



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 4QY1 / pdb_00004qy1
Title : Structure of H10 from human-infecting H10N8 in complex with avian receptor
Authors : Wang, M.; Zhang, W.; Qi, J.; Wang, F.; Zhou, J.; Bi, Y.; Wu, Y.; Sun, H.;
Liu, J.; Huang, C.; Li, X.; Yan, J.; Shu, Y.; Shi, Y.; Gao, G.F.
Deposited on : 2014-07-23
Resolution : 2.59 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

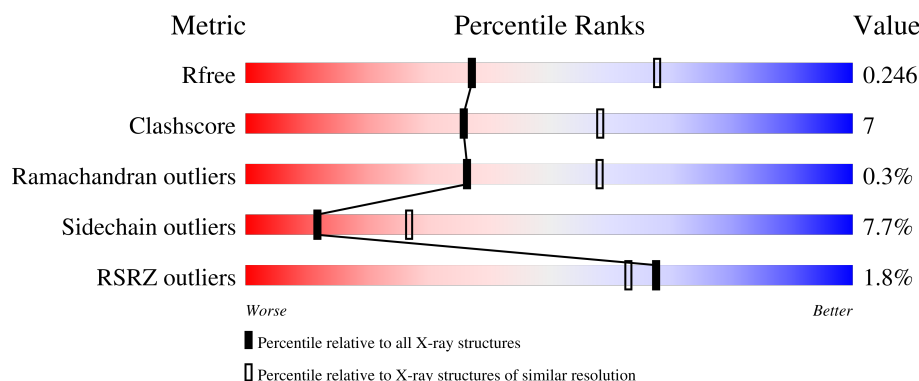
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	318	 76% 21% .
1	C	318	 79% 19% .
1	E	318	 77% 20% .
1	G	318	 81% 18% .
1	I	318	 81% 17% .

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Mol	Chain	Length	Quality of chain
1	K	318	80% 19% .
1	M	318	6% 82% 16% .
1	O	318	3% 76% 22% .
1	Q	318	74% 24% .
1	S	318	3% 81% 17% .
1	U	318	79% 18% .
1	W	318	2% 78% 19% .
2	B	174	3% 83% 14% .
2	D	174	2% 80% 16% .
2	F	174	3% 80% 16% .
2	H	174	79% 20% .
2	J	174	5% 84% 13% .
2	L	174	3% 81% 16% .
2	N	174	3% 84% 14% ..
2	P	174	2% 80% 17% ..
2	R	174	2% 80% 18% .
2	T	174	2% 82% 15% .
2	V	174	2% 76% 21% .
2	X	174	4% 80% 18% .
3	Y	2	50% 50%
4	Z	3	67% 33%
4	a	3	67% 33%
4	b	3	33% 33% 33%
4	c	3	33% 33% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48138 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	C	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	E	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	G	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	I	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	K	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	M	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	O	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	Q	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	S	318	Total	C	N	O	S	0	0	0
			2436	1506	449	464	17			
1	U	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			
1	W	318	Total	C	N	O	S	0	0	0
			2437	1506	449	465	17			

- Molecule 2 is a protein called hemagglutinin.

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

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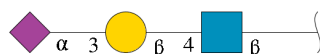
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	L	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	N	174	Total	C	N	O	S	0	0	0
			1402	866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

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



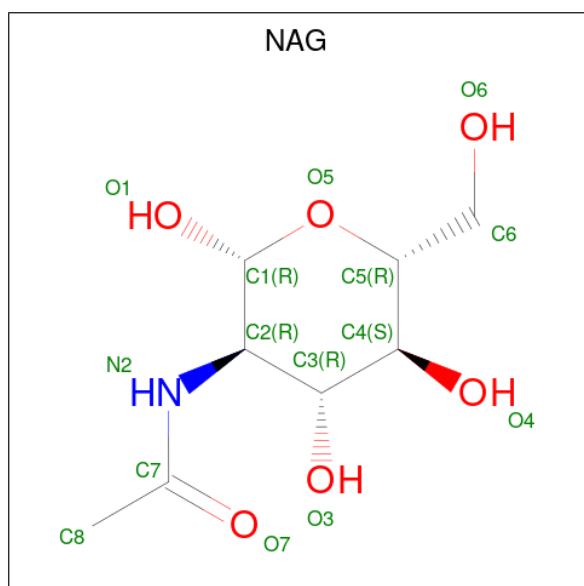
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Z	3	Total	C	N	O	0	0	0
			45	25	2	18			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	a	3	Total	C	N	O	0	0	0
			45	25	2	18			
4	b	3	Total	C	N	O	0	0	0
			45	25	2	18			
4	c	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	R	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	T	1	Total	C	N	O	0	0
			14	8	1	5		
5	U	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	W	1	Total	C	N	O	0	0
			14	8	1	5		
5	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	70	Total	O	0	0
			70	70		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	71	Total 71	O 71	0	0
6	D	87	Total 87	O 87	0	0
6	E	93	Total 93	O 93	0	0
6	F	64	Total 64	O 64	0	0
6	G	80	Total 80	O 80	0	0
6	H	53	Total 53	O 53	0	0
6	I	102	Total 102	O 102	0	0
6	J	43	Total 43	O 43	0	0
6	K	93	Total 93	O 93	0	0
6	L	53	Total 53	O 53	0	0
6	M	27	Total 27	O 27	0	0
6	N	46	Total 46	O 46	0	0
6	O	40	Total 40	O 40	0	0
6	P	48	Total 48	O 48	0	0
6	Q	84	Total 84	O 84	0	0
6	R	42	Total 42	O 42	0	0
6	S	64	Total 64	O 64	0	0
6	T	49	Total 49	O 49	0	0
6	U	76	Total 76	O 76	0	0
6	V	44	Total 44	O 44	0	0
6	W	50	Total 50	O 50	0	0

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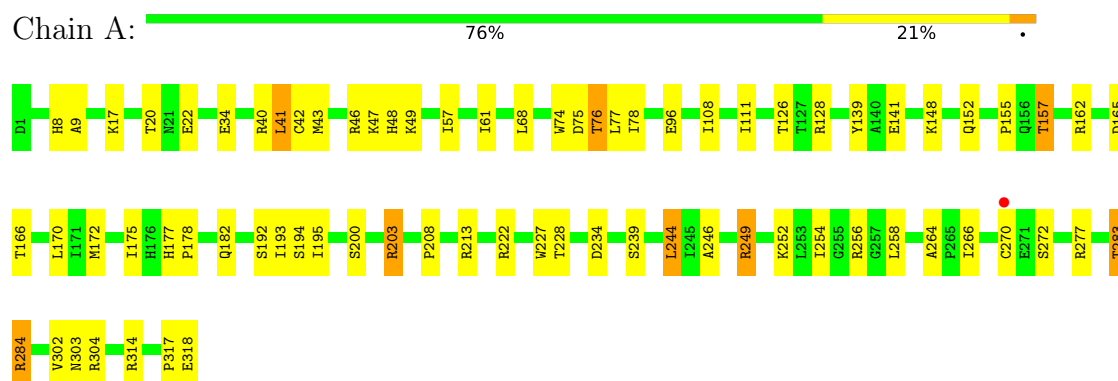
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	28	Total	O	0	0
			28	28		

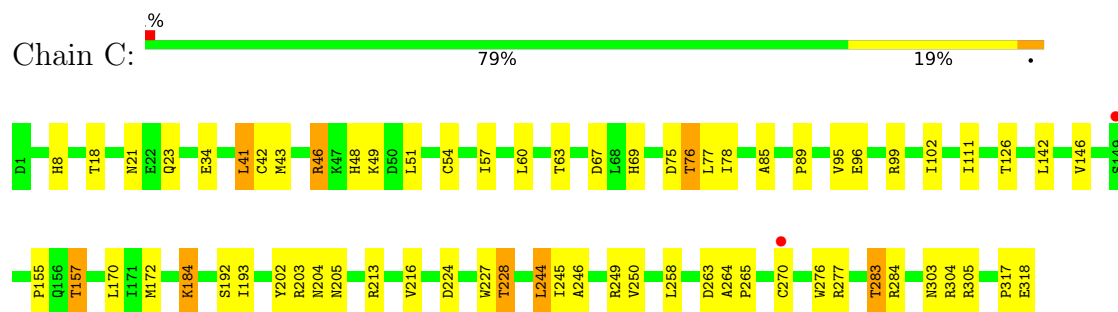
3 Residue-property plots

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.

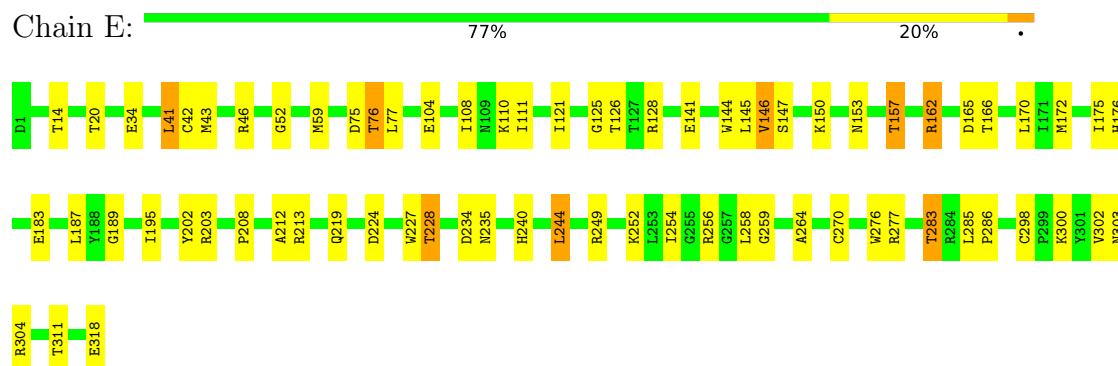
- Molecule 1: hemagglutinin



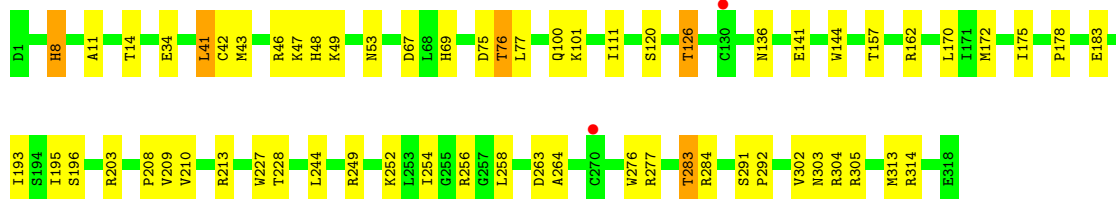
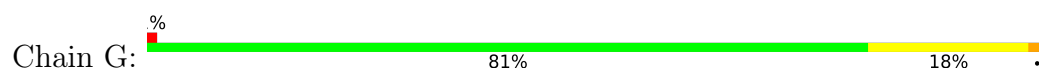
- Molecule 1: hemagglutinin



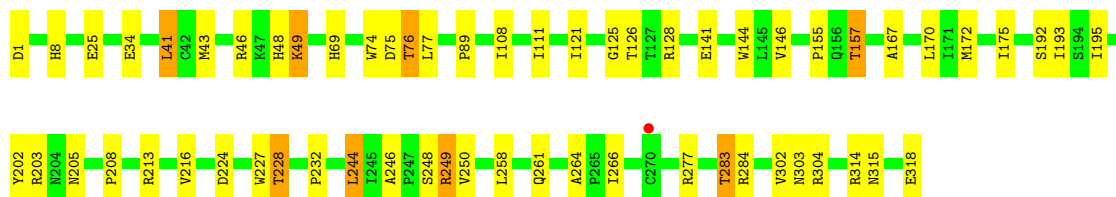
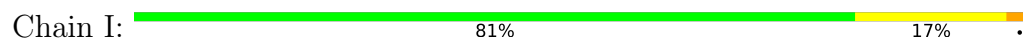
- Molecule 1: hemagglutinin



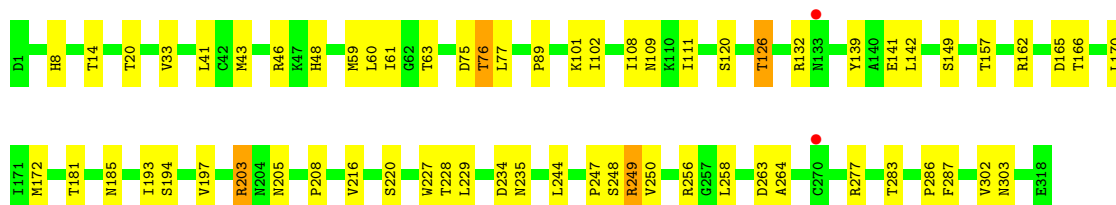
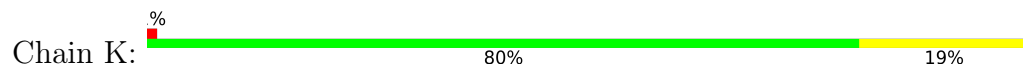
- Molecule 1: hemagglutinin



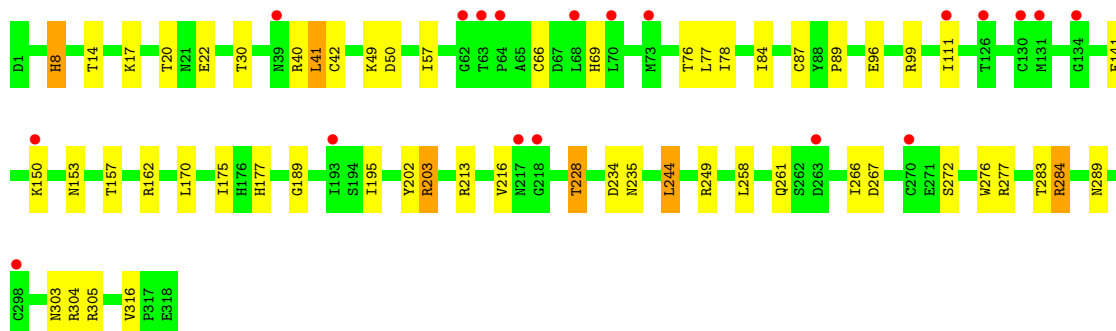
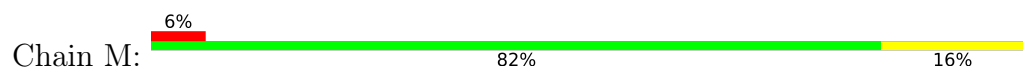
- Molecule 1: hemagglutinin



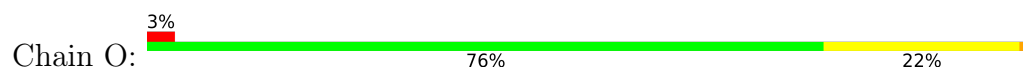
- Molecule 1: hemagglutinin

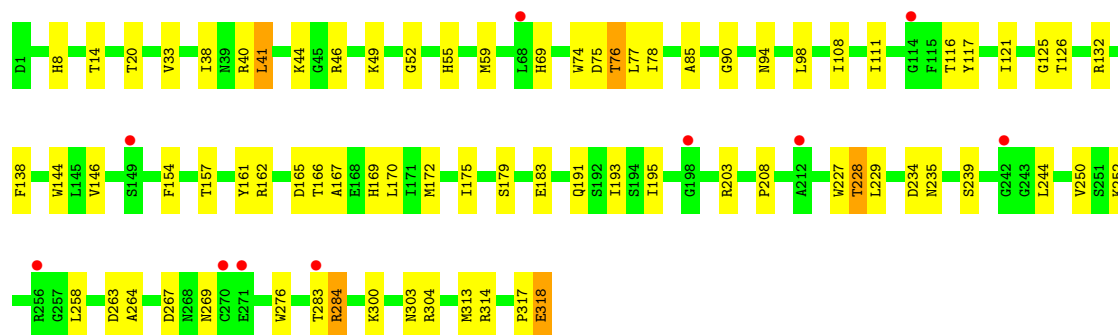


- Molecule 1: hemagglutinin

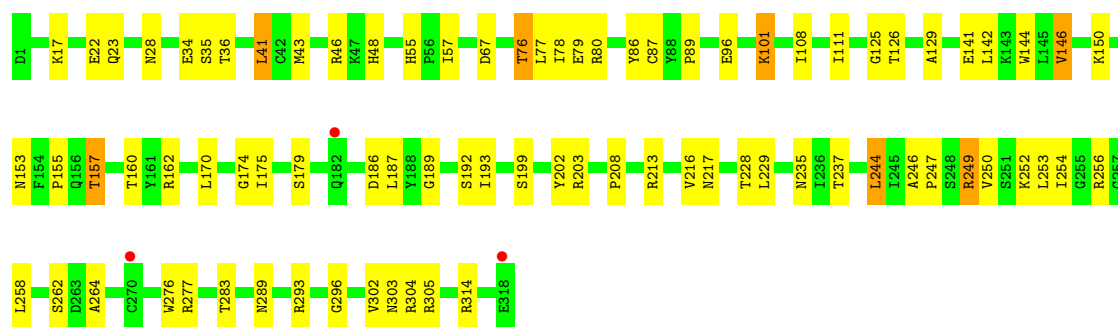
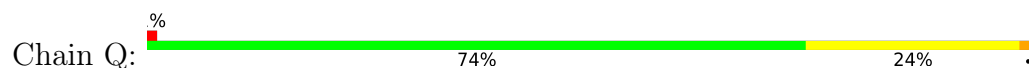


- Molecule 1: hemagglutinin

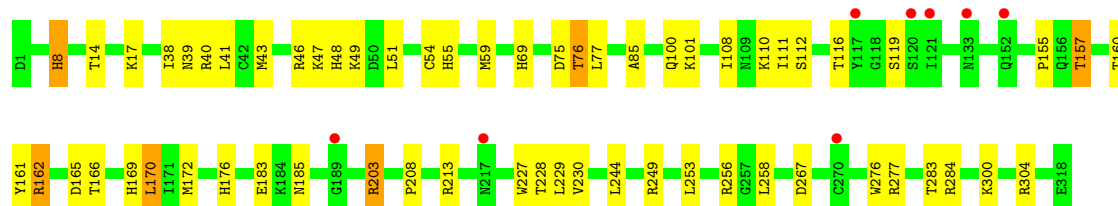
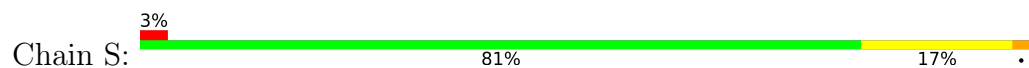




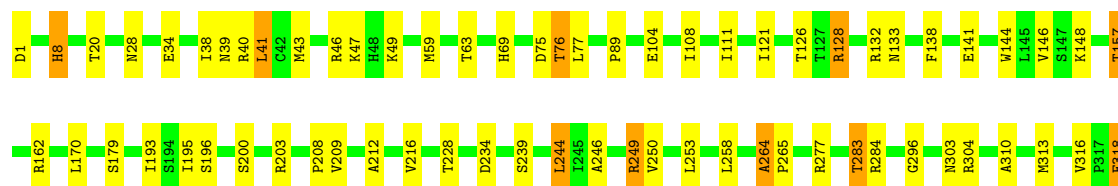
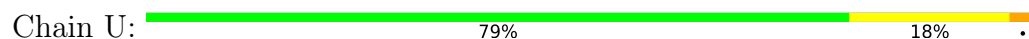
• Molecule 1: hemagglutinin



