Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:02 AM BST

PDB ID	:	4JUG
Title	:	Crystal structure of 1918 pandemic influenza virus hemagglutinin mutant D225G
Authors	:	Zhang, W.; Shi, Y.; Qi, J.; Gao, F.; Li, Q.; Fan, Z.; Yan, J.; Gao, G.F.
Deposited on	:	2013-03-24
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

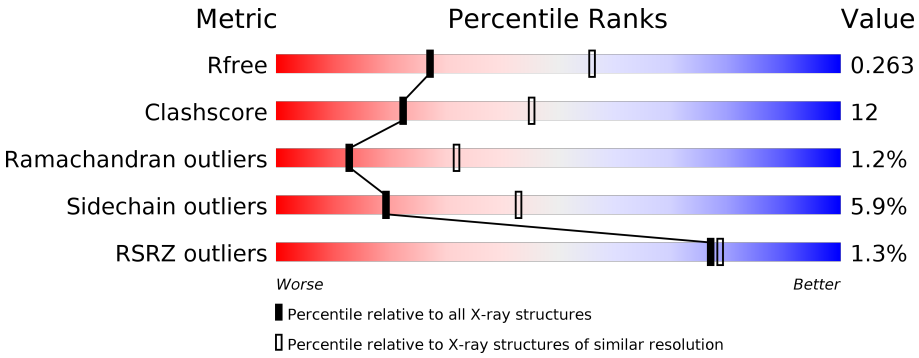
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	324	2% 76% 22%
1	C	324	77% 19%
1	E	324	% 77% 22%
1	G	324	2% 77% 19%
1	I	324	76% 21%
1	K	324	2% 75% 23%

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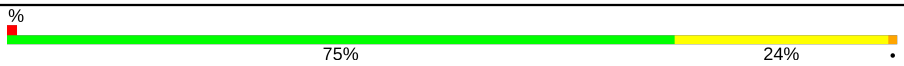
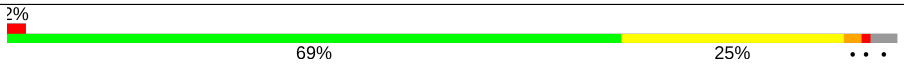
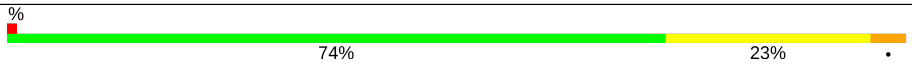
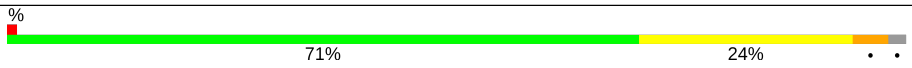
Mol	Chain	Length	Quality of chain
2	B	170	
2	D	170	
2	F	170	
2	H	170	
2	J	170	
2	L	170	
3	M	2	
3	N	2	
3	P	2	
3	Q	2	
3	R	2	
3	T	2	
4	O	3	
4	S	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23611 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	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	C	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	E	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	G	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	I	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			
1	K	324	Total	C	N	O	S	0	0	0
			2512	1584	434	483	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLY	ASP	engineered mutation	UNP Q9WFX3
A	326	ALA	-	expression tag	UNP Q9WFX3
A	327	ARG	-	expression tag	UNP Q9WFX3
C	225	GLY	ASP	engineered mutation	UNP Q9WFX3
C	326	ALA	-	expression tag	UNP Q9WFX3
C	327	ARG	-	expression tag	UNP Q9WFX3
E	225	GLY	ASP	engineered mutation	UNP Q9WFX3
E	326	ALA	-	expression tag	UNP Q9WFX3
E	327	ARG	-	expression tag	UNP Q9WFX3
G	225	GLY	ASP	engineered mutation	UNP Q9WFX3
G	326	ALA	-	expression tag	UNP Q9WFX3
G	327	ARG	-	expression tag	UNP Q9WFX3
I	225	GLY	ASP	engineered mutation	UNP Q9WFX3
I	326	ALA	-	expression tag	UNP Q9WFX3
I	327	ARG	-	expression tag	UNP Q9WFX3
K	225	GLY	ASP	engineered mutation	UNP Q9WFX3
K	326	ALA	-	expression tag	UNP Q9WFX3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	327	ARG	-	expression tag	UNP Q9WFX3

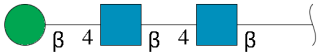
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1368	855	236	271	6			
2	D	169	Total	C	N	O	S	0	0	0
			1357	849	232	270	6			
2	F	165	Total	C	N	O	S	0	0	0
			1326	830	226	264	6			
2	H	170	Total	C	N	O	S	0	0	0
			1368	855	236	271	6			
2	J	167	Total	C	N	O	S	0	0	0
			1341	839	229	267	6			
2	L	165	Total	C	N	O	S	0	0	0
			1326	830	226	264	6			

- 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	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	O	3	Total C N O 39 22 2 15	0	0	0
4	S	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is water.

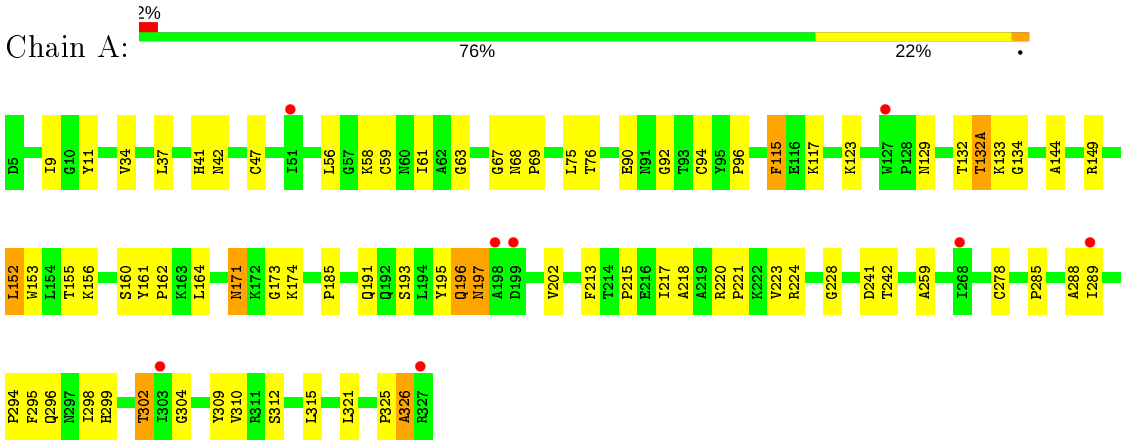
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	6	Total O 6 6	0	0
5	C	35	Total O 35 35	0	0
5	D	19	Total O 19 19	0	0
5	E	18	Total O 18 18	0	0
5	F	6	Total O 6 6	0	0
5	G	14	Total O 14 14	0	0
5	H	5	Total O 5 5	0	0
5	I	45	Total O 45 45	0	0
5	J	24	Total O 24 24	0	0
5	K	12	Total O 12 12	0	0
5	L	7	Total O 7 7	0	0

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.

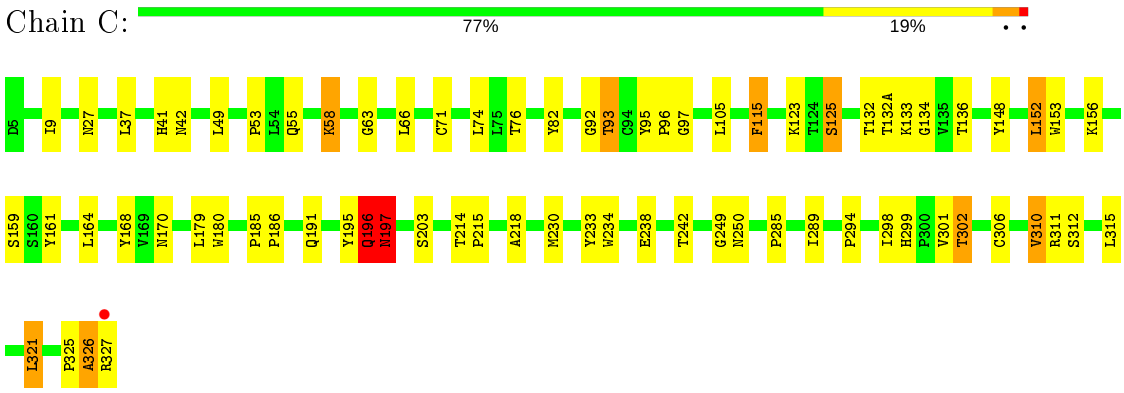
- Molecule 1: Hemagglutinin

Chain A:



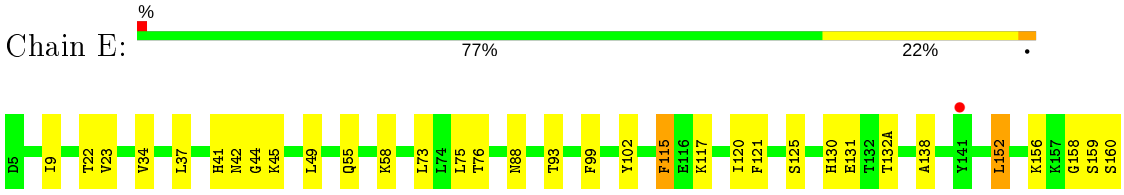
- Molecule 1: Hemagglutinin

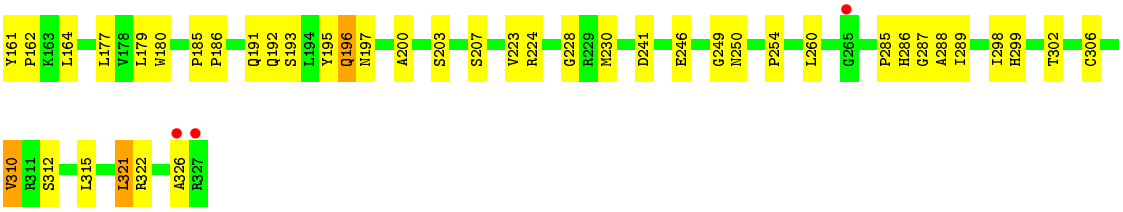
Chain C:



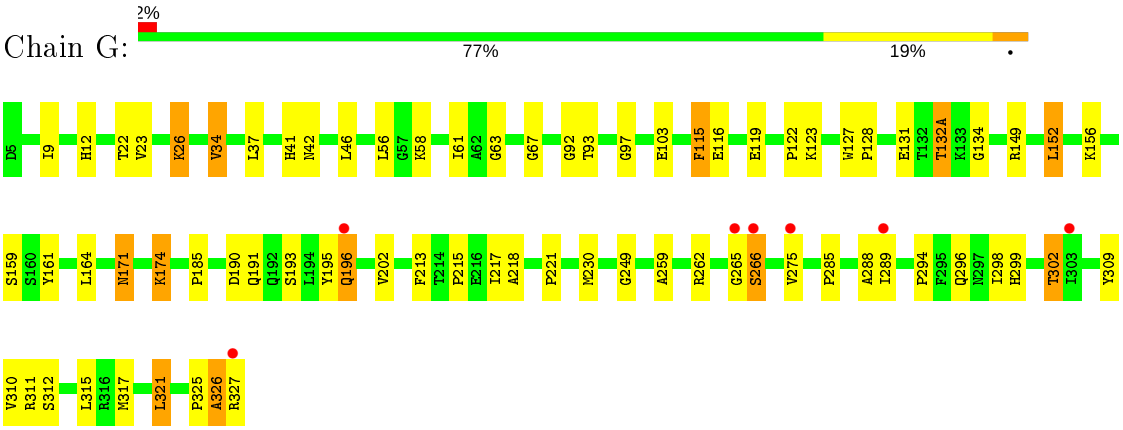
- Molecule 1: Hemagglutinin

Chain E:

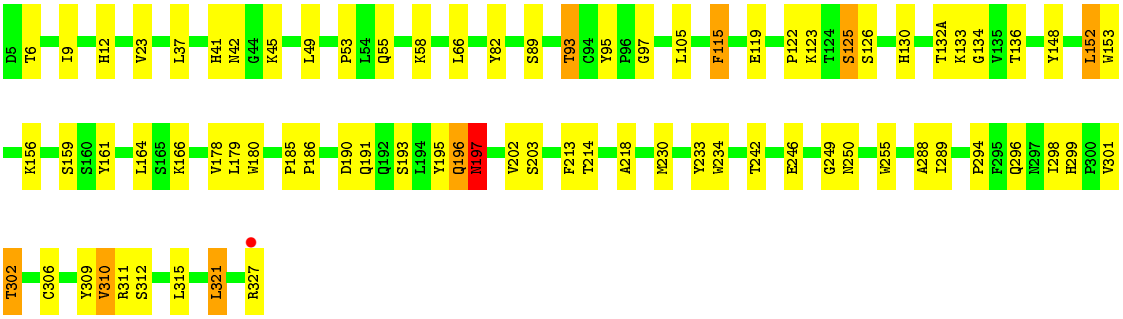




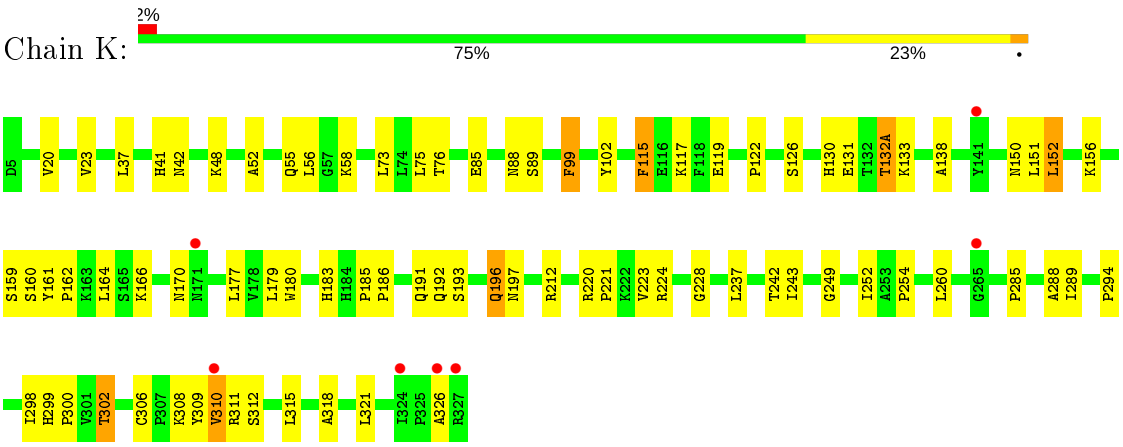
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

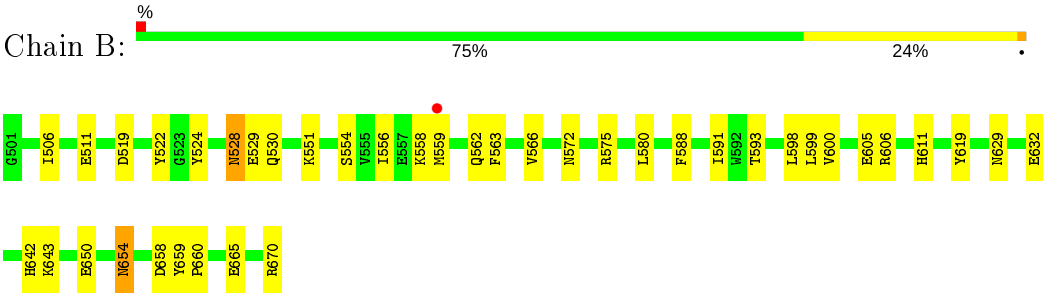


• Molecule 1: Hemagglutinin



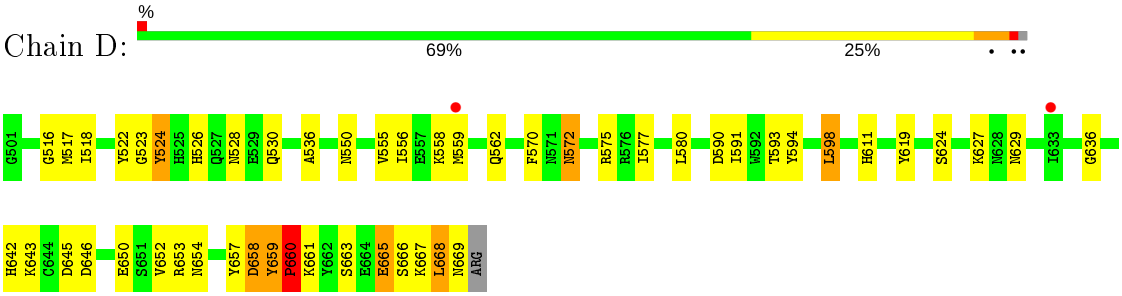
• Molecule 2: Hemagglutinin

Chain B:



