Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:28 PM EST

PDB ID	:	4UBD
Title	:	Crystal structure of a neutralizing human monoclonal antibody with 1968 H3 HA
Authors	:	Shore, D.A.; Yang, H.; Cho, M.; Donis, R.O.; Stevens, J.
Deposited on	:	2014-08-12
Resolution	:	3.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

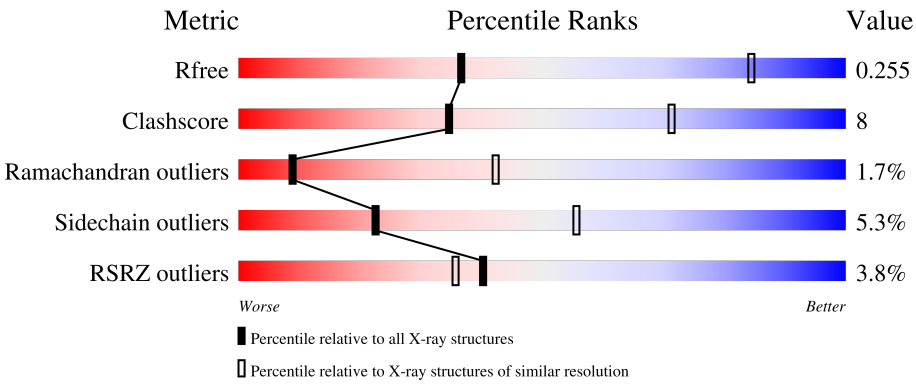
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	321	% 83% 14% • •
1	E	321	81% 17% •
1	I	321	84% 13% • •
1	M	321	83% 15% •
1	Q	321	81% 16% •

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Mol	Chain	Length	Quality of chain
1	U	321	.% 83% 16% •
2	B	175	.% 77% 13% 5% 6%
2	F	175	73% 17% • 7%
2	J	175	2% 77% 14% • • 6%
2	N	175	.% 77% 14% • • 7%
2	R	175	.% 75% 15% • • 5%
2	V	175	.% 77% 15% • 6%
3	C	226	73% 18% • • •
3	G	226	2% 74% 18% • • •
3	K	226	19% 75% 18% • • •
3	O	226	24% 73% 19% • • •
3	S	226	2% 74% 19% • • •
3	Y	226	74% 19% • • •
4	D	215	82% 16% • •
4	H	215	81% 16% • •
4	L	215	14% 84% 14% • •
4	P	215	21% 82% 16% •
4	T	215	2% 82% 15% • •
4	X	215	.% 83% 15% • •
5	W	4	100%
5	b	4	100%
5	c	4	100%
5	d	4	100%
5	e	4	100%
5	g	4	100%

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Mol	Chain	Length	Quality of chain
6	Z	2	50% 50%
6	a	2	100%
6	f	2	100%

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
5	MAN	W	4	X	-	-	-
5	MAN	b	4	X	-	-	-
5	MAN	c	4	X	-	-	-
5	MAN	d	4	X	-	-	-
5	MAN	e	4	X	-	-	-
5	MAN	g	4	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 43086 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2470	1546	434	477	13	0	0	0
1	U	320	2470	1546	434	477	13	0	0	0
1	I	317	2445	1531	429	472	13	0	0	0
1	M	320	2470	1546	434	477	13	0	0	0
1	Q	320	2470	1546	434	477	13	0	0	0
1	E	320	2470	1546	434	477	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	GLN	-	expression tag	UNP Q91MA7
U	329	GLN	-	expression tag	UNP Q91MA7
I	329	GLN	-	expression tag	UNP Q91MA7
M	329	GLN	-	expression tag	UNP Q91MA7
Q	329	GLN	-	expression tag	UNP Q91MA7
E	329	GLN	-	expression tag	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	V	164	1346	831	238	271	6	0	0	0
2	F	163	1338	825	237	270	6	0	0	0
2	B	165	1357	840	239	272	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	164	1349	834	238	271	6	0	0	0
			Total	C	N	O	S			
2	N	163	1338	825	237	270	6	0	0	0
			Total	C	N	O	S			
2	R	166	1359	839	241	273	6	0	0	0

- Molecule 3 is a protein called monoclonal antibody H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	Y	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	G	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	S	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	O	219	1637	1036	278	319	4	0	0	0
			Total	C	N	O	S			
3	K	219	1637	1036	278	319	4	0	0	0

- Molecule 4 is a protein called monoclonal antibody L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	X	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	H	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	T	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	P	213	1650	1029	290	327	4	0	0	0
			Total	C	N	O	S			
4	L	213	1650	1029	290	327	4	0	0	0

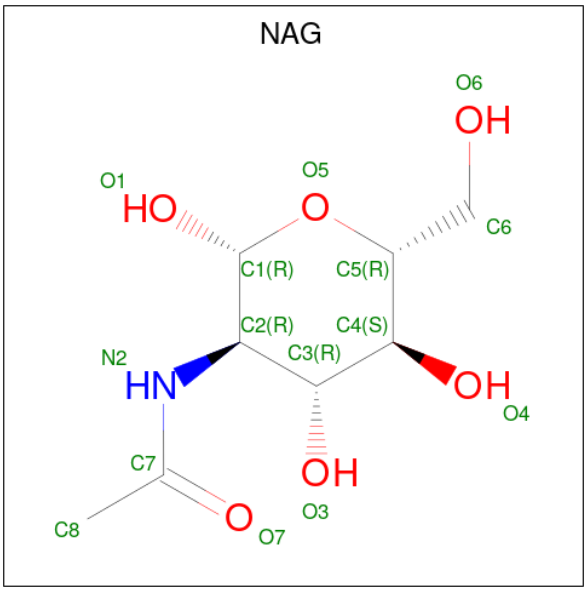
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	W	4	50	28	2	20	0	0	0
5	b	4	50	28	2	20	0	0	0
5	c	4	50	28	2	20	0	0	0
5	d	4	50	28	2	20	0	0	0
5	e	4	50	28	2	20	0	0	0
5	g	4	50	28	2	20	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	Z	2	28	16	2	10	0	0	0
6	a	2	28	16	2	10	0	0	0
6	f	2	28	16	2	10	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



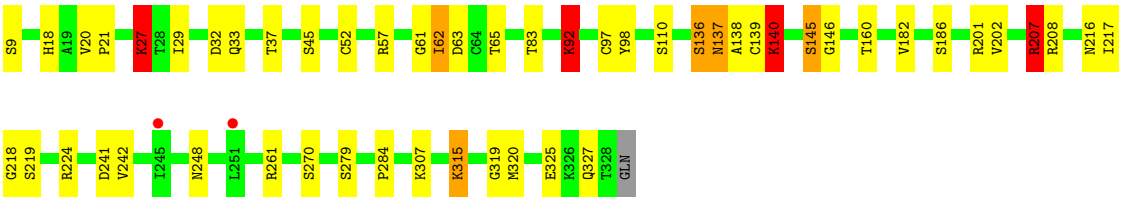
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	U	1	14	8	1	5	0	0
			Total	C	N	O		
7	V	1	14	8	1	5	0	0
			Total	C	N	O		
7	I	1	14	8	1	5	0	0
			Total	C	N	O		
7	M	1	14	8	1	5	0	0
			Total	C	N	O		
7	Q	1	14	8	1	5	0	0
			Total	C	N	O		
7	F	1	14	8	1	5	0	0

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.

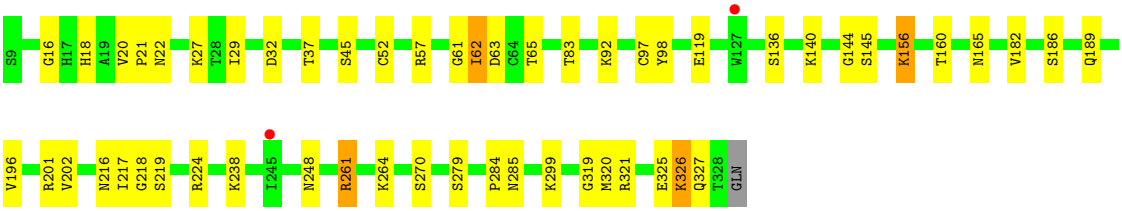
• Molecule 1: Hemagglutinin HA1 chain

Chain A:



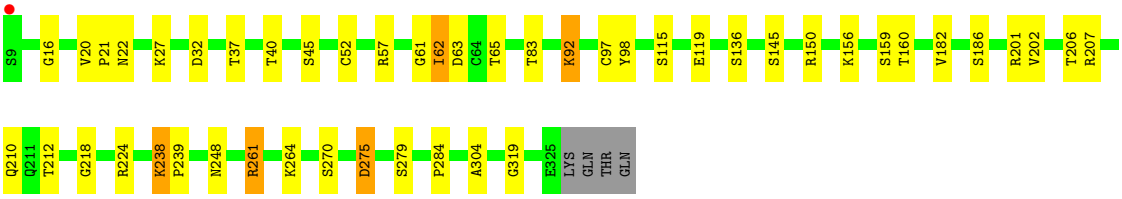
• Molecule 1: Hemagglutinin HA1 chain

Chain U:



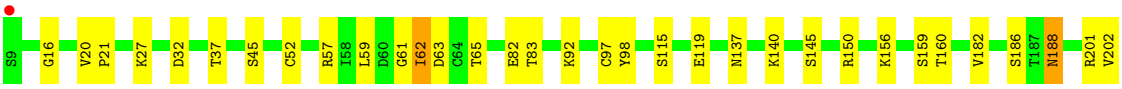
• Molecule 1: Hemagglutinin HA1 chain

Chain I:



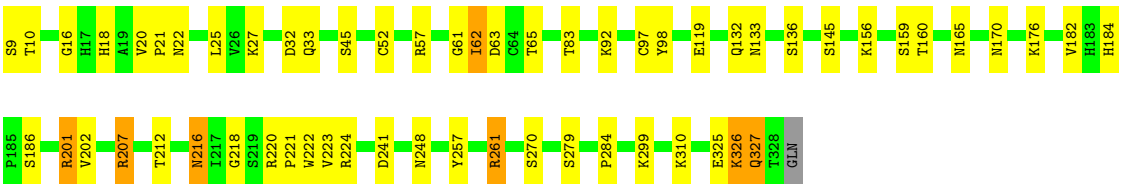
• Molecule 1: Hemagglutinin HA1 chain

Chain M:



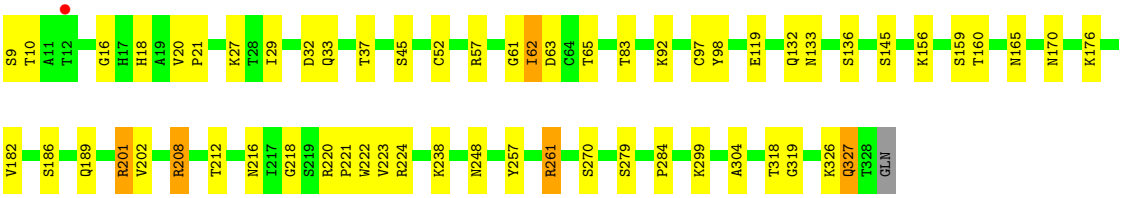
• Molecule 1: Hemagglutinin HA1 chain

Chain Q:



