



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:28 PM UTC

PDB ID : 4WSX / pdb_00004wsx
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

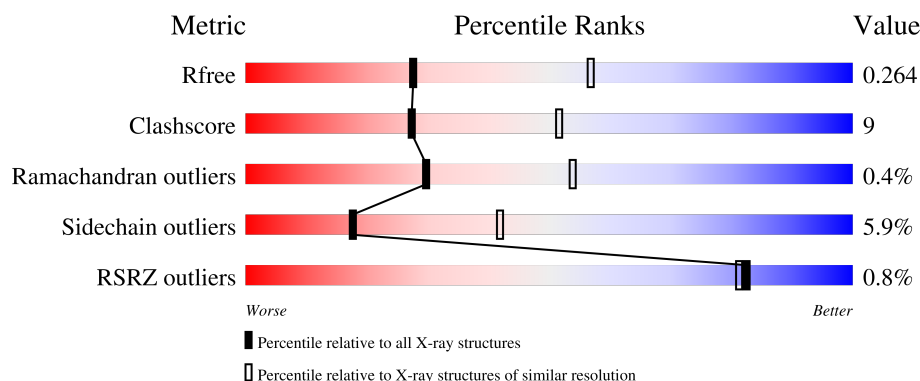
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

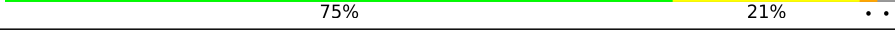
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	
1	C	327	
1	E	327	
1	G	327	
1	I	327	

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Mol	Chain	Length	Quality of chain
1	K	327	74% 21% ...
1	M	327	76% 20% ...
1	O	327	74% 22% ..
1	Q	327	74% 22% ..
1	S	327	74% 21% ..
1	U	327	75% 21% ..
1	W	327	76% 20% ..
2	B	174	3% 77% 17% 5% .
2	D	174	3% 75% 19% 5% .
2	F	174	2% 76% 18% 5% .
2	H	174	2% 76% 18% 5% .
2	J	174	2% 74% 20% 5% .
2	L	174	2% 75% 20% . ..
2	N	174	3% 75% 20% 5% .
2	P	174	78% 16% 5% .
2	R	174	76% 18% 5% .
2	T	174	77% 17% 5% .
2	V	174	77% 17% 5% .
2	X	174	3% 75% 20% 5% .

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.

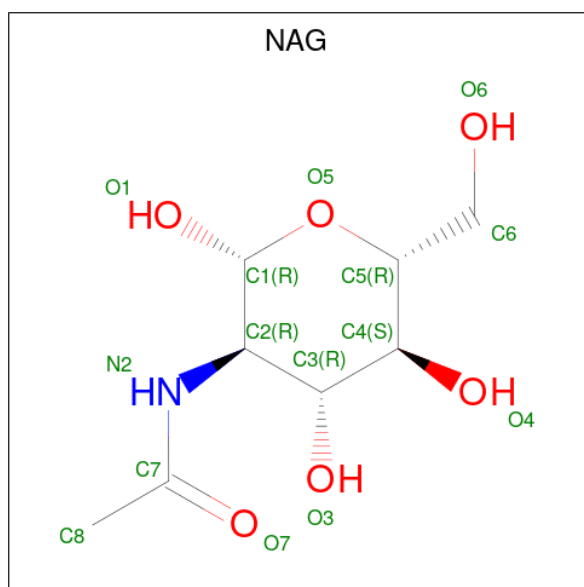
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			
2	D	172	Total	C	N	O	S	0	0	0
			1386	856	240	282	8			

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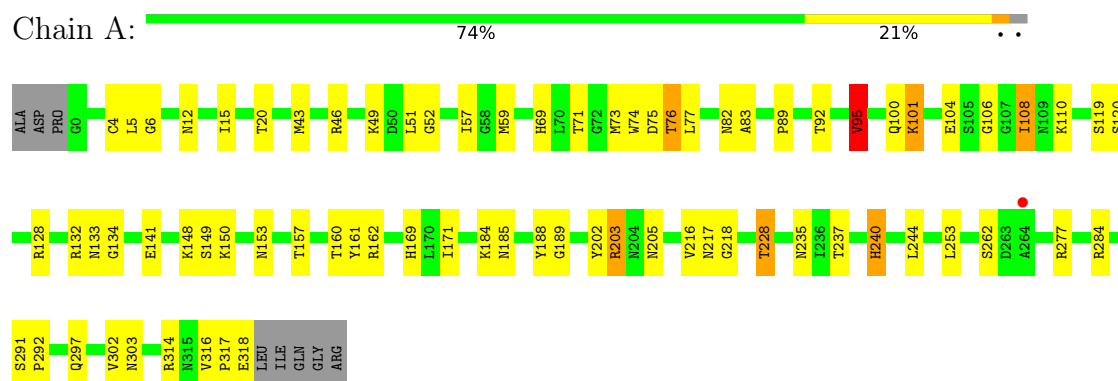
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	W	1	Total	C	N	O	0	0
			14	8	1	5		
3	X	1	Total	C	N	O	0	0
			14	8	1	5		

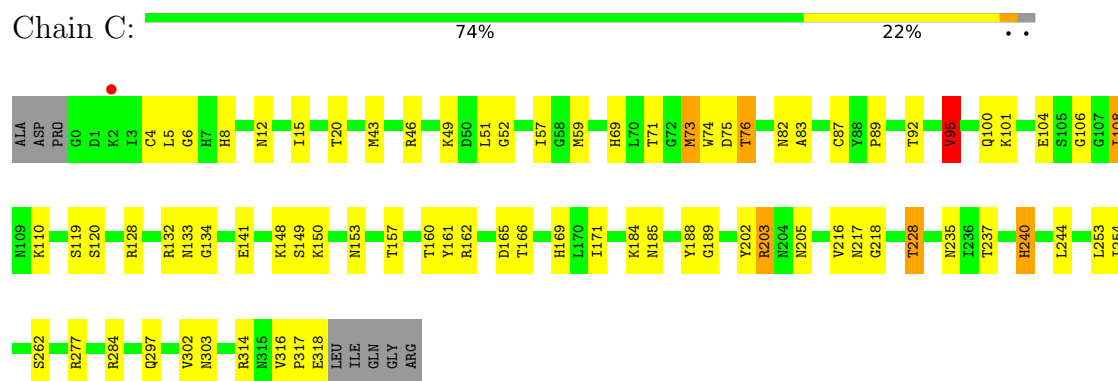
3 Residue-property plots

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

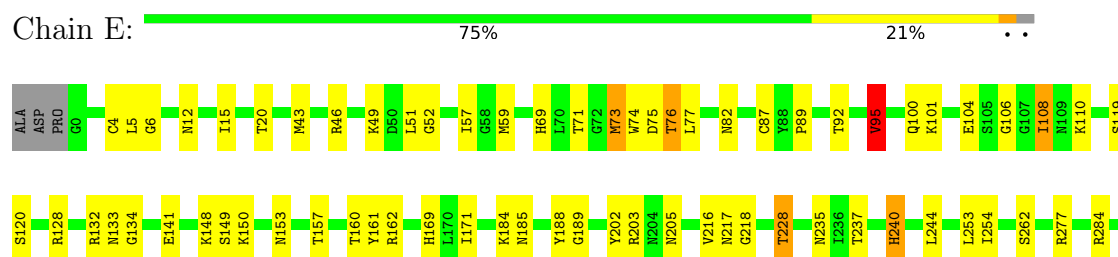
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain



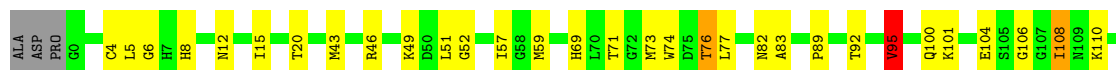
• Molecule 1: Hemagglutinin HA1 chain





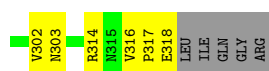
- Molecule 1: Hemagglutinin HA1 chain

Chain G: 75% 21% ..



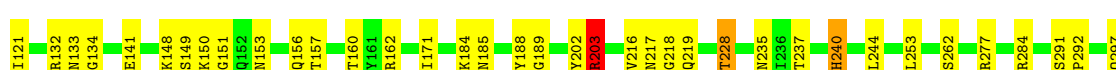
- Molecule 1: Hemagglutinin HA1 chain

Chain I: 75% 21% ..



- Molecule 1: Hemagglutinin HA1 chain

Chain K: 74% 21% ..



- Molecule 1: Hemagglutinin HA1 chain

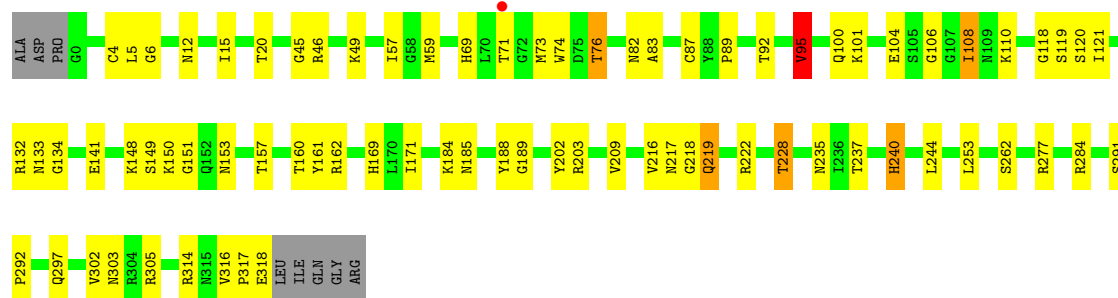
Chain M: 76% 20% ..





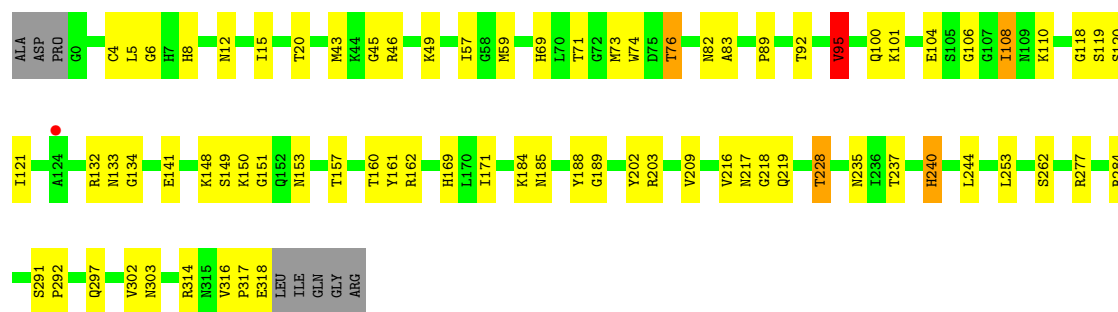
- Molecule 1: Hemagglutinin HA1 chain

Chain O: 74% 22% ..



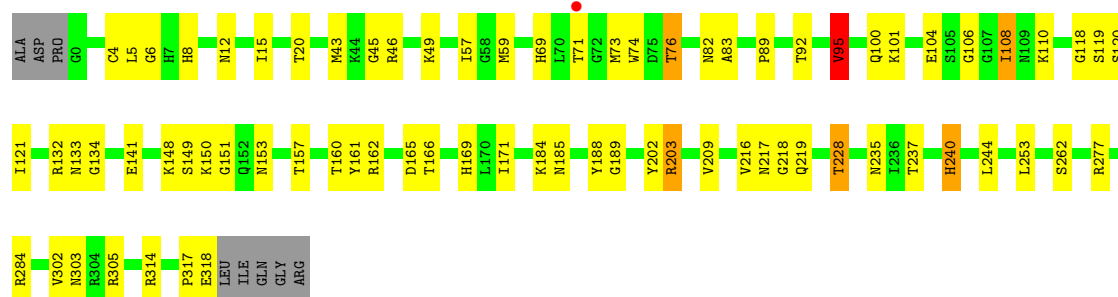
- Molecule 1: Hemagglutinin HA1 chain

Chain Q: 74% 22% ..



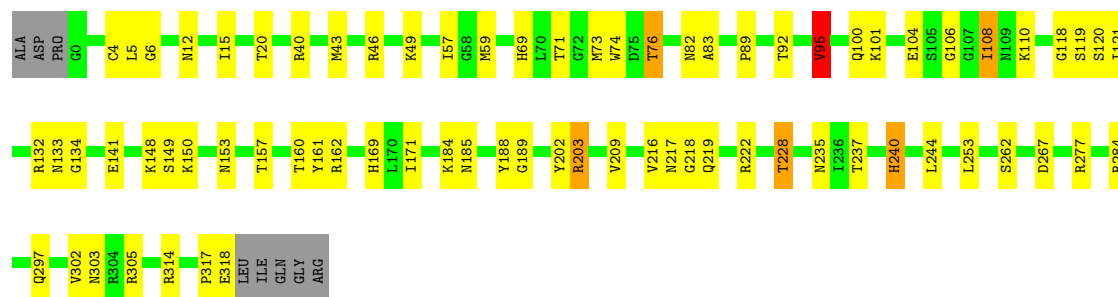
- Molecule 1: Hemagglutinin HA1 chain

Chain S: 74% 21% ..



