



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:09 AM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

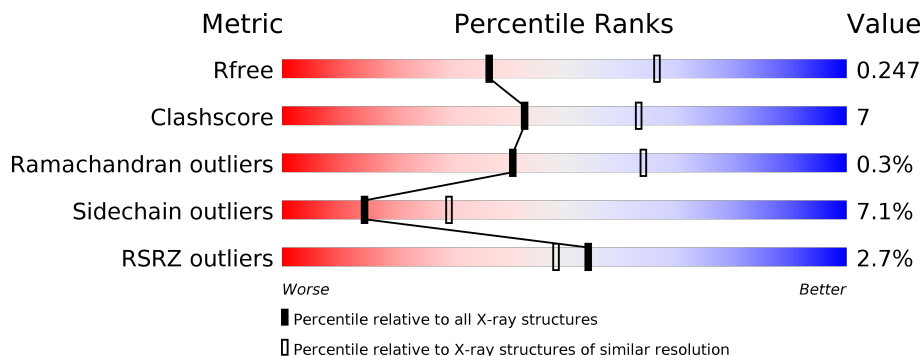
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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.



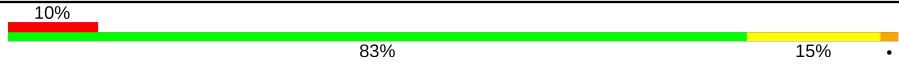
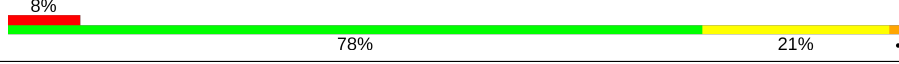



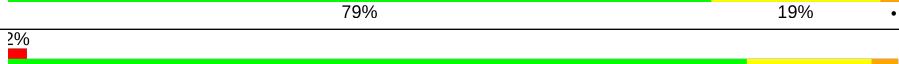
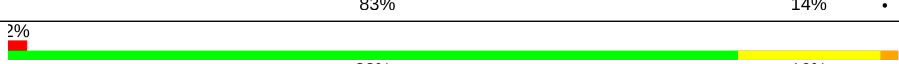
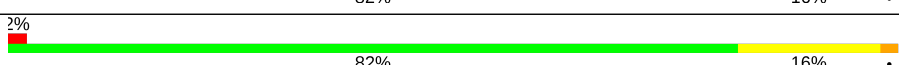
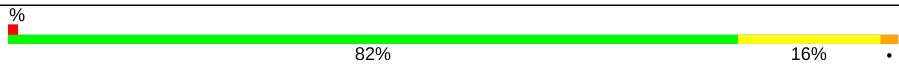

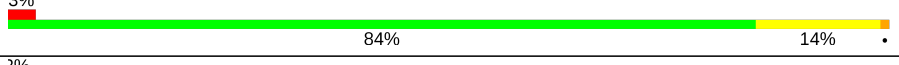
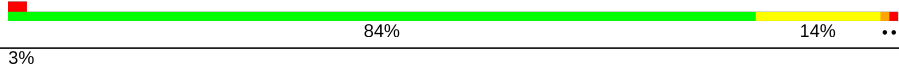

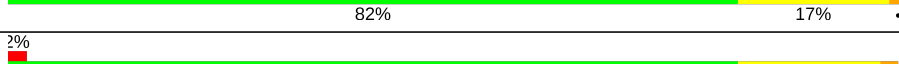
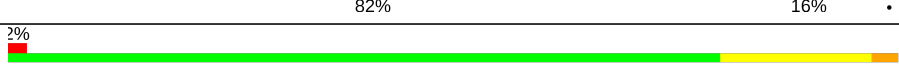

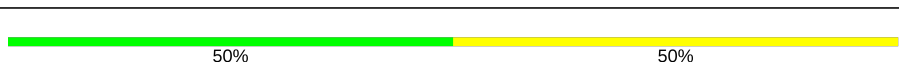

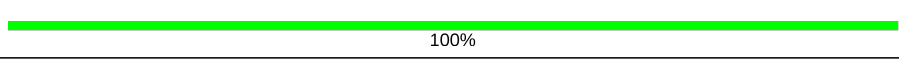



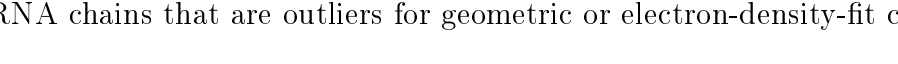
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	C	318	
1	E	318	
1	G	318	
1	I	318	
1	K	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	318	
1	O	318	
1	Q	318	
1	S	318	
1	U	318	
1	W	318	
2	B	174	
2	D	174	
2	F	174	
2	H	174	
2	J	174	
2	L	174	
2	N	174	
2	P	174	
2	R	174	
2	T	174	
2	V	174	
2	X	174	
3	Y	2	
4	Z	3	
4	a	3	
4	b	3	
4	c	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	Z	1	-	-	-	X
4	NAG	a	1	-	-	-	X
4	NAG	b	1	-	-	-	X
4	NAG	c	1	-	-	-	X

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	318	2437	1506	449	465	17	0	0	0
1	C	318	2437	1506	449	465	17	0	0	0
1	E	318	2437	1506	449	465	17	0	0	0
1	G	318	2437	1506	449	465	17	0	0	0
1	I	318	2437	1506	449	465	17	0	0	0
1	K	318	2437	1506	449	465	17	0	0	0
1	M	318	2437	1506	449	465	17	0	0	0
1	O	318	2437	1506	449	465	17	0	0	0
1	Q	318	2437	1506	449	465	17	0	0	0
1	S	318	2436	1506	449	464	17	0	0	0
1	U	318	2437	1506	449	465	17	0	0	0
1	W	318	2437	1506	449	465	17	0	0	0

- Molecule 2 is a protein called hemagglutinin.

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

Continued on next page...

Continued from previous page...

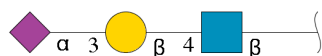
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	H	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	J	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	L	174	Total	C	N	O	S	0	0	0
			1402	866	243	285	8			
2	N	174	Total	C	N	O	S	0	0	0
			1402	866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



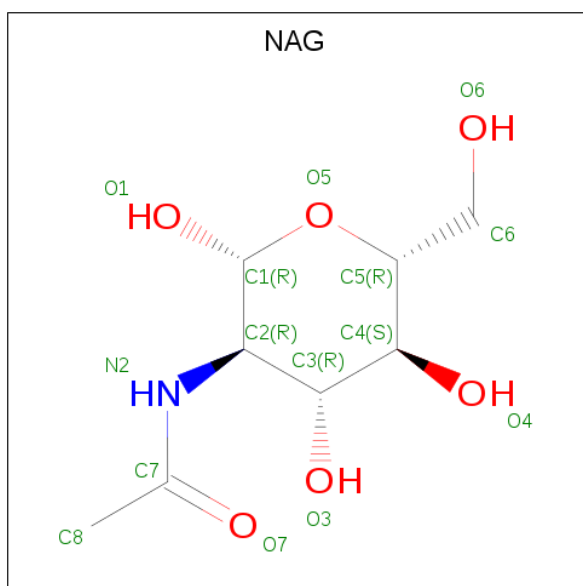
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Z	3	Total	C	N	O	0	0	0
			45	25	2	18			

Continued on next page...

Continued from previous page...

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 (three-letter code: 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	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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

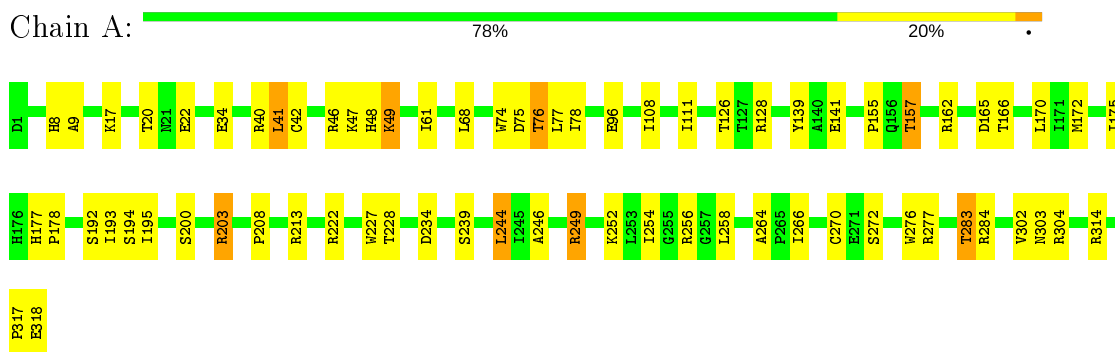
Continued from previous page...

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

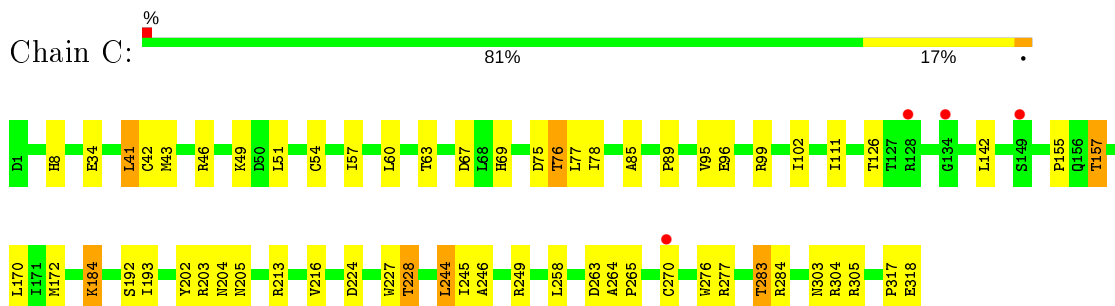
3 Residue-property plots [i](#)

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

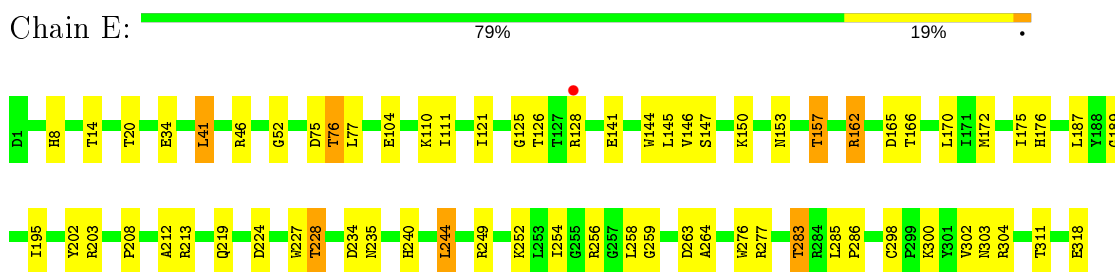
- Molecule 1: hemagglutinin



- Molecule 1: hemagglutinin

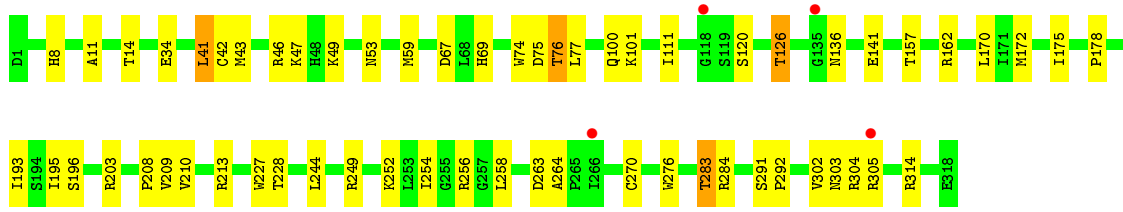


- Molecule 1: hemagglutinin

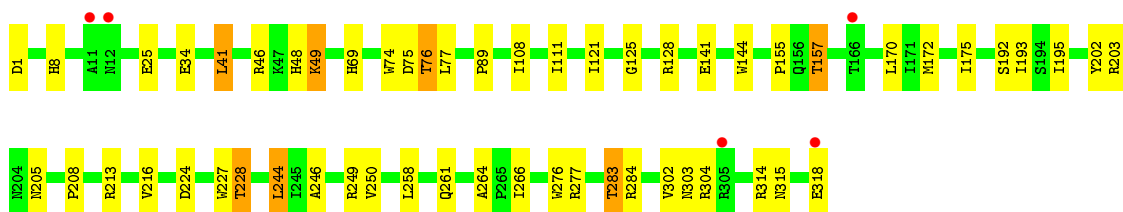
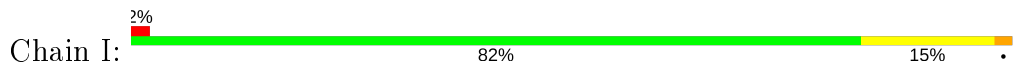


- Molecule 1: hemagglutinin

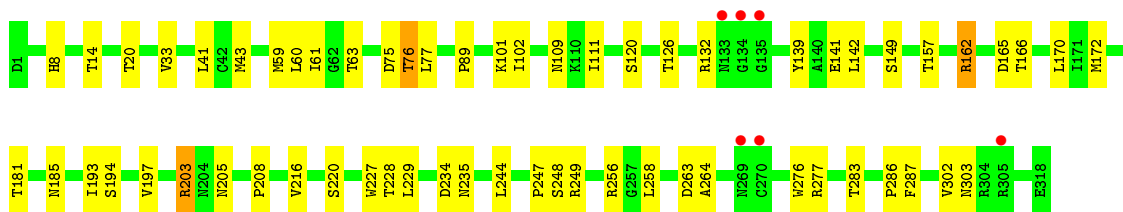
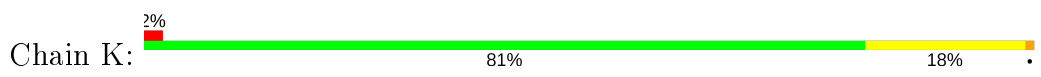