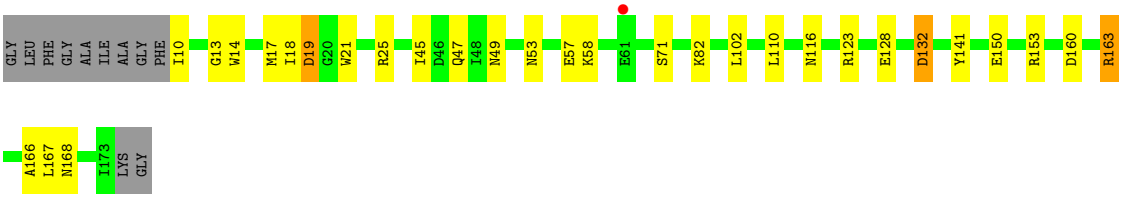
• Molecule 1: Hemagglutinin HA1 chain

Chain E:



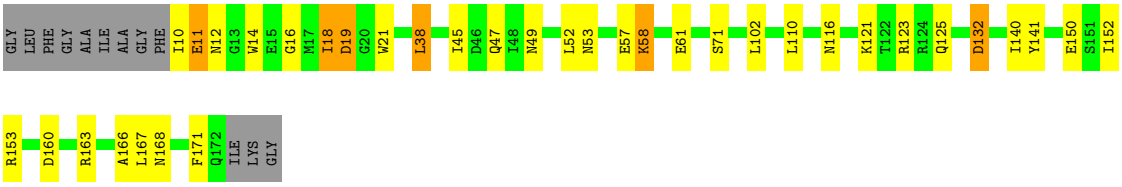
• Molecule 2: Hemagglutinin HA2 chain

Chain V:



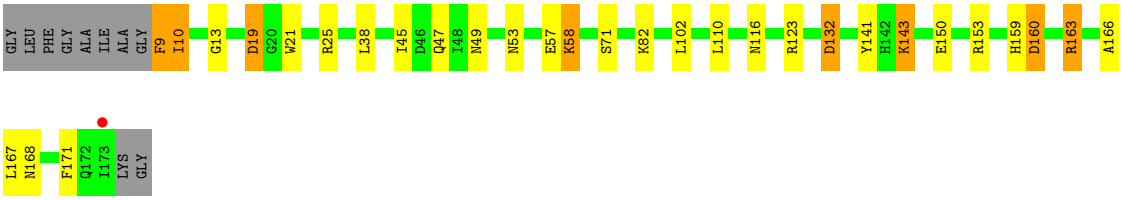
• Molecule 2: Hemagglutinin HA2 chain

Chain F:



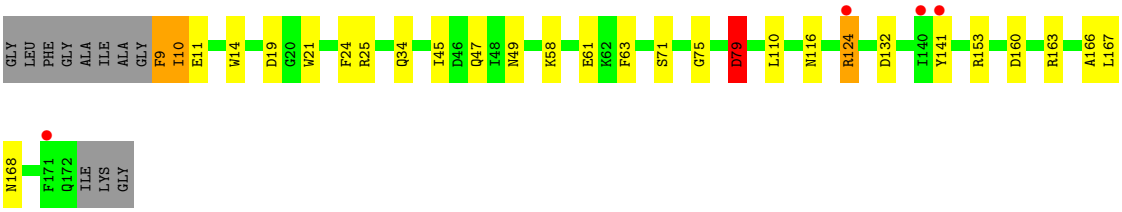
• Molecule 2: Hemagglutinin HA2 chain

Chain B:



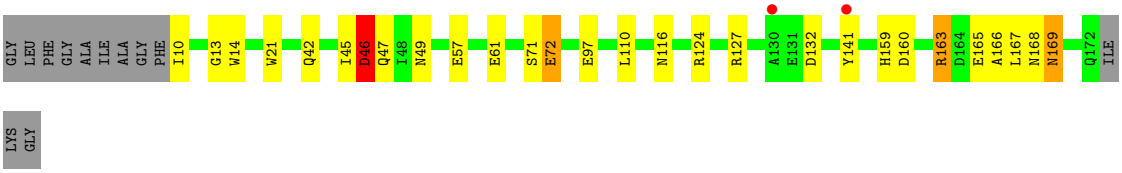
• Molecule 2: Hemagglutinin HA2 chain

Chain J:



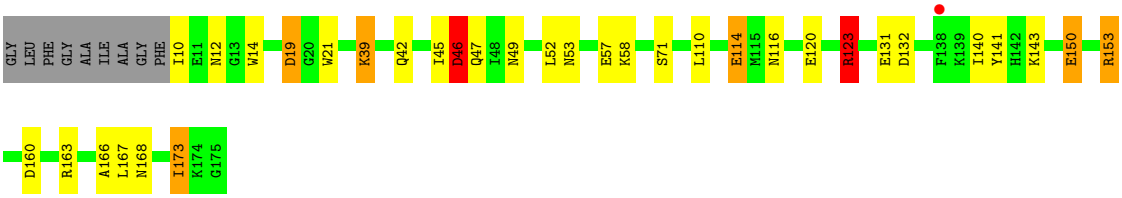
• Molecule 2: Hemagglutinin HA2 chain

Chain N:



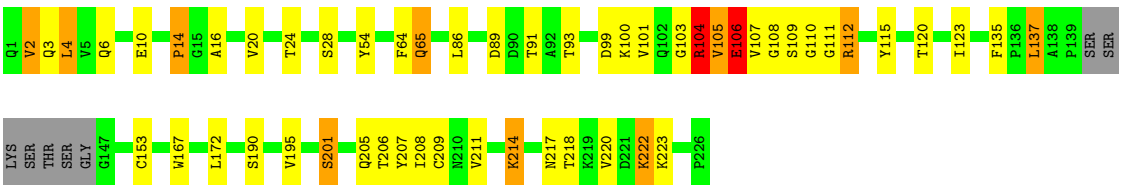
• Molecule 2: Hemagglutinin HA2 chain

Chain R:



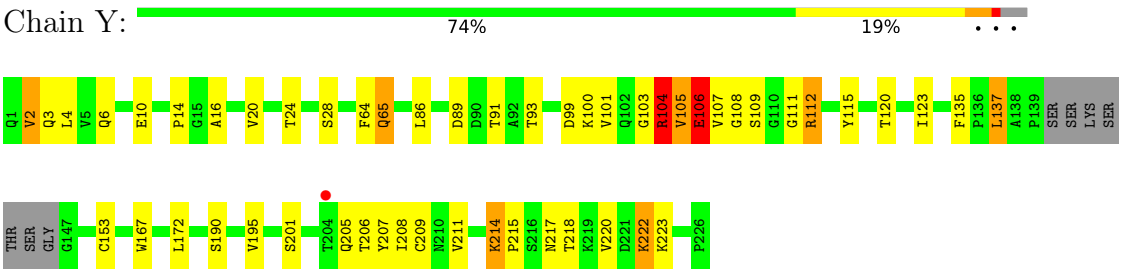
• Molecule 3: monoclonal antibody H chain

Chain C:



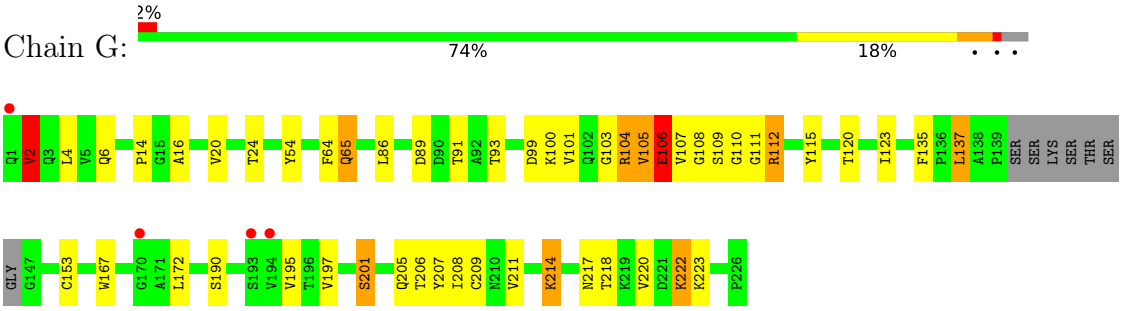
• Molecule 3: monoclonal antibody H chain

Chain Y:



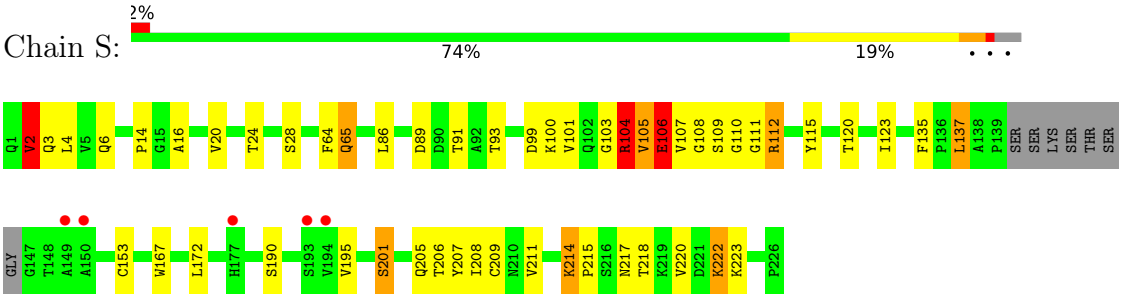
• Molecule 3: monoclonal antibody H chain

Chain G:



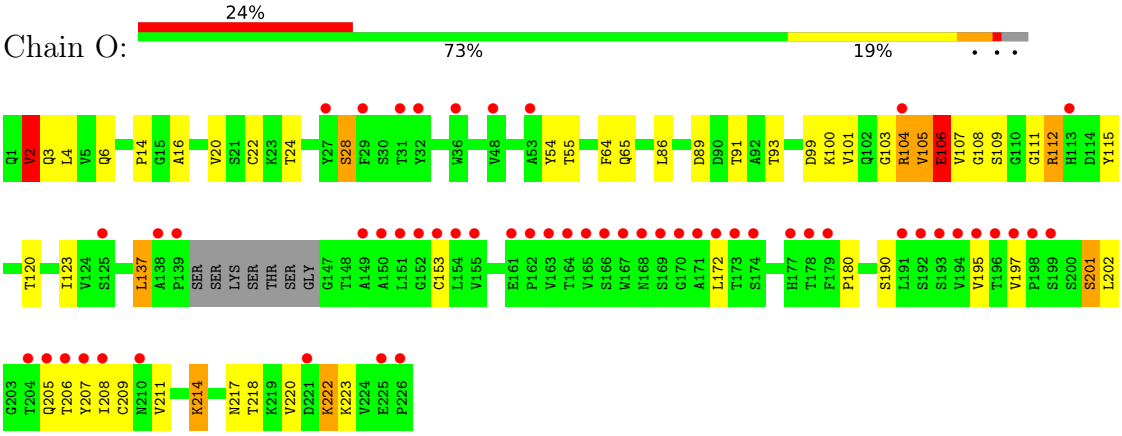
• Molecule 3: monoclonal antibody H chain

