2:X:57:GLU:O	2.21	0.58
2:J:168:LEU:HG	2:J:169:ASN:N	2.18	0.58
2:N:57:GLU:O	2:N:57:GLU:OE1	2.21	0.58
2:R:57:GLU:O	2:R:57:GLU:OE1	2.21	0.58
2:V:127:ARG:HD3	2:V:159:HIS:CE1	2.39	0.58
2:F:25:ARG:NH1	2:F:34:GLN:OE1	2.36	0.58
2:J:10:LEU:CD1	2:J:115:MET:HE3	2.33	0.58
1:A:46:ARG:HE	1:A:76:THR:CG2	2.16	0.57
2:L:57:GLU:O	2:L:57:GLU:OE1	2.21	0.57
1:S:46:ARG:NE	1:S:76:THR:HG21	2.18	0.57
2:J:57:GLU:O	2:J:57:GLU:OE1	2.21	0.57
2:L:168:LEU:HG	2:L:169:ASN:N	2.18	0.57
2:H:25:ARG:NH1	2:H:34:GLN:OE1	2.36	0.57
2:J:124:LYS:HA	2:J:124:LYS:HE3	1.87	0.57
1:Q:46:ARG:NE	1:Q:76:THR:HG21	2.19	0.57
2:T:127:ARG:HD3	2:T:159:HIS:CE1	2.39	0.57
1:U:46:ARG:NE	1:U:76:THR:HG21	2.19	0.57
2:V:47:GLN:NE2	2:V:110:MET:HE3	2.19	0.57
2:L:124:LYS:HA	2:L:124:LYS:HE3	1.87	0.57
1:C:297:GLN:HG3	2:D:62:GLU:HG2	1.87	0.57
1:S:240:HIS:CD2	1:S:244:LEU:HD23	2.38	0.57
2:R:47:GLN:NE2	2:R:110:MET:HE3	2.20	0.57
1:E:133:ASN:N	1:E:134:GLY:O	2.37	0.56
1:S:202:TYR:CD1	1:S:228:THR:HG21	2.40	0.56
2:X:124:LYS:HA	2:X:124:LYS:HE3	1.87	0.56
2:N:79:ASN:OD1	3:N:301:NAG:H81	2.06	0.56
1:Q:133:ASN:N	1:Q:134:GLY:O	2.39	0.56
2:J:110:MET:HE2	2:J:114:GLU:HG2	1.88	0.56
2:N:47:GLN:NE2	2:N:110:MET:HE3	2.19	0.56
2:N:10:LEU:CD1	2:N:115:MET:HE3	2.36	0.56
2:N:124:LYS:HE3	2:N:124:LYS:HA	1.87	0.56
1:A:202:TYR:CD1	1:A:228:THR:HG21	2.41	0.56
2:R:10:LEU:HD13	2:R:115:MET:HE3	1.87	0.56
1:E:5:LEU:HD22	2:F:119:TYR:HA	1.88	0.56
2:T:10:LEU:HD13	2:T:115:MET:HE3	1.88	0.56
1:A:297:GLN:HG3	2:B:62:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:TYR:CD1	1:C:228:THR:HG21	2.41	0.56
1:O:202:TYR:CD1	1:O:228:THR:HG21	2.41	0.56
1:Q:12:ASN:OD1	1:Q:12:ASN:N	2.39	0.56
2:B:168:LEU:HG	2:B:169:ASN:N	2.21	0.56
1:I:12:ASN:OD1	1:I:12:ASN:N	2.39	0.56
1:O:12:ASN:N	1:O:12:ASN:OD1	2.39	0.56
1:Q:202:TYR:CD1	1:Q:228:THR:HG21	2.41	0.56
1:U:133:ASN:N	1:U:134:GLY:O	2.39	0.56
1:U:202:TYR:CD1	1:U:228:THR:HG21	2.40	0.56
2:D:168:LEU:HG	2:D:169:ASN:N	2.21	0.55
2:D:88:ILE:HD13	2:V:87:SER:HB3	1.89	0.55
1:M:46:ARG:NE	1:M:76:THR:HG21	2.21	0.55
1:A:133:ASN:N	1:A:134:GLY:O	2.39	0.55
2:B:124:LYS:HA	2:B:124:LYS:HE3	1.89	0.55
2:F:124:LYS:HA	2:F:124:LYS:HE3	1.89	0.55
1:S:12:ASN:OD1	1:S:12:ASN:N	2.39	0.55
1:E:202:TYR:CD1	1:E:228:THR:HG21	2.41	0.55
1:E:317:PRO:O	1:E:318:GLU:HB2	2.07	0.55
1:A:12:ASN:N	1:A:12:ASN:OD1	2.40	0.55
1:G:133:ASN:N	1:G:134:GLY:O	2.39	0.55
2:H:168:LEU:HG	2:H:169:ASN:N	2.21	0.55
1:K:133:ASN:N	1:K:134:GLY:O	2.40	0.55
1:E:12:ASN:OD1	1:E:12:ASN:N	2.40	0.55
1:I:240:HIS:HD2	1:I:244:LEU:HB3	1.72	0.55
1:U:12:ASN:OD1	1:U:12:ASN:N	2.39	0.55
1:W:12:ASN:OD1	1:W:12:ASN:N	2.39	0.55
1:I:46:ARG:NE	1:I:76:THR:HG21	2.22	0.55
1:M:12:ASN:OD1	1:M:12:ASN:N	2.39	0.55
1:O:46:ARG:NE	1:O:76:THR:HG21	2.20	0.55
1:W:46:ARG:NE	1:W:76:THR:HG21	2.22	0.55
1:C:317:PRO:O	1:C:318:GLU:HB2	2.07	0.55
1:I:133:ASN:N	1:I:134:GLY:O	2.40	0.55
2:R:124:LYS:HE3	2:R:124:LYS:HA	1.89	0.55
1:G:202:TYR:CD1	1:G:228:THR:HG21	2.41	0.54
1:G:46:ARG:NE	1:G:76:THR:HG21	2.22	0.54
1:M:133:ASN:N	1:M:134:GLY:O	2.40	0.54
1:C:12:ASN:N	1:C:12:ASN:OD1	2.40	0.54
2:D:124:LYS:HE3	2:D:124:LYS:HA	1.89	0.54
1:G:317:PRO:O	1:G:318:GLU:HB2	2.07	0.54
2:H:124:LYS:HA	2:H:124:LYS:HE3	1.89	0.54
1:I:217:ASN:N	1:I:218:GLY:HA3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:ASN:OD1	1:K:12:ASN:N	2.40	0.54
2:F:168:LEU:HG	2:F:169:ASN:N	2.21	0.54
2:P:124:LYS:HA	2:P:124:LYS:HE3	1.90	0.54
1:W:133:ASN:N	1:W:134:GLY:O	2.40	0.54
1:G:12:ASN:N	1:G:12:ASN:OD1	2.40	0.54
2:J:79:ASN:OD1	3:J:301:NAG:H81	2.08	0.54
1:K:317:PRO:O	1:K:318:GLU:HB2	2.08	0.54
1:G:284:ARG:HB3	2:H:56:VAL:HG13	1.90	0.54
1:K:46:ARG:NE	1:K:76:THR:HG21	2.22	0.54
1:O:133:ASN:N	1:O:134:GLY:O	2.40	0.54
1:S:133:ASN:N	1:S:134:GLY:O	2.40	0.54
1:A:89:PRO:HG3	1:A:216:VAL:O	2.08	0.54
1:K:240:HIS:HD2	1:K:244:LEU:HB3	1.73	0.54
1:W:92:THR:HB	1:W:95:VAL:HG13	1.90	0.54
1:E:49:LYS:HE2	1:E:69:HIS:ND1	2.23	0.54
1:G:5:LEU:HD22	2:H:119:TYR:HA	1.90	0.54
1:M:317:PRO:O	1:M:318:GLU:HB2	2.08	0.54
1:Q:317:PRO:O	1:Q:318:GLU:HB2	2.08	0.54
1:A:317:PRO:O	1:A:318:GLU:HB2	2.07	0.54
2:D:47:GLN:NE2	2:D:110:MET:HE3	2.23	0.54
1:E:297:GLN:HG3	2:F:62:GLU:HG2	1.89	0.54
2:L:79:ASN:OD1	3:L:301:NAG:H81	2.08	0.54
2:T:124:LYS:HA	2:T:124:LYS:HE3	1.90	0.54
2:B:10:LEU:HD13	2:B:115:MET:HE3	1.90	0.53
1:E:89:PRO:HG3	1:E:216:VAL:O	2.09	0.53
1:I:92:THR:HB	1:I:95:VAL:HG13	1.90	0.53
2:P:119:TYR:OH	2:P:132:GLU:HG2	2.08	0.53
2:R:119:TYR:OH	2:R:132:GLU:HG2	2.08	0.53
1:O:305:ARG:NH1	1:S:45:GLY:O	2.41	0.53
2:T:119:TYR:OH	2:T:132:GLU:HG2	2.08	0.53
2:V:119:TYR:OH	2:V:132:GLU:HG2	2.09	0.53
2:F:47:GLN:NE2	2:F:110:MET:HE3	2.23	0.53
1:I:317:PRO:O	1:I:318:GLU:HB2	2.07	0.53
1:A:303:ASN:HB2	2:B:93:THR:HG21	1.89	0.53
2:R:110:MET:HE2	2:R:114:GLU:HG2	1.90	0.53
1:S:317:PRO:O	1:S:318:GLU:HB2	2.08	0.53
2:V:124:LYS:HA	2:V:124:LYS:HE3	1.90	0.53
1:W:217:ASN:N	1:W:218:GLY:HA3	2.22	0.53
1:C:46:ARG:NE	1:C:76:THR:HG21	2.24	0.53
2:F:88:ILE:HD13	2:T:87:SER:HB3	1.91	0.53
1:M:217:ASN:N	1:M:218:GLY:HA3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:THR:HB	1:M:95:VAL:HG13	1.90	0.53
1:U:317:PRO:O	1:U:318:GLU:HB2	2.08	0.53
2:H:88:ILE:HD13	2:R:87:SER:HB3	1.91	0.53
1:M:240:HIS:HD2	1:M:244:LEU:HB3	1.73	0.53
1:C:5:LEU:HD22	2:D:119:TYR:HA	1.91	0.53
1:G:89:PRO:HG3	1:G:216:VAL:O	2.08	0.53
1:O:185:ASN:O	1:O:188:TYR:O	2.27	0.53
1:U:119:SER:O	1:U:120:SER:OG	2.27	0.53
1:W:317:PRO:O	1:W:318:GLU:HB2	2.08	0.53
1:A:5:LEU:HD22	2:B:119:TYR:HA	1.91	0.53
2:B:88:ILE:HD13	2:P:87:SER:HB3	1.91	0.53
2:H:47:GLN:NE2	2:H:110:MET:HE3	2.23	0.53
2:N:110:MET:HE2	2:N:114:GLU:HG2	1.91	0.53
1:G:185:ASN:O	1:G:188:TYR:O	2.27	0.53
1:K:92:THR:HB	1:K:95:VAL:HG13	1.91	0.53
2:P:170:ARG:CZ	2:P:171:LEU:HB3	2.39	0.53
1:E:303:ASN:HB2	2:F:93:THR:HG21	1.90	0.53
1:C:89:PRO:HG3	1:C:216:VAL:O	2.08	0.52
2:L:119:TYR:OH	2:L:132:GLU:HG2	2.09	0.52
1:Q:45:GLY:O	1:S:305:ARG:NH1	2.41	0.52
1:U:185:ASN:O	1:U:188:TYR:O	2.27	0.52
1:A:46:ARG:NE	1:A:76:THR:HG21	2.24	0.52
1:G:297:GLN:HG3	2:H:62:GLU:HG2	1.90	0.52
2:N:119:TYR:OH	2:N:132:GLU:HG2	2.10	0.52
1:W:240:HIS:HD2	1:W:244:LEU:HB3	1.73	0.52
2:B:110:MET:HE2	2:B:114:GLU:HG2	1.90	0.52
1:E:46:ARG:NE	1:E:76:THR:HG21	2.24	0.52
2:J:47:GLN:NE2	2:J:110:MET:HE3	2.24	0.52
2:V:170:ARG:CZ	2:V:171:LEU:HB3	2.39	0.52
1:Q:185:ASN:O	1:Q:188:TYR:O	2.28	0.52
2:X:119:TYR:OH	2:X:132:GLU:HG2	2.09	0.52
1:K:185:ASN:O	1:K:188:TYR:O	2.28	0.52
1:S:185:ASN:O	1:S:188:TYR:O	2.27	0.52
2:T:170:ARG:CZ	2:T:171:LEU:HB3	2.39	0.52
1:E:217:ASN:N	1:E:218:GLY:HA3	2.25	0.52
1:O:317:PRO:O	1:O:318:GLU:HB2	2.08	0.52
1:A:185:ASN:O	1:A:188:TYR:O	2.27	0.52
1:C:49:LYS:HE2	1:C:69:HIS:ND1	2.25	0.52
1:S:89:PRO:HG3	1:S:216:VAL:O	2.10	0.52
1:W:89:PRO:HG3	1:W:216:VAL:O	2.10	0.52
2:X:79:ASN:OD1	3:X:301:NAG:H81	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ARG:HD3	2:B:159:HIS:CE1	2.45	0.52
1:K:217:ASN:N	1:K:218:GLY:HA3	2.23	0.52
1:M:89:PRO:HG3	1:M:216:VAL:O	2.10	0.52
1:Q:92:THR:HB	1:Q:95:VAL:HG13	1.92	0.52
1:C:303:ASN:HB2	2:D:93:THR:HG21	1.92	0.52
1:U:89:PRO:HG3	1:U:216:VAL:O	2.10	0.52
1:W:185:ASN:O	1:W:188:TYR:O	2.28	0.52
1:A:217:ASN:N	1:A:218:GLY:HA3	2.25	0.52
1:I:284:ARG:HB3	2:J:56:VAL:HG13	1.92	0.52
2:R:10:LEU:HD11	2:R:115:MET:HE3	1.92	0.52
2:F:10:LEU:HD13	2:F:115:MET:HE3	1.91	0.51
1:G:303:ASN:HB2	2:H:93:THR:HG21	1.92	0.51
2:L:145:ASP:OD1	2:L:146:ASP:N	2.44	0.51
1:C:185:ASN:O	1:C:188:TYR:O	2.27	0.51
1:E:284:ARG:HB3	2:F:56:VAL:HG13	1.92	0.51
1:G:240:HIS:HD2	1:G:244:LEU:HB3	1.76	0.51
2:N:145:ASP:OD1	2:N:146:ASP:N	2.43	0.51
1:O:89:PRO:HG3	1:O:216:VAL:O	2.10	0.51
2:R:170:ARG:CZ	2:R:171:LEU:HB3	2.39	0.51
1:U:92:THR:HB	1:U:95:VAL:HG13	1.92	0.51
2:H:110:MET:HE2	2:H:114:GLU:HG2	1.93	0.51
1:K:89:PRO:HG3	1:K:216:VAL:O	2.10	0.51
1:A:92:THR:HB	1:A:95:VAL:HG13	1.93	0.51
1:C:119:SER:O	1:C:120:SER:OG	2.26	0.51
1:C:217:ASN:N	1:C:218:GLY:HA3	2.25	0.51
2:D:127:ARG:HD3	2:D:159:HIS:CE1	2.45	0.51
1:S:92:THR:HB	1:S:95:VAL:HG13	1.93	0.51
1:E:240:HIS:HD2	1:E:244:LEU:HB3	1.76	0.51
2:F:119:TYR:OH	2:F:132:GLU:HG2	2.11	0.51
1:G:4:CYS:HA	2:H:137:CYS:HA	1.93	0.51
1:I:185:ASN:O	1:I:188:TYR:O	2.28	0.51
1:A:49:LYS:HE2	1:A:69:HIS:ND1	2.26	0.51
1:C:240:HIS:HD2	1:C:244:LEU:HB3	1.75	0.51
1:C:92:THR:HB	1:C:95:VAL:HG13	1.93	0.51
2:J:119:TYR:OH	2:J:132:GLU:HG2	2.10	0.51
2:R:168:LEU:HG	2:R:169:ASN:N	2.25	0.51
2:T:168:LEU:HG	2:T:169:ASN:N	2.26	0.51
2:X:110:MET:HE2	2:X:114:GLU:HG2	1.92	0.51
2:X:10:LEU:HD13	2:X:115:MET:HE3	1.93	0.51
1:A:240:HIS:HD2	1:A:244:LEU:HB3	1.75	0.51
1:K:303:ASN:HB2	2:L:93:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:THR:O	2:L:50:GLY:HA3	2.11	0.51
2:P:145:ASP:OD1	2:P:146:ASP:N	2.44	0.51
1:Q:89:PRO:HG3	1:Q:216:VAL:O	2.11	0.51
2:X:145:ASP:OD1	2:X:146:ASP:N	2.43	0.51
1:I:49:LYS:HE2	1:I:69:HIS:ND1	2.26	0.51
1:K:6:GLY:CA	2:L:115:MET:HE1	2.41	0.51
1:Q:303:ASN:HB2	2:R:93:THR:HG21	1.91	0.51
1:W:284:ARG:HB3	2:X:56:VAL:HG13	1.93	0.51
2:D:119:TYR:OH	2:D:132:GLU:HG2	2.11	0.51
1:K:6:GLY:C	2:L:115:MET:HE1	2.31	0.51
1:O:240:HIS:HD2	1:O:244:LEU:HB3	1.75	0.51
1:O:92:THR:HB	1:O:95:VAL:HG13	1.93	0.51
2:P:168:LEU:HG	2:P:169:ASN:N	2.26	0.51
2:R:145:ASP:OD1	2:R:146:ASP:N	2.44	0.51
2:T:145:ASP:OD1	2:T:146:ASP:N	2.44	0.51
2:D:110:MET:HE2	2:D:114:GLU:HG2	1.92	0.50
1:G:217:ASN:N	1:G:218:GLY:HA3	2.25	0.50
2:J:145:ASP:OD1	2:J:146:ASP:N	2.43	0.50
2:V:110:MET:HE2	2:V:114:GLU:HG2	1.92	0.50
2:V:145:ASP:OD1	2:V:146:ASP:N	2.44	0.50