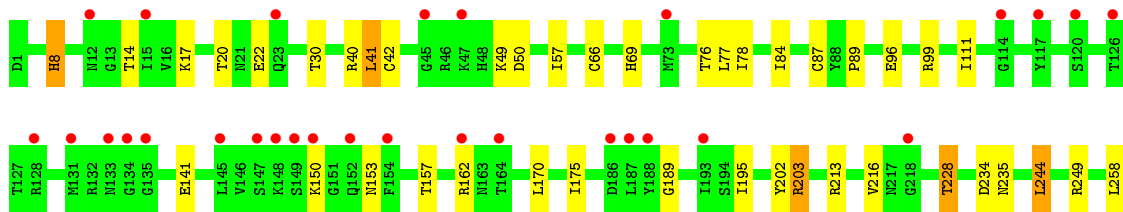
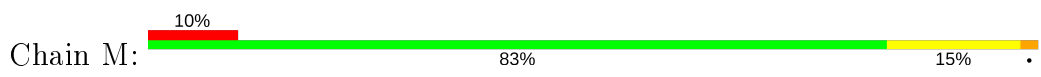
• Molecule 1: hemagglutinin



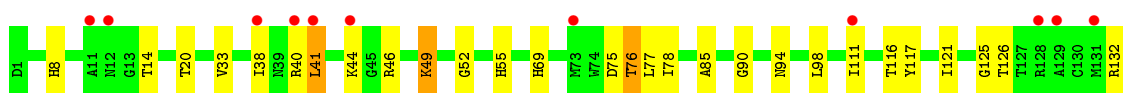
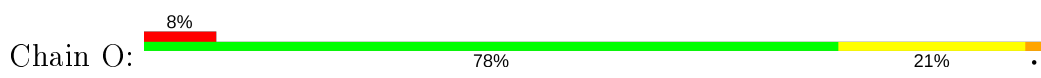
• Molecule 1: hemagglutinin

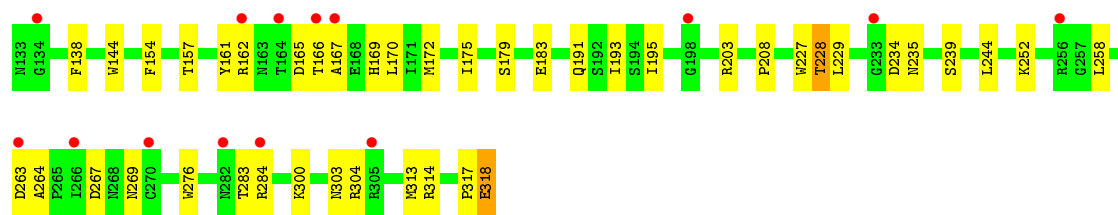


• Molecule 1: hemagglutinin

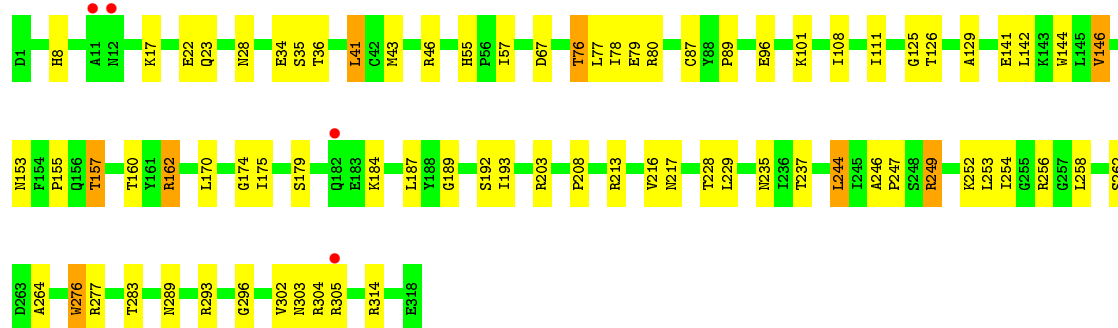
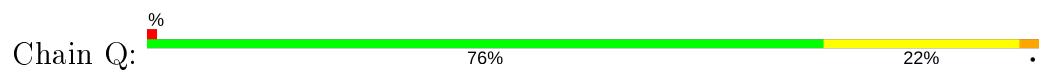


• Molecule 1: hemagglutinin

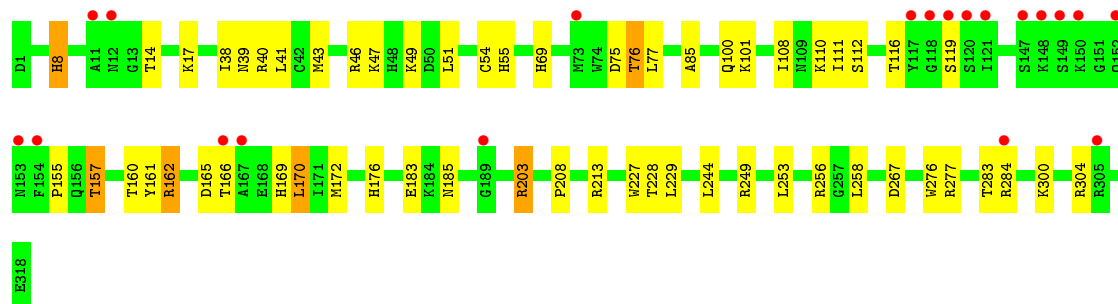
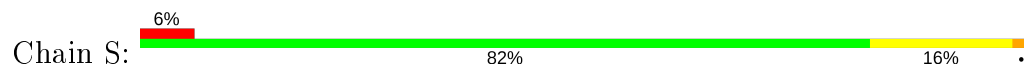




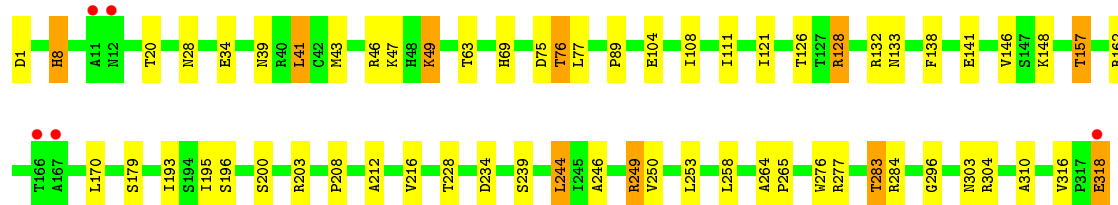
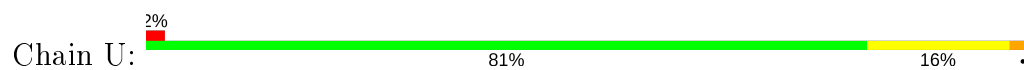
- Molecule 1: hemagglutinin



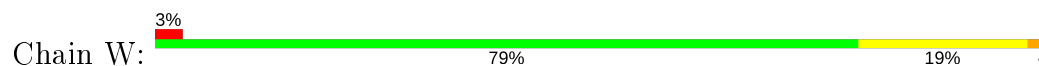
- Molecule 1: hemagglutinin

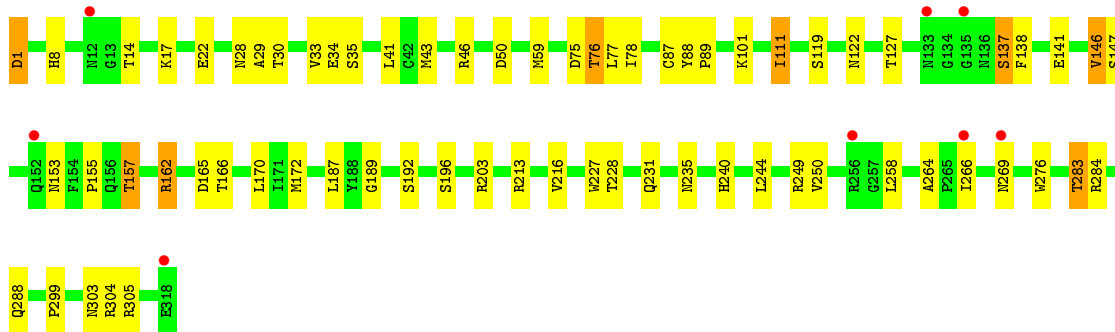


- Molecule 1: hemagglutinin

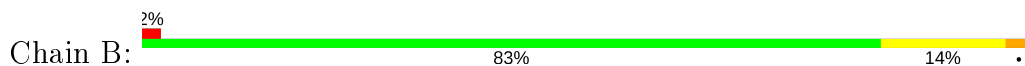


- Molecule 1: hemagglutinin

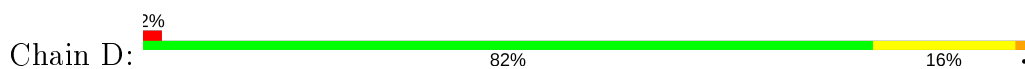




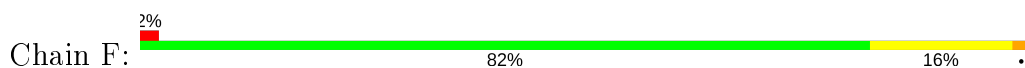
• Molecule 2: hemagglutinin



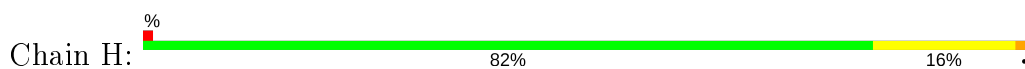
• Molecule 2: hemagglutinin



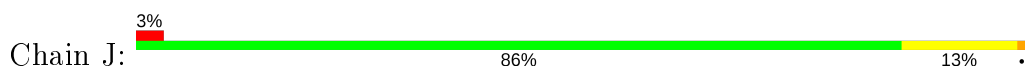
• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin

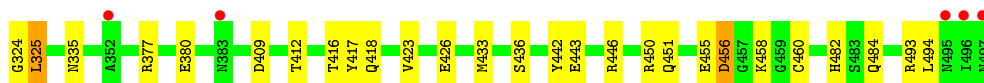
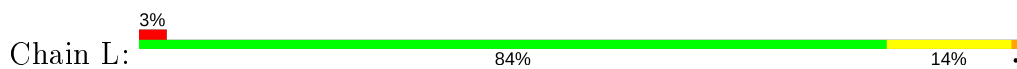


• Molecule 2: hemagglutinin

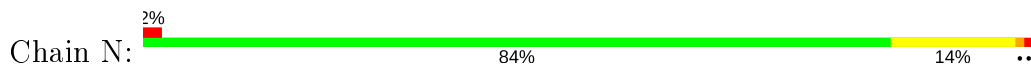


• Molecule 2: hemagglutinin

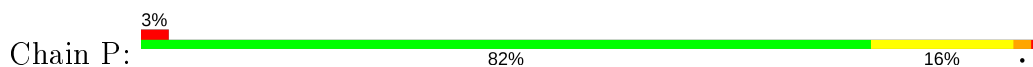




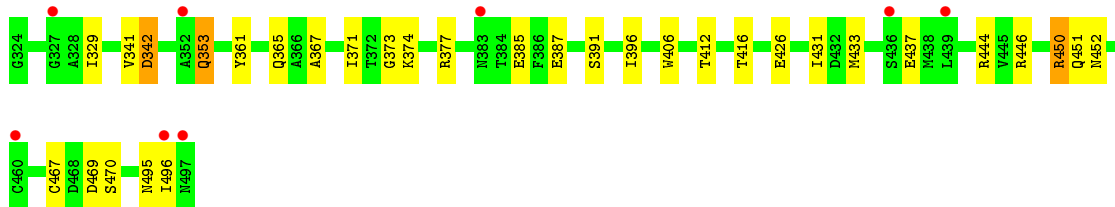
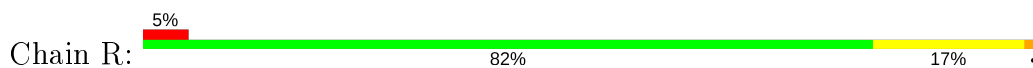
• Molecule 2: hemagglutinin



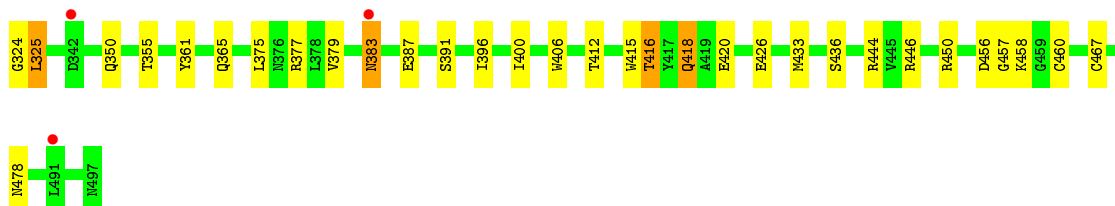
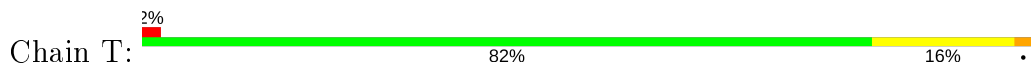
• Molecule 2: hemagglutinin