Chain S:



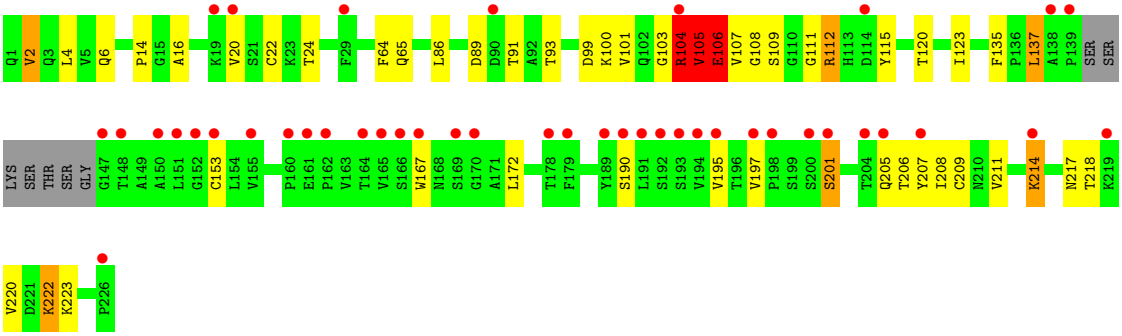
• Molecule 3: monoclonal antibody H chain

Chain O:



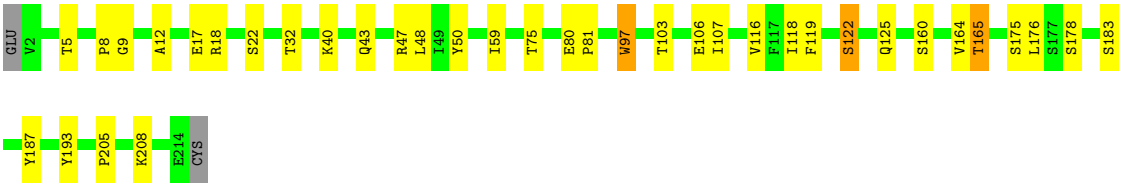
• Molecule 3: monoclonal antibody H chain

Chain K:



• Molecule 4: monoclonal antibody L chain

Chain D:

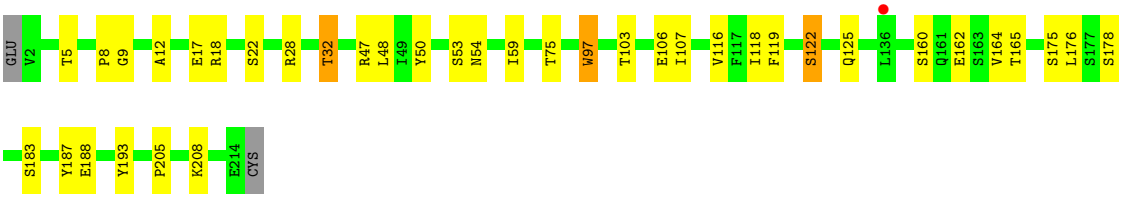


• Molecule 4: monoclonal antibody L chain

Chain X:

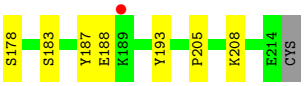
• Molecule 4: monoclonal antibody L chain

Chain H:



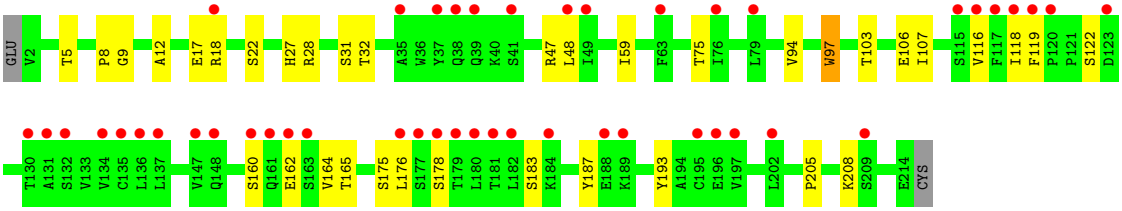
• Molecule 4: monoclonal antibody L chain

Chain T:



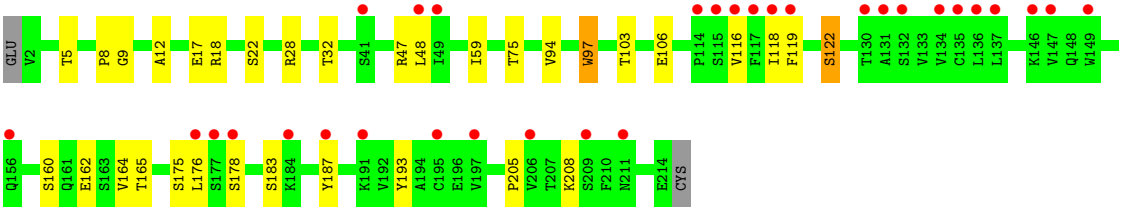
• Molecule 4: monoclonal antibody L chain

Chain P:



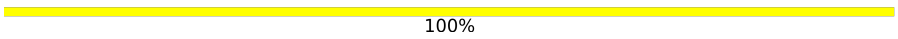
• Molecule 4: monoclonal antibody L chain

Chain L:



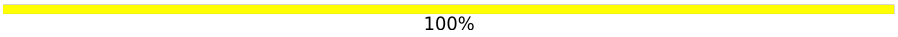
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



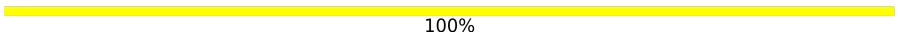
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%

NAG1
NAG2
BMA3
MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 100%

NAG1
NAG2
BMA3
MAN4

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%

NAG1
NAG2
BMA3
MAN4

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 50% 50%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 100%

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	128.70Å 128.70Å 428.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.50 48.26 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.50) 99.4 (48.26-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.258 0.216 , 0.255	Depositor DCC
R_{free} test set	4962 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	97.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.410 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	43086	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.60	0/2526	0.80	5/3442 (0.1%)
1	E	0.61	0/2526	0.76	1/3442 (0.0%)
1	I	0.64	1/2501 (0.0%)	0.77	2/3409 (0.1%)
1	M	0.62	1/2526 (0.0%)	0.77	2/3442 (0.1%)
1	Q	0.61	0/2526	0.78	2/3442 (0.1%)
1	U	0.61	0/2526	0.78	1/3442 (0.0%)
2	B	0.77	3/1380 (0.2%)	0.92	6/1855 (0.3%)
2	F	0.74	3/1360 (0.2%)	0.92	4/1828 (0.2%)
2	J	0.72	1/1372 (0.1%)	0.89	5/1844 (0.3%)
2	N	0.74	1/1360 (0.1%)	0.95	5/1828 (0.3%)
2	R	0.74	2/1381 (0.1%)	1.05	10/1855 (0.5%)
2	V	0.78	4/1368 (0.3%)	0.92	6/1839 (0.3%)
3	C	0.62	0/1677	0.79	3/2289 (0.1%)
3	G	0.59	0/1677	0.78	1/2289 (0.0%)
3	K	0.53	0/1677	0.75	2/2289 (0.1%)
3	O	0.53	0/1677	0.75	1/2289 (0.0%)
3	S	0.59	0/1677	0.78	2/2289 (0.1%)
3	Y	0.62	0/1677	0.79	3/2289 (0.1%)
4	D	0.61	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	H	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	L	0.49	1/1687 (0.1%)	0.71	1/2292 (0.0%)
4	P	0.50	1/1687 (0.1%)	0.72	1/2292 (0.0%)
4	T	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
4	X	0.62	1/1687 (0.1%)	0.76	1/2292 (0.0%)
All	All	0.63	22/43536 (0.1%)	0.80	67/59154 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	G	0	1
3	K	0	1
3	O	0	1
3	S	0	1
3	Y	0	1
All	All	0	6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	275	ASP	CB-CG	7.09	1.66	1.51
4	L	97	TRP	CB-CG	6.63	1.62	1.50
1	M	275	ASP	CB-CG	6.58	1.65	1.51
2	V	10	ILE	CA-CB	6.55	1.70	1.54
2	V	19	ASP	CB-CG	6.29	1.65	1.51
2	J	160	ASP	CB-CG	6.16	1.64	1.51
4	P	97	TRP	CB-CG	6.14	1.61	1.50
2	N	160	ASP	CB-CG	6.13	1.64	1.51
4	T	97	TRP	CB-CG	6.13	1.61	1.50
2	B	160	ASP	CB-CG	6.04	1.64	1.51
4	H	97	TRP	CB-CG	5.99	1.61	1.50
2	B	19	ASP	CB-CG	5.94	1.64	1.51
2	V	160	ASP	CB-CG	5.87	1.64	1.51
2	R	160	ASP	CB-CG	5.79	1.64	1.51
2	R	19	ASP	CB-CG	5.78	1.63	1.51
2	F	160	ASP	CB-CG	5.76	1.63	1.51
2	V	150	GLU	CG-CD	5.73	1.60	1.51
2	B	150	GLU	CG-CD	5.61	1.60	1.51
2	F	19	ASP	CB-CG	5.47	1.63	1.51
4	D	97	TRP	CB-CG	5.24	1.59	1.50
4	X	97	TRP	CB-CG	5.23	1.59	1.50
2	F	150	GLU	CG-CD	5.01	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	19	ASP	CB-CG-OD2	16.74	133.37	118.30
1	U	156	LYS	CB-CA-C	-8.49	93.43	110.40
2	V	82	LYS	CD-CE-NZ	8.34	130.89	111.70
2	R	123	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	R	46	ASP	N-CA-CB	8.28	125.51	110.60
2	N	46	ASP	N-CA-CB	8.13	125.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	163	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	J	124	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	Q	207	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	27	LYS	CD-CE-NZ	6.90	127.57	111.70
2	N	160	ASP	CB-CG-OD2	6.46	124.11	118.30
2	B	160	ASP	CB-CG-OD2	6.42	124.08	118.30
2	F	160	ASP	CB-CG-OD2	6.39	124.05	118.30
2	B	163	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	N	163	ARG	NE-CZ-NH2	-6.19	117.21	120.30
2	R	160	ASP	CB-CG-OD2	6.17	123.85	118.30
2	R	114	GLU	N-CA-CB	6.06	121.50	110.60
2	J	11	GLU	CB-CA-C	-6.04	98.33	110.40
3	Y	104	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	R	123	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	R	153	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	V	163	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	92	LYS	CB-CA-C	-5.82	98.76	110.40
2	J	79	ASP	N-CA-CB	5.80	121.03	110.60
2	V	160	ASP	CB-CG-OD2	5.79	123.51	118.30
2	R	19	ASP	OD1-CG-OD2	-5.75	112.38	123.30
1	M	275	ASP	CB-CG-OD2	5.71	123.44	118.30
1	I	275	ASP	CB-CG-OD2	5.70	123.43	118.30
3	C	104	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	Y	10	GLU	OE1-CD-OE2	-5.64	116.53	123.30
3	Y	2	VAL	CB-CA-C	-5.63	100.69	111.40
3	G	2	VAL	CB-CA-C	-5.62	100.72	111.40
2	V	153	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	R	39	LYS	CB-CA-C	5.59	121.58	110.40
3	C	2	VAL	CB-CA-C	-5.59	100.78	111.40
3	O	2	VAL	CB-CA-C	-5.53	100.89	111.40
2	V	25	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	153	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	I	150	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	163	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	307	LYS	CD-CE-NZ	5.41	124.15	111.70
4	T	97	TRP	CA-CB-CG	5.40	123.95	113.70
2	J	160	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	140	LYS	CA-CB-CG	-5.37	101.58	113.40
1	M	150	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	S	104	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	S	2	VAL	CB-CA-C	-5.32	101.30	111.40
4	X	97	TRP	CA-CB-CG	5.31	123.80	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	222	TRP	CA-CB-CG	5.30	123.78	113.70
3	K	2	VAL	CB-CA-C	-5.30	101.32	111.40
2	F	153	ARG	NE-CZ-NH2	-5.26	117.67	120.30
4	H	97	TRP	CA-CB-CG	5.25	123.68	113.70
2	F	132	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	132	ASP	CB-CG-OD2	5.23	123.00	118.30
2	V	132	ASP	CB-CG-OD2	5.21	122.99	118.30
2	N	132	ASP	CB-CG-OD2	5.20	122.98	118.30
2	J	132	ASP	CB-CG-OD2	5.19	122.97	118.30
4	L	97	TRP	CA-CB-CG	5.19	123.56	113.70
2	F	150	GLU	OE1-CD-OE2	-5.18	117.08	123.30
2	R	132	ASP	CB-CG-OD2	5.18	122.96	118.30
4	P	97	TRP	CA-CB-CG	5.17	123.53	113.70
1	Q	207	ARG	N-CA-CB	5.16	119.89	110.60
4	D	97	TRP	CA-CB-CG	5.16	123.50	113.70
3	C	10	GLU	OE1-CD-OE2	-5.09	117.19	123.30
2	B	25	ARG	NE-CZ-NH1	5.09	122.85	120.30
3	K	104	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	207	ARG	N-CA-CB	5.05	119.70	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	106	GLU	Peptide
3	G	106	GLU	Peptide
3	K	106	GLU	Peptide
3	O	106	GLU	Peptide
3	S	106	GLU	Peptide
3	Y	106	GLU	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	2470	0	2419	57	0
1	E	2470	0	2422	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2445	0	2393	29	1
1	M	2470	0	2421	36	1
1	Q	2470	0	2420	45	0
1	U	2470	0	2421	46	0
2	B	1357	0	1275	23	0
2	F	1338	0	1255	26	0
2	J	1349	0	1264	17	0
2	N	1338	0	1255	20	0
2	R	1359	0	1282	23	0
2	V	1346	0	1265	13	0
3	C	1637	0	1610	55	0
3	G	1637	0	1610	52	0
3	K	1637	0	1610	48	0
3	O	1637	0	1610	48	0
3	S	1637	0	1610	52	0
3	Y	1637	0	1610	52	0
4	D	1650	0	1602	20	0
4	H	1650	0	1602	24	1
4	L	1650	0	1602	23	0
4	P	1650	0	1602	23	0
4	T	1650	0	1602	23	1
4	X	1650	0	1602	17	0
5	W	50	0	43	0	0
5	b	50	0	43	0	0
5	c	50	0	43	0	0
5	d	50	0	43	0	0
5	e	50	0	43	0	0
5	g	50	0	43	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	f	28	0	25	0	0
7	A	14	0	13	0	0
7	F	14	0	13	0	0
7	I	14	0	13	2	0
7	M	14	0	13	0	0
7	Q	14	0	13	0	0
7	U	14	0	13	5	0
7	V	14	0	13	0	0
All	All	43086	0	41788	693	2