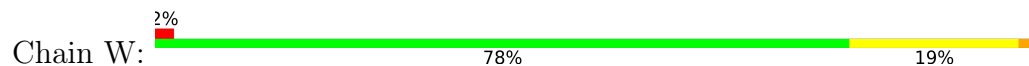
• Molecule 1: hemagglutinin



• Molecule 1: hemagglutinin

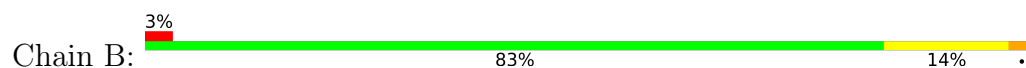


• Molecule 1: hemagglutinin

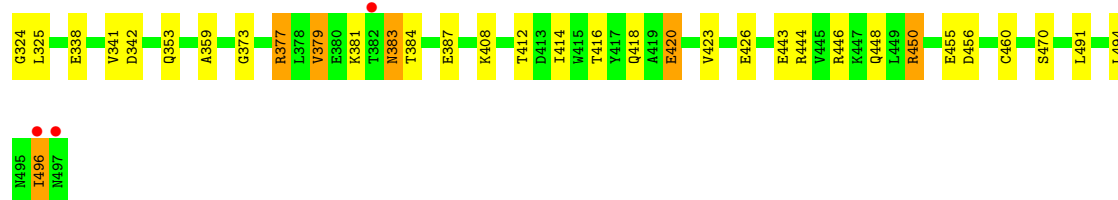
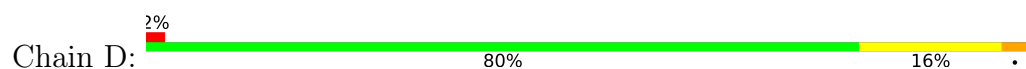




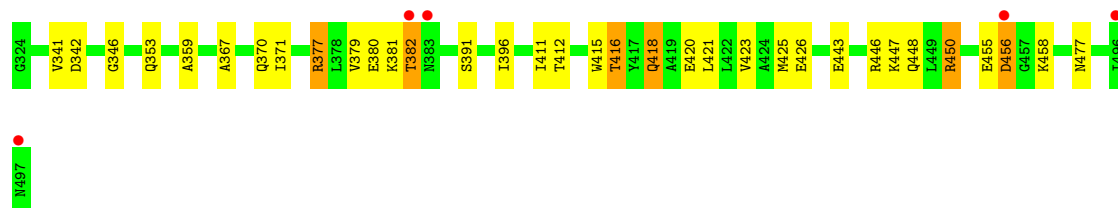
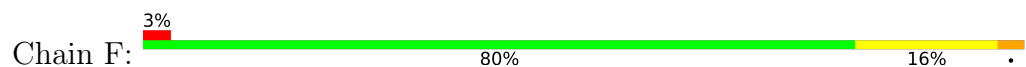
• Molecule 2: hemagglutinin



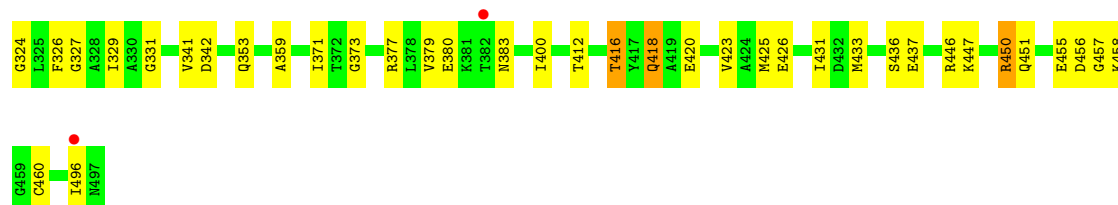
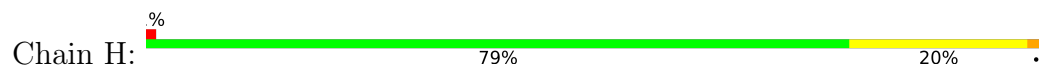
• Molecule 2: hemagglutinin