2:D:170:ARG:CZ	2:D:171:LEU:HB3	2.42	0.50
1:G:92:THR:HB	1:G:95:VAL:HG13	1.93	0.50
2:H:119:TYR:OH	2:H:132:GLU:HG2	2.11	0.50
1:I:89:PRO:HG3	1:I:216:VAL:O	2.10	0.50
2:T:10:LEU:HD11	2:T:115:MET:HE3	1.93	0.50
2:B:10:LEU:HD11	2:B:115:MET:HE3	1.93	0.50
1:C:284:ARG:HB3	2:D:56:VAL:HG13	1.94	0.50
1:E:92:THR:HB	1:E:95:VAL:HG13	1.93	0.50
2:F:127:ARG:HD3	2:F:159:HIS:CE1	2.46	0.50
1:M:185:ASN:O	1:M:188:TYR:O	2.28	0.50
2:N:170:ARG:CZ	2:N:171:LEU:HB3	2.41	0.50
1:S:5:LEU:HD22	2:T:119:TYR:HA	1.94	0.50
1:U:240:HIS:HD2	1:U:244:LEU:HB3	1.76	0.50
1:A:20:THR:O	2:X:50:GLY:HA3	2.12	0.50
1:A:284:ARG:HB3	2:B:56:VAL:HG13	1.93	0.50
1:C:132:ARG:O	1:C:134:GLY:HA2	2.12	0.50
1:G:132:ARG:O	1:G:134:GLY:HA2	2.12	0.50
1:M:284:ARG:HB3	2:N:56:VAL:HG13	1.92	0.50
1:E:4:CYS:HA	2:F:137:CYS:HA	1.94	0.50
2:L:110:MET:HE2	2:L:114:GLU:HG2	1.94	0.50
1:S:240:HIS:HD2	1:S:244:LEU:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:303:ASN:HB2	2:V:93:THR:HG21	1.94	0.50
2:B:119:TYR:OH	2:B:132:GLU:HG2	2.12	0.50
2:P:124:LYS:HE2	2:X:132:GLU:CD	2.32	0.50
1:S:132:ARG:O	1:S:134:GLY:HA2	2.12	0.50
2:N:132:GLU:CD	2:V:124:LYS:HE2	2.31	0.50
1:A:119:SER:O	1:A:120:SER:OG	2.26	0.50
1:G:6:GLY:CA	2:H:115:MET:HE1	2.41	0.50
1:E:132:ARG:O	1:E:134:GLY:HA2	2.12	0.50
1:E:185:ASN:O	1:E:188:TYR:O	2.27	0.50
1:K:284:ARG:HB3	2:L:56:VAL:HG13	1.94	0.50
1:O:45:GLY:O	1:U:305:ARG:NH1	2.45	0.50
1:Q:132:ARG:O	1:Q:134:GLY:HA2	2.11	0.50
1:Q:240:HIS:HD2	1:Q:244:LEU:HB3	1.76	0.50
1:G:49:LYS:HE2	1:G:69:HIS:ND1	2.26	0.50
2:V:170:ARG:NH2	2:V:171:LEU:HB3	2.27	0.50
2:F:110:MET:HE2	2:F:114:GLU:HG2	1.93	0.49
1:I:132:ARG:O	1:I:134:GLY:HA2	2.12	0.49
1:M:49:LYS:HE2	1:M:69:HIS:ND1	2.27	0.49
2:V:168:LEU:HG	2:V:169:ASN:N	2.27	0.49
1:W:49:LYS:HE2	1:W:69:HIS:ND1	2.27	0.49
1:O:303:ASN:HB2	2:P:93:THR:HG21	1.94	0.49
2:X:170:ARG:CZ	2:X:171:LEU:HB3	2.42	0.49
1:A:4:CYS:HA	2:B:137:CYS:HA	1.93	0.49
1:C:20:THR:O	2:N:50:GLY:HA3	2.11	0.49
2:D:10:LEU:HD13	2:D:115:MET:HE3	1.93	0.49
1:M:303:ASN:HB2	2:N:93:THR:HG21	1.94	0.49
1:A:132:ARG:O	1:A:134:GLY:HA2	2.12	0.49
2:B:170:ARG:CZ	2:B:171:LEU:HB3	2.42	0.49
1:I:303:ASN:HB2	2:J:93:THR:HG21	1.95	0.49
2:D:10:LEU:HD11	2:D:115:MET:HE3	1.94	0.49
2:H:127:ARG:HD3	2:H:159:HIS:CE1	2.47	0.49
1:K:49:LYS:HE2	1:K:69:HIS:ND1	2.27	0.49
1:O:49:LYS:HE2	1:O:69:HIS:ND1	2.27	0.49
2:V:10:LEU:HD11	2:V:115:MET:HE3	1.95	0.49
2:X:10:LEU:HD11	2:X:115:MET:HE3	1.94	0.49
2:P:110:MET:HE2	2:P:114:GLU:HG2	1.94	0.49
1:C:6:GLY:CA	2:D:115:MET:HE1	2.43	0.49
2:P:10:LEU:HD11	2:P:115:MET:HE3	1.94	0.49
2:P:170:ARG:NH2	2:P:171:LEU:HB3	2.27	0.49
2:D:145:ASP:OD1	2:D:146:ASP:N	2.46	0.49
2:H:170:ARG:CZ	2:H:171:LEU:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:170:ARG:NH2	2:R:171:LEU:HB3	2.28	0.49
1:W:132:ARG:O	1:W:134:GLY:HA2	2.13	0.49
1:W:303:ASN:HB2	2:X:93:THR:HG21	1.95	0.49
1:O:132:ARG:O	1:O:134:GLY:HA2	2.12	0.48
1:Q:49:LYS:HE2	1:Q:69:HIS:ND1	2.28	0.48
2:B:47:GLN:NE2	2:B:110:MET:HE3	2.28	0.48
1:I:1:ASP:OD1	2:J:28:ASN:HA	2.12	0.48
1:K:153:ASN:HA	1:K:189:GLY:CA	2.44	0.48
1:K:160:THR:HG22	1:K:237:THR:HG23	1.95	0.48
1:M:132:ARG:O	1:M:134:GLY:HA2	2.12	0.48
1:K:203:ARG:HG3	1:K:203:ARG:O	2.13	0.48
2:P:10:LEU:HD13	2:P:115:MET:HE3	1.94	0.48
1:E:119:SER:O	1:E:120:SER:OG	2.26	0.48
1:I:233:GLY:O	3:I:401:NAG:H82	2.13	0.48
1:Q:5:LEU:HD22	2:R:119:TYR:HA	1.96	0.48
1:U:132:ARG:O	1:U:134:GLY:HA2	2.12	0.48
1:G:302:VAL:HA	2:H:93:THR:HG22	1.96	0.48
2:H:10:LEU:HD13	2:H:115:MET:HE3	1.94	0.48
2:H:145:ASP:OD1	2:H:146:ASP:N	2.47	0.48
1:K:132:ARG:O	1:K:134:GLY:HA2	2.12	0.48
1:S:303:ASN:HB2	2:T:93:THR:HG21	1.95	0.48
2:F:170:ARG:CZ	2:F:171:LEU:HB3	2.42	0.48
2:F:170:ARG:NH2	2:F:171:LEU:HB3	2.29	0.48
2:L:132:GLU:CD	2:T:124:LYS:HE2	2.34	0.48
1:M:5:LEU:HD22	2:N:119:TYR:HA	1.96	0.48
2:T:170:ARG:NH2	2:T:171:LEU:HB3	2.28	0.48
1:C:160:THR:HG22	1:C:237:THR:HG23	1.95	0.48
2:J:132:GLU:CD	2:R:124:LYS:HE2	2.33	0.48
1:G:20:THR:O	2:J:50:GLY:HA3	2.13	0.48
1:U:217:ASN:N	1:U:218:GLY:HA3	2.29	0.48
1:W:153:ASN:HA	1:W:189:GLY:CA	2.44	0.48
2:B:127:ARG:HH21	2:P:131:GLU:HG3	1.79	0.48
2:D:170:ARG:NH2	2:D:171:LEU:HB3	2.28	0.48
2:L:127:ARG:HD3	2:L:159:HIS:CE1	2.49	0.48
1:O:119:SER:O	1:O:120:SER:OG	2.27	0.48
1:Q:302:VAL:HA	2:R:93:THR:HG22	1.95	0.48
2:P:88:ILE:HD13	2:X:87:SER:HB3	1.96	0.48
1:E:302:VAL:HA	2:F:93:THR:HG22	1.96	0.48
2:H:10:LEU:HD11	2:H:115:MET:HE3	1.95	0.48
1:W:160:THR:HG22	1:W:237:THR:HG23	1.96	0.48
1:E:6:GLY:CA	2:F:115:MET:HE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217:ASN:N	1:O:218:GLY:HA3	2.29	0.48
1:U:6:GLY:CA	2:V:115:MET:HE1	2.44	0.48
2:T:47:GLN:HE22	2:T:110:MET:HE3	1.79	0.47
1:S:284:ARG:HB3	2:T:56:VAL:HG13	1.96	0.47
1:U:5:LEU:HD22	2:V:119:TYR:HA	1.96	0.47
2:F:10:LEU:HD11	2:F:115:MET:HE3	1.94	0.47
1:O:160:THR:HG22	1:O:237:THR:HG23	1.96	0.47
1:S:49:LYS:HE2	1:S:69:HIS:ND1	2.29	0.47
1:U:160:THR:HG22	1:U:237:THR:HG23	1.96	0.47
1:U:49:LYS:HE2	1:U:69:HIS:ND1	2.29	0.47
1:W:5:LEU:HD22	2:X:119:TYR:HA	1.96	0.47
1:M:297:GLN:HG3	2:N:62:GLU:HG2	1.96	0.47
1:Q:153:ASN:HA	1:Q:189:GLY:CA	2.44	0.47
1:Q:217:ASN:N	1:Q:218:GLY:HA3	2.29	0.47
1:A:303:ASN:H	2:B:93:THR:CG2	2.28	0.47
2:T:110:MET:HE2	2:T:114:GLU:HG2	1.96	0.47
1:A:160:THR:HG22	1:A:237:THR:HG23	1.96	0.47
1:C:4:CYS:HA	2:D:137:CYS:HA	1.96	0.47
2:D:87:SER:HB3	2:N:88:ILE:HD13	1.97	0.47
2:L:10:LEU:CD1	2:L:115:MET:HE3	2.44	0.47
2:N:10:LEU:HD11	2:N:115:MET:HE3	1.97	0.47
1:O:302:VAL:HA	2:P:93:THR:HG22	1.95	0.47
1:S:217:ASN:N	1:S:218:GLY:HA3	2.29	0.47
1:S:160:THR:HG22	1:S:237:THR:HG23	1.96	0.47
2:B:170:ARG:NH2	2:B:171:LEU:HB3	2.29	0.47
1:E:203:ARG:O	1:E:203:ARG:HG3	2.15	0.47
2:J:10:LEU:HD11	2:J:115:MET:HE3	1.96	0.47
1:M:153:ASN:HA	1:M:189:GLY:CA	2.44	0.47
1:O:153:ASN:HA	1:O:189:GLY:CA	2.44	0.47
1:O:5:LEU:HD22	2:P:119:TYR:HA	1.97	0.47
2:D:127:ARG:HH21	2:V:131:GLU:HG3	1.80	0.47
2:H:170:ARG:NH2	2:H:171:LEU:HB3	2.29	0.47
1:I:160:THR:HG22	1:I:237:THR:HG23	1.96	0.47
1:A:302:VAL:HA	2:B:93:THR:HG22	1.95	0.47
1:E:303:ASN:H	2:F:93:THR:CG2	2.28	0.47
1:I:153:ASN:HA	1:I:189:GLY:CA	2.44	0.47
2:J:10:LEU:HD13	2:J:115:MET:HE3	1.96	0.47
1:M:6:GLY:CA	2:N:115:MET:HE1	2.45	0.47
2:L:87:SER:HB3	2:T:88:ILE:HD13	1.96	0.47
1:U:153:ASN:HA	1:U:189:GLY:CA	2.45	0.47
1:U:302:VAL:HA	2:V:93:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:127:ARG:HD3	2:X:159:HIS:CE1	2.50	0.47
1:C:302:VAL:HA	2:D:93:THR:HG22	1.96	0.47
1:E:160:THR:HG22	1:E:237:THR:HG23	1.96	0.47
1:M:160:THR:HG22	1:M:237:THR:HG23	1.96	0.47
2:N:127:ARG:HD3	2:N:159:HIS:CE1	2.49	0.47
1:S:119:SER:O	1:S:120:SER:OG	2.27	0.47
1:S:302:VAL:HA	2:T:93:THR:HG22	1.97	0.47
2:B:145:ASP:OD1	2:B:146:ASP:N	2.47	0.46
2:F:145:ASP:OD1	2:F:146:ASP:N	2.47	0.46
1:G:153:ASN:HA	1:G:189:GLY:CA	2.46	0.46
1:W:4:CYS:HA	2:X:137:CYS:HA	1.96	0.46
1:U:284:ARG:HB3	2:V:56:VAL:HG13	1.96	0.46
1:A:153:ASN:HA	1:A:189:GLY:CA	2.46	0.46
1:G:160:THR:HG22	1:G:237:THR:HG23	1.96	0.46
2:J:127:ARG:HD3	2:J:159:HIS:CE1	2.50	0.46
2:B:50:GLY:HA3	1:O:20:THR:O	2.16	0.46
1:G:119:SER:O	1:G:120:SER:OG	2.27	0.46
2:J:87:SER:HB3	2:R:88:ILE:HD13	1.97	0.46
2:N:170:ARG:NH2	2:N:171:LEU:HB3	2.31	0.46
2:P:141:TYR:HB3	2:P:169:ASN:HB2	1.98	0.46
1:C:153:ASN:HA	1:C:189:GLY:CA	2.45	0.46
1:K:297:GLN:HG3	2:L:62:GLU:HG2	1.97	0.46
2:V:10:LEU:HD13	2:V:115:MET:HE3	1.96	0.46
2:V:141:TYR:HB3	2:V:169:ASN:HB2	1.98	0.46
1:W:203:ARG:O	1:W:203:ARG:HG3	2.14	0.46
1:G:303:ASN:H	2:H:93:THR:CG2	2.29	0.46
2:N:87:SER:HB3	2:V:88:ILE:HD13	1.97	0.46
2:V:133:ASP:HB3	2:V:137:CYS:O	2.16	0.46
1:E:153:ASN:HA	1:E:189:GLY:CA	2.46	0.46
2:R:133:ASP:HB3	2:R:137:CYS:O	2.15	0.46
1:I:4:CYS:HA	2:J:137:CYS:HA	1.97	0.46
2:T:133:ASP:HB3	2:T:137:CYS:O	2.16	0.46
2:F:50:GLY:HA3	1:S:20:THR:O	2.16	0.46
1:K:119:SER:HA	1:K:148:LYS:NZ	2.31	0.46
1:K:4:CYS:HA	2:L:137:CYS:HA	1.96	0.46
2:P:133:ASP:HB3	2:P:137:CYS:O	2.15	0.46
1:S:153:ASN:HA	1:S:189:GLY:CA	2.46	0.46
2:X:102:MET:HG3	2:X:103:GLU:N	2.31	0.46
2:J:133:ASP:HB3	2:J:137:CYS:O	2.16	0.46
1:Q:160:THR:HG22	1:Q:237:THR:HG23	1.97	0.46
1:G:6:GLY:C	2:H:115:MET:HE1	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:CYS:HA	2:N:137:CYS:HA	1.98	0.45
2:L:47:GLN:HE22	2:L:110:MET:HE3	1.81	0.45
1:M:203:ARG:O	1:M:203:ARG:HG3	2.15	0.45
1:O:284:ARG:HB3	2:P:56:VAL:HG13	1.97	0.45
2:P:47:GLN:HE22	2:P:110:MET:HE3	1.80	0.45
1:I:203:ARG:O	1:I:203:ARG:HG3	2.14	0.45
2:L:133:ASP:HB3	2:L:137:CYS:O	2.17	0.45
2:N:141:TYR:HB3	2:N:169:ASN:HB2	1.99	0.45
1:W:119:SER:O	1:W:120:SER:OG	2.27	0.45
2:P:11:GLU:OE2	1:Q:133:ASN:O	2.34	0.45
2:X:170:ARG:NH2	2:X:171:LEU:HB3	2.31	0.45
1:A:6:GLY:CA	2:B:115:MET:HE1	2.47	0.45
1:I:297:GLN:HG3	2:J:62:GLU:HG2	1.99	0.45
1:C:119:SER:HA	1:C:148:LYS:NZ	2.32	0.45
1:I:5:LEU:HD22	2:J:119:TYR:HA	1.98	0.45
1:S:110:LYS:HE2	1:S:141:GLU:HG3	1.99	0.45
1:I:6:GLY:CA	2:J:115:MET:HE1	2.47	0.45
2:X:47:GLN:HE22	2:X:110:MET:HE3	1.81	0.45
2:B:133:ASP:HB3	2:B:137:CYS:O	2.17	0.44
2:J:141:TYR:HB3	2:J:169:ASN:HB2	1.99	0.44
2:N:133:ASP:HB3	2:N:137:CYS:O	2.16	0.44
1:A:205:ASN:ND2	1:O:209:VAL:HG21	2.31	0.44
2:X:133:ASP:HB3	2:X:137:CYS:O	2.17	0.44
2:B:141:TYR:HB3	2:B:169:ASN:HB2	2.00	0.44
1:G:119:SER:HA	1:G:148:LYS:NZ	2.32	0.44
2:L:141:TYR:HB3	2:L:169:ASN:HB2	1.99	0.44
1:Q:303:ASN:H	2:R:93:THR:CG2	2.30	0.44
1:Q:110:LYS:HE2	1:Q:141:GLU:HG3	2.00	0.44
2:R:141:TYR:HB3	2:R:169:ASN:HB2	1.99	0.44
2:T:141:TYR:HB3	2:T:169:ASN:HB2	1.99	0.44
1:U:110:LYS:HE2	1:U:141:GLU:HG3	2.00	0.44
2:D:141:TYR:HB3	2:D:169:ASN:HB2	1.99	0.44