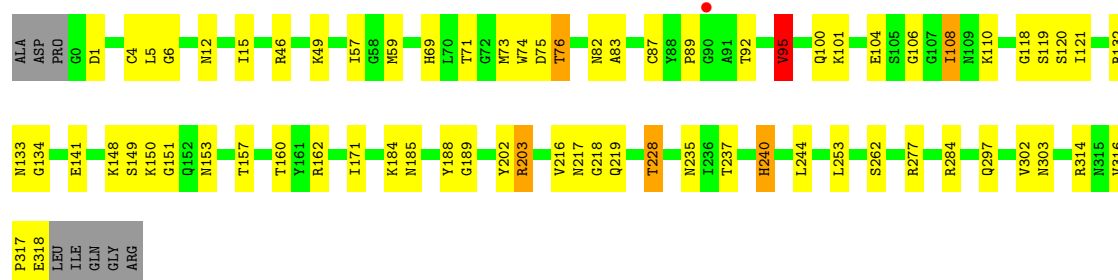
- Molecule 1: Hemagglutinin HA1 chain

Chain U: 75% 21% ..



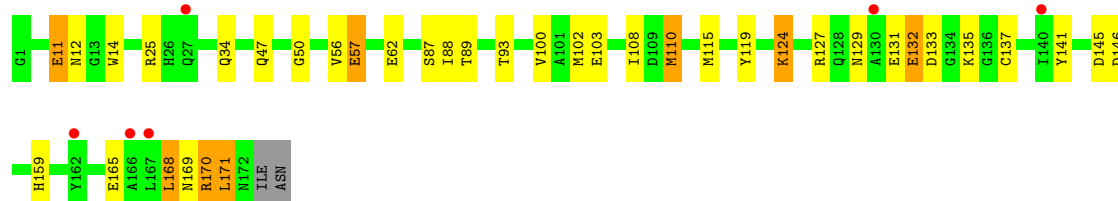
• Molecule 1: Hemagglutinin HA1 chain

Chain W: 76% 20% . .



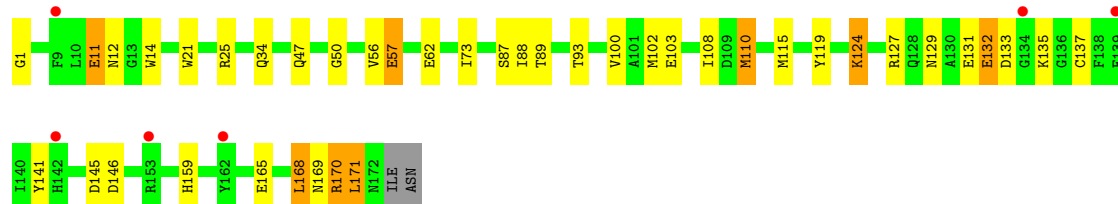
• Molecule 2: Hemagglutinin HA2 chain

Chain B: 77% 17% 5% .



• Molecule 2: Hemagglutinin HA2 chain

Chain D: 75% 19% 5% .

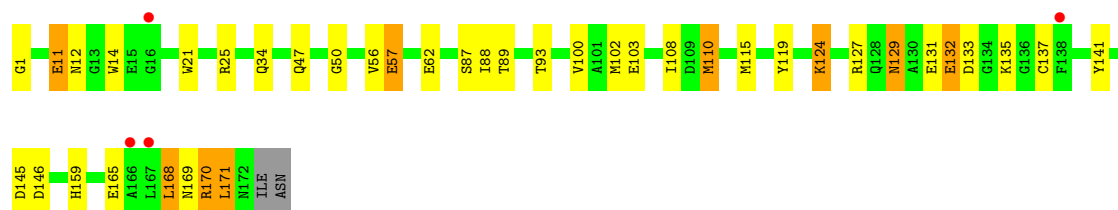
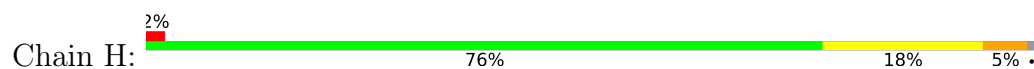


• Molecule 2: Hemagglutinin HA2 chain

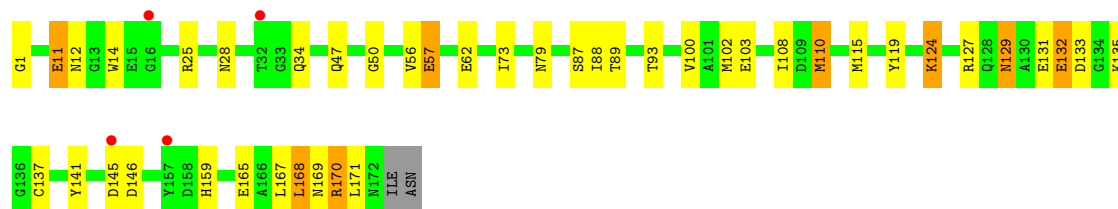
Chain F: 76% 18% 5% .



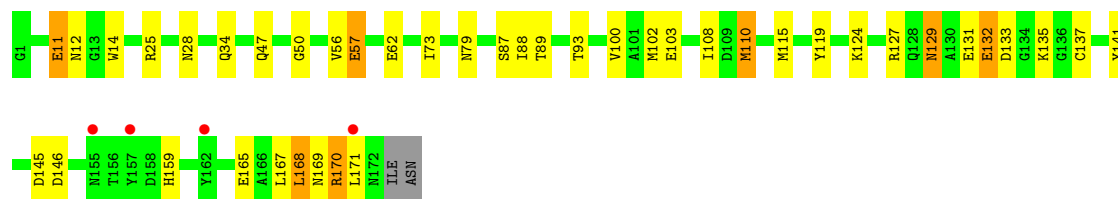
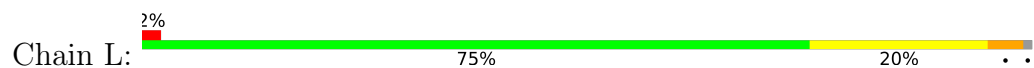
• Molecule 2: Hemagglutinin HA2 chain



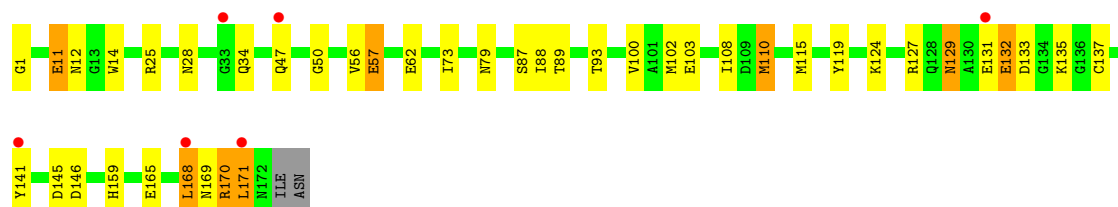
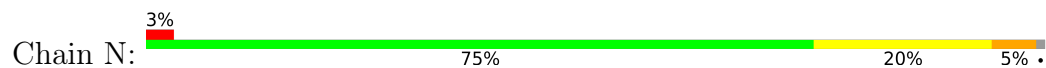
• Molecule 2: Hemagglutinin HA2 chain



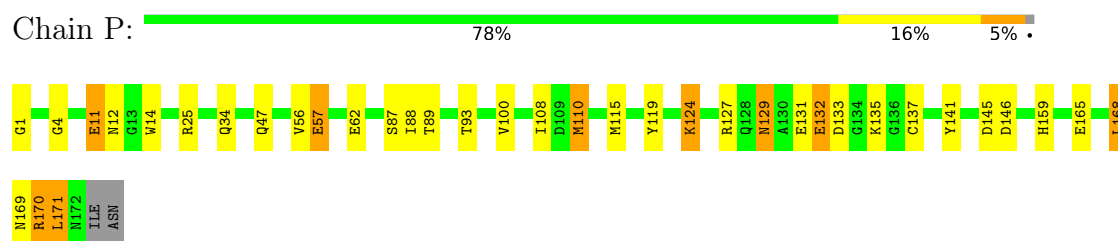
• Molecule 2: Hemagglutinin HA2 chain



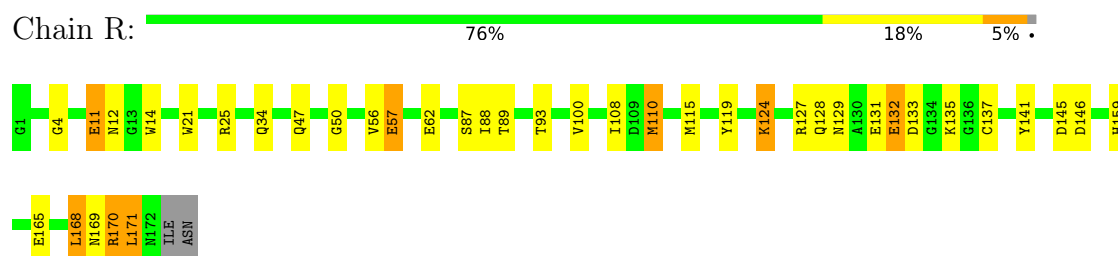
• Molecule 2: Hemagglutinin HA2 chain



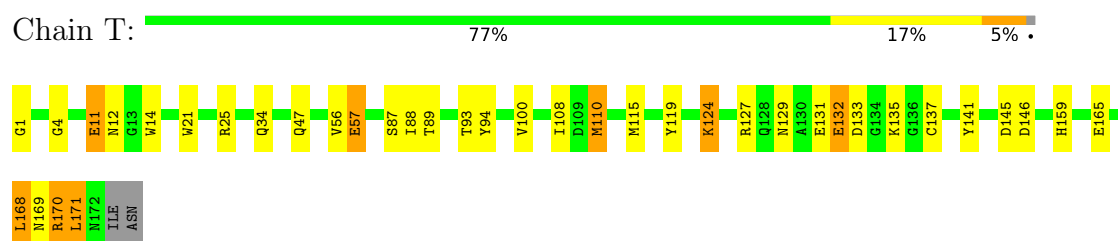
- Molecule 2: Hemagglutinin HA2 chain



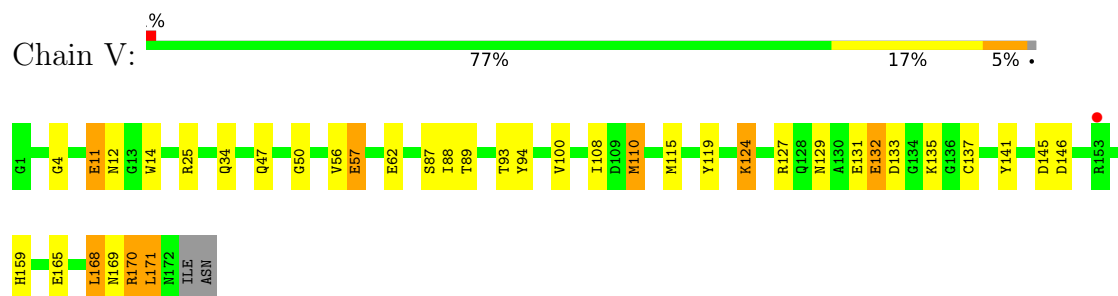
- Molecule 2: Hemagglutinin HA2 chain



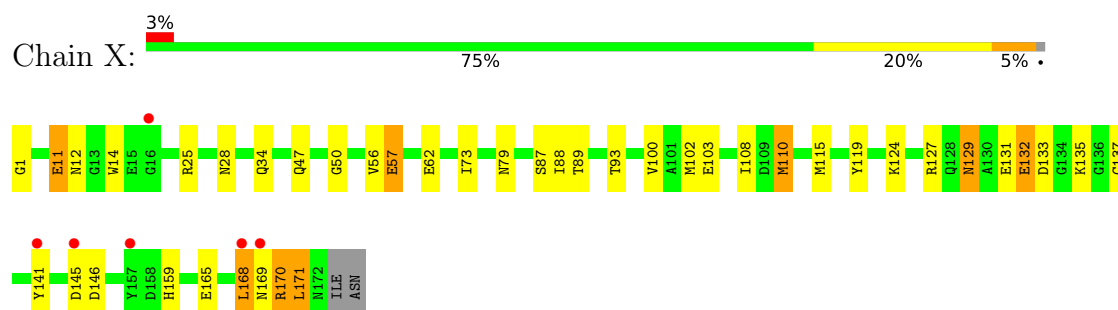
- Molecule 2: Hemagglutinin HA2 chain



- 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, α , β , γ	217.40Å 217.61Å 146.27Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	48.76 – 2.70 48.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-2.70) 99.6 (48.76-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.243 , 0.266 0.243 , 0.264	Depositor DCC
R_{free} test set	9317 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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	0.94	EDS
Total number of atoms	46260	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

¹Intensities estimated from amplitudes.