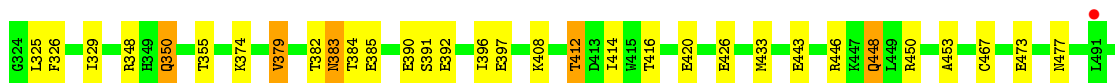
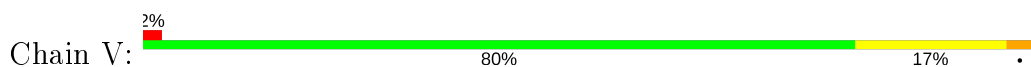
• Molecule 2: hemagglutinin



• Molecule 2: hemagglutinin

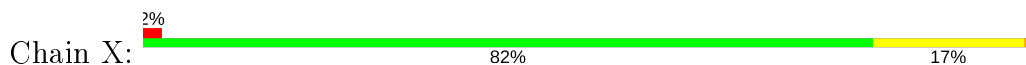


• Molecule 2: hemagglutinin





- 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



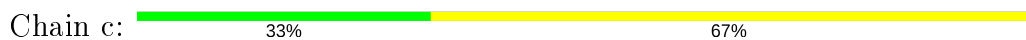
- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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) 89.1 (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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.197 , 0.246 0.197 , 0.247	Depositor DCC
R_{free} test set	13242 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtrriage
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

Xtrriage'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: SIA, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/2486	0.50	0/3368
1	C	0.30	0/2486	0.48	0/3368
1	E	0.31	0/2486	0.49	0/3368
1	G	0.31	0/2486	0.48	0/3368
1	I	0.31	0/2486	0.49	0/3368
1	K	0.31	0/2486	0.49	0/3368
1	M	0.27	0/2486	0.45	0/3368
1	O	0.28	0/2486	0.46	0/3368
1	Q	0.31	0/2486	0.47	0/3368
1	S	0.29	0/2485	0.49	0/3366
1	U	0.30	0/2486	0.48	0/3368
1	W	0.29	0/2486	0.47	0/3368
2	B	0.33	0/1427	0.46	0/1926
2	D	0.34	0/1427	0.50	0/1926
2	F	0.34	0/1427	0.48	0/1926
2	H	0.33	0/1427	0.46	0/1926
2	J	0.31	0/1427	0.47	0/1926
2	L	0.32	0/1427	0.46	0/1926
2	N	0.31	0/1427	0.45	0/1926
2	P	0.33	0/1427	0.47	0/1926
2	R	0.31	0/1427	0.45	0/1926
2	T	0.32	0/1427	0.45	0/1926
2	V	0.31	0/1427	0.48	0/1926
2	X	0.30	0/1427	0.45	0/1926
All	All	0.31	0/46955	0.47	0/63526

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2389	41	0
1	C	2437	0	2389	31	0
1	E	2437	0	2387	40	0
1	G	2437	0	2389	33	0
1	I	2437	0	2389	33	0
1	K	2437	0	2389	27	0
1	M	2437	0	2389	26	0
1	O	2437	0	2389	39	0
1	Q	2437	0	2389	38	0
1	S	2436	0	2389	33	0
1	U	2437	0	2389	34	0
1	W	2437	0	2389	37	0
2	B	1402	0	1298	21	0
2	D	1402	0	1298	27	0
2	F	1402	0	1298	20	0
2	H	1402	0	1298	29	0
2	J	1402	0	1298	20	0
2	L	1402	0	1298	21	0
2	N	1402	0	1298	19	0
2	P	1402	0	1298	22	0
2	R	1402	0	1298	26	0
2	T	1402	0	1298	23	0
2	V	1402	0	1298	26	0
2	X	1402	0	1298	23	0
3	Y	28	0	25	1	0
4	Z	45	0	38	4	0
4	a	45	0	38	0	0
4	b	45	0	38	0	0
4	c	45	0	38	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
6	B	70	0	0	2	0
6	C	71	0	0	5	0
6	D	87	0	0	9	0
6	E	93	0	0	11	0
6	F	64	0	0	3	0
6	G	80	0	0	11	0
6	H	53	0	0	6	0
6	I	102	0	0	8	0
6	J	43	0	0	8	0
6	K	93	0	0	3	0
6	L	53	0	0	3	0
6	M	27	0	0	5	0
6	N	46	0	0	4	0
6	O	40	0	0	5	0
6	P	48	0	0	6	0
6	Q	84	0	0	5	0
6	R	42	0	0	8	0
6	S	64	0	0	7	0
6	T	49	0	0	3	0
6	U	76	0	0	7	0
6	V	44	0	0	9	0
6	W	50	0	0	11	0
6	X	28	0	0	4	0
All	All	48138	0	44744	609	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 (609) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:17:LYS:HE3	1:Q:22:GLU:HG3	1.69	0.74
1:Q:67:ASP:O	6:Q:713:HOH:O	2.05	0.74
2:R:437:GLU:OE1	6:R:719:HOH:O	2.06	0.74
1:S:203:ARG:NH1	6:S:750:HOH:O	2.20	0.74
1:G:252:LYS:HE3	1:G:254:ILE:HD11	1.69	0.73
1:I:41:LEU:HD13	1:I:264:ALA:HB3	1.71	0.73
1:I:314:ARG:NH1	6:I:753:HOH:O	2.21	0.73
2:J:397:GLU:OE2	6:J:738:HOH:O	2.06	0.72
1:I:304:ARG:NH1	2:J:420:GLU:OE1	2.22	0.72
1:E:252:LYS:HE3	1:E:254:ILE:HD11	1.72	0.71
1:M:84:ILE:O	6:M:721:HOH:O	2.07	0.71
2:V:374:LYS:NZ	2:V:426:GLU:OE1	2.20	0.71
5:N:601:NAG:O7	6:N:731:HOH:O	2.08	0.71
1:E:104:GLU:OE1	6:E:770:HOH:O	2.08	0.70
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:C:305:ARG:O	6:C:703:HOH:O	2.11	0.68
1:M:153:ASN:HA	1:M:189:GLY:HA3	1.75	0.68
1:G:314:ARG:NH1	6:G:756:HOH:O	2.27	0.68
1:S:40:ARG:HD2	1:S:267:ASP:HB2	1.76	0.68
1:S:304:ARG:NH1	2:T:420:GLU:OE1	2.27	0.68
1:S:46:ARG:HE	1:S:76:THR:HG21	1.59	0.68
2:X:443:GLU:OE2	2:X:446:ARG:NH1	2.26	0.68
1:W:137:SER:O	6:W:733:HOH:O	2.13	0.67
2:D:443:GLU:OE1	2:D:446:ARG:NH1	2.27	0.67
1:S:185:ASN:OD1	6:S:709:HOH:O	2.13	0.67
1:G:256:ARG:O	6:G:723:HOH:O	2.12	0.67
2:N:377:ARG:NH2	2:N:426:GLU:OE2	2.28	0.67
5:D:601:NAG:O7	6:E:770:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:33:VAL:O	6:W:740:HOH:O	2.12	0.66
1:E:298:CYS:O	6:E:722:HOH:O	2.12	0.66
2:N:443:GLU:OE2	2:N:446:ARG:NH1	2.28	0.66
2:X:377:ARG:NH2	2:X:426:GLU:OE2	2.27	0.66
1:E:286:PRO:O	6:E:767:HOH:O	2.12	0.66
2:V:392:GLU:OE1	6:V:701:HOH:O	2.14	0.66
1:E:212:ALA:O	6:E:721:HOH:O	2.13	0.65
2:P:350:GLN:HG2	2:P:355:THR:HG22	1.76	0.65
1:E:110:LYS:NZ	1:E:141:GLU:OE2	2.26	0.65
1:C:224:ASP:OD1	6:C:729:HOH:O	2.11	0.65
1:K:193:ILE:HG22	1:K:208:PRO:HD2	1.77	0.65
2:J:377:ARG:NH2	2:J:426:GLU:OE2	2.29	0.65
1:M:195:ILE:HG12	1:M:244:LEU:HB2	1.78	0.65
2:N:391:SER:H	2:N:396:ILE:HD11	1.62	0.65
1:I:261:GLN:O	6:I:770:HOH:O	2.14	0.65
2:T:350:GLN:HG3	2:T:355:THR:HG22	1.79	0.65
1:U:212:ALA:O	6:U:728:HOH:O	2.14	0.65
2:D:338:GLU:OE2	6:D:779:HOH:O	2.14	0.65
2:B:450:ARG:HG3	2:B:451:GLN:H	1.62	0.64
2:J:394:SER:OG	6:J:740:HOH:O	2.09	0.64
2:V:412:THR:O	2:V:416:THR:HG23	1.96	0.64
2:R:431:ILE:O	6:R:714:HOH:O	2.15	0.64
1:E:304:ARG:NH1	2:F:420:GLU:OE1	2.31	0.64
1:M:66:CYS:SG	6:M:721:HOH:O	2.55	0.64
2:L:412:THR:O	2:L:416:THR:HG23	1.98	0.64
2:V:348:ARG:NH1	6:V:735:HOH:O	2.29	0.64
1:G:304:ARG:NH1	2:H:420:GLU:OE1	2.31	0.64
1:A:252:LYS:HE3	1:A:254:ILE:HD11	1.80	0.63
1:K:172:MET:HG2	1:K:227:TRP:HB3	1.80	0.63
2:V:494:LEU:HB3	2:V:496:ILE:HG12	1.78	0.63
2:N:470:SER:O	6:N:722:HOH:O	2.16	0.63
1:Q:96:GLU:OE1	6:Q:742:HOH:O	2.15	0.63
2:B:381:LYS:NZ	2:B:382:THR:O	2.32	0.63
2:D:420:GLU:HG3	6:D:728:HOH:O	1.99	0.63
1:I:1:ASP:N	6:I:729:HOH:O	2.32	0.63
1:W:101:LYS:O	6:W:735:HOH:O	2.15	0.63
1:U:41:LEU:HD13	1:U:264:ALA:HB3	1.80	0.62
1:E:283:THR:HG22	1:E:285:LEU:H	1.64	0.62
2:R:377:ARG:NH2	2:R:426:GLU:OE2	2.33	0.62
1:G:196:SER:OG	6:G:745:HOH:O	2.16	0.62
2:J:412:THR:O	2:J:416:THR:HG23	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:443:GLU:OE2	2:L:446:ARG:NH1	2.32	0.62
2:D:412:THR:O	2:D:416:THR:HG23	2.01	0.61
2:F:412:THR:O	2:F:416:THR:HG23	2.01	0.61
1:U:28:ASN:ND2	6:U:761:HOH:O	2.32	0.61
2:H:418:GLN:HG2	2:L:417:TYR:CE1	2.36	0.61
1:O:125:GLY:HA3	1:O:144:TRP:HB3	1.83	0.61
2:D:408:LYS:NZ	6:D:716:HOH:O	2.04	0.61
2:F:418:GLN:NE2	6:F:734:HOH:O	2.25	0.61
2:P:443:GLU:OE1	2:P:446:ARG:NH1	2.33	0.60
1:A:41:LEU:HD23	1:A:78:ILE:HD13	1.82	0.60
2:R:452:ASN:OD1	6:R:707:HOH:O	2.16	0.60
1:E:34:GLU:HB2	1:E:283:THR:HG21	1.84	0.60
2:J:387:GLU:HB2	6:J:728:HOH:O	2.01	0.60
1:U:304:ARG:NH1	2:V:420:GLU:OE1	2.34	0.60
1:O:117:TYR:HB3	1:O:121:ILE:HD12	1.84	0.60
1:A:46:ARG:HE	1:A:76:THR:HG21	1.66	0.60
2:B:418:GLN:OE1	2:D:418:GLN:NE2	2.34	0.60
1:C:41:LEU:HD23	1:C:78:ILE:HD13	1.82	0.60
1:U:8:HIS:HD2	6:V:731:HOH:O	1.84	0.60
1:O:304:ARG:NH1	2:P:420:GLU:OE1	2.34	0.59
1:S:256:ARG:NH2	2:T:387:GLU:OE1	2.36	0.59
1:A:172:MET:HG2	1:A:227:TRP:HB3	1.84	0.59
2:R:469:ASP:OD1	6:R:718:HOH:O	2.17	0.59
2:N:455:GLU:OE1	2:P:446:ARG:NH2	2.36	0.59
1:Q:41:LEU:HD13	1:Q:264:ALA:HB3	1.85	0.59
1:O:55:HIS:HB3	1:O:85:ALA:HB2	1.84	0.59
2:N:412:THR:O	2:N:416:THR:HG23	2.03	0.59
2:T:412:THR:O	2:T:416:THR:HG22	2.02	0.59
2:J:349:HIS:HE1	6:J:729:HOH:O	1.85	0.58
1:S:165:ASP:OD1	1:S:166:THR:N	2.36	0.58
1:M:303:ASN:H	2:N:416:THR:HG22	1.69	0.58
1:C:96:GLU:OE2	1:C:99:ARG:NH2	2.35	0.58
1:K:234:ASP:HA	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:O:161:TYR:HH	1:O:169:HIS:HD1	1.52	0.58
1:W:304:ARG:NH1	2:X:420:GLU:OE1	2.37	0.58
1:I:34:GLU:HB2	1:I:283:THR:HG21	1.85	0.57
1:K:141:GLU:OE1	1:K:249:ARG:HD3	2.03	0.57