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 8.

All (693) 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:U:285:ASN:ND2	7:U:405:NAG:C1	1.71	1.51
1:U:156:LYS:HE2	1:U:196:VAL:CG2	1.66	1.25
1:A:140:LYS:HD2	1:A:140:LYS:N	1.33	1.22
1:U:156:LYS:CE	1:U:196:VAL:HG23	1.75	1.16
3:G:208:ILE:HA	3:G:223:LYS:HD3	1.21	1.11
3:S:208:ILE:HA	3:S:223:LYS:HD3	1.22	1.10
3:Y:208:ILE:HA	3:Y:223:LYS:HD3	1.21	1.10
3:C:208:ILE:HA	3:C:223:LYS:HD3	1.20	1.10
3:O:208:ILE:HA	3:O:223:LYS:HD3	1.23	1.09
2:R:120:GLU:OE1	2:R:123:ARG:NH1	1.86	1.08
3:K:208:ILE:HA	3:K:223:LYS:HD3	1.22	1.07
1:A:137:ASN:HA	1:A:140:LYS:HE2	1.39	1.03
2:V:49:ASN:OD1	3:Y:106:GLU:HB3	1.60	1.01
2:B:49:ASN:OD1	3:C:106:GLU:HB3	1.63	0.98
1:A:140:LYS:N	1:A:140:LYS:CD	2.27	0.97
1:U:156:LYS:HE2	1:U:196:VAL:HG23	0.98	0.96
1:A:27:LYS:HD2	1:A:32:ASP:O	1.66	0.96
3:S:107:VAL:HB	3:S:108:GLY:HA2	1.47	0.95
3:C:208:ILE:HA	3:C:223:LYS:CD	1.97	0.94
1:M:212:THR:HB	1:Q:216:ASN:HD22	1.32	0.94
3:Y:208:ILE:HA	3:Y:223:LYS:CD	1.97	0.93
3:G:107:VAL:HB	3:G:108:GLY:HA2	1.49	0.93
2:V:49:ASN:OD1	3:Y:106:GLU:CB	2.17	0.93
3:G:208:ILE:HA	3:G:223:LYS:CD	1.99	0.92
3:S:208:ILE:HA	3:S:223:LYS:CD	1.99	0.92
3:O:208:ILE:HA	3:O:223:LYS:CD	2.00	0.91
1:A:136:SER:O	1:A:140:LYS:NZ	2.02	0.91
1:A:139:CYS:C	1:A:140:LYS:HD2	1.91	0.91
3:C:107:VAL:HB	3:C:108:GLY:HA2	1.50	0.91
3:O:107:VAL:HB	3:O:108:GLY:HA2	1.50	0.91
3:K:107:VAL:HB	3:K:108:GLY:HA2	1.49	0.90
3:Y:107:VAL:HB	3:Y:108:GLY:HA2	1.49	0.90
3:K:208:ILE:HA	3:K:223:LYS:CD	2.00	0.90
2:B:49:ASN:OD1	3:C:106:GLU:CB	2.20	0.90
2:B:9:PHE:CE1	2:B:10:ILE:HD11	2.07	0.89
1:Q:27:LYS:HE3	4:P:28:ARG:HG3	1.55	0.89
2:J:9:PHE:CE1	2:J:10:ILE:HD11	2.09	0.88
2:R:150:GLU:OE1	2:R:150:GLU:HA	1.71	0.87
1:A:27:LYS:HE2	1:A:33:GLN:HE22	1.41	0.85
1:A:140:LYS:HE2	1:A:145:SER:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LYS:HE3	4:L:28:ARG:HG3	1.59	0.84
1:E:33:GLN:HB2	4:L:94:VAL:HG22	1.61	0.83
3:S:107:VAL:HB	3:S:108:GLY:CA	2.09	0.83
2:R:49:ASN:OD1	3:S:106:GLU:HB3	1.78	0.82
2:F:49:ASN:OD1	3:G:106:GLU:HB3	1.80	0.82
2:N:127:ARG:HE	2:N:159:HIS:CE1	1.97	0.82
1:U:285:ASN:ND2	7:U:405:NAG:O5	2.10	0.82
3:Y:107:VAL:HB	3:Y:108:GLY:CA	2.09	0.81
3:G:107:VAL:HB	3:G:108:GLY:CA	2.10	0.81
1:U:285:ASN:CG	7:U:405:NAG:C1	2.48	0.81
1:I:40:THR:HA	7:I:405:NAG:H82	1.63	0.80
3:C:107:VAL:HB	3:C:108:GLY:CA	2.11	0.80
1:U:156:LYS:HE3	1:U:196:VAL:N	1.97	0.79
2:R:150:GLU:OE1	2:R:150:GLU:CA	2.32	0.78
2:J:49:ASN:OD1	3:K:106:GLU:HB3	1.83	0.77
3:K:107:VAL:HB	3:K:108:GLY:CA	2.14	0.77
1:U:156:LYS:CD	1:U:196:VAL:HG23	2.13	0.77
3:O:107:VAL:HB	3:O:108:GLY:CA	2.14	0.77
1:A:137:ASN:C	1:A:140:LYS:HD3	2.06	0.75
1:E:33:GLN:HG2	4:L:94:VAL:HG21	1.68	0.75
3:C:208:ILE:CA	3:C:223:LYS:HD3	2.11	0.74
2:R:150:GLU:OE2	2:R:153:ARG:NH2	2.21	0.74
1:A:27:LYS:HE3	4:H:28:ARG:HG3	1.70	0.74
1:A:216:ASN:CG	1:E:212:THR:HG21	2.09	0.74
1:A:137:ASN:HA	1:A:140:LYS:CE	2.15	0.73
1:A:207:ARG:NH1	1:A:242:VAL:HG12	2.04	0.72
3:G:209:CYS:SG	3:G:223:LYS:NZ	2.63	0.72
3:S:209:CYS:SG	3:S:223:LYS:NZ	2.63	0.72
1:U:216:ASN:CG	1:Q:212:THR:HG21	2.11	0.72
3:O:209:CYS:SG	3:O:223:LYS:NZ	2.63	0.72
1:A:140:LYS:HE3	1:A:145:SER:HA	1.72	0.71
2:R:49:ASN:OD1	3:S:106:GLU:CB	2.37	0.71
3:K:209:CYS:SG	3:K:223:LYS:NZ	2.63	0.71
1:A:27:LYS:HE2	1:A:33:GLN:NE2	2.03	0.71
3:G:208:ILE:CA	3:G:223:LYS:HD3	2.12	0.70
3:C:209:CYS:SG	3:C:223:LYS:NZ	2.64	0.70
3:S:208:ILE:CA	3:S:223:LYS:HD3	2.13	0.70
1:U:238:LYS:HE3	2:N:72:GLU:OE1	1.92	0.70
3:Y:209:CYS:SG	3:Y:223:LYS:NZ	2.64	0.70
2:N:49:ASN:OD1	3:O:106:GLU:HB3	1.92	0.70
2:N:127:ARG:NH2	2:R:131:GLU:OE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:33:GLN:HB2	4:P:94:VAL:HG22	1.73	0.69
2:F:49:ASN:OD1	3:G:106:GLU:CB	2.39	0.69
3:Y:99:ASP:OD1	3:Y:112:ARG:HD3	1.92	0.69
1:E:33:GLN:CB	4:L:94:VAL:HG22	2.22	0.69
1:A:140:LYS:HE3	1:A:145:SER:CA	2.23	0.69
1:A:137:ASN:O	1:A:140:LYS:HD3	1.92	0.69
3:Y:208:ILE:CA	3:Y:223:LYS:HD3	2.12	0.69
3:G:99:ASP:OD1	3:G:112:ARG:HD3	1.93	0.69
3:S:99:ASP:OD1	3:S:112:ARG:HD3	1.93	0.69
3:O:208:ILE:CA	3:O:223:LYS:HD3	2.14	0.69
3:K:208:ILE:CA	3:K:223:LYS:HD3	2.13	0.68
3:C:99:ASP:OD1	3:C:112:ARG:HD3	1.94	0.68
3:K:99:ASP:OD1	3:K:112:ARG:HD3	1.94	0.68
1:A:140:LYS:CE	1:A:145:SER:HB2	2.23	0.67
3:C:207:TYR:C	3:C:223:LYS:HE2	2.14	0.67
3:O:99:ASP:OD1	3:O:112:ARG:HD3	1.95	0.66
3:S:207:TYR:C	3:S:223:LYS:HE2	2.16	0.66
1:M:212:THR:CB	1:Q:216:ASN:HD22	2.07	0.66
3:G:207:TYR:C	3:G:223:LYS:HE2	2.16	0.66
1:U:156:LYS:CE	1:U:196:VAL:N	2.57	0.66
3:Y:207:TYR:C	3:Y:223:LYS:HE2	2.15	0.66
1:A:136:SER:C	1:A:140:LYS:NZ	2.48	0.66
3:G:137:LEU:CD1	4:H:119:PHE:CG	2.78	0.65
1:Q:207:ARG:HG2	1:Q:241:ASP:OD1	1.96	0.65
1:A:137:ASN:CA	1:A:140:LYS:HE2	2.23	0.64
1:A:219:SER:HB2	1:E:165:ASN:OD1	1.98	0.64
1:A:207:ARG:HG2	1:A:241:ASP:OD1	1.96	0.64
3:S:137:LEU:CD1	4:T:119:PHE:CG	2.80	0.64
1:A:27:LYS:CE	1:A:33:GLN:HE22	2.11	0.64
2:J:75:GLY:O	2:J:79:ASP:OD1	2.16	0.64
1:U:219:SER:HB2	1:Q:165:ASN:OD1	1.98	0.63
1:M:27:LYS:HE3	2:N:97:GLU:OE2	1.99	0.63
3:G:137:LEU:HD11	4:H:119:PHE:CG	2.33	0.63
1:A:217:ILE:O	1:E:201:ARG:CZ	2.45	0.63
1:U:140:LYS:HG2	1:U:144:GLY:O	1.98	0.63
2:B:9:PHE:CE1	2:B:10:ILE:CD1	2.80	0.63
2:J:9:PHE:CE1	2:J:10:ILE:CD1	2.82	0.63
3:K:207:TYR:C	3:K:223:LYS:HE2	2.20	0.62