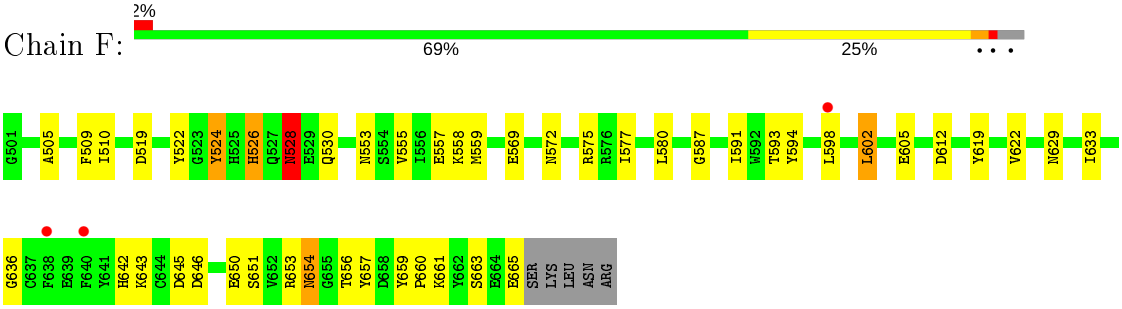
• Molecule 2: Hemagglutinin

Chain D:



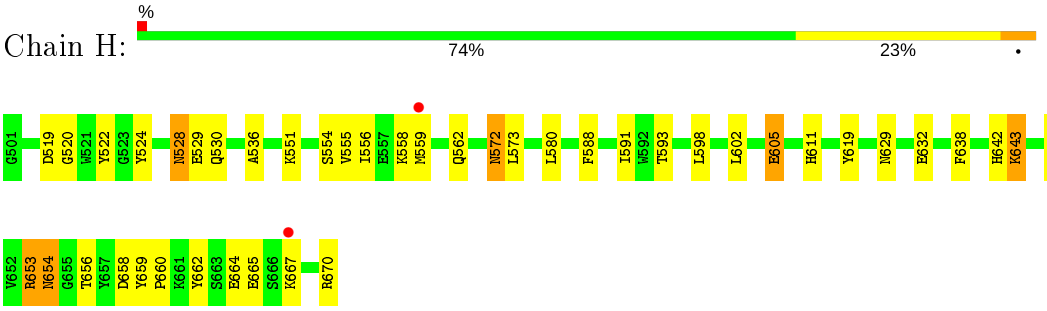
• Molecule 2: Hemagglutinin

Chain F:



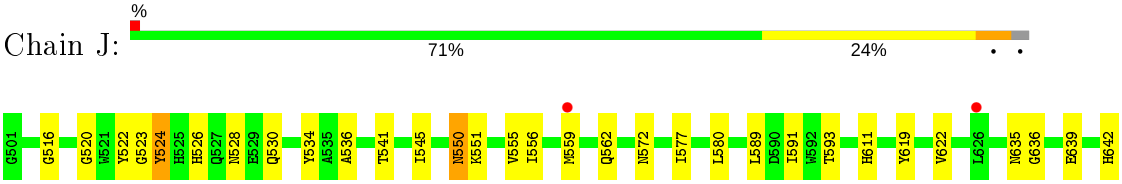
• Molecule 2: Hemagglutinin

Chain H:



• Molecule 2: Hemagglutinin

Chain J:



• Molecule 2: Hemagglutinin

Chain L:

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

Chain M:

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

Chain N:

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

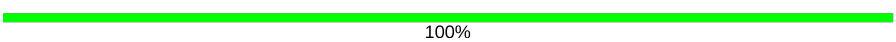
Chain P:

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

Chain Q:

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

Chain R:



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

Chain T:

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

Chain O:

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

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	120.86Å 120.86Å 235.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.90 – 2.70 47.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (47.90-2.70) 98.6 (47.90-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.207 , 0.267 0.207 , 0.263	Depositor DCC
R_{free} test set	5228 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.028 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23611	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7261e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, 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	0.27	0/2576	0.43	0/3508
1	C	0.30	0/2576	0.44	1/3508 (0.0%)
1	E	0.31	0/2576	0.49	1/3508 (0.0%)
1	G	0.29	0/2576	0.45	2/3508 (0.1%)
1	I	0.30	0/2576	0.46	1/3508 (0.0%)
1	K	0.31	0/2576	0.45	3/3508 (0.1%)
2	B	0.24	0/1395	0.39	0/1878
2	D	0.28	0/1384	0.52	2/1864 (0.1%)
2	F	0.26	0/1353	0.48	1/1823 (0.1%)
2	H	0.23	0/1395	0.40	0/1878
2	J	0.30	0/1368	0.45	0/1842
2	L	0.25	0/1353	0.54	2/1823 (0.1%)
All	All	0.28	0/23704	0.46	13/32156 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	197	ASN	N-CA-CB	14.84	137.31	110.60
2	L	663	SER	N-CA-C	12.43	144.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	196	GLN	N-CA-C	8.54	134.06	111.00
2	D	660	PRO	N-CA-C	8.42	133.98	112.10
2	F	528	ASN	CB-CA-C	7.41	125.21	110.40
2	L	663	SER	CB-CA-C	-7.22	96.38	110.10
1	C	196	GLN	N-CA-C	6.47	128.48	111.00
1	K	196	GLN	N-CA-C	6.38	128.23	111.00
2	D	660	PRO	CB-CA-C	-6.30	96.24	112.00
1	G	196	GLN	CB-CA-C	-5.96	98.48	110.40
1	I	89	SER	N-CA-C	-5.73	95.53	111.00
1	K	89	SER	N-CA-C	-5.54	96.05	111.00
1	K	196	GLN	CB-CA-C	-5.11	100.19	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	GLN	Peptide
1	I	196	GLN	Peptide

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	2512	0	2440	68	0
1	C	2512	0	2440	59	0
1	E	2512	0	2440	50	0
1	G	2512	0	2440	63	0
1	I	2512	0	2440	69	0
1	K	2512	0	2440	49	0
2	B	1368	0	1285	33	0
2	D	1357	0	1270	46	0
2	F	1326	0	1237	33	0
2	H	1368	0	1285	46	0
2	J	1341	0	1253	51	0
2	L	1326	0	1237	37	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	28	0	25	1	0
3	Q	28	0	25	2	0
3	R	28	0	25	0	0
3	T	28	0	25	1	0
4	O	39	0	34	0	0
4	S	39	0	34	0	0
5	A	16	0	0	1	0
5	B	6	0	0	0	0
5	C	35	0	0	0	0
5	D	19	0	0	0	0
5	E	18	0	0	1	0
5	F	6	0	0	0	0
5	G	14	0	0	0	0
5	H	5	0	0	0	0
5	I	45	0	0	1	0
5	J	24	0	0	0	0
5	K	12	0	0	0	0
5	L	7	0	0	0	0
All	All	23611	0	22425	530	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 12.