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:LEU:HD13	1:I:246:ALA:HB2	1.89	0.55
2:X:488:GLU:O	2:X:492:ASN:ND2	2.40	0.55
1:O:162:ARG:NH2	5:O:601:NAG:O6	2.40	0.54
2:P:412:THR:O	2:P:416:THR:HG23	2.05	0.54
1:I:284:ARG:HB3	2:J:379:VAL:HG22	1.89	0.54
1:O:132:ARG:NH1	1:O:138:PHE:O	2.39	0.54
2:P:496:ILE:HD12	2:P:497:ASN:HB2	1.89	0.54
2:T:377:ARG:NH2	2:T:426:GLU:OE2	2.41	0.54
1:A:304:ARG:NH1	2:B:420:GLU:OE1	2.40	0.54
1:I:89:PRO:HB3	1:I:216:VAL:HB	1.89	0.54
1:O:161:TYR:OH	1:O:169:HIS:ND1	2.37	0.54
2:J:473:GLU:O	2:J:477:ASN:HB2	2.08	0.54
1:Q:193:ILE:HG22	1:Q:208:PRO:HD2	1.87	0.54
2:R:450:ARG:HG3	2:R:451:GLN:H	1.73	0.54
1:U:89:PRO:HB3	1:U:216:VAL:HB	1.89	0.54
1:A:47:LYS:NZ	6:A:804:HOH:O	2.41	0.54
1:S:161:TYR:OH	1:S:169:HIS:ND1	2.41	0.54
1:U:162:ARG:NH2	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:E:302:VAL:HA	2:F:416:THR:HG22	1.91	0.53
1:K:303:ASN:H	2:L:416:THR:HG22	1.73	0.53
1:O:90:GLY:O	6:O:709:HOH:O	2.18	0.53
1:U:195:ILE:HG12	1:U:244:LEU:HB2	1.91	0.53
2:J:420:GLU:HG3	6:J:720:HOH:O	2.08	0.53
2:J:494:LEU:HD22	2:L:494:LEU:HD11	1.90	0.53
1:U:49:LYS:HD2	1:U:69:HIS:ND1	2.24	0.53
1:O:52:GLY:O	6:O:712:HOH:O	2.19	0.53
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:161:TYR:HH	1:S:169:HIS:HD1	1.58	0.52
1:U:20:THR:O	2:X:373:GLY:HA3	2.09	0.52
1:C:75:ASP:OD2	1:C:76:THR:HG22	2.09	0.52
1:E:234:ASP:HA	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:111:ILE:HG23	1:W:250:VAL:HG12	1.91	0.51
1:W:141:GLU:OE1	1:W:249:ARG:HD3	2.10	0.51
2:F:443:GLU:OE2	2:F:446:ARG:NH1	2.44	0.51
1:I:25:GLU:HG2	1:I:315:ASN:HB3	1.91	0.51
1:O:317:PRO:O	1:O:318:GLU:HB2	2.10	0.51
2:X:442:TYR:OH	2:X:455:GLU:OE2	2.20	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
2:N:381:LYS:NZ	2:N:382:THR:O	2.44	0.51
1:E:128:ARG:HG2	4:Z:3:SIA:O1A	2.10	0.51
1:K:75:ASP:OD2	1:K:76:THR:HG22	2.11	0.50
2:N:450:ARG:HB3	6:R:704:HOH:O	2.11	0.50
2:R:329:ILE:O	6:R:701:HOH:O	2.19	0.50
2:V:355:THR:O	6:V:722:HOH:O	2.19	0.50
1:I:46:ARG:NH2	6:I:739:HOH:O	2.45	0.50
1:M:41:LEU:HD23	1:M:78:ILE:HD13	1.94	0.50
2:X:377:ARG:NH1	6:X:707:HOH:O	2.41	0.50
1:G:178:PRO:HB2	1:G:210:VAL:HG22	1.94	0.50
1:K:303:ASN:H	2:L:416:THR:CG2	2.24	0.50
1:M:89:PRO:HB3	1:M:216:VAL:HB	1.92	0.50
1:Q:244:LEU:HD13	1:Q:246:ALA:HB2	1.92	0.50
1:W:46:ARG:NH2	6:W:739:HOH:O	2.44	0.50
1:A:175:ILE:HD12	1:A:195:ILE:HD13	1.93	0.50
1:A:203:ARG:NH2	1:E:224:ASP:OD2	2.43	0.50
2:H:446:ARG:HH12	2:H:447:LYS:HE3	1.77	0.50
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:387:GLU:N	6:P:713:HOH:O	2.15	0.47
1:Q:141:GLU:OE1	1:Q:249:ARG:HD3	2.13	0.47
1:U:141:GLU:OE1	1:U:249:ARG:HD3	2.13	0.47
1:U:1:ASP:HA	2:V:350:GLN:O	2.14	0.47
1:W:41:LEU:HD23	1:W:78:ILE:HD13	1.95	0.47
2:X:450:ARG:HG3	2:X:451:GLN:H	1.79	0.47
2:B:344:TRP:HH2	2:B:371:ILE:HD12	1.78	0.47
2:H:418:GLN:HG2	2:L:417:TYR:HE1	1.77	0.47
1:W:172:MET:HG2	1:W:227:TRP:HB3	1.96	0.47
1:A:244:LEU:HD13	1:A:246:ALA:HB2	1.97	0.47
1:K:101:LYS:HE3	1:K:229:LEU:HD11	1.96	0.47
1:O:98:LEU:HD13	1:O:227:TRP:CD2	2.50	0.47
2:R:374:LYS:NZ	2:R:426:GLU:O	2.48	0.47
1:S:155:PRO:O	1:S:157:THR:HG22	2.13	0.47
1:W:14:THR:HG21	1:W:29:ALA:HB3	1.96	0.47
1:A:303:ASN:H	2:B:416:THR:HG21	1.80	0.47
1:E:41:LEU:HD13	1:E:264:ALA:HB3	1.97	0.47
1:G:43:MET:HE2	1:G:43:MET:HB3	1.83	0.47
1:I:303:ASN:H	2:J:416:THR:CG2	2.27	0.47
1:U:318:GLU:OE2	6:U:736:HOH:O	2.21	0.47
1:E:234:ASP:OD1	1:E:235:ASN:N	2.47	0.47
1:E:153:ASN:HA	1:E:189:GLY:HA3	1.97	0.47
2:F:446:ARG:HH12	2:F:447:LYS:HE3	1.79	0.47
1:G:193:ILE:HG22	1:G:208:PRO:HD2	1.97	0.47
1:O:41:LEU:HD13	1:O:264:ALA:HB3	1.96	0.47
1:S:17:LYS:NZ	2:T:420:GLU:OE2	2.39	0.47
2:B:446:ARG:NH2	2:F:455:GLU:OE1	2.48	0.47
1:E:125:GLY:HA3	1:E:144:TRP:HB3	1.96	0.47
2:L:377:ARG:O	2:L:380:GLU:HG2	2.15	0.47
1:I:49:LYS:HD2	1:I:69:HIS:ND1	2.30	0.47
1:O:40:ARG:NE	1:O:267:ASP:OD2	2.48	0.47
1:W:122:ASN:HB3	1:W:146:VAL:HG12	1.95	0.47
1:G:284:ARG:HB3	2:H:379:VAL:HG13	1.97	0.47
2:R:391:SER:O	6:R:737:HOH:O	2.20	0.47
2:F:342:ASP:HB3	2:F:359:ALA:HB2	1.97	0.46
1:Q:146:VAL:HG22	1:Q:187:LEU:HB3	1.96	0.46
2:N:408:LYS:HG2	2:R:406:TRP:CH2	2.50	0.46
2:L:446:ARG:HD2	2:L:455:GLU:OE1	2.14	0.46
1:M:40:ARG:NE	1:M:267:ASP:OD2	2.45	0.46
2:V:408:LYS:O	2:V:412:THR:HG23	2.15	0.46
2:F:391:SER:H	2:F:396:ILE:HD11	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:ASN:H	2:F:416:THR:HG21	1.80	0.46
2:H:329:ILE:O	6:H:701:HOH:O	2.21	0.46
2:H:412:THR:O	2:H:416:THR:HG23	2.15	0.46
2:B:406:TRP:CZ2	2:D:408:LYS:HE2	2.51	0.46
1:E:141:GLU:OE1	1:E:249:ARG:HD3	2.16	0.46
1:A:193:ILE:HG21	1:A:208:PRO:HG2	1.95	0.46
1:K:162:ARG:HG3	1:K:235:ASN:OD1	2.15	0.46
1:Q:34:GLU:OE2	1:Q:36:THR:N	2.33	0.46
1:W:146:VAL:HG22	1:W:187:LEU:HB3	1.96	0.46
1:W:153:ASN:HA	1:W:189:GLY:HA3	1.98	0.46
1:I:175:ILE:HD12	1:I:195:ILE:HD13	1.97	0.46
1:Q:108:ILE:HG12	1:Q:253:LEU:HD23	1.97	0.46
1:Q:296:GLY:HA2	2:R:385:GLU:HG3	1.97	0.46
1:A:128:ARG:NH1	1:U:133:ASN:O	2.49	0.46
1:E:303:ASN:H	2:F:416:THR:CG2	2.29	0.46
1:G:41:LEU:HD13	1:G:264:ALA:HB3	1.97	0.46
1:K:194:SER:OG	1:K:205:ASN:ND2	2.46	0.46
2:T:456:ASP:HB2	2:T:460:CYS:O	2.15	0.46
2:D:383:ASN:HA	2:D:384:THR:HB	1.98	0.46
1:M:202:TYR:CD2	1:M:228:THR:HG21	2.51	0.46
2:X:448:GLN:NE2	2:X:478:ASN:HA	2.30	0.46
2:T:400:ILE:HD12	2:T:400:ILE:HA	1.87	0.46
1:C:172:MET:HG2	1:C:227:TRP:HB3	1.98	0.45
1:C:317:PRO:O	1:C:318:GLU:HB2	2.16	0.45
1:C:60:LEU:HD11	1:C:102:ILE:HD11	1.97	0.45
2:N:448:GLN:OE1	2:N:478:ASN:HA	2.15	0.45
2:N:478:ASN:O	2:N:478:ASN:ND2	2.49	0.45
1:W:59:MET:HE2	1:W:59:MET:HB3	1.87	0.45
1:E:162:ARG:HE	1:E:162:ARG:HB2	1.59	0.45
1:G:303:ASN:H	2:H:416:THR:HG21	1.81	0.45
1:O:303:ASN:H	2:P:416:THR:HG21	1.81	0.45
2:T:446:ARG:NH2	2:X:455:GLU:OE1	2.49	0.45
1:M:289:ASN:HD22	1:M:305:ARG:HA	1.81	0.45
2:P:446:ARG:HH12	2:P:447:LYS:HE3	1.80	0.45
1:Q:155:PRO:O	1:Q:157:THR:HG22	2.17	0.45
2:T:456:ASP:HB3	2:T:458:LYS:H	1.81	0.45
1:A:74:TRP:CH2	1:A:108:ILE:HG13	2.50	0.45
1:A:34:GLU:HB2	1:A:283:THR:HG21	1.99	0.45
2:P:450:ARG:HB3	6:P:710:HOH:O	2.15	0.45
1:S:55:HIS:HB3	1:S:85:ALA:HB2	1.98	0.45
1:C:202:TYR:CD2	1:C:228:THR:HG21	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:302:VAL:HA	2:R:416:THR:HG22	1.98	0.45
1:S:8:HIS:CE1	6:S:701:HOH:O	2.67	0.45
1:W:288:GLN:HG3	1:W:299:PRO:HB2	1.99	0.45
2:D:383:ASN:HA	2:D:384:THR:CB	2.46	0.45
2:H:342:ASP:HB3	2:H:359:ALA:HB2	1.98	0.45
1:Q:34:GLU:OE2	1:Q:35:SER:N	2.49	0.45
1: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:E:219:GLN:NE2	4:Z:3:SIA:C1	2.79	0.45
1:A:165:ASP:OD1	1:A:166:THR:N	2.44	0.45
1:G:209:VAL:HG21	1:I:205:ASN:ND2	2.32	0.45
1:M:8:HIS:HE1	6:M:707:HOH:O	2.00	0.45
1:A:256:ARG:NE	6:A:776:HOH:O	2.47	0.45
1:E:300:LYS:HG3	2:F:415:TRP:CE2	2.51	0.45
2:H:383:ASN:ND2	2:H:383:ASN:O	2.50	0.45
1:I:193:ILE:HG21	1:I:208:PRO:HG2	1.98	0.45
1:Q:80:ARG:NH1	1:Q:262:SER:O	2.43	0.45
1:A:61:ILE:O	1:A:139:TYR:HB3	2.18	0.44
1:E:202:TYR:CD2	1:E:228:THR:HG21	2.52	0.44
1:W:17:LYS:NZ	2:X:420:GLU:OE2	2.39	0.44
1:E:75:ASP:OD2	1:E:76:THR:HG22	2.17	0.44
1:Q:162:ARG:HG3	1:Q:235:ASN:OD1	2.17	0.44
1:C:142:LEU:HB3	1:C:245:ILE:HG22	2.00	0.44
2:B:373:GLY:HA3	1:E:20:THR:O	2.18	0.44
1:O:49:LYS:HD2	1:O:69:HIS:ND1	2.32	0.44
1:O:20:THR:O	2:R:373:GLY:HA3	2.17	0.44
1:U:121:ILE:HD11	1:U:157:THR:HG21	1.99	0.44
2:R:361:TYR:CZ	2:R:365:GLN:HG3	2.53	0.44
2:F:367:ALA:O	2:F:371:ILE:HG12	2.18	0.44
2:H:377:ARG:O	2:H:380:GLU:HG2	2.18	0.44
2:T:391:SER:H	2:T:396:ILE:HD11	1.82	0.44
2:B:473:GLU:O	2:B:477:ASN:HB2	2.18	0.44
1:G:175:ILE:HD12	1:G:195:ILE:HD13	1.98	0.44
1:C:155:PRO:O	1:C:157:THR:HG22	2.16	0.44
1:E:52:GLY:O	6:E:704:HOH:O	2.21	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:170:LEU:HD22	1:S:229:LEU:HD21	2.01	0.43
1:A:9:ALA:HB2	2:B:336:GLY:HA3	2.00	0.43
1:A:20:THR:O	2:D:373:GLY:HA3	2.18	0.43
1:E:176:HIS:O	1:E:208:PRO:HB3	2.18	0.43
2:H:327:GLY:O	2:H:331:GLY:HA3	2.18	0.43
1:M:203:ARG:O	1:M:203:ARG:HG3	2.18	0.43
1:O:167:ALA:HB3	1:O:252:LYS:HE3	2.00	0.43
1:S:46:ARG:HB2	1:S:75:ASP:OD2	2.19	0.43
1:A:49:LYS:NZ	6:A:740:HOH:O	2.40	0.43
1:S:300:LYS:HG3	2:T:415:TRP:CE2	2.53	0.43
1:A:213:ARG:HD2	1:A:222:ARG:HG2	2.00	0.43
2:D:342:ASP:HB3	2:D:359:ALA:HB2	2.00	0.43
1:G:314:ARG:HG3	2:H:431:ILE:HG23	2.01	0.43
2:H:450:ARG:HB3	6:H:721:HOH:O	2.18	0.43
1:M:49:LYS:HD2	1:M:69:HIS:ND1	2.34	0.43
1:A:317:PRO:O	1:A:318:GLU:HB2	2.18	0.43
1:U:264:ALA:HA	1:U:265:PRO:HD3	1.91	0.43
1:W:165:ASP:OD1	1:W:166:THR:N	2.43	0.43
1:O:44:LYS:HD2	1:O:269:ASN:O	2.18	0.43
1:Q:252:LYS:HE3	1:Q:254:ILE:HD11	1.99	0.43
2:L:456:ASP:CG	2:L:460:CYS:HB2	2.39	0.43
1:Q:174:GLY:O	1:Q:175:ILE:HD13	2.18	0.43
1:Q:46:ARG:HE	1:Q:76:THR:HG21	1.84	0.43
1:A:42:CYS:HB3	1:A:270:CYS:O	2.19	0.43
1:S:101:LYS:HE3	1:S:229:LEU:HD11	2.01	0.43
1:U:34:GLU:HB2	1:U:283:THR:HG21	2.01	0.43
2:D:414:ILE:O	2:D:418:GLN:HG3	2.19	0.43
1:S:110:LYS:HB2	1:S:249:ARG:HH21	1.83	0.43
1:S:160:THR:HG22	1:S:162:ARG:HD2	2.00	0.42
1:W:41:LEU:O	1:W:43:MET:HG2	2.19	0.42
1:G:302:VAL:HA	2:H:416:THR:HG22	2.01	0.42
1:K:197:VAL:O	1:K:203:ARG:HA	2.19	0.42
1:S:47:LYS:HB3	1:S:47:LYS:HE2	1.86	0.42
1:G:34:GLU:HB2	1:G:283:THR:HG21	2.00	0.42
1:G:67:ASP:CG	6:G:743:HOH:O	2.50	0.42
2:T:457:GLY:N	6:T:725:HOH:O	2.38	0.42
1:O:300:LYS:HD3	1:O:300:LYS:HA	1.83	0.42
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:A:200:SER:OG	1:A:234:ASP:OD1	2.29	0.42
1:G:101:LYS:O	6:G:764:HOH:O	2.21	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:303:ASN:H	2:X:416:THR:CG2	2.32	0.42
1:A:48:HIS:CD2	1:A:266:ILE:HD13	2.55	0.42
1:G:193:ILE:HG21	1:G:208:PRO:HG2	2.00	0.42
1:I:74:TRP:CH2	1:I:108:ILE:HG13	2.55	0.42
2:J:381:LYS:HA	2:J:381:LYS:HD2	1.83	0.42
1:K:165:ASP:OD1	1:K:166:THR:N	2.42	0.42
1:O:313:MET:HG3	1:O:314:ARG:O	2.20	0.42
1:C:284:ARG:HB3	2:D:379:VAL:HG22	2.02	0.42
1:O:175:ILE:HD12	1:O:195:ILE:HD13	2.01	0.42
1:C:51:LEU:HB3	1:C:54:CYS:O	2.20	0.42
1:G:46:ARG:HB2	1:G:75:ASP:OD2	2.19	0.42
2:H:400:ILE:HD12	2:H:400:ILE:HA	1.89	0.42
1:K:41:LEU:HD13	1:K:264:ALA:HB3	2.02	0.42
1:M:96:GLU:OE2	1:M:99:ARG:NH2	2.37	0.42
1:O:75:ASP:OD2	1:O:76:THR:HG22	2.20	0.42
1:Q:276:TRP:HB2	1:Q:293:ARG:O	2.19	0.42
2:B:422:LEU:O	2:B:426:GLU:HG2	2.18	0.42
1:I:75:ASP:OD2	1:I:76:THR:HG22	2.19	0.42
1:Q:101:LYS:HE3	1:Q:229:LEU:HD11	2.02	0.42
1:Q:43:MET:HB3	1:Q:43:MET:HE2	1.96	0.42
1:A:40:ARG:NH2	6:A:800:HOH:O	2.30	0.42
1:O:33:VAL:O	6:O:706:HOH:O	2.21	0.42
1:Q:55:HIS:CE1	1:Q:57:ILE:HG12	2.55	0.42
1:C:89:PRO:HB3	1:C:216:VAL:HB	2.02	0.41
1:C:244:LEU:HD13	1:C:246:ALA:HB2	2.02	0.41
1:C:42:CYS:HB3	1:C:270:CYS:O	2.20	0.41
1:I:48:HIS:CD2	1:I:266:ILE:HD13	2.55	0.41
1:M:284:ARG:HB3	2:N:379:VAL:HG13	2.02	0.41
2:R:367:ALA:O	2:R:371:ILE:HG12	2.19	0.41
1:U:296:GLY:HA2	2:V:385:GLU:HG3	2.01	0.41
1:W:127:THR:HG22	6:W:733:HOH:O	2.19	0.41
1:K:172:MET:O	1:K:247:PRO:HB3	2.19	0.41
1:A:17:LYS:HE2	1:A:22:GLU:HG3	2.02	0.41
1:E:240:HIS:CE1	1:E:244:LEU:HD12	2.55	0.41
2:F:377:ARG:O	2:F:380:GLU:HG2	2.20	0.41
1:K:61:ILE:HD12	1:K:139:TYR:CE1	2.55	0.41
2:H:446:ARG:NH2	2:L:455:GLU:OE1	2.53	0.41
1:O:193:ILE:HG21	1:O:208:PRO:HG2	2.01	0.41
2:P:386:PHE:HA	6:P:713:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HA	2:B:416:THR:HG22	2.03	0.41
1:A:42:CYS:HB2	1:A:272:SER:HB3	2.02	0.41
1:A:68:LEU:HB2	6:A:739:HOH:O	2.20	0.41
1:C:57:ILE:HD12	1:C:95:VAL:HG23	2.02	0.41
2:L:324:GLY:HA3	6:L:740:HOH:O	2.20	0.41
1:M:42:CYS:HB2	1:M:272:SER:HB2	2.02	0.41
2:N:451:GLN:O	2:N:493:ARG:NH1	2.48	0.41
2:X:444:ARG:HD3	2:X:478:ASN:OD1	2.20	0.41
2:J:377:ARG:NH2	6:J:714:HOH:O	2.52	0.41
1:K:302:VAL:HA	2:L:416:THR:HG22	2.02	0.41
6:P:708:HOH:O	2:R:450:ARG:HB3	2.20	0.41
1:A:177:HIS:HA	1:A:178:PRO:HD3	1.84	0.41
1:A:46:ARG:HB2	1:A:75:ASP:OD2	2.21	0.41
1:C:303:ASN:HB2	2:D:416:THR:HG21	2.02	0.41
1:E:175:ILE:HD12	1:E:195:ILE:HD13	2.01	0.41
1:E:172:MET:HG2	1:E:227:TRP:HB3	2.03	0.41
1:E:311:THR:HG21	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:318:GLU:O	6:E:708:HOH:O	2.22	0.41
2:H:433:MET:O	2:H:436:SER:HB3	2.21	0.41
2:H:455:GLU:OE1	2:J:446:ARG:NH2	2.54	0.41
1:O:234:ASP:OD1	1:O:235:ASN:N	2.54	0.41
1:I:125:GLY:HA3	1:I:144:TRP:HB3	2.03	0.41
1:K:181:THR:HG22	1:K:185:ASN:ND2	2.36	0.41
1:Q:289:ASN:ND2	1:Q:305:ARG:HA	2.36	0.41
1:U:75:ASP:OD2	1:U:76:THR:HG22	2.21	0.41
1:C:43:MET:HE2	1:C:43:MET:HB3	1.94	0.41
1:G:59:MET:HE1	1:G:74:TRP:CH2	2.55	0.41
2:J:400:ILE:HA	2:J:400:ILE:HD12	1.91	0.41
1:Q:153:ASN:HA	1:Q:189:GLY:HA3	2.01	0.41
1:Q:142:LEU:HD23	1:Q:247:PRO:HA	2.03	0.41
1:E:145:LEU:HB2	6:E:715:HOH:O	2.20	0.41
2:H:456:ASP:HB2	2:H:460:CYS:HB2	2.02	0.41
1:I:74:TRP:HH2	1:I:108:ILE:HG13	1.85	0.41
1:I:155:PRO:O	1:I:157:THR:HG22	2.21	0.41
1:K:286:PRO:HG2	1:K:287:PHE:CD2	2.56	0.41
1:S:176:HIS:O	1:S:208:PRO:HB3	2.20	0.41
1:S:43:MET:O	1:S:46:ARG:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:ASN:OD1	6:K:779:HOH:O	2.22	0.41
1:K:43:MET:HE2	1:K:43:MET:HB3	1.94	0.41
1:M:20:THR:O	2:P:373:GLY:HA3	2.21	0.41
1:C:63:THR:OG1	1:C:85:ALA:O	2.33	0.40
1:G:291:SER:HA	1:G:292:PRO:HD3	1.87	0.40
1:O:179:SER:OG	1:O:183:GLU:OE1	2.38	0.40
2:P:381:LYS:HD2	2:P:381:LYS:HA	1.91	0.40
1:Q:87:CYS:HB2	1:Q:129:ALA:O	2.20	0.40
4:Z:3:SIA:O10	4:Z:3:SIA:O7	2.32	0.40
1:O:228:THR:HG22	1:O:229:LEU:H	1.86	0.40
2:P:377:ARG:O	2:P:380:GLU:HG2	2.21	0.40
2:N:410:SER:HB3	2:P:411:ILE:HD13	2.03	0.40
1:Q:125:GLY:HA3	1:Q:144:TRP:HB3	2.03	0.40
2:T:375:LEU:HD23	2:T:375:LEU:HA	1.89	0.40
2:B:344:TRP:CH2	2:B:371:ILE:HD12	2.56	0.40
2:F:456:ASP:HB3	2:F:458:LYS:H	1.86	0.40
1:M:234:ASP:OD1	1:M:235:ASN:N	2.54	0.40
1:O:172:MET:HG2	1:O:227:TRP:HB3	2.03	0.40
1:S:110:LYS:HB3	1:S:249:ARG:HE	1.86	0.40
1:S:284:ARG:HB3	2:T:379:VAL:HG13	2.03	0.40
1:U:132:ARG:NH1	1:U:138:PHE:O	2.54	0.40
1:U:43:MET:HE2	1:U:43:MET:HB3	1.94	0.40
1:U:46:ARG:HB2	1:U:75:ASP:OD2	2.21	0.40
2:V:383:ASN:HA	2:V:384:THR:HB	2.04	0.40
1:W:87:CYS:SG	1:W:88:TYR:N	2.93	0.40
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.93	0.40
1:G:172:MET:HG2	1:G:227:TRP:HB3	2.03	0.40
1:K:59:MET:HE2	1:K:59:MET:HB3	1.98	0.40
2:P:455:GLU:OE1	2:R:446:ARG:NH2	2.53	0.40
1:Q:303:ASN:O	1:Q:304:ARG:NE	2.52	0.40
1:S:172:MET:HG2	1:S:227:TRP:HB3	2.04	0.40
1:W:50:ASP:HB2	1:W:266:ILE:HD11	2.03	0.40
1:E:146:VAL:HG21	1:E:187:LEU:HD22	2.04	0.40
1:K:60:LEU:HD11	1:K:102:ILE:HD11	2.03	0.40
2:H:373:GLY:HA3	1:K:20:THR:O	2.21	0.40
1:S:51:LEU:HB3	1:S:54:CYS:O	2.21	0.40
2:T:406:TRP:CH2	2:V:408:LYS:HG2	2.56	0.40
1:W:162:ARG:HG3	1:W:235:ASN:CG	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
1	C	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	E	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	G	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
1	I	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	K	316/318 (99%)	306 (97%)	10 (3%)	0	100	100
1	M	316/318 (99%)	302 (96%)	13 (4%)	1 (0%)	41	64
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%)	41	64
1	U	316/318 (99%)	307 (97%)	8 (2%)	1 (0%)	41	64
1	W	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
2	B	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	25	47
2	D	172/174 (99%)	166 (96%)	4 (2%)	2 (1%)	13	27
2	F	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	25	47
2	H	172/174 (99%)	168 (98%)	3 (2%)	1 (1%)	25	47
2	J	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	25	47
2	L	172/174 (99%)	169 (98%)	2 (1%)	1 (1%)	25	47
2	N	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	25	47
2	P	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	25	47
2	R	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	47
2	T	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	47
2	V	172/174 (99%)	163 (95%)	8 (5%)	1 (1%)	25	47
2	X	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	25	47
All	All	5856/5904 (99%)	5662 (97%)	178 (3%)	16 (0%)	41	64