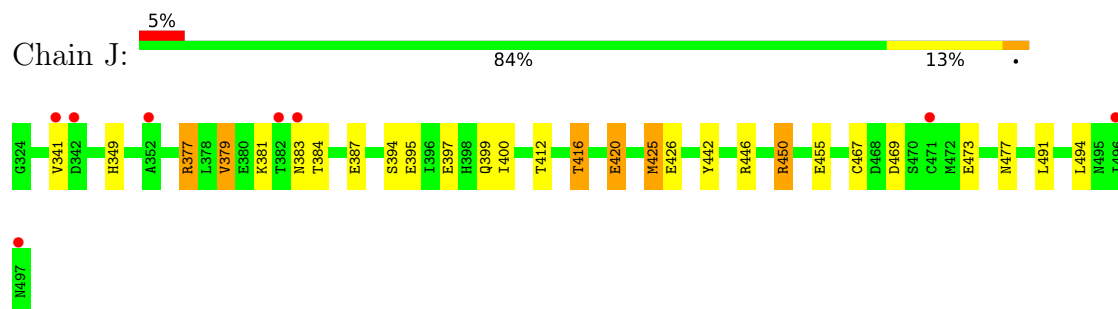
• Molecule 2: hemagglutinin



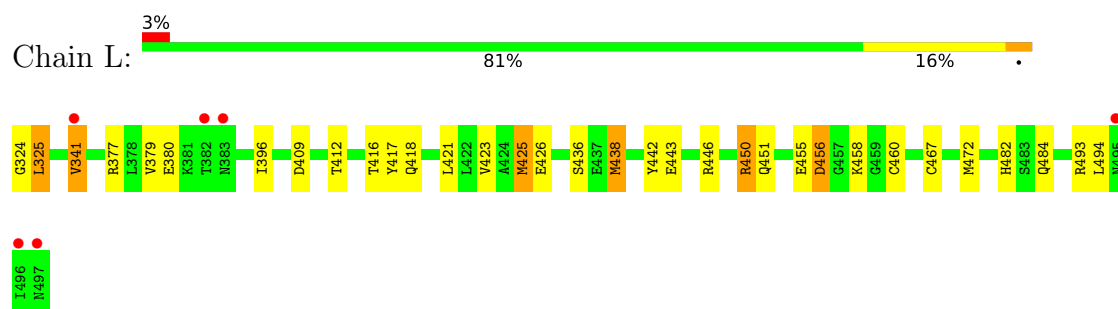
• Molecule 2: hemagglutinin



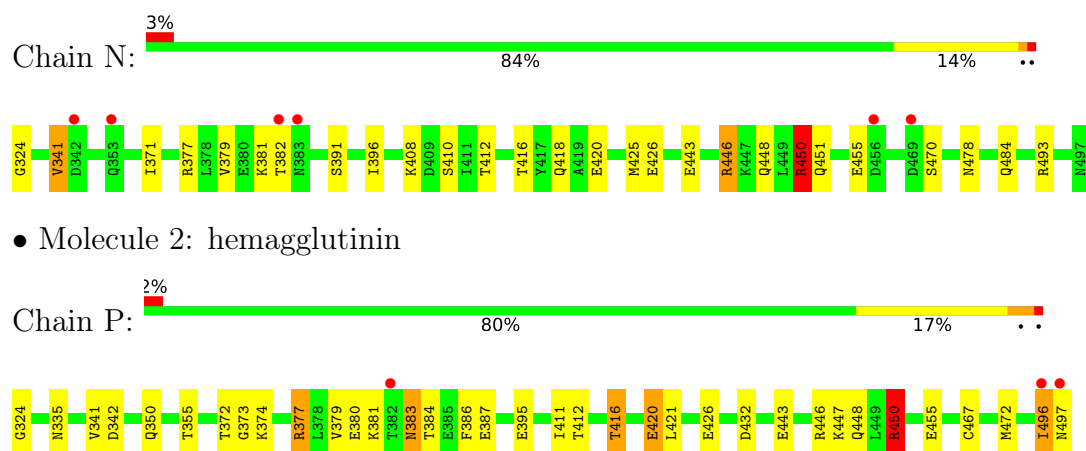
- Molecule 2: hemagglutinin



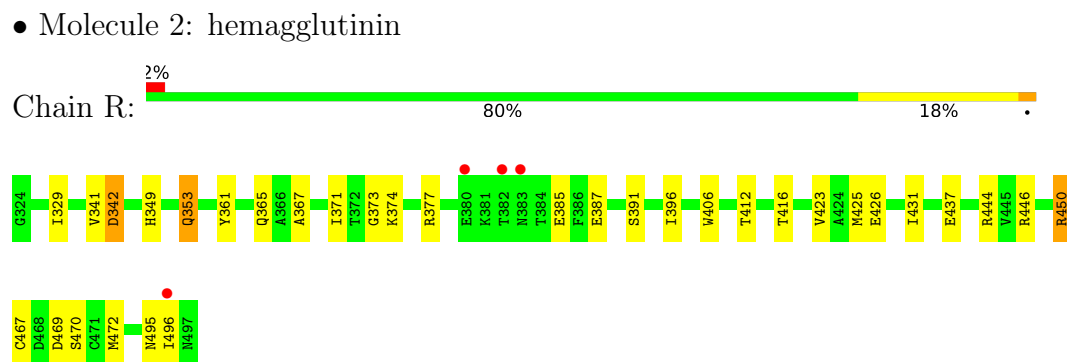
- Molecule 2: hemagglutinin



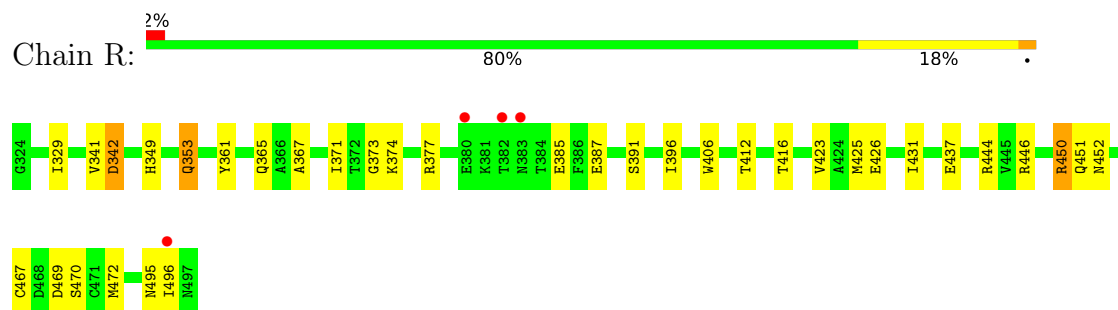
- Molecule 2: hemagglutinin



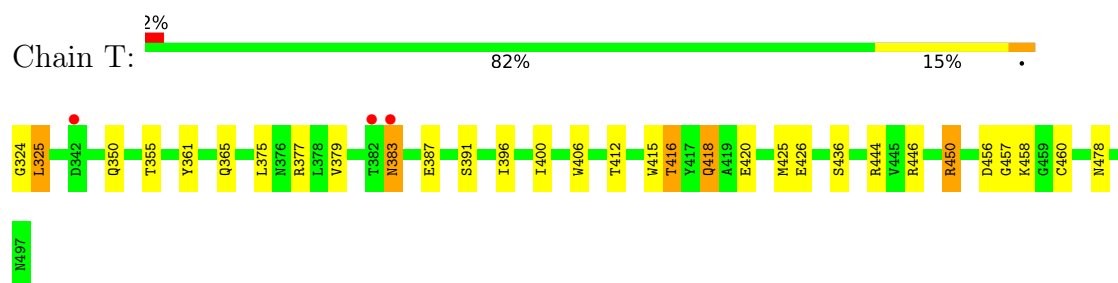
- Molecule 2: hemagglutinin



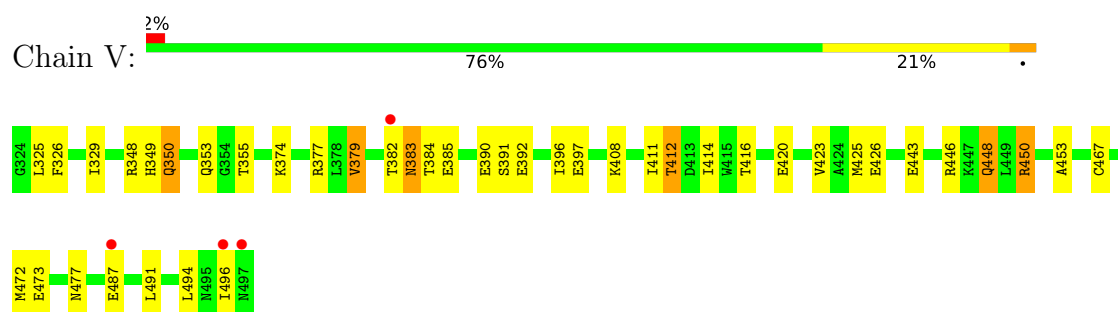
- Molecule 2: hemagglutinin



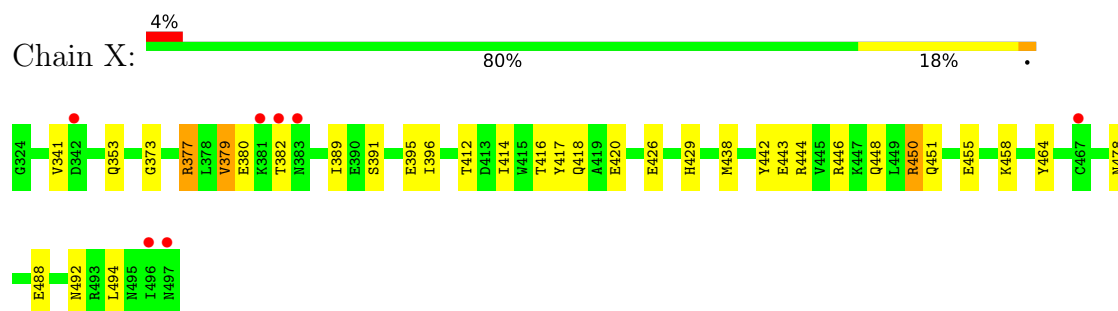
- Molecule 2: hemagglutinin



- Molecule 2: hemagglutinin



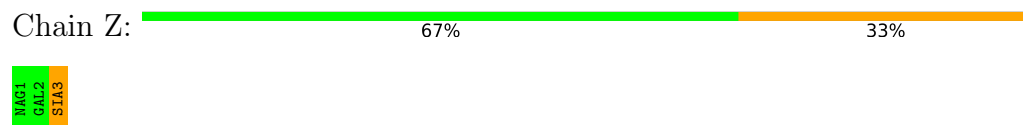
- Molecule 2: hemagglutinin



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.26Å 111.44Å 222.35Å 94.96° 101.17° 91.90°	Depositor
Resolution (Å)	37.07 – 2.59 37.07 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.07-2.59) 89.0 (37.07-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.246	Depositor DCC
R_{free} test set	13242 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	48138	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/2486	0.77	1/3368 (0.0%)
1	C	0.36	0/2486	0.79	0/3368
1	E	0.38	0/2486	0.77	0/3368
1	G	0.37	0/2486	0.76	0/3368
1	I	0.38	0/2486	0.77	0/3368
1	K	0.38	0/2486	0.77	0/3368
1	M	0.35	0/2486	0.75	3/3368 (0.1%)
1	O	0.35	0/2486	0.76	1/3368 (0.0%)
1	Q	0.37	0/2486	0.77	0/3368
1	S	0.37	0/2485	0.77	0/3366
1	U	0.36	0/2486	0.77	2/3368 (0.1%)
1	W	0.35	0/2486	0.77	1/3368 (0.0%)
2	B	0.39	0/1427	0.75	0/1926
2	D	0.40	0/1427	0.78	0/1926
2	F	0.39	0/1427	0.77	1/1926 (0.1%)
2	H	0.39	0/1427	0.74	1/1926 (0.1%)
2	J	0.36	0/1427	0.75	0/1926
2	L	0.37	0/1427	0.75	1/1926 (0.1%)
2	N	0.36	0/1427	0.74	1/1926 (0.1%)
2	P	0.38	0/1427	0.77	0/1926
2	R	0.37	0/1427	0.74	0/1926
2	T	0.38	0/1427	0.71	0/1926
2	V	0.36	0/1427	0.78	0/1926
2	X	0.36	0/1427	0.76	2/1926 (0.1%)
All	All	0.37	0/46955	0.76	14/63526 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	389	ILE	N-CA-C	-7.35	106.14	113.20
2	X	341	VAL	N-CA-C	-6.25	106.90	112.90
1	O	284	ARG	N-CA-C	-5.58	106.31	113.23
2	H	457	GLY	N-CA-C	-5.56	107.34	114.85
2	L	341	VAL	N-CA-C	-5.40	107.86	113.10
1	A	284	ARG	N-CA-C	-5.26	106.37	112.89
1	M	284	ARG	N-CA-C	-5.23	106.75	113.23
1	U	264	ALA	CA-C-N	5.22	125.14	119.76
1	U	264	ALA	C-N-CA	5.22	125.14	119.76
2	N	341	VAL	N-CA-C	-5.21	107.22	112.17
1	M	177	HIS	CA-C-N	5.18	125.11	119.78
1	M	177	HIS	C-N-CA	5.18	125.11	119.78
2	F	346	GLY	N-CA-C	5.14	118.65	111.19
1	W	284	ARG	N-CA-C	-5.02	107.16	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2389	45	0
1	C	2437	0	2389	34	0
1	E	2437	0	2387	45	0
1	G	2437	0	2389	38	0
1	I	2437	0	2389	38	0
1	K	2437	0	2389	28	0
1	M	2437	0	2389	26	0
1	O	2437	0	2389	40	0
1	Q	2437	0	2389	42	0
1	S	2436	0	2389	37	0
1	U	2437	0	2389	40	0
1	W	2437	0	2389	39	0
2	B	1402	0	1298	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1402	0	1298	29	0
2	F	1402	0	1298	21	0
2	H	1402	0	1298	30	0
2	J	1402	0	1298	22	0
2	L	1402	0	1298	25	0
2	N	1402	0	1298	19	0
2	P	1402	0	1298	24	0
2	R	1402	0	1298	28	0
2	T	1402	0	1298	23	0
2	V	1402	0	1298	28	0
2	X	1402	0	1298	24	0
3	Y	28	0	25	1	0
4	Z	45	0	38	5	0
4	a	45	0	38	5	0
4	b	45	0	38	3	0
4	c	45	0	38	4	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	1	0
5	E	28	0	26	1	0
5	F	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	1	0
5	K	14	0	13	1	0
5	L	14	0	13	0	0
5	M	14	0	13	0	0
5	N	14	0	13	1	0
5	O	14	0	13	1	0
5	P	14	0	13	0	0
5	Q	14	0	13	0	0
5	R	14	0	13	0	0
5	S	14	0	13	0	0
5	T	14	0	13	1	0
5	U	14	0	13	1	0
5	V	14	0	13	0	0
5	W	14	0	13	0	0
5	X	14	0	13	0	0
6	A	106	0	0	9	0
6	B	70	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	71	0	0	5	0
6	D	87	0	0	9	0
6	E	93	0	0	11	0
6	F	64	0	0	3	0
6	G	80	0	0	11	0
6	H	53	0	0	6	0
6	I	102	0	0	8	0
6	J	43	0	0	8	0
6	K	93	0	0	3	0
6	L	53	0	0	3	0
6	M	27	0	0	5	0
6	N	46	0	0	4	0
6	O	40	0	0	5	0
6	P	48	0	0	6	0
6	Q	84	0	0	6	0
6	R	42	0	0	8	0
6	S	64	0	0	7	0
6	T	49	0	0	3	0
6	U	76	0	0	7	0
6	V	44	0	0	9	0
6	W	50	0	0	11	0
6	X	28	0	0	4	0
All	All	48138	0	44744	667	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (667) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:409:ASP:OD2	6:L:738:HOH:O	1.81	0.98
1:A:96:GLU:OE1	6:A:712:HOH:O	1.86	0.92
2:R:444:ARG:O	6:R:723:HOH:O	1.89	0.89
2:V:390:GLU:OE2	6:V:709:HOH:O	1.90	0.89
1:G:11:ALA:O	6:G:712:HOH:O	1.91	0.88
2:B:383:ASN:ND2	6:B:757:HOH:O	2.05	0.88
2:N:324:GLY:N	6:N:733:HOH:O	2.04	0.88
1:G:67:ASP:OD1	6:G:743:HOH:O	1.91	0.87
1:A:318:GLU:OE1	6:A:759:HOH:O	1.91	0.87
2:D:377:ARG:NH2	2:D:426:GLU:OE2	2.09	0.86
1:I:202:TYR:OH	6:I:724:HOH:O	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:437:GLU:OE1	6:H:752:HOH:O	1.94	0.85
1:C:67:ASP:O	6:C:726:HOH:O	1.94	0.84
1:U:318:GLU:HA	6:U:736:HOH:O	1.76	0.84
1:W:1:ASP:N	6:W:713:HOH:O	2.08	0.83
2:X:391:SER:H	2:X:396:ILE:HD11	1.44	0.83
1:Q:179:SER:OG	6:Q:740:HOH:O	1.99	0.81
2:H:353:GLN:OE1	6:H:745:HOH:O	1.98	0.81
1:W:231:GLN:OE1	6:W:725:HOH:O	1.98	0.81
2:B:444:ARG:O	6:B:727:HOH:O	1.98	0.80
2:N:446:ARG:O	6:N:704:HOH:O	2.00	0.80
1:G:305:ARG:O	6:G:706:HOH:O	1.99	0.80
2:V:448:GLN:OE1	6:V:707:HOH:O	2.01	0.79
1:A:194:SER:OG	6:A:792:HOH:O	2.00	0.78
2:L:377:ARG:NH2	2:L:426:GLU:OE2	2.17	0.78
1:G:42:CYS:O	6:G:705:HOH:O	2.00	0.78
1:M:261:GLN:O	6:M:719:HOH:O	2.01	0.78
1:S:100:GLN:OE1	6:S:742:HOH:O	2.01	0.77
2:X:464:TYR:OH	6:X:711:HOH:O	2.03	0.77
1:W:240:HIS:ND1	6:W:709:HOH:O	2.16	0.77
1:C:43:MET:HE3	1:C:46:ARG:HG3	1.67	0.76
1:E:104:GLU:OE2	6:E:725:HOH:O	2.04	0.76
2:X:442:TYR:OH	6:X:710:HOH:O	2.01	0.76
1:E:147:SER:O	6:E:712:HOH:O	2.02	0.75
2:V:391:SER:H	2:V:396:ILE:HD11	1.52	0.75
2:H:377:ARG:NH2	2:H:426:GLU:OE2	2.21	0.74
1:Q:160:THR:HG1	1:Q:237:THR:HG1	1.33	0.74
1:S:183:GLU:OE2	6:S:741:HOH:O	2.06	0.74
2:B:443:GLU:OE2	2:B:446:ARG:NH1	2.21	0.74
1:Q:17:LYS:HE3	1:Q:22:GLU:HG3	1.69	0.74
1:Q:67:ASP:O	6:Q:713:HOH:O	2.05	0.74
2:R:437:GLU:OE1	6:R:719:HOH:O	2.06	0.74
4:c:3:SIA:O10	4:c:3:SIA:O7	2.05	0.74
1:S:203:ARG:NH1	6:S:750:HOH:O	2.20	0.74
1:G:252:LYS:HE3	1:G:254:ILE:HD11	1.69	0.73
1:I:41:LEU:HD13	1:I:264:ALA:HB3	1.71	0.73
1:I:314:ARG:NH1	6:I:753:HOH:O	2.21	0.73
2:J:397:GLU:OE2	6:J:738:HOH:O	2.06	0.72
1:I:304:ARG:NH1	2:J:420:GLU:OE1	2.22	0.72
1:E:252:LYS:HE3	1:E:254:ILE:HD11	1.72	0.71
1:M:84:ILE:O	6:M:721:HOH:O	2.07	0.71
2:V:374:LYS:NZ	2:V:426:GLU:OE1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:601:NAG:O7	6:N:731:HOH:O	2.08	0.71
2:J:394:SER:OG	6:J:740:HOH:O	2.09	0.70
1:E:104:GLU:OE1	6:E:770:HOH:O	2.08	0.70
5:J:601:NAG:O7	6:J:726:HOH:O	2.08	0.70
1:O:121:ILE:HD11	1:O:157:THR:HG21	1.73	0.70
2:D:448:GLN:O	6:D:758:HOH:O	2.10	0.70
1:I:318:GLU:O	6:I:715:HOH:O	2.10	0.70
1:W:305:ARG:NH2	6:W:724:HOH:O	2.24	0.70
1:G:100:GLN:OE1	6:G:720:HOH:O	2.10	0.70
2:F:370:GLN:OE1	6:F:754:HOH:O	2.09	0.69
1:G:46:ARG:HE	1:G:76:THR:HG21	1.55	0.69
2:P:324:GLY:N	6:P:737:HOH:O	2.24	0.69
1:G:53:ASN:OD1	6:G:742:HOH:O	2.11	0.69
1:O:284:ARG:HB3	2:P:379:VAL:HG13	1.75	0.69
2:V:443:GLU:OE1	2:V:446:ARG:NH1	2.25	0.69
2:V:397:GLU:OE2	6:V:705:HOH:O	2.10	0.68
2:B:391:SER:H	2:B:396:ILE:HD11	1.57	0.68
1:Q:43:MET:HE3	1:Q:46:ARG:HG3	1.76	0.68
1:C:305:ARG:O	6:C:703:HOH:O	2.11	0.68
1:M:153:ASN:HA	1:M:189:GLY:HA3	1.75	0.68
1:G:314:ARG:NH1	6:G:756:HOH:O	2.27	0.68
1:S:40:ARG:HD2	1:S:267:ASP:HB2	1.76	0.68
1:S:46:ARG:HE	1:S:76:THR:HG21	1.59	0.68
1:S:304:ARG:NH1	2:T:420:GLU:OE1	2.27	0.68
2:X:443:GLU:OE2	2:X:446:ARG:NH1	2.26	0.68
1:W:137:SER:O	6:W:733:HOH:O	2.13	0.67
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.27	0.67
1:S:185:ASN:OD1	6:S:709:HOH:O	2.13	0.67
1:G:256:ARG:O	6:G:723:HOH:O	2.12	0.67
2:N:377:ARG:NH2	2:N:426:GLU:OE2	2.28	0.67
1:A:43:MET:HE3	1:A:46:ARG:HG3	1.77	0.66
5:D:601:NAG:O7	6:E:770:HOH:O	2.13	0.66
1:W:33:VAL:O	6:W:740:HOH:O	2.12	0.66
1:E:298:CYS:O	6:E:722:HOH:O	2.12	0.66
2:N:443:GLU:OE2	2:N:446:ARG:NH1	2.28	0.66
2:X:377:ARG:NH2	2:X:426:GLU:OE2	2.27	0.66
1:E:286:PRO:O	6:E:767:HOH:O	2.12	0.66
2:V:392:GLU:OE1	6:V:701:HOH:O	2.14	0.66
1:E:212:ALA:O	6:E:721:HOH:O	2.13	0.65
2:P:350:GLN:HG2	2:P:355:THR:HG22	1.76	0.65
1:E:110:LYS:NZ	1:E:141:GLU:OE2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASP:OD1	6:C:729:HOH:O	2.11	0.65
1:K:193:ILE:HG22	1:K:208:PRO:HD2	1.77	0.65
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.29	0.65
1:M:195:ILE:HG12	1:M:244:LEU:HB2	1.78	0.65
2:N:391:SER:H	2:N:396:ILE:HD11	1.62	0.65
1:I:261:GLN:O	6:I:770:HOH:O	2.14	0.65
2:T:350:GLN:HG3	2:T:355:THR:HG22	1.79	0.65
1:U:212:ALA:O	6:U:728:HOH:O	2.14	0.65
2:D:338:GLU:OE2	6:D:779:HOH:O	2.14	0.65
2:B:450:ARG:HG3	2:B:451:GLN:H	1.62	0.64
2:V:412:THR:O	2:V:416:THR:HG23	1.96	0.64
2:R:431:ILE:O	6:R:714:HOH:O	2.15	0.64
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.31	0.64
1:M:66:CYS:SG	6:M:721:HOH:O	2.55	0.64
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.64
2:V:348:ARG:NH1	6:V:735:HOH:O	2.29	0.64
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.31	0.64
1:A:252:LYS:HE3	1:A:254:ILE:HD11	1.80	0.63
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.80	0.63
2:V:494:LEU:HB3	2:V:496:ILE:HG12	1.78	0.63
2:N:470:SER:O	6:N:722:HOH:O	2.16	0.63
1:Q:96:GLU:OE1	6:Q:742:HOH:O	2.15	0.63
2:B:381:LYS:NZ	2:B:382:THR:O	2.32	0.63
2:D:420:GLU:HG3	6:D:728:HOH:O	1.99	0.63
1:W:101:LYS:O	6:W:735:HOH:O	2.15	0.63
1:U:41:LEU:HD13	1:U:264:ALA:HB3	1.80	0.62
1:E:283:THR:HG22	1:E:285:LEU:H	1.64	0.62
2:R:377:ARG:NH2	2:R:426:GLU:OE2	2.33	0.62
1:G:196:SER:OG	6:G:745:HOH:O	2.16	0.62
2:J:412:THR:O	2:J:416:THR:HG23	2.00	0.62
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.32	0.62
2:D:412:THR:O	2:D:416:THR:HG23	2.01	0.61
1:I:43:MET:HE3	1:I:46:ARG:HG3	1.82	0.61
2:F:412:THR:O	2:F:416:THR:HG23	2.01	0.61
1:U:28:ASN:ND2	6:U:761:HOH:O	2.32	0.61
1:G:43:MET:HE2	1:G:48:HIS:HB3	1.82	0.61
2:H:418:GLN:HG2	2:L:417:TYR:CE1	2.36	0.61
1:O:125:GLY:HA3	1:O:144:TRP:HB3	1.83	0.61
2:D:408:LYS:NZ	6:D:716:HOH:O	2.04	0.61
1:E:43:MET:HE3	1:E:46:ARG:HG3	1.82	0.61
2:F:418:GLN:NE2	6:F:734:HOH:O	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:443:GLU:OE1	2:P:446:ARG:NH1	2.33	0.60
1:A:41:LEU:HD23	1:A:78:ILE:HD13	1.82	0.60
2:R:452:ASN:OD1	6:R:707:HOH:O	2.16	0.60
1:E:34:GLU:HB2	1:E:283:THR:HG21	1.84	0.60
2:J:387:GLU:HB2	6:J:728:HOH:O	2.01	0.60
1:U:304:ARG:NH1	2:V:420:GLU:OE1	2.34	0.60
1:O:117:TYR:HB3	1:O:121:ILE:HD12	1.84	0.60
2:L:442:TYR:OH	2:L:455:GLU:OE2	2.18	0.60
1:A:46:ARG:HE	1:A:76:THR:HG21	1.66	0.60
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.34	0.60
1:C:41:LEU:HD23	1:C:78:ILE:HD13	1.82	0.60
1:U:8:HIS:HD2	6:V:731:HOH:O	1.84	0.60
1:O:304:ARG:NH1	2:P:420:GLU:OE1	2.34	0.59
1:I:1:ASP:N	6:I:729:HOH:O	2.32	0.59
1:S:256:ARG:NH2	2:T:387:GLU:OE1	2.36	0.59
1:A:172:MET:HG2	1:A:227:TRP:HB3	1.84	0.59
2:R:469:ASP:OD1	6:R:718:HOH:O	2.17	0.59
2:N:455:GLU:OE1	2:P:446:ARG:NH2	2.36	0.59
1:Q:41:LEU:HD13	1:Q:264:ALA:HB3	1.85	0.59
1:O:55:HIS:HB3	1:O:85:ALA:HB2	1.84	0.59
2:N:412:THR:O	2:N:416:THR:HG23	2.03	0.59
2:T:412:THR:O	2:T:416:THR:HG22	2.02	0.59
2:J:349:HIS:HE1	6:J:729:HOH:O	1.85	0.58
1:Q:86:TYR:OH	6:Q:726:HOH:O	2.10	0.58
1:S:165:ASP:OD1	1:S:166:THR:N	2.36	0.58
1:A:43:MET:HE2	1:A:48:HIS:HB3	1.85	0.58
1:M:303:ASN:H	2:N:416:THR:HG22	1.69	0.58
1:C:96:GLU:OE2	1:C:99:ARG:NH2	2.35	0.58
2:X:442:TYR:OH	2:X:455:GLU:OE2	2.20	0.58
1:K:234:ASP:HA	5:K:601:NAG:H82	1.84	0.58
1:M:303:ASN:H	2:N:416:THR:CG2	2.17	0.58
1:M:304:ARG:NH2	6:M:702:HOH:O	2.37	0.58
2:R:412:THR:O	2:R:416:THR:HG23	2.04	0.58
1:U:303:ASN:H	2:V:416:THR:CG2	2.16	0.58
1:W:304:ARG:NH1	2:X:420:GLU:OE1	2.37	0.58
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.85	0.57
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.03	0.57
1:S:8:HIS:HE1	6:S:701:HOH:O	1.87	0.57
1:C:304:ARG:NH1	2:D:420:GLU:OE1	2.37	0.57
2:F:377:ARG:NH2	2:F:426:GLU:OE2	2.36	0.57
1:M:304:ARG:NH1	2:N:420:GLU:OE1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE1	1:A:249:ARG:HD3	2.04	0.57
2:R:353:GLN:H	2:R:353:GLN:HE21	1.52	0.57
1:W:28:ASN:ND2	6:W:708:HOH:O	2.22	0.57
2:L:456:ASP:HB3	2:L:458:LYS:H	1.70	0.57
2:D:383:ASN:OD1	2:D:383:ASN:N	2.38	0.57
1:C:303:ASN:H	2:D:416:THR:CG2	2.18	0.57
2:L:482:HIS:ND1	6:L:716:HOH:O	2.13	0.57
1:O:38:ILE:HG22	1:O:40:ARG:H	1.70	0.57
1:C:318:GLU:OE1	6:C:728:HOH:O	2.16	0.56
1:M:50:ASP:HB2	1:M:266:ILE:HD11	1.86	0.56
2:H:456:ASP:HB3	2:H:458:LYS:H	1.69	0.56
1:O:46:ARG:NH2	6:O:733:HOH:O	2.38	0.56
1:O:154:PHE:O	1:O:191:GLN:NE2	2.38	0.56
1:W:34:GLU:HB2	1:W:283:THR:HG21	1.87	0.56
1:O:41:LEU:HD23	1:O:78:ILE:HD13	1.87	0.56
2:X:412:THR:O	2:X:416:THR:HG23	2.06	0.56
2:B:412:THR:O	2:B:416:THR:HG23	2.05	0.56
2:D:455:GLU:OE1	2:F:446:ARG:NH2	2.38	0.56
1:Q:256:ARG:NH2	2:R:387:GLU:OE1	2.39	0.56
1:K:33:VAL:O	6:K:709:HOH:O	2.18	0.56
1:G:144:TRP:CH2	4:a:3:SIA:H91	2.41	0.56
1:G:43:MET:HE3	1:G:46:ARG:HG3	1.88	0.56
1:I:49:LYS:NZ	6:I:732:HOH:O	2.38	0.55
1:E:259:GLY:O	6:E:745:HOH:O	2.18	0.55
2:J:399:GLN:OE1	6:J:732:HOH:O	2.17	0.55
1:O:165:ASP:OD1	1:O:166:THR:N	2.36	0.55
2:D:377:ARG:NH1	6:D:738:HOH:O	2.39	0.55
2:P:383:ASN:HA	2:P:384:THR:HB	1.88	0.55
2:D:387:GLU:HB2	6:D:706:HOH:O	2.05	0.55
1:U:303:ASN:H	2:V:416:THR:HG22	1.72	0.55
2:D:324:GLY:N	6:D:709:HOH:O	2.40	0.55
1:S:119:SER:N	6:S:720:HOH:O	2.40	0.55
1:A:41:LEU:HD13	1:A:264:ALA:HB3	1.87	0.55
2:D:381:LYS:HG3	2:D:383:ASN:OD1	2.07	0.55
2:D:448:GLN:OE1	6:D:739:HOH:O	2.18	0.55
2:H:450:ARG:HG3	2:H:451:GLN:H	1.72	0.55
2:H:455:GLU:O	6:H:705:HOH:O	2.17	0.55
2:V:414:ILE:HD13	2:X:414:ILE:HG21	1.89	0.55
1:I:244:LEU:HD13	1:I:246:ALA:HB2	1.89	0.55
1:K:43:MET:HE3	1:K:46:ARG:HG3	1.89	0.55
2:X:488:GLU:O	2:X:492:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:162:ARG:NH2	5:O:601:NAG:O6	2.40	0.54
2:P:374:LYS:NZ	2:P:426:GLU:OE1	2.39	0.54
2:P:412:THR:O	2:P:416:THR:HG23	2.05	0.54
1:I:284:ARG:HB3	2:J:379:VAL:HG22	1.89	0.54
1:O:132:ARG:NH1	1:O:138:PHE:O	2.39	0.54
2:P:496:ILE:HD12	2:P:497:ASN:HB2	1.89	0.54
1:S:59:MET:HE2	1:S:108:ILE:HD12	1.89	0.54
1:S:161:TYR:HH	1:S:169:HIS:HD1	1.56	0.54
2:T:377:ARG:NH2	2:T:426:GLU:OE2	2.41	0.54
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.40	0.54
1:I:89:PRO:HB3	1:I:216:VAL:HB	1.89	0.54
1:O:161:TYR:OH	1:O:169:HIS:ND1	2.37	0.54
2:J:473:GLU:O	2:J:477:ASN:HB2	2.08	0.54
1:Q:193:ILE:HG22	1:Q:208:PRO:HD2	1.87	0.54
2:R:450:ARG:HG3	2:R:451:GLN:H	1.73	0.54
1:U:89:PRO:HB3	1:U:216:VAL:HB	1.89	0.54
1:A:47:LYS:NZ	6:A:804:HOH:O	2.41	0.54
1:S:161:TYR:OH	1:S:169:HIS:ND1	2.41	0.54
1:U:162:ARG:NH2	5:U:601:NAG:O6	2.41	0.54
1:A:74:TRP:HH2	1:A:108:ILE:HG13	1.73	0.54
1:A:155:PRO:O	1:A:157:THR:HG22	2.08	0.54
1:Q:41:LEU:HD23	1:Q:78:ILE:HD13	1.90	0.54
2:V:329:ILE:O	6:V:714:HOH:O	2.17	0.54
1:A:284:ARG:HB3	2:B:379:VAL:HG22	1.91	0.53
1:E:121:ILE:HD11	1:E:157:THR:HG21	1.90	0.53
1:E:165:ASP:OD1	1:E:166:THR:N	2.37	0.53
1:Q:79:GLU:OE2	6:Q:730:HOH:O	2.17	0.53
1:U:193:ILE:HG22	1:U:208:PRO:HD2	1.90	0.53
1:M:141:GLU:OE1	1:M:249:ARG:HD3	2.08	0.53
1:I:202:TYR:CD2	1:I:228:THR:HG21	2.43	0.53
1:I:303:ASN:H	2:J:416:THR:HG21	1.73	0.53
1:C:204:ASN:OD1	1:C:205:ASN:N	2.38	0.53
1:A:49:LYS:NZ	6:A:740:HOH:O	2.40	0.53
1:E:302:VAL:HA	2:F:416:THR:HG22	1.91	0.53
1:K:303:ASN:H	2:L:416:THR:HG22	1.73	0.53
1:O:90:GLY:O	6:O:709:HOH:O	2.18	0.53
1:C:43:MET:HE2	1:C:48:HIS:HB3	1.89	0.53
1:U:195:ILE:HG12	1:U:244:LEU:HB2	1.91	0.53
2:J:420:GLU:HG3	6:J:720:HOH:O	2.08	0.53
2:J:494:LEU:HD22	2:L:494:LEU:HD11	1.90	0.53
1:U:49:LYS:HD2	1:U:69:HIS:ND1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:MET:HE2	1:I:48:HIS:HB3	1.91	0.53
1:O:52:GLY:O	6:O:712:HOH:O	2.19	0.53
2:V:473:GLU:O	2:V:477:ASN:HB2	2.09	0.53
1:C:49:LYS:HD2	1:C:69:HIS:ND1	2.25	0.52
2:P:421:LEU:HD11	2:R:425:MET:HE1	1.89	0.52
1:U:20:THR:O	2:X:373:GLY:HA3	2.09	0.52
1:C:75:ASP:OD2	1:C:76:THR:HG22	2.09	0.52
2:R:349:HIS:HB2	2:R:472:MET:HE3	1.91	0.52
2:L:467:CYS:HB3	2:L:472:MET:HE2	1.90	0.52
1:U:43:MET:HE3	1:U:46:ARG:HG3	1.90	0.52
1:E:234:ASP:HA	5:E:601:NAG:H82	1.92	0.52
1:S:38:ILE:O	1:S:40:ARG:N	2.43	0.52
2:T:324:GLY:N	6:T:701:HOH:O	2.42	0.52
1:W:41:LEU:HD13	1:W:264:ALA:HB3	1.92	0.52
1:S:49:LYS:HD2	1:S:69:HIS:ND1	2.25	0.52
1:C:249:ARG:O	6:C:757:HOH:O	2.19	0.52
1:O:20:THR:HG22	2:R:374:LYS:HG3	1.92	0.52
1:W:59:MET:HE2	1:W:108:ILE:HD12	1.92	0.51
1:W:111:ILE:HG23	1:W:250:VAL:HG12	1.91	0.51
4:b:3:SIA:O10	4:b:3:SIA:O7	2.17	0.51
2:V:349:HIS:HB2	2:V:472:MET:HE3	1.91	0.51
1:W:141:GLU:OE1	1:W:249:ARG:HD3	2.10	0.51
2:F:443:GLU:OE2	2:F:446:ARG:NH1	2.44	0.51
1:I:25:GLU:HG2	1:I:315:ASN:HB3	1.91	0.51
1:O:317:PRO:O	1:O:318:GLU:HB2	2.10	0.51
1:C:303:ASN:H	2:D:416:THR:HG22	1.75	0.51
1:Q:87:CYS:O	1:Q:217:ASN:ND2	2.38	0.51
1:C:184:LYS:HE3	1:C:193:ILE:HD11	1.93	0.51
1:G:49:LYS:HD2	1:G:69:HIS:ND1	2.26	0.51
1:E:128:ARG:HG2	4:Z:3:SIA:O1A	2.10	0.51
1:G:144:TRP:HH2	4:a:3:SIA:H91	1.76	0.51
2:N:381:LYS:NZ	2:N:382:THR:O	2.44	0.51
1:U:59:MET:HE2	1:U:108:ILE:HD12	1.91	0.51
2:B:425:MET:HE1	2:F:421:LEU:HD11	1.93	0.51
1:K:75:ASP:OD2	1:K:76:THR:HG22	2.11	0.50
2:N:450:ARG:HB3	6:R:704:HOH:O	2.11	0.50
2:R:329:ILE:O	6:R:701:HOH:O	2.19	0.50
2:V:355:THR:O	6:V:722:HOH:O	2.19	0.50
1:I:46:ARG:NH2	6:I:739:HOH:O	2.45	0.50
1:M:41:LEU:HD23	1:M:78:ILE:HD13	1.94	0.50
2:X:377:ARG:NH1	6:X:707:HOH:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:TRP:CH2	4:a:3:SIA:H7	2.46	0.50
1:G:178:PRO:HB2	1:G:210:VAL:HG22	1.94	0.50
1:K:303:ASN:H	2:L:416:THR:CG2	2.24	0.50