1:O:297:GLN:HG3	2:P:62:GLU:HG2	1.99	0.44
1:W:119:SER:HA	1:W:148:LYS:NZ	2.33	0.44
1:A:291:SER:HA	1:A:292:PRO:HD3	1.87	0.44
1:M:110:LYS:HE2	1:M:141:GLU:HG3	1.99	0.44
1:M:162:ARG:HG3	1:M:235:ASN:OD1	2.18	0.44
1:C:203:ARG:HG3	1:C:203:ARG:O	2.15	0.44
2:H:133:ASP:HB3	2:H:137:CYS:O	2.18	0.44
1:I:110:LYS:HE2	1:I:141:GLU:HG3	1.99	0.44
1:I:119:SER:HA	1:I:148:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:102:MET:HG3	2:J:103:GLU:N	2.32	0.44
1:O:203:ARG:O	1:O:203:ARG:HG3	2.17	0.44
1:S:203:ARG:O	1:S:203:ARG:HG3	2.16	0.44
2:F:56:VAL:HG12	2:F:57:GLU:N	2.33	0.44
1:K:1:ASP:OD1	2:L:28:ASN:HA	2.17	0.44
2:F:87:SER:HB3	2:L:88:ILE:HD13	1.99	0.44
1:O:110:LYS:HE2	1:O:141:GLU:HG3	2.00	0.44
1:Q:4:CYS:HA	2:R:137:CYS:HA	2.00	0.44
1:G:203:ARG:O	1:G:203:ARG:HG3	2.15	0.44
1:G:57:ILE:CD1	1:G:95:VAL:HG12	2.48	0.44
1:S:57:ILE:CD1	1:S:95:VAL:HG12	2.48	0.44
1:I:162:ARG:HG3	1:I:235:ASN:OD1	2.18	0.43
2:J:129:ASN:OD1	2:J:129:ASN:N	2.51	0.43
2:D:50:GLY:HA3	1:U:20:THR:O	2.17	0.43
1:W:110:LYS:HE2	1:W:141:GLU:HG3	1.98	0.43
2:X:141:TYR:HB3	2:X:169:ASN:HB2	1.99	0.43
2:J:165:GLU:O	2:J:168:LEU:HB3	2.18	0.43
1:M:119:SER:HA	1:M:148:LYS:NZ	2.32	0.43
1:G:205:ASN:ND2	1:Q:209:VAL:HG21	2.32	0.43
1:U:57:ILE:CD1	1:U:95:VAL:HG12	2.48	0.43
1:C:303:ASN:H	2:D:93:THR:CG2	2.31	0.43
2:F:133:ASP:HB3	2:F:137:CYS:O	2.18	0.43
2:F:141:TYR:HB3	2:F:169:ASN:HB2	1.99	0.43
2:H:141:TYR:HB3	2:H:169:ASN:HB2	1.99	0.43
1:I:302:VAL:HA	2:J:93:THR:HG22	2.00	0.43
2:R:47:GLN:HE22	2:R:110:MET:HE3	1.82	0.43
1:E:205:ASN:ND2	1:S:209:VAL:HG21	2.33	0.43
1:A:119:SER:HA	1:A:148:LYS:NZ	2.33	0.43
1:E:57:ILE:CD1	1:E:95:VAL:HG12	2.48	0.43
2:N:10:LEU:HD13	2:N:115:MET:HE3	1.99	0.43
1:S:119:SER:HA	1:S:148:LYS:NZ	2.33	0.43
1:W:302:VAL:HA	2:X:93:THR:HG22	2.00	0.43
1:E:119:SER:HA	1:E:148:LYS:NZ	2.32	0.43
2:L:165:GLU:O	2:L:168:LEU:HB3	2.18	0.43
1:O:153:ASN:HA	1:O:189:GLY:HA3	2.01	0.43
1:A:203:ARG:HD3	1:O:222:ARG:HG3	2.01	0.43
1:O:57:ILE:CD1	1:O:95:VAL:HG12	2.48	0.43
1:Q:57:ILE:CD1	1:Q:95:VAL:HG12	2.48	0.43
1:O:305:ARG:HH12	1:S:46:ARG:HA	1.83	0.43
2:D:133:ASP:HB3	2:D:137:CYS:O	2.18	0.43
1:O:162:ARG:HG3	1:O:235:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:262:SER:OG	1:Q:277:ARG:O	2.29	0.43
1:S:162:ARG:HG3	1:S:235:ASN:OD1	2.19	0.43
1:I:20:THR:O	2:R:50:GLY:HA3	2.19	0.43
1:K:5:LEU:HD22	2:L:119:TYR:HA	1.99	0.43
2:N:165:GLU:O	2:N:168:LEU:HB3	2.19	0.43
1:O:6:GLY:CA	2:P:115:MET:HE1	2.49	0.43
1:C:6:GLY:C	2:D:115:MET:HE1	2.39	0.43
1:K:162:ARG:HG3	1:K:235:ASN:OD1	2.18	0.43
1:Q:119:SER:HA	1:Q:148:LYS:NZ	2.33	0.43
1:C:57:ILE:CD1	1:C:95:VAL:HG12	2.49	0.43
1:G:110:LYS:HE2	1:G:141:GLU:HG3	2.00	0.43
1:G:162:ARG:HG3	1:G:235:ASN:OD1	2.19	0.43
2:H:165:GLU:O	2:H:168:LEU:HB3	2.19	0.43
1:Q:284:ARG:HB3	2:R:56:VAL:HG13	2.01	0.43
1:U:119:SER:HA	1:U:148:LYS:NZ	2.33	0.43
1:C:110:LYS:HE2	1:C:141:GLU:HG3	2.01	0.43
2:H:102:MET:HG3	2:H:103:GLU:N	2.33	0.43
2:N:129:ASN:N	2:N:129:ASN:OD1	2.52	0.43
1:O:303:ASN:H	2:P:93:THR:CG2	2.32	0.43
2:X:165:GLU:O	2:X:168:LEU:HB3	2.19	0.43
2:B:56:VAL:HG12	2:B:57:GLU:N	2.34	0.42
1:C:162:ARG:HG3	1:C:235:ASN:OD1	2.18	0.42
1:K:110:LYS:HE2	1:K:141:GLU:HG3	2.00	0.42
1:Q:161:TYR:OH	1:Q:169:HIS:CD2	2.72	0.42
1:S:133:ASN:O	2:V:11:GLU:OE2	2.37	0.42
1:A:57:ILE:CD1	1:A:95:VAL:HG12	2.49	0.42
2:B:165:GLU:O	2:B:168:LEU:HB3	2.19	0.42
1:C:205:ASN:ND2	1:U:209:VAL:HG21	2.34	0.42
1:E:162:ARG:HG3	1:E:235:ASN:OD1	2.19	0.42
1:I:57:ILE:CD1	1:I:95:VAL:HG12	2.49	0.42
2:L:129:ASN:N	2:L:129:ASN:OD1	2.51	0.42
1:M:153:ASN:HA	1:M:189:GLY:HA3	2.01	0.42
1:M:302:VAL:HA	2:N:93:THR:HG22	2.00	0.42
1:O:119:SER:HA	1:O:148:LYS:NZ	2.33	0.42
1:Q:153:ASN:HA	1:Q:189:GLY:HA3	2.00	0.42
2:R:56:VAL:HG12	2:R:57:GLU:N	2.34	0.42
1:W:297:GLN:HG3	2:X:62:GLU:HG2	2.00	0.42
1:W:57:ILE:CD1	1:W:95:VAL:HG12	2.50	0.42
2:X:129:ASN:N	2:X:129:ASN:OD1	2.53	0.42
2:B:87:SER:HB3	2:X:88:ILE:HD13	2.00	0.42
2:L:131:GLU:HG3	2:T:127:ARG:NH2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:CYS:HA	2:P:137:CYS:HA	2.01	0.42
1:Q:162:ARG:HG3	1:Q:235:ASN:OD1	2.19	0.42
1:Q:46:ARG:HA	1:S:305:ARG:HH12	1.84	0.42
1:W:162:ARG:HG3	1:W:235:ASN:OD1	2.18	0.42
1:A:162:ARG:HG3	1:A:235:ASN:OD1	2.19	0.42
2:H:56:VAL:HG12	2:H:57:GLU:N	2.34	0.42
2:N:47:GLN:HE22	2:N:110:MET:HE3	1.83	0.42
1:O:291:SER:HA	1:O:292:PRO:HD3	1.89	0.42
1:Q:8:HIS:CD2	2:R:21:TRP:HA	2.55	0.42
1:U:162:ARG:HG3	1:U:235:ASN:OD1	2.19	0.42
2:H:87:SER:HB3	2:J:88:ILE:HD13	2.01	0.42
1:K:291:SER:HA	1:K:292:PRO:HD3	1.88	0.42
1:Q:119:SER:O	1:Q:120:SER:OG	2.27	0.42
1:A:262:SER:OG	1:A:277:ARG:O	2.29	0.42
1:K:153:ASN:HA	1:K:189:GLY:HA3	2.01	0.42
2:R:165:GLU:O	2:R:168:LEU:HB3	2.20	0.42
1:U:161:TYR:OH	1:U:169:HIS:CD2	2.72	0.42
1:A:203:ARG:O	1:A:203:ARG:HG3	2.16	0.42
2:D:165:GLU:O	2:D:168:LEU:HB3	2.19	0.42
1:E:161:TYR:OH	1:E:169:HIS:CD2	2.73	0.42
2:L:102:MET:HG3	2:L:103:GLU:N	2.34	0.42
1:M:1:ASP:OD1	2:N:28:ASN:HA	2.19	0.42
1:Q:297:GLN:HG3	2:R:62:GLU:HG2	2.02	0.42
1:S:8:HIS:CD2	2:T:21:TRP:HA	2.54	0.42
2:T:165:GLU:O	2:T:168:LEU:HB3	2.20	0.42
1:A:110:LYS:HE2	1:A:141:GLU:HG3	2.01	0.42
1:S:161:TYR:OH	1:S:169:HIS:CD2	2.73	0.42
1:W:100:GLN:O	1:W:104:GLU:HG2	2.20	0.42
1:K:100:GLN:O	1:K:104:GLU:HG2	2.20	0.42
1:M:100:GLN:O	1:M:104:GLU:HG2	2.20	0.42
1:S:4:CYS:HA	2:T:137:CYS:HA	2.01	0.42
1:U:153:ASN:HA	1:U:189:GLY:HA3	2.02	0.42
1:C:100:GLN:O	1:C:104:GLU:HG2	2.20	0.41
1:E:6:GLY:C	2:F:115:MET:HE1	2.40	0.41
2:H:50:GLY:HA3	1:Q:20:THR:O	2.18	0.41
1:K:57:ILE:CD1	1:K:95:VAL:HG12	2.50	0.41
1:O:161:TYR:OH	1:O:169:HIS:CD2	2.72	0.41
1:U:303:ASN:H	2:V:93:THR:CG2	2.33	0.41
2:X:56:VAL:HG12	2:X:57:GLU:N	2.35	0.41
2:D:56:VAL:HG12	2:D:57:GLU:N	2.35	0.41
1:E:110:LYS:HE2	1:E:141:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:GLN:O	1:I:104:GLU:HG2	2.20	0.41
2:P:56:VAL:HG12	2:P:57:GLU:N	2.35	0.41
1:U:4:CYS:HA	2:V:137:CYS:HA	2.01	0.41
1:E:100:GLN:O	1:E:104:GLU:HG2	2.20	0.41
1:G:8:HIS:CD2	2:H:21:TRP:HA	2.56	0.41
2:J:47:GLN:HE22	2:J:110:MET:HE3	1.85	0.41
2:L:170:ARG:CZ	2:L:171:LEU:HB2	2.51	0.41
2:P:129:ASN:N	2:P:129:ASN:OD1	2.53	0.41
1:Q:291:SER:HA	1:Q:292:PRO:HD3	1.90	0.41
2:F:127:ARG:HH21	2:T:131:GLU:HG3	1.85	0.41
2:F:165:GLU:O	2:F:168:LEU:HB3	2.19	0.41
2:N:56:VAL:HG12	2:N:57:GLU:N	2.35	0.41
1:S:100:GLN:O	1:S:104:GLU:HG2	2.21	0.41
1:A:161:TYR:OH	1:A:169:HIS:CD2	2.74	0.41
2:B:56:VAL:CG1	2:B:57:GLU:N	2.84	0.41
1:C:153:ASN:HA	1:C:189:GLY:HA3	2.03	0.41
1:C:161:TYR:OH	1:C:169:HIS:CD2	2.73	0.41
2:F:56:VAL:CG1	2:F:57:GLU:N	2.83	0.41
1:G:100:GLN:O	1:G:104:GLU:HG2	2.20	0.41
1:M:57:ILE:CD1	1:M:95:VAL:HG12	2.50	0.41
2:V:165:GLU:O	2:V:168:LEU:HB3	2.20	0.41
1:W:153:ASN:HA	1:W:189:GLY:HA3	2.02	0.41
2:F:129:ASN:OD1	2:F:129:ASN:N	2.54	0.41
2:F:170:ARG:NH1	2:L:167:LEU:HD23	2.36	0.41
2:J:170:ARG:CZ	2:J:171:LEU:HB2	2.50	0.41
1:M:118:GLY:O	1:M:121:ILE:HG23	2.21	0.41
2:T:56:VAL:HG12	2:T:57:GLU:N	2.36	0.41
1:S:303:ASN:H	2:T:93:THR:CG2	2.34	0.41
1:U:203:ARG:HG3	1:U:203:ARG:O	2.16	0.41
1:W:118:GLY:O	1:W:121:ILE:HG23	2.21	0.41
2:H:170:ARG:NH1	2:J:167:LEU:HD23	2.36	0.41
2:L:56:VAL:HG12	2:L:57:GLU:N	2.35	0.41
1:M:20:THR:O	2:V:50:GLY:HA3	2.20	0.41
1:O:100:GLN:O	1:O:104:GLU:HG2	2.21	0.41
2:P:165:GLU:O	2:P:168:LEU:HB3	2.20	0.41
1:U:100:GLN:O	1:U:104:GLU:HG2	2.21	0.41
1:U:118:GLY:O	1:U:121:ILE:HG23	2.21	0.41
1:W:1:ASP:OD1	2:X:28:ASN:HA	2.21	0.41
2:P:127:ARG:NH2	2:X:131:GLU:HG3	2.32	0.41
2:F:47:GLN:HE22	2:F:110:MET:HE3	1.85	0.41
1:W:6:GLY:CA	2:X:115:MET:HE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:O	1:A:104:GLU:HG2	2.20	0.41
1:A:153:ASN:HA	1:A:189:GLY:HA3	2.03	0.41
1:C:165:ASP:OD1	1:C:166:THR:N	2.49	0.41
1:C:8:HIS:CD2	2:D:21:TRP:HA	2.56	0.41
1:G:51:LEU:O	1:G:52:GLY:C	2.57	0.41
2:H:56:VAL:CG1	2:H:57:GLU:N	2.84	0.41
1:K:302:VAL:HA	2:L:93:THR:HG22	2.03	0.41
2:L:170:ARG:NH2	2:L:171:LEU:HD13	2.36	0.41
1:Q:100:GLN:O	1:Q:104:GLU:HG2	2.21	0.41
1:S:118:GLY:O	1:S:121:ILE:HG23	2.21	0.41
2:V:47:GLN:HE22	2:V:110:MET:HE3	1.83	0.41
2:B:102:MET:HG3	2:B:103:GLU:N	2.36	0.41
1:C:203:ARG:HD3	1:U:222:ARG:HG3	2.03	0.41
1:C:73:MET:SD	1:C:254:ILE:HD13	2.61	0.41
1:I:153:ASN:HA	1:I:189:GLY:HA3	2.02	0.41
1:Q:118:GLY:O	1:Q:121:ILE:HG23	2.21	0.41
1:S:153:ASN:HA	1:S:189:GLY:HA3	2.02	0.41
2:L:10:LEU:HD11	2:L:115:MET:HE3	2.03	0.40
2:N:102:MET:HG3	2:N:103:GLU:N	2.36	0.40
2:N:131:GLU:HG3	2:V:127:ARG:NH2	2.29	0.40
1:E:73:MET:SD	1:E:254:ILE:HD13	2.62	0.40
1:G:161:TYR:OH	1:G:169:HIS:CD2	2.73	0.40
2:J:119:TYR:HH	2:J:132:GLU:HG2	1.85	0.40
1:K:119:SER:O	1:K:120:SER:OG	2.27	0.40
1:K:118:GLY:O	1:K:121:ILE:HG23	2.21	0.40
1:M:40:ARG:NH1	1:M:267:ASP:OD2	2.55	0.40
1:U:40:ARG:NH1	1:U:267:ASP:OD2	2.54	0.40
1:E:51:LEU:O	1:E:52:GLY:C	2.59	0.40
2:H:127:ARG:HH21	2:R:131:GLU:HG3	1.86	0.40
2:J:170:ARG:NH2	2:J:171:LEU:HB2	2.36	0.40
2:D:102:MET:HG3	2:D:103:GLU:N	2.36	0.40
2:H:129:ASN:OD1	2:H:129:ASN:N	2.54	0.40
1:I:118:GLY:O	1:I:121:ILE:HG23	2.21	0.40
1:O:118:GLY:O	1:O:121:ILE:HG23	2.21	0.40
1:S:165:ASP:OD1	1:S:166:THR:N	2.51	0.40
1:U:297:GLN:HG3	2:V:62:GLU:HG2	2.04	0.40
2:F:102:MET:HG3	2:F:103:GLU:N	2.37	0.40
1:G:291:SER:HA	1:G:292:PRO:HD3	1.88	0.40
1:I:161:TYR:OH	1:I:169:HIS:CD2	2.75	0.40
2:J:56:VAL:HG12	2:J:57:GLU:N	2.36	0.40
1:O:305:ARG:NH1	1:S:46:ARG:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:131:GLU:OE2	2:R:128:GLN:CG	2.70	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)
2:N:171:LEU:CG	2:N:171:LEU:CD1[2_656]	1.80	0.40