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/269 (100%)	248 (92%)	21 (8%)	12	25
1	C	269/269 (100%)	249 (93%)	20 (7%)	13	28
1	E	269/269 (100%)	247 (92%)	22 (8%)	11	22
1	G	269/269 (100%)	248 (92%)	21 (8%)	12	25
1	I	269/269 (100%)	250 (93%)	19 (7%)	14	29
1	K	269/269 (100%)	246 (91%)	23 (9%)	10	20
1	M	269/269 (100%)	250 (93%)	19 (7%)	14	29
1	O	269/269 (100%)	249 (93%)	20 (7%)	13	28
1	Q	269/269 (100%)	246 (91%)	23 (9%)	10	20
1	S	269/269 (100%)	250 (93%)	19 (7%)	14	29
1	U	269/269 (100%)	241 (90%)	28 (10%)	7	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	269/269 (100%)	245 (91%)	24 (9%)	9	19
2	B	148/148 (100%)	139 (94%)	9 (6%)	18	38
2	D	148/148 (100%)	138 (93%)	10 (7%)	16	32
2	F	148/148 (100%)	137 (93%)	11 (7%)	13	28
2	H	148/148 (100%)	144 (97%)	4 (3%)	44	71
2	J	148/148 (100%)	140 (95%)	8 (5%)	22	44
2	L	148/148 (100%)	140 (95%)	8 (5%)	22	44
2	N	148/148 (100%)	141 (95%)	7 (5%)	26	50
2	P	148/148 (100%)	137 (93%)	11 (7%)	13	28
2	R	148/148 (100%)	141 (95%)	7 (5%)	26	50
2	T	148/148 (100%)	141 (95%)	7 (5%)	26	50
2	V	148/148 (100%)	139 (94%)	9 (6%)	18	38
2	X	148/148 (100%)	143 (97%)	5 (3%)	37	63
All	All	5004/5004 (100%)	4649 (93%)	355 (7%)	14	29