1:M:89:PRO:HB3	1:M:216:VAL:HB	1.92	0.50
1:Q:244:LEU:HD13	1:Q:246:ALA:HB2	1.92	0.50
1:W:46:ARG:NH2	6:W:739:HOH:O	2.44	0.50
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.93	0.50
1:A:203:ARG:NH2	1:E:224:ASP:OD2	2.43	0.50
1:C:49:LYS:HD2	1:C:69:HIS:HD1	1.76	0.50
2:H:446:ARG:HH12	2:H:447:LYS:HE3	1.77	0.50
4:b:3:SIA:O1B	4:b:3:SIA:H6	2.12	0.50
2:R:391:SER:H	2:R:396:ILE:HD11	1.76	0.50
1:I:224:ASP:HB2	6:I:718:HOH:O	2.11	0.50
1:U:284:ARG:HB3	2:V:379:VAL:HG22	1.94	0.50
1:U:200:SER:OG	1:U:234:ASP:OD1	2.25	0.50
1:W:75:ASP:OD2	1:W:76:THR:HG22	2.12	0.50
1:W:284:ARG:HB3	2:X:379:VAL:HG22	1.94	0.49
1:W:138:PHE:HA	6:W:733:HOH:O	2.12	0.49
2:D:418:GLN:HB3	6:D:764:HOH:O	2.12	0.49
2:R:342:ASP:OD1	2:R:342:ASP:N	2.44	0.49
1:A:303:ASN:H	2:B:416:THR:CG2	2.26	0.49
2:L:451:GLN:O	2:L:493:ARG:NH1	2.40	0.49
1:S:43:MET:HE3	1:S:46:ARG:HG3	1.94	0.49
2:T:325:LEU:HD13	2:V:326:PHE:HZ	1.78	0.49
1:O:303:ASN:H	2:P:416:THR:CG2	2.26	0.49
2:H:324:GLY:N	6:H:701:HOH:O	2.46	0.49
2:V:494:LEU:HD22	2:X:494:LEU:HD11	1.95	0.49
1:W:43:MET:HE3	1:W:46:ARG:HG3	1.95	0.49
1:C:18:THR:HG1	1:C:21:ASN:H	1.60	0.49
1:K:126:THR:HG23	6:K:712:HOH:O	2.11	0.49
1:W:88:TYR:HD1	1:W:127:THR:HG21	1.78	0.49
1:K:89:PRO:HB3	1:K:216:VAL:HB	1.93	0.49
2:T:377:ARG:NH1	6:T:730:HOH:O	2.32	0.49
2:T:383:ASN:ND2	2:T:383:ASN:O	2.45	0.49
1:I:46:ARG:HE	1:I:76:THR:HG21	1.77	0.48
1:I:302:VAL:HA	2:J:416:THR:HG22	1.93	0.48
1:K:43:MET:HE2	1:K:48:HIS:HB3	1.95	0.48
2:L:456:ASP:HB2	2:L:460:CYS:O	2.12	0.48
1:Q:303:ASN:H	2:R:416:THR:CG2	2.25	0.48
1:S:108:ILE:HG12	1:S:253:LEU:HD23	1.94	0.48
1:U:108:ILE:HG12	1:U:253:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:GLU:OE1	1:G:249:ARG:HD3	2.14	0.48
1:M:175:ILE:HD12	1:M:195:ILE:HD13	1.96	0.48
1:U:244:LEU:HD13	1:U:246:ALA:HB2	1.95	0.48
2:F:381:LYS:NZ	2:F:382:THR:O	2.35	0.48
1:G:67:ASP:CG	6:G:743:HOH:O	2.50	0.48
1:M:17:LYS:HE2	1:M:22:GLU:HG3	1.96	0.48
1:C:34:GLU:HB2	1:C:283:THR:HG21	1.95	0.48
1:O:314:ARG:NH1	6:O:716:HOH:O	2.22	0.48
2:R:495:ASN:O	2:R:495:ASN:ND2	2.47	0.48
2:T:418:GLN:HG2	2:X:417:TYR:CE1	2.49	0.48
1:U:128:ARG:HE	1:U:128:ARG:HB2	1.43	0.48
4:Z:3:SIA:O1B	4:Z:3:SIA:H6	2.13	0.48
1:I:172:MET:HG2	1:I:227:TRP:HB3	1.95	0.48
1:U:310:ALA:O	6:U:714:HOH:O	2.20	0.48
4:Z:3:SIA:O10	4:Z:3:SIA:O7	2.32	0.48
2:J:469:ASP:O	2:J:473:GLU:HB2	2.13	0.48
1:Q:28:ASN:ND2	6:Q:708:HOH:O	2.47	0.48
2:V:453:ALA:O	6:V:730:HOH:O	2.20	0.48
1:W:17:LYS:HE3	1:W:22:GLU:HG3	1.96	0.48
2:H:326:PHE:HZ	2:L:325:LEU:HD13	1.79	0.47
2:L:456:ASP:CG	2:L:460:CYS:HB2	2.39	0.47
2:P:387:GLU:N	6:P:713:HOH:O	2.15	0.47
1:Q:141:GLU:OE1	1:Q:249:ARG:HD3	2.13	0.47
1:U:1:ASP:HA	2:V:350:GLN:O	2.14	0.47
1:U:141:GLU:OE1	1:U:249:ARG:HD3	2.13	0.47
1:W:41:LEU:HD23	1:W:78:ILE:HD13	1.95	0.47
2:X:450:ARG:HG3	2:X:451:GLN:H	1.79	0.47
2:B:344:TRP:HH2	2:B:371:ILE:HD12	1.78	0.47
2:H:418:GLN:HG2	2:L:417:TYR:HE1	1.77	0.47
1:W:172:MET:HG2	1:W:227:TRP:HB3	1.96	0.47
1:A:244:LEU:HD13	1:A:246:ALA:HB2	1.97	0.47
1:K:101:LYS:HE3	1:K:229:LEU:HD11	1.96	0.47
1:O:98:LEU:HD13	1:O:227:TRP:CD2	2.50	0.47
2:R:374:LYS:NZ	2:R:426:GLU:O	2.48	0.47
1:S:155:PRO:O	1:S:157:THR:HG22	2.13	0.47
1:W:14:THR:HG21	1:W:29:ALA:HB3	1.96	0.47
1:A:303:ASN:H	2:B:416:THR:HG21	1.80	0.47
1:E:41:LEU:HD13	1:E:264:ALA:HB3	1.97	0.47
1:I:303:ASN:H	2:J:416:THR:CG2	2.27	0.47
1:U:318:GLU:OE2	6:U:736:HOH:O	2.21	0.47
1:E:153:ASN:HA	1:E:189:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:ASP:OD1	1:E:235:ASN:N	2.47	0.47
2:F:446:ARG:HH12	2:F:447:LYS:HE3	1.79	0.47
1:G:193:ILE:HG22	1:G:208:PRO:HD2	1.97	0.47
2:H:425:MET:HE1	2:L:421:LEU:HD11	1.96	0.47
1:O:41:LEU:HD13	1:O:264:ALA:HB3	1.96	0.47
1:Q:199:SER:HG	1:Q:202:TYR:H	1.62	0.47
1:S:17:LYS:NZ	2:T:420:GLU:OE2	2.39	0.47
2:B:446:ARG:NH2	2:F:455:GLU:OE1	2.48	0.47
1:E:125:GLY:HA3	1:E:144:TRP:HB3	1.96	0.47
2:L:377:ARG:O	2:L:380:GLU:HG2	2.15	0.47
1:Q:43:MET:HE2	1:Q:48:HIS:CB	2.45	0.47
1:I:49:LYS:HD2	1:I:69:HIS:ND1	2.30	0.47
1:O:40:ARG:NE	1:O:267:ASP:OD2	2.48	0.47
1:W:122:ASN:HB3	1:W:146:VAL:HG12	1.95	0.47
1:G:284:ARG:HB3	2:H:379:VAL:HG13	1.97	0.47
2:R:391:SER:O	6:R:737:HOH:O	2.20	0.47
2:F:342:ASP:HB3	2:F:359:ALA:HB2	1.97	0.46
2:N:408:LYS:HG2	2:R:406:TRP:CH2	2.50	0.46
1:Q:146:VAL:HG22	1:Q:187:LEU:HB3	1.96	0.46
2:J:425:MET:HE2	2:L:425:MET:HE2	1.96	0.46
2:L:446:ARG:HD2	2:L:455:GLU:OE1	2.14	0.46
1:M:40:ARG:NE	1:M:267:ASP:OD2	2.45	0.46
2:V:408:LYS:O	2:V:412:THR:HG23	2.15	0.46
1:E:303:ASN:H	2:F:416:THR:HG21	1.80	0.46
2:F:391:SER:H	2:F:396:ILE:HD11	1.81	0.46
2:H:329:ILE:O	6:H:701:HOH:O	2.21	0.46
2:H:412:THR:O	2:H:416:THR:HG23	2.15	0.46
2:B:406:TRP:CZ2	2:D:408:LYS:HE2	2.51	0.46
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.16	0.46
1:A:193:ILE:HG21	1:A:208:PRO:HG2	1.95	0.46
1:K:59:MET:HE2	1:K:108:ILE:HD12	1.97	0.46
1:K:162:ARG:HG3	1:K:235:ASN:OD1	2.15	0.46
1:Q:34:GLU:OE2	1:Q:36:THR:N	2.33	0.46
1:W:146:VAL:HG22	1:W:187:LEU:HB3	1.96	0.46
1:W:153:ASN:HA	1:W:189:GLY:HA3	1.98	0.46
1:A:128:ARG:NH1	1:U:133:ASN:O	2.49	0.46
1:I:175:ILE:HD12	1:I:195:ILE:HD13	1.97	0.46
1:Q:108:ILE:HG12	1:Q:253:LEU:HD23	1.97	0.46
1:Q:296:GLY:HA2	2:R:385:GLU:HG3	1.97	0.46
1:E:303:ASN:H	2:F:416:THR:CG2	2.29	0.46
1:G:41:LEU:HD13	1:G:264:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:SER:OG	1:K:205:ASN:ND2	2.46	0.46
2:T:456:ASP:HB2	2:T:460:CYS:O	2.15	0.46
2:D:383:ASN:HA	2:D:384:THR:HB	1.98	0.46
1:M:202:TYR:CD2	1:M:228:THR:HG21	2.51	0.46
2:X:448:GLN:NE2	2:X:478:ASN:HA	2.30	0.46
2:T:400:ILE:HD12	2:T:400:ILE:HA	1.87	0.46
1:C:60:LEU:HD11	1:C:102:ILE:HD11	1.97	0.45
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.98	0.45
1:C:317:PRO:O	1:C:318:GLU:HB2	2.16	0.45
2:N:448:GLN:OE1	2:N:478:ASN:HA	2.15	0.45
2:N:478:ASN:ND2	2:N:478:ASN:O	2.49	0.45
1:E:162:ARG:HE	1:E:162:ARG:HB2	1.59	0.45
1:G:303:ASN:H	2:H:416:THR:HG21	1.81	0.45
1:O:303:ASN:H	2:P:416:THR:HG21	1.81	0.45
2:T:446:ARG:NH2	2:X:455:GLU:OE1	2.49	0.45
1:M:289:ASN:HD22	1:M:305:ARG:HA	1.81	0.45
2:P:446:ARG:HH12	2:P:447:LYS:HE3	1.80	0.45
1:Q:155:PRO:O	1:Q:157:THR:HG22	2.17	0.45
2:T:456:ASP:HB3	2:T:458:LYS:H	1.81	0.45
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.99	0.45
1:A:74:TRP:CH2	1:A:108:ILE:HG13	2.50	0.45
2:P:450:ARG:HB3	6:P:710:HOH:O	2.15	0.45
1:S:55:HIS:HB3	1:S:85:ALA:HB2	1.98	0.45
1:C:202:TYR:CD2	1:C:228:THR:HG21	2.52	0.45
2:P:467:CYS:HB3	2:P:472:MET:HE2	1.98	0.45
1:Q:302:VAL:HA	2:R:416:THR:HG22	1.98	0.45
1:S:8:HIS:CE1	6:S:701:HOH:O	2.67	0.45
1:W:288:GLN:HG3	1:W:299:PRO:HB2	1.99	0.45
1:A:43:MET:HE2	1:A:48:HIS:CB	2.47	0.45
2:D:383:ASN:HA	2:D:384:THR:CB	2.46	0.45
2:H:342:ASP:HB3	2:H:359:ALA:HB2	1.98	0.45
1:Q:34:GLU:OE2	1:Q:35:SER:N	2.49	0.45
1:E:219:GLN:NE2	4:Z:3:SIA:C1	2.79	0.45
1:U:104:GLU:OE1	6:U:757:HOH:O	2.21	0.45
1:W:89:PRO:HB3	1:W:216:VAL:HB	1.99	0.45
1:W:162:ARG:HG3	1:W:235:ASN:CG	2.41	0.45
1:A:165:ASP:OD1	1:A:166:THR:N	2.44	0.45
1:G:209:VAL:HG21	1:I:205:ASN:ND2	2.32	0.45
1:M:8:HIS:HE1	6:M:707:HOH:O	2.00	0.45
1:A:256:ARG:NE	6:A:776:HOH:O	2.47	0.45
1:E:300:LYS:HG3	2:F:415:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:383:ASN:O	2:H:383:ASN:ND2	2.50	0.45
1:I:193:ILE:HG21	1:I:208:PRO:HG2	1.98	0.45
1:Q:80:ARG:NH1	1:Q:262:SER:O	2.43	0.45
1:G:183:GLU:OE2	4:a:3:SIA:O9	2.32	0.44
2:V:487:GLU:H	2:V:487:GLU:CD	2.25	0.44
1:A:61:ILE:O	1:A:139:TYR:HB3	2.18	0.44
1:E:202:TYR:CD2	1:E:228:THR:HG21	2.52	0.44
1:I:144:TRP:CH2	4:b:3:SIA:H7	2.52	0.44
1:W:17:LYS:NZ	2:X:420:GLU:OE2	2.39	0.44
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.17	0.44
1:Q:162:ARG:HG3	1:Q:235:ASN:OD1	2.17	0.44
2:B:373:GLY:HA3	1:E:20:THR:O	2.18	0.44
1:C:142:LEU:HB3	1:C:245:ILE:HG22	2.00	0.44
1:O:20:THR:O	2:R:373:GLY:HA3	2.17	0.44
1:O:49:LYS:HD2	1:O:69:HIS:ND1	2.32	0.44
1:U:209:VAL:HG21	1:W:205:ASN:CG	2.42	0.44
1:U:121:ILE:HD11	1:U:157:THR:HG21	1.99	0.44
1:A:148:LYS:NZ	6:A:763:HOH:O	2.47	0.44
1:Q:150:LYS:HE3	1:Q:186:ASP:CG	2.42	0.44
2:R:361:TYR:CZ	2:R:365:GLN:HG3	2.53	0.44
2:F:367:ALA:O	2:F:371:ILE:HG12	2.18	0.44
2:H:377:ARG:O	2:H:380:GLU:HG2	2.18	0.44
2:T:391:SER:H	2:T:396:ILE:HD11	1.82	0.44
2:B:473:GLU:O	2:B:477:ASN:HB2	2.18	0.44
2:D:456:ASP:CG	2:D:460:CYS:HB2	2.43	0.44
1:G:8:HIS:CE1	1:G:313:MET:HE3	2.52	0.44
1:G:175:ILE:HD12	1:G:195:ILE:HD13	1.98	0.44
1:C:155:PRO:O	1:C:157:THR:HG22	2.16	0.44
1:E:52:GLY:O	6:E:704:HOH:O	2.21	0.44
2:F:448:GLN:NE2	6:F:730:HOH:O	2.47	0.44
1:W:155:PRO:O	1:W:157:THR:HG22	2.18	0.44
1:I:121:ILE:HD11	1:I:157:THR:HG21	2.00	0.43
1:K:142:LEU:HD23	1:K:247:PRO:HA	2.00	0.43
2:P:432:ASP:OD1	6:P:729:HOH:O	2.21	0.43
1:U:46:ARG:HE	1:U:76:THR:HG21	1.83	0.43
1:S:170:LEU:HD22	1:S:229:LEU:HD21	2.01	0.43
1:A:9:ALA:HB2	2:B:336:GLY:HA3	2.00	0.43
1:A:20:THR:O	2:D:373:GLY:HA3	2.18	0.43
1:E:176:HIS:O	1:E:208:PRO:HB3	2.18	0.43
2:H:327:GLY:O	2:H:331:GLY:HA3	2.18	0.43
1:M:203:ARG:O	1:M:203:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:167:ALA:HB3	1:O:252:LYS:HE3	2.00	0.43
1:S:38:ILE:C	1:S:40:ARG:H	2.26	0.43
1:S:46:ARG:HB2	1:S:75:ASP:OD2	2.19	0.43
2:D:494:LEU:C	2:D:496:ILE:H	2.26	0.43
1:S:300:LYS:HG3	2:T:415:TRP:CE2	2.53	0.43
1:A:213:ARG:HD2	1:A:222:ARG:HG2	2.00	0.43
2:D:342:ASP:HB3	2:D:359:ALA:HB2	2.00	0.43
1:G:314:ARG:HG3	2:H:431:ILE:HG23	2.01	0.43
2:H:450:ARG:HB3	6:H:721:HOH:O	2.18	0.43
1:M:49:LYS:HD2	1:M:69:HIS:ND1	2.34	0.43
1:O:59:MET:HE2	1:O:108:ILE:HD12	2.00	0.43
1:U:8:HIS:CE1	1:U:313:MET:HE3	2.54	0.43
1:A:317:PRO:O	1:A:318:GLU:HB2	2.18	0.43
1:U:264:ALA:HA	1:U:265:PRO:HD3	1.91	0.43
1:W:165:ASP:OD1	1:W:166:THR:N	2.43	0.43
1:O:44:LYS:HD2	1:O:269:ASN:O	2.18	0.43
1:Q:252:LYS:HE3	1:Q:254:ILE:HD11	1.99	0.43
1:Q:46:ARG:HE	1:Q:76:THR:HG21	1.84	0.43
1:Q:174:GLY:O	1:Q:175:ILE:HD13	2.18	0.43
4:a:3:SIA:O10	4:a:3:SIA:O7	2.24	0.43
1:A:42:CYS:HB3	1:A:270:CYS:O	2.19	0.43
1:S:43:MET:HE2	1:S:48:HIS:HB3	2.00	0.43
1:S:101:LYS:HE3	1:S:229:LEU:HD11	2.01	0.43
1:U:34:GLU:HB2	1:U:283:THR:HG21	2.01	0.43
2:D:414:ILE:O	2:D:418:GLN:HG3	2.19	0.43
1:S:110:LYS:HB2	1:S:249:ARG:HH21	1.83	0.43
1:S:160:THR:HG22	1:S:162:ARG:HD2	2.00	0.42
1:W:41:LEU:O	1:W:43:MET:HG2	2.19	0.42
1:G:302:VAL:HA	2:H:416:THR:HG22	2.01	0.42
1:K:197:VAL:O	1:K:203:ARG:HA	2.19	0.42
1:S:47:LYS:HE2	1:S:47:LYS:HB3	1.86	0.42
1:U:144:TRP:HH2	4:c:3:SIA:H91	1.84	0.42
1:G:34:GLU:HB2	1:G:283:THR:HG21	2.00	0.42
2:T:457:GLY:N	6:T:725:HOH:O	2.38	0.42
1:O:300:LYS:HA	1:O:300:LYS:HD3	1.83	0.42
5:T:601:NAG:O7	6:U:757:HOH:O	2.21	0.42
2:X:429:HIS:NE2	6:X:721:HOH:O	2.05	0.42
1:G:101:LYS:O	6:G:764:HOH:O	2.21	0.42
1:G:126:THR:HG23	1:G:136:ASN:HB3	2.01	0.42
2:T:361:TYR:CZ	2:T:365:GLN:HG3	2.54	0.42
1:U:144:TRP:CH2	4:c:3:SIA:H7	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:303:ASN:H	2:X:416:THR:CG2	2.32	0.42
1:A:48:HIS:CD2	1:A:266:ILE:HD13	2.55	0.42
1:G:193:ILE:HG21	1:G:208:PRO:HG2	2.00	0.42
1:I:74:TRP:CH2	1:I:108:ILE:HG13	2.55	0.42
2:J:381:LYS:HD2	2:J:381:LYS:HA	1.83	0.42
1:K:165:ASP:OD1	1:K:166:THR:N	2.42	0.42
1:O:313:MET:HG3	1:O:314:ARG:O	2.20	0.42
1:C:284:ARG:HB3	2:D:379:VAL:HG22	2.02	0.42
1:O:175:ILE:HD12	1:O:195:ILE:HD13	2.01	0.42
1:U:38:ILE:C	1:U:40:ARG:H	2.27	0.42
2:X:438:MET:HE3	2:X:438:MET:HA	2.02	0.42
1:A:200:SER:OG	1:A:234:ASP:OD1	2.29	0.42
1:C:51:LEU:HB3	1:C:54:CYS:O	2.20	0.42
1:G:46:ARG:HB2	1:G:75:ASP:OD2	2.19	0.42
2:H:400:ILE:HD12	2:H:400:ILE:HA	1.89	0.42
1:K:41:LEU:HD13	1:K:264:ALA:HB3	2.02	0.42
1:M:96:GLU:OE2	1:M:99:ARG:NH2	2.37	0.42
1:O:75:ASP:OD2	1:O:76:THR:HG22	2.20	0.42
1:Q:276:TRP:HB2	1:Q:293:ARG:O	2.19	0.42
2:B:422:LEU:O	2:B:426:GLU:HG2	2.18	0.42
1:I:75:ASP:OD2	1:I:76:THR:HG22	2.19	0.42
1:Q:101:LYS:HE3	1:Q:229:LEU:HD11	2.02	0.42
1:A:40:ARG:NH2	6:A:800:HOH:O	2.30	0.42
2:J:442:TYR:OH	2:J:455:GLU:OE2	2.29	0.42
1:O:33:VAL:O	6:O:706:HOH:O	2.21	0.42
1:Q:55:HIS:CE1	1:Q:57:ILE:HG12	2.55	0.42
1:C:42:CYS:HB3	1:C:270:CYS:O	2.20	0.41
1:C:89:PRO:HB3	1:C:216:VAL:HB	2.02	0.41
1:C:244:LEU:HD13	1:C:246:ALA:HB2	2.02	0.41
1:I:48:HIS:CD2	1:I:266:ILE:HD13	2.55	0.41
1:M:284:ARG:HB3	2:N:379:VAL:HG13	2.02	0.41
2:R:367:ALA:O	2:R:371:ILE:HG12	2.19	0.41
1:U:296:GLY:HA2	2:V:385:GLU:HG3	2.01	0.41
1:W:127:THR:HG22	6:W:733:HOH:O	2.19	0.41
1:K:172:MET:O	1:K:247:PRO:HB3	2.19	0.41
1:A:17:LYS:HE2	1:A:22:GLU:HG3	2.02	0.41
1:E:240:HIS:CE1	1:E:244:LEU:HD12	2.55	0.41
2:F:377:ARG:O	2:F:380:GLU:HG2	2.20	0.41
2:H:446:ARG:NH2	2:L:455:GLU:OE1	2.53	0.41
1:K:61:ILE:HD12	1:K:139:TYR:CE1	2.55	0.41
2:L:438:MET:HE3	2:L:438:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:ILE:HG21	1:O:208:PRO:HG2	2.01	0.41
2:P:386:PHE:HA	6:P:713:HOH:O	2.19	0.41
1:A:42:CYS:HB2	1:A:272:SER:HB3	2.02	0.41
1:A:68:LEU:HB2	6:A:739:HOH:O	2.20	0.41
1:A:302:VAL:HA	2:B:416:THR:HG22	2.03	0.41
1:C:57:ILE:HD12	1:C:95:VAL:HG23	2.02	0.41
1:E:162:ARG:HG3	1:E:235:ASN:CG	2.45	0.41
1:E:183:GLU:OE2	4:Z:3:SIA:O9	2.35	0.41
2:L:324:GLY:HA3	6:L:740:HOH:O	2.20	0.41
1:M:42:CYS:HB2	1:M:272:SER:HB2	2.02	0.41
2:N:451:GLN:O	2:N:493:ARG:NH1	2.48	0.41
2:X:444:ARG:HD3	2:X:478:ASN:OD1	2.20	0.41
2:J:377:ARG:NH2	6:J:714:HOH:O	2.52	0.41
1:K:302:VAL:HA	2:L:416:THR:HG22	2.02	0.41
6:P:708:HOH:O	2:R:450:ARG:HB3	2.20	0.41
1:A:46:ARG:HB2	1:A:75:ASP:OD2	2.21	0.41
1:A:177:HIS:HA	1:A:178:PRO:HD3	1.84	0.41
1:C:303:ASN:HB2	2:D:416:THR:HG21	2.02	0.41
1:E:59:MET:HE2	1:E:108:ILE:HD12	2.02	0.41
1:E:172:MET:HG2	1:E:227:TRP:HB3	2.03	0.41
1:E:175:ILE:HD12	1:E:195:ILE:HD13	2.01	0.41
1:E:311:THR:HG21	3:Y:1:NAG:O6	2.21	0.41
1:I:141:GLU:OE1	1:I:249:ARG:HD3	2.20	0.41
1:Q:89:PRO:HB3	1:Q:216:VAL:HB	2.03	0.41
2:T:444:ARG:HD3	2:T:478:ASN:OD1	2.21	0.41
2:X:377:ARG:O	2:X:380:GLU:HG2	2.20	0.41
1:E:42:CYS:HB3	1:E:270:CYS:C	2.46	0.41
1:E:318:GLU:O	6:E:708:HOH:O	2.22	0.41
2:H:433:MET:O	2:H:436:SER:HB3	2.21	0.41
2:H:455:GLU:OE1	2:J:446:ARG:NH2	2.54	0.41
1:O:234:ASP:OD1	1:O:235:ASN:N	2.54	0.41
1:I:125:GLY:HA3	1:I:144:TRP:HB3	2.03	0.41
1:K:181:THR:HG22	1:K:185:ASN:ND2	2.36	0.41
1:Q:289:ASN:ND2	1:Q:305:ARG:HA	2.36	0.41
1:U:75:ASP:OD2	1:U:76:THR:HG22	2.21	0.41
1:E:145:LEU:HB2	6:E:715:HOH:O	2.20	0.41
2:H:456:ASP:HB2	2:H:460:CYS:HB2	2.02	0.41
1:I:74:TRP:HH2	1:I:108:ILE:HG13	1.85	0.41
1:I:155:PRO:O	1:I:157:THR:HG22	2.21	0.41
1:I:167:ALA:C	1:I:232:PRO:HG3	2.46	0.41
2:J:400:ILE:HD12	2:J:400:ILE:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:PRO:HG2	1:K:287:PHE:CD2	2.56	0.41
1:Q:142:LEU:HD23	1:Q:247:PRO:HA	2.03	0.41
1:Q:153:ASN:HA	1:Q:189:GLY:HA3	2.01	0.41
1:S:43:MET:O	1:S:46:ARG:HG2	2.21	0.41
1:S:176:HIS:O	1:S:208:PRO:HB3	2.20	0.41
1:K:109:ASN:OD1	6:K:779:HOH:O	2.22	0.41
1:M:20:THR:O	2:P:373:GLY:HA3	2.21	0.41
1:C:63:THR:OG1	1:C:85:ALA:O	2.33	0.40
1:G:291:SER:HA	1:G:292:PRO:HD3	1.87	0.40
1:I:43:MET:HE2	1:I:48:HIS:CB	2.50	0.40
1:O:179:SER:OG	1:O:183:GLU:OE1	2.38	0.40
2:P:381:LYS:HD2	2:P:381:LYS:HA	1.91	0.40
1:Q:87:CYS:HB2	1:Q:129:ALA:O	2.20	0.40
2:N:410:SER:HB3	2:P:411:ILE:HD13	2.03	0.40
1:O:228:THR:HG22	1:O:229:LEU:H	1.86	0.40
2:P:377:ARG:O	2:P:380:GLU:HG2	2.21	0.40
1:Q:125:GLY:HA3	1:Q:144:TRP:HB3	2.03	0.40
2:T:375:LEU:HD23	2:T:375:LEU:HA	1.89	0.40
2:B:344:TRP:CH2	2:B:371:ILE:HD12	2.56	0.40
2:F:456:ASP:HB3	2:F:458:LYS:H	1.86	0.40
1:M:234:ASP:OD1	1:M:235:ASN:N	2.54	0.40
1:O:172:MET:HG2	1:O:227:TRP:HB3	2.03	0.40
1:S:110:LYS:HB3	1:S:249:ARG:HE	1.86	0.40
1:S:284:ARG:HB3	2:T:379:VAL:HG13	2.03	0.40
1:U:46:ARG:HB2	1:U:75:ASP:OD2	2.21	0.40
1:U:132:ARG:NH1	1:U:138:PHE:O	2.54	0.40
2:V:383:ASN:HA	2:V:384:THR:HB	2.04	0.40
1:W:87:CYS:SG	1:W:88:TYR:N	2.93	0.40
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.93	0.40
1:G:172:MET:HG2	1:G:227:TRP:HB3	2.03	0.40
1:O:59:MET:HE1	1:O:74:TRP:CH2	2.56	0.40
2:P:455:GLU:OE1	2:R:446:ARG:NH2	2.53	0.40
1:Q:303:ASN:O	1:Q:304:ARG:NE	2.52	0.40
1:S:172:MET:HG2	1:S:227:TRP:HB3	2.04	0.40
1:W:50:ASP:HB2	1:W:266:ILE:HD11	2.03	0.40
4:c:3:SIA:O10	4:c:3:SIA:C7	2.69	0.40
1:E:146:VAL:HG21	1:E:187:LEU:HD22	2.04	0.40
2:H:373:GLY:HA3	1:K:20:THR:O	2.21	0.40
1:K:60:LEU:HD11	1:K:102:ILE:HD11	2.03	0.40
1:S:51:LEU:HB3	1:S:54:CYS:O	2.21	0.40
2:T:406:TRP:CH2	2:V:408:LYS:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
1	C	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	E	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	G	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
1	I	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	K	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	M	316/318 (99%)	302 (96%)	13 (4%)	1 (0%)	36	58
1	O	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
1	Q	316/318 (99%)	304 (96%)	12 (4%)	0	100	100
1	S	316/318 (99%)	305 (96%)	10 (3%)	1 (0%)	36	58
1	U	316/318 (99%)	307 (97%)	8 (2%)	1 (0%)	36	58
1	W	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
2	B	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	21	42
2	D	172/174 (99%)	166 (96%)	4 (2%)	2 (1%)	10	23
2	F	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	21	42
2	H	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	21	42
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	21	42
2	L	172/174 (99%)	169 (98%)	2 (1%)	1 (1%)	21	42
2	N	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	21	42
2	P	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	21	42
2	R	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	42
2	T	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	21	42
2	X	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	42
All	All	5856/5904 (99%)	5662 (97%)	178 (3%)	16 (0%)	36	58