## 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	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	C	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	E	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	G	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	I	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	41	66
1	K	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	M	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	41	66
1	O	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	Q	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
1	S	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	41	66
1	U	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	41	66
1	W	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	41	66
2	B	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50
2	D	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50
2	F	170/174 (98%)	157 (92%)	12 (7%)	1 (1%)	25	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
2	H	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	J	170/174 (98%)	157 (92%)	12 (7%)	1 (1%)	25	50	
2	L	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	N	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	P	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	R	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	T	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	V	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
2	X	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	25	50	
All	All	5844/6012 (97%)	5490 (94%)	330 (6%)	24 (0%)	34	60	

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	LYS
2	B	170	ARG
1	C	150	LYS
2	D	170	ARG
1	E	150	LYS
2	F	170	ARG
1	G	150	LYS
2	H	170	ARG
1	I	150	LYS
2	J	170	ARG
1	K	150	LYS
2	L	170	ARG
1	M	150	LYS
2	N	170	ARG
1	O	150	LYS
2	P	170	ARG
1	Q	150	LYS
2	R	170	ARG
1	S	150	LYS
2	T	170	ARG
1	U	150	LYS
2	V	170	ARG
1	W	150	LYS
2	X	170	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	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	C	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	E	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	G	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	I	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	K	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	M	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	O	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	Q	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	S	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	U	269/275 (98%)	257 (96%)	12 (4%)	27	55
1	W	269/275 (98%)	257 (96%)	12 (4%)	27	55
2	B	146/148 (99%)	140 (96%)	6 (4%)	30	59
2	D	146/148 (99%)	140 (96%)	6 (4%)	30	59
2	F	146/148 (99%)	139 (95%)	7 (5%)	25	53
2	H	146/148 (99%)	140 (96%)	6 (4%)	30	59
2	J	146/148 (99%)	141 (97%)	5 (3%)	37	66
2	L	146/148 (99%)	140 (96%)	6 (4%)	30	59
2	N	146/148 (99%)	140 (96%)	6 (4%)	30	59
2	P	146/148 (99%)	139 (95%)	7 (5%)	25	53
2	R	146/148 (99%)	139 (95%)	7 (5%)	25	53
2	T	146/148 (99%)	139 (95%)	7 (5%)	25	53
2	V	146/148 (99%)	139 (95%)	7 (5%)	25	53
2	X	146/148 (99%)	140 (96%)	6 (4%)	30	59
All	All	4980/5076 (98%)	4760 (96%)	220 (4%)	28	56