1:U:217:ILE:O	1:Q:201:ARG:CZ	2.46	0.62
1:I:27:LYS:HG2	1:I:32:ASP:O	1.99	0.62
1:Q:33:GLN:HG2	4:P:94:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LYS:HG2	1:E:32:ASP:O	1.98	0.62
1:U:27:LYS:HG2	1:U:32:ASP:O	1.98	0.62
1:Q:27:LYS:HG2	1:Q:32:ASP:O	1.98	0.62
3:Y:201:SER:O	3:Y:205:GLN:NE2	2.32	0.62
3:C:201:SER:O	3:C:205:GLN:NE2	2.32	0.62
3:O:137:LEU:CD1	4:P:119:PHE:CG	2.83	0.62
2:V:53:ASN:HD21	3:Y:108:GLY:HA2	1.64	0.61
3:O:207:TYR:C	3:O:223:LYS:HE2	2.20	0.61
3:C:137:LEU:CD1	4:D:119:PHE:CG	2.84	0.61
3:O:201:SER:O	3:O:205:GLN:NE2	2.34	0.61
1:M:212:THR:HB	1:Q:216:ASN:ND2	2.12	0.60
3:G:201:SER:O	3:G:205:GLN:NE2	2.34	0.60
3:S:201:SER:O	3:S:205:GLN:NE2	2.34	0.60
1:U:156:LYS:HE3	1:U:196:VAL:H	1.63	0.60
1:I:97:CYS:O	1:I:224:ARG:NH1	2.35	0.60
3:S:137:LEU:HD11	4:T:119:PHE:CG	2.36	0.60
1:A:37:THR:HG23	1:A:319:GLY:HA3	1.83	0.60
3:C:207:TYR:O	3:C:223:LYS:HG3	2.02	0.60
3:K:201:SER:O	3:K:205:GLN:NE2	2.34	0.60
3:O:111:GLY:HA2	3:O:112:ARG:HB2	1.84	0.60
1:A:140:LYS:HE3	1:A:146:GLY:H	1.67	0.60
3:O:223:LYS:HA	3:O:223:LYS:CE	2.32	0.60
1:M:97:CYS:O	1:M:224:ARG:NH1	2.35	0.60
3:Y:207:TYR:O	3:Y:223:LYS:HG3	2.02	0.60
3:C:105:VAL:CG1	6:Z:1:NAG:O7	2.50	0.60
1:U:156:LYS:HD2	1:U:196:VAL:HG23	1.84	0.59
1:A:182:VAL:HG22	1:A:202:VAL:HG21	1.84	0.59
1:U:37:THR:HG23	1:U:319:GLY:HA3	1.84	0.59
3:O:137:LEU:HD11	4:P:119:PHE:CG	2.38	0.59
3:G:137:LEU:HD11	4:H:119:PHE:CD2	2.38	0.59
3:O:207:TYR:O	3:O:223:LYS:HG3	2.03	0.59
3:K:111:GLY:HA2	3:K:112:ARG:HB2	1.85	0.59
3:K:223:LYS:HA	3:K:223:LYS:CE	2.32	0.59
1:E:10:THR:HB	2:F:140:ILE:O	2.03	0.59
3:K:207:TYR:O	3:K:223:LYS:HG3	2.02	0.59
3:C:137:LEU:HD11	4:D:119:PHE:CD2	2.37	0.59
3:G:207:TYR:O	3:G:223:LYS:HG3	2.02	0.59
3:S:207:TYR:O	3:S:223:LYS:HG3	2.02	0.59
3:O:4:LEU:HD13	3:O:24:THR:HG22	1.84	0.59
1:U:325:GLU:HG3	2:V:13:GLY:O	2.03	0.59
3:C:223:LYS:CE	3:C:223:LYS:HA	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:104:ARG:O	3:G:105:VAL:O	2.21	0.59
3:G:223:LYS:HA	3:G:223:LYS:CE	2.33	0.59
2:N:57:GLU:OE2	4:P:31:SER:N	2.34	0.58
3:S:104:ARG:O	3:S:105:VAL:O	2.21	0.58
1:I:182:VAL:HG22	1:I:202:VAL:HG21	1.85	0.58
1:Q:184:HIS:CE1	1:Q:216:ASN:OD1	2.56	0.58
3:Y:137:LEU:CD1	4:X:119:PHE:CG	2.86	0.58
4:L:164:VAL:HG22	4:L:176:LEU:HD13	1.85	0.58
1:A:97:CYS:O	1:A:224:ARG:NH1	2.36	0.58
1:U:182:VAL:HG22	1:U:202:VAL:HG21	1.86	0.58
1:E:37:THR:HG23	1:E:319:GLY:HA3	1.85	0.58
1:E:97:CYS:O	1:E:224:ARG:NH1	2.35	0.58
3:Y:4:LEU:HD13	3:Y:24:THR:HG22	1.85	0.58
7:I:405:NAG:H5	3:K:105:VAL:HG11	1.85	0.58
1:Q:33:GLN:CB	4:P:94:VAL:HG22	2.34	0.58
1:U:97:CYS:O	1:U:224:ARG:NH1	2.36	0.58
1:M:182:VAL:HG22	1:M:202:VAL:HG21	1.86	0.58
1:Q:97:CYS:O	1:Q:224:ARG:NH1	2.35	0.58
3:G:4:LEU:HD13	3:G:24:THR:HG22	1.84	0.58
3:S:4:LEU:HD13	3:S:24:THR:HG22	1.85	0.58
3:S:218:THR:HG22	3:S:220:VAL:HG23	1.84	0.58
4:P:164:VAL:HG22	4:P:176:LEU:HD13	1.86	0.58
1:I:37:THR:HG23	1:I:319:GLY:HA3	1.86	0.58
1:M:27:LYS:HG2	1:M:32:ASP:O	2.04	0.58
1:M:37:THR:HG23	1:M:319:GLY:HA3	1.86	0.58
3:G:218:THR:HG22	3:G:220:VAL:HG23	1.84	0.58
3:S:137:LEU:HD11	4:T:119:PHE:CD2	2.39	0.57
1:Q:182:VAL:HG22	1:Q:202:VAL:HG21	1.86	0.57
3:S:223:LYS:HA	3:S:223:LYS:CE	2.34	0.57
3:K:4:LEU:HD13	3:K:24:THR:HG22	1.85	0.57
1:U:216:ASN:CB	1:Q:212:THR:HG21	2.34	0.57
3:C:207:TYR:O	3:C:223:LYS:HE2	2.04	0.57
2:B:53:ASN:HD21	3:C:108:GLY:HA2	1.68	0.57
4:H:164:VAL:HG22	4:H:176:LEU:HD13	1.85	0.57
3:Y:207:TYR:O	3:Y:223:LYS:HE2	2.04	0.57
3:G:110:GLY:HA2	4:H:50:TYR:CE1	2.39	0.57
3:O:218:THR:HG22	3:O:220:VAL:HG23	1.87	0.57
2:N:42:GLN:O	2:N:46:ASP:OD1	2.23	0.57
1:A:216:ASN:CB	1:E:212:THR:HG21	2.34	0.57
1:E:176:LYS:HE3	1:E:257:TYR:CD2	2.39	0.57
1:E:182:VAL:HG22	1:E:202:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:THR:HG22	3:C:220:VAL:HG23	1.86	0.57
3:Y:223:LYS:CE	3:Y:223:LYS:HA	2.33	0.57
4:T:164:VAL:HG22	4:T:176:LEU:HD13	1.86	0.57
3:K:104:ARG:O	3:K:105:VAL:O	2.23	0.57
3:K:218:THR:HG22	3:K:220:VAL:HG23	1.87	0.57
2:F:38:LEU:HG	3:G:54:TYR:CZ	2.39	0.57
3:C:4:LEU:HD13	3:C:24:THR:HG22	1.86	0.57
3:S:207:TYR:O	3:S:223:LYS:HE2	2.05	0.57
3:Y:104:ARG:O	3:Y:105:VAL:O	2.23	0.56
3:Y:137:LEU:HD11	4:X:119:PHE:CD2	2.40	0.56
3:G:207:TYR:O	3:G:223:LYS:HE2	2.05	0.56
3:Y:218:THR:HG22	3:Y:220:VAL:HG23	1.86	0.56
3:K:103:GLY:O	3:K:104:ARG:O	2.23	0.56
3:K:207:TYR:O	3:K:223:LYS:HE2	2.06	0.56
1:A:325:GLU:HG3	2:B:13:GLY:O	2.05	0.56
1:M:304:ALA:HB2	2:N:61:GLU:HG2	1.88	0.56
3:C:103:GLY:O	3:C:104:ARG:O	2.22	0.56
3:S:107:VAL:CB	3:S:108:GLY:CA	2.83	0.56
3:Y:103:GLY:O	3:Y:104:ARG:O	2.23	0.56
3:S:107:VAL:CB	3:S:108:GLY:HA2	2.29	0.56
3:O:207:TYR:O	3:O:223:LYS:HE2	2.06	0.56
3:C:111:GLY:HA2	3:C:112:ARG:HB2	1.87	0.56
2:J:49:ASN:OD1	3:K:106:GLU:CB	2.54	0.56
3:G:107:VAL:CB	3:G:108:GLY:CA	2.84	0.56
3:Y:107:VAL:CB	3:Y:108:GLY:HA2	2.30	0.56
3:Y:111:GLY:HA2	3:Y:112:ARG:HB2	1.87	0.56
2:R:42:GLN:O	2:R:46:ASP:OD1	2.23	0.56
3:K:137:LEU:CD1	4:L:119:PHE:CG	2.89	0.56
2:F:57:GLU:OE2	4:H:32:THR:HG22	2.05	0.55
3:O:104:ARG:O	3:O:105:VAL:O	2.23	0.55
3:K:137:LEU:HD11	4:L:119:PHE:CG	2.41	0.55
3:C:104:ARG:O	3:C:105:VAL:O	2.24	0.55
4:D:164:VAL:HG22	4:D:176:LEU:HD13	1.87	0.55
3:G:107:VAL:CB	3:G:108:GLY:HA2	2.29	0.55
1:Q:176:LYS:HE3	1:Q:257:TYR:CD2	2.41	0.55
2:J:25:ARG:HD3	2:J:34:GLN:OE1	2.07	0.55
4:X:164:VAL:HG22	4:X:176:LEU:HD13	1.88	0.55