All (16) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	247 (92%)	22 (8%)	10	24
1	C	269/269 (100%)	246 (91%)	23 (9%)	10	22
1	E	269/269 (100%)	249 (93%)	20 (7%)	13	29
1	G	269/269 (100%)	248 (92%)	21 (8%)	11	26
1	I	269/269 (100%)	247 (92%)	22 (8%)	10	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	269/269 (100%)	245 (91%)	24 (9%)	9	20
1	M	269/269 (100%)	248 (92%)	21 (8%)	11	26
1	O	269/269 (100%)	248 (92%)	21 (8%)	11	26
1	Q	269/269 (100%)	248 (92%)	21 (8%)	11	26
1	S	269/269 (100%)	249 (93%)	20 (7%)	13	29
1	U	269/269 (100%)	243 (90%)	26 (10%)	8	17
1	W	269/269 (100%)	245 (91%)	24 (9%)	9	20
2	B	148/148 (100%)	138 (93%)	10 (7%)	14	32
2	D	148/148 (100%)	136 (92%)	12 (8%)	11	24
2	F	148/148 (100%)	135 (91%)	13 (9%)	9	21
2	H	148/148 (100%)	142 (96%)	6 (4%)	27	54
2	J	148/148 (100%)	136 (92%)	12 (8%)	11	24
2	L	148/148 (100%)	136 (92%)	12 (8%)	11	24
2	N	148/148 (100%)	141 (95%)	7 (5%)	23	48
2	P	148/148 (100%)	136 (92%)	12 (8%)	11	24
2	R	148/148 (100%)	141 (95%)	7 (5%)	23	48
2	T	148/148 (100%)	141 (95%)	7 (5%)	23	48
2	V	148/148 (100%)	133 (90%)	15 (10%)	7	15
2	X	148/148 (100%)	141 (95%)	7 (5%)	23	48
All	All	5004/5004 (100%)	4619 (92%)	385 (8%)	12	27