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	15	ILE
1	A	71	THR
1	A	73	MET
1	A	76	THR
1	A	77	LEU
1	A	95	VAL
1	A	101	LYS
1	A	128	ARG
1	A	228	THR
1	A	240	HIS
1	A	314	ARG
2	B	57	GLU
2	B	110	MET
2	B	129	ASN
2	B	132	GLU
2	B	168	LEU
2	B	171	LEU
1	C	8	HIS
1	C	15	ILE
1	C	71	THR
1	C	73	MET
1	C	76	THR
1	C	77	LEU
1	C	95	VAL
1	C	101	LYS
1	C	128	ARG
1	C	228	THR
1	C	240	HIS
1	C	314	ARG
2	D	57	GLU
2	D	110	MET
2	D	129	ASN
2	D	132	GLU
2	D	168	LEU
2	D	171	LEU
1	E	8	HIS
1	E	15	ILE
1	E	71	THR
1	E	73	MET
1	E	76	THR
1	E	77	LEU
1	E	95	VAL

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Mol	Chain	Res	Type
1	E	101	LYS
1	E	128	ARG
1	E	228	THR
1	E	240	HIS
1	E	314	ARG
2	F	57	GLU
2	F	110	MET
2	F	129	ASN
2	F	132	GLU
2	F	160	SER
2	F	168	LEU
2	F	171	LEU
1	G	8	HIS
1	G	15	ILE
1	G	71	THR
1	G	73	MET
1	G	76	THR
1	G	77	LEU
1	G	95	VAL
1	G	101	LYS
1	G	128	ARG
1	G	228	THR
1	G	240	HIS
1	G	314	ARG
2	H	57	GLU
2	H	110	MET
2	H	129	ASN
2	H	132	GLU
2	H	168	LEU
2	H	171	LEU
1	I	8	HIS
1	I	15	ILE
1	I	71	THR
1	I	73	MET
1	I	76	THR
1	I	77	LEU
1	I	95	VAL
1	I	101	LYS
1	I	128	ARG
1	I	228	THR
1	I	240	HIS
1	I	314	ARG

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Mol	Chain	Res	Type
2	J	57	GLU
2	J	110	MET
2	J	129	ASN
2	J	132	GLU
2	J	168	LEU
1	K	8	HIS
1	K	15	ILE
1	K	71	THR
1	K	73	MET
1	K	76	THR
1	K	77	LEU
1	K	95	VAL
1	K	101	LYS
1	K	128	ARG
1	K	228	THR
1	K	240	HIS
1	K	314	ARG
2	L	57	GLU
2	L	110	MET
2	L	129	ASN
2	L	132	GLU
2	L	160	SER
2	L	168	LEU
1	M	8	HIS
1	M	15	ILE
1	M	71	THR
1	M	73	MET
1	M	76	THR
1	M	77	LEU
1	M	95	VAL
1	M	101	LYS
1	M	128	ARG
1	M	228	THR
1	M	240	HIS
1	M	314	ARG
2	N	57	GLU
2	N	110	MET
2	N	129	ASN
2	N	132	GLU
2	N	168	LEU
2	N	171	LEU
1	O	8	HIS

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Mol	Chain	Res	Type
1	O	15	ILE
1	O	71	THR
1	O	73	MET
1	O	76	THR
1	O	77	LEU
1	O	95	VAL
1	O	101	LYS
1	O	128	ARG
1	O	228	THR
1	O	240	HIS
1	O	314	ARG
2	P	57	GLU
2	P	110	MET
2	P	129	ASN
2	P	132	GLU
2	P	160	SER
2	P	168	LEU
2	P	171	LEU
1	Q	8	HIS
1	Q	15	ILE
1	Q	71	THR
1	Q	73	MET
1	Q	76	THR
1	Q	77	LEU
1	Q	95	VAL
1	Q	101	LYS
1	Q	128	ARG
1	Q	228	THR
1	Q	240	HIS
1	Q	314	ARG
2	R	57	GLU
2	R	110	MET
2	R	129	ASN
2	R	132	GLU
2	R	160	SER
2	R	168	LEU
2	R	171	LEU
1	S	8	HIS
1	S	15	ILE
1	S	71	THR
1	S	73	MET
1	S	76	THR

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Mol	Chain	Res	Type
1	S	77	LEU
1	S	95	VAL
1	S	101	LYS
1	S	128	ARG
1	S	228	THR
1	S	240	HIS
1	S	314	ARG
2	T	57	GLU
2	T	110	MET
2	T	129	ASN
2	T	132	GLU
2	T	160	SER
2	T	168	LEU
2	T	171	LEU
1	U	8	HIS
1	U	15	ILE
1	U	71	THR
1	U	73	MET
1	U	76	THR
1	U	77	LEU
1	U	95	VAL
1	U	101	LYS
1	U	128	ARG
1	U	228	THR
1	U	240	HIS
1	U	314	ARG
2	V	57	GLU
2	V	110	MET
2	V	129	ASN
2	V	132	GLU
2	V	160	SER
2	V	168	LEU
2	V	171	LEU
1	W	8	HIS
1	W	15	ILE
1	W	71	THR
1	W	73	MET
1	W	76	THR
1	W	77	LEU
1	W	95	VAL
1	W	101	LYS
1	W	128	ARG

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Mol	Chain	Res	Type
1	W	228	THR
1	W	240	HIS
1	W	314	ARG
2	X	57	GLU
2	X	110	MET
2	X	129	ASN
2	X	132	GLU
2	X	168	LEU
2	X	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	159	ASN
1	A	169	HIS
1	A	240	HIS
2	B	47	GLN
1	C	8	HIS
1	C	159	ASN
1	C	169	HIS
1	C	240	HIS
2	D	47	GLN
1	E	8	HIS
1	E	159	ASN
1	E	169	HIS
1	E	240	HIS
2	F	47	GLN
1	G	8	HIS
1	G	159	ASN
1	G	169	HIS
1	G	240	HIS
2	H	47	GLN
1	I	8	HIS
1	I	159	ASN
1	I	169	HIS
1	I	219	GLN
1	I	240	HIS
2	J	47	GLN
2	J	172	ASN
1	K	8	HIS
1	K	159	ASN

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Mol	Chain	Res	Type
1	K	169	HIS
1	K	240	HIS
2	L	47	GLN
2	L	172	ASN
1	M	8	HIS
1	M	159	ASN
1	M	169	HIS
1	M	240	HIS
2	N	47	GLN
2	N	172	ASN
1	O	8	HIS
1	O	159	ASN
1	O	169	HIS
1	O	240	HIS
2	P	47	GLN
1	Q	8	HIS
1	Q	159	ASN
1	Q	169	HIS
1	Q	240	HIS
2	R	47	GLN
1	S	8	HIS
1	S	159	ASN
1	S	169	HIS
1	S	240	HIS
2	T	47	GLN
1	U	8	HIS
1	U	159	ASN
1	U	169	HIS
1	U	240	HIS
2	V	47	GLN
1	W	8	HIS
1	W	159	ASN
1	W	169	HIS
1	W	240	HIS
2	X	47	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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	X	301	2	14,14,15	0.78	0	17,19,21	2.57	6 (35%)
3	NAG	W	401	1	14,14,15	0.47	0	17,19,21	2.85	6 (35%)
3	NAG	F	301	2	14,14,15	1.18	1 (7%)	17,19,21	2.99	9 (52%)
3	NAG	B	301	2	14,14,15	1.26	1 (7%)	17,19,21	3.00	9 (52%)
3	NAG	O	401	1	14,14,15	0.49	0	17,19,21	1.61	2 (11%)
3	NAG	N	301	2	14,14,15	0.75	0	17,19,21	2.41	4 (23%)
3	NAG	S	401	1	14,14,15	0.52	0	17,19,21	1.51	3 (17%)
3	NAG	P	301	2	14,14,15	0.77	0	17,19,21	1.52	3 (17%)
3	NAG	K	401	1	14,14,15	0.46	0	17,19,21	2.78	3 (17%)
3	NAG	T	301	2	14,14,15	0.80	1 (7%)	17,19,21	1.84	4 (23%)
3	NAG	Q	401	1	14,14,15	0.52	0	17,19,21	1.61	3 (17%)
3	NAG	U	401	1	14,14,15	0.49	0	17,19,21	1.54	3 (17%)
3	NAG	M	401	1	14,14,15	0.48	0	17,19,21	2.99	8 (47%)
3	NAG	G	401	1	14,14,15	0.63	0	17,19,21	2.06	3 (17%)
3	NAG	V	301	2	14,14,15	0.83	0	17,19,21	2.03	3 (17%)
3	NAG	R	301	2	14,14,15	0.95	1 (7%)	17,19,21	1.89	4 (23%)
3	NAG	C	401	1	14,14,15	0.46	0	17,19,21	1.81	3 (17%)
3	NAG	H	301	2	14,14,15	1.19	1 (7%)	17,19,21	2.61	7 (41%)
3	NAG	I	401	1	14,14,15	0.56	0	17,19,21	2.70	5 (29%)
3	NAG	A	401	1	14,14,15	0.56	0	17,19,21	2.18	6 (35%)
3	NAG	L	301	2	14,14,15	0.84	0	17,19,21	2.55	5 (29%)
3	NAG	E	401	1	14,14,15	0.55	0	17,19,21	1.90	4 (23%)
3	NAG	D	301	2	14,14,15	1.25	2 (14%)	17,19,21	3.10	9 (52%)
3	NAG	J	301	2	14,14,15	0.72	0	17,19,21	2.05	3 (17%)

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	X	301	2	-	2/6/23/26	0/1/1/1
3	NAG	W	401	1	-	2/6/23/26	0/1/1/1
3	NAG	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	B	301	2	-	1/6/23/26	0/1/1/1
3	NAG	O	401	1	-	0/6/23/26	0/1/1/1
3	NAG	N	301	2	-	2/6/23/26	0/1/1/1
3	NAG	S	401	1	-	2/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	K	401	1	-	2/6/23/26	0/1/1/1
3	NAG	T	301	2	-	2/6/23/26	0/1/1/1
3	NAG	Q	401	1	-	1/6/23/26	0/1/1/1
3	NAG	U	401	1	-	1/6/23/26	0/1/1/1
3	NAG	M	401	1	-	2/6/23/26	0/1/1/1
3	NAG	G	401	1	-	2/6/23/26	0/1/1/1
3	NAG	V	301	2	-	2/6/23/26	0/1/1/1
3	NAG	R	301	2	-	2/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	H	301	2	-	2/6/23/26	0/1/1/1
3	NAG	I	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	L	301	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	D	301	2	-	2/6/23/26	0/1/1/1
3	NAG	J	301	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	NAG	O7-C7	3.19	1.30	1.23
3	B	301	NAG	O7-C7	3.06	1.30	1.23
3	F	301	NAG	O7-C7	2.88	1.29	1.23
3	D	301	NAG	O7-C7	2.83	1.29	1.23
3	D	301	NAG	O5-C1	2.28	1.47	1.43
3	R	301	NAG	O7-C7	2.11	1.28	1.23
3	T	301	NAG	O7-C7	2.10	1.28	1.23