All (530) 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)
1:C:196:GLN:CG	1:C:196:GLN:O	1.94	1.07
2:D:629:ASN:HA	2:D:665:GLU:HG2	1.36	1.05
2:F:528:ASN:ND2	2:F:646:ASP:OD1	1.93	1.00
1:G:196:GLN:HG2	1:G:196:GLN:O	1.61	1.00
1:E:41:HIS:HB3	1:E:298:ILE:HD13	1.45	0.96
1:I:196:GLN:HG3	1:I:196:GLN:O	1.67	0.95
2:B:528:ASN:HD22	2:B:529:GLU:H	1.14	0.94
1:C:196:GLN:O	1:C:196:GLN:HG3	1.11	0.92
2:D:642:HIS:HB3	2:D:665:GLU:OE1	1.69	0.92
2:B:528:ASN:HD22	2:B:529:GLU:N	1.69	0.90
1:K:41:HIS:HB3	1:K:298:ILE:HD13	1.51	0.89
1:I:156:LYS:HD2	1:I:196:GLN:HB2	1.56	0.87
1:I:159:SER:CA	1:I:196:GLN:HE21	1.87	0.86
2:D:629:ASN:HA	2:D:665:GLU:CG	2.04	0.85
1:C:156:LYS:CD	1:C:196:GLN:HB2	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132(A):THR:HG22	1:C:133:LYS:H	1.42	0.84
1:G:22:THR:HB	2:H:605:GLU:HG2	1.60	0.83
2:D:526:HIS:CD2	2:D:526:HIS:O	2.35	0.80
2:J:577:ILE:HD11	2:L:577:ILE:HD13	1.63	0.80
1:C:156:LYS:HD2	1:C:196:GLN:HB2	1.63	0.79
2:J:663:SER:C	2:J:665:GLU:H	1.87	0.79
2:J:643:LYS:CD	2:J:643:LYS:N	2.46	0.78
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.65	0.77
1:A:123:LYS:HG3	1:A:152:LEU:HD11	1.66	0.77
2:J:642:HIS:HE1	2:J:657:TYR:OH	1.68	0.77
2:D:667:LYS:C	2:D:669:ASN:H	1.89	0.76
1:I:156:LYS:CD	1:I:196:GLN:HB2	2.16	0.76
1:I:310:VAL:HG13	1:I:312:SER:H	1.48	0.76
1:I:132(A):THR:HG22	1:I:133:LYS:H	1.51	0.75
2:B:629:ASN:ND2	2:B:665:GLU:HG2	2.01	0.75
1:G:195:TYR:O	1:G:196:GLN:HB3	1.84	0.75
2:J:650:GLU:O	2:J:654:ASN:HB2	1.86	0.74
2:J:526:HIS:O	2:J:526:HIS:CD2	2.41	0.74
1:I:159:SER:HA	1:I:196:GLN:HE21	1.52	0.74
2:H:528:ASN:HD22	2:H:529:GLU:N	1.85	0.73
1:K:310:VAL:HG13	1:K:312:SER:H	1.53	0.73
1:G:41:HIS:HB3	1:G:298:ILE:HD13	1.71	0.72
1:I:159:SER:HB2	1:I:196:GLN:NE2	2.05	0.72
1:G:285:PRO:HG2	1:G:299:HIS:CE1	2.24	0.72
2:L:662:TYR:CD1	2:L:664:GLU:OE2	2.42	0.72
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.72	0.72
2:D:650:GLU:O	2:D:654:ASN:HB2	1.89	0.71
1:G:34:VAL:HG23	1:G:317:MET:HB3	1.73	0.71
1:G:9:ILE:HD13	2:H:619:TYR:HA	1.71	0.71
1:K:186:PRO:HG3	1:K:228:GLY:N	2.06	0.71
1:C:302:THR:HB	2:D:562:GLN:HE21	1.57	0.70
2:H:591:ILE:HD13	2:J:591:ILE:HG21	1.74	0.70
1:C:310:VAL:HG13	1:C:312:SER:H	1.55	0.70
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.73	0.70
2:H:524:TYR:CE1	2:H:653:ARG:HB3	2.27	0.70
1:E:195:TYR:C	1:E:196:GLN:O	2.28	0.69
1:E:186:PRO:HG3	1:E:228:GLY:N	2.08	0.69
2:D:665:GLU:OE1	2:D:665:GLU:HA	1.92	0.69
2:D:526:HIS:CD2	2:D:526:HIS:C	2.66	0.69
1:G:123:LYS:HG3	1:G:152:LEU:HD11	1.75	0.68
1:G:171:ASN:HD22	1:G:171:ASN:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:643:LYS:N	2:J:643:LYS:HD3	2.09	0.67
1:A:37:LEU:HB2	1:A:315:LEU:HB2	1.76	0.67
1:C:195:TYR:O	1:C:197:ASN:HB2	1.93	0.67
2:J:526:HIS:C	2:J:526:HIS:CD2	2.68	0.67
2:L:664:GLU:CA	2:L:664:GLU:OE1	2.43	0.66
1:I:159:SER:C	1:I:196:GLN:HE21	1.99	0.66
2:L:629:ASN:N	2:L:629:ASN:HD22	1.94	0.65
1:A:195:TYR:C	1:A:196:GLN:O	2.29	0.65
1:E:302:THR:HG23	1:E:306:CYS:SG	2.36	0.65
1:I:302:THR:HB	2:J:562:GLN:HE21	1.61	0.65
1:K:159:SER:HA	1:K:196:GLN:HG3	1.78	0.65
2:D:658:ASP:O	2:D:659:TYR:O	2.15	0.65
1:G:171:ASN:N	1:G:171:ASN:HD22	1.94	0.65
2:H:530:GLN:HE22	2:H:646:ASP:H	1.43	0.65
1:A:161:TYR:N	1:A:196:GLN:OE1	2.23	0.65
1:A:9:ILE:CD1	2:B:619:TYR:HA	2.25	0.65
2:L:664:GLU:N	2:L:664:GLU:OE1	2.29	0.65
1:K:285:PRO:HG2	1:K:299:HIS:CE1	2.31	0.65
2:D:629:ASN:ND2	2:D:665:GLU:HG2	2.13	0.64
1:G:46:LEU:HB2	1:G:275:VAL:HG22	1.78	0.64
1:K:302:THR:HG23	1:K:306:CYS:SG	2.38	0.64
2:H:642:HIS:HB3	2:H:665:GLU:HB3	1.78	0.64
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.80	0.64
1:I:161:TYR:CZ	1:I:249:GLY:HA2	2.33	0.64
2:J:662:TYR:CD1	2:J:662:TYR:N	2.65	0.63
1:A:196:GLN:HG2	1:A:197:ASN:H	1.64	0.63
1:G:23:VAL:HG13	2:H:605:GLU:HG3	1.80	0.63
1:K:160:SER:O	1:K:162:PRO:HD3	1.99	0.62
1:C:93:THR:O	1:C:93:THR:HG22	1.98	0.62
1:I:41:HIS:HB3	1:I:298:ILE:HD13	1.80	0.62
1:I:186:PRO:HA	1:I:218:ALA:O	2.00	0.62
1:A:285:PRO:HG2	1:A:299:HIS:CE1	2.35	0.62
1:E:42:ASN:HB3	1:E:288:ALA:H	1.64	0.61
1:G:9:ILE:CD1	2:H:619:TYR:HA	2.29	0.61
2:H:650:GLU:O	2:H:654:ASN:HB2	2.00	0.61
1:K:185:PRO:HG2	1:K:191:GLN:NE2	2.15	0.61
1:C:156:LYS:HD3	1:C:196:GLN:HB2	1.83	0.61
2:F:651:SER:HB2	2:F:656:THR:O	1.99	0.61
2:H:528:ASN:HD22	2:H:529:GLU:H	1.48	0.61
2:L:651:SER:HB2	2:L:656:THR:O	1.98	0.61
1:G:294:PRO:HG3	2:H:556:ILE:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:HA3	1:A:92:GLY:HA2	1.82	0.61
2:F:524:TYR:CD1	2:F:653:ARG:HD3	2.36	0.61
2:D:642:HIS:HB3	2:D:665:GLU:CD	2.22	0.60
1:E:138:ALA:O	1:E:224:ARG:NH1	2.34	0.60
1:I:159:SER:CA	1:I:196:GLN:NE2	2.61	0.60
2:L:664:GLU:CD	2:L:664:GLU:N	2.54	0.60
2:L:662:TYR:HD1	2:L:664:GLU:OE2	1.83	0.60
2:B:591:ILE:HD13	2:D:591:ILE:HG21	1.83	0.60
1:G:174:LYS:HD2	1:G:259:ALA:HB1	1.83	0.60
1:I:130:HIS:HD2	5:I:930:HOH:O	1.84	0.60
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.84	0.60
1:C:97:GLY:HA3	1:C:230:MET:O	2.01	0.60
1:C:159:SER:O	1:C:196:GLN:HG2	2.02	0.59
1:I:93:THR:HG22	1:I:93:THR:O	2.01	0.59
1:I:159:SER:HA	1:I:196:GLN:NE2	2.17	0.59
2:J:524:TYR:CE1	2:J:653:ARG:HB2	2.38	0.59
2:H:591:ILE:HG21	2:L:591:ILE:HD13	1.85	0.59
1:I:123:LYS:HG3	1:I:152:LEU:HD11	1.85	0.59
1:A:185:PRO:HG2	1:A:191:GLN:NE2	2.18	0.59
2:F:659:TYR:N	2:F:660:PRO:HD2	2.18	0.59
1:A:9:ILE:HD13	2:B:619:TYR:HA	1.85	0.58
1:C:289:ILE:HD11	1:C:298:ILE:HD12	1.85	0.58
1:A:63:GLY:CA	1:A:92:GLY:HA2	2.32	0.58
1:C:186:PRO:HA	1:C:218:ALA:O	2.03	0.58
2:L:662:TYR:CE1	2:L:664:GLU:OE2	2.57	0.58
1:A:132(A):THR:C	1:A:134:GLY:H	2.07	0.58
1:I:97:GLY:HA3	1:I:230:MET:O	2.04	0.58
1:G:218:ALA:CB	1:I:203:SER:HB2	2.33	0.58
1:G:23:VAL:HG21	2:J:551:LYS:HE2	1.86	0.58
2:H:530:GLN:NE2	2:H:646:ASP:H	2.00	0.58
1:E:99:PHE:HB3	1:E:102:TYR:HB2	1.86	0.57
2:H:662:TYR:O	2:H:665:GLU:HG3	2.05	0.57
2:D:667:LYS:C	2:D:669:ASN:N	2.57	0.57
1:E:285:PRO:HG2	1:E:299:HIS:CE1	2.39	0.57
2:J:642:HIS:C	2:J:643:LYS:CD	2.73	0.57
2:L:664:GLU:HA	2:L:664:GLU:OE1	2.03	0.57
1:A:156:LYS:HE2	1:A:193:SER:O	2.04	0.57
1:A:302:THR:HB	2:B:562:GLN:HE21	1.70	0.57
1:C:123:LYS:HG3	1:C:152:LEU:HD11	1.86	0.57
1:I:195:TYR:O	1:I:197:ASN:HB2	2.04	0.57
2:D:629:ASN:CA	2:D:665:GLU:HG2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:642:HIS:CG	2:L:642:HIS:O	2.58	0.56
1:C:185:PRO:HG2	1:C:191:GLN:NE2	2.20	0.56
2:H:629:ASN:HD22	2:H:629:ASN:N	2.01	0.56
2:B:629:ASN:N	2:B:629:ASN:HD22	2.03	0.56
1:G:265:GLY:O	1:G:266:SER:HB2	2.06	0.56
2:J:663:SER:C	2:J:665:GLU:N	2.55	0.56
2:J:642:HIS:C	2:J:643:LYS:HD2	2.26	0.56
1:K:138:ALA:O	1:K:224:ARG:NH1	2.39	0.56
1:K:310:VAL:HG22	2:L:593:THR:HA	1.88	0.56
1:E:130:HIS:HE1	1:E:162:PRO:O	1.89	0.56
2:J:659:TYR:C	2:J:661:LYS:O	2.44	0.56
1:I:159:SER:CB	1:I:196:GLN:NE2	2.69	0.56
1:K:164:LEU:O	1:K:164:LEU:HD12	2.05	0.56
1:E:321:LEU:HD12	1:E:322:ARG:O	2.06	0.55
2:H:528:ASN:ND2	2:H:529:GLU:H	2.04	0.55
2:J:619:TYR:CE1	2:J:636:GLY:HA2	2.41	0.55
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.41	0.55
1:I:255:TRP:CD1	1:I:255:TRP:O	2.59	0.55
1:C:41:HIS:HB3	1:C:298:ILE:HD13	1.88	0.55
2:D:591:ILE:HD13	2:F:591:ILE:HG21	1.88	0.55
2:D:663:SER:C	2:D:665:GLU:H	2.10	0.55
2:D:624:SER:O	2:D:627:LYS:HE3	2.07	0.55
1:E:75:LEU:HD22	1:E:117:LYS:NZ	2.21	0.55
2:F:526:HIS:HD1	2:F:526:HIS:C	2.09	0.55
1:C:156:LYS:HD2	1:C:196:GLN:CB	2.34	0.55
2:D:530:GLN:NE2	2:D:645:ASP:HB2	2.22	0.55
2:B:606:ARG:NH2	2:F:605:GLU:HG2	2.22	0.54
2:F:553:ASN:O	2:F:557:GLU:HG3	2.07	0.54
1:K:294:PRO:HG3	2:L:556:ILE:HG12	1.88	0.54
2:L:594:TYR:O	2:L:598:LEU:HB2	2.07	0.54
2:B:619:TYR:CE1	2:B:636:GLY:HA2	2.43	0.54
1:C:302:THR:HB	2:D:562:GLN:NE2	2.23	0.54
2:B:591:ILE:HG21	2:F:591:ILE:HD13	1.90	0.54
1:E:164:LEU:O	1:E:164:LEU:HD12	2.06	0.54
1:G:296:GLN:O	1:G:309:TYR:HA	2.08	0.54
1:G:63:GLY:HA3	1:G:92:GLY:HA2	1.90	0.54
1:C:185:PRO:HG2	1:C:191:GLN:HE21	1.73	0.54
1:G:310:VAL:CG2	2:H:593:THR:HA	2.38	0.54
1:K:37:LEU:HB2	1:K:315:LEU:HB2	1.89	0.54
2:L:553:ASN:O	2:L:557:GLU:HG3	2.08	0.54
1:A:196:GLN:HG2	1:A:197:ASN:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:VAL:HB	1:G:213:PHE:HB2	1.89	0.53
2:H:629:ASN:ND2	2:H:665:GLU:HG2	2.24	0.53
2:J:591:ILE:HD13	2:L:591:ILE:HG21	1.90	0.53
1:A:195:TYR:O	1:A:196:GLN:HB3	2.08	0.53
1:I:6:THR:HG22	2:J:639:GLU:HA	1.90	0.53
1:G:195:TYR:O	1:G:196:GLN:CB	2.56	0.53
1:K:180:TRP:HB3	1:K:254:PRO:HG3	1.91	0.53
1:G:116:GLU:OE1	1:G:174:LYS:HE3	2.09	0.53
1:G:185:PRO:HG2	1:G:191:GLN:NE2	2.24	0.53
1:A:221:PRO:HG3	1:C:242:THR:HB	1.90	0.53
1:E:254:PRO:HB3	5:E:916:HOH:O	2.08	0.53
2:J:662:TYR:HD1	2:J:662:TYR:N	2.06	0.53
1:A:218:ALA:CB	1:C:203:SER:HB2	2.39	0.53
1:A:294:PRO:HG3	2:B:556:ILE:HG12	1.90	0.52
1:I:132(A):THR:HG22	1:I:133:LYS:N	2.23	0.52
1:K:308:LYS:HA	2:L:562:GLN:HB2	1.91	0.52
2:L:663:SER:O	2:L:665:GLU:N	2.39	0.52
1:A:310:VAL:CG2	2:B:593:THR:HA	2.39	0.52
1:I:196:GLN:CG	1:I:196:GLN:O	2.40	0.52
1:A:310:VAL:HG13	1:A:312:SER:H	1.74	0.52
1:E:115:PHE:HB3	1:E:260:LEU:HD23	1.91	0.52
1:G:22:THR:HB	2:H:605:GLU:CG	2.37	0.52
1:I:310:VAL:HG22	2:J:593:THR:HA	1.92	0.52
1:G:171:ASN:H	1:G:171:ASN:ND2	2.07	0.52
2:D:642:HIS:CD2	2:D:665:GLU:OE2	2.63	0.52
1:E:44:GLY:H	1:E:287:GLY:HA3	1.75	0.52
2:H:629:ASN:HB3	2:H:642:HIS:HD2	1.75	0.52
1:E:37:LEU:HB2	1:E:315:LEU:HB2	1.91	0.52
2:F:526:HIS:ND1	2:F:526:HIS:C	2.62	0.52
5:A:901:HOH:O	2:F:577:ILE:HG13	2.09	0.52
1:I:302:THR:HB	2:J:562:GLN:NE2	2.25	0.51
1:K:42:ASN:HB3	1:K:288:ALA:H	1.75	0.51
1:E:310:VAL:HG13	1:E:312:SER:H	1.74	0.51
1:C:302:THR:HG23	1:C:306:CYS:SG	2.50	0.51
1:G:63:GLY:CA	1:G:92:GLY:HA2	2.41	0.51
1:I:159:SER:O	1:I:196:GLN:HG2	2.11	0.51
2:H:572:ASN:HD22	2:H:573:LEU:N	2.08	0.51
2:F:642:HIS:NE2	2:F:657:TYR:OH	2.44	0.51
1:I:95:TYR:CD2	1:I:230:MET:HB2	2.46	0.51
2:D:516:GLY:O	2:D:518:ILE:HG23	2.11	0.51
1:E:223:VAL:HG12	1:E:224:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LYS:HE2	1:G:193:SER:O	2.10	0.51
1:G:325:PRO:O	1:G:326:ALA:C	2.48	0.51
1:A:144:ALA:HB1	2:H:667:LYS:NZ	2.26	0.51
1:E:185:PRO:HG2	1:E:191:GLN:NE2	2.26	0.51
1:I:302:THR:CB	2:J:562:GLN:HE21	2.22	0.51
1:A:9:ILE:HD12	2:B:619:TYR:HA	1.92	0.51
1:I:159:SER:HB2	1:I:196:GLN:HE22	1.72	0.51
1:K:224:ARG:NH2	3:T:1:NAG:O3	2.44	0.50
1:A:325:PRO:O	1:A:326:ALA:C	2.49	0.50
1:E:177:LEU:HG	1:E:179:LEU:HD11	1.92	0.50
2:L:650:GLU:O	2:L:654:ASN:HB2	2.11	0.50
1:E:224:ARG:NH2	3:P:1:NAG:O3	2.44	0.50
1:A:115:PHE:CD1	1:A:115:PHE:C	2.85	0.50
2:J:661:LYS:C	2:J:662:TYR:CD1	2.85	0.50
1:A:115:PHE:HD1	1:A:115:PHE:C	2.14	0.50
1:A:47:CYS:HB3	1:A:278:CYS:O	2.11	0.50
1:G:218:ALA:HB2	1:I:203:SER:HB2	1.92	0.50
1:A:94:CYS:HB2	1:A:224:ARG:HH12	1.75	0.50
1:G:302:THR:HB	2:H:562:GLN:NE2	2.26	0.50
1:K:132(A):THR:HG22	1:K:133:LYS:H	1.76	0.50
3:Q:1:NAG:H61	3:Q:2:NAG:H82	1.94	0.50
2:H:528:ASN:HD22	2:H:530:GLN:H	1.60	0.50
1:A:195:TYR:O	1:A:196:GLN:O	2.30	0.50
2:D:660:PRO:O	2:D:663:SER:N	2.45	0.50
2:F:555:VAL:O	2:F:559:MET:HG2	2.12	0.49
1:A:196:GLN:O	1:A:197:ASN:O	2.30	0.49
2:F:619:TYR:CE1	2:F:636:GLY:HA2	2.47	0.49
1:G:310:VAL:HG23	2:H:593:THR:HA	1.93	0.49
2:F:505:ALA:HB3	2:F:612:ASP:OD2	2.13	0.49
2:B:632:GLU:HG2	2:B:638:PHE:CE2	2.48	0.49
1:A:315:LEU:HD22	2:B:600:VAL:HG21	1.94	0.49
2:H:555:VAL:O	2:H:559:MET:HG2	2.11	0.49
2:H:629:ASN:HB3	2:H:642:HIS:CD2	2.48	0.49
2:J:642:HIS:C	2:J:643:LYS:HD3	2.33	0.49
1:E:180:TRP:HB3	1:E:254:PRO:HG3	1.95	0.49
1:E:130:HIS:CE1	1:E:162:PRO:O	2.66	0.49
2:F:524:TYR:CE1	2:F:653:ARG:HB3	2.47	0.49
1:A:171:ASN:HD22	1:A:171:ASN:H	1.59	0.49
1:K:170:ASN:HB2	1:K:237:LEU:HD23	1.95	0.49
1:C:156:LYS:CD	1:C:196:GLN:CB	2.87	0.48
2:J:530:GLN:NE2	2:J:646:ASP:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLY:O	2:B:563:PHE:HA	2.13	0.48
1:E:160:SER:O	1:E:162:PRO:HD3	2.13	0.48
1:G:132(A):THR:C	1:G:134:GLY:H	2.17	0.48
2:J:659:TYR:N	2:J:660:PRO:HD2	2.28	0.48
1:A:132(A):THR:O	1:A:133:LYS:HB2	2.12	0.48
2:B:629:ASN:CG	2:B:665:GLU:HG2	2.33	0.48
1:K:156:LYS:HD2	1:K:196:GLN:CG	2.44	0.48
1:C:180:TRP:CE2	1:C:233:TYR:HB2	2.49	0.48
1:E:195:TYR:O	1:E:196:GLN:HB2	2.13	0.48
1:A:285:PRO:HG2	1:A:299:HIS:ND1	2.28	0.48
1:C:95:TYR:CD2	1:C:230:MET:HB2	2.48	0.48
1:C:159:SER:HA	1:C:196:GLN:HE21	1.78	0.48