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

Mol	Chain	Res	Type
1	A	8	HIS
1	A	41	LEU
1	A	49	LYS
1	A	76	THR
1	A	77	LEU
1	A	111	ILE
1	A	126	THR
1	A	157	THR
1	A	162	ARG
1	A	170	LEU
1	A	192	SER
1	A	203	ARG
1	A	228	THR
1	A	239	SER
1	A	244	LEU
1	A	249	ARG
1	A	258	LEU
1	A	276	TRP
1	A	277	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	283	THR
1	A	314	ARG
2	B	341	VAL
2	B	382	THR
2	B	416	THR
2	B	420	GLU
2	B	433	MET
2	B	456	ASP
2	B	470	SER
2	B	477	ASN
2	B	492	ASN
1	C	8	HIS
1	C	41	LEU
1	C	46	ARG
1	C	76	THR
1	C	77	LEU
1	C	111	ILE
1	C	126	THR
1	C	157	THR
1	C	170	LEU
1	C	184	LYS
1	C	192	SER
1	C	203	ARG
1	C	213	ARG
1	C	228	THR
1	C	244	LEU
1	C	258	LEU
1	C	263	ASP
1	C	276	TRP
1	C	277	ARG
1	C	283	THR
2	D	341	VAL
2	D	353	GLN
2	D	377	ARG
2	D	383	ASN
2	D	433	MET
2	D	444	ARG
2	D	450	ARG
2	D	470	SER
2	D	491	LEU
2	D	495	ASN
1	E	8	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	14	THR
1	E	41	LEU
1	E	46	ARG
1	E	76	THR
1	E	77	LEU
1	E	111	ILE
1	E	126	THR
1	E	150	LYS
1	E	157	THR
1	E	162	ARG
1	E	170	LEU
1	E	203	ARG
1	E	213	ARG
1	E	228	THR
1	E	244	LEU
1	E	256	ARG
1	E	258	LEU
1	E	263	ASP
1	E	276	TRP
1	E	277	ARG
1	E	283	THR
2	F	353	GLN
2	F	379	VAL
2	F	382	THR
2	F	411	ILE
2	F	416	THR
2	F	418	GLN
2	F	425	MET
2	F	433	MET
2	F	456	ASP
2	F	467	CYS
2	F	477	ASN
1	G	8	HIS
1	G	14	THR
1	G	41	LEU
1	G	47	LYS
1	G	76	THR
1	G	77	LEU
1	G	111	ILE
1	G	120	SER
1	G	126	THR
1	G	157	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	162	ARG
1	G	170	LEU
1	G	203	ARG
1	G	213	ARG
1	G	228	THR
1	G	244	LEU
1	G	258	LEU
1	G	263	ASP
1	G	270	CYS
1	G	276	TRP
1	G	283	THR
2	H	341	VAL
2	H	416	THR
2	H	418	GLN
2	H	433	MET
1	I	8	HIS
1	I	41	LEU
1	I	49	LYS
1	I	76	THR
1	I	77	LEU
1	I	111	ILE
1	I	128	ARG
1	I	157	THR
1	I	170	LEU
1	I	192	SER
1	I	203	ARG
1	I	213	ARG
1	I	228	THR
1	I	244	LEU
1	I	250	VAL
1	I	258	LEU
1	I	276	TRP
1	I	277	ARG
1	I	283	THR
2	J	341	VAL
2	J	379	VAL
2	J	383	ASN
2	J	384	THR
2	J	416	THR
2	J	433	MET
2	J	467	CYS
2	J	495	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	8	HIS
1	K	14	THR
1	K	63	THR
1	K	76	THR
1	K	77	LEU
1	K	111	ILE
1	K	120	SER
1	K	132	ARG
1	K	149	SER
1	K	157	THR
1	K	162	ARG
1	K	170	LEU
1	K	203	ARG
1	K	220	SER
1	K	228	THR
1	K	244	LEU
1	K	248	SER
1	K	256	ARG
1	K	258	LEU
1	K	263	ASP
1	K	276	TRP
1	K	277	ARG
1	K	283	THR
2	L	325	LEU
2	L	335	ASN
2	L	418	GLN
2	L	423	VAL
2	L	433	MET
2	L	436	SER
2	L	456	ASP
2	L	484	GLN
1	M	8	HIS
1	M	14	THR
1	M	30	THR
1	M	41	LEU
1	M	57	ILE
1	M	76	THR
1	M	77	LEU
1	M	87	CYS
1	M	111	ILE
1	M	157	THR
1	M	162	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	170	LEU
1	M	203	ARG
1	M	213	ARG
1	M	228	THR
1	M	244	LEU
1	M	258	LEU
1	M	276	TRP
1	M	283	THR
2	N	335	ASN
2	N	371	ILE
2	N	418	GLN
2	N	433	MET
2	N	446	ARG
2	N	450	ARG
2	N	484	GLN
1	O	8	HIS
1	O	14	THR
1	O	41	LEU
1	O	49	LYS
1	O	76	THR
1	O	77	LEU
1	O	94	ASN
1	O	111	ILE
1	O	116	THR
1	O	126	THR
1	O	170	LEU
1	O	203	ARG
1	O	228	THR
1	O	239	SER
1	O	244	LEU
1	O	258	LEU
1	O	263	ASP
1	O	276	TRP
1	O	283	THR
1	O	318	GLU
2	P	335	ASN
2	P	341	VAL
2	P	342	ASP
2	P	372	THR
2	P	377	ARG
2	P	383	ASN
2	P	395	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	416	THR
2	P	420	GLU
2	P	433	MET
2	P	450	ARG
1	Q	8	HIS
1	Q	23	GLN
1	Q	41	LEU
1	Q	76	THR
1	Q	77	LEU
1	Q	111	ILE
1	Q	126	THR
1	Q	146	VAL
1	Q	157	THR
1	Q	162	ARG
1	Q	170	LEU
1	Q	184	LYS
1	Q	192	SER
1	Q	203	ARG
1	Q	213	ARG
1	Q	228	THR
1	Q	244	LEU
1	Q	249	ARG
1	Q	258	LEU
1	Q	276	TRP
1	Q	277	ARG
1	Q	283	THR
1	Q	314	ARG
2	R	341	VAL
2	R	342	ASP
2	R	353	GLN
2	R	433	MET
2	R	467	CYS
2	R	470	SER
2	R	496	ILE
1	S	8	HIS
1	S	14	THR
1	S	41	LEU
1	S	76	THR
1	S	77	LEU
1	S	111	ILE
1	S	112	SER
1	S	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	157	THR
1	S	162	ARG
1	S	170	LEU
1	S	203	ARG
1	S	213	ARG
1	S	228	THR
1	S	244	LEU
1	S	258	LEU
1	S	276	TRP
1	S	277	ARG
1	S	283	THR
2	T	325	LEU
2	T	383	ASN
2	T	416	THR
2	T	418	GLN
2	T	433	MET
2	T	436	SER
2	T	467	CYS
1	U	8	HIS
1	U	41	LEU
1	U	47	LYS
1	U	49	LYS
1	U	63	THR
1	U	76	THR
1	U	77	LEU
1	U	111	ILE
1	U	126	THR
1	U	128	ARG
1	U	146	VAL
1	U	148	LYS
1	U	157	THR
1	U	170	LEU
1	U	179	SER
1	U	196	SER
1	U	203	ARG
1	U	228	THR
1	U	239	SER
1	U	244	LEU
1	U	249	ARG
1	U	250	VAL
1	U	258	LEU
1	U	276	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	277	ARG
1	U	283	THR
1	U	316	VAL
1	U	318	GLU
2	V	325	LEU
2	V	350	GLN
2	V	379	VAL
2	V	382	THR
2	V	383	ASN
2	V	412	THR
2	V	433	MET
2	V	448	GLN
2	V	467	CYS
1	W	1	ASP
1	W	8	HIS
1	W	30	THR
1	W	35	SER
1	W	76	THR
1	W	77	LEU
1	W	111	ILE
1	W	119	SER
1	W	137	SER
1	W	146	VAL
1	W	147	SER
1	W	157	THR
1	W	162	ARG
1	W	170	LEU
1	W	192	SER
1	W	196	SER
1	W	203	ARG
1	W	213	ARG
1	W	228	THR
1	W	244	LEU
1	W	258	LEU
1	W	269	ASN
1	W	276	TRP
1	W	283	THR
2	X	353	GLN
2	X	382	THR
2	X	395	GLU
2	X	418	GLN
2	X	433	MET

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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	0.44	0
3	NAG	Y	2	3	14,14,15	0.84	0	17,19,21	0.70	0
4	NAG	Z	1	4	14,14,15	0.31	0	17,19,21	0.39	0
4	GAL	Z	2	4	11,11,12	0.78	0	15,15,17	1.02	0
4	SIA	Z	3	4	17,20,21	0.27	0	21,28,31	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	a	1	4	14,14,15	0.26	0	17,19,21	0.35	0
4	GAL	a	2	4	11,11,12	0.28	0	15,15,17	0.77	0
4	SIA	a	3	4	17,20,21	0.27	0	21,28,31	0.53	0
4	NAG	b	1	4	14,14,15	0.38	0	17,19,21	0.47	0
4	GAL	b	2	4	11,11,12	0.91	0	15,15,17	1.30	2 (13%)
4	SIA	b	3	4	17,20,21	0.26	0	21,28,31	0.53	0
4	NAG	c	1	4	14,14,15	0.24	0	17,19,21	0.48	0
4	GAL	c	2	4	11,11,12	0.76	0	15,15,17	1.12	1 (6%)
4	SIA	c	3	4	17,20,21	2.09	9 (52%)	21,28,31	3.08	11 (52%)

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	-	0/14/34/38	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	-	0/14/34/38	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	-	0/14/34/38	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	-	6/14/34/38	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	3	SIA	C8-C7	-3.48	1.46	1.53
4	c	3	SIA	C4-C5	-3.08	1.50	1.53
4	c	3	SIA	O10-C10	-3.03	1.16	1.23
4	c	3	SIA	C7-C6	-2.71	1.49	1.53
4	c	3	SIA	C3-C4	2.59	1.57	1.52
4	c	3	SIA	C3-C2	2.42	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	3	SIA	C11-C10	-2.15	1.46	1.50
4	c	3	SIA	O8-C8	-2.09	1.38	1.43
4	c	3	SIA	O4-C4	-2.03	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	3	SIA	O6-C2-C3	-6.80	97.95	109.87
4	c	3	SIA	C6-O6-C2	5.52	123.15	111.34
4	c	3	SIA	O9-C9-C8	-5.34	99.45	111.07
4	c	3	SIA	C3-C2-C1	-4.93	101.16	111.93
4	c	3	SIA	O10-C10-C11	-4.01	114.62	122.06
4	c	3	SIA	C11-C10-N5	3.86	122.63	116.10
4	b	2	GAL	C1-C2-C3	3.19	113.59	109.67
4	c	2	GAL	C1-C2-C3	2.97	113.32	109.67
4	c	3	SIA	C3-C4-C5	2.58	114.58	111.46
4	c	3	SIA	O8-C8-C9	-2.35	103.62	109.14
4	c	3	SIA	C6-C5-N5	2.28	114.71	110.91
4	b	2	GAL	C1-O5-C5	2.28	115.28	112.19
4	c	3	SIA	O4-C4-C3	2.22	115.45	109.94
4	c	3	SIA	C9-C8-C7	-2.14	107.77	112.41

There are no chirality outliers.