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	41	LEU
1	A	57	ILE
1	A	76	THR
1	A	77	LEU
1	A	111	ILE
1	A	126	THR
1	A	152	GLN
1	A	157	THR
1	A	162	ARG
1	A	170	LEU

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	192	SER
1	A	203	ARG
1	A	228	THR
1	A	239	SER
1	A	244	LEU
1	A	249	ARG
1	A	258	LEU
1	A	277	ARG
1	A	283	THR
1	A	314	ARG
2	B	341	VAL
2	B	377	ARG
2	B	379	VAL
2	B	382	THR
2	B	416	THR
2	B	420	GLU
2	B	456	ASP
2	B	470	SER
2	B	477	ASN
2	B	492	ASN
1	C	8	HIS
1	C	23	GLN
1	C	41	LEU
1	C	46	ARG
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	126	THR
1	C	146	VAL
1	C	157	THR
1	C	170	LEU
1	C	184	LYS
1	C	192	SER
1	C	203	ARG
1	C	213	ARG
1	C	228	THR
1	C	244	LEU
1	C	250	VAL
1	C	258	LEU
1	C	263	ASP
1	C	276	TRP

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Mol	Chain	Res	Type
1	C	277	ARG
1	C	283	THR
2	D	325	LEU
2	D	341	VAL
2	D	353	GLN
2	D	377	ARG
2	D	379	VAL
2	D	383	ASN
2	D	420	GLU
2	D	423	VAL
2	D	444	ARG
2	D	450	ARG
2	D	470	SER
2	D	491	LEU
1	E	14	THR
1	E	41	LEU
1	E	76	THR
1	E	77	LEU
1	E	111	ILE
1	E	126	THR
1	E	146	VAL
1	E	150	LYS
1	E	157	THR
1	E	162	ARG
1	E	170	LEU
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	256	ARG
1	E	258	LEU
1	E	276	TRP
1	E	277	ARG
1	E	283	THR
2	F	341	VAL
2	F	353	GLN
2	F	377	ARG
2	F	379	VAL
2	F	382	THR
2	F	411	ILE
2	F	416	THR
2	F	418	GLN

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Mol	Chain	Res	Type
2	F	423	VAL
2	F	425	MET
2	F	450	ARG
2	F	456	ASP
2	F	477	ASN
1	G	8	HIS
1	G	14	THR
1	G	41	LEU
1	G	47	LYS
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	120	SER
1	G	126	THR
1	G	157	THR
1	G	162	ARG
1	G	170	LEU
1	G	203	ARG
1	G	213	ARG
1	G	228	THR
1	G	244	LEU
1	G	258	LEU
1	G	263	ASP
1	G	276	TRP
1	G	277	ARG
1	G	283	THR
2	H	341	VAL
2	H	371	ILE
2	H	416	THR
2	H	418	GLN
2	H	423	VAL
2	H	496	ILE
1	I	8	HIS
1	I	41	LEU
1	I	49	LYS
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	126	THR
1	I	128	ARG
1	I	146	VAL
1	I	157	THR

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Mol	Chain	Res	Type
1	I	170	LEU
1	I	192	SER
1	I	203	ARG
1	I	213	ARG
1	I	228	THR
1	I	244	LEU
1	I	248	SER
1	I	249	ARG
1	I	250	VAL
1	I	258	LEU
1	I	277	ARG
1	I	283	THR
2	J	341	VAL
2	J	377	ARG
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	395	GLU
2	J	416	THR
2	J	420	GLU
2	J	425	MET
2	J	450	ARG
2	J	467	CYS
2	J	491	LEU
1	K	8	HIS
1	K	14	THR
1	K	63	THR
1	K	76	THR
1	K	77	LEU
1	K	111	ILE
1	K	120	SER
1	K	126	THR
1	K	132	ARG
1	K	149	SER
1	K	157	THR
1	K	170	LEU
1	K	203	ARG
1	K	220	SER
1	K	228	THR
1	K	244	LEU
1	K	248	SER
1	K	249	ARG

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Mol	Chain	Res	Type
1	K	250	VAL
1	K	256	ARG
1	K	258	LEU
1	K	263	ASP
1	K	277	ARG
1	K	283	THR
2	L	325	LEU
2	L	341	VAL
2	L	379	VAL
2	L	396	ILE
2	L	418	GLN
2	L	423	VAL
2	L	425	MET
2	L	436	SER
2	L	438	MET
2	L	450	ARG
2	L	456	ASP
2	L	484	GLN
1	M	8	HIS
1	M	14	THR
1	M	30	THR
1	M	41	LEU
1	M	57	ILE
1	M	76	THR
1	M	77	LEU
1	M	87	CYS
1	M	111	ILE
1	M	157	THR
1	M	162	ARG
1	M	170	LEU
1	M	203	ARG
1	M	213	ARG
1	M	228	THR
1	M	244	LEU
1	M	258	LEU
1	M	276	TRP
1	M	277	ARG
1	M	283	THR
1	M	316	VAL
2	N	341	VAL
2	N	371	ILE
2	N	418	GLN

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Mol	Chain	Res	Type
2	N	425	MET
2	N	446	ARG
2	N	450	ARG
2	N	484	GLN
1	O	8	HIS
1	O	14	THR
1	O	41	LEU
1	O	76	THR
1	O	77	LEU
1	O	94	ASN
1	O	111	ILE
1	O	116	THR
1	O	126	THR
1	O	146	VAL
1	O	170	LEU
1	O	203	ARG
1	O	228	THR
1	O	239	SER
1	O	244	LEU
1	O	250	VAL
1	O	258	LEU
1	O	263	ASP
1	O	276	TRP
1	O	283	THR
1	O	318	GLU
2	P	335	ASN
2	P	341	VAL
2	P	342	ASP
2	P	372	THR
2	P	377	ARG
2	P	383	ASN
2	P	395	GLU
2	P	416	THR
2	P	420	GLU
2	P	448	GLN
2	P	450	ARG
2	P	496	ILE
1	Q	23	GLN
1	Q	41	LEU
1	Q	76	THR
1	Q	77	LEU
1	Q	101	LYS

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Mol	Chain	Res	Type
1	Q	111	ILE
1	Q	126	THR
1	Q	146	VAL
1	Q	157	THR
1	Q	170	LEU
1	Q	192	SER
1	Q	203	ARG
1	Q	213	ARG
1	Q	228	THR
1	Q	244	LEU
1	Q	249	ARG
1	Q	250	VAL
1	Q	258	LEU
1	Q	277	ARG
1	Q	283	THR
1	Q	314	ARG
2	R	341	VAL
2	R	342	ASP
2	R	353	GLN
2	R	423	VAL
2	R	467	CYS
2	R	470	SER
2	R	496	ILE
1	S	8	HIS
1	S	14	THR
1	S	41	LEU
1	S	76	THR
1	S	77	LEU
1	S	111	ILE
1	S	112	SER
1	S	116	THR
1	S	157	THR
1	S	162	ARG
1	S	170	LEU
1	S	203	ARG
1	S	213	ARG
1	S	228	THR
1	S	230	VAL
1	S	244	LEU
1	S	258	LEU
1	S	276	TRP
1	S	277	ARG

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Mol	Chain	Res	Type
1	S	283	THR
2	T	325	LEU
2	T	383	ASN
2	T	416	THR
2	T	418	GLN
2	T	425	MET
2	T	436	SER
2	T	450	ARG
1	U	8	HIS
1	U	41	LEU
1	U	47	LYS
1	U	63	THR
1	U	76	THR
1	U	77	LEU
1	U	111	ILE
1	U	126	THR
1	U	128	ARG
1	U	146	VAL
1	U	148	LYS
1	U	157	THR
1	U	170	LEU
1	U	179	SER
1	U	196	SER
1	U	203	ARG
1	U	228	THR
1	U	239	SER
1	U	244	LEU
1	U	249	ARG
1	U	250	VAL
1	U	258	LEU
1	U	277	ARG
1	U	283	THR
1	U	316	VAL
1	U	318	GLU
2	V	325	LEU
2	V	350	GLN
2	V	353	GLN
2	V	377	ARG
2	V	379	VAL
2	V	382	THR
2	V	383	ASN
2	V	411	ILE

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Mol	Chain	Res	Type
2	V	412	THR
2	V	423	VAL
2	V	425	MET
2	V	448	GLN
2	V	450	ARG
2	V	467	CYS
2	V	491	LEU
1	W	8	HIS
1	W	30	THR
1	W	35	SER
1	W	41	LEU
1	W	76	THR
1	W	77	LEU
1	W	111	ILE
1	W	119	SER
1	W	146	VAL
1	W	147	SER
1	W	157	THR
1	W	170	LEU
1	W	192	SER
1	W	196	SER
1	W	203	ARG
1	W	213	ARG
1	W	228	THR
1	W	244	LEU
1	W	249	ARG
1	W	250	VAL
1	W	258	LEU
1	W	269	ASN
1	W	276	TRP
1	W	283	THR
2	X	353	GLN
2	X	377	ARG
2	X	379	VAL
2	X	382	THR
2	X	395	GLU
2	X	418	GLN
2	X	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	418	GLN
1	C	82	ASN
2	D	418	GLN
2	D	448	GLN
1	E	39	ASN
1	E	156	GLN
1	E	219	GLN
2	F	370	GLN
1	G	8	HIS
1	G	94	ASN
1	G	182	GLN
1	G	219	GLN
1	I	7	HIS
1	I	136	ASN
1	I	152	GLN
1	I	205	ASN
2	J	335	ASN
2	J	399	GLN
2	J	492	ASN
1	K	185	ASN
1	K	205	ASN
2	L	398	HIS
1	M	21	ASN
1	M	182	GLN
1	M	205	ASN
1	M	226	HIS
1	M	269	ASN
2	N	350	GLN
2	N	353	GLN
2	N	398	HIS
1	O	153	ASN
1	O	226	HIS
2	P	428	GLN
1	Q	205	ASN
1	Q	303	ASN
2	R	365	GLN
2	R	398	HIS
1	S	8	HIS
1	S	152	GLN
1	S	163	ASN
2	T	418	GLN
1	U	8	HIS
1	U	159	ASN

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Mol	Chain	Res	Type
1	U	297	GLN
2	V	335	ASN
2	V	418	GLN
2	V	428	GLN
2	V	448	GLN
2	V	477	ASN
1	W	156	GLN
1	W	231	GLN
2	X	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 monosaccharides 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	Y	1	1,3	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	Y	2	3	14,14,15	0.84	0	17,19,21	0.73	0
4	NAG	Z	1	4	14,14,15	0.30	0	17,19,21	0.41	0
4	GAL	Z	2	4	11,11,12	0.77	0	15,15,17	0.96	0
4	SIA	Z	3	4	20,20,21	0.55	0	21,28,31	0.84	2 (9%)
4	NAG	a	1	4	14,14,15	0.26	0	17,19,21	0.37	0
4	GAL	a	2	4	11,11,12	0.28	0	15,15,17	0.66	0
4	SIA	a	3	4	20,20,21	0.55	0	21,28,31	0.84	2 (9%)
4	NAG	b	1	4	14,14,15	0.36	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	b	2	4	11,11,12	0.90	0	15,15,17	1.20	2 (13%)
4	SIA	b	3	4	20,20,21	0.54	0	21,28,31	0.83	1 (4%)
4	NAG	c	1	4	14,14,15	0.25	0	17,19,21	0.50	0
4	GAL	c	2	4	11,11,12	0.75	0	15,15,17	1.02	1 (6%)
4	SIA	c	3	4	20,20,21	2.01	11 (55%)	21,28,31	3.03	9 (42%)

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	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	1/6/23/26	0/1/1/1
4	NAG	Z	1	4	-	2/6/23/26	0/1/1/1
4	GAL	Z	2	4	-	2/2/19/22	0/1/1/1
4	SIA	Z	3	4	-	0/18/34/38	0/1/1/1
4	NAG	a	1	4	-	2/6/23/26	0/1/1/1
4	GAL	a	2	4	-	0/2/19/22	0/1/1/1
4	SIA	a	3	4	-	0/18/34/38	0/1/1/1
4	NAG	b	1	4	-	2/6/23/26	0/1/1/1
4	GAL	b	2	4	-	2/2/19/22	0/1/1/1
4	SIA	b	3	4	-	0/18/34/38	0/1/1/1
4	NAG	c	1	4	-	2/6/23/26	0/1/1/1
4	GAL	c	2	4	-	0/2/19/22	0/1/1/1
4	SIA	c	3	4	-	7/18/34/38	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	3	SIA	C8-C7	-3.72	1.46	1.53
4	c	3	SIA	C4-C5	-3.08	1.50	1.53
4	c	3	SIA	O10-C10	-3.06	1.16	1.23
4	c	3	SIA	C7-C6	-2.76	1.49	1.52
4	c	3	SIA	C3-C2	2.42	1.56	1.52
4	c	3	SIA	C3-C4	2.39	1.57	1.52
4	c	3	SIA	C11-C10	-2.16	1.46	1.50
4	c	3	SIA	O8-C8	-2.11	1.38	1.43
4	c	3	SIA	C9-C8	-2.10	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	3	SIA	O1B-C1	-2.08	1.24	1.30
4	c	3	SIA	O4-C4	-2.05	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	3	SIA	O6-C2-C3	-9.38	97.95	110.56
4	c	3	SIA	O9-C9-C8	-5.58	99.45	111.16
4	c	3	SIA	O10-C10-C11	-4.18	114.62	122.05
4	c	3	SIA	C11-C10-N5	3.93	122.63	116.12
4	c	3	SIA	O6-C2-C1	3.11	113.59	107.72
4	b	2	GAL	C1-C2-C3	2.71	113.59	109.64
4	c	2	GAL	C1-C2-C3	2.53	113.32	109.64
4	c	3	SIA	C6-C5-N5	2.38	114.71	110.91
4	c	3	SIA	O8-C8-C9	-2.38	103.62	109.03
4	b	2	GAL	C1-O5-C5	2.31	115.28	112.19
4	c	3	SIA	O4-C4-C3	2.25	115.45	109.86
4	a	3	SIA	O1B-C1-C2	2.24	118.52	112.71
4	Z	3	SIA	O1B-C1-C2	2.22	118.49	112.71
4	b	3	SIA	O1B-C1-C2	2.22	118.48	112.71
4	c	3	SIA	C9-C8-C7	-2.16	107.77	112.17
4	a	3	SIA	O1A-C1-C2	-2.02	118.48	122.85
4	Z	3	SIA	O1A-C1-C2	-2.02	118.48	122.85

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	c	3	SIA	O6-C6-C7-C8
4	c	3	SIA	O6-C6-C7-O7
4	b	2	GAL	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	Z	2	GAL	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	b	2	GAL	C4-C5-C6-O6
4	Z	2	GAL	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6

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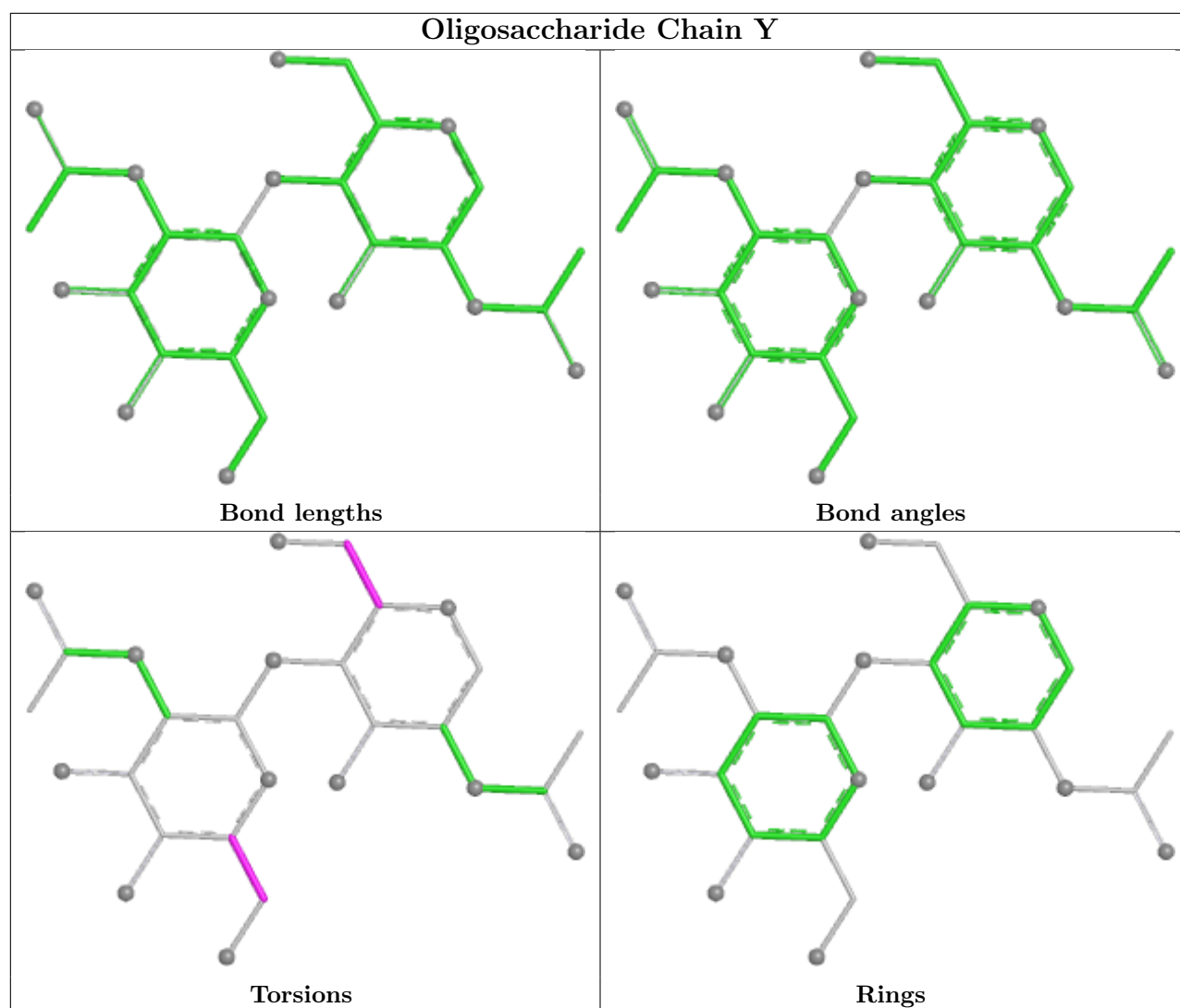
Mol	Chain	Res	Type	Atoms
4	Z	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	c	3	SIA	C6-C7-C8-C9
4	c	3	SIA	O7-C7-C8-C9
3	Y	2	NAG	C4-C5-C6-O6
4	c	3	SIA	C4-C5-N5-C10
4	c	3	SIA	C5-C6-C7-O7
4	c	3	SIA	C6-C5-N5-C10