2:H:632:GLU:HG2	2:H:638:PHE:CE2	2.48	0.48
1:I:180:TRP:CE2	1:I:233:TYR:HB2	2.48	0.48
1:E:156:LYS:NZ	1:E:196:GLN:HE21	2.12	0.47
1:G:221:PRO:HG3	1:I:242:THR:HB	1.95	0.47
1:I:37:LEU:HB2	1:I:315:LEU:HB2	1.96	0.47
1:I:289:ILE:HD11	1:I:298:ILE:HD12	1.96	0.47
2:J:642:HIS:CE1	2:J:657:TYR:OH	2.58	0.47
1:K:56:LEU:HD12	1:K:85:GLU:HG2	1.96	0.47
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.95	0.47
2:B:528:ASN:ND2	2:B:529:GLU:H	1.95	0.47
2:H:554:SER:O	2:H:558:LYS:HG2	2.14	0.47
2:J:659:TYR:N	2:J:660:PRO:CD	2.77	0.47
1:K:242:THR:HG22	1:K:243:ILE:N	2.29	0.47
1:C:325:PRO:O	1:C:326:ALA:C	2.52	0.47
1:I:53:PRO:HB3	1:I:82:TYR:CZ	2.50	0.47
2:L:555:VAL:O	2:L:559:MET:HG2	2.14	0.47
1:A:196:GLN:O	1:A:197:ASN:HB2	2.13	0.47
1:C:294:PRO:HG3	2:D:556:ILE:HG12	1.95	0.47
2:D:629:ASN:ND2	2:D:659:TYR:CE1	2.83	0.47
1:G:115:PHE:C	1:G:115:PHE:CD1	2.88	0.47
2:F:509:PHE:CE1	2:F:510:ILE:HG13	2.50	0.47
2:J:665:GLU:HA	2:J:665:GLU:OE1	2.15	0.47
2:D:665:GLU:OE1	2:D:665:GLU:CA	2.62	0.47
1:K:115:PHE:C	1:K:115:PHE:CD1	2.88	0.47
1:E:195:TYR:O	1:E:196:GLN:C	2.54	0.47
1:E:310:VAL:CG2	2:F:593:THR:HA	2.44	0.47
1:K:177:LEU:HG	1:K:179:LEU:HD11	1.96	0.47
1:A:115:PHE:HD1	1:A:115:PHE:O	1.98	0.46
2:B:650:GLU:O	2:B:654:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:572:ASN:HD22	2:H:572:ASN:C	2.18	0.46
1:I:255:TRP:O	1:I:255:TRP:HD1	1.98	0.46
1:K:48:LYS:HG2	1:K:52:ALA:HA	1.96	0.46
1:A:133:LYS:HE2	2:H:660:PRO:HB2	1.97	0.46
2:F:509:PHE:CD1	2:F:510:ILE:HG13	2.50	0.46
1:G:67:GLY:O	1:G:149:ARG:HG2	2.16	0.46
1:G:97:GLY:HA3	1:G:230:MET:O	2.14	0.46
1:I:190:ASP:HA	1:I:193:SER:OG	2.15	0.46
2:J:642:HIS:CD2	2:J:642:HIS:C	2.89	0.46
1:K:99:PHE:HB3	1:K:102:TYR:HB2	1.97	0.46
1:C:66:LEU:O	1:C:148:TYR:HB3	2.16	0.46
1:C:310:VAL:HG22	2:D:593:THR:HA	1.96	0.46
2:F:650:GLU:O	2:F:654:ASN:HB2	2.15	0.46
1:I:115:PHE:CD1	1:I:115:PHE:C	2.89	0.46
1:A:289:ILE:HD11	1:A:298:ILE:HD12	1.96	0.46
1:E:115:PHE:HD1	1:E:115:PHE:C	2.19	0.46
2:L:516:GLY:HA3	2:L:534:TYR:CE1	2.50	0.46
2:B:629:ASN:ND2	2:B:659:TYR:CE2	2.84	0.46
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.98	0.46
2:D:598:LEU:HD22	2:D:598:LEU:HA	1.70	0.46
2:F:528:ASN:HD21	2:F:646:ASP:N	2.14	0.46
2:H:629:ASN:CG	2:H:665:GLU:HG2	2.36	0.46
1:I:42:ASN:HB2	1:I:288:ALA:H	1.81	0.46
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.50	0.46
2:B:554:SER:O	2:B:558:LYS:HG2	2.16	0.46
2:B:588:PHE:CZ	2:F:587:GLY:HA3	2.50	0.46
2:D:555:VAL:O	2:D:559:MET:HG2	2.16	0.46
1:E:115:PHE:CD1	1:E:115:PHE:C	2.89	0.46
2:D:570:PHE:CE1	2:D:577:ILE:HG22	2.51	0.46
1:E:42:ASN:ND2	1:E:45:LYS:HB2	2.30	0.46
2:H:528:ASN:ND2	2:H:529:GLU:N	2.57	0.46
2:B:654:ASN:HD22	2:B:654:ASN:HA	1.58	0.46
2:D:629:ASN:HD22	2:D:665:GLU:HG2	1.81	0.46
1:K:308:LYS:HE3	2:L:592:TRP:CD1	2.51	0.46
1:A:123:LYS:HE3	1:A:132:THR:O	2.16	0.45
1:G:115:PHE:HD1	1:G:115:PHE:C	2.18	0.45
1:G:56:LEU:HD11	1:G:61:ILE:HD13	1.98	0.45
1:I:134:GLY:HA3	1:I:153:TRP:HB3	1.99	0.45
1:K:185:PRO:HG2	1:K:191:GLN:HE21	1.80	0.45
2:L:659:TYR:N	2:L:660:PRO:HD3	2.31	0.45
1:C:115:PHE:HD1	1:C:115:PHE:C	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132(A):THR:HG22	1:C:133:LYS:N	2.19	0.45
1:A:218:ALA:HB2	1:C:203:SER:HB2	1.98	0.45
1:C:299:HIS:CE1	1:C:301:VAL:HB	2.51	0.45
1:C:71:CYS:HB3	1:C:74:LEU:HD12	1.98	0.45
1:K:58:LYS:HA	1:K:88:ASN:O	2.16	0.45
1:A:195:TYR:O	1:A:196:GLN:C	2.53	0.45
1:A:56:LEU:HD11	1:A:61:ILE:HD13	1.98	0.45
1:C:164:LEU:O	1:C:164:LEU:HD12	2.16	0.45
2:D:619:TYR:CE1	2:D:636:GLY:HA2	2.51	0.45
2:L:509:PHE:CD1	2:L:510:ILE:HG13	2.52	0.45
2:F:598:LEU:HD13	2:F:602:LEU:HD22	1.98	0.45
1:G:161:TYR:CB	1:G:195:TYR:O	2.64	0.45
2:H:658:ASP:OD2	2:H:660:PRO:HD2	2.16	0.45
1:I:115:PHE:HD1	1:I:115:PHE:C	2.19	0.45
2:B:629:ASN:HB3	2:B:642:HIS:HD2	1.82	0.45
1:G:215:PRO:O	1:G:217:ILE:HD12	2.17	0.45
2:L:524:TYR:CE1	2:L:653:ARG:HB3	2.52	0.45
2:D:594:TYR:O	2:D:598:LEU:HB2	2.16	0.45
2:D:642:HIS:O	2:D:643:LYS:CB	2.63	0.45
2:L:619:TYR:CE1	2:L:636:GLY:HA2	2.52	0.45
2:L:528:ASN:HD21	2:L:646:ASP:N	2.15	0.45
1:I:311:ARG:NH1	2:J:589:LEU:HG	2.32	0.45
1:G:26:LYS:HD3	2:J:550:ASN:HD21	1.82	0.45
1:K:115:PHE:HD1	1:K:115:PHE:C	2.20	0.45
1:A:321:LEU:HB3	2:B:611:HIS:CG	2.52	0.45
2:J:658:ASP:OD1	2:J:660:PRO:HD2	2.16	0.45
2:D:652:VAL:HA	2:D:657:TYR:HB2	1.99	0.45
1:E:9:ILE:HD11	2:F:622:VAL:HG21	1.99	0.45
1:E:310:VAL:HG22	2:F:593:THR:HA	1.99	0.45
1:I:9:ILE:N	1:I:9:ILE:HD12	2.32	0.45
2:J:523:GLY:HA3	2:J:536:ALA:HA	1.98	0.45
2:B:599:LEU:HD22	2:F:594:TYR:OH	2.17	0.44
1:C:9:ILE:N	1:C:9:ILE:HD12	2.31	0.44
2:D:524:TYR:CE1	2:D:653:ARG:HB2	2.52	0.44
2:L:572:ASN:HD22	2:L:572:ASN:N	2.15	0.44
1:C:115:PHE:CD1	1:C:115:PHE:C	2.91	0.44
2:D:666:SER:HA	2:D:668:LEU:HB2	1.99	0.44
1:E:207:SER:HB2	1:E:241:ASP:OD1	2.18	0.44
1:G:321:LEU:HB3	2:H:611:HIS:CG	2.52	0.44
2:D:598:LEU:HD23	2:F:558:LYS:HG3	1.98	0.44
2:L:634:GLY:O	2:L:636:GLY:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:572:ASN:C	2:D:572:ASN:HD22	2.21	0.44
1:G:42:ASN:HB3	1:G:288:ALA:H	1.82	0.44
1:G:37:LEU:HD21	1:G:312:SER:O	2.17	0.44
1:A:173:GLY:C	1:A:174:LYS:HG3	2.37	0.44
1:A:241:ASP:OD2	1:A:242:THR:N	2.50	0.44
2:D:530:GLN:NE2	2:D:646:ASP:H	2.15	0.44
1:E:289:ILE:HD11	1:E:298:ILE:HD12	1.99	0.44
2:H:643:LYS:HB3	2:H:643:LYS:HE2	1.87	0.44
1:A:295:PHE:CZ	2:B:559:MET:HG3	2.53	0.44
1:I:156:LYS:HD3	1:I:196:GLN:HB2	1.97	0.44
2:J:577:ILE:HD11	2:L:577:ILE:HG21	2.00	0.44
2:J:530:GLN:NE2	2:J:645:ASP:HB2	2.33	0.44
1:K:20:VAL:HG11	1:K:318:ALA:HB2	1.99	0.44
1:A:37:LEU:HD21	1:A:312:SER:O	2.18	0.44
1:K:156:LYS:HE2	1:K:193:SER:O	2.18	0.44
1:K:220:ARG:HB3	1:K:221:PRO:HD2	2.00	0.44
1:A:129:ASN:HB3	1:A:162:PRO:HG2	2.00	0.43
1:E:58:LYS:HA	1:E:88:ASN:O	2.18	0.43
1:G:171:ASN:N	1:G:171:ASN:ND2	2.64	0.43
1:A:321:LEU:HD23	1:A:321:LEU:H	1.83	0.43
1:K:300:PRO:HG3	1:K:309:TYR:CE2	2.53	0.43
1:I:126:SER:HB3	1:I:166:LYS:HE2	2.00	0.43
2:J:541:THR:O	2:J:545:ILE:HG13	2.18	0.43
1:K:315:LEU:HD21	2:L:597:GLU:HG2	1.99	0.43
1:A:42:ASN:HB3	1:A:288:ALA:H	1.83	0.43
2:H:659:TYR:HB3	2:H:660:PRO:HD3	2.00	0.43
1:A:11:TYR:CZ	2:B:506:ILE:HG23	2.53	0.43
1:C:55:GLN:O	1:C:74:LEU:HD21	2.19	0.43
2:J:661:LYS:HA	2:J:662:TYR:HA	1.81	0.43
1:A:56:LEU:HB3	1:A:59:CYS:O	2.18	0.43
1:I:321:LEU:HB3	2:J:611:HIS:CG	2.53	0.43
2:D:517:MET:SD	2:D:523:GLY:HA3	2.59	0.43
1:G:302:THR:HB	2:H:562:GLN:HE21	1.82	0.43
2:H:551:LYS:HG3	1:K:23:VAL:CG2	2.49	0.43
2:D:523:GLY:HA3	2:D:536:ALA:HA	2.01	0.43
2:B:606:ARG:HH21	2:F:605:GLU:HG2	1.84	0.43
1:I:119:GLU:HG2	1:I:122:PRO:HA	1.99	0.43
1:I:159:SER:O	1:I:196:GLN:NE2	2.51	0.43
1:I:42:ASN:HB3	1:I:45:LYS:HB2	2.01	0.43
1:C:285:PRO:HG2	1:C:299:HIS:CE1	2.54	0.43
2:J:516:GLY:HA3	2:J:534:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:LEU:HD22	1:K:117:LYS:NZ	2.34	0.43
1:C:249:GLY:O	1:C:250:ASN:HB2	2.19	0.42
1:E:230:MET:HB2	1:E:230:MET:HE2	1.89	0.42
1:G:321:LEU:N	1:G:321:LEU:HD23	2.34	0.42
1:K:150:ASN:O	1:K:151:LEU:HD12	2.19	0.42
1:A:220:ARG:NH1	1:A:228:GLY:HA2	2.34	0.42
1:C:164:LEU:HD12	1:C:164:LEU:C	2.39	0.42
2:F:530:GLN:NE2	2:F:645:ASP:HB2	2.34	0.42
1:G:321:LEU:H	1:G:321:LEU:HD23	1.84	0.42
1:K:126:SER:HB3	1:K:166:LYS:HE2	2.01	0.42
2:L:509:PHE:CE1	2:L:510:ILE:HG13	2.55	0.42
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.55	0.42
2:F:642:HIS:HE2	2:F:657:TYR:HH	1.60	0.42
1:G:164:LEU:HD12	1:G:164:LEU:C	2.39	0.42
1:I:249:GLY:C	1:I:250:ASN:HD22	2.23	0.42
2:J:528:ASN:HB3	2:J:530:GLN:H	1.84	0.42
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.82	0.42
1:G:115:PHE:HD1	1:G:115:PHE:O	2.02	0.42
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.55	0.42
2:J:664:GLU:O	2:J:664:GLU:HG2	2.20	0.42
3:Q:1:NAG:H61	3:Q:2:NAG:C7	2.49	0.42
1:A:132(A):THR:C	1:A:134:GLY:N	2.73	0.42
2:B:551:LYS:HG3	1:E:23:VAL:CG2	2.50	0.42
1:I:294:PRO:HG3	2:J:556:ILE:HG12	2.02	0.42
1:C:327:ARG:C	1:C:327:ARG:HD2	2.40	0.42
1:G:127:TRP:N	1:G:128:PRO:HD3	2.34	0.42
2:H:629:ASN:ND2	2:H:659:TYR:CE2	2.88	0.42
1:C:123:LYS:HE3	1:C:132:THR:O	2.20	0.42
1:C:95:TYR:HA	1:C:96:PRO:HD3	1.85	0.42
1:I:164:LEU:O	1:I:246:GLU:HA	2.20	0.42
1:A:202:VAL:O	1:A:213:PHE:HD1	2.03	0.42
1:A:215:PRO:O	1:A:217:ILE:HD12	2.20	0.42
1:A:75:LEU:HD22	1:A:117:LYS:NZ	2.34	0.42
1:C:105:LEU:HD13	1:C:234:TRP:CD2	2.55	0.42
1:E:203:SER:HB3	1:E:246:GLU:HB3	2.01	0.42
2:H:519:ASP:OD2	2:H:536:ALA:HB2	2.19	0.42
1:K:115:PHE:HB3	1:K:260:LEU:HD23	2.01	0.42
1:C:249:GLY:C	1:C:250:ASN:HD22	2.24	0.41
1:G:12:HIS:HB2	2:H:520:GLY:O	2.20	0.41
1:G:289:ILE:HD11	1:G:298:ILE:HD12	2.01	0.41
1:I:296:GLN:NE2	1:I:309:TYR:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:558:LYS:HA	2:D:558:LYS:HD3	1.84	0.41
1:E:152:LEU:HD23	1:E:152:LEU:HA	1.86	0.41
1:E:185:PRO:HA	1:E:186:PRO:HD3	1.84	0.41
1:E:44:GLY:HA2	1:E:286:HIS:O	2.20	0.41
1:I:105:LEU:HD13	1:I:234:TRP:CD2	2.55	0.41
1:C:214:THR:HA	1:C:215:PRO:HD3	1.85	0.41
1:E:9:ILE:N	1:E:9:ILE:HD12	2.35	0.41
2:J:528:ASN:OD1	2:J:644:CYS:O	2.39	0.41
2:J:662:TYR:HB2	2:J:665:GLU:OE2	2.20	0.41
2:L:524:TYR:CE1	2:L:653:ARG:CB	3.03	0.41
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.85	0.41
1:A:296:GLN:O	1:A:309:TYR:HA	2.21	0.41
1:G:119:GLU:OE2	1:G:122:PRO:HA	2.20	0.41
1:G:310:VAL:HG22	1:G:311:ARG:N	2.34	0.41
1:I:178:VAL:O	1:I:234:TRP:HA	2.20	0.41
1:C:63:GLY:N	1:C:92:GLY:HA2	2.36	0.41
2:D:665:GLU:C	2:D:667:LYS:H	2.24	0.41
1:G:103:GLU:H	1:G:103:GLU:CD	2.23	0.41
2:J:555:VAL:O	2:J:559:MET:HG2	2.20	0.41
2:H:588:PHE:CZ	2:L:587:GLY:HA3	2.55	0.41
2:B:559:MET:SD	2:F:594:TYR:CE1	3.14	0.41
1:C:321:LEU:HB3	2:D:611:HIS:CG	2.56	0.41
2:H:651:SER:HB2	2:H:656:THR:O	2.20	0.41
2:J:526:HIS:ND1	2:J:653:ARG:NH2	2.68	0.41
1:K:183:HIS:HB2	1:K:252:ILE:HD11	2.03	0.41
1:C:37:LEU:HB2	1:C:315:LEU:HB2	2.01	0.41
1:I:66:LEU:O	1:I:148:TYR:HB3	2.21	0.41
1:I:185:PRO:HG2	1:I:191:GLN:NE2	2.36	0.41
1:K:152:LEU:HA	1:K:152:LEU:HD23	1.87	0.41
1:K:156:LYS:HD2	1:K:196:GLN:HG3	2.01	0.41
2:L:629:ASN:N	2:L:629:ASN:ND2	2.62	0.41
1:E:120:ILE:HG23	1:E:121:PHE:N	2.36	0.41
1:I:122:PRO:HB2	1:I:125:SER:HB3	2.03	0.41
1:A:164:LEU:C	1:A:164:LEU:HD12	2.42	0.41
1:A:68:ASN:HA	1:A:69:PRO:HD3	1.94	0.41
1:C:58:LYS:HG3	1:C:58:LYS:H	1.61	0.41
1:E:200:ALA:HB3	1:E:250:ASN:ND2	2.36	0.41
1:G:285:PRO:HG2	1:G:299:HIS:ND1	2.36	0.41
1:I:12:HIS:HB2	2:J:520:GLY:O	2.21	0.41
1:I:164:LEU:O	1:I:164:LEU:HD12	2.20	0.41
1:I:299:HIS:CE1	1:I:301:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PRO:HG3	1:C:82:TYR:CE2	2.56	0.41
1:E:22:THR:HB	2:F:605:GLU:OE1	2.21	0.41
1:K:223:VAL:HG12	1:K:224:ARG:HG3	2.03	0.41
1:K:311:ARG:NH1	2:L:590:ASP:OD1	2.53	0.41
1:A:96:PRO:HG3	1:A:223:VAL:O	2.21	0.41
2:F:629:ASN:HB3	2:F:642:HIS:CD2	2.55	0.41
1:I:202:VAL:O	1:I:213:PHE:N	2.47	0.40
1:K:130:HIS:CE1	1:K:162:PRO:O	2.74	0.40
1:K:289:ILE:HD11	1:K:298:ILE:HD12	2.02	0.40
1:C:168:TYR:CE2	1:C:170:ASN:HA	2.56	0.40
1:E:156:LYS:HE2	1:E:193:SER:O	2.21	0.40
1:G:161:TYR:HB2	1:G:195:TYR:O	2.21	0.40
1:G:93:THR:O	1:G:93:THR:HG22	2.21	0.40
2:H:629:ASN:ND2	2:H:629:ASN:N	2.68	0.40
1:I:249:GLY:O	1:I:250:ASN:HB2	2.21	0.40
1:K:119:GLU:OE2	1:K:122:PRO:HA	2.21	0.40
1:A:115:PHE:HB2	1:A:259:ALA:O	2.21	0.40
2:B:658:ASP:OD2	2:B:660:PRO:HD2	2.22	0.40
1:I:9:ILE:HD11	2:J:622:VAL:HG21	2.03	0.40
1:C:311:ARG:NH1	2:D:590:ASP:OD1	2.54	0.40
1:E:195:TYR:O	1:E:196:GLN:O	2.39	0.40
1:I:302:THR:HG23	1:I:306:CYS:SG	2.61	0.40
1:A:67:GLY:O	1:A:149:ARG:HG2	2.22	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	322/324 (99%)	298 (92%)	21 (6%)	3 (1%)	17	40
1	C	322/324 (99%)	301 (94%)	18 (6%)	3 (1%)	17	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	322/324 (99%)	299 (93%)	18 (6%)	5 (2%)	9 24
1	G	322/324 (99%)	296 (92%)	23 (7%)	3 (1%)	17 40
1	I	322/324 (99%)	303 (94%)	17 (5%)	2 (1%)	25 50
1	K	322/324 (99%)	296 (92%)	24 (8%)	2 (1%)	25 50
2	B	168/170 (99%)	156 (93%)	10 (6%)	2 (1%)	13 32
2	D	167/170 (98%)	149 (89%)	13 (8%)	5 (3%)	4 10
2	F	163/170 (96%)	145 (89%)	13 (8%)	5 (3%)	4 9
2	H	168/170 (99%)	156 (93%)	11 (6%)	1 (1%)	25 50
2	J	165/170 (97%)	151 (92%)	13 (8%)	1 (1%)	25 50
2	L	163/170 (96%)	147 (90%)	12 (7%)	4 (2%)	5 14
All	All	2926/2964 (99%)	2697 (92%)	193 (7%)	36 (1%)	13 32