All (21) 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
3	Y	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	b	2	GAL	O5-C5-C6-O6
4	Z	2	GAL	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	b	2	GAL	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	Z	2	GAL	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

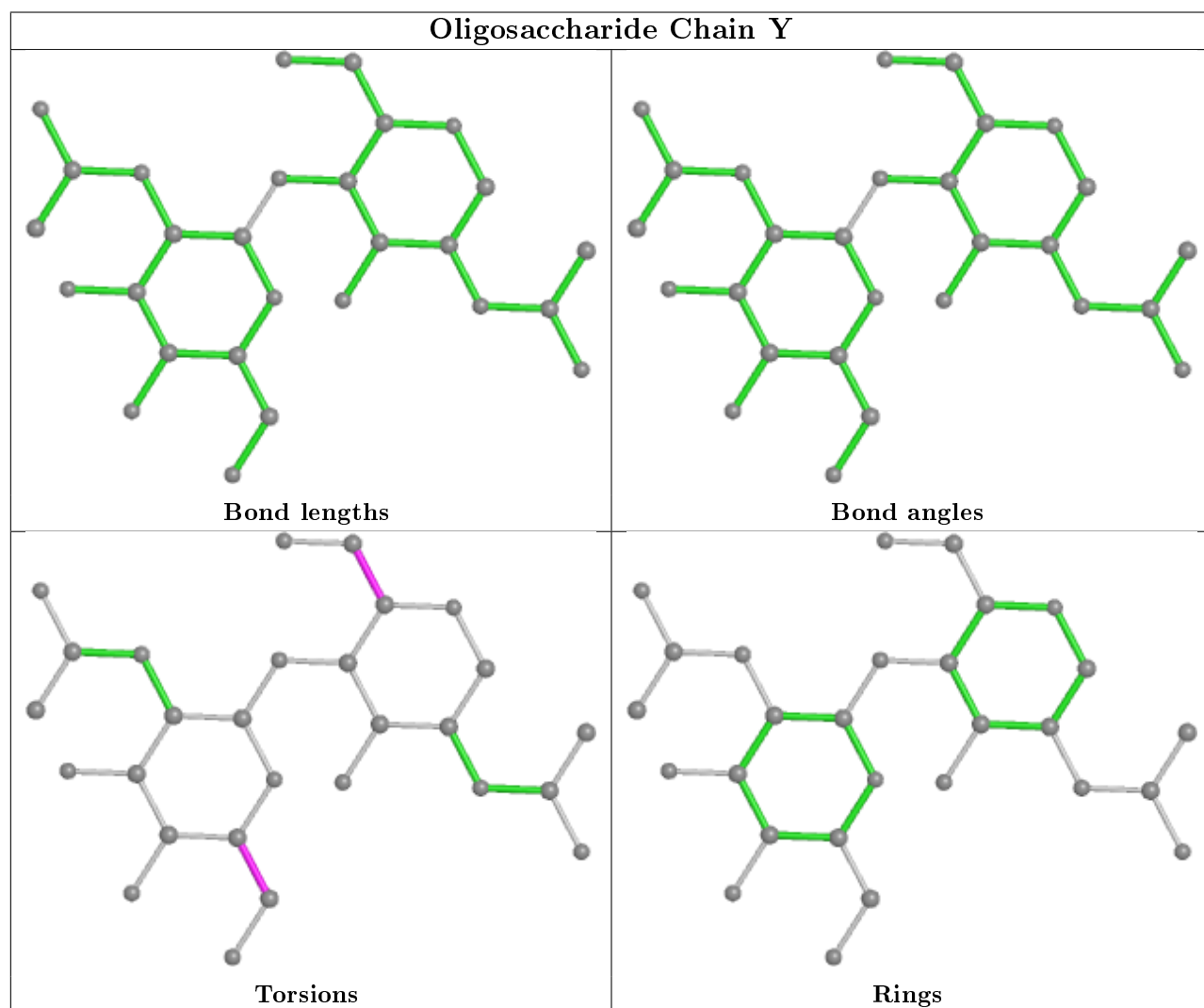
Mol	Chain	Res	Type	Atoms
4	c	3	SIA	C6-C7-C8-C9
3	Y	2	NAG	C4-C5-C6-O6
4	c	3	SIA	O7-C7-C8-C9
4	c	3	SIA	C4-C5-N5-C10
4	c	3	SIA	C6-C5-N5-C10

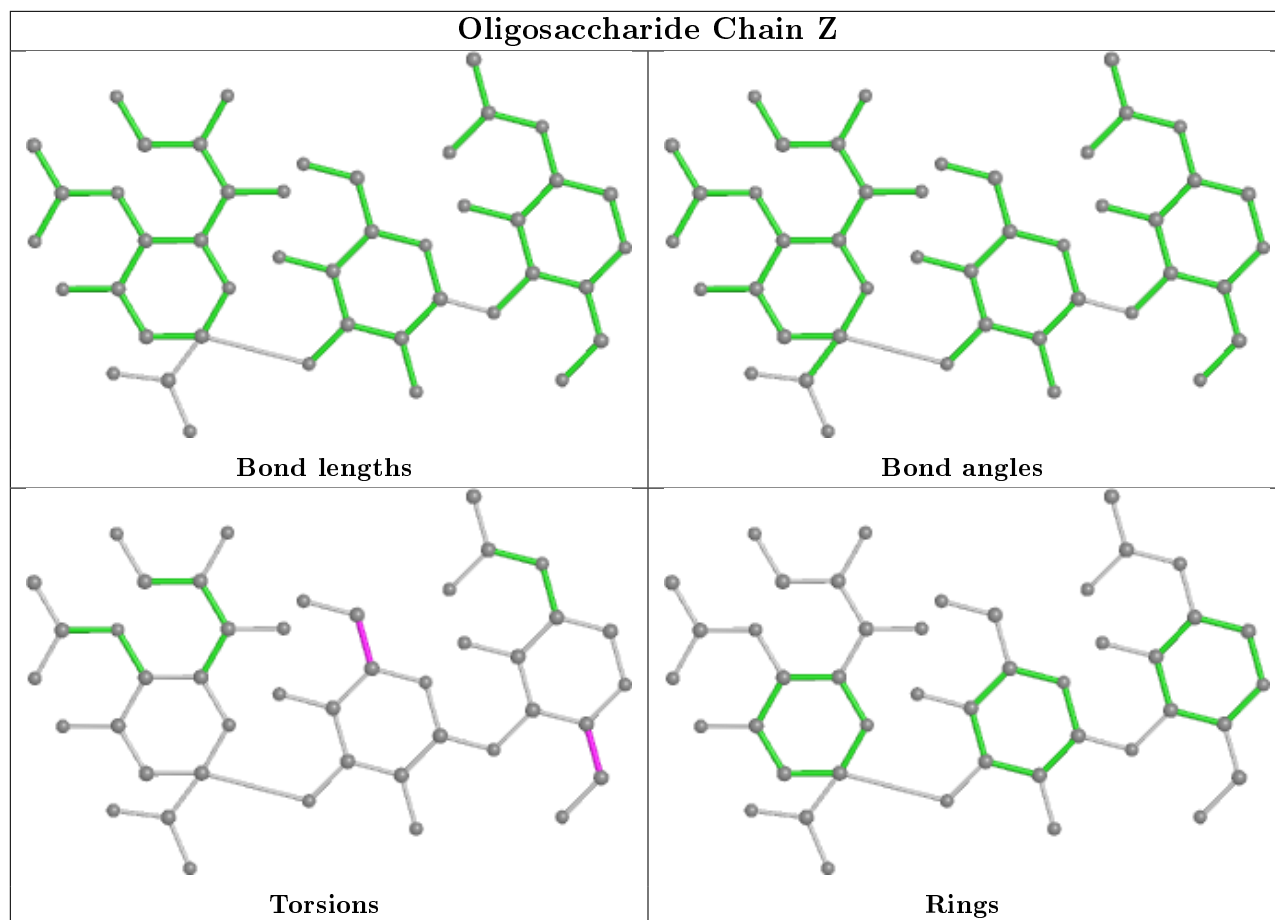
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	1	NAG	1	0
4	Z	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	C	601	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	601	2	14,14,15	0.35	0	17,19,21	0.51	0
5	NAG	X	601	2	14,14,15	0.51	0	17,19,21	0.54	0
5	NAG	K	601	1	14,14,15	0.35	0	17,19,21	0.54	0
5	NAG	J	601	2	14,14,15	0.70	0	17,19,21	0.76	0
5	NAG	S	601	1	14,14,15	0.28	0	17,19,21	0.55	0
5	NAG	T	601	2	14,14,15	0.55	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	Q	601	1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	R	601	2	14,14,15	0.21	0	17,19,21	0.62	0
5	NAG	L	601	2	14,14,15	0.37	0	17,19,21	0.47	0
5	NAG	W	601	1	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	V	601	2	14,14,15	0.40	0	17,19,21	0.51	0
5	NAG	E	602	1	14,14,15	0.90	1 (7%)	17,19,21	0.93	0
5	NAG	D	601	2	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	I	601	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	O	601	1	14,14,15	0.20	0	17,19,21	0.37	0
5	NAG	N	601	2	14,14,15	0.47	0	17,19,21	0.44	0
5	NAG	P	601	2	14,14,15	0.36	0	17,19,21	0.48	0
5	NAG	G	601	1	14,14,15	0.18	0	17,19,21	0.46	0
5	NAG	E	601	1	14,14,15	0.38	0	17,19,21	0.50	0
5	NAG	F	601	2	14,14,15	0.31	0	17,19,21	0.61	0
5	NAG	M	601	1	14,14,15	0.36	0	17,19,21	0.57	0
5	NAG	H	601	2	14,14,15	0.42	0	17,19,21	0.59	0
5	NAG	U	601	1	14,14,15	0.42	0	17,19,21	0.43	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	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	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	K	601	1	-	2/6/23/26	0/1/1/1
5	NAG	J	601	2	-	0/6/23/26	0/1/1/1
5	NAG	S	601	1	-	0/6/23/26	0/1/1/1
5	NAG	T	601	2	-	2/6/23/26	0/1/1/1
5	NAG	Q	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	L	601	2	-	2/6/23/26	0/1/1/1
5	NAG	W	601	1	-	4/6/23/26	0/1/1/1
5	NAG	V	601	2	-	0/6/23/26	0/1/1/1
5	NAG	E	602	1	-	0/6/23/26	0/1/1/1
5	NAG	D	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	I	601	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	601	1	-	2/6/23/26	0/1/1/1
5	NAG	N	601	2	-	0/6/23/26	0/1/1/1
5	NAG	P	601	2	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	0/1/1/1
5	NAG	F	601	2	-	0/6/23/26	0/1/1/1
5	NAG	M	601	1	-	0/6/23/26	0/1/1/1
5	NAG	H	601	2	-	0/6/23/26	0/1/1/1
5	NAG	U	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	2.26	1.50	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	G	601	NAG	C4-C5-C6-O6
5	G	601	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.19	0 100 100	10, 25, 42, 69	0
1	C	318/318 (100%)	0.11	4 (1%) 77 73	10, 36, 64, 95	0
1	E	318/318 (100%)	-0.05	1 (0%) 94 93	11, 30, 48, 70	0
1	G	318/318 (100%)	0.04	4 (1%) 77 73	15, 34, 54, 80	0
1	I	318/318 (100%)	-0.03	5 (1%) 72 68	11, 29, 52, 101	0
1	K	318/318 (100%)	-0.08	6 (1%) 66 62	13, 29, 52, 84	0
1	M	318/318 (100%)	0.63	31 (9%) 7 5	24, 56, 87, 123	0
1	O	318/318 (100%)	0.48	25 (7%) 12 9	22, 52, 82, 112	0
1	Q	318/318 (100%)	-0.10	4 (1%) 77 73	12, 33, 54, 92	0
1	S	318/318 (100%)	0.31	20 (6%) 20 15	17, 43, 70, 107	0
1	U	318/318 (100%)	-0.05	5 (1%) 72 68	16, 31, 53, 83	0
1	W	318/318 (100%)	0.22	8 (2%) 57 51	24, 44, 71, 94	0
2	B	174/174 (100%)	0.23	3 (1%) 70 66	12, 26, 54, 108	0
2	D	174/174 (100%)	0.24	3 (1%) 70 66	11, 25, 52, 130	0
2	F	174/174 (100%)	0.17	4 (2%) 60 54	10, 27, 56, 101	0
2	H	174/174 (100%)	0.18	2 (1%) 80 78	12, 29, 55, 125	0
2	J	174/174 (100%)	0.40	5 (2%) 51 45	12, 37, 74, 132	0
2	L	174/174 (100%)	0.31	5 (2%) 51 45	14, 35, 67, 108	0
2	N	174/174 (100%)	0.31	3 (1%) 70 66	23, 38, 71, 109	0
2	P	174/174 (100%)	0.36	5 (2%) 51 45	18, 37, 66, 125	0
2	R	174/174 (100%)	0.29	8 (4%) 32 26	16, 33, 55, 110	0
2	T	174/174 (100%)	0.19	3 (1%) 70 66	13, 37, 61, 119	0
2	V	174/174 (100%)	0.29	3 (1%) 70 66	14, 39, 71, 127	0
2	X	174/174 (100%)	0.35	3 (1%) 70 66	19, 45, 69, 119	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5904/5904 (100%)	0.17	160 (2%) 54 48	10, 35, 69, 132	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	497	ASN	13.2
2	P	497	ASN	12.7
2	J	497	ASN	11.3
2	V	496	ILE	10.5
2	X	497	ASN	10.3
2	L	497	ASN	10.1
2	H	497	ASN	9.6
2	H	496	ILE	9.4
2	D	496	ILE	9.1
2	X	496	ILE	9.0
2	V	497	ASN	8.5
2	P	496	ILE	7.3
2	F	497	ASN	6.8
2	B	496	ILE	6.8
2	F	496	ILE	6.7
2	J	496	ILE	6.7
2	F	383	ASN	5.4
2	R	496	ILE	5.3
2	B	497	ASN	5.2
2	L	496	ILE	5.0
1	S	120	SER	4.5
1	M	131	MET	4.1
1	M	134	GLY	3.9
1	W	318	GLU	3.8
1	K	269	ASN	3.8
1	O	256	ARG	3.8
2	T	383	ASN	3.8
1	O	128	ARG	3.7
1	O	12	ASN	3.7
1	M	305	ARG	3.7
2	N	496	ILE	3.6
1	M	135	GLY	3.6
1	M	152	GLN	3.6
1	S	152	GLN	3.6
1	M	150	LYS	3.5
1	I	318	GLU	3.5
1	O	167	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	270	CYS	3.4
2	P	324	GLY	3.4
1	O	134	GLY	3.3
2	R	497	ASN	3.3
1	O	270	CYS	3.3
2	L	495	ASN	3.2
1	O	166	THR	3.2
1	K	133	ASN	3.2
2	X	383	ASN	3.2
2	T	342	ASP	3.2
1	M	45	GLY	3.1
1	O	129	ALA	3.1
1	E	128	ARG	3.0
1	M	120	SER	3.0
1	S	121	ILE	3.0
1	S	150	LYS	3.0
1	G	135	GLY	2.9
1	C	149	SER	2.9
1	M	117	TYR	2.9
1	G	305	ARG	2.9
1	O	233	GLY	2.9
1	S	305	ARG	2.9
1	O	131	MET	2.8
1	M	187	LEU	2.8
1	O	284	ARG	2.8
1	M	12	ASN	2.8
2	L	383	ASN	2.8
1	M	128	ARG	2.8
1	S	167	ALA	2.8
1	S	149	SER	2.8
1	O	198	GLY	2.8
1	I	166	THR	2.7
1	M	15	ILE	2.7
1	O	11	ALA	2.7
1	O	38	ILE	2.7
1	U	166	THR	2.7
1	C	128	ARG	2.7
2	J	356	GLY	2.7
1	O	164	THR	2.7
1	M	23	GLN	2.7
1	K	305	ARG	2.6
1	M	162	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	12	ASN	2.6
1	M	145	LEU	2.6
1	S	153	ASN	2.6
1	W	256	ARG	2.6
1	M	154	PHE	2.6
1	S	284	ARG	2.5
1	W	152	GLN	2.5
1	Q	11	ALA	2.5
2	T	491	LEU	2.5
1	M	133	ASN	2.5
1	O	41	LEU	2.5
1	W	133	ASN	2.5
1	M	114	GLY	2.5
1	M	218	GLY	2.5
1	O	44	LYS	2.4
1	S	117	TYR	2.4
1	O	111	ILE	2.4
1	I	11	ALA	2.4
2	N	378	LEU	2.4
1	M	188	TYR	2.4
2	L	352	ALA	2.4
1	O	40	ARG	2.4
2	N	361	TYR	2.4
1	S	148	LYS	2.4
1	M	149	SER	2.4
1	S	12	ASN	2.3
1	O	266	ILE	2.3
1	Q	182	GLN	2.3
1	M	147	SER	2.3
1	O	73	MET	2.3
1	G	266	ILE	2.3
2	R	439	LEU	2.3
2	P	382	THR	2.3
1	S	73	MET	2.3
1	W	12	ASN	2.3
1	S	166	THR	2.3
2	D	324	GLY	2.3
1	M	186	ASP	2.3
1	O	263	ASP	2.3
1	M	126	THR	2.3
2	R	383	ASN	2.2
2	F	324	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	167	ALA	2.2
1	C	270	CYS	2.2
2	R	436	SER	2.2
1	I	305	ARG	2.2
1	S	118	GLY	2.2
1	S	189	GLY	2.2
1	M	148	LYS	2.2
2	R	352	ALA	2.2
2	P	326	PHE	2.2
1	K	134	GLY	2.2
1	S	11	ALA	2.2
1	U	12	ASN	2.2
2	B	383	ASN	2.2
1	K	135	GLY	2.2
2	J	491	LEU	2.2
1	Q	12	ASN	2.1
1	M	193	ILE	2.1
1	S	154	PHE	2.1
1	M	47	LYS	2.1
1	W	269	ASN	2.1
1	G	118	GLY	2.1
1	O	162	ARG	2.1
1	C	134	GLY	2.1
1	O	305	ARG	2.1
1	S	119	SER	2.1
1	W	135	GLY	2.1
1	U	11	ALA	2.1
1	M	164	THR	2.1
2	J	378	LEU	2.1
1	U	318	GLU	2.0
2	V	491	LEU	2.0
2	R	327	GLY	2.0
1	K	270	CYS	2.0
2	R	460	CYS	2.0
1	O	282	ASN	2.0
1	Q	305	ARG	2.0
1	S	147	SER	2.0
1	W	266	ILE	2.0
1	M	73	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