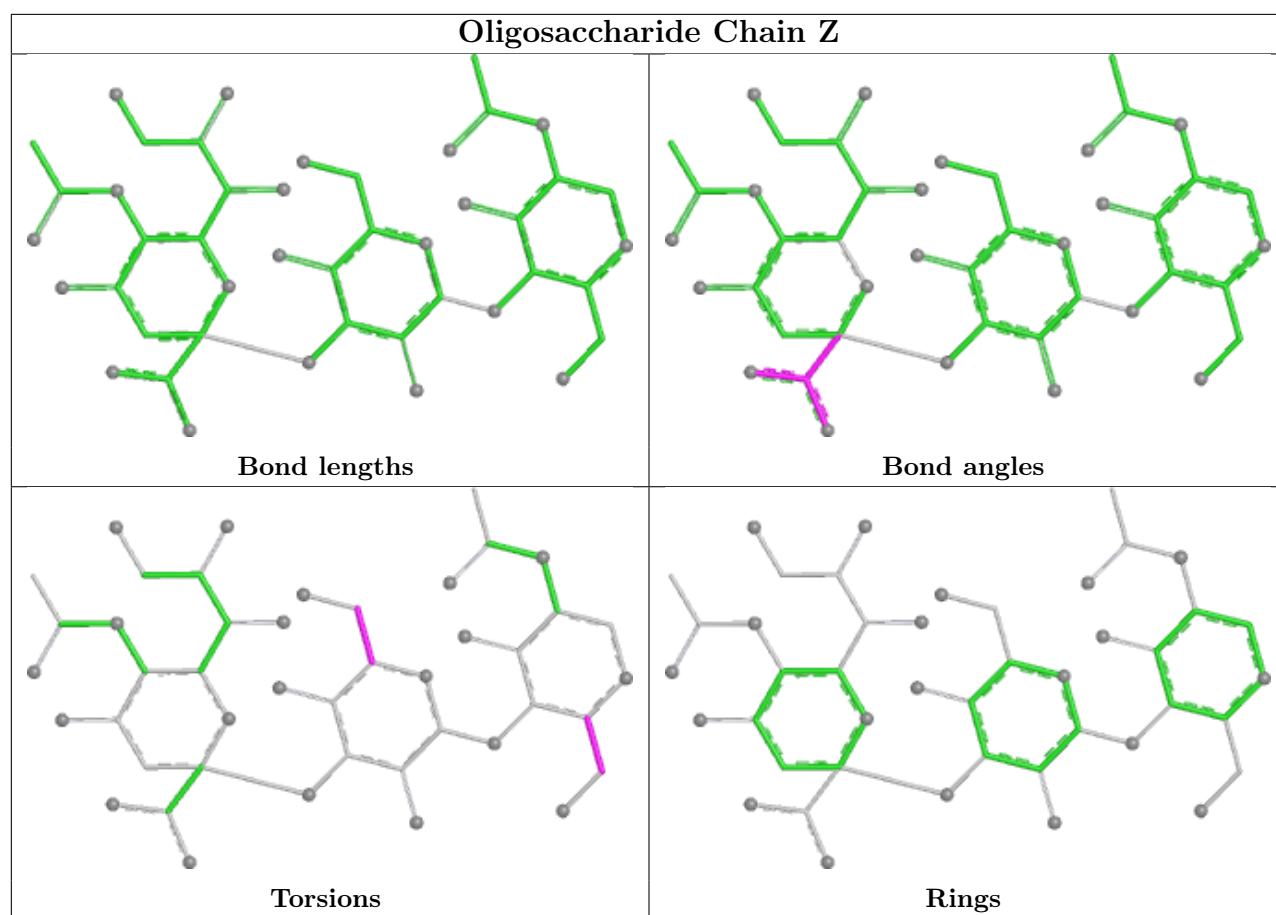
There are no ring outliers.

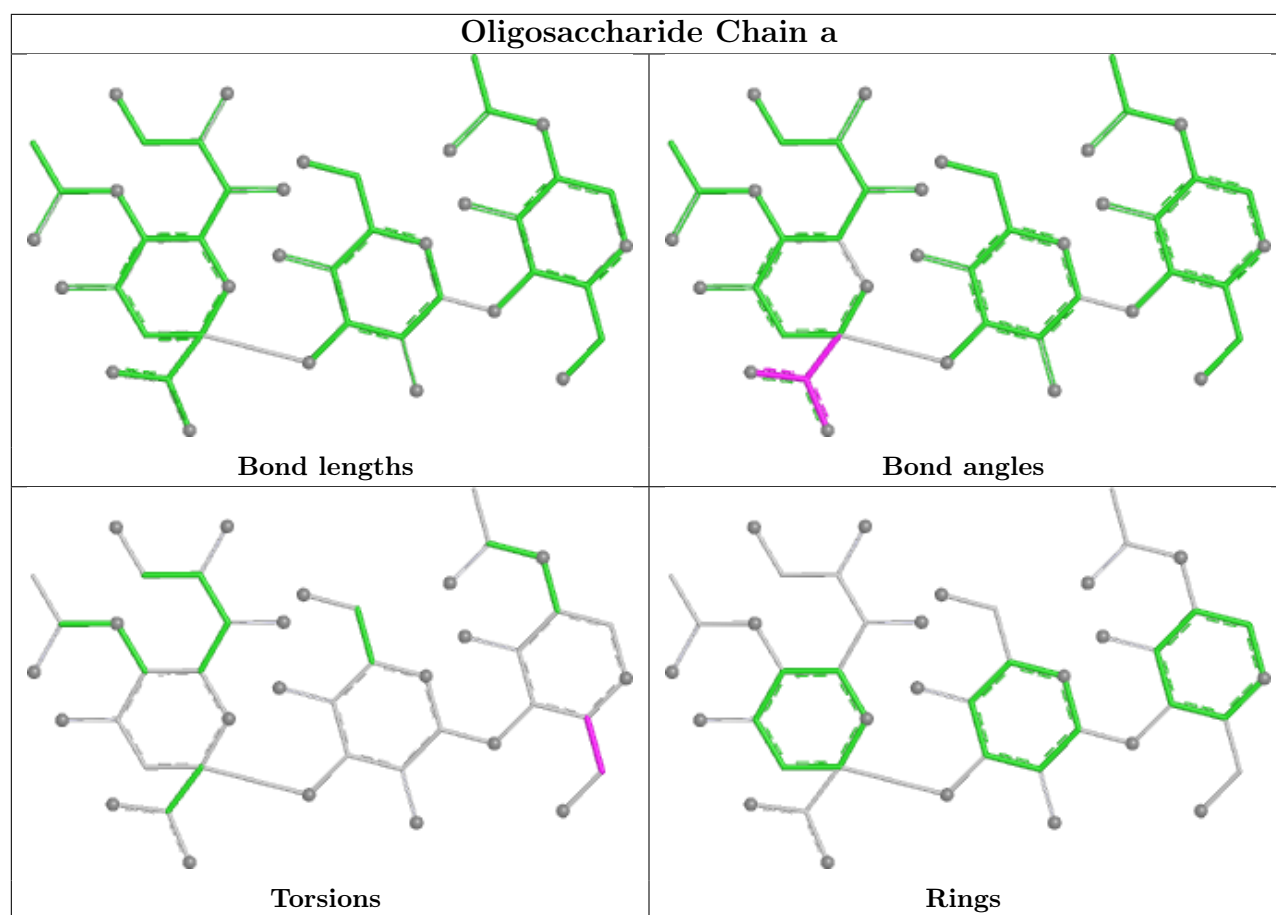
5 monomers are involved in 18 short contacts:

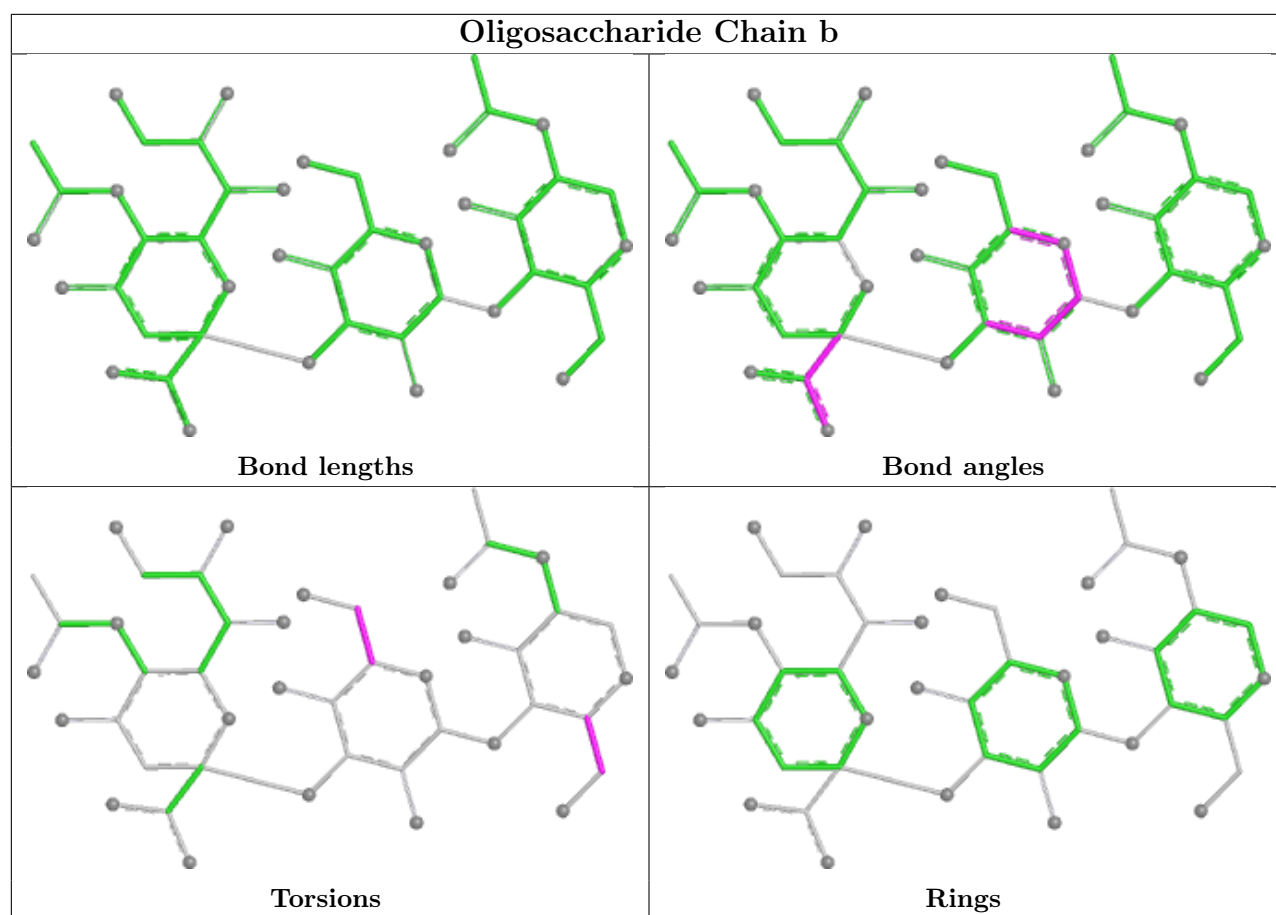
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	1	NAG	1	0
4	a	3	SIA	5	0
4	b	3	SIA	3	0
4	Z	3	SIA	5	0
4	c	3	SIA	4	0

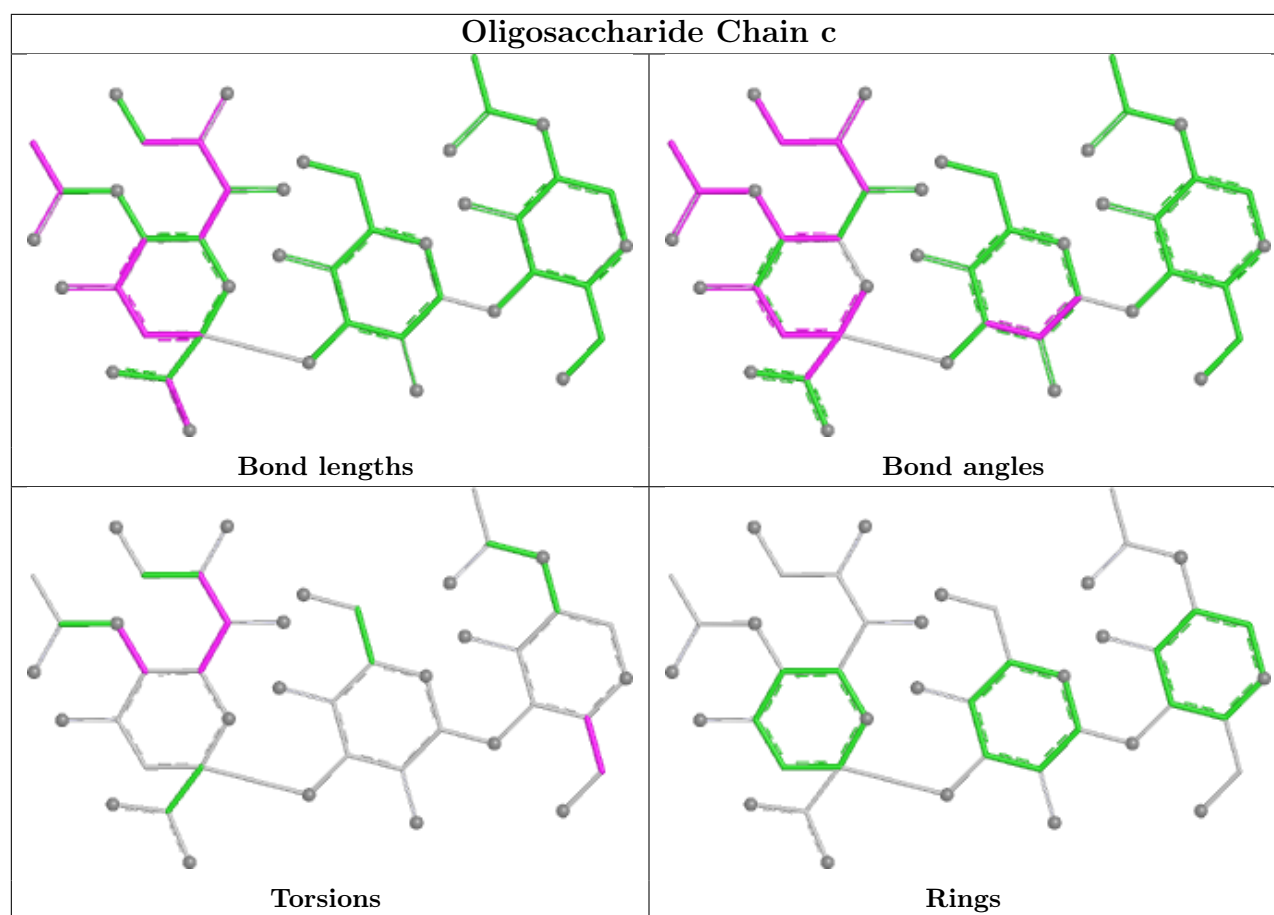
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	P	601	2	14,14,15	0.37	0	17,19,21	0.50	0
5	NAG	X	601	2	14,14,15	0.54	0	17,19,21	0.56	0
5	NAG	T	601	2	14,14,15	0.59	0	17,19,21	0.41	0
5	NAG	M	601	1	14,14,15	0.36	0	17,19,21	0.59	0
5	NAG	F	601	2	14,14,15	0.32	0	17,19,21	0.63	0
5	NAG	W	601	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	E	602	1	14,14,15	0.92	1 (7%)	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	601	1	14,14,15	0.18	0	17,19,21	0.48	0
5	NAG	B	601	2	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	D	601	2	14,14,15	0.32	0	17,19,21	0.45	0
5	NAG	J	601	2	14,14,15	0.71	0	17,19,21	0.79	0
5	NAG	Q	601	1	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	O	601	1	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	V	601	2	14,14,15	0.40	0	17,19,21	0.53	0
5	NAG	I	601	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	L	601	2	14,14,15	0.39	0	17,19,21	0.49	0
5	NAG	E	601	1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	C	601	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	S	601	1	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	N	601	2	14,14,15	0.49	0	17,19,21	0.46	0
5	NAG	U	601	1	14,14,15	0.43	0	17,19,21	0.44	0
5	NAG	R	601	2	14,14,15	0.21	0	17,19,21	0.64	0
5	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	H	601	2	14,14,15	0.44	0	17,19,21	0.61	0
5	NAG	K	601	1	14,14,15	0.35	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	601	2	-	0/6/23/26	0/1/1/1
5	NAG	X	601	2	-	2/6/23/26	0/1/1/1
5	NAG	T	601	2	-	2/6/23/26	0/1/1/1
5	NAG	M	601	1	-	0/6/23/26	0/1/1/1
5	NAG	F	601	2	-	0/6/23/26	0/1/1/1
5	NAG	W	601	1	-	4/6/23/26	0/1/1/1
5	NAG	E	602	1	-	1/6/23/26	0/1/1/1
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	B	601	2	-	0/6/23/26	0/1/1/1
5	NAG	D	601	2	-	0/6/23/26	0/1/1/1
5	NAG	J	601	2	-	0/6/23/26	0/1/1/1
5	NAG	Q	601	1	-	2/6/23/26	0/1/1/1
5	NAG	O	601	1	-	2/6/23/26	0/1/1/1
5	NAG	V	601	2	-	0/6/23/26	0/1/1/1
5	NAG	I	601	1	-	0/6/23/26	0/1/1/1
5	NAG	L	601	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	S	601	1	-	1/6/23/26	0/1/1/1
5	NAG	N	601	2	-	0/6/23/26	0/1/1/1
5	NAG	U	601	1	-	2/6/23/26	0/1/1/1
5	NAG	R	601	2	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	H	601	2	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	602	NAG	C2-N2	2.36	1.50	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	602	NAG	O7-C7-N2	2.02	125.55	121.98