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

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	0.88	0/2490	0.98	2/3373 (0.1%)
1	C	0.90	0/2490	0.97	3/3373 (0.1%)
1	E	0.89	0/2490	0.97	2/3373 (0.1%)
1	G	0.89	0/2490	0.97	3/3373 (0.1%)
1	I	0.81	0/2490	0.96	5/3373 (0.1%)
1	K	0.82	0/2490	0.96	7/3373 (0.2%)
1	M	0.81	0/2490	0.96	6/3373 (0.2%)
1	O	0.79	1/2490 (0.0%)	0.96	5/3373 (0.1%)
1	Q	0.78	0/2490	0.96	4/3373 (0.1%)
1	S	0.79	0/2490	0.96	4/3373 (0.1%)
1	U	0.79	0/2490	0.96	3/3373 (0.1%)
1	W	0.82	0/2490	0.97	5/3373 (0.1%)
2	B	0.88	0/1411	0.98	1/1904 (0.1%)
2	D	0.88	1/1411 (0.1%)	0.98	1/1904 (0.1%)
2	F	0.88	1/1411 (0.1%)	0.98	1/1904 (0.1%)
2	H	0.88	1/1411 (0.1%)	0.98	1/1904 (0.1%)
2	J	0.81	1/1411 (0.1%)	0.94	1/1904 (0.1%)
2	L	0.81	0/1411	0.95	1/1904 (0.1%)
2	N	0.82	1/1411 (0.1%)	0.95	1/1904 (0.1%)
2	P	0.84	1/1411 (0.1%)	0.99	2/1904 (0.1%)
2	R	0.84	0/1411	0.99	2/1904 (0.1%)
2	T	0.85	1/1411 (0.1%)	1.00	2/1904 (0.1%)
2	V	0.85	0/1411	1.00	2/1904 (0.1%)
2	X	0.80	1/1411 (0.1%)	0.94	1/1904 (0.1%)
All	All	0.84	9/46812 (0.0%)	0.97	65/63324 (0.1%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	219	GLN	CA-C	8.40	1.63	1.52
2	F	1	GLY	N-CA	5.77	1.54	1.45
2	H	1	GLY	N-CA	5.35	1.54	1.45
2	N	1	GLY	N-CA	5.29	1.54	1.45
2	J	1	GLY	N-CA	5.26	1.53	1.45
2	P	1	GLY	N-CA	5.11	1.53	1.45
2	D	1	GLY	N-CA	5.05	1.53	1.45
2	T	1	GLY	N-CA	5.03	1.53	1.45
2	X	1	GLY	N-CA	5.03	1.53	1.45

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	95	VAL	CB-CA-C	-8.37	101.17	111.88
1	W	95	VAL	CB-CA-C	-8.34	101.20	111.88
1	A	95	VAL	CB-CA-C	-8.06	101.56	111.88
1	K	95	VAL	CB-CA-C	-7.97	101.67	111.88
1	M	95	VAL	CB-CA-C	-7.91	101.75	111.88
1	G	95	VAL	CB-CA-C	-7.89	101.78	111.88
1	S	95	VAL	CB-CA-C	-7.89	101.77	111.88
1	C	95	VAL	CB-CA-C	-7.84	101.84	111.88
1	Q	95	VAL	CB-CA-C	-7.73	101.98	111.88
1	U	95	VAL	CB-CA-C	-7.71	102.02	111.88
1	E	95	VAL	CB-CA-C	-7.70	102.03	111.88
1	O	95	VAL	CB-CA-C	-7.51	102.26	111.88
2	P	12	ASN	N-CA-C	6.31	117.82	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	12	ASN	N-CA-C	6.29	117.78	108.60
1	S	219	GLN	N-CA-C	6.27	119.35	110.14
2	T	12	ASN	N-CA-C	6.15	117.58	108.60
2	V	12	ASN	N-CA-C	6.13	117.55	108.60
1	U	219	GLN	N-CA-C	6.05	119.04	110.14
1	Q	219	GLN	N-CA-C	5.98	118.94	110.14
2	N	12	ASN	N-CA-C	5.90	117.82	108.79
2	X	12	ASN	N-CA-C	5.78	117.63	108.79
2	J	12	ASN	N-CA-C	5.78	117.63	108.79
2	L	12	ASN	N-CA-C	5.77	117.62	108.79
1	M	83	ALA	N-CA-C	5.57	117.92	110.35
1	Q	83	ALA	N-CA-C	5.55	117.91	110.35
1	U	83	ALA	N-CA-C	5.52	117.86	110.35
1	W	151	GLY	N-CA-C	-5.52	100.10	113.18
1	W	83	ALA	N-CA-C	5.48	117.80	110.35
1	M	151	GLY	N-CA-C	-5.48	100.20	113.18
1	I	87	CYS	N-CA-C	-5.45	105.26	111.14
1	O	83	ALA	N-CA-C	5.45	117.76	110.35
1	K	83	ALA	N-CA-C	5.44	117.75	110.35
2	B	12	ASN	N-CA-C	5.43	117.10	108.79
1	M	87	CYS	N-CA-C	-5.42	105.28	111.14
1	K	151	GLY	N-CA-C	-5.41	100.35	113.18
2	R	4	GLY	N-CA-C	5.37	122.50	115.47
2	F	12	ASN	N-CA-C	5.35	116.97	108.79
1	S	83	ALA	N-CA-C	5.34	117.62	110.35
1	I	83	ALA	N-CA-C	5.33	118.02	110.50
1	I	151	GLY	N-CA-C	-5.33	100.56	113.18
1	W	219	GLN	N-CA-C	5.28	117.91	110.14
2	H	12	ASN	N-CA-C	5.28	116.87	108.79
2	T	4	GLY	N-CA-C	5.28	122.39	115.47
1	W	87	CYS	N-CA-C	-5.23	105.50	111.14
2	D	12	ASN	N-CA-C	5.22	116.77	108.79
1	I	203	ARG	CG-CD-NE	-5.21	100.54	112.00
1	K	219	GLN	N-CA-C	5.19	117.77	110.14
1	M	156	GLN	N-CA-C	-5.18	102.23	109.96
2	P	4	GLY	N-CA-C	5.18	122.26	115.47
1	K	87	CYS	N-CA-C	-5.18	105.55	111.14
1	O	219	GLN	CB-CA-C	5.18	119.57	110.36
2	V	4	GLY	N-CA-C	5.17	122.25	115.47
1	E	87	CYS	N-CA-C	-5.15	105.58	111.14
1	Q	151	GLY	N-CA-C	-5.14	101.00	113.18
1	S	151	GLY	N-CA-C	-5.08	101.13	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ALA	N-CA-C	5.06	117.24	110.35
1	O	87	CYS	N-CA-C	-5.06	105.67	111.14
1	M	203	ARG	CG-CD-NE	-5.06	100.87	112.00
1	G	83	ALA	N-CA-C	5.04	117.61	110.50
1	K	203	ARG	CG-CD-NE	-5.04	100.91	112.00
1	C	83	ALA	N-CA-C	5.02	117.58	110.50
1	O	151	GLY	N-CA-C	-5.01	101.31	113.18
1	C	87	CYS	N-CA-C	-5.01	105.73	111.14
1	G	151	GLY	N-CA-C	-5.01	101.31	113.18
1	K	156	GLN	N-CA-C	-5.01	102.50	109.96