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	ASN
2	D	658	ASP
2	D	659	TYR
2	D	661	LYS
2	D	668	LEU
2	F	661	LYS
1	G	326	ALA
1	I	125	SER
1	I	197	ASN
2	L	633	ILE
1	A	326	ALA
2	B	643	LYS
1	C	125	SER
1	C	326	ALA
1	E	125	SER
2	F	663	SER
2	H	643	LYS
2	J	664	GLU
1	K	197	ASN
1	K	326	ALA
2	L	635	ASN
2	L	643	LYS
2	L	664	GLU

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Mol	Chain	Res	Type
1	A	197	ASN
1	E	159	SER
1	E	196	GLN
2	F	633	ILE
2	F	643	LYS
1	G	266	SER
1	A	196	GLN
1	E	326	ALA
2	F	528	ASN
1	G	262	ARG
1	E	158	GLY
2	B	566	VAL
2	D	660	PRO

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	278/278 (100%)	267 (96%)	11 (4%)	31	60
1	C	278/278 (100%)	263 (95%)	15 (5%)	22	47
1	E	278/278 (100%)	265 (95%)	13 (5%)	26	54
1	G	278/278 (100%)	264 (95%)	14 (5%)	24	51
1	I	278/278 (100%)	264 (95%)	14 (5%)	24	51
1	K	278/278 (100%)	265 (95%)	13 (5%)	26	54
2	B	145/145 (100%)	132 (91%)	13 (9%)	9	22
2	D	144/145 (99%)	135 (94%)	9 (6%)	18	40
2	F	140/145 (97%)	129 (92%)	11 (8%)	12	28
2	H	145/145 (100%)	134 (92%)	11 (8%)	13	30
2	J	142/145 (98%)	133 (94%)	9 (6%)	18	40
2	L	140/145 (97%)	125 (89%)	15 (11%)	6	15
All	All	2524/2538 (99%)	2376 (94%)	148 (6%)	19	43

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	58	LYS
1	A	76	THR
1	A	90	GLU
1	A	115	PHE
1	A	132(A)	THR
1	A	152	LEU
1	A	155	THR
1	A	160	SER
1	A	171	ASN
1	A	302	THR
2	B	511	GLU
2	B	519	ASP
2	B	522	TYR
2	B	524	TYR
2	B	528	ASN
2	B	530	GLN
2	B	572	ASN
2	B	575	ARG
2	B	580	LEU
2	B	598	LEU
2	B	605	GLU
2	B	654	ASN
2	B	670	ARG
1	C	27	ASN
1	C	42	ASN
1	C	49	LEU
1	C	58	LYS
1	C	76	THR
1	C	93	THR
1	C	115	PHE
1	C	125	SER
1	C	136	THR
1	C	152	LEU
1	C	197	ASN
1	C	238	GLU
1	C	302	THR
1	C	310	VAL
1	C	321	LEU
2	D	522	TYR
2	D	524	TYR
2	D	528	ASN

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Mol	Chain	Res	Type
2	D	550	ASN
2	D	572	ASN
2	D	575	ARG
2	D	580	LEU
2	D	598	LEU
2	D	665	GLU
1	E	34	VAL
1	E	49	LEU
1	E	55	GLN
1	E	73	LEU
1	E	76	THR
1	E	93	THR
1	E	115	PHE
1	E	131	GLU
1	E	132(A)	THR
1	E	152	LEU
1	E	192	GLN
1	E	310	VAL
1	E	321	LEU
2	F	519	ASP
2	F	522	TYR
2	F	524	TYR
2	F	526	HIS
2	F	569	GLU
2	F	572	ASN
2	F	575	ARG
2	F	580	LEU
2	F	602	LEU
2	F	654	ASN
2	F	665	GLU
1	G	26	LYS
1	G	34	VAL
1	G	58	LYS
1	G	115	PHE
1	G	131	GLU
1	G	132(A)	THR
1	G	152	LEU
1	G	159	SER
1	G	171	ASN
1	G	174	LYS
1	G	190	ASP
1	G	302	THR

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Mol	Chain	Res	Type
1	G	321	LEU
1	G	327	ARG
2	H	522	TYR
2	H	528	ASN
2	H	572	ASN
2	H	580	LEU
2	H	598	LEU
2	H	602	LEU
2	H	605	GLU
2	H	653	ARG
2	H	654	ASN
2	H	664	GLU
2	H	670	ARG
1	I	23	VAL
1	I	49	LEU
1	I	55	GLN
1	I	58	LYS
1	I	93	THR
1	I	115	PHE
1	I	136	THR
1	I	152	LEU
1	I	197	ASN
1	I	214	THR
1	I	302	THR
1	I	310	VAL
1	I	321	LEU
1	I	327	ARG
2	J	522	TYR
2	J	524	TYR
2	J	550	ASN
2	J	572	ASN
2	J	580	LEU
2	J	635	ASN
2	J	643	LYS
2	J	661	LYS
2	J	662	TYR
1	K	55	GLN
1	K	73	LEU
1	K	76	THR
1	K	99	PHE
1	K	115	PHE
1	K	131	GLU

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Mol	Chain	Res	Type
1	K	132(A)	THR
1	K	152	LEU
1	K	192	GLN
1	K	212	ARG
1	K	302	THR
1	K	310	VAL
1	K	321	LEU
2	L	522	TYR
2	L	524	TYR
2	L	526	HIS
2	L	569	GLU
2	L	572	ASN
2	L	580	LEU
2	L	598	LEU
2	L	602	LEU
2	L	629	ASN
2	L	642	HIS
2	L	643	LYS
2	L	653	ARG
2	L	654	ASN
2	L	661	LYS
2	L	664	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	88	ASN
1	A	171	ASN
1	A	191	GLN
1	A	250	ASN
2	B	528	ASN
2	B	530	GLN
2	B	572	ASN
2	B	625	GLN
2	B	629	ASN
2	B	635	ASN
2	B	654	ASN
1	C	35	ASN
1	C	88	ASN
1	C	130	HIS
1	C	191	GLN

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Mol	Chain	Res	Type
1	C	196	GLN
1	C	250	ASN
1	C	276	HIS
2	D	528	ASN
2	D	530	GLN
2	D	550	ASN
2	D	562	GLN
2	D	572	ASN
2	D	625	GLN
2	D	629	ASN
1	E	35	ASN
1	E	42	ASN
1	E	130	HIS
1	E	191	GLN
1	E	196	GLN
1	E	250	ASN
2	F	530	GLN
2	F	560	ASN
2	F	572	ASN
2	F	625	GLN
2	F	629	ASN
2	F	654	ASN
1	G	35	ASN
1	G	130	HIS
1	G	171	ASN
1	G	191	GLN
1	G	250	ASN
2	H	528	ASN
2	H	530	GLN
2	H	572	ASN
2	H	625	GLN
2	H	629	ASN
2	H	654	ASN
1	I	35	ASN
1	I	88	ASN
1	I	130	HIS
1	I	191	GLN
1	I	196	GLN
1	I	250	ASN
1	I	276	HIS
2	J	528	ASN
2	J	530	GLN

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Mol	Chain	Res	Type
2	J	550	ASN
2	J	562	GLN
2	J	572	ASN
2	J	625	GLN
2	J	629	ASN
2	J	642	HIS
1	K	35	ASN
1	K	130	HIS
1	K	191	GLN
1	K	250	ASN
2	L	528	ASN
2	L	530	GLN
2	L	572	ASN
2	L	625	GLN
2	L	629	ASN
2	L	654	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

18 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	M	1	1,3	14,14,15	0.57	0	17,19,21	0.62	0
3	NAG	M	2	3	14,14,15	0.53	0	17,19,21	0.89	0
3	NAG	N	1	1,3	14,14,15	0.50	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	N	2	3	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
4	NAG	O	1	2,4	14,14,15	0.49	0	17,19,21	1.20	2 (11%)
4	NAG	O	2	4	14,14,15	0.59	0	17,19,21	0.84	0
4	BMA	O	3	4	11,11,12	0.27	0	15,15,17	0.63	0
3	NAG	P	1	1,3	14,14,15	0.55	0	17,19,21	0.75	0
3	NAG	P	2	3	14,14,15	0.51	0	17,19,21	0.72	0
3	NAG	Q	1	1,3	14,14,15	0.59	0	17,19,21	0.64	0
3	NAG	Q	2	3	14,14,15	0.46	0	17,19,21	1.02	0
3	NAG	R	1	1,3	14,14,15	0.49	0	17,19,21	0.83	0
3	NAG	R	2	3	14,14,15	0.53	0	17,19,21	0.64	0
4	NAG	S	1	2,4	14,14,15	0.50	0	17,19,21	1.26	2 (11%)
4	NAG	S	2	4	14,14,15	0.58	0	17,19,21	0.75	0
4	BMA	S	3	4	11,11,12	0.27	0	15,15,17	0.64	0
3	NAG	T	1	1,3	14,14,15	0.54	0	17,19,21	0.85	0
3	NAG	T	2	3	14,14,15	0.51	0	17,19,21	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
4	NAG	O	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	BMA	O	3	4	-	1/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
4	NAG	S	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	NAG	C1-O5-C5	3.55	117.00	112.19
4	S	1	NAG	C1-O5-C5	3.01	116.27	112.19
4	S	1	NAG	C4-C3-C2	3.00	115.42	111.02
3	N	2	NAG	C1-O5-C5	2.39	115.42	112.19
4	O	1	NAG	C4-C3-C2	2.01	113.97	111.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	3	BMA	C4-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6

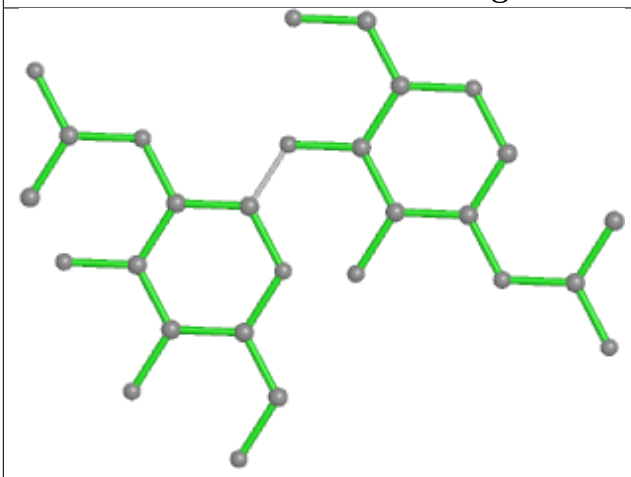
There are no ring outliers.

4 monomers are involved in 4 short contacts:

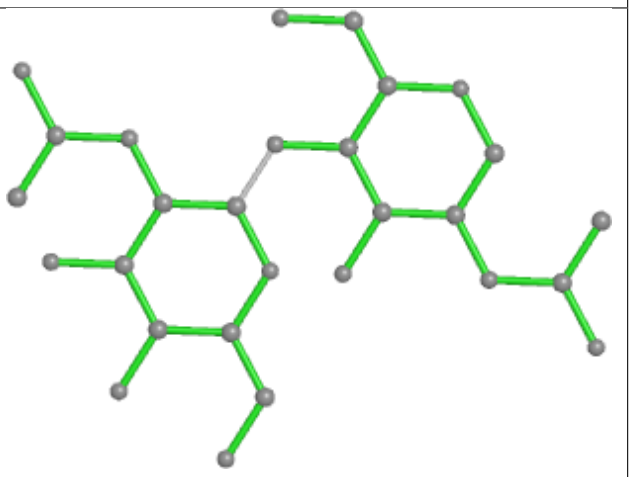
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1	NAG	2	0
3	P	1	NAG	1	0
3	T	1	NAG	1	0
3	Q	2	NAG	2	0