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	401	NAG	C1-O5-C5	9.68	125.31	112.19
3	K	401	NAG	C1-O5-C5	9.58	125.17	112.19
3	I	401	NAG	C1-O5-C5	9.57	125.16	112.19
3	W	401	NAG	C1-O5-C5	8.92	124.28	112.19
3	X	301	NAG	C1-O5-C5	8.57	123.80	112.19
3	L	301	NAG	C1-O5-C5	7.96	122.98	112.19
3	N	301	NAG	C1-O5-C5	7.01	121.69	112.19
3	J	301	NAG	C1-O5-C5	6.28	120.70	112.19
3	A	401	NAG	C1-O5-C5	6.26	120.67	112.19
3	E	401	NAG	C1-O5-C5	6.15	120.53	112.19
3	D	301	NAG	C1-O5-C5	6.06	120.41	112.19
3	B	301	NAG	O7-C7-N2	6.01	133.00	121.95
3	G	401	NAG	C1-O5-C5	5.78	120.02	112.19
3	T	301	NAG	C1-O5-C5	5.69	119.89	112.19
3	V	301	NAG	C1-O5-C5	5.68	119.89	112.19
3	C	401	NAG	C1-O5-C5	5.67	119.88	112.19
3	B	301	NAG	C2-N2-C7	5.61	130.90	122.90
3	F	301	NAG	O7-C7-N2	5.52	132.09	121.95
3	D	301	NAG	O7-C7-N2	5.41	131.90	121.95
3	R	301	NAG	C1-O5-C5	5.38	119.49	112.19
3	H	301	NAG	C8-C7-N2	-5.30	107.13	116.10
3	F	301	NAG	C1-O5-C5	5.21	119.25	112.19
3	F	301	NAG	C8-C7-N2	-4.88	107.84	116.10
3	B	301	NAG	C8-C7-N2	-4.81	107.95	116.10
3	D	301	NAG	C2-N2-C7	4.77	129.69	122.90
3	O	401	NAG	C1-O5-C5	4.76	118.65	112.19
3	U	401	NAG	C1-O5-C5	4.60	118.43	112.19
3	H	301	NAG	C1-O5-C5	4.60	118.42	112.19
3	D	301	NAG	C8-C7-N2	-4.52	108.44	116.10
3	B	301	NAG	C1-O5-C5	4.52	118.32	112.19
3	H	301	NAG	O7-C7-N2	4.23	129.73	121.95
3	Q	401	NAG	C1-O5-C5	4.05	117.68	112.19
3	N	301	NAG	C8-C7-N2	-4.00	109.33	116.10
3	K	401	NAG	O5-C1-C2	3.94	117.52	111.29
3	F	301	NAG	C2-N2-C7	3.92	128.49	122.90
3	G	401	NAG	O5-C5-C6	3.81	113.18	107.20
3	F	301	NAG	O5-C1-C2	3.79	117.28	111.29
3	M	401	NAG	O5-C1-C2	3.77	117.24	111.29
3	N	301	NAG	O5-C1-C2	-3.62	105.57	111.29
3	W	401	NAG	O5-C1-C2	3.61	116.99	111.29
3	P	301	NAG	C1-O5-C5	3.54	116.99	112.19
3	A	401	NAG	O5-C5-C6	3.53	112.73	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	NAG	O5-C1-C2	-3.40	105.93	111.29
3	V	301	NAG	O7-C7-N2	3.33	128.07	121.95
3	D	301	NAG	O5-C1-C2	3.32	116.52	111.29
3	R	301	NAG	O7-C7-N2	3.25	127.92	121.95
3	D	301	NAG	C1-C2-N2	3.23	116.01	110.49
3	L	301	NAG	C8-C7-N2	-3.22	110.66	116.10
3	P	301	NAG	O5-C5-C6	3.11	112.09	107.20
3	B	301	NAG	O5-C5-C4	3.04	118.23	110.83
3	Q	401	NAG	C3-C4-C5	-3.02	104.84	110.24
3	B	301	NAG	O5-C1-C2	2.98	115.99	111.29
3	M	401	NAG	C4-C3-C2	-2.98	106.66	111.02
3	S	401	NAG	C1-O5-C5	2.97	116.22	112.19
3	O	401	NAG	C3-C4-C5	-2.96	104.96	110.24
3	F	301	NAG	O5-C5-C4	2.94	117.97	110.83
3	H	301	NAG	C1-C2-N2	2.91	115.45	110.49
3	M	401	NAG	C3-C4-C5	-2.91	105.06	110.24
3	W	401	NAG	O5-C5-C6	-2.90	102.66	107.20
3	X	301	NAG	C8-C7-N2	-2.86	111.26	116.10
3	S	401	NAG	C3-C4-C5	-2.81	105.23	110.24
3	W	401	NAG	O4-C4-C5	2.73	116.07	109.30
3	D	301	NAG	O5-C5-C4	2.71	117.42	110.83
3	H	301	NAG	C4-C3-C2	-2.69	107.07	111.02
3	J	301	NAG	C8-C7-N2	-2.67	111.57	116.10
3	F	301	NAG	O3-C3-C2	2.65	114.95	109.47
3	I	401	NAG	O7-C7-C8	-2.65	117.14	122.06
3	W	401	NAG	O7-C7-C8	-2.61	117.20	122.06
3	J	301	NAG	O5-C1-C2	-2.61	107.16	111.29
3	Q	401	NAG	O5-C1-C2	-2.59	107.19	111.29
3	I	401	NAG	C8-C7-N2	2.57	120.45	116.10
3	M	401	NAG	C8-C7-N2	2.57	120.45	116.10
3	B	301	NAG	O3-C3-C2	2.55	114.75	109.47
3	M	401	NAG	O7-C7-C8	-2.53	117.35	122.06
3	K	401	NAG	O7-C7-C8	-2.53	117.35	122.06
3	W	401	NAG	C3-C4-C5	-2.53	105.72	110.24
3	C	401	NAG	C4-C3-C2	-2.53	107.32	111.02
3	H	301	NAG	O5-C5-C4	2.52	116.97	110.83
3	H	301	NAG	C2-N2-C7	2.51	126.48	122.90
3	X	301	NAG	O5-C5-C6	2.50	111.13	107.20
3	A	401	NAG	C4-C3-C2	2.49	114.66	111.02
3	X	301	NAG	O5-C1-C2	-2.48	107.37	111.29
3	T	301	NAG	O7-C7-N2	2.47	126.50	121.95
3	F	301	NAG	C1-C2-N2	2.47	114.70	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	NAG	C4-C3-C2	-2.46	107.41	111.02
3	D	301	NAG	C4-C3-C2	-2.45	107.43	111.02
3	T	301	NAG	O3-C3-C4	-2.39	104.83	110.35
3	C	401	NAG	O3-C3-C4	2.38	115.85	110.35
3	V	301	NAG	O3-C3-C4	-2.38	104.86	110.35
3	D	301	NAG	O5-C5-C6	2.37	110.92	107.20
3	E	401	NAG	O5-C5-C6	2.37	110.91	107.20
3	R	301	NAG	O5-C5-C6	2.36	110.90	107.20
3	P	301	NAG	O7-C7-N2	2.32	126.21	121.95
3	B	301	NAG	C1-C2-N2	2.23	114.30	110.49
3	S	401	NAG	O5-C1-C2	-2.23	107.77	111.29
3	A	401	NAG	C3-C4-C5	2.21	114.18	110.24
3	X	301	NAG	O7-C7-N2	2.18	125.96	121.95
3	L	301	NAG	C6-C5-C4	-2.15	107.98	113.00
3	N	301	NAG	O7-C7-N2	2.14	125.89	121.95
3	L	301	NAG	O5-C5-C4	2.14	116.02	110.83
3	I	401	NAG	O5-C1-C2	2.11	114.62	111.29
3	T	301	NAG	C2-N2-C7	-2.11	119.90	122.90
3	E	401	NAG	C4-C3-C2	-2.10	107.94	111.02
3	B	301	NAG	C3-C4-C5	2.10	113.98	110.24
3	A	401	NAG	C6-C5-C4	-2.10	108.09	113.00
3	M	401	NAG	O3-C3-C2	2.09	113.80	109.47
3	R	301	NAG	C8-C7-N2	-2.07	112.59	116.10
3	G	401	NAG	C4-C3-C2	-2.06	108.00	111.02
3	U	401	NAG	C6-C5-C4	-2.06	108.19	113.00
3	I	401	NAG	O3-C3-C4	-2.05	105.61	110.35
3	E	401	NAG	O3-C3-C4	2.05	115.08	110.35
3	X	301	NAG	O3-C3-C2	2.04	113.68	109.47
3	M	401	NAG	O4-C4-C5	2.04	114.35	109.30
3	U	401	NAG	C3-C4-C5	-2.03	106.62	110.24
3	A	401	NAG	O3-C3-C4	-2.01	105.70	110.35

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	301	NAG	O5-C5-C6-O6
3	M	401	NAG	O5-C5-C6-O6
3	P	301	NAG	O5-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6
3	N	301	NAG	O5-C5-C6-O6
3	K	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	T	301	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	H	301	NAG	O5-C5-C6-O6
3	I	401	NAG	O5-C5-C6-O6
3	J	301	NAG	O5-C5-C6-O6
3	X	301	NAG	C4-C5-C6-O6
3	W	401	NAG	O5-C5-C6-O6
3	G	401	NAG	O5-C5-C6-O6
3	R	301	NAG	O5-C5-C6-O6
3	D	301	NAG	O5-C5-C6-O6
3	K	401	NAG	C4-C5-C6-O6
3	P	301	NAG	C4-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	M	401	NAG	C4-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	V	301	NAG	O5-C5-C6-O6
3	I	401	NAG	C4-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	J	301	NAG	C4-C5-C6-O6
3	N	301	NAG	C4-C5-C6-O6
3	W	401	NAG	C4-C5-C6-O6
3	R	301	NAG	C4-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
3	V	301	NAG	C4-C5-C6-O6
3	T	301	NAG	C4-C5-C6-O6
3	G	401	NAG	C4-C5-C6-O6
3	D	301	NAG	C4-C5-C6-O6
3	H	301	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	S	401	NAG	O5-C5-C6-O6
3	F	301	NAG	O5-C5-C6-O6
3	S	401	NAG	C4-C5-C6-O6
3	U	401	NAG	O5-C5-C6-O6
3	Q	401	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	301	NAG	1	0
3	N	301	NAG	1	0
3	I	401	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	301	NAG	1	0
3	J	301	NAG	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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	X	301	2	14,14,15	0.78	0	17,19,21	2.57	6 (35%)
3	NAG	W	401	1	14,14,15	0.47	0	17,19,21	2.85	6 (35%)
3	NAG	F	301	2	14,14,15	1.18	1 (7%)	17,19,21	2.99	9 (52%)
3	NAG	B	301	2	14,14,15	1.26	1 (7%)	17,19,21	3.00	9 (52%)
3	NAG	O	401	1	14,14,15	0.49	0	17,19,21	1.61	2 (11%)
3	NAG	N	301	2	14,14,15	0.75	0	17,19,21	2.41	4 (23%)
3	NAG	S	401	1	14,14,15	0.52	0	17,19,21	1.51	3 (17%)
3	NAG	P	301	2	14,14,15	0.77	0	17,19,21	1.52	3 (17%)
3	NAG	K	401	1	14,14,15	0.46	0	17,19,21	2.78	3 (17%)
3	NAG	T	301	2	14,14,15	0.80	1 (7%)	17,19,21	1.84	4 (23%)
3	NAG	Q	401	1	14,14,15	0.52	0	17,19,21	1.61	3 (17%)
3	NAG	U	401	1	14,14,15	0.49	0	17,19,21	1.54	3 (17%)
3	NAG	M	401	1	14,14,15	0.48	0	17,19,21	2.99	8 (47%)
3	NAG	G	401	1	14,14,15	0.63	0	17,19,21	2.06	3 (17%)
3	NAG	V	301	2	14,14,15	0.83	0	17,19,21	2.03	3 (17%)
3	NAG	R	301	2	14,14,15	0.95	1 (7%)	17,19,21	1.89	4 (23%)
3	NAG	C	401	1	14,14,15	0.46	0	17,19,21	1.81	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	H	301	2	14,14,15	1.19	1 (7%)	17,19,21	2.61	7 (41%)
3	NAG	I	401	1	14,14,15	0.56	0	17,19,21	2.70	5 (29%)
3	NAG	A	401	1	14,14,15	0.56	0	17,19,21	2.18	6 (35%)
3	NAG	L	301	2	14,14,15	0.84	0	17,19,21	2.55	5 (29%)
3	NAG	E	401	1	14,14,15	0.55	0	17,19,21	1.90	4 (23%)
3	NAG	D	301	2	14,14,15	1.25	2 (14%)	17,19,21	3.10	9 (52%)
3	NAG	J	301	2	14,14,15	0.72	0	17,19,21	2.05	3 (17%)

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	X	301	2	-	2/6/23/26	0/1/1/1
3	NAG	W	401	1	-	2/6/23/26	0/1/1/1
3	NAG	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	B	301	2	-	1/6/23/26	0/1/1/1
3	NAG	O	401	1	-	0/6/23/26	0/1/1/1
3	NAG	N	301	2	-	2/6/23/26	0/1/1/1
3	NAG	S	401	1	-	2/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	K	401	1	-	2/6/23/26	0/1/1/1
3	NAG	T	301	2	-	2/6/23/26	0/1/1/1
3	NAG	Q	401	1	-	1/6/23/26	0/1/1/1
3	NAG	U	401	1	-	1/6/23/26	0/1/1/1
3	NAG	M	401	1	-	2/6/23/26	0/1/1/1
3	NAG	G	401	1	-	2/6/23/26	0/1/1/1
3	NAG	V	301	2	-	2/6/23/26	0/1/1/1
3	NAG	R	301	2	-	2/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	H	301	2	-	2/6/23/26	0/1/1/1
3	NAG	I	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	L	301	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	D	301	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	301	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	NAG	O7-C7	3.19	1.30	1.23
3	B	301	NAG	O7-C7	3.06	1.30	1.23
3	F	301	NAG	O7-C7	2.88	1.29	1.23
3	D	301	NAG	O7-C7	2.83	1.29	1.23
3	D	301	NAG	O5-C1	2.28	1.47	1.43
3	R	301	NAG	O7-C7	2.11	1.28	1.23
3	T	301	NAG	O7-C7	2.10	1.28	1.23