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	48	0
1	C	2441	0	2392	49	0
1	E	2441	0	2392	44	0
1	G	2441	0	2392	45	0
1	I	2441	0	2392	44	0
1	K	2441	0	2392	43	0
1	M	2441	0	2392	41	0
1	O	2441	0	2392	48	0
1	Q	2441	0	2392	49	0
1	S	2441	0	2392	51	0
1	U	2441	0	2392	47	0
1	W	2441	0	2392	41	0
2	B	1386	0	1284	36	0
2	D	1386	0	1284	36	0
2	F	1386	0	1284	38	0
2	H	1386	0	1284	39	0
2	J	1386	0	1284	42	0
2	L	1386	0	1284	43	0
2	N	1386	0	1284	40	1
2	P	1386	0	1284	35	0
2	R	1386	0	1284	35	0
2	T	1386	0	1284	35	0
2	V	1386	0	1284	35	0
2	X	1386	0	1284	39	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	2	0
3	M	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	14	0	13	2	0
3	O	14	0	13	0	0
3	P	14	0	13	0	0
3	Q	14	0	13	0	0
3	R	14	0	13	0	0
3	S	14	0	13	0	0
3	T	14	0	13	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	825	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 (825) 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
1:E:6:GLY:C	2:F:115:MET:HE1	2.09	0.77
1:G:6:GLY:C	2:H:115:MET:HE1	2.10	0.77
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:F:132:GLU:CD	2:L:124:LYS:HE2	2.11	0.76
2:L:170:ARG:NH2	2:L:171:LEU:HD22	2.01	0.75
2:D:132:GLU:CD	2:N:124:LYS:HE2	2.12	0.75
1:C:6:GLY:C	2:D:115:MET:HE1	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:C	2:B:115:MET:HE1	2.12	0.74
2:B:132:GLU:CD	2:X:124:LYS:HE2	2.12	0.74
2:T:47:GLN:NE2	2:T:110:MET:HE3	2.02	0.74
2:J:170:ARG:NH2	2:J:171:LEU:HD22	2.01	0.74
2:X:47:GLN:NE2	2:X:110:MET:HE3	2.02	0.74
2:H:132:GLU:CD	2:J:124:LYS:HE2	2.12	0.74
2:P:47:GLN:NE2	2:P:110:MET:HE3	2.03	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
2:N:47:GLN:NE2	2:N:110:MET:HE3	2.04	0.73
1:A:74:TRP:CD1	1:A:106:GLY:HA2	2.23	0.72
2:L:47:GLN:NE2	2:L:110:MET:HE3	2.04	0.72
1:C:74:TRP:CD1	1:C:106:GLY:HA2	2.23	0.72
2:R:47:GLN:NE2	2:R:110:MET:HE3	2.04	0.72
2:J:47:GLN:NE2	2:J:110:MET:HE3	2.05	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
2:V:47:GLN:NE2	2:V:110:MET:HE3	2.03	0.72
1:E:74:TRP:CD1	1:E:106:GLY:HA2	2.25	0.71
2:J:131:GLU:HG3	2:R:127:ARG:HH21	1.55	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
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
1:U:74:TRP:CD1	1:U:106:GLY:HA2	2.27	0.69
1:S:6:GLY:C	2:T:115:MET:HE1	2.18	0.69
1:O:74:TRP:CD1	1:O:106:GLY:HA2	2.27	0.69
1:U:6:GLY:C	2:V:115:MET:HE1	2.18	0.69
1:U:108:ILE:HG22	1:U:253:LEU:HD23	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:GLY:C	2:P:115:MET:HE1	2.19	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:Q:6:GLY:C	2:R:115:MET:HE1	2.19	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:H:47:GLN:NE2	2:H:110:MET:HE3	2.10	0.66
2:F:47:GLN:NE2	2:F:110:MET:HE3	2.11	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
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
2:D:47:GLN:NE2	2:D:110:MET:HE3	2.10	0.65
1:K:6:GLY:C	2:L:115:MET:HE1	2.22	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
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:W:6:GLY:C	2:X:115:MET:HE1	2.23	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
2:B:47:GLN:NE2	2:B:110:MET:HE3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:GLY:C	2:N:115:MET:HE1	2.24	0.62
1:I:6:GLY:C	2:J:115:MET:HE1	2.23	0.62
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: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
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
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
1:I:46:ARG:HE	1:I:76:THR:CG2	2.14	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
2:X:47:GLN:CD	2:X:110:MET:HE3	2.26	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
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:57:GLU:OE1	2:H:57:GLU:O	2.20	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:6:GLY:CA	2:F:115:MET:HE1	2.32	0.59
1:E:240:HIS:CD2	1:E:244:LEU:HD23	2.37	0.59
2:B:57:GLU:OE1	2:B:57:GLU:O	2.20	0.59
2:F:11:GLU:OE2	2:F:135:LYS:HE3	2.02	0.59
1:G:6:GLY:CA	2:H:115:MET:HE1	2.33	0.59
2:V:57:GLU:OE1	2:V:57:GLU:O	2.21	0.59
2:F:57:GLU:O	2:F:57:GLU:OE1	2.20	0.59
1:G:240:HIS:CD2	1:G:244:LEU:HD23	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:47:GLN:CD	2:L:110:MET:HE3	2.28	0.59
2:N:47:GLN:CD	2:N:110:MET:HE3	2.28	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:OE1	2:T:57:GLU:O	2.21	0.59
2:P:47:GLN:CD	2:P:110:MET:HE3	2.27	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:6:GLY:CA	2:D:115:MET:HE1	2.33	0.58
2:T:47:GLN:CD	2:T:110:MET:HE3	2.27	0.58
1:C:46:ARG:HE	1:C:76:THR:CG2	2.16	0.58
2:V:47:GLN:CD	2:V:110:MET:HE3	2.28	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
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:J:47:GLN:CD	2:J:110:MET:HE3	2.29	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:R:47:GLN:CD	2:R:110:MET:HE3	2.28	0.58
1:A:6:GLY:CA	2:B:115:MET:HE1	2.34	0.57
1:A:46:ARG:HE	1:A:76:THR:CG2	2.16	0.57
2:L:57:GLU:OE1	2:L:57:GLU:O	2.21	0.57
1:S:46:ARG:NE	1:S:76:THR:HG21	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:GLU:OE1	2:J:57:GLU:O	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:L:124:LYS:HE3	2:L:124:LYS:HA	1.87	0.57
1:C:297:GLN:HG3	2:D:62:GLU:HG2	1.87	0.57
1:Q:6:GLY:CA	2:R:115:MET:HE1	2.35	0.57
1:S:240:HIS:CD2	1:S:244:LEU:HD23	2.38	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
1:U:6:GLY:CA	2:V:115:MET:HE1	2.35	0.56
2:X:124:LYS:HE3	2:X:124:LYS:HA	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: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
1:E:5:LEU:HD22	2:F:119:TYR:HA	1.88	0.56
1:A:297:GLN:HG3	2:B:62:GLU:HG2	1.87	0.56
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
1:I:12:ASN:N	1:I:12:ASN:OD1	2.39	0.56
1:O:12:ASN:OD1	1:O:12:ASN:N	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:88:ILE:HD13	2:V:87:SER:HB3	1.89	0.55
2:D:168:LEU:HG	2:D:169:ASN:N	2.21	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:HE3	2:B:124:LYS:HA	1.89	0.55
2:F:124:LYS:HE3	2:F:124:LYS:HA	1.89	0.55
1:S:6:GLY:CA	2:T:115:MET:HE1	2.35	0.55
1:S:12:ASN:N	1:S:12:ASN:OD1	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:OD1	1:A:12:ASN:N	2.40	0.55
1:G:133:ASN:N	1:G:134:GLY:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:U:12:ASN:OD1	2.39	0.55
1:W:12:ASN:OD1	1:W:12:ASN:N	2.39	0.55
2:D:47:GLN:CD	2:D:110:MET:HE3	2.32	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:O:6:GLY:CA	2:P:115:MET:HE1	2.36	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:N:132:GLU:CD	2:V:124:LYS:HE2	2.31	0.55
2:P:124:LYS:HE2	2:X:132:GLU:CD	2.32	0.55
2:R:124:LYS:HE3	2:R:124:LYS:HA	1.89	0.55
2:B:168:LEU:HG	2:B:169:ASN:N	2.21	0.54
1:G:46:ARG:NE	1:G:76:THR:HG21	2.22	0.54
1:G:202:TYR:CD1	1:G:228:THR:HG21	2.41	0.54
2:H:47:GLN:CD	2:H:110:MET:HE3	2.32	0.54
1:M:133:ASN:N	1:M:134:GLY:O	2.40	0.54
1:C:12:ASN:OD1	1:C:12:ASN:N	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:HE3	2:H:124:LYS:HA	1.89	0.54
1:I:217:ASN:N	1:I:218:GLY:HA3	2.22	0.54
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:HE3	2:P:124:LYS:HA	1.90	0.54
1:W:133:ASN:N	1:W:134:GLY:O	2.40	0.54
1:G:12:ASN:OD1	1:G:12:ASN:N	2.40	0.54
1:I:6:GLY:CA	2:J:115:MET:HE1	2.38	0.54
2:J:79:ASN:OD1	3:J:301:NAG:H81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:297:GLN:HG3	2:F:62:GLU:HG2	1.89	0.54
1:K:317:PRO:O	1:K:318:GLU:HB2	2.08	0.54
2:L:79:ASN:OD1	3:L:301:NAG:H81	2.08	0.54
2:T:124:LYS:HE3	2:T:124:LYS:HA	1.90	0.54
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
1:O:305:ARG:NH1	1:S:45:GLY:O	2.41	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
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
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: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:92:THR:HB	1:M:95:VAL:HG13	1.90	0.53
1:M:217:ASN:N	1:M:218:GLY:HA3	2.23	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:6:GLY:CA	2:N:115:MET:HE1	2.38	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:K:6:GLY:CA	2:L:115:MET:HE1	2.38	0.53
1:O:185:ASN:O	1:O:188:TYR:O	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:L:132:GLU:CD	2:T:124:LYS:HE2	2.34	0.53
1:G:185:ASN:O	1:G:188:TYR:O	2.27	0.53
2:J:132:GLU:CD	2:R:124:LYS:HE2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:46:ARG:NE	1:E:76:THR:HG21	2.24	0.52
2:V:170:ARG:CZ	2:V:171:LEU:HB3	2.39	0.52
1:W:6:GLY:CA	2:X:115:MET:HE1	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
1:S:317:PRO:O	1:S:318:GLU:HB2	2.08	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
2:F:47:GLN:CD	2:F:110:MET:HE3	2.34	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
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
1:G:303:ASN:HB2	2:H:93:THR:HG21	1.92	0.51
2:B:47:GLN:CD	2:B:110:MET:HE3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:92:THR:HB	1:C:95:VAL:HG13	1.93	0.51
1:C:240:HIS:HD2	1:C:244:LEU:HB3	1.75	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
1:A:240:HIS:HD2	1:A:244:LEU:HB3	1.75	0.51
1:E:20:THR:O	2:L:50:GLY:HA3	2.11	0.51
1:K:303:ASN:HB2	2:L:93:THR:HG21	1.93	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: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:O:92:THR:HB	1:O:95:VAL:HG13	1.93	0.51
1:O:240:HIS:HD2	1:O:244:LEU:HB3	1.75	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
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: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
1:I:119:SER:O	1:I:120:SER:OG	2.27	0.50
1:C:284:ARG:HB3	2:D:56:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:T:168:LEU:HG	2:T:169:ASN:N	2.26	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
1:S:240:HIS:HD2	1:S:244:LEU:HB3	1.77	0.50
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
1:S:132:ARG:O	1:S:134:GLY:HA2	2.12	0.50
1:A:119:SER:O	1:A:120:SER:OG	2.26	0.50
1:C:262:SER:OG	1:C:277:ARG:O	2.29	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
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
1:E:59:MET:HE2	1:E:108:ILE:HD11	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:H:127:ARG:HD3	2:H:159:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:59:MET:HE2	1:G:108:ILE:HD11	1.93	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
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:M:119:SER:O	1:M:120:SER:OG	2.27	0.48
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
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:59:MET:HE2	1:M:108:ILE:HD11	1.95	0.48
1:M:132:ARG:O	1:M:134:GLY:HA2	2.12	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:C:59:MET:HE2	1:C:108:ILE:HD11	1.94	0.48
1:G:302:VAL:HA	2:H:93:THR:HG22	1.96	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
1:I:59:MET:HE2	1:I:108:ILE:HD11	1.95	0.48
1:M:5:LEU:HD22	2:N:119:TYR:HA	1.96	0.48
1:O:59:MET:HE2	1:O:108:ILE:HD11	1.95	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
1:G:20:THR:O	2:J:50:GLY:HA3	2.13	0.48
1:K:59:MET:HE2	1:K:108:ILE:HD11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:88:ILE:HD13	2:X:87:SER:HB3	1.96	0.48
1:Q:302:VAL:HA	2:R:93:THR:HG22	1.95	0.48
1:W:59:MET:HE2	1:W:108:ILE:HD11	1.95	0.48
1:E:302:VAL:HA	2:F:93:THR:HG22	1.96	0.48
1:S:59:MET:HE2	1:S:108:ILE:HD11	1.96	0.48
1:W:160:THR:HG22	1:W:237:THR:HG23	1.96	0.48
1:A:262:SER:OG	1:A:277:ARG:O	2.29	0.48
1:O:217:ASN:N	1:O:218:GLY:HA3	2.29	0.48
1:O:262:SER:OG	1:O:277:ARG:O	2.29	0.48
1:S:262:SER:OG	1:S:277:ARG:O	2.29	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
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:49:LYS:HE2	1:U:69:HIS:ND1	2.29	0.47
1:U:160:THR:HG22	1:U:237:THR:HG23	1.96	0.47
1:W:5:LEU:HD22	2:X:119:TYR:HA	1.96	0.47
1:A:59:MET:HE2	1:A:108:ILE:HD11	1.94	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
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
1:O:302:VAL:HA	2:P:93:THR:HG22	1.95	0.47
1:S:160:THR:HG22	1:S:237:THR:HG23	1.96	0.47
1:S:217:ASN:N	1:S:218:GLY:HA3	2.29	0.47
2:B:170:ARG:NH2	2:B:171:LEU:HB3	2.29	0.47
2:D:127:ARG:HH21	2:V:131:GLU:HG3	1.80	0.47
1:M:153:ASN:HA	1:M:189:GLY:CA	2.44	0.47
1:O:5:LEU:HD22	2:P:119:TYR:HA	1.97	0.47
1:O:153:ASN:HA	1:O:189:GLY:CA	2.44	0.47
1:A:302:VAL:HA	2:B:93:THR:HG22	1.95	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:U:59:MET:HE2	1:U:108:ILE:HD11	1.96	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
1:Q:59:MET:HE2	1:Q:108:ILE:HD11	1.96	0.47
2:L:87:SER:HB3	2:T:88:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:153:ASN:HA	1:U:189:GLY:CA	2.45	0.47
1:U:262:SER:OG	1:U:277:ARG:O	2.29	0.47
1:U:302:VAL:HA	2:V:93:THR:HG22	1.97	0.47
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
1:Q:262:SER:OG	1:Q:277:ARG:O	2.29	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:4:CYS:HA	2:L:137:CYS:HA	1.96	0.46
1:K:119:SER:HA	1:K:148:LYS:NZ	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:SER:OG	1:I:277:ARG:O	2.29	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:M:4:CYS:HA	2:N:137:CYS:HA	1.98	0.45
1:G:51:LEU:O	1:G:52:GLY:C	2.57	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
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
2:T:14:TRP:CD1	2:T:25:ARG:HH21	2.35	0.45
1:W:119:SER:O	1:W:120:SER:OG	2.27	0.45
1:E:51:LEU:O	1:E:52:GLY:C	2.59	0.45
2:P:11:GLU:OE2	1:Q:133:ASN:O	2.34	0.45
1:W:262:SER:OG	1:W:277:ARG:O	2.29	0.45
2:X:170:ARG:NH2	2:X:171:LEU:HB3	2.31	0.45
1:I:297:GLN:HG3	2:J:62:GLU:HG2	1.99	0.45
1:A:51:LEU:O	1:A:52:GLY:C	2.57	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:A:205:ASN:ND2	1:O:209:VAL:HG21	2.31	0.44
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
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:D:14:TRP:CD1	2:D:25:ARG:HH21	2.35	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
2:L:79:ASN:CG	3:L:301:NAG:H81	2.43	0.44
1:M:110:LYS:HE2	1:M:141:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:162:ARG:HG3	1:M:235:ASN:OD1	2.18	0.44
1:C:203:ARG:O	1:C:203:ARG:HG3	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
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
2:F:87:SER:HB3	2:L:88:ILE:HD13	1.99	0.44
2:J:14:TRP:CD1	2:J:25:ARG:HH21	2.36	0.44
1:K:1:ASP:OD1	2:L:28:ASN:HA	2.17	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:57:ILE:CD1	1:G:95:VAL:HG12	2.48	0.44
1:G:203:ARG:O	1:G:203:ARG:HG3	2.15	0.44
1:S:57:ILE:CD1	1:S:95:VAL:HG12	2.48	0.44
2:D:50:GLY:HA3	1:U:20:THR:O	2.17	0.43
1:I:162:ARG:HG3	1:I:235:ASN:OD1	2.18	0.43
2:J:129:ASN:N	2:J:129:ASN:OD1	2.51	0.43
1:K:262:SER:OG	1:K:277:ARG:O	2.29	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
1:G:205:ASN:ND2	1:Q:209:VAL:HG21	2.32	0.43
2:J:102:MET:HG3	2:J:103:GLU:N	2.32	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: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
1:E:205:ASN:ND2	1:S:209:VAL:HG21	2.33	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:14:TRP:CD1	2:H:25:ARG:HH21	2.36	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
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:14:TRP:CD1	2:N:25:ARG:HH21	2.36	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:A:203:ARG:HD3	1:O:222:ARG:HG3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:57:ILE:CD1	1:O:95:VAL:HG12	2.48	0.43
1:O:153:ASN:HA	1:O:189:GLY:HA3	2.01	0.43
1:O:305:ARG:HH12	1:S:46:ARG:HA	1.83	0.43
1:Q:57:ILE:CD1	1:Q:95:VAL:HG12	2.48	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
1:S:162:ARG:HG3	1:S:235:ASN:OD1	2.19	0.43
1:U:119:SER:O	1:U:120:SER:OG	2.27	0.43
2:X:14:TRP:CD1	2:X:25:ARG:HH21	2.36	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: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
2:L:14:TRP:CD1	2:L:25:ARG:HH21	2.36	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:OD1	2:N:129:ASN:N	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:51:LEU:O	1:C:52:GLY:C	2.59	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:14:TRP:CD1	2:B:25:ARG:HH21	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:W:57:ILE:CD1	1:W:95:VAL:HG12	2.50	0.42
1:W:297:GLN:HG3	2:X:62:GLU:HG2	2.00	0.42
2:X:129:ASN:OD1	2:X:129:ASN:N	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
1:O:4:CYS:HA	2:P:137:CYS:HA	2.01	0.42
1:Q:46:ARG:HA	1:S:305:ARG:HH12	1.84	0.42
1:Q:162:ARG:HG3	1:Q:235:ASN:OD1	2.19	0.42
2:R:14:TRP:CD1	2:R:25:ARG:HH21	2.37	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:F:14:TRP:CD1	2:F:25:ARG:HH21	2.37	0.42
2:H:56:VAL:HG12	2:H:57:GLU:N	2.34	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:K:153:ASN:HA	1:K:189:GLY:HA3	2.01	0.42
2:P:14:TRP:CD1	2:P:25:ARG:HH21	2.37	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
2:V:14:TRP:CD1	2:V:25:ARG:HH21	2.37	0.42
1:A:203:ARG:O	1:A:203:ARG:HG3	2.16	0.42
1:C:119:SER:O	1:C:120:SER:OG	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASP:OD1	1:C:75:ASP:C	2.63	0.41
1:C:100:GLN:O	1:C:104:GLU:HG2	2.20	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
1:E:262:SER:OG	1:E:277:ARG:O	2.29	0.41
1:I:100:GLN:O	1:I:104:GLU:HG2	2.20	0.41
1:K:203:ARG:O	1:K:203:ARG:HG3	2.13	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:75:ASP:OD1	1:E:75:ASP:C	2.63	0.41
1:E:100:GLN:O	1:E:104:GLU:HG2	2.20	0.41
2:F:127:ARG:HH21	2:T:131:GLU:HG3	1.85	0.41
1:G:8:HIS:CD2	2:H:21:TRP:HA	2.56	0.41
2:L:170:ARG:CZ	2:L:171:LEU:HB2	2.51	0.41
2:P:129:ASN:OD1	2:P:129:ASN:N	2.53	0.41
1:Q:291:SER:HA	1:Q:292:PRO:HD3	1.90	0.41
2:F:165:GLU:O	2:F:168:LEU:HB3	2.19	0.41
1:G:43:MET:HE1	1:G:76:THR:OG1	2.21	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
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: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
1:S:303:ASN:H	2:T:93:THR:CG2	2.34	0.41
2:T:56:VAL:HG12	2:T:57:GLU:N	2.36	0.41
1:U:203:ARG:O	1:U:203:ARG:HG3	2.16	0.41
1:W:118:GLY:O	1:W:121:ILE:HG23	2.21	0.41
2:B:56:VAL:CG1	2:B:57:GLU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:79:ASN:CG	3:N:301:NAG:H81	2.45	0.41
1:O:100:GLN:O	1:O:104:GLU:HG2	2.21	0.41
2:P:127:ARG:NH2	2:X:131:GLU:HG3	2.32	0.41
2:P:165:GLU:O	2:P:168:LEU:HB3	2.20	0.41
1:Q:43:MET:HE1	1:Q:76:THR:OG1	2.21	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
1:A:75:ASP:OD1	1:A:75:ASP:C	2.63	0.41
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:8:HIS:CD2	2:D:21:TRP:HA	2.56	0.41
1:C:165:ASP:OD1	1:C:166:THR:N	2.49	0.41
2:F:124:LYS:HE2	2:T:132:GLU:CD	2.46	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:B:102:MET:HG3	2:B:103:GLU:N	2.36	0.41
1:C:73:MET:SD	1:C:254:ILE:HD13	2.61	0.41
1:C:203:ARG:HD3	1:U:222:ARG:HG3	2.03	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
2:R:56:VAL:HG12	2:R:57:GLU:N	2.34	0.41
1:S:153:ASN:HA	1:S:189:GLY:HA3	2.02	0.41
2:L:102:MET:HG3	2:L:103:GLU:N	2.34	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:U:43:MET:HE1	1:U:76:THR:OG1	2.21	0.40
1:E:43:MET:HE1	1:E:76:THR:OG1	2.22	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
1:K:118:GLY:O	1:K:121:ILE:HG23	2.21	0.40
1:K:119:SER:O	1:K:120:SER:OG	2.27	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
2:H:127:ARG:HH21	2:R:131:GLU:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:170:ARG:NH2	2:J:171:LEU:HB2	2.36	0.40
1:K:75:ASP:OD1	1:K:75:ASP:C	2.64	0.40
2:V:94:TYR:CD2	2:V:94:TYR:C	3.00	0.40
1:W:75:ASP:OD1	1:W:75:ASP:C	2.64	0.40
1:A:43:MET:HE1	1:A:76:THR:OG1	2.21	0.40
1:A:100:GLN:O	1:A:101:LYS:C	2.65	0.40
1:C:43:MET:HE1	1:C:76:THR:OG1	2.21	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:K:51:LEU:O	1:K:52:GLY:C	2.64	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:119:SER:HA	1:G:148:LYS:HZ1	1.86	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
2:J:131:GLU:OE2	2:R:128:GLN:CG	2.70	0.40
1:O:305:ARG:NH1	1:S:46:ARG:HA	2.36	0.40
1:Q:119:SER:HA	1:Q:148:LYS:HZ1	1.85	0.40
1:S:43:MET:HE1	1:S:76:THR:OG1	2.21	0.40
2:T:94:TYR:CD2	2:T:94:TYR:C	3.00	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%)	36	60
1	C	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	E	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	G	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	I	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	36	60
1	K	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	M	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	36	60
1	O	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	Q	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
1	S	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	36	60
1	U	317/327 (97%)	299 (94%)	17 (5%)	1 (0%)	36	60
1	W	317/327 (97%)	300 (95%)	16 (5%)	1 (0%)	36	60
2	B	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	D	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	F	170/174 (98%)	157 (92%)	12 (7%)	1 (1%)	21	44
2	H	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	J	170/174 (98%)	157 (92%)	12 (7%)	1 (1%)	21	44
2	L	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	N	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	P	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	R	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	T	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	V	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
2	X	170/174 (98%)	158 (93%)	11 (6%)	1 (1%)	21	44
All	All	5844/6012 (97%)	5490 (94%)	330 (6%)	24 (0%)	30	54