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	W	601	NAG	C1-C2-N2-C7
5	W	601	NAG	C8-C7-N2-C2
5	W	601	NAG	O7-C7-N2-C2
5	O	601	NAG	O5-C5-C6-O6
5	T	601	NAG	O5-C5-C6-O6
5	X	601	NAG	O5-C5-C6-O6
5	K	601	NAG	O5-C5-C6-O6
5	Q	601	NAG	O5-C5-C6-O6
5	U	601	NAG	O5-C5-C6-O6
5	L	601	NAG	O5-C5-C6-O6
5	O	601	NAG	C4-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	T	601	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	X	601	NAG	C4-C5-C6-O6
5	U	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	Q	601	NAG	C4-C5-C6-O6
5	K	601	NAG	C4-C5-C6-O6
5	L	601	NAG	C4-C5-C6-O6
5	W	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	G	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6
5	S	601	NAG	C1-C2-N2-C7
5	E	602	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	601	NAG	1	0
5	D	601	NAG	1	0
5	J	601	NAG	1	0
5	O	601	NAG	1	0
5	E	601	NAG	1	0
5	N	601	NAG	1	0
5	U	601	NAG	1	0
5	K	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/318 (100%)	-0.32	1 (0%) 90 88	10, 25, 42, 69	0
1	C	318/318 (100%)	-0.00	2 (0%) 85 83	10, 36, 64, 95	0
1	E	318/318 (100%)	-0.22	0 100 100	11, 30, 48, 70	0
1	G	318/318 (100%)	-0.13	2 (0%) 85 83	15, 34, 54, 80	0
1	I	318/318 (100%)	-0.18	1 (0%) 90 88	11, 29, 52, 101	0
1	K	318/318 (100%)	-0.24	2 (0%) 85 83	13, 29, 52, 84	0
1	M	318/318 (100%)	0.64	19 (5%) 27 22	24, 56, 87, 123	0
1	O	318/318 (100%)	0.50	10 (3%) 51 45	22, 52, 82, 112	0
1	Q	318/318 (100%)	-0.11	3 (0%) 81 78	12, 33, 54, 92	0
1	S	318/318 (100%)	0.27	8 (2%) 58 52	17, 43, 70, 107	0
1	U	318/318 (100%)	-0.19	0 100 100	16, 31, 53, 83	0
1	W	318/318 (100%)	0.29	5 (1%) 70 66	24, 44, 71, 94	0
2	B	174/174 (100%)	-0.16	5 (2%) 53 48	12, 26, 54, 108	0
2	D	174/174 (100%)	-0.14	3 (1%) 69 64	11, 25, 52, 130	0
2	F	174/174 (100%)	-0.13	5 (2%) 53 48	10, 27, 56, 101	0
2	H	174/174 (100%)	-0.13	2 (1%) 78 74	12, 29, 55, 125	0
2	J	174/174 (100%)	0.19	8 (4%) 37 32	12, 37, 74, 132	0
2	L	174/174 (100%)	0.13	6 (3%) 48 42	14, 35, 67, 108	0
2	N	174/174 (100%)	0.17	6 (3%) 48 42	23, 38, 71, 109	0
2	P	174/174 (100%)	0.05	3 (1%) 69 64	18, 37, 66, 125	0
2	R	174/174 (100%)	-0.01	4 (2%) 61 55	16, 33, 55, 110	0
2	T	174/174 (100%)	0.01	3 (1%) 69 64	13, 37, 61, 119	0
2	V	174/174 (100%)	0.12	4 (2%) 61 55	14, 39, 71, 127	0
2	X	174/174 (100%)	0.19	7 (4%) 42 37	19, 45, 69, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5904/5904 (100%)	0.03	109 (1%) 67 63	10, 35, 69, 132	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	496	ILE	8.4
2	F	496	ILE	7.8
2	L	496	ILE	7.8
2	V	496	ILE	7.7
2	L	497	ASN	7.6
2	X	496	ILE	6.3
2	D	497	ASN	4.9
2	N	382	THR	4.6
2	J	496	ILE	4.5
2	H	496	ILE	4.4
2	X	497	ASN	4.4
1	O	270	CYS	4.3
2	R	496	ILE	4.3
2	T	382	THR	4.0
1	Q	182	GLN	3.9
2	F	382	THR	3.9
2	B	496	ILE	3.9
1	W	270	CYS	3.8
2	R	382	THR	3.7
1	O	198	GLY	3.6
2	P	497	ASN	3.5
1	O	114	GLY	3.5
2	J	382	THR	3.4
1	Q	270	CYS	3.4
1	Q	318	GLU	3.3
2	J	341	VAL	3.3
2	L	382	THR	3.3
1	S	120	SER	3.3
1	K	270	CYS	3.2
1	S	152	GLN	3.2
2	F	383	ASN	3.2
2	V	487	GLU	3.2
2	V	497	ASN	3.2
2	D	382	THR	3.2
2	P	496	ILE	3.2
2	L	383	ASN	3.1
1	M	270	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	T	342	ASP	3.1
1	M	130	CYS	2.9
2	J	497	ASN	2.8
2	X	383	ASN	2.8
1	C	270	CYS	2.8
1	O	283	THR	2.8
1	O	68	LEU	2.8
2	P	382	THR	2.8
1	O	149	SER	2.8
2	F	497	ASN	2.7
2	N	383	ASN	2.7
1	G	270	CYS	2.7
1	M	126	THR	2.7
2	X	381	LYS	2.6
2	B	381	LYS	2.6
2	N	353	GLN	2.6
1	I	270	CYS	2.6
1	O	242	GLY	2.6
1	W	256	ARG	2.6
2	T	383	ASN	2.6
1	M	64	PRO	2.5
2	X	382	THR	2.5
1	S	217	ASN	2.5
2	X	467	CYS	2.5
2	N	469	ASP	2.5
1	G	130	CYS	2.4
1	M	62	GLY	2.4
1	M	134	GLY	2.4
2	B	383	ASN	2.4
2	B	382	THR	2.4
2	V	382	THR	2.4
1	M	263	ASP	2.4
1	M	217	ASN	2.4
1	S	133	ASN	2.4
1	M	218	GLY	2.4
1	M	131	MET	2.4
1	A	270	CYS	2.3
1	C	149	SER	2.3
1	O	256	ARG	2.3
2	N	342	ASP	2.3
1	W	130	CYS	2.3
1	M	39	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	68	LEU	2.2
1	O	271	GLU	2.2
2	J	383	ASN	2.2
1	M	73	MET	2.2
1	M	63	THR	2.2
2	F	456	ASP	2.2
2	J	352	ALA	2.1
1	S	121	ILE	2.1
2	N	456	ASP	2.1
1	M	150	LYS	2.1
2	L	341	VAL	2.1
1	K	133	ASN	2.1
2	L	495	ASN	2.1
1	S	189	GLY	2.1
1	W	134	GLY	2.1
2	H	382	THR	2.1
1	M	193	ILE	2.1
2	B	342	ASP	2.1
2	X	342	ASP	2.1
1	O	212	ALA	2.1
2	R	383	ASN	2.1
1	S	270	CYS	2.1
1	M	70	LEU	2.1
1	M	111	ILE	2.1
2	J	471	CYS	2.1
2	R	380	GLU	2.0
1	W	149	SER	2.0
1	M	298	CYS	2.0
2	J	342	ASP	2.0
1	S	117	TYR	2.0

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

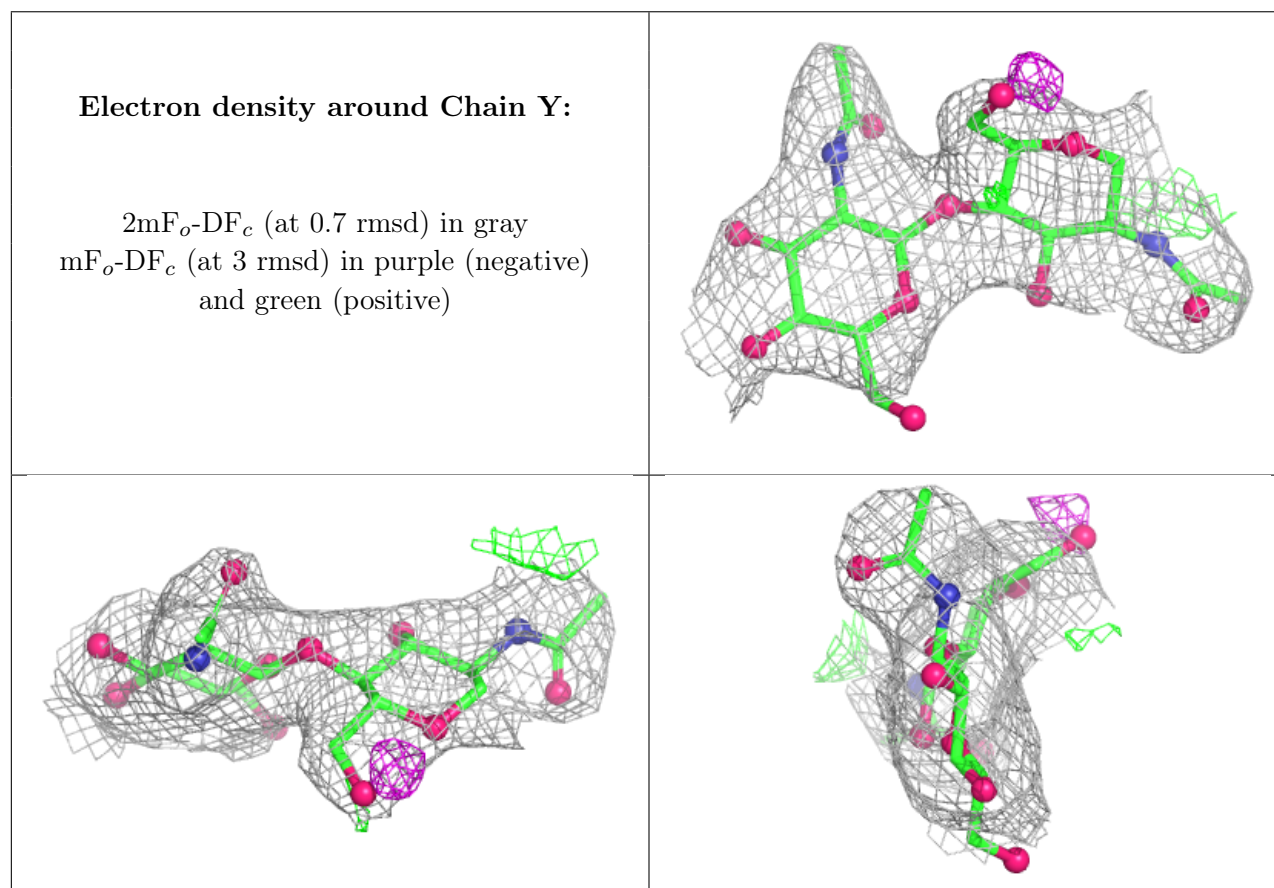
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.

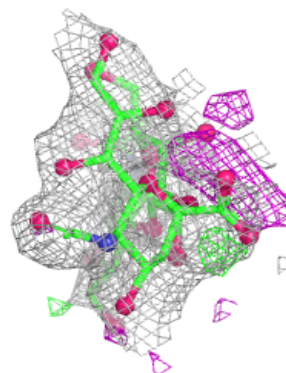
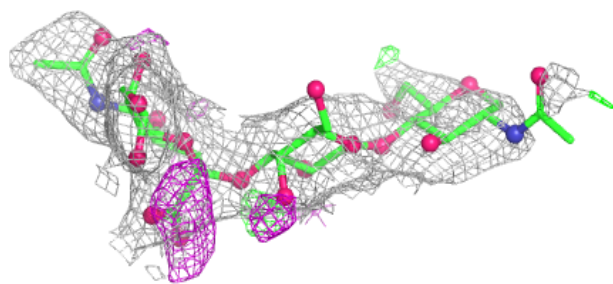
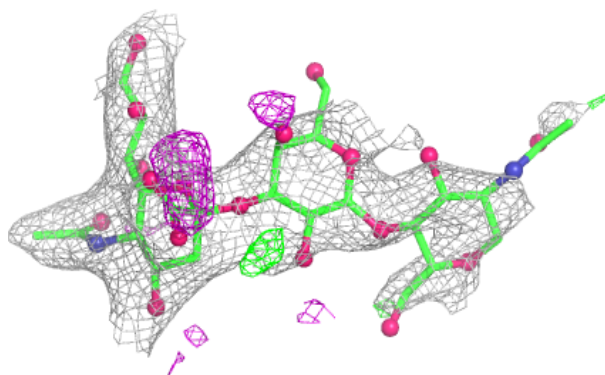
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	Z	1	14/15	0.51	0.18	100,109,111,112	0
4	GAL	Z	2	11/12	0.57	0.20	90,98,116,120	0
3	NAG	Y	2	14/15	0.81	0.11	48,69,77,80	0
4	SIA	Z	3	20/21	0.83	0.13	34,45,58,60	0
3	NAG	Y	1	14/15	0.88	0.11	46,54,64,68	0
4	NAG	a	1	14/15	-	-	125,140,147,147	0
4	GAL	a	2	11/12	-	-	72,90,112,114	0
4	SIA	a	3	20/21	-	-	44,57,71,72	0
4	NAG	b	1	14/15	-	-	97,103,110,110	0
4	GAL	b	2	11/12	-	-	66,76,99,100	0
4	SIA	b	3	20/21	-	-	26,35,46,47	0
4	NAG	c	1	14/15	-	-	99,115,125,128	0
4	GAL	c	2	11/12	-	-	58,69,81,85	0
4	SIA	c	3	20/21	-	-	24,34,46,47	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

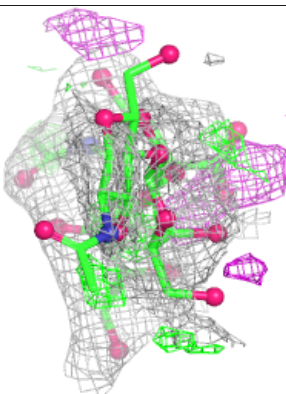
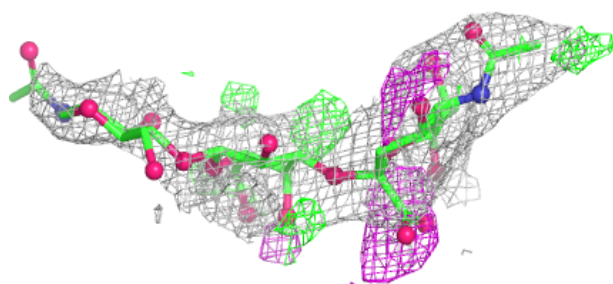
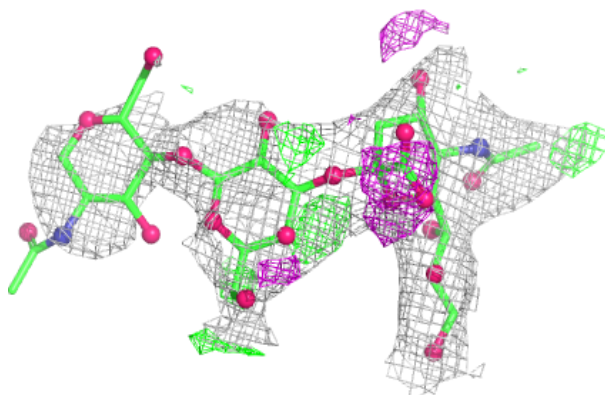


Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

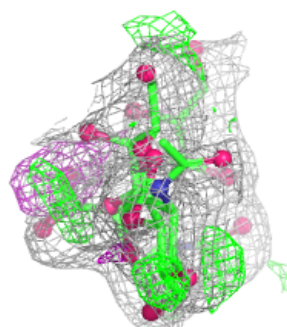
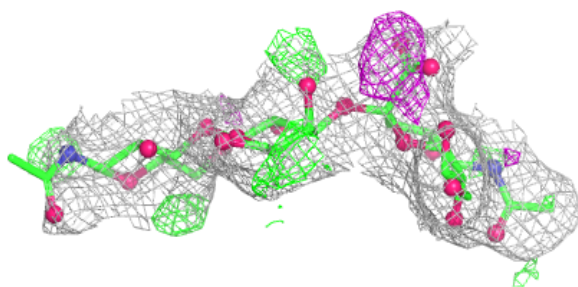
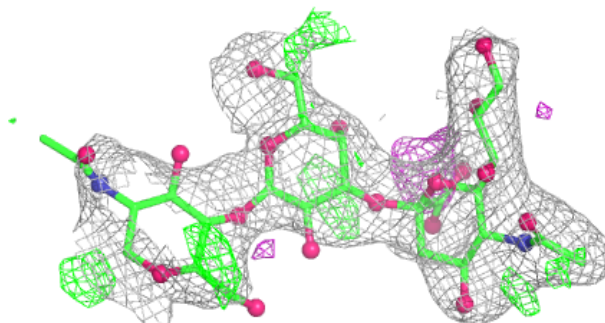
**Electron density around Chain a:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

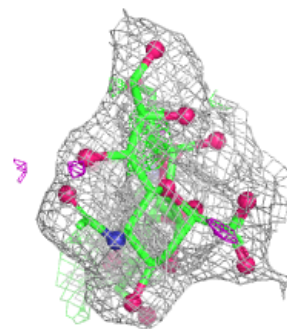
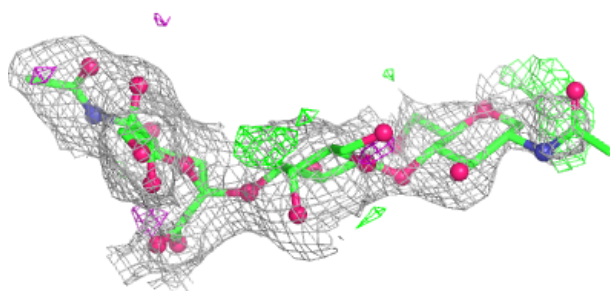
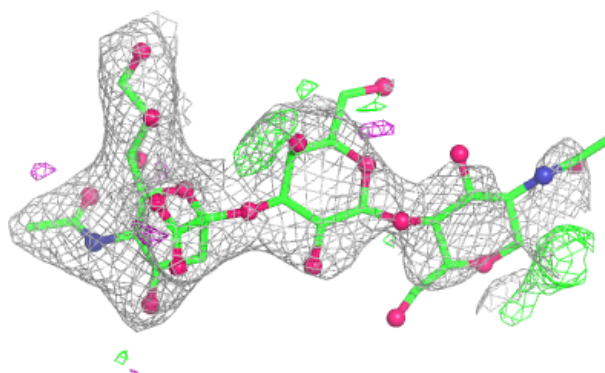


Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain c:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(Å ²)	Q<0.9
5	NAG	W	601	14/15	0.59	0.23	79,87,91,92	0
5	NAG	E	602	14/15	0.62	0.16	54,58,73,77	0
5	NAG	S	601	14/15	0.66	0.17	54,75,88,92	0
5	NAG	O	601	14/15	0.66	0.18	61,88,97,101	0
5	NAG	U	601	14/15	0.70	0.16	80,98,105,113	0
5	NAG	M	601	14/15	0.73	0.15	66,83,89,92	0
5	NAG	Q	601	14/15	0.74	0.15	76,87,98,99	0
5	NAG	K	601	14/15	0.75	0.13	46,71,77,79	0
5	NAG	R	601	14/15	0.76	0.11	32,39,49,50	0
5	NAG	B	601	14/15	0.78	0.10	29,38,43,50	0
5	NAG	C	601	14/15	0.80	0.12	46,67,77,77	0
5	NAG	G	601	14/15	0.82	0.11	43,64,72,74	0
5	NAG	A	601	14/15	0.82	0.10	34,57,68,74	0
5	NAG	V	601	14/15	0.82	0.10	28,38,40,44	0
5	NAG	F	601	14/15	0.82	0.08	25,30,33,36	0
5	NAG	L	601	14/15	0.83	0.10	23,32,38,38	0
5	NAG	E	601	14/15	0.84	0.11	48,62,69,70	0
5	NAG	H	601	14/15	0.85	0.09	22,30,33,33	0
5	NAG	I	601	14/15	0.86	0.10	52,62,65,65	0
5	NAG	X	601	14/15	0.86	0.10	37,46,54,54	0
5	NAG	N	601	14/15	0.88	0.09	40,50,51,54	0
5	NAG	P	601	14/15	0.91	0.07	34,38,44,44	0
5	NAG	D	601	14/15	0.91	0.07	20,28,36,37	0
5	NAG	J	601	14/15	0.92	0.08	18,28,36,38	0
5	NAG	T	601	14/15	0.92	0.07	23,34,41,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.