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

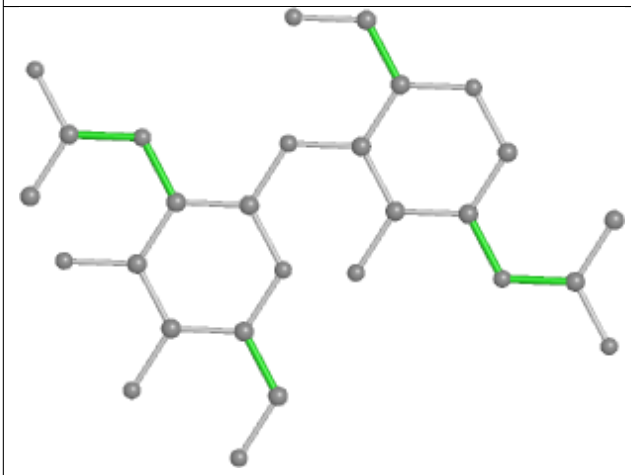
Oligosaccharide Chain M



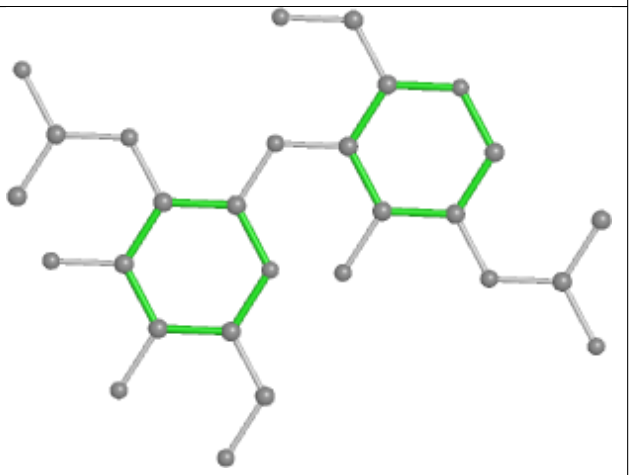
Bond lengths



Bond angles

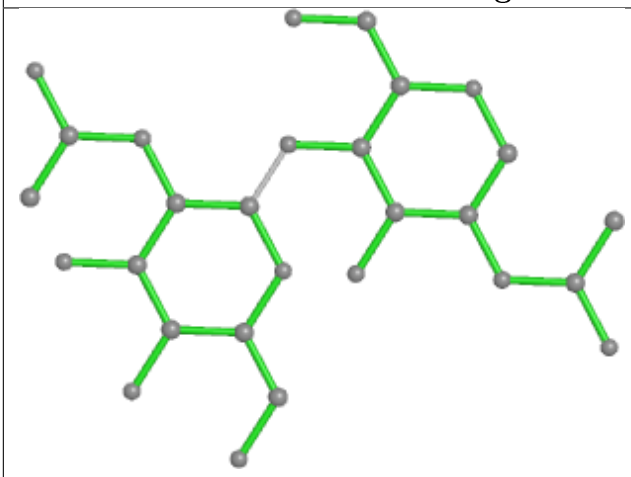


Torsions

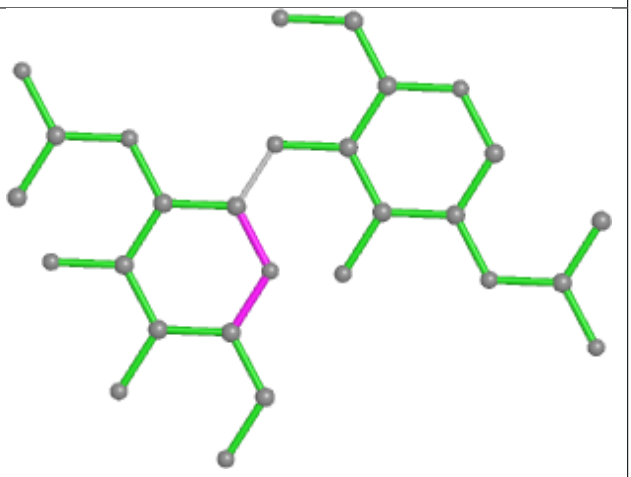


Rings

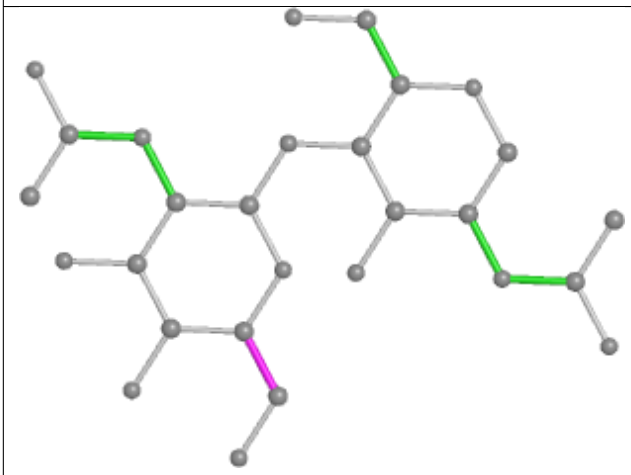
Oligosaccharide Chain N



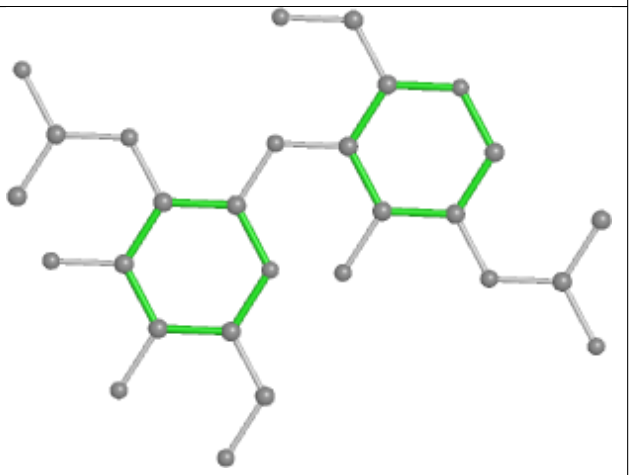
Bond lengths



Bond angles

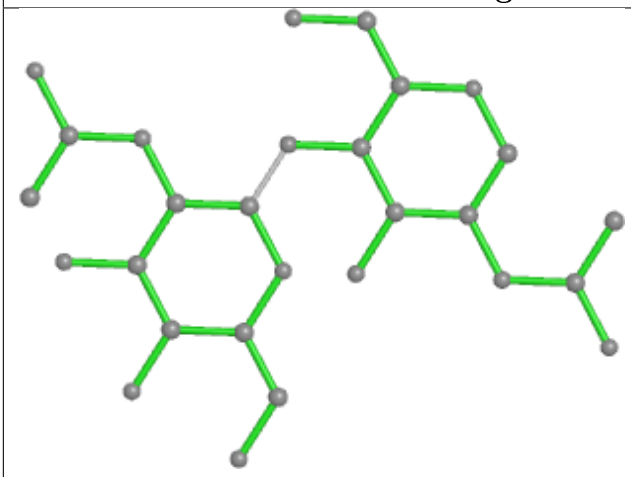


Torsions

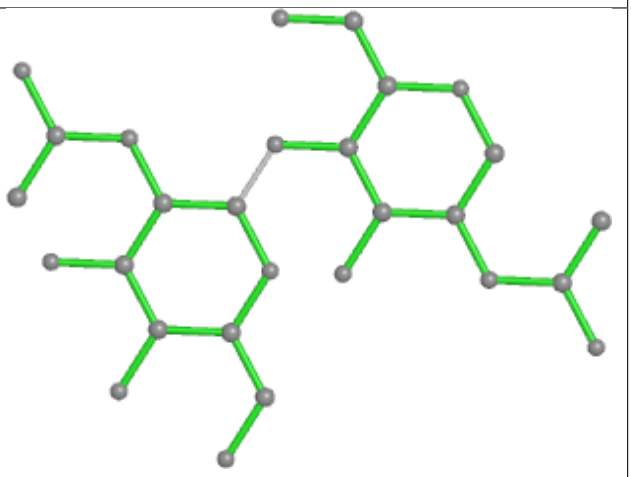


Rings

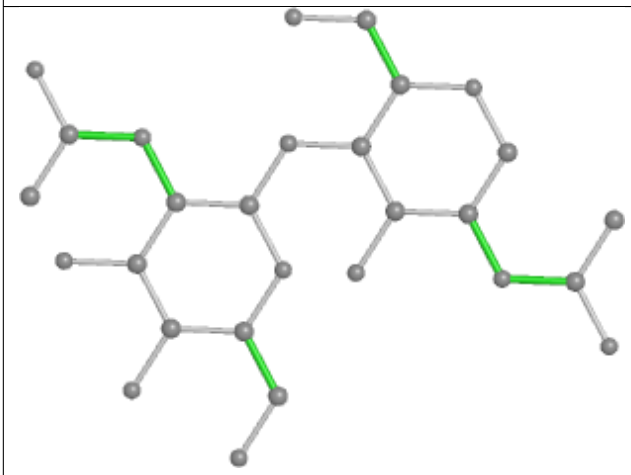
Oligosaccharide Chain P



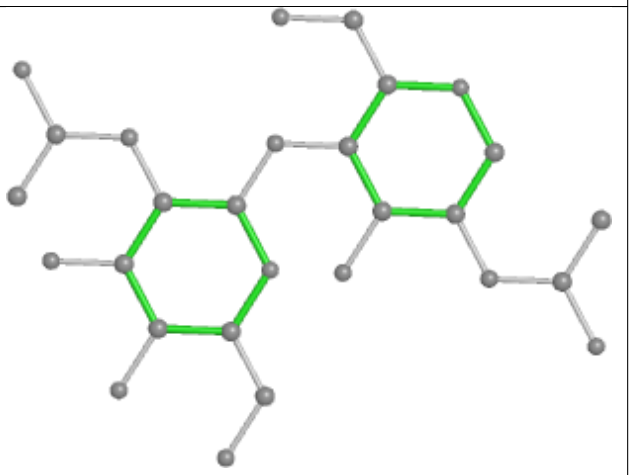
Bond lengths



Bond angles

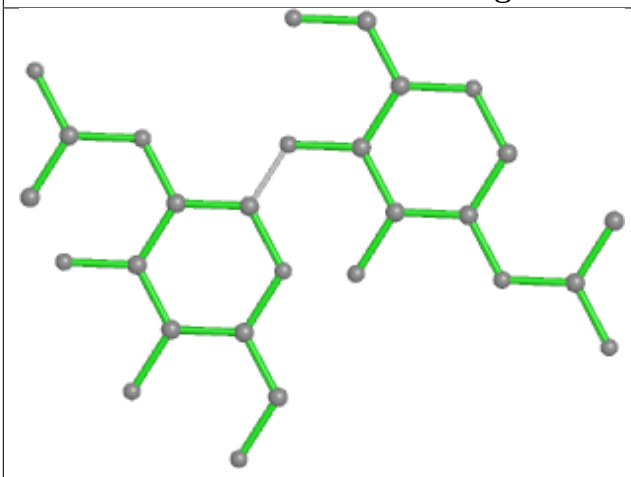


Torsions

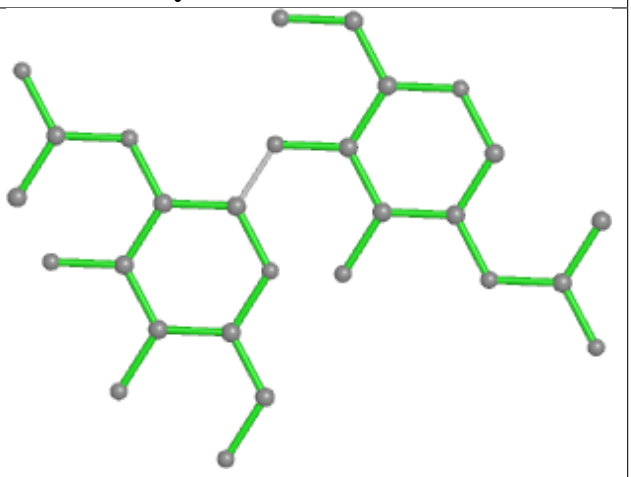


Rings

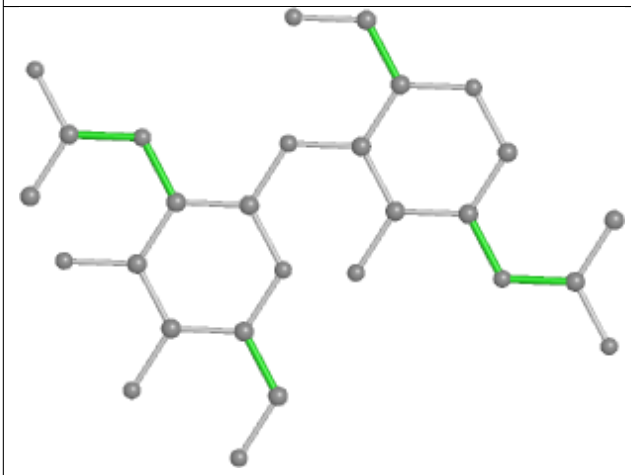
Oligosaccharide Chain Q



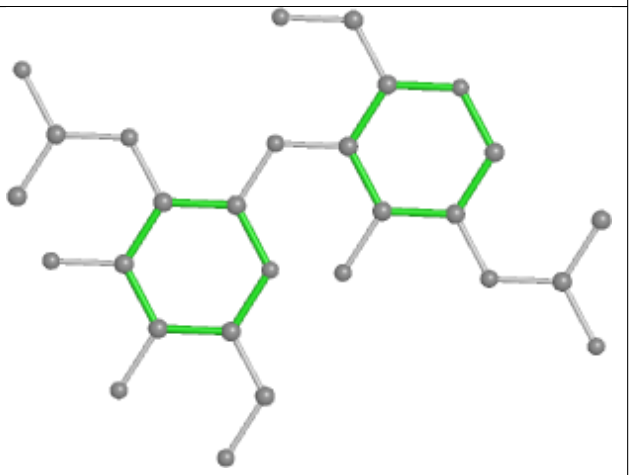
Bond lengths



Bond angles

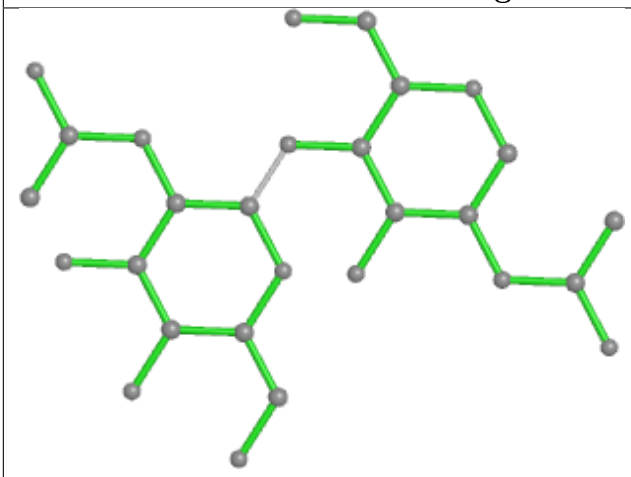


Torsions

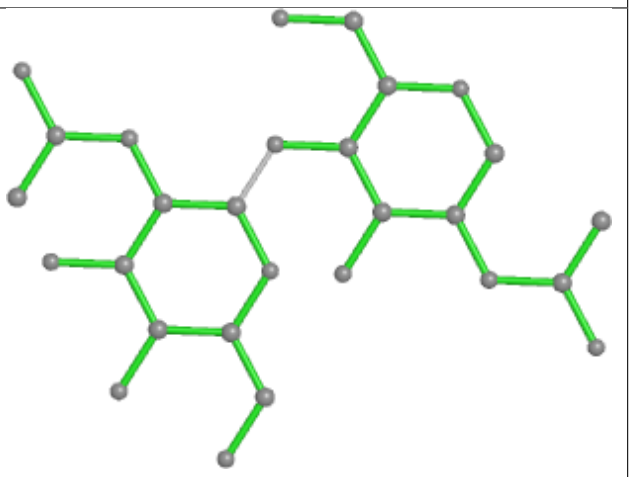


Rings

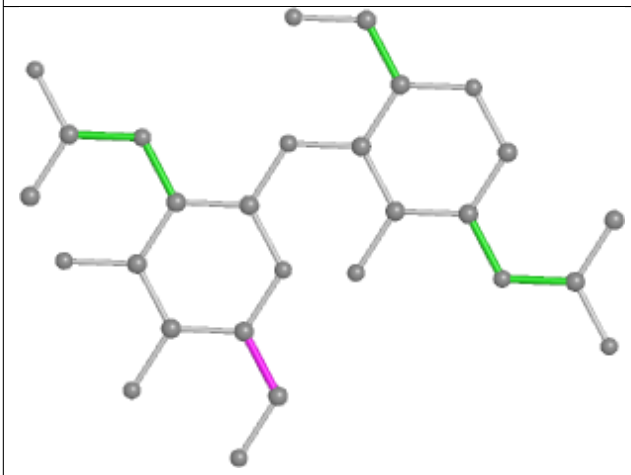
Oligosaccharide Chain R



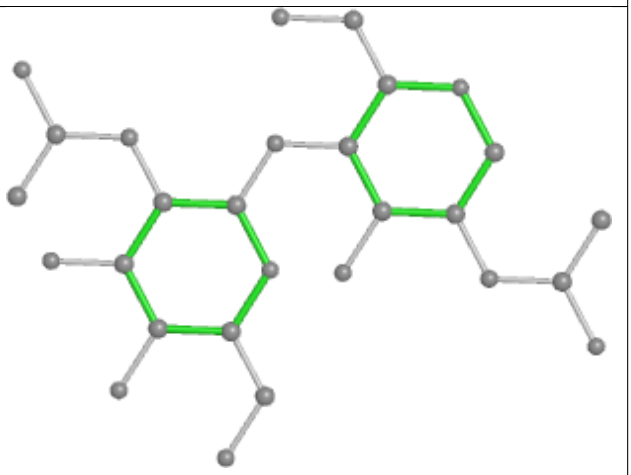
Bond lengths



Bond angles

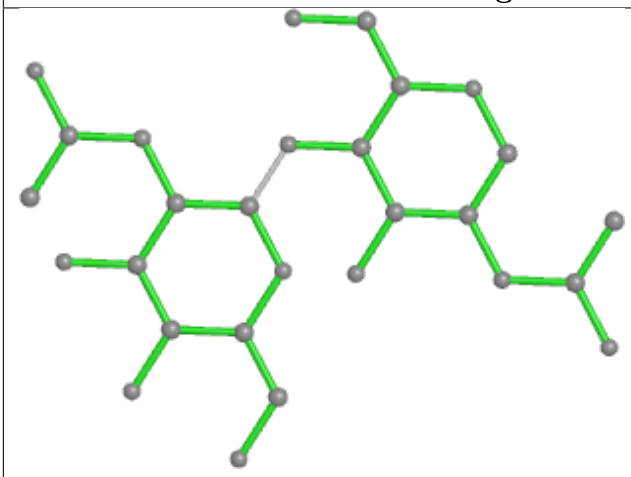


Torsions

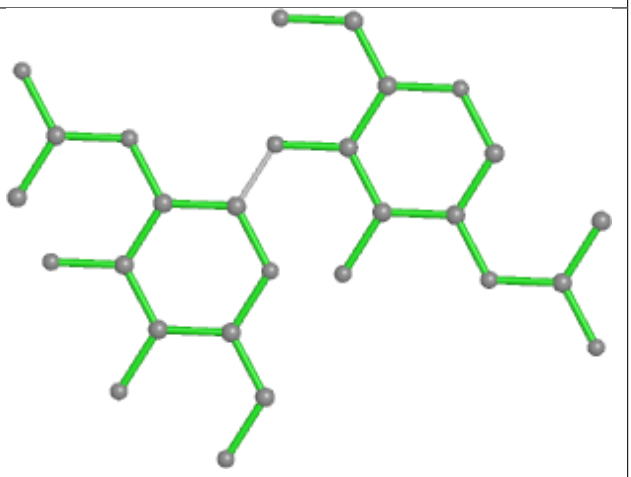


Rings

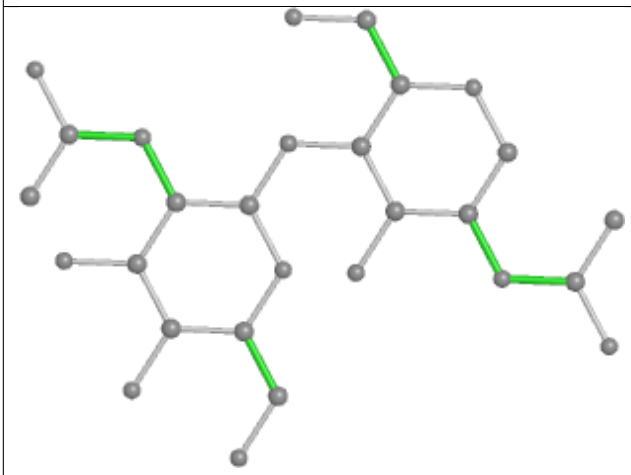
Oligosaccharide Chain T



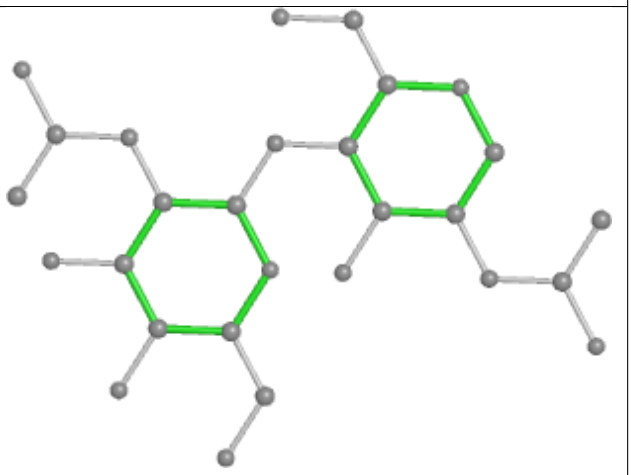
Bond lengths



Bond angles

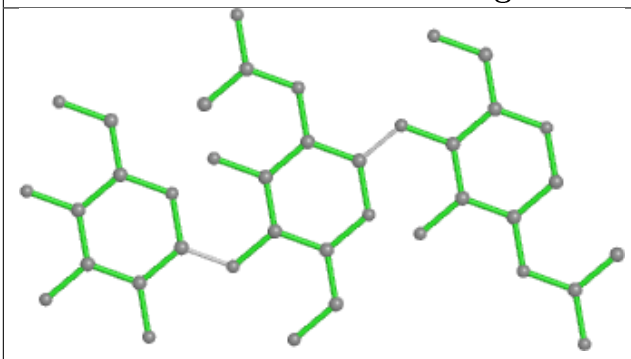


Torsions

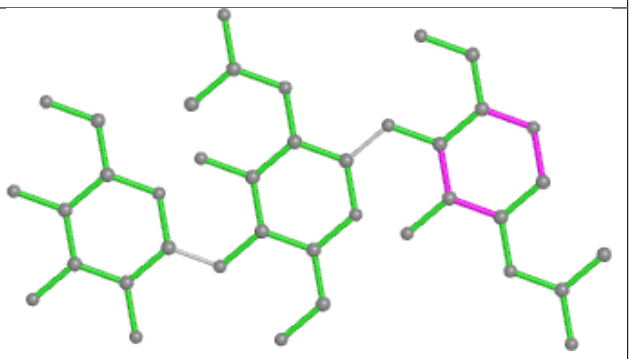


Rings

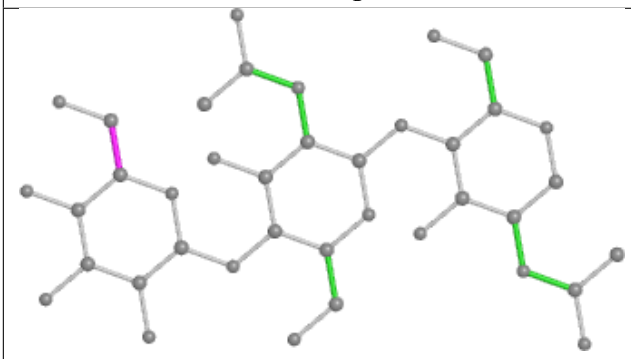
Oligosaccharide Chain O



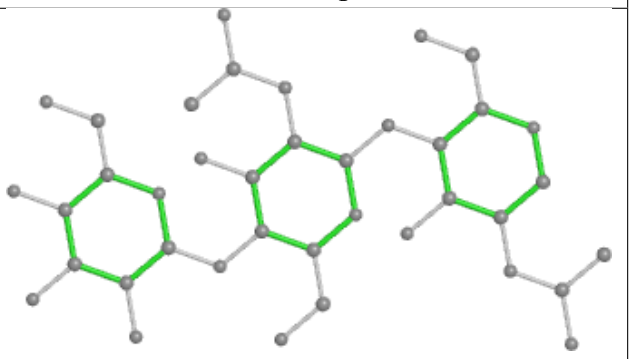
Bond lengths



Bond angles

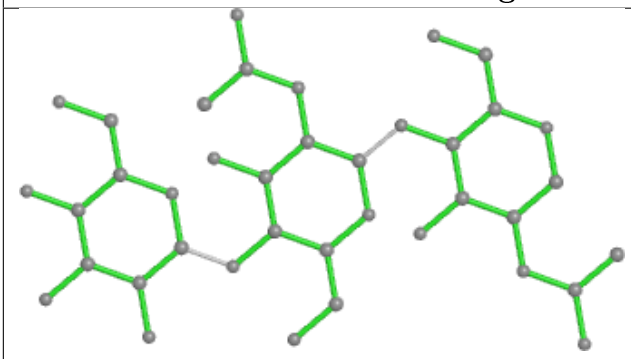


Torsions



Rings

Oligosaccharide Chain S



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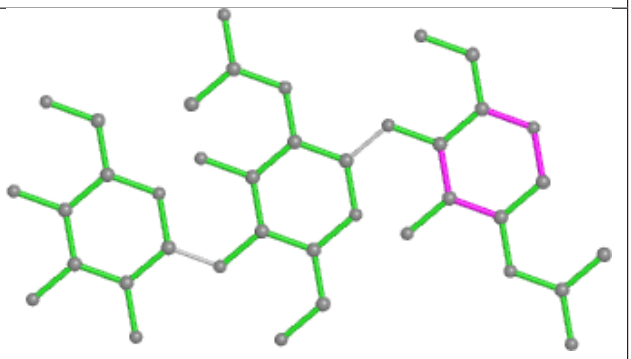
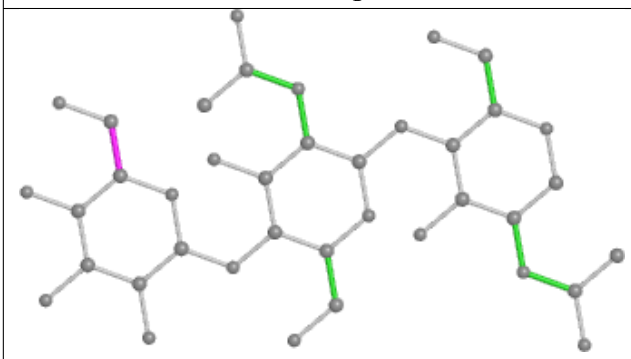
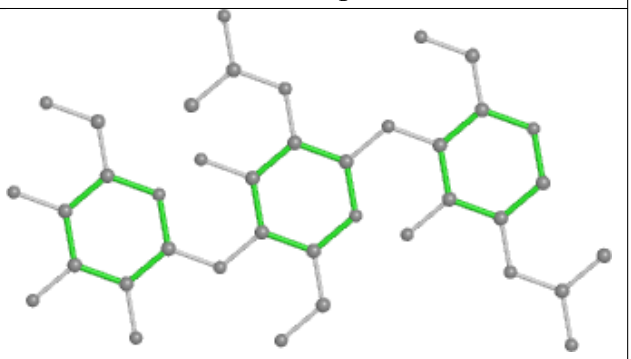


Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	324/324 (100%)	0.31	8 (2%) 57 59	43, 70, 106, 159	0
1	C	324/324 (100%)	0.01	1 (0%) 94 95	27, 46, 68, 153	0
1	E	324/324 (100%)	0.17	4 (1%) 79 80	38, 65, 94, 153	0
1	G	324/324 (100%)	0.23	7 (2%) 62 63	44, 69, 106, 146	0
1	I	324/324 (100%)	0.01	1 (0%) 94 95	25, 47, 70, 143	0