4:X:165:THR:HG22	4:X:175:SER:N	2.21	0.55
3:S:103:GLY:O	3:S:104:ARG:O	2.25	0.55
3:O:103:GLY:O	3:O:104:ARG:O	2.23	0.55
1:M:206:THR:C	1:Q:221:PRO:HG2	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:216:ASN:OD1	1:Q:216:ASN:N	2.39	0.55
4:D:165:THR:HG22	4:D:175:SER:N	2.21	0.55
3:G:103:GLY:O	3:G:104:ARG:O	2.25	0.55
3:C:107:VAL:CB	3:C:108:GLY:HA2	2.31	0.55
1:I:304:ALA:HB2	2:J:61:GLU:HG2	1.89	0.55
3:C:137:LEU:HD11	4:D:119:PHE:CG	2.42	0.55
1:Q:248:ASN:C	1:Q:248:ASN:OD1	2.45	0.54
2:B:21:TRP:CE2	2:B:45:ILE:HD11	2.42	0.54
2:N:72:GLU:OE1	2:N:72:GLU:CA	2.54	0.54
3:K:107:VAL:CB	3:K:108:GLY:HA2	2.31	0.54
3:O:137:LEU:HD11	4:P:119:PHE:CD2	2.42	0.54
3:C:208:ILE:HA	3:C:223:LYS:CE	2.39	0.53
3:C:223:LYS:HA	3:C:223:LYS:HE3	1.90	0.53
3:O:111:GLY:CA	3:O:112:ARG:HB2	2.38	0.53
2:V:21:TRP:CE2	2:V:45:ILE:HD11	2.43	0.53
1:E:248:ASN:C	1:E:248:ASN:OD1	2.45	0.53
3:Y:137:LEU:HD11	4:X:119:PHE:CG	2.44	0.53
2:B:49:ASN:OD1	3:C:107:VAL:HG13	2.08	0.53
2:V:49:ASN:OD1	3:Y:107:VAL:HG13	2.09	0.53
3:Y:208:ILE:HA	3:Y:223:LYS:CE	2.39	0.53
3:G:111:GLY:HA2	3:G:112:ARG:HB2	1.90	0.53
3:S:111:GLY:HA2	3:S:112:ARG:HB2	1.90	0.53
4:P:165:THR:HG22	4:P:175:SER:N	2.24	0.53
2:F:53:ASN:HD21	3:G:108:GLY:HA2	1.74	0.53
2:N:141:TYR:O	2:N:166:ALA:HA	2.09	0.53
1:U:165:ASN:OD1	1:M:219:SER:OG	2.26	0.52
1:M:27:LYS:CE	2:N:97:GLU:OE2	2.57	0.52
1:Q:10:THR:HB	2:R:140:ILE:O	2.08	0.52
2:J:141:TYR:O	2:J:166:ALA:HA	2.09	0.52
3:G:105:VAL:O	3:G:106:GLU:OE1	2.27	0.52
1:E:156:LYS:HD2	1:E:159:SER:HA	1.91	0.52
3:O:107:VAL:CB	3:O:108:GLY:CA	2.87	0.52
3:O:107:VAL:CB	3:O:108:GLY:HA2	2.32	0.52
1:M:27:LYS:NZ	2:N:97:GLU:OE2	2.39	0.52
1:E:33:GLN:HG2	4:L:94:VAL:CG2	2.37	0.52
4:L:165:THR:HG22	4:L:175:SER:N	2.25	0.52
1:U:27:LYS:HE3	4:T:28:ARG:HG3	1.91	0.52
1:M:16:GLY:HA3	2:N:14:TRP:CZ2	2.45	0.52
3:K:105:VAL:O	3:K:106:GLU:OE1	2.28	0.52
4:D:165:THR:HG22	4:D:175:SER:H	1.74	0.52
4:P:18:ARG:O	4:P:18:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ARG:HD2	1:E:238:LYS:HE2	1.92	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.09	0.52
2:R:114:GLU:O	2:R:114:GLU:HG3	2.08	0.52
3:O:101:VAL:HG11	3:O:104:ARG:HD3	1.92	0.52
3:C:2:VAL:HG11	3:C:115:TYR:CD2	2.45	0.52
4:X:165:THR:HG22	4:X:175:SER:H	1.74	0.52
4:P:48:LEU:HA	4:P:59:ILE:CD1	2.40	0.52
1:M:59:LEU:HD11	1:M:82:GLU:HG2	1.91	0.52
1:Q:22:ASN:N	1:Q:22:ASN:OD1	2.43	0.52
4:T:165:THR:HG22	4:T:175:SER:N	2.25	0.52
1:E:326:LYS:HG3	2:F:12:ASN:HB3	1.91	0.51
3:K:111:GLY:CA	3:K:112:ARG:HB2	2.40	0.51
1:Q:156:LYS:HD2	1:Q:159:SER:HA	1.92	0.51
3:Y:223:LYS:HA	3:Y:223:LYS:HE3	1.92	0.51
3:S:105:VAL:O	3:S:106:GLU:OE1	2.28	0.51
4:T:18:ARG:HG3	4:T:18:ARG:O	2.09	0.51
3:O:223:LYS:HA	3:O:223:LYS:HE3	1.92	0.51
1:U:22:ASN:OD1	1:U:22:ASN:N	2.41	0.51
3:G:223:LYS:HA	3:G:223:LYS:HE3	1.92	0.51
4:T:48:LEU:HA	4:T:59:ILE:CD1	2.40	0.51
4:P:12:ALA:HA	4:P:106:GLU:O	2.10	0.51
1:M:210:GLN:HG3	1:Q:220:ARG:HE	1.74	0.51
4:X:48:LEU:HA	4:X:59:ILE:CD1	2.40	0.51
2:N:21:TRP:CE2	2:N:45:ILE:HD11	2.45	0.51
4:D:18:ARG:O	4:D:18:ARG:HG3	2.10	0.51
4:H:165:THR:HG22	4:H:175:SER:N	2.26	0.51
4:L:18:ARG:O	4:L:18:ARG:HG3	2.10	0.51
4:D:48:LEU:HA	4:D:59:ILE:CD1	2.40	0.51
4:X:18:ARG:O	4:X:18:ARG:HG3	2.10	0.51
4:L:48:LEU:HA	4:L:59:ILE:CD1	2.41	0.51
4:H:12:ALA:HA	4:H:106:GLU:O	2.11	0.51
4:H:187:TYR:HA	4:H:193:TYR:OH	2.10	0.51
4:T:12:ALA:HA	4:T:106:GLU:O	2.11	0.51
3:O:6:GLN:NE2	3:O:120:THR:HG22	2.25	0.51
3:O:105:VAL:O	3:O:106:GLU:OE1	2.28	0.51
3:K:101:VAL:HG11	3:K:104:ARG:HD3	1.93	0.51
3:K:223:LYS:HA	3:K:223:LYS:HE3	1.91	0.51
4:L:12:ALA:HA	4:L:106:GLU:O	2.10	0.51
4:H:18:ARG:HG3	4:H:18:ARG:O	2.10	0.51
4:H:48:LEU:HA	4:H:59:ILE:CD1	2.40	0.51
3:S:223:LYS:HA	3:S:223:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:THR:C	1:E:221:PRO:HG2	2.30	0.51
2:B:143:LYS:N	2:B:143:LYS:HD2	2.26	0.51
2:R:141:TYR:O	2:R:166:ALA:HA	2.10	0.51
4:X:187:TYR:HA	4:X:193:TYR:OH	2.10	0.51
3:G:101:VAL:HG11	3:G:104:ARG:HD3	1.92	0.51
3:S:135:PHE:HB3	4:T:122:SER:OG	2.11	0.51
4:T:187:TYR:HA	4:T:193:TYR:OH	2.11	0.51
1:E:27:LYS:CE	4:L:28:ARG:HG3	2.36	0.50
3:Y:2:VAL:HG11	3:Y:115:TYR:CD2	2.46	0.50
4:P:48:LEU:HA	4:P:59:ILE:HD13	1.93	0.50
1:M:325:GLU:HG3	2:N:13:GLY:O	2.11	0.50
1:U:186:SER:HA	1:U:218:GLY:O	2.12	0.50
1:M:238:LYS:HD2	1:M:239:PRO:HD2	1.93	0.50
3:S:101:VAL:HG11	3:S:104:ARG:HD3	1.92	0.50
1:E:16:GLY:HA3	2:F:14:TRP:CZ2	2.46	0.50
3:C:101:VAL:HG11	3:C:104:ARG:HD3	1.93	0.50
1:A:186:SER:HA	1:A:218:GLY:O	2.12	0.50
1:U:285:ASN:ND2	7:U:405:NAG:C2	2.65	0.50
3:Y:111:GLY:CA	3:Y:112:ARG:HB2	2.42	0.50
3:G:135:PHE:HB3	4:H:122:SER:OG	2.12	0.50
1:E:132:GLN:CB	1:E:133:ASN:HD22	2.24	0.50
3:C:105:VAL:O	3:C:106:GLU:OE1	2.30	0.50
1:A:97:CYS:SG	1:A:98:TYR:N	2.84	0.50
3:C:111:GLY:CA	3:C:112:ARG:HB2	2.42	0.50
3:C:222:LYS:C	3:C:223:LYS:HD2	2.32	0.50
3:C:20:VAL:CG1	3:C:120:THR:HG21	2.42	0.49
2:V:141:TYR:O	2:V:166:ALA:HA	2.11	0.49
1:I:238:LYS:HD2	1:I:239:PRO:HD2	1.93	0.49
1:M:188:ASN:OD1	1:M:188:ASN:N	2.42	0.49
3:S:110:GLY:HA2	4:T:50:TYR:CE1	2.47	0.49
3:Y:6:GLN:NE2	3:Y:120:THR:HG22	2.27	0.49
3:Y:101:VAL:HG11	3:Y:104:ARG:HD3	1.94	0.49
3:Y:105:VAL:O	3:Y:106:GLU:OE1	2.30	0.49
3:O:20:VAL:CG1	3:O:120:THR:HG21	2.42	0.49
1:Q:132:GLN:CB	1:Q:133:ASN:HD22	2.25	0.49
4:X:12:ALA:HA	4:X:106:GLU:O	2.11	0.49