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

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Mol	Chain	Res	Type
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%)	253 (94%)	16 (6%)	18	42
1	C	269/275 (98%)	254 (94%)	15 (6%)	19	44
1	E	269/275 (98%)	253 (94%)	16 (6%)	18	42
1	G	269/275 (98%)	253 (94%)	16 (6%)	18	42
1	I	269/275 (98%)	255 (95%)	14 (5%)	21	47
1	K	269/275 (98%)	255 (95%)	14 (5%)	21	47
1	M	269/275 (98%)	255 (95%)	14 (5%)	21	47
1	O	269/275 (98%)	254 (94%)	15 (6%)	19	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	269/275 (98%)	255 (95%)	14 (5%)	21	47
1	S	269/275 (98%)	256 (95%)	13 (5%)	23	50
1	U	269/275 (98%)	256 (95%)	13 (5%)	23	50
1	W	269/275 (98%)	255 (95%)	14 (5%)	21	47
2	B	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	D	146/148 (99%)	135 (92%)	11 (8%)	12	31
2	F	146/148 (99%)	135 (92%)	11 (8%)	12	31
2	H	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	J	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	L	146/148 (99%)	137 (94%)	9 (6%)	16	39
2	N	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	P	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	R	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	T	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	V	146/148 (99%)	136 (93%)	10 (7%)	14	35
2	X	146/148 (99%)	136 (93%)	10 (7%)	14	35
All	All	4980/5076 (98%)	4685 (94%)	295 (6%)	18	42

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	108	ILE
1	A	128	ARG
1	A	171	ILE
1	A	184	LYS
1	A	203	ARG
1	A	228	THR
1	A	240	HIS
1	A	314	ARG

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Mol	Chain	Res	Type
1	A	316	VAL
2	B	11	GLU
2	B	57	GLU
2	B	100	VAL
2	B	108	ILE
2	B	110	MET
2	B	124	LYS
2	B	129	ASN
2	B	132	GLU
2	B	168	LEU
2	B	171	LEU
1	C	15	ILE
1	C	71	THR
1	C	73	MET
1	C	76	THR
1	C	95	VAL
1	C	101	LYS
1	C	108	ILE
1	C	128	ARG
1	C	171	ILE
1	C	184	LYS
1	C	203	ARG
1	C	228	THR
1	C	240	HIS
1	C	314	ARG
1	C	316	VAL
2	D	11	GLU
2	D	57	GLU
2	D	73	ILE
2	D	100	VAL
2	D	108	ILE
2	D	110	MET
2	D	124	LYS
2	D	129	ASN
2	D	132	GLU
2	D	168	LEU
2	D	171	LEU
1	E	15	ILE
1	E	71	THR
1	E	73	MET
1	E	76	THR
1	E	77	LEU

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Mol	Chain	Res	Type
1	E	95	VAL
1	E	101	LYS
1	E	108	ILE
1	E	128	ARG
1	E	171	ILE
1	E	184	LYS
1	E	203	ARG
1	E	228	THR
1	E	240	HIS
1	E	314	ARG
1	E	316	VAL
2	F	11	GLU
2	F	57	GLU
2	F	73	ILE
2	F	100	VAL
2	F	108	ILE
2	F	110	MET
2	F	124	LYS
2	F	129	ASN
2	F	132	GLU
2	F	168	LEU
2	F	171	LEU
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	108	ILE
1	G	128	ARG
1	G	171	ILE
1	G	184	LYS
1	G	203	ARG
1	G	228	THR
1	G	240	HIS
1	G	314	ARG
1	G	316	VAL
2	H	11	GLU
2	H	57	GLU
2	H	100	VAL
2	H	108	ILE

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Mol	Chain	Res	Type
2	H	110	MET
2	H	124	LYS
2	H	129	ASN
2	H	132	GLU
2	H	168	LEU
2	H	171	LEU
1	I	15	ILE
1	I	71	THR
1	I	73	MET
1	I	76	THR
1	I	95	VAL
1	I	101	LYS
1	I	108	ILE
1	I	171	ILE
1	I	184	LYS
1	I	203	ARG
1	I	228	THR
1	I	240	HIS
1	I	314	ARG
1	I	316	VAL
2	J	11	GLU
2	J	57	GLU
2	J	73	ILE
2	J	100	VAL
2	J	108	ILE
2	J	110	MET
2	J	124	LYS
2	J	129	ASN
2	J	132	GLU
2	J	168	LEU
1	K	15	ILE
1	K	71	THR
1	K	73	MET
1	K	76	THR
1	K	95	VAL
1	K	101	LYS
1	K	108	ILE
1	K	171	ILE
1	K	184	LYS
1	K	203	ARG
1	K	228	THR
1	K	240	HIS

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Mol	Chain	Res	Type
1	K	314	ARG
1	K	316	VAL
2	L	11	GLU
2	L	57	GLU
2	L	73	ILE
2	L	100	VAL
2	L	108	ILE
2	L	110	MET
2	L	129	ASN
2	L	132	GLU
2	L	168	LEU
1	M	15	ILE
1	M	71	THR
1	M	73	MET
1	M	76	THR
1	M	95	VAL
1	M	101	LYS
1	M	108	ILE
1	M	171	ILE
1	M	184	LYS
1	M	203	ARG
1	M	228	THR
1	M	240	HIS
1	M	314	ARG
1	M	316	VAL
2	N	11	GLU
2	N	57	GLU
2	N	73	ILE
2	N	100	VAL
2	N	108	ILE
2	N	110	MET
2	N	129	ASN
2	N	132	GLU
2	N	168	LEU
2	N	171	LEU
1	O	15	ILE
1	O	71	THR
1	O	73	MET
1	O	76	THR
1	O	95	VAL
1	O	101	LYS
1	O	108	ILE