1	K	324/324 (100%)	0.14	7 (2%) 62 63	40, 63, 93, 135	0
2	B	170/170 (100%)	0.16	1 (0%) 89 91	33, 70, 107, 129	0
2	D	169/170 (99%)	0.04	2 (1%) 79 80	37, 55, 81, 116	0
2	F	165/170 (97%)	0.26	3 (1%) 68 70	40, 67, 102, 133	0
2	H	170/170 (100%)	0.11	2 (1%) 79 80	35, 66, 105, 129	0
2	J	167/170 (98%)	0.10	2 (1%) 79 80	35, 54, 84, 112	0
2	L	165/170 (97%)	0.16	0 100 100	39, 62, 96, 130	0
All	All	2950/2964 (99%)	0.14	38 (1%) 77 78	25, 61, 99, 159	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	ARG	9.8
1	C	327	ARG	9.1
1	E	327	ARG	7.3
1	I	327	ARG	6.7
1	G	327	ARG	5.6
1	K	327	ARG	5.2
1	K	326	ALA	4.9
1	A	303	ILE	3.7
1	E	265	GLY	3.6
2	B	559	MET	3.5
1	E	326	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	141	TYR	2.9
1	G	275	VAL	2.9
1	G	303	ILE	2.7
1	K	324	ILE	2.7
1	K	265	GLY	2.6
2	F	640	PHE	2.5
2	H	559	MET	2.5
2	D	559	MET	2.5
2	H	667	LYS	2.5
1	G	289	ILE	2.4
1	A	199	ASP	2.4
1	A	268	ILE	2.4
1	G	266	SER	2.3
1	A	198	ALA	2.3
2	J	626	LEU	2.3
2	D	633	ILE	2.3
1	G	196	GLN	2.3
1	K	171	ASN	2.2
1	A	51	ILE	2.1
2	F	638	PHE	2.1
1	K	310	VAL	2.1
2	J	559	MET	2.1
2	F	598	LEU	2.0
1	A	289	ILE	2.0
1	K	141	TYR	2.0
1	G	265	GLY	2.0
1	A	127	TRP	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, 95^{th} 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	BMA	O	3	11/12	0.75	0.19	91,104,110,121	0

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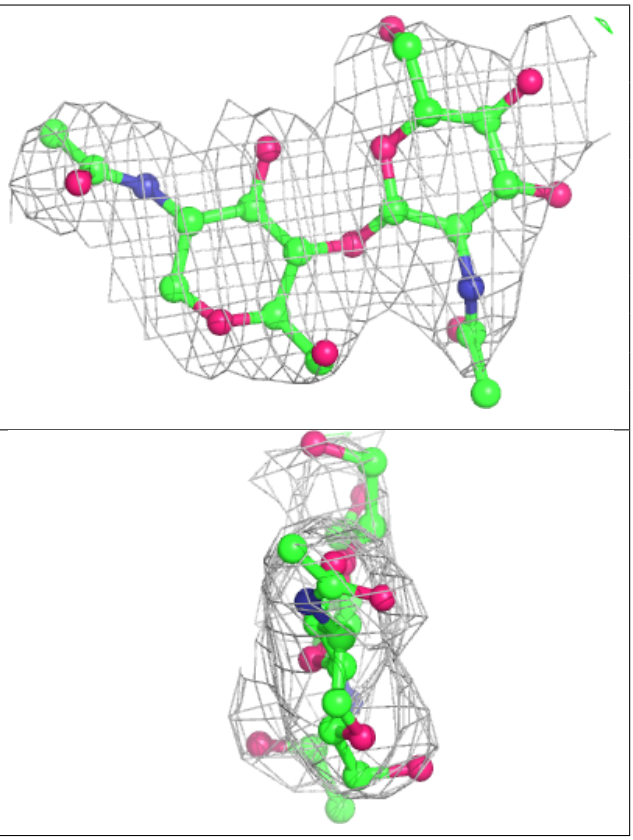
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	Q	2	14/15	0.81	0.35	100,120,126,131	0
3	NAG	T	2	14/15	0.84	0.26	106,111,117,122	0
4	BMA	S	3	11/12	0.86	0.21	97,112,119,130	0
3	NAG	R	2	14/15	0.88	0.18	69,80,87,91	0
3	NAG	M	2	14/15	0.89	0.19	103,115,126,129	0
4	NAG	S	2	14/15	0.89	0.25	78,92,99,100	0
3	NAG	P	2	14/15	0.89	0.15	107,117,122,125	0
4	NAG	O	1	14/15	0.89	0.23	72,79,84,89	0
4	NAG	O	2	14/15	0.90	0.19	65,76,81,83	0
4	NAG	S	1	14/15	0.92	0.25	73,80,87,90	0
3	NAG	N	2	14/15	0.94	0.14	66,73,78,81	0
3	NAG	T	1	14/15	0.95	0.20	65,79,94,98	0
3	NAG	Q	1	14/15	0.96	0.17	59,69,81,83	0
3	NAG	P	1	14/15	0.96	0.21	71,81,99,105	0
3	NAG	M	1	14/15	0.96	0.15	60,70,82,86	0
3	NAG	R	1	14/15	0.96	0.14	39,45,53,54	0
3	NAG	N	1	14/15	0.97	0.14	40,48,59,60	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.