4:X:48:LEU:HA	4:X:59:ILE:HD13	1.93	0.49
1:Q:186:SER:HA	1:Q:218:GLY:O	2.12	0.49
4:D:187:TYR:HA	4:D:193:TYR:OH	2.12	0.49
3:S:208:ILE:HA	3:S:223:LYS:CE	2.42	0.49
4:P:187:TYR:HA	4:P:193:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:97:CYS:SG	1:U:98:TYR:N	2.84	0.49
3:G:208:ILE:HA	3:G:223:LYS:CE	2.42	0.49
3:K:20:VAL:CG1	3:K:120:THR:HG21	2.43	0.49
3:G:2:VAL:HG11	3:G:115:TYR:CD2	2.47	0.49
1:U:326:LYS:O	1:U:327:GLN:HB2	2.13	0.49
2:J:21:TRP:CE2	2:J:45:ILE:HD11	2.48	0.49
3:Y:20:VAL:CG1	3:Y:120:THR:HG21	2.42	0.49
4:L:187:TYR:HA	4:L:193:TYR:OH	2.12	0.49
1:A:139:CYS:H	1:A:140:LYS:HZ3	1.61	0.49
1:A:140:LYS:CE	1:A:145:SER:CB	2.89	0.49
4:X:116:VAL:O	4:X:208:LYS:HD2	2.13	0.49
3:S:6:GLN:NE2	3:S:120:THR:HG22	2.28	0.49
4:D:48:LEU:HA	4:D:59:ILE:HD13	1.93	0.49
4:D:116:VAL:O	4:D:208:LYS:HD2	2.13	0.49
4:T:118:ILE:CG2	4:T:119:PHE:N	2.75	0.49
3:O:208:ILE:HA	3:O:223:LYS:CE	2.42	0.49
4:P:165:THR:HG22	4:P:175:SER:H	1.77	0.49
2:B:141:TYR:O	2:B:166:ALA:HA	2.12	0.48
1:A:37:THR:CG2	1:A:319:GLY:HA3	2.43	0.48
1:I:16:GLY:HA3	2:J:14:TRP:CZ2	2.49	0.48
3:C:6:GLN:NE2	3:C:120:THR:HG22	2.28	0.48
3:Y:222:LYS:C	3:Y:223:LYS:HD2	2.34	0.48
4:L:48:LEU:HA	4:L:59:ILE:HD13	1.94	0.48
1:A:248:ASN:OD1	1:A:248:ASN:C	2.51	0.48
4:T:165:THR:HG22	4:T:175:SER:H	1.78	0.48
1:E:186:SER:HA	1:E:218:GLY:O	2.13	0.48
1:I:248:ASN:OD1	1:I:248:ASN:C	2.52	0.48
3:G:111:GLY:CA	3:G:112:ARG:HB2	2.44	0.48
4:L:165:THR:HG22	4:L:175:SER:H	1.78	0.48
1:Q:170:ASN:CG	1:Q:176:LYS:HD3	2.33	0.48
2:F:171:PHE:CE2	2:B:171:PHE:CE2	3.01	0.48
1:I:210:GLN:HG3	1:E:220:ARG:HE	1.78	0.48
3:Y:64:PHE:O	3:Y:65:GLN:C	2.52	0.48
1:A:140:LYS:NZ	1:A:146:GLY:O	2.47	0.48
1:M:20:VAL:HB	1:M:21:PRO:HD2	1.96	0.48
1:A:327:GLN:N	1:A:327:GLN:OE1	2.47	0.47
1:E:170:ASN:CG	1:E:176:LYS:HD3	2.34	0.47
4:D:12:ALA:HA	4:D:106:GLU:O	2.13	0.47
1:I:37:THR:CG2	1:I:319:GLY:HA3	2.44	0.47
1:M:248:ASN:OD1	1:M:248:ASN:C	2.52	0.47
2:N:165:GLU:O	2:N:169:ASN:OD1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:48:LEU:HA	4:H:59:ILE:HD13	1.95	0.47
4:T:48:LEU:HA	4:T:59:ILE:HD13	1.94	0.47
3:K:6:GLN:NE2	3:K:120:THR:HG22	2.29	0.47
1:M:37:THR:CG2	1:M:319:GLY:HA3	2.44	0.47
1:M:326:LYS:O	1:M:327:GLN:CB	2.61	0.47
3:C:64:PHE:O	3:C:65:GLN:C	2.52	0.47
3:S:2:VAL:HG11	3:S:115:TYR:CD2	2.49	0.47
2:R:150:GLU:CD	2:R:153:ARG:NH2	2.66	0.47
4:H:165:THR:HG22	4:H:175:SER:H	1.79	0.47
3:S:111:GLY:CA	3:S:112:ARG:HB2	2.44	0.47
3:K:208:ILE:HA	3:K:223:LYS:CE	2.43	0.47
4:L:116:VAL:O	4:L:208:LYS:HD2	2.15	0.47
1:E:37:THR:CG2	1:E:319:GLY:HA3	2.44	0.47
3:G:20:VAL:CG1	3:G:120:THR:HG21	2.43	0.47
3:S:135:PHE:CE2	4:T:125:GLN:HG3	2.49	0.47
1:U:16:GLY:HA3	2:V:14:TRP:CZ2	2.50	0.47
1:I:22:ASN:OD1	1:I:22:ASN:O	2.32	0.47
2:B:58:LYS:HD2	2:B:58:LYS:HA	1.76	0.47
2:J:75:GLY:C	2:J:79:ASP:OD1	2.52	0.47
3:G:14:PRO:O	3:G:86:LEU:O	2.33	0.47
1:A:137:ASN:HA	1:A:140:LYS:CD	2.43	0.47
1:U:248:ASN:OD1	1:U:248:ASN:C	2.52	0.47
1:Q:326:LYS:O	1:Q:327:GLN:CB	2.62	0.47
1:E:52:CYS:HB2	1:E:279:SER:HB3	1.96	0.47
3:S:20:VAL:CG1	3:S:120:THR:HG21	2.44	0.47
4:P:116:VAL:O	4:P:208:LYS:HD2	2.15	0.47
1:U:37:THR:CG2	1:U:319:GLY:HA3	2.44	0.47
1:I:20:VAL:HB	1:I:21:PRO:HD2	1.97	0.47
1:I:119:GLU:OE1	1:I:261:ARG:NH2	2.48	0.47
1:M:186:SER:HA	1:M:218:GLY:O	2.14	0.47
2:R:53:ASN:HB3	4:T:32:THR:HG21	1.97	0.47
1:M:119:GLU:OE1	1:M:261:ARG:NH2	2.48	0.47
3:Y:14:PRO:O	3:Y:86:LEU:O	2.31	0.47
1:Q:325:GLU:HB2	2:R:12:ASN:HD22	1.80	0.47
1:E:326:LYS:O	1:E:327:GLN:HG2	2.15	0.47
3:O:2:VAL:HG11	3:O:115:TYR:CD2	2.50	0.47
1:A:140:LYS:HE3	1:A:145:SER:CB	2.45	0.46
1:Q:52:CYS:HB2	1:Q:279:SER:HB3	1.97	0.46
2:F:21:TRP:CE2	2:F:45:ILE:HD11	2.51	0.46
2:B:9:PHE:CZ	2:B:10:ILE:HD11	2.50	0.46
3:Y:172:LEU:HD21	3:Y:195:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:116:VAL:O	4:T:208:LYS:HD2	2.14	0.46
1:Q:326:LYS:O	1:Q:327:GLN:HB2	2.15	0.46
2:B:171:PHE:CD1	2:B:171:PHE:N	2.83	0.46
3:S:14:PRO:O	3:S:86:LEU:O	2.34	0.46
3:S:222:LYS:C	3:S:223:LYS:HD2	2.36	0.46
3:K:14:PRO:O	3:K:86:LEU:O	2.34	0.46
1:U:119:GLU:OE1	1:U:261:ARG:NH2	2.48	0.46
1:U:217:ILE:O	1:Q:201:ARG:NH1	2.49	0.46
4:H:116:VAL:O	4:H:208:LYS:HD2	2.14	0.46
3:O:14:PRO:O	3:O:86:LEU:O	2.33	0.46
1:I:186:SER:HA	1:I:218:GLY:O	2.15	0.46
2:R:21:TRP:CE2	2:R:45:ILE:HD11	2.51	0.46
3:C:14:PRO:O	3:C:86:LEU:O	2.32	0.46
1:A:29:ILE:HD11	2:B:102:LEU:HD23	1.96	0.46
3:K:2:VAL:HG11	3:K:115:TYR:CD2	2.50	0.46
1:U:156:LYS:HE2	1:U:196:VAL:CB	2.41	0.46
2:V:163:ARG:O	2:V:167:LEU:HB2	2.16	0.46
1:E:20:VAL:HB	1:E:21:PRO:HD2	1.97	0.46
4:H:118:ILE:CG2	4:H:119:PHE:N	2.78	0.46
2:V:17:MET:O	2:V:18:ILE:HD13	2.15	0.46
1:I:156:LYS:HD2	1:I:159:SER:HA	1.96	0.46
1:E:97:CYS:SG	1:E:98:TYR:N	2.86	0.46
3:C:172:LEU:HD21	3:C:195:VAL:HG11	1.98	0.46
3:S:28:SER:O	3:S:28:SER:OG	2.34	0.46
1:A:9:SER:N	2:B:143:LYS:HE3	2.31	0.46
1:U:52:CYS:HB2	1:U:279:SER:HB3	1.98	0.46
1:M:97:CYS:SG	1:M:98:TYR:N	2.86	0.46
1:E:119:GLU:OE1	1:E:261:ARG:NH2	2.49	0.46
1:A:57:ARG:NH1	1:A:83:THR:O	2.49	0.45
1:M:137:ASN:OD1	1:M:140:LYS:HE3	2.16	0.45
1:E:29:ILE:HD11	2:F:102:LEU:HD23	1.96	0.45
2:J:9:PHE:CZ	2:J:10:ILE:HD11	2.51	0.45
1:A:270:SER:HB2	1:A:284:PRO:HA	1.98	0.45
1:I:63:ASP:OD1	1:I:92:LYS:HE3	2.16	0.45
1:I:210:GLN:HE21	1:E:220:ARG:NH2	2.14	0.45
1:E:326:LYS:HE2	2:F:11:GLU:OE1	2.16	0.45
2:B:159:HIS:ND1	2:B:160:ASP:N	2.64	0.45