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	401	NAG	C1-O5-C5	9.68	125.31	112.19
3	K	401	NAG	C1-O5-C5	9.58	125.17	112.19
3	I	401	NAG	C1-O5-C5	9.57	125.16	112.19
3	W	401	NAG	C1-O5-C5	8.92	124.28	112.19
3	X	301	NAG	C1-O5-C5	8.57	123.80	112.19
3	L	301	NAG	C1-O5-C5	7.96	122.98	112.19
3	N	301	NAG	C1-O5-C5	7.01	121.69	112.19
3	J	301	NAG	C1-O5-C5	6.28	120.70	112.19
3	A	401	NAG	C1-O5-C5	6.26	120.67	112.19
3	E	401	NAG	C1-O5-C5	6.15	120.53	112.19
3	D	301	NAG	C1-O5-C5	6.06	120.41	112.19
3	B	301	NAG	O7-C7-N2	6.01	133.00	121.95
3	G	401	NAG	C1-O5-C5	5.78	120.02	112.19
3	T	301	NAG	C1-O5-C5	5.69	119.89	112.19
3	V	301	NAG	C1-O5-C5	5.68	119.89	112.19
3	C	401	NAG	C1-O5-C5	5.67	119.88	112.19
3	B	301	NAG	C2-N2-C7	5.61	130.90	122.90
3	F	301	NAG	O7-C7-N2	5.52	132.09	121.95
3	D	301	NAG	O7-C7-N2	5.41	131.90	121.95
3	R	301	NAG	C1-O5-C5	5.38	119.49	112.19
3	H	301	NAG	C8-C7-N2	-5.30	107.13	116.10
3	F	301	NAG	C1-O5-C5	5.21	119.25	112.19
3	F	301	NAG	C8-C7-N2	-4.88	107.84	116.10
3	B	301	NAG	C8-C7-N2	-4.81	107.95	116.10
3	D	301	NAG	C2-N2-C7	4.77	129.69	122.90
3	O	401	NAG	C1-O5-C5	4.76	118.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	401	NAG	C1-O5-C5	4.60	118.43	112.19
3	H	301	NAG	C1-O5-C5	4.60	118.42	112.19
3	D	301	NAG	C8-C7-N2	-4.52	108.44	116.10
3	B	301	NAG	C1-O5-C5	4.52	118.32	112.19
3	H	301	NAG	O7-C7-N2	4.23	129.73	121.95
3	Q	401	NAG	C1-O5-C5	4.05	117.68	112.19
3	N	301	NAG	C8-C7-N2	-4.00	109.33	116.10
3	K	401	NAG	O5-C1-C2	3.94	117.52	111.29
3	F	301	NAG	C2-N2-C7	3.92	128.49	122.90
3	G	401	NAG	O5-C5-C6	3.81	113.18	107.20
3	F	301	NAG	O5-C1-C2	3.79	117.28	111.29
3	M	401	NAG	O5-C1-C2	3.77	117.24	111.29
3	N	301	NAG	O5-C1-C2	-3.62	105.57	111.29
3	W	401	NAG	O5-C1-C2	3.61	116.99	111.29
3	P	301	NAG	C1-O5-C5	3.54	116.99	112.19
3	A	401	NAG	O5-C5-C6	3.53	112.73	107.20
3	L	301	NAG	O5-C1-C2	-3.40	105.93	111.29
3	V	301	NAG	O7-C7-N2	3.33	128.07	121.95
3	D	301	NAG	O5-C1-C2	3.32	116.52	111.29
3	R	301	NAG	O7-C7-N2	3.25	127.92	121.95
3	D	301	NAG	C1-C2-N2	3.23	116.01	110.49
3	L	301	NAG	C8-C7-N2	-3.22	110.66	116.10
3	P	301	NAG	O5-C5-C6	3.11	112.09	107.20
3	B	301	NAG	O5-C5-C4	3.04	118.23	110.83
3	Q	401	NAG	C3-C4-C5	-3.02	104.84	110.24
3	B	301	NAG	O5-C1-C2	2.98	115.99	111.29
3	M	401	NAG	C4-C3-C2	-2.98	106.66	111.02
3	S	401	NAG	C1-O5-C5	2.97	116.22	112.19
3	O	401	NAG	C3-C4-C5	-2.96	104.96	110.24
3	F	301	NAG	O5-C5-C4	2.94	117.97	110.83
3	H	301	NAG	C1-C2-N2	2.91	115.45	110.49
3	M	401	NAG	C3-C4-C5	-2.91	105.06	110.24
3	W	401	NAG	O5-C5-C6	-2.90	102.66	107.20
3	X	301	NAG	C8-C7-N2	-2.86	111.26	116.10
3	S	401	NAG	C3-C4-C5	-2.81	105.23	110.24
3	W	401	NAG	O4-C4-C5	2.73	116.07	109.30
3	D	301	NAG	O5-C5-C4	2.71	117.42	110.83
3	H	301	NAG	C4-C3-C2	-2.69	107.07	111.02
3	J	301	NAG	C8-C7-N2	-2.67	111.57	116.10
3	F	301	NAG	O3-C3-C2	2.65	114.95	109.47
3	I	401	NAG	O7-C7-C8	-2.65	117.14	122.06
3	W	401	NAG	O7-C7-C8	-2.61	117.20	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	301	NAG	O5-C1-C2	-2.61	107.16	111.29
3	Q	401	NAG	O5-C1-C2	-2.59	107.19	111.29
3	I	401	NAG	C8-C7-N2	2.57	120.45	116.10
3	M	401	NAG	C8-C7-N2	2.57	120.45	116.10
3	B	301	NAG	O3-C3-C2	2.55	114.75	109.47
3	M	401	NAG	O7-C7-C8	-2.53	117.35	122.06
3	K	401	NAG	O7-C7-C8	-2.53	117.35	122.06
3	W	401	NAG	C3-C4-C5	-2.53	105.72	110.24
3	C	401	NAG	C4-C3-C2	-2.53	107.32	111.02
3	H	301	NAG	O5-C5-C4	2.52	116.97	110.83
3	H	301	NAG	C2-N2-C7	2.51	126.48	122.90
3	X	301	NAG	O5-C5-C6	2.50	111.13	107.20
3	A	401	NAG	C4-C3-C2	2.49	114.66	111.02
3	X	301	NAG	O5-C1-C2	-2.48	107.37	111.29
3	T	301	NAG	O7-C7-N2	2.47	126.50	121.95
3	F	301	NAG	C1-C2-N2	2.47	114.70	110.49
3	F	301	NAG	C4-C3-C2	-2.46	107.41	111.02
3	D	301	NAG	C4-C3-C2	-2.45	107.43	111.02
3	T	301	NAG	O3-C3-C4	-2.39	104.83	110.35
3	C	401	NAG	O3-C3-C4	2.38	115.85	110.35
3	V	301	NAG	O3-C3-C4	-2.38	104.86	110.35
3	D	301	NAG	O5-C5-C6	2.37	110.92	107.20
3	E	401	NAG	O5-C5-C6	2.37	110.91	107.20
3	R	301	NAG	O5-C5-C6	2.36	110.90	107.20
3	P	301	NAG	O7-C7-N2	2.32	126.21	121.95
3	B	301	NAG	C1-C2-N2	2.23	114.30	110.49
3	S	401	NAG	O5-C1-C2	-2.23	107.77	111.29
3	A	401	NAG	C3-C4-C5	2.21	114.18	110.24
3	X	301	NAG	O7-C7-N2	2.18	125.96	121.95
3	L	301	NAG	C6-C5-C4	-2.15	107.98	113.00
3	N	301	NAG	O7-C7-N2	2.14	125.89	121.95
3	L	301	NAG	O5-C5-C4	2.14	116.02	110.83
3	I	401	NAG	O5-C1-C2	2.11	114.62	111.29
3	T	301	NAG	C2-N2-C7	-2.11	119.90	122.90
3	E	401	NAG	C4-C3-C2	-2.10	107.94	111.02
3	B	301	NAG	C3-C4-C5	2.10	113.98	110.24
3	A	401	NAG	C6-C5-C4	-2.10	108.09	113.00
3	M	401	NAG	O3-C3-C2	2.09	113.80	109.47
3	R	301	NAG	C8-C7-N2	-2.07	112.59	116.10
3	G	401	NAG	C4-C3-C2	-2.06	108.00	111.02
3	U	401	NAG	C6-C5-C4	-2.06	108.19	113.00
3	I	401	NAG	O3-C3-C4	-2.05	105.61	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	NAG	O3-C3-C4	2.05	115.08	110.35
3	X	301	NAG	O3-C3-C2	2.04	113.68	109.47
3	M	401	NAG	O4-C4-C5	2.04	114.35	109.30
3	U	401	NAG	C3-C4-C5	-2.03	106.62	110.24
3	A	401	NAG	O3-C3-C4	-2.01	105.70	110.35