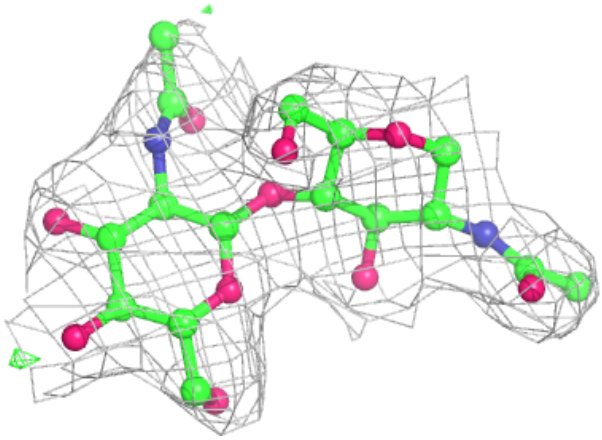
Electron density around Chain M:

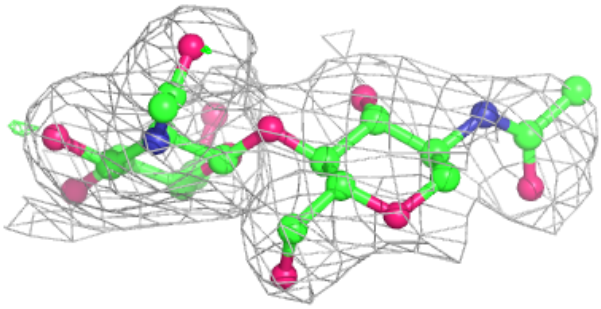
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

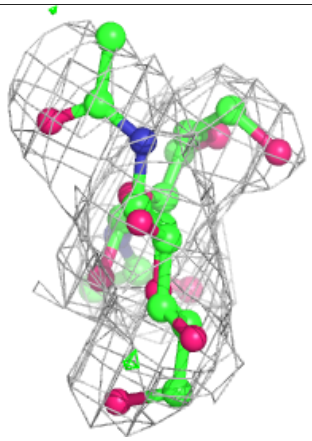


Electron density around Chain N:

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

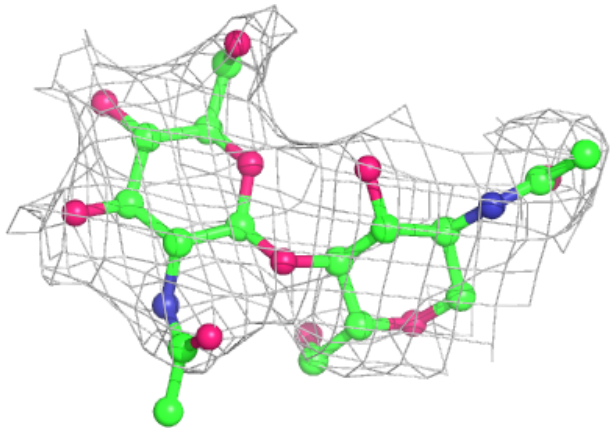


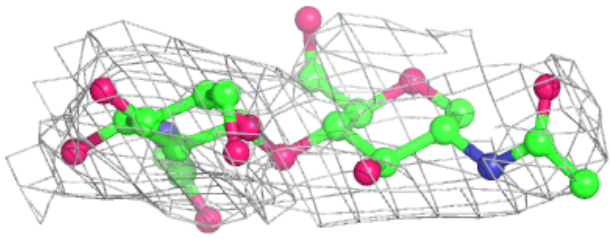


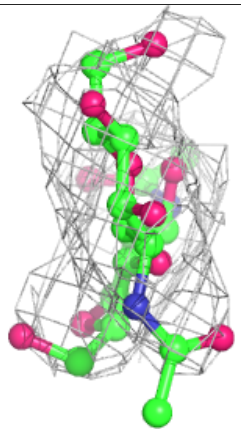


Electron density around Chain P:

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

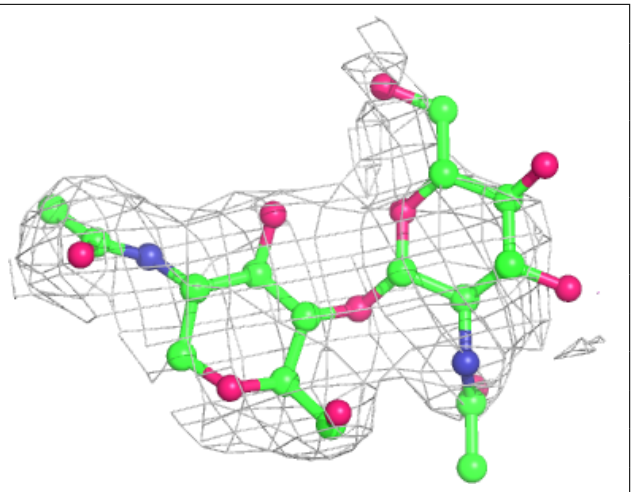


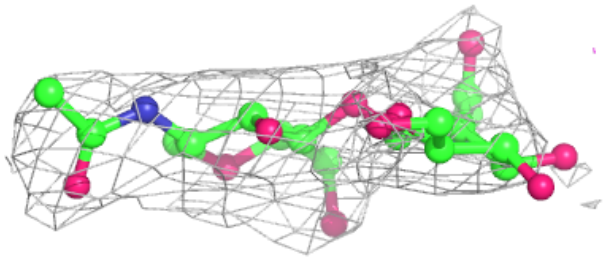


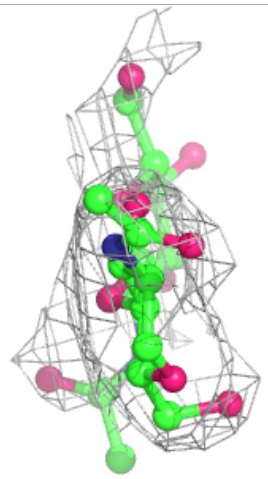


Electron density around Chain Q:

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

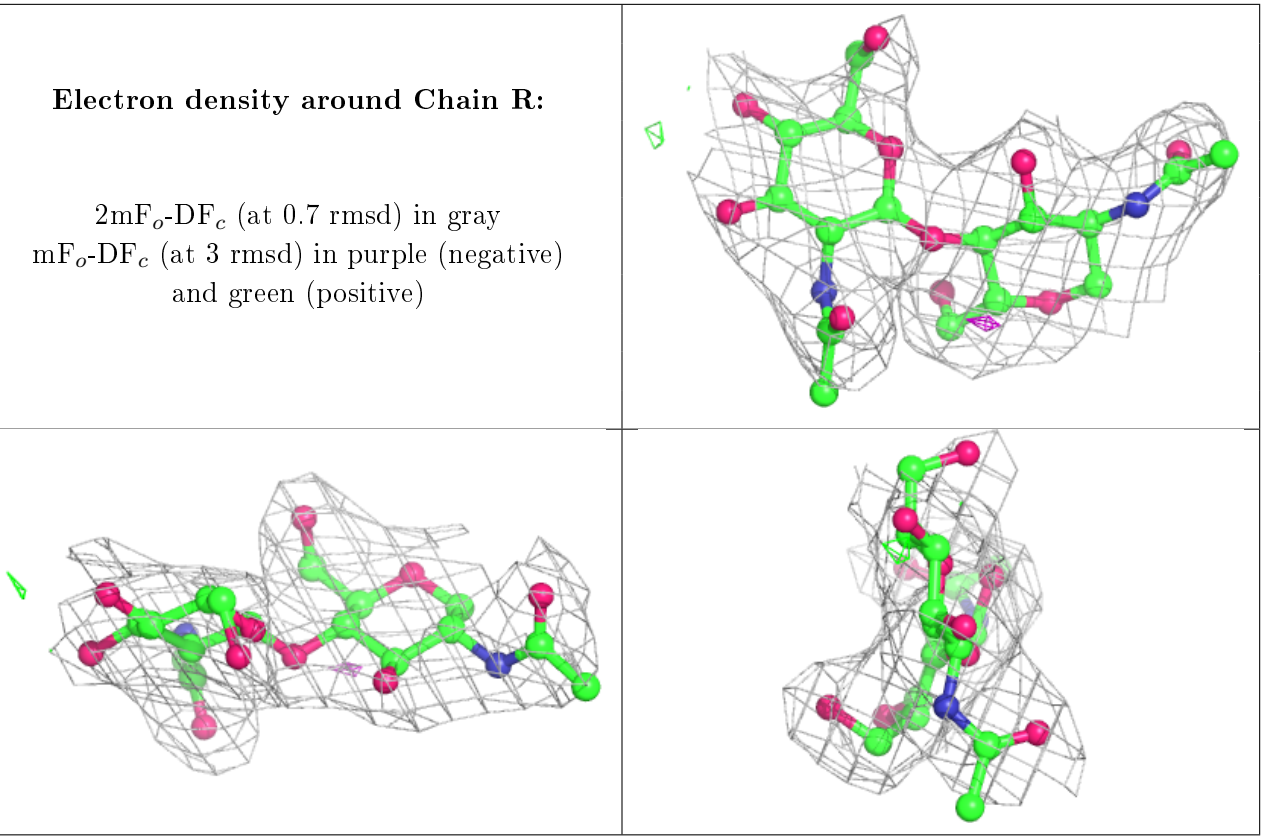






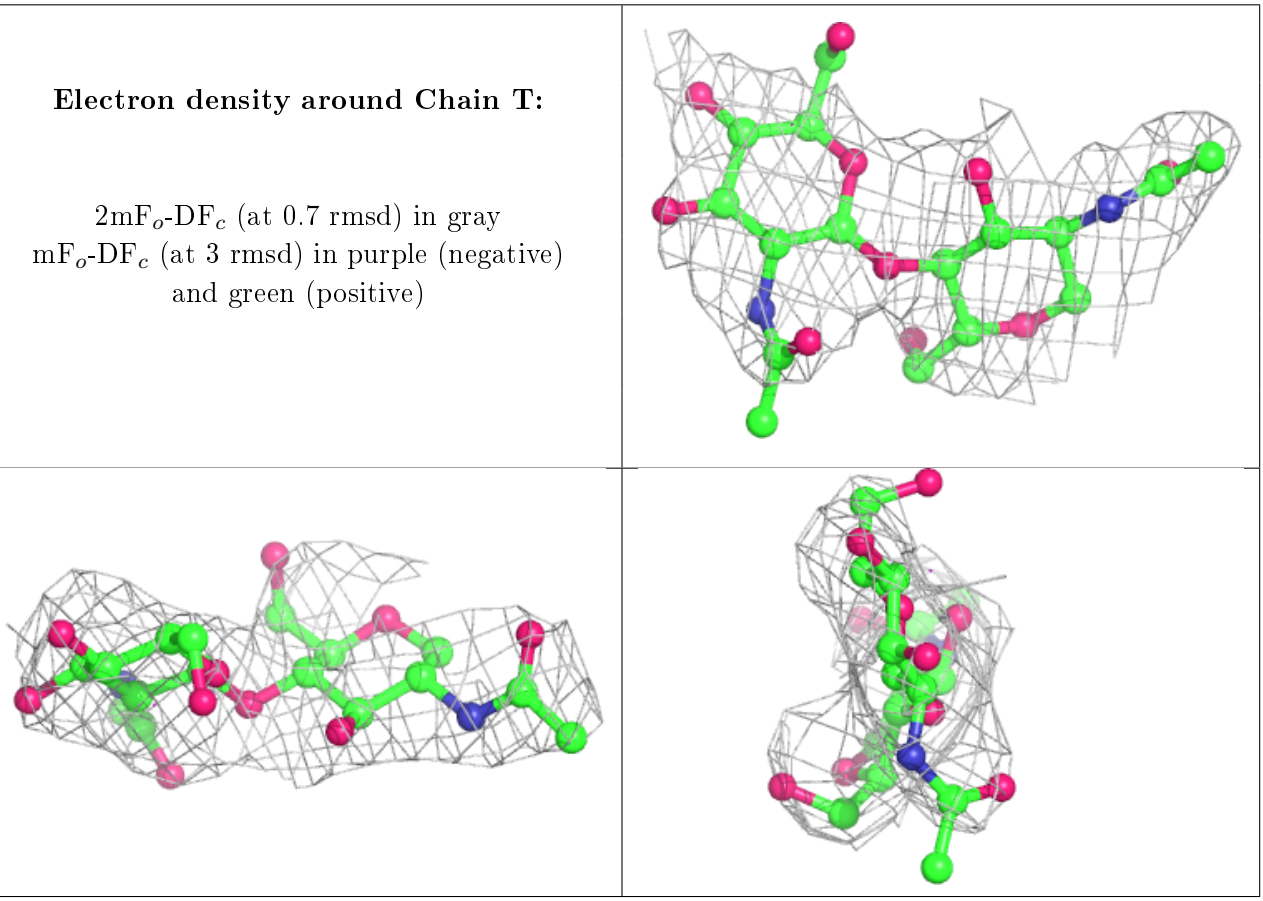
Electron density around Chain R:

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



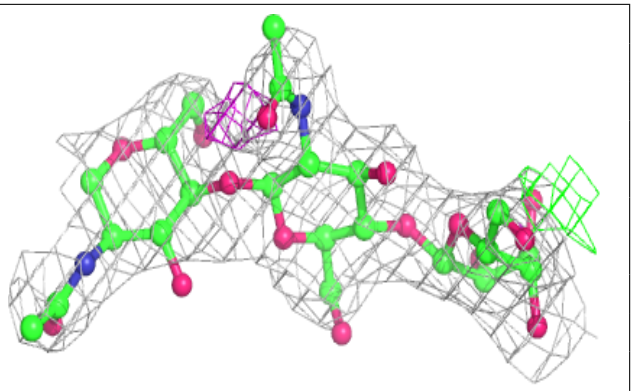
Electron density around Chain T:

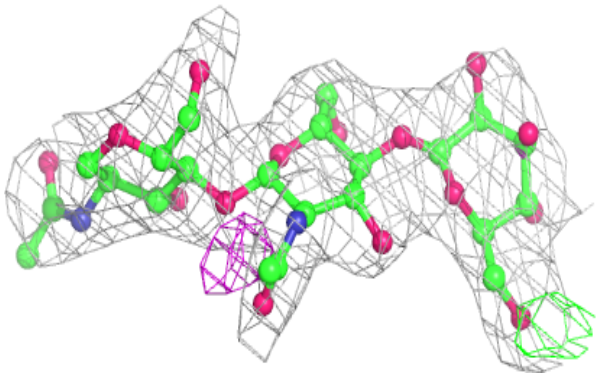
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

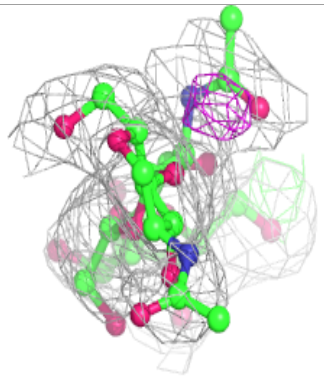


Electron density around Chain O:

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

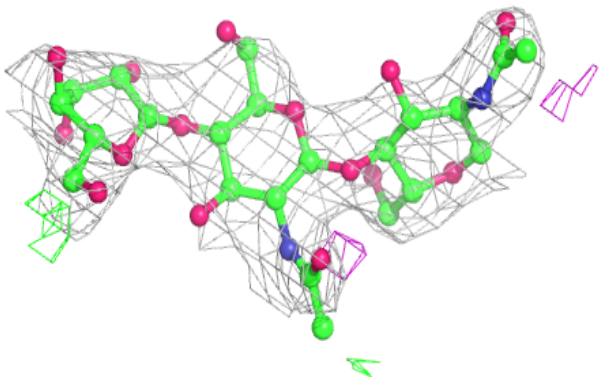


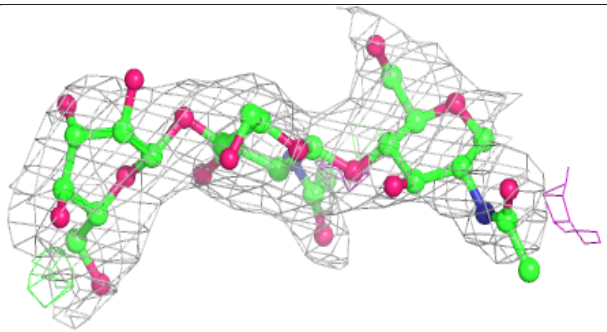


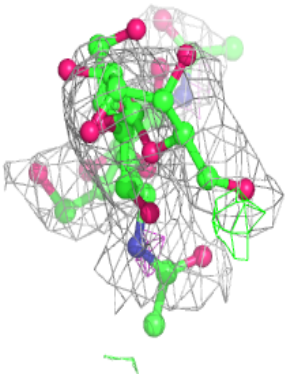


Electron density around Chain S:

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







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.