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Mol	Chain	Res	Type
1	O	171	ILE
1	O	184	LYS
1	O	203	ARG
1	O	219	GLN
1	O	228	THR
1	O	240	HIS
1	O	314	ARG
1	O	316	VAL
2	P	11	GLU
2	P	57	GLU
2	P	100	VAL
2	P	108	ILE
2	P	110	MET
2	P	124	LYS
2	P	129	ASN
2	P	132	GLU
2	P	168	LEU
2	P	171	LEU
1	Q	15	ILE
1	Q	71	THR
1	Q	73	MET
1	Q	76	THR
1	Q	95	VAL
1	Q	101	LYS
1	Q	108	ILE
1	Q	171	ILE
1	Q	184	LYS
1	Q	203	ARG
1	Q	228	THR
1	Q	240	HIS
1	Q	314	ARG
1	Q	316	VAL
2	R	11	GLU
2	R	57	GLU
2	R	100	VAL
2	R	108	ILE
2	R	110	MET
2	R	124	LYS
2	R	129	ASN
2	R	132	GLU
2	R	168	LEU
2	R	171	LEU

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Mol	Chain	Res	Type
1	S	15	ILE
1	S	71	THR
1	S	73	MET
1	S	76	THR
1	S	95	VAL
1	S	101	LYS
1	S	108	ILE
1	S	171	ILE
1	S	184	LYS
1	S	203	ARG
1	S	228	THR
1	S	240	HIS
1	S	314	ARG
2	T	11	GLU
2	T	57	GLU
2	T	100	VAL
2	T	108	ILE
2	T	110	MET
2	T	124	LYS
2	T	129	ASN
2	T	132	GLU
2	T	168	LEU
2	T	171	LEU
1	U	15	ILE
1	U	71	THR
1	U	73	MET
1	U	76	THR
1	U	95	VAL
1	U	101	LYS
1	U	108	ILE
1	U	171	ILE
1	U	184	LYS
1	U	203	ARG
1	U	228	THR
1	U	240	HIS
1	U	314	ARG
2	V	11	GLU
2	V	57	GLU
2	V	100	VAL
2	V	108	ILE
2	V	110	MET
2	V	124	LYS

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Mol	Chain	Res	Type
2	V	129	ASN
2	V	132	GLU
2	V	168	LEU
2	V	171	LEU
1	W	15	ILE
1	W	71	THR
1	W	73	MET
1	W	76	THR
1	W	95	VAL
1	W	101	LYS
1	W	108	ILE
1	W	171	ILE
1	W	184	LYS
1	W	203	ARG
1	W	228	THR
1	W	240	HIS
1	W	314	ARG
1	W	316	VAL
2	X	11	GLU
2	X	57	GLU
2	X	73	ILE
2	X	100	VAL
2	X	108	ILE
2	X	110	MET
2	X	129	ASN
2	X	132	GLU
2	X	168	LEU
2	X	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	159	ASN
1	A	169	HIS
1	A	217	ASN
1	A	240	HIS
2	B	47	GLN
1	C	8	HIS
1	C	159	ASN
1	C	169	HIS
1	C	217	ASN

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Mol	Chain	Res	Type
1	C	240	HIS
2	D	47	GLN
1	E	8	HIS
1	E	159	ASN
1	E	169	HIS
1	E	217	ASN
1	E	240	HIS
2	F	47	GLN
1	G	8	HIS
1	G	159	ASN
1	G	169	HIS
1	G	217	ASN
1	G	231	GLN
1	G	240	HIS
2	H	47	GLN
1	I	159	ASN
1	I	169	HIS
1	I	217	ASN
1	I	219	GLN
1	I	240	HIS
2	J	47	GLN
2	J	105	GLN
2	J	172	ASN
1	K	8	HIS
1	K	159	ASN
1	K	169	HIS
1	K	217	ASN
1	K	240	HIS
2	L	47	GLN
2	L	105	GLN
2	L	172	ASN
1	M	8	HIS
1	M	159	ASN
1	M	169	HIS
1	M	217	ASN
1	M	240	HIS
2	N	47	GLN
2	N	105	GLN
1	O	8	HIS
1	O	39	ASN
1	O	159	ASN
1	O	169	HIS

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Mol	Chain	Res	Type
1	O	217	ASN
1	O	240	HIS
2	P	47	GLN
2	P	95	GLN
1	Q	8	HIS
1	Q	159	ASN
1	Q	169	HIS
1	Q	217	ASN
1	Q	240	HIS
2	R	47	GLN
1	S	8	HIS
1	S	39	ASN
1	S	159	ASN
1	S	169	HIS
1	S	217	ASN
1	S	240	HIS
2	T	47	GLN
1	U	8	HIS
1	U	39	ASN
1	U	159	ASN
1	U	169	HIS
1	U	217	ASN
1	U	240	HIS
2	V	47	GLN
1	W	159	ASN
1	W	169	HIS
1	W	217	ASN
1	W	240	HIS
2	X	47	GLN
2	X	105	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	H	301	2	14,14,15	1.20	1 (7%)	17,19,21	2.67	7 (41%)
3	NAG	I	401	1	14,14,15	0.56	0	17,19,21	2.73	5 (29%)
3	NAG	Q	401	1	14,14,15	0.52	0	17,19,21	1.63	3 (17%)
3	NAG	X	301	2	14,14,15	0.79	0	17,19,21	2.57	5 (29%)
3	NAG	M	401	1	14,14,15	0.48	0	17,19,21	3.03	8 (47%)
3	NAG	J	301	2	14,14,15	0.72	0	17,19,21	2.06	3 (17%)
3	NAG	K	401	1	14,14,15	0.47	0	17,19,21	2.81	3 (17%)
3	NAG	L	301	2	14,14,15	0.83	0	17,19,21	2.55	5 (29%)
3	NAG	B	301	2	14,14,15	1.28	1 (7%)	17,19,21	3.10	9 (52%)
3	NAG	D	301	2	14,14,15	1.26	2 (14%)	17,19,21	3.16	9 (52%)
3	NAG	R	301	2	14,14,15	0.97	1 (7%)	17,19,21	1.88	3 (17%)
3	NAG	V	301	2	14,14,15	0.85	0	17,19,21	2.03	3 (17%)
3	NAG	S	401	1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
3	NAG	E	401	1	14,14,15	0.57	0	17,19,21	1.87	2 (11%)
3	NAG	N	301	2	14,14,15	0.76	0	17,19,21	2.43	4 (23%)
3	NAG	C	401	1	14,14,15	0.46	0	17,19,21	1.80	3 (17%)
3	NAG	F	301	2	14,14,15	1.19	1 (7%)	17,19,21	3.06	9 (52%)
3	NAG	P	301	2	14,14,15	0.79	0	17,19,21	1.45	3 (17%)
3	NAG	U	401	1	14,14,15	0.48	0	17,19,21	1.52	1 (5%)
3	NAG	T	301	2	14,14,15	0.82	1 (7%)	17,19,21	1.85	4 (23%)
3	NAG	G	401	1	14,14,15	0.66	0	17,19,21	1.98	3 (17%)
3	NAG	A	401	1	14,14,15	0.58	0	17,19,21	2.11	5 (29%)
3	NAG	W	401	1	14,14,15	0.46	0	17,19,21	2.86	6 (35%)
3	NAG	O	401	1	14,14,15	0.49	0	17,19,21	1.61	2 (11%)

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	H	301	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	401	1	-	2/6/23/26	0/1/1/1
3	NAG	Q	401	1	-	1/6/23/26	0/1/1/1
3	NAG	X	301	2	-	2/6/23/26	0/1/1/1
3	NAG	M	401	1	-	2/6/23/26	0/1/1/1
3	NAG	J	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	L	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	1/6/23/26	0/1/1/1
3	NAG	D	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	V	301	2	-	3/6/23/26	0/1/1/1
3	NAG	S	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	N	301	2	-	2/6/23/26	0/1/1/1
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1
3	NAG	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	U	401	1	-	1/6/23/26	0/1/1/1
3	NAG	T	301	2	-	3/6/23/26	0/1/1/1
3	NAG	G	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	W	401	1	-	2/6/23/26	0/1/1/1
3	NAG	O	401	1	-	0/6/23/26	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	3.22	1.30	1.23
3	B	301	NAG	O7-C7	3.09	1.30	1.23
3	F	301	NAG	O7-C7	2.91	1.29	1.23
3	D	301	NAG	O7-C7	2.86	1.29	1.23
3	D	301	NAG	O5-C1	2.18	1.47	1.43
3	R	301	NAG	O7-C7	2.13	1.28	1.23
3	T	301	NAG	O7-C7	2.12	1.28	1.23