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	301	NAG	O5-C5-C6-O6
3	M	401	NAG	O5-C5-C6-O6
3	P	301	NAG	O5-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6
3	N	301	NAG	O5-C5-C6-O6
3	K	401	NAG	O5-C5-C6-O6
3	T	301	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	H	301	NAG	O5-C5-C6-O6
3	I	401	NAG	O5-C5-C6-O6
3	J	301	NAG	O5-C5-C6-O6
3	X	301	NAG	C4-C5-C6-O6
3	W	401	NAG	O5-C5-C6-O6
3	G	401	NAG	O5-C5-C6-O6
3	R	301	NAG	O5-C5-C6-O6
3	D	301	NAG	O5-C5-C6-O6
3	K	401	NAG	C4-C5-C6-O6
3	P	301	NAG	C4-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	M	401	NAG	C4-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	V	301	NAG	O5-C5-C6-O6
3	I	401	NAG	C4-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	J	301	NAG	C4-C5-C6-O6
3	N	301	NAG	C4-C5-C6-O6
3	W	401	NAG	C4-C5-C6-O6
3	R	301	NAG	C4-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
3	V	301	NAG	C4-C5-C6-O6
3	T	301	NAG	C4-C5-C6-O6
3	G	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	301	NAG	C4-C5-C6-O6
3	H	301	NAG	C4-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	S	401	NAG	O5-C5-C6-O6
3	F	301	NAG	O5-C5-C6-O6
3	S	401	NAG	C4-C5-C6-O6
3	U	401	NAG	O5-C5-C6-O6
3	Q	401	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	301	NAG	1	0
3	N	301	NAG	1	0
3	I	401	NAG	1	0
3	L	301	NAG	1	0
3	J	301	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	319/327 (97%)	0.04	6 (1%) 66 69	44, 62, 87, 130	0
1	C	319/327 (97%)	0.09	8 (2%) 57 59	44, 63, 87, 131	0
1	E	319/327 (97%)	0.08	7 (2%) 62 63	43, 62, 87, 132	0
1	G	319/327 (97%)	0.03	6 (1%) 66 69	42, 63, 86, 131	0
1	I	319/327 (97%)	0.40	19 (5%) 21 20	53, 80, 117, 165	0
1	K	319/327 (97%)	0.39	17 (5%) 26 25	53, 80, 117, 158	0
1	M	319/327 (97%)	0.37	21 (6%) 18 16	53, 79, 117, 161	0
1	O	319/327 (97%)	0.47	20 (6%) 20 19	55, 88, 122, 149	0
1	Q	319/327 (97%)	0.44	23 (7%) 15 13	55, 88, 121, 154	0
1	S	319/327 (97%)	0.55	28 (8%) 10 8	56, 89, 121, 151	0
1	U	319/327 (97%)	0.55	31 (9%) 7 6	56, 89, 120, 151	0
1	W	319/327 (97%)	0.42	19 (5%) 21 20	51, 80, 116, 162	0
2	B	172/174 (98%)	0.56	8 (4%) 31 30	64, 96, 146, 193	0
2	D	172/174 (98%)	0.55	11 (6%) 19 18	65, 99, 145, 188	0
2	F	172/174 (98%)	0.59	12 (6%) 16 14	63, 97, 140, 182	0
2	H	172/174 (98%)	0.48	10 (5%) 23 22	55, 93, 138, 184	0
2	J	172/174 (98%)	1.03	33 (19%) 1 0	65, 115, 175, 219	0
2	L	172/174 (98%)	0.99	25 (14%) 2 1	64, 113, 173, 211	0
2	N	172/174 (98%)	1.16	31 (18%) 1 1	65, 116, 180, 219	0
2	P	172/174 (98%)	0.51	13 (7%) 13 12	48, 81, 124, 184	0
2	R	172/174 (98%)	0.45	10 (5%) 23 22	46, 82, 124, 185	0
2	T	172/174 (98%)	0.40	12 (6%) 16 14	46, 81, 124, 194	0
2	V	172/174 (98%)	0.36	11 (6%) 19 18	47, 83, 125, 178	0
2	X	172/174 (98%)	0.93	30 (17%) 1 1	60, 108, 168, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5892/6012 (98%)	0.44	411 (6%) 16 14	42, 81, 140, 219	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	33	GLY	19.6
2	L	33	GLY	13.1
2	X	33	GLY	8.6
2	J	33	GLY	8.1
2	V	153	ARG	6.8
2	N	23	GLY	6.5
2	J	23	GLY	6.4
2	F	27	GLN	6.4
2	X	157	TYR	6.1
1	G	0	GLY	6.1
2	N	21	TRP	6.1
2	X	23	GLY	5.8
2	N	152	ILE	5.8
2	L	140	ILE	5.7
2	N	31	GLY	5.5
2	R	153	ARG	5.3
2	D	27	GLN	5.1
2	B	27	GLN	5.1
2	N	59	THR	5.0
2	N	170	ARG	4.9
2	N	32	THR	4.9
2	T	153	ARG	4.9
2	J	170	ARG	4.8
1	U	74	TRP	4.8
2	L	21	TRP	4.8
2	L	157	TYR	4.8
1	S	146	VAL	4.7
1	E	162	ARG	4.6
2	N	168	LEU	4.6
2	L	170	ARG	4.5
2	P	153	ARG	4.5
2	L	152	ILE	4.5
2	J	171	LEU	4.5
2	P	172	ASN	4.5
2	X	32	THR	4.5
2	J	32	THR	4.4
2	J	152	ILE	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	V	138	PHE	4.3
2	J	121	ARG	4.3
2	N	157	TYR	4.3
2	L	31	GLY	4.3
1	U	146	VAL	4.3
2	X	31	GLY	4.2
2	N	26	HIS	4.2
2	J	31	GLY	4.2
1	Q	77	LEU	4.2
2	N	172	ASN	4.1
2	X	168	LEU	4.1
1	Q	74	TRP	4.1
1	S	74	TRP	4.0
2	J	168	LEU	4.0
2	J	21	TRP	4.0
2	J	59	THR	4.0
1	I	2	LYS	3.9
2	B	130	ALA	3.9
2	N	140	ILE	3.9
2	J	157	TYR	3.9
2	H	27	GLN	3.9
2	X	21	TRP	3.9
1	E	2	LYS	3.9
1	W	2	LYS	3.9
2	J	143	ALA	3.8
2	J	24	PHE	3.8
2	N	153	ARG	3.8
2	X	140	ILE	3.8
1	C	2	LYS	3.8
1	I	312	GLY	3.8
1	G	162	ARG	3.8
2	V	59	THR	3.8
2	L	23	GLY	3.8
2	V	168	LEU	3.7
1	M	13	GLY	3.7
1	W	90	GLY	3.6
2	J	140	ILE	3.6
1	C	162	ARG	3.6
1	O	118	GLY	3.6
2	N	141	TYR	3.6
1	O	82	ASN	3.6
1	O	77	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	J	16	GLY	3.6
2	D	153	ARG	3.6
2	H	138	PHE	3.6
2	L	168	LEU	3.6
2	V	172	ASN	3.5
1	A	150	LYS	3.5
1	U	127	THR	3.5
2	X	121	ARG	3.5
1	E	0	GLY	3.5
1	K	82	ASN	3.5
2	L	59	THR	3.5
2	X	170	ARG	3.5
2	F	11	GLU	3.5
1	S	266	ILE	3.5
2	H	32	THR	3.5
1	S	77	LEU	3.5
1	S	258	LEU	3.5
2	N	121	ARG	3.5
2	R	164	GLU	3.5
1	U	72	GLY	3.4
1	M	12	ASN	3.4
2	X	152	ILE	3.4
2	X	144	CYS	3.4
2	P	59	THR	3.4
2	N	143	ALA	3.4
1	I	316	VAL	3.4
2	L	32	THR	3.4
1	O	162	ARG	3.3
2	R	32	THR	3.3
1	U	77	LEU	3.3
2	D	138	PHE	3.3
1	I	128	ARG	3.3
2	D	11	GLU	3.3
1	U	216	VAL	3.3
2	R	59	THR	3.3
2	R	138	PHE	3.3
1	O	74	TRP	3.3
1	O	117	TYR	3.3
1	W	15	ILE	3.3
2	F	130	ALA	3.3
1	I	68	LEU	3.3
1	C	0	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	139	GLU	3.2
2	B	140	ILE	3.2
2	N	34	GLN	3.2
2	F	33	GLY	3.2
2	B	138	PHE	3.2
2	P	138	PHE	3.2
1	S	216	VAL	3.2
1	Q	150	LYS	3.2
1	M	162	ARG	3.2
2	L	24	PHE	3.2
1	S	139	TYR	3.2
1	I	196	SER	3.2
1	I	217	ASN	3.2
2	X	172	ASN	3.2
1	I	14	THR	3.2
1	K	162	ARG	3.2
1	W	23	GLN	3.2
1	O	146	VAL	3.2
1	M	85	ALA	3.2
1	K	221	GLY	3.2
1	A	162	ARG	3.2
2	D	122	VAL	3.1
2	J	149	MET	3.1
2	X	153	ARG	3.1
1	U	162	ARG	3.1
1	U	238	PHE	3.1
2	T	59	THR	3.1
1	I	3	ILE	3.1
1	I	23	GLN	3.1
2	L	171	LEU	3.0
1	S	117	TYR	3.0
2	X	38	TYR	3.0
2	R	172	ASN	3.0
1	C	150	LYS	3.0
1	I	162	ARG	3.0
2	J	153	ARG	3.0
2	X	25	ARG	3.0
2	X	24	PHE	3.0
1	Q	162	ARG	3.0
1	K	15	ILE	3.0
1	W	82	ASN	3.0
2	L	172	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	121	ILE	2.9
2	J	26	HIS	2.9
2	N	67	GLU	2.9
2	X	141	TYR	2.9
1	M	317	PRO	2.9
2	T	27	GLN	2.9
1	M	15	ILE	2.9
2	L	138	PHE	2.9
2	X	16	GLY	2.9
1	O	139	TYR	2.9
2	X	26	HIS	2.9
1	K	23	GLN	2.9
1	U	88	TYR	2.9
2	H	140	ILE	2.9
2	H	130	ALA	2.9
1	W	162	ARG	2.9
1	K	90	GLY	2.9
1	M	2	LYS	2.9
2	L	143	ALA	2.9
1	Q	236	ILE	2.9
2	D	130	ALA	2.9
2	F	122	VAL	2.9
1	M	82	ASN	2.9
2	B	139	GLU	2.8
1	S	88	TYR	2.8
1	S	118	GLY	2.8
1	W	14	THR	2.8
2	J	141	TYR	2.8
2	J	57	GLU	2.8
2	J	172	ASN	2.8
1	S	129	ALA	2.8
2	J	156	THR	2.8
2	L	22	TYR	2.8
2	X	162	TYR	2.8
1	U	258	LEU	2.8
1	M	312	GLY	2.8
1	U	76	THR	2.8
2	P	124	LYS	2.8
1	K	296	GLY	2.8
1	M	254	ILE	2.8
1	Q	254	ILE	2.8
2	R	60	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	262	SER	2.7
1	A	41	LEU	2.7
1	O	238	PHE	2.7
1	K	107	GLY	2.7
1	S	76	THR	2.7
1	Q	216	VAL	2.7
1	U	167	ALA	2.7
1	A	0	GLY	2.7
2	J	138	PHE	2.7
2	T	164	GLU	2.7
2	L	26	HIS	2.7
1	S	236	ILE	2.7
1	O	76	THR	2.7
1	Q	268	ASN	2.7
2	P	29	ALA	2.7
2	H	11	GLU	2.7
2	T	171	LEU	2.6
2	V	171	LEU	2.6
1	G	150	LYS	2.6
1	K	60	LEU	2.6
1	K	13	GLY	2.6
2	F	124	LYS	2.6
2	X	28	ASN	2.6
2	N	24	PHE	2.6
1	Q	139	TYR	2.6
1	U	236	ILE	2.6
1	W	107	GLY	2.6
2	X	67	GLU	2.6
1	S	264	ALA	2.6
2	L	153	ARG	2.6
2	P	164	GLU	2.6
1	M	84	ILE	2.6
2	N	56	VAL	2.6
2	N	57	GLU	2.6
1	W	312	GLY	2.6
1	A	128	ARG	2.6
1	W	304	ARG	2.6
1	I	317	PRO	2.5
1	U	117	TYR	2.5
2	N	38	TYR	2.5
1	Q	146	VAL	2.5
2	T	168	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	25	ARG	2.5
1	Q	167	ALA	2.5
1	Q	72	GLY	2.5
1	Q	312	GLY	2.5
1	S	128	ARG	2.5
1	S	268	ASN	2.5
1	U	109	ASN	2.5
1	U	15	ILE	2.5
1	U	212	ALA	2.5
2	N	47	GLN	2.5
2	J	144	CYS	2.5
1	W	269	ASN	2.5
1	C	128	ARG	2.5
1	E	150	LYS	2.5
1	Q	238	PHE	2.5
1	I	12	ASN	2.5
1	I	304	ARG	2.5
2	J	25	ARG	2.5
1	U	108	ILE	2.5
2	L	162	TYR	2.5
2	T	24	PHE	2.5
1	M	284	ARG	2.5
2	F	132	GLU	2.4
2	X	34	GLN	2.4
1	S	126	THR	2.4
2	T	32	THR	2.4
2	P	171	LEU	2.4
1	G	128	ARG	2.4
2	T	170	ARG	2.4
1	U	47	LYS	2.4
2	L	141	TYR	2.4
1	C	266	ILE	2.4
1	U	78	ILE	2.4
2	F	126	LEU	2.4
1	K	128	ARG	2.4
2	J	55	LEU	2.4
1	S	102	ILE	2.4
2	D	140	ILE	2.4
1	A	23	GLN	2.4
2	X	139	GLU	2.4
1	E	41	LEU	2.4
2	T	138	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	293	ARG	2.4
1	S	82	ASN	2.4
1	W	128	ARG	2.4
1	U	244	LEU	2.4
2	X	44	ALA	2.4
1	S	78	ILE	2.4
1	S	162	ARG	2.4
2	N	150	GLU	2.4
2	J	22	TYR	2.3
2	N	149	MET	2.3
2	N	22	TYR	2.3
1	S	127	THR	2.3
1	U	264	ALA	2.3
2	X	59	THR	2.3
1	Q	15	ILE	2.3
1	M	216	VAL	2.3
2	N	138	PHE	2.3
1	U	150	LYS	2.3
1	O	267	ASP	2.3
2	R	171	LEU	2.3
1	K	12	ASN	2.3
2	T	140	ILE	2.3
1	U	138	PHE	2.3
1	E	128	ARG	2.3
1	M	277	ARG	2.3
1	K	14	THR	2.3
1	C	38	ILE	2.3
2	F	138	PHE	2.3
2	L	121	ARG	2.3
1	W	13	GLY	2.3
1	W	196	SER	2.3
2	P	168	LEU	2.3
2	R	170	ARG	2.3
1	U	121	ILE	2.3
1	I	197	VAL	2.3
1	O	216	VAL	2.3
2	J	145	ASP	2.3
2	F	8	GLY	2.2
1	U	129	ALA	2.2
2	D	32	THR	2.2
1	U	41	LEU	2.2
2	P	170	ARG	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	V	141	TYR	2.2
1	W	1	ASP	2.2
2	H	139	GLU	2.2
1	O	62	GLY	2.2
2	V	32	THR	2.2
1	K	118	GLY	2.2
1	I	284	ARG	2.2
1	W	192	SER	2.2
1	Q	5	LEU	2.2
1	I	85	ALA	2.2
2	H	115	MET	2.2
1	O	0	GLY	2.2
1	Q	76	THR	2.2
1	Q	258	LEU	2.2
1	S	41	LEU	2.2
1	S	167	ALA	2.2
2	P	102	MET	2.2
2	X	149	MET	2.2
1	M	14	THR	2.2
1	U	126	THR	2.2
1	M	3	ILE	2.2
1	G	43	MET	2.2
2	D	25	ARG	2.2
2	V	60	ASN	2.1
2	J	167	LEU	2.1
2	T	172	ASN	2.1
1	W	254	ILE	2.1
2	X	125	GLN	2.1
1	M	1	ASP	2.1
2	L	67	GLU	2.1
2	V	132	GLU	2.1
1	Q	82	ASN	2.1
1	K	316	VAL	2.1
1	U	188	TYR	2.1
2	R	166	ALA	2.1
2	N	28	ASN	2.1
1	W	4	CYS	2.1
1	E	6	GLY	2.1
1	O	125	GLY	2.1
2	N	124	LYS	2.1
2	B	59	THR	2.1
2	H	102	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	150	LYS	2.1
1	G	38	ILE	2.1
1	I	15	ILE	2.1
1	O	142	LEU	2.1
1	Q	78	ILE	2.1
2	F	139	GLU	2.1
2	F	164	GLU	2.1
2	J	67	GLU	2.1
1	M	23	GLN	2.1
1	W	131	MET	2.1
2	V	9	PHE	2.1
1	Q	88	TYR	2.1
2	J	162	TYR	2.1
1	S	59	MET	2.1
1	O	258	LEU	2.1
2	D	171	LEU	2.1
1	Q	117	TYR	2.1
1	S	150	LYS	2.1
2	J	34	GLN	2.1
1	U	85	ALA	2.1
2	L	156	THR	2.1
2	L	16	GLY	2.1
1	S	170	LEU	2.0
2	P	27	GLN	2.0
1	O	188	TYR	2.0
1	M	25	GLU	2.0
1	C	41	LEU	2.0
1	U	293	ARG	2.0
1	M	90	GLY	2.0
1	S	47	LYS	2.0
2	H	31	GLY	2.0
1	I	82	ASN	2.0
2	P	157	TYR	2.0
2	X	22	TYR	2.0
1	K	46	ARG	2.0
1	O	5	LEU	2.0
2	B	153	ARG	2.0
2	B	171	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	P	301	14/15	0.49	0.31	83,87,94,97	0
3	NAG	V	301	14/15	0.53	0.30	86,90,95,96	0
3	NAG	X	301	14/15	0.63	0.31	91,95,102,102	0
3	NAG	N	301	14/15	0.63	0.27	92,96,102,103	0
3	NAG	R	301	14/15	0.64	0.28	82,84,88,89	0
3	NAG	T	301	14/15	0.70	0.24	80,85,89,90	0
3	NAG	L	301	14/15	0.70	0.23	91,95,102,103	0
3	NAG	H	301	14/15	0.71	0.18	80,84,86,86	0
3	NAG	J	301	14/15	0.72	0.23	97,101,108,108	0
3	NAG	B	301	14/15	0.73	0.17	81,84,87,88	0
3	NAG	D	301	14/15	0.75	0.17	85,88,92,92	0
3	NAG	F	301	14/15	0.79	0.15	81,84,89,89	0
3	NAG	G	401	14/15	0.81	0.19	100,107,110,110	0
3	NAG	E	401	14/15	0.81	0.18	97,105,107,110	0
3	NAG	Q	401	14/15	0.82	0.21	99,112,116,117	0
3	NAG	A	401	14/15	0.82	0.17	103,110,114,118	0
3	NAG	C	401	14/15	0.83	0.19	95,105,109,109	0
3	NAG	U	401	14/15	0.85	0.20	101,114,121,121	0
3	NAG	O	401	14/15	0.86	0.20	97,111,116,117	0
3	NAG	S	401	14/15	0.88	0.20	97,111,117,119	0
3	NAG	W	401	14/15	0.90	0.13	64,72,75,78	0
3	NAG	I	401	14/15	0.91	0.13	63,71,76,77	0
3	NAG	M	401	14/15	0.92	0.12	63,72,76,78	0
3	NAG	K	401	14/15	0.93	0.10	67,75,81,82	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	P	301	14/15	0.49	0.31	83,87,94,97	0
3	NAG	V	301	14/15	0.53	0.30	86,90,95,96	0
3	NAG	X	301	14/15	0.63	0.31	91,95,102,102	0
3	NAG	N	301	14/15	0.63	0.27	92,96,102,103	0
3	NAG	R	301	14/15	0.64	0.28	82,84,88,89	0
3	NAG	T	301	14/15	0.70	0.24	80,85,89,90	0
3	NAG	L	301	14/15	0.70	0.23	91,95,102,103	0
3	NAG	H	301	14/15	0.71	0.18	80,84,86,86	0
3	NAG	J	301	14/15	0.72	0.23	97,101,108,108	0
3	NAG	B	301	14/15	0.73	0.17	81,84,87,88	0
3	NAG	D	301	14/15	0.75	0.17	85,88,92,92	0
3	NAG	F	301	14/15	0.79	0.15	81,84,89,89	0
3	NAG	G	401	14/15	0.81	0.19	100,107,110,110	0
3	NAG	E	401	14/15	0.81	0.18	97,105,107,110	0
3	NAG	Q	401	14/15	0.82	0.21	99,112,116,117	0
3	NAG	A	401	14/15	0.82	0.17	103,110,114,118	0
3	NAG	C	401	14/15	0.83	0.19	95,105,109,109	0
3	NAG	U	401	14/15	0.85	0.20	101,114,121,121	0
3	NAG	O	401	14/15	0.86	0.20	97,111,116,117	0
3	NAG	S	401	14/15	0.88	0.20	97,111,117,119	0
3	NAG	W	401	14/15	0.90	0.13	64,72,75,78	0
3	NAG	I	401	14/15	0.91	0.13	63,71,76,77	0
3	NAG	M	401	14/15	0.92	0.12	63,72,76,78	0
3	NAG	K	401	14/15	0.93	0.10	67,75,81,82	0

## 6.5 Other polymers

There are no such residues in this entry.