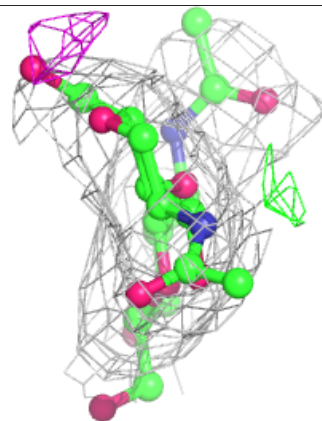
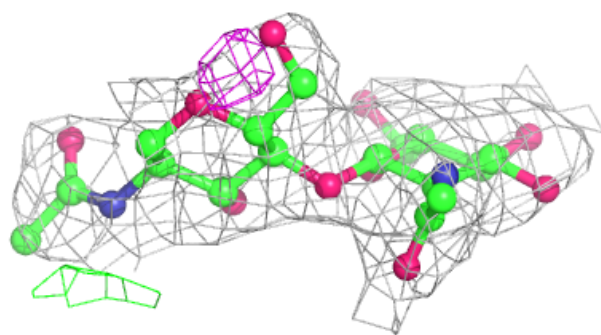
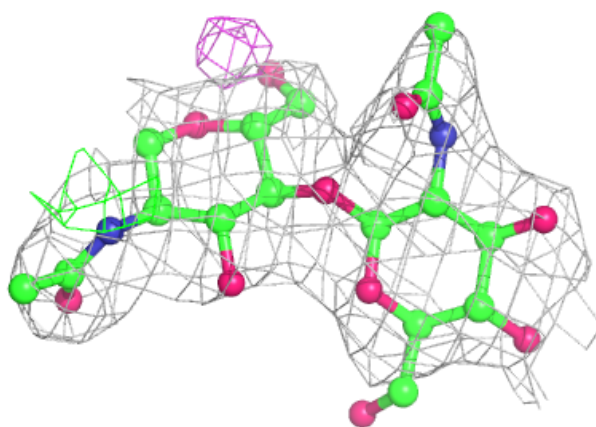
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	a	1	14/15	0.70	0.78	125,140,147,147	0
4	NAG	Z	1	14/15	0.72	0.56	100,109,111,112	0
4	GAL	a	2	11/12	0.74	0.24	72,90,112,114	0
4	NAG	c	1	14/15	0.76	0.58	99,115,125,128	0
4	NAG	b	1	14/15	0.77	0.49	97,103,110,110	0
4	GAL	b	2	11/12	0.78	0.24	66,76,99,100	0
4	GAL	c	2	11/12	0.78	0.27	58,69,81,85	0
4	GAL	Z	2	11/12	0.86	0.24	90,98,116,120	0
4	SIA	Z	3	20/21	0.87	0.19	34,45,58,60	0
4	SIA	a	3	20/21	0.87	0.24	44,57,71,72	0
3	NAG	Y	2	14/15	0.89	0.26	48,69,77,80	0
4	SIA	b	3	20/21	0.90	0.19	26,35,46,47	0
4	SIA	c	3	20/21	0.93	0.15	24,34,46,47	0
3	NAG	Y	1	14/15	0.94	0.22	46,54,64,68	0

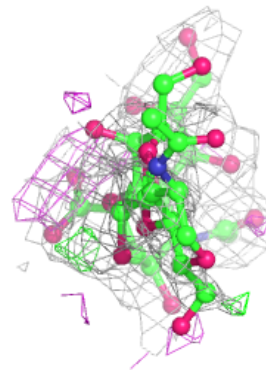
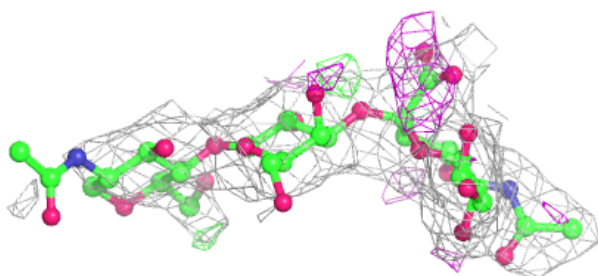
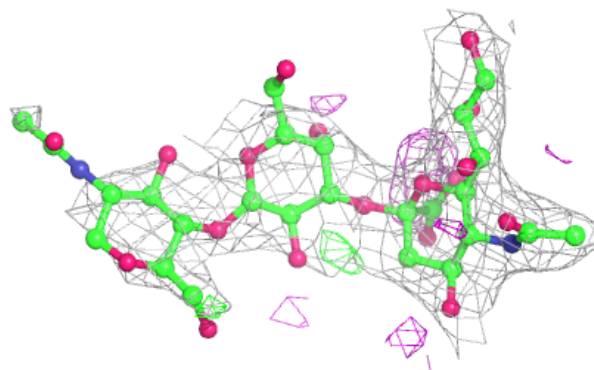
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

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

**Electron density around Chain Z:**

$2mF_o-DF_c$ (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	0.72	0.30	79,87,91,92	0
5	NAG	O	601	14/15	0.72	0.30	61,88,97,101	0
5	NAG	S	601	14/15	0.79	0.20	54,75,88,92	0
5	NAG	U	601	14/15	0.84	0.32	80,98,105,113	0
5	NAG	L	601	14/15	0.85	0.17	23,32,38,38	0
5	NAG	G	601	14/15	0.86	0.17	43,64,72,74	0
5	NAG	R	601	14/15	0.86	0.15	32,39,49,50	0
5	NAG	C	601	14/15	0.87	0.19	46,67,77,77	0
5	NAG	Q	601	14/15	0.87	0.20	76,87,98,99	0
5	NAG	X	601	14/15	0.87	0.16	37,46,54,54	0
5	NAG	M	601	14/15	0.87	0.28	66,83,89,92	0
5	NAG	K	601	14/15	0.87	0.26	46,71,77,79	0
5	NAG	E	602	14/15	0.88	0.27	54,58,73,77	0
5	NAG	F	601	14/15	0.88	0.14	25,30,33,36	0
5	NAG	V	601	14/15	0.90	0.17	28,38,40,44	0
5	NAG	N	601	14/15	0.90	0.13	40,50,51,54	0
5	NAG	H	601	14/15	0.91	0.13	22,30,33,33	0
5	NAG	E	601	14/15	0.91	0.14	48,62,69,70	0
5	NAG	I	601	14/15	0.92	0.17	52,62,65,65	0
5	NAG	A	601	14/15	0.93	0.18	34,57,68,74	0
5	NAG	P	601	14/15	0.93	0.13	34,38,44,44	0
5	NAG	B	601	14/15	0.93	0.10	29,38,43,50	0
5	NAG	T	601	14/15	0.93	0.12	23,34,41,43	0
5	NAG	D	601	14/15	0.95	0.11	20,28,36,37	0
5	NAG	J	601	14/15	0.95	0.13	18,28,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.