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	401	NAG	C1-O5-C5	9.79	125.31	112.19
3	K	401	NAG	C1-O5-C5	9.69	125.17	112.19
3	I	401	NAG	C1-O5-C5	9.68	125.16	112.19
3	W	401	NAG	C1-O5-C5	9.03	124.28	112.19
3	X	301	NAG	C1-O5-C5	8.66	123.80	112.19
3	L	301	NAG	C1-O5-C5	8.06	122.98	112.19
3	N	301	NAG	C1-O5-C5	7.09	121.69	112.19
3	J	301	NAG	C1-O5-C5	6.35	120.70	112.19
3	A	401	NAG	C1-O5-C5	6.33	120.67	112.19
3	B	301	NAG	O7-C7-N2	6.24	133.00	121.98
3	E	401	NAG	C1-O5-C5	6.22	120.53	112.19
3	D	301	NAG	C1-O5-C5	6.13	120.41	112.19
3	B	301	NAG	C2-N2-C7	5.97	130.90	122.90
3	G	401	NAG	C1-O5-C5	5.84	120.02	112.19
3	T	301	NAG	C1-O5-C5	5.75	119.89	112.19
3	V	301	NAG	C1-O5-C5	5.75	119.89	112.19
3	C	401	NAG	C1-O5-C5	5.74	119.88	112.19
3	F	301	NAG	O7-C7-N2	5.72	132.09	121.98
3	D	301	NAG	O7-C7-N2	5.61	131.90	121.98
3	R	301	NAG	C1-O5-C5	5.45	119.49	112.19
3	H	301	NAG	C8-C7-N2	-5.42	107.13	116.12
3	F	301	NAG	C1-O5-C5	5.27	119.25	112.19
3	D	301	NAG	C2-N2-C7	5.07	129.69	122.90
3	F	301	NAG	C8-C7-N2	-4.99	107.84	116.12
3	B	301	NAG	C8-C7-N2	-4.92	107.95	116.12
3	O	401	NAG	C1-O5-C5	4.82	118.65	112.19
3	U	401	NAG	C1-O5-C5	4.66	118.43	112.19
3	H	301	NAG	C1-O5-C5	4.66	118.42	112.19
3	D	301	NAG	C8-C7-N2	-4.63	108.44	116.12
3	B	301	NAG	C1-O5-C5	4.57	118.32	112.19
3	H	301	NAG	O7-C7-N2	4.38	129.73	121.98
3	F	301	NAG	C2-N2-C7	4.17	128.49	122.90
3	Q	401	NAG	C1-O5-C5	4.10	117.68	112.19
3	N	301	NAG	C8-C7-N2	-4.09	109.33	116.12
3	K	401	NAG	O5-C1-C2	4.02	117.52	111.29
3	F	301	NAG	O5-C1-C2	3.87	117.28	111.29
3	M	401	NAG	O5-C1-C2	3.85	117.24	111.29
3	N	301	NAG	O5-C1-C2	-3.70	105.57	111.29
3	W	401	NAG	O5-C1-C2	3.68	116.99	111.29
3	P	301	NAG	C1-O5-C5	3.58	116.99	112.19
3	D	301	NAG	C1-C2-N2	3.54	116.01	110.43
3	L	301	NAG	O5-C1-C2	-3.47	105.93	111.29
3	V	301	NAG	O7-C7-N2	3.44	128.07	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAG	O5-C1-C2	3.38	116.52	111.29
3	R	301	NAG	O7-C7-N2	3.36	127.92	121.98
3	L	301	NAG	C8-C7-N2	-3.29	110.66	116.12
3	H	301	NAG	C1-C2-N2	3.19	115.45	110.43
3	B	301	NAG	O5-C5-C4	3.04	118.23	110.83
3	B	301	NAG	O5-C1-C2	3.04	115.99	111.29
3	S	401	NAG	C1-O5-C5	3.01	116.22	112.19
3	M	401	NAG	C4-C3-C2	-2.98	106.66	111.02
3	Q	401	NAG	C3-C4-C5	-2.97	104.84	110.23
3	F	301	NAG	O5-C5-C4	2.94	117.97	110.83
3	X	301	NAG	C8-C7-N2	-2.93	111.26	116.12
3	O	401	NAG	C3-C4-C5	-2.91	104.96	110.23
3	M	401	NAG	C3-C4-C5	-2.86	105.06	110.23
3	G	401	NAG	O5-C5-C6	2.84	113.18	107.66
3	I	401	NAG	O7-C7-C8	-2.76	117.14	122.05
3	S	401	NAG	C3-C4-C5	-2.76	105.23	110.23
3	J	301	NAG	C8-C7-N2	-2.74	111.57	116.12
3	W	401	NAG	O4-C4-C5	2.74	116.07	109.32
3	W	401	NAG	O7-C7-C8	-2.73	117.20	122.05
3	F	301	NAG	C1-C2-N2	2.71	114.70	110.43
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	F	301	NAG	O3-C3-C2	2.67	114.95	109.40
3	J	301	NAG	O5-C1-C2	-2.67	107.16	111.29
3	H	301	NAG	C2-N2-C7	2.67	126.48	122.90
3	Q	401	NAG	O5-C1-C2	-2.65	107.19	111.29
3	M	401	NAG	O7-C7-C8	-2.64	117.35	122.05
3	K	401	NAG	O7-C7-C8	-2.64	117.35	122.05
3	I	401	NAG	C8-C7-N2	2.61	120.45	116.12
3	M	401	NAG	C8-C7-N2	2.61	120.45	116.12
3	A	401	NAG	O5-C5-C6	2.60	112.73	107.66
3	B	301	NAG	O3-C3-C2	2.57	114.75	109.40
3	W	401	NAG	O5-C5-C6	-2.57	102.66	107.66
3	T	301	NAG	O7-C7-N2	2.56	126.50	121.98
3	X	301	NAG	O5-C1-C2	-2.54	107.37	111.29
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	W	401	NAG	C3-C4-C5	-2.49	105.72	110.23
3	A	401	NAG	C4-C3-C2	2.49	114.66	111.02
3	F	301	NAG	C4-C3-C2	-2.46	107.41	111.02
3	B	301	NAG	C1-C2-N2	2.45	114.30	110.43
3	D	301	NAG	C4-C3-C2	-2.45	107.43	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	301	NAG	O7-C7-N2	2.39	126.21	121.98
3	T	301	NAG	O3-C3-C4	-2.35	104.83	110.38
3	V	301	NAG	O3-C3-C4	-2.34	104.86	110.38
3	C	401	NAG	O3-C3-C4	2.32	115.85	110.38
3	S	401	NAG	O5-C1-C2	-2.27	107.77	111.29
3	P	301	NAG	O5-C5-C6	2.27	112.09	107.66
3	X	301	NAG	O7-C7-N2	2.25	125.96	121.98
3	T	301	NAG	C2-N2-C7	-2.24	119.90	122.90
3	N	301	NAG	O7-C7-N2	2.21	125.89	121.98
3	A	401	NAG	C3-C4-C5	2.18	114.18	110.23
3	I	401	NAG	O5-C1-C2	2.15	114.62	111.29
3	L	301	NAG	O5-C5-C4	2.14	116.02	110.83
3	R	301	NAG	C8-C7-N2	-2.13	112.59	116.12
3	M	401	NAG	O3-C3-C2	2.12	113.80	109.40
3	E	401	NAG	C4-C3-C2	-2.10	107.94	111.02
3	B	301	NAG	C3-C4-C5	2.07	113.98	110.23
3	G	401	NAG	C4-C3-C2	-2.06	108.00	111.02
3	X	301	NAG	O3-C3-C2	2.06	113.68	109.40
3	L	301	NAG	C6-C5-C4	-2.05	107.98	113.02
3	M	401	NAG	O4-C4-C5	2.04	114.35	109.32
3	I	401	NAG	O3-C3-C4	-2.02	105.61	110.38
3	A	401	NAG	C6-C5-C4	-2.01	108.09	113.02
3	D	301	NAG	O3-C3-C2	2.00	113.56	109.40

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	G	401	NAG	O5-C5-C6-O6
3	W	401	NAG	O5-C5-C6-O6
3	K	401	NAG	C4-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	P	301	NAG	C4-C5-C6-O6
3	V	301	NAG	O5-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	M	401	NAG	C4-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	A	401	NAG	C4-C5-C6-O6
3	R	301	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	C	401	NAG	C1-C2-N2-C7
3	T	301	NAG	C1-C2-N2-C7
3	V	301	NAG	C1-C2-N2-C7
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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	401	NAG	1	0
3	X	301	NAG	1	0
3	J	301	NAG	1	0
3	L	301	NAG	2	0
3	N	301	NAG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	H	301	2	14,14,15	1.20	1 (7%)	17,19,21	2.67	7 (41%)
3	NAG	I	401	1	14,14,15	0.56	0	17,19,21	2.73	5 (29%)
3	NAG	Q	401	1	14,14,15	0.52	0	17,19,21	1.63	3 (17%)
3	NAG	X	301	2	14,14,15	0.79	0	17,19,21	2.57	5 (29%)
3	NAG	M	401	1	14,14,15	0.48	0	17,19,21	3.03	8 (47%)
3	NAG	J	301	2	14,14,15	0.72	0	17,19,21	2.06	3 (17%)
3	NAG	K	401	1	14,14,15	0.47	0	17,19,21	2.81	3 (17%)
3	NAG	L	301	2	14,14,15	0.83	0	17,19,21	2.55	5 (29%)
3	NAG	B	301	2	14,14,15	1.28	1 (7%)	17,19,21	3.10	9 (52%)
3	NAG	D	301	2	14,14,15	1.26	2 (14%)	17,19,21	3.16	9 (52%)
3	NAG	R	301	2	14,14,15	0.97	1 (7%)	17,19,21	1.88	3 (17%)
3	NAG	V	301	2	14,14,15	0.85	0	17,19,21	2.03	3 (17%)
3	NAG	S	401	1	14,14,15	0.51	0	17,19,21	1.53	3 (17%)
3	NAG	E	401	1	14,14,15	0.57	0	17,19,21	1.87	2 (11%)
3	NAG	N	301	2	14,14,15	0.76	0	17,19,21	2.43	4 (23%)
3	NAG	C	401	1	14,14,15	0.46	0	17,19,21	1.80	3 (17%)
3	NAG	F	301	2	14,14,15	1.19	1 (7%)	17,19,21	3.06	9 (52%)
3	NAG	P	301	2	14,14,15	0.79	0	17,19,21	1.45	3 (17%)
3	NAG	U	401	1	14,14,15	0.48	0	17,19,21	1.52	1 (5%)
3	NAG	T	301	2	14,14,15	0.82	1 (7%)	17,19,21	1.85	4 (23%)
3	NAG	G	401	1	14,14,15	0.66	0	17,19,21	1.98	3 (17%)
3	NAG	A	401	1	14,14,15	0.58	0	17,19,21	2.11	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	W	401	1	14,14,15	0.46	0	17,19,21	2.86	6 (35%)
3	NAG	O	401	1	14,14,15	0.49	0	17,19,21	1.61	2 (11%)

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	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	Q	401	1	-	1/6/23/26	0/1/1/1
3	NAG	X	301	2	-	2/6/23/26	0/1/1/1
3	NAG	M	401	1	-	2/6/23/26	0/1/1/1
3	NAG	J	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	L	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	1/6/23/26	0/1/1/1
3	NAG	D	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	V	301	2	-	3/6/23/26	0/1/1/1
3	NAG	S	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	N	301	2	-	2/6/23/26	0/1/1/1
3	NAG	C	401	1	-	3/6/23/26	0/1/1/1
3	NAG	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	U	401	1	-	1/6/23/26	0/1/1/1
3	NAG	T	301	2	-	3/6/23/26	0/1/1/1
3	NAG	G	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	W	401	1	-	2/6/23/26	0/1/1/1
3	NAG	O	401	1	-	0/6/23/26	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	3.22	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAG	O7-C7	3.09	1.30	1.23
3	F	301	NAG	O7-C7	2.91	1.29	1.23
3	D	301	NAG	O7-C7	2.86	1.29	1.23
3	D	301	NAG	O5-C1	2.18	1.47	1.43
3	R	301	NAG	O7-C7	2.13	1.28	1.23
3	T	301	NAG	O7-C7	2.12	1.28	1.23

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	401	NAG	C1-O5-C5	9.79	125.31	112.19
3	K	401	NAG	C1-O5-C5	9.69	125.17	112.19
3	I	401	NAG	C1-O5-C5	9.68	125.16	112.19
3	W	401	NAG	C1-O5-C5	9.03	124.28	112.19
3	X	301	NAG	C1-O5-C5	8.66	123.80	112.19
3	L	301	NAG	C1-O5-C5	8.06	122.98	112.19
3	N	301	NAG	C1-O5-C5	7.09	121.69	112.19
3	J	301	NAG	C1-O5-C5	6.35	120.70	112.19
3	A	401	NAG	C1-O5-C5	6.33	120.67	112.19
3	B	301	NAG	O7-C7-N2	6.24	133.00	121.98
3	E	401	NAG	C1-O5-C5	6.22	120.53	112.19
3	D	301	NAG	C1-O5-C5	6.13	120.41	112.19
3	B	301	NAG	C2-N2-C7	5.97	130.90	122.90
3	G	401	NAG	C1-O5-C5	5.84	120.02	112.19
3	T	301	NAG	C1-O5-C5	5.75	119.89	112.19
3	V	301	NAG	C1-O5-C5	5.75	119.89	112.19
3	C	401	NAG	C1-O5-C5	5.74	119.88	112.19
3	F	301	NAG	O7-C7-N2	5.72	132.09	121.98
3	D	301	NAG	O7-C7-N2	5.61	131.90	121.98
3	R	301	NAG	C1-O5-C5	5.45	119.49	112.19
3	H	301	NAG	C8-C7-N2	-5.42	107.13	116.12
3	F	301	NAG	C1-O5-C5	5.27	119.25	112.19
3	D	301	NAG	C2-N2-C7	5.07	129.69	122.90
3	F	301	NAG	C8-C7-N2	-4.99	107.84	116.12
3	B	301	NAG	C8-C7-N2	-4.92	107.95	116.12
3	O	401	NAG	C1-O5-C5	4.82	118.65	112.19
3	U	401	NAG	C1-O5-C5	4.66	118.43	112.19
3	H	301	NAG	C1-O5-C5	4.66	118.42	112.19
3	D	301	NAG	C8-C7-N2	-4.63	108.44	116.12
3	B	301	NAG	C1-O5-C5	4.57	118.32	112.19
3	H	301	NAG	O7-C7-N2	4.38	129.73	121.98
3	F	301	NAG	C2-N2-C7	4.17	128.49	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	401	NAG	C1-O5-C5	4.10	117.68	112.19
3	N	301	NAG	C8-C7-N2	-4.09	109.33	116.12
3	K	401	NAG	O5-C1-C2	4.02	117.52	111.29
3	F	301	NAG	O5-C1-C2	3.87	117.28	111.29
3	M	401	NAG	O5-C1-C2	3.85	117.24	111.29
3	N	301	NAG	O5-C1-C2	-3.70	105.57	111.29
3	W	401	NAG	O5-C1-C2	3.68	116.99	111.29
3	P	301	NAG	C1-O5-C5	3.58	116.99	112.19
3	D	301	NAG	C1-C2-N2	3.54	116.01	110.43
3	L	301	NAG	O5-C1-C2	-3.47	105.93	111.29
3	V	301	NAG	O7-C7-N2	3.44	128.07	121.98
3	D	301	NAG	O5-C1-C2	3.38	116.52	111.29
3	R	301	NAG	O7-C7-N2	3.36	127.92	121.98
3	L	301	NAG	C8-C7-N2	-3.29	110.66	116.12
3	H	301	NAG	C1-C2-N2	3.19	115.45	110.43
3	B	301	NAG	O5-C5-C4	3.04	118.23	110.83
3	B	301	NAG	O5-C1-C2	3.04	115.99	111.29
3	S	401	NAG	C1-O5-C5	3.01	116.22	112.19
3	M	401	NAG	C4-C3-C2	-2.98	106.66	111.02
3	Q	401	NAG	C3-C4-C5	-2.97	104.84	110.23
3	F	301	NAG	O5-C5-C4	2.94	117.97	110.83
3	X	301	NAG	C8-C7-N2	-2.93	111.26	116.12
3	O	401	NAG	C3-C4-C5	-2.91	104.96	110.23
3	M	401	NAG	C3-C4-C5	-2.86	105.06	110.23
3	G	401	NAG	O5-C5-C6	2.84	113.18	107.66
3	I	401	NAG	O7-C7-C8	-2.76	117.14	122.05
3	S	401	NAG	C3-C4-C5	-2.76	105.23	110.23
3	J	301	NAG	C8-C7-N2	-2.74	111.57	116.12
3	W	401	NAG	O4-C4-C5	2.74	116.07	109.32
3	W	401	NAG	O7-C7-C8	-2.73	117.20	122.05
3	F	301	NAG	C1-C2-N2	2.71	114.70	110.43
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	F	301	NAG	O3-C3-C2	2.67	114.95	109.40
3	J	301	NAG	O5-C1-C2	-2.67	107.16	111.29
3	H	301	NAG	C2-N2-C7	2.67	126.48	122.90
3	Q	401	NAG	O5-C1-C2	-2.65	107.19	111.29
3	M	401	NAG	O7-C7-C8	-2.64	117.35	122.05
3	K	401	NAG	O7-C7-C8	-2.64	117.35	122.05
3	I	401	NAG	C8-C7-N2	2.61	120.45	116.12
3	M	401	NAG	C8-C7-N2	2.61	120.45	116.12
3	A	401	NAG	O5-C5-C6	2.60	112.73	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAG	O3-C3-C2	2.57	114.75	109.40
3	W	401	NAG	O5-C5-C6	-2.57	102.66	107.66
3	T	301	NAG	O7-C7-N2	2.56	126.50	121.98
3	X	301	NAG	O5-C1-C2	-2.54	107.37	111.29
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	W	401	NAG	C3-C4-C5	-2.49	105.72	110.23
3	A	401	NAG	C4-C3-C2	2.49	114.66	111.02
3	F	301	NAG	C4-C3-C2	-2.46	107.41	111.02
3	B	301	NAG	C1-C2-N2	2.45	114.30	110.43
3	D	301	NAG	C4-C3-C2	-2.45	107.43	111.02
3	P	301	NAG	O7-C7-N2	2.39	126.21	121.98
3	T	301	NAG	O3-C3-C4	-2.35	104.83	110.38
3	V	301	NAG	O3-C3-C4	-2.34	104.86	110.38
3	C	401	NAG	O3-C3-C4	2.32	115.85	110.38
3	S	401	NAG	O5-C1-C2	-2.27	107.77	111.29
3	P	301	NAG	O5-C5-C6	2.27	112.09	107.66
3	X	301	NAG	O7-C7-N2	2.25	125.96	121.98
3	T	301	NAG	C2-N2-C7	-2.24	119.90	122.90
3	N	301	NAG	O7-C7-N2	2.21	125.89	121.98
3	A	401	NAG	C3-C4-C5	2.18	114.18	110.23
3	I	401	NAG	O5-C1-C2	2.15	114.62	111.29
3	L	301	NAG	O5-C5-C4	2.14	116.02	110.83
3	R	301	NAG	C8-C7-N2	-2.13	112.59	116.12
3	M	401	NAG	O3-C3-C2	2.12	113.80	109.40
3	E	401	NAG	C4-C3-C2	-2.10	107.94	111.02
3	B	301	NAG	C3-C4-C5	2.07	113.98	110.23
3	G	401	NAG	C4-C3-C2	-2.06	108.00	111.02
3	X	301	NAG	O3-C3-C2	2.06	113.68	109.40
3	L	301	NAG	C6-C5-C4	-2.05	107.98	113.02
3	M	401	NAG	O4-C4-C5	2.04	114.35	109.32
3	I	401	NAG	O3-C3-C4	-2.02	105.61	110.38
3	A	401	NAG	C6-C5-C4	-2.01	108.09	113.02
3	D	301	NAG	O3-C3-C2	2.00	113.56	109.40

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	401	NAG	O5-C5-C6-O6
3	K	401	NAG	O5-C5-C6-O6
3	N	301	NAG	O5-C5-C6-O6
3	H	301	NAG	O5-C5-C6-O6
3	T	301	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	I	401	NAG	O5-C5-C6-O6
3	J	301	NAG	O5-C5-C6-O6
3	R	301	NAG	O5-C5-C6-O6
3	X	301	NAG	C4-C5-C6-O6
3	D	301	NAG	O5-C5-C6-O6
3	G	401	NAG	O5-C5-C6-O6
3	W	401	NAG	O5-C5-C6-O6
3	K	401	NAG	C4-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	P	301	NAG	C4-C5-C6-O6
3	V	301	NAG	O5-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	M	401	NAG	C4-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	A	401	NAG	C4-C5-C6-O6
3	R	301	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	C	401	NAG	C1-C2-N2-C7
3	T	301	NAG	C1-C2-N2-C7
3	V	301	NAG	C1-C2-N2-C7
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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	401	NAG	1	0
3	X	301	NAG	1	0
3	J	301	NAG	1	0
3	L	301	NAG	2	0
3	N	301	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/327 (97%)	-0.93	1 (0%) 90 89	44, 62, 87, 130	0
1	C	319/327 (97%)	-0.86	1 (0%) 90 89	44, 63, 87, 131	0
1	E	319/327 (97%)	-0.89	0 100 100	43, 62, 87, 132	0
1	G	319/327 (97%)	-0.93	0 100 100	42, 63, 86, 131	0
1	I	319/327 (97%)	-0.58	0 100 100	53, 80, 117, 165	0
1	K	319/327 (97%)	-0.57	2 (0%) 85 85	53, 80, 117, 158	0
1	M	319/327 (97%)	-0.62	1 (0%) 90 89	53, 79, 117, 161	0
1	O	319/327 (97%)	-0.52	1 (0%) 90 89	55, 88, 122, 149	0
1	Q	319/327 (97%)	-0.48	1 (0%) 90 89	55, 88, 121, 154	0
1	S	319/327 (97%)	-0.42	1 (0%) 90 89	56, 89, 121, 151	0
1	U	319/327 (97%)	-0.40	0 100 100	56, 89, 120, 151	0
1	W	319/327 (97%)	-0.64	1 (0%) 90 89	51, 80, 116, 162	0
2	B	172/174 (98%)	-0.08	6 (3%) 47 43	64, 96, 146, 193	0
2	D	172/174 (98%)	-0.11	6 (3%) 47 43	65, 99, 145, 188	0
2	F	172/174 (98%)	-0.15	4 (2%) 61 58	63, 97, 140, 182	0
2	H	172/174 (98%)	-0.24	4 (2%) 61 58	55, 93, 138, 184	0
2	J	172/174 (98%)	0.09	4 (2%) 61 58	65, 115, 175, 219	0
2	L	172/174 (98%)	0.03	4 (2%) 61 58	64, 113, 173, 211	0
2	N	172/174 (98%)	0.21	6 (3%) 47 43	65, 116, 180, 219	0
2	P	172/174 (98%)	-0.58	0 100 100	48, 81, 124, 184	0
2	R	172/174 (98%)	-0.61	0 100 100	46, 82, 124, 185	0
2	T	172/174 (98%)	-0.51	0 100 100	46, 81, 124, 194	0
2	V	172/174 (98%)	-0.50	1 (0%) 85 85	47, 82, 125, 178	0
2	X	172/174 (98%)	-0.02	6 (3%) 47 43	60, 108, 168, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5892/6012 (98%)	-0.50	50 (0%) 82 81	42, 81, 140, 219	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	27	GLN	4.6
2	J	16	GLY	4.2
2	J	145	ASP	3.6
2	F	143	ALA	3.3
1	K	107	GLY	3.3
2	F	16	GLY	3.3
2	X	168	LEU	3.1
2	D	139	GLU	3.1
2	D	153	ARG	3.1
1	C	2	LYS	3.0
2	B	140	ILE	3.0
2	L	155	ASN	2.9
2	B	167	LEU	2.8
2	D	9	PHE	2.7
2	X	157	TYR	2.7
2	B	130	ALA	2.7
2	X	16	GLY	2.6
2	D	162	TYR	2.6
1	O	71	THR	2.6
2	N	168	LEU	2.5
2	B	166	ALA	2.5
2	N	33	GLY	2.5
1	Q	124	ALA	2.4
2	L	171	LEU	2.4
2	B	162	TYR	2.4
2	N	131	GLU	2.3
2	D	134	GLY	2.3
1	A	264	ALA	2.3
2	H	167	LEU	2.3
2	H	138	PHE	2.3
2	H	166	ALA	2.2
2	X	141	TYR	2.2
2	L	162	TYR	2.2
1	W	90	GLY	2.2
1	K	11	ALA	2.2
2	J	32	THR	2.2
2	D	142	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	169	ASN	2.2
2	N	47	GLN	2.2
2	X	145	ASP	2.2
2	L	157	TYR	2.1
2	F	167	LEU	2.1
2	N	141	TYR	2.1
1	M	58	GLY	2.0
2	J	157	TYR	2.0
2	V	153	ARG	2.0
2	F	133	ASP	2.0
1	S	71	THR	2.0
2	N	171	LEU	2.0
2	H	16	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	J	301	14/15	0.90	0.12	97,101,108,108	0
3	NAG	X	301	14/15	0.95	0.09	91,95,102,102	0
3	NAG	E	401	14/15	0.96	0.07	97,105,107,110	0
3	NAG	H	301	14/15	0.96	0.07	80,84,86,86	0
3	NAG	A	401	14/15	0.96	0.09	103,110,114,118	0
3	NAG	K	401	14/15	0.96	0.06	67,75,81,82	0
3	NAG	O	401	14/15	0.96	0.08	97,111,116,117	0
3	NAG	P	301	14/15	0.96	0.07	83,87,94,97	0
3	NAG	R	301	14/15	0.96	0.08	82,84,88,89	0
3	NAG	S	401	14/15	0.96	0.07	97,111,117,119	0
3	NAG	D	301	14/15	0.96	0.07	85,88,92,92	0
3	NAG	C	401	14/15	0.97	0.08	95,105,109,109	0
3	NAG	Q	401	14/15	0.97	0.09	99,112,116,117	0
3	NAG	L	301	14/15	0.97	0.07	91,95,102,103	0
3	NAG	M	401	14/15	0.97	0.06	63,72,76,78	0
3	NAG	U	401	14/15	0.97	0.08	101,114,121,121	0
3	NAG	V	301	14/15	0.97	0.06	86,90,95,96	0
3	NAG	W	401	14/15	0.97	0.04	64,72,75,78	0
3	NAG	G	401	14/15	0.97	0.07	100,107,110,110	0
3	NAG	T	301	14/15	0.98	0.05	80,85,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	I	401	14/15	0.98	0.06	63,71,76,77	0
3	NAG	B	301	14/15	0.98	0.06	81,84,87,88	0
3	NAG	N	301	14/15	0.98	0.08	92,96,102,103	0
3	NAG	F	301	14/15	0.98	0.05	81,84,89,89	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	J	301	14/15	0.90	0.12	97,101,108,108	0
3	NAG	X	301	14/15	0.95	0.09	91,95,102,102	0
3	NAG	E	401	14/15	0.96	0.07	97,105,107,110	0
3	NAG	H	301	14/15	0.96	0.07	80,84,86,86	0
3	NAG	A	401	14/15	0.96	0.09	103,110,114,118	0
3	NAG	K	401	14/15	0.96	0.06	67,75,81,82	0
3	NAG	O	401	14/15	0.96	0.08	97,111,116,117	0
3	NAG	P	301	14/15	0.96	0.07	83,87,94,97	0
3	NAG	R	301	14/15	0.96	0.08	82,84,88,89	0
3	NAG	S	401	14/15	0.96	0.07	97,111,117,119	0
3	NAG	D	301	14/15	0.96	0.07	85,88,92,92	0
3	NAG	C	401	14/15	0.97	0.08	95,105,109,109	0
3	NAG	Q	401	14/15	0.97	0.09	99,112,116,117	0
3	NAG	L	301	14/15	0.97	0.07	91,95,102,103	0
3	NAG	M	401	14/15	0.97	0.06	63,72,76,78	0
3	NAG	U	401	14/15	0.97	0.08	101,114,121,121	0
3	NAG	V	301	14/15	0.97	0.06	86,90,95,96	0
3	NAG	W	401	14/15	0.97	0.04	64,72,75,78	0
3	NAG	G	401	14/15	0.97	0.07	100,107,110,110	0
3	NAG	T	301	14/15	0.98	0.05	80,85,89,90	0
3	NAG	I	401	14/15	0.98	0.06	63,71,76,77	0
3	NAG	B	301	14/15	0.98	0.06	81,84,87,88	0
3	NAG	N	301	14/15	0.98	0.08	92,96,102,103	0
3	NAG	F	301	14/15	0.98	0.05	81,84,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.