3:K:172:LEU:HD21	3:K:195:VAL:HG11	1.98	0.45
1:A:52:CYS:HB2	1:A:279:SER:HB3	1.99	0.45
1:A:217:ILE:O	1:E:201:ARG:NH1	2.50	0.45
2:B:163:ARG:O	2:B:167:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:GLN:NE2	3:G:120:THR:HG22	2.31	0.45
3:G:222:LYS:C	3:G:223:LYS:HD2	2.37	0.45
3:O:172:LEU:HD21	3:O:195:VAL:HG11	1.98	0.45
1:I:97:CYS:SG	1:I:98:TYR:N	2.87	0.45
1:M:57:ARG:NH1	1:M:83:THR:O	2.49	0.45
1:E:326:LYS:O	1:E:327:GLN:CB	2.64	0.45
3:G:105:VAL:C	3:G:106:GLU:CD	2.75	0.45
3:K:214:LYS:HA	3:K:214:LYS:HD2	1.68	0.45
1:A:136:SER:O	1:A:138:ALA:N	2.50	0.45
2:J:163:ARG:O	2:J:167:LEU:HB2	2.16	0.45
3:O:222:LYS:C	3:O:223:LYS:HD2	2.37	0.45
1:A:140:LYS:HE3	1:A:146:GLY:N	2.30	0.45
1:U:156:LYS:HE2	1:U:196:VAL:CA	2.46	0.45
1:Q:184:HIS:ND1	1:Q:216:ASN:OD1	2.50	0.45
2:R:57:GLU:OE2	4:T:32:THR:HG22	2.16	0.45
1:Q:97:CYS:SG	1:Q:98:TYR:N	2.87	0.45
2:B:47:GLN:HB3	2:B:110:LEU:HD11	1.99	0.45
2:R:163:ARG:O	2:R:167:LEU:HB2	2.17	0.45
4:D:80:GLU:HB3	4:D:81:PRO:HD2	1.99	0.45
3:S:172:LEU:HD21	3:S:195:VAL:HG11	1.99	0.45
3:O:20:VAL:HG11	3:O:120:THR:HG21	1.99	0.45
1:I:270:SER:HB2	1:I:284:PRO:HA	1.98	0.45
1:Q:57:ARG:NH1	1:Q:83:THR:O	2.50	0.45
2:F:123:ARG:HH21	2:F:132:ASP:HB2	1.81	0.45
3:K:222:LYS:C	3:K:223:LYS:HD2	2.37	0.45
1:Q:20:VAL:HB	1:Q:21:PRO:HD2	1.98	0.45
3:O:99:ASP:OD1	3:O:112:ARG:HA	2.17	0.45
1:Q:119:GLU:OE1	1:Q:261:ARG:NH2	2.50	0.44
3:G:135:PHE:CE2	4:H:125:GLN:HG3	2.52	0.44
1:U:57:ARG:NH1	1:U:83:THR:O	2.50	0.44
1:M:52:CYS:HB2	1:M:279:SER:HB3	1.98	0.44
1:M:270:SER:HB2	1:M:284:PRO:HA	1.98	0.44
2:R:49:ASN:OD1	3:S:107:VAL:HG13	2.17	0.44
3:O:28:SER:O	3:O:28:SER:OG	2.36	0.44
1:M:156:LYS:HD2	1:M:159:SER:HA	1.98	0.44
1:E:33:GLN:HB3	4:L:94:VAL:HG13	1.98	0.44
2:F:38:LEU:HD12	2:F:38:LEU:HA	1.82	0.44
2:F:163:ARG:O	2:F:167:LEU:HB2	2.18	0.44
2:N:163:ARG:O	2:N:167:LEU:HB2	2.17	0.44
4:X:80:GLU:HB3	4:X:81:PRO:HD2	1.99	0.44
3:S:91:THR:HG23	3:S:123:ILE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:20:VAL:HG11	3:K:120:THR:HG21	2.00	0.44
3:K:91:THR:HG23	3:K:123:ILE:HA	2.00	0.44
1:U:29:ILE:HD11	2:V:102:LEU:HD23	1.98	0.44
3:S:99:ASP:OD1	3:S:112:ARG:HA	2.17	0.44
4:P:118:ILE:CG2	4:P:119:PHE:N	2.81	0.44
1:M:62:ILE:HG22	1:M:63:ASP:N	2.32	0.44
1:Q:16:GLY:HA3	2:R:14:TRP:CZ2	2.51	0.44
1:E:61:GLY:O	1:E:62:ILE:C	2.56	0.44
3:Y:28:SER:O	3:Y:28:SER:OG	2.35	0.44
3:G:99:ASP:OD1	3:G:112:ARG:HA	2.17	0.44
3:G:172:LEU:HD21	3:G:195:VAL:HG11	1.99	0.44
2:V:47:GLN:HB3	2:V:110:LEU:HD11	2.00	0.44
1:I:57:ARG:NH1	1:I:83:THR:O	2.51	0.44
3:C:20:VAL:HG11	3:C:120:THR:HG21	1.99	0.44
3:Y:111:GLY:HA2	3:Y:112:ARG:CB	2.47	0.44
1:A:20:VAL:HB	1:A:21:PRO:HD2	1.99	0.44
1:E:57:ARG:NH1	1:E:83:THR:O	2.51	0.44
3:C:3:GLN:C	3:C:4:LEU:HD22	2.38	0.44
3:C:28:SER:O	3:C:28:SER:OG	2.35	0.44
3:K:99:ASP:OD1	3:K:112:ARG:HA	2.18	0.44
3:K:105:VAL:C	3:K:106:GLU:CD	2.76	0.44
1:I:52:CYS:HB2	1:I:279:SER:HB3	1.98	0.44
2:F:38:LEU:HG	3:G:54:TYR:CE2	2.53	0.44
3:Y:214:LYS:HD2	3:Y:214:LYS:HA	1.66	0.44
3:G:64:PHE:O	3:G:65:GLN:C	2.55	0.44
1:U:20:VAL:HB	1:U:21:PRO:HD2	2.00	0.43
2:J:47:GLN:HB3	2:J:110:LEU:HD11	2.00	0.43
2:R:150:GLU:CD	2:R:153:ARG:HH21	2.20	0.43
3:C:111:GLY:HA2	3:C:112:ARG:CB	2.47	0.43
3:K:64:PHE:O	3:K:65:GLN:C	2.56	0.43
1:M:207:ARG:HG3	1:Q:223:VAL:HG22	2.00	0.43
2:F:125:GLN:HE22	2:F:152:ILE:HA	1.83	0.43
2:B:38:LEU:HD22	3:C:54:TYR:CZ	2.53	0.43
3:O:91:THR:HG23	3:O:123:ILE:HA	2.00	0.43
4:L:118:ILE:CG2	4:L:119:PHE:N	2.81	0.43
1:U:62:ILE:HG22	1:U:63:ASP:N	2.33	0.43
2:N:47:GLN:HB3	2:N:110:LEU:HD11	2.00	0.43
2:R:150:GLU:OE1	2:R:153:ARG:NE	2.52	0.43
3:G:167:TRP:HA	3:G:208:ILE:O	2.19	0.43
2:F:171:PHE:CE2	2:B:171:PHE:HE2	2.36	0.43
3:C:214:LYS:HD2	3:C:214:LYS:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:20:VAL:HG11	3:Y:120:THR:HG21	2.00	0.43
3:S:64:PHE:O	3:S:65:GLN:C	2.55	0.43
1:I:62:ILE:HG22	1:I:63:ASP:N	2.33	0.43
3:K:137:LEU:HD11	4:L:119:PHE:CD2	2.53	0.43
1:A:27:LYS:CE	1:A:33:GLN:NE2	2.77	0.43
1:U:270:SER:HB2	1:U:284:PRO:HA	2.01	0.43
2:F:49:ASN:OD1	3:G:107:VAL:HG13	2.19	0.43
2:F:58:LYS:NZ	4:H:54:ASN:HD21	2.16	0.43
3:G:91:THR:HG23	3:G:123:ILE:HA	1.99	0.43
3:S:167:TRP:HA	3:S:208:ILE:O	2.19	0.43
2:R:47:GLN:HB3	2:R:110:LEU:HD11	2.00	0.43
3:O:64:PHE:O	3:O:65:GLN:C	2.57	0.43
1:I:61:GLY:O	1:I:62:ILE:C	2.56	0.43
1:Q:270:SER:HB2	1:Q:284:PRO:HA	2.00	0.43
3:Y:99:ASP:OD1	3:Y:112:ARG:HA	2.18	0.43
1:Q:25:LEU:HB2	4:P:27:HIS:CE1	2.54	0.42
3:C:91:THR:HG23	3:C:123:ILE:HA	2.00	0.42
4:X:40:LYS:O	4:X:43:GLN:HG2	2.19	0.42
2:F:16:GLY:O	2:F:18:ILE:HD12	2.19	0.42
2:N:72:GLU:OE1	2:N:72:GLU:N	2.52	0.42
3:S:20:VAL:HG11	3:S:120:THR:HG21	2.01	0.42
2:F:47:GLN:HB3	2:F:110:LEU:HD11	2.00	0.42
2:N:72:GLU:OE1	2:N:72:GLU:HA	2.18	0.42
1:U:37:THR:HG22	1:U:320:MET:N	2.34	0.42
1:E:62:ILE:HG22	1:E:63:ASP:N	2.34	0.42
3:Y:91:THR:HG23	3:Y:123:ILE:HA	2.00	0.42
3:G:214:LYS:HD2	3:G:214:LYS:HA	1.66	0.42
3:O:54:TYR:HD2	3:O:55:THR:HG23	1.84	0.42
1:Q:61:GLY:O	1:Q:62:ILE:C	2.58	0.42
1:A:92:LYS:HB2	1:A:92:LYS:HE2	1.78	0.42
3:G:20:VAL:HG11	3:G:120:THR:HG21	2.01	0.42
4:T:162:GLU:HB2	4:T:176:LEU:HD11	2.01	0.42
1:Q:62:ILE:HG22	1:Q:63:ASP:N	2.35	0.42
3:C:99:ASP:OD1	3:C:112:ARG:HA	2.19	0.42
3:C:209:CYS:HB3	3:C:211:VAL:HG23	2.01	0.42
4:D:118:ILE:CG2	4:D:119:PHE:N	2.82	0.42
3:Y:209:CYS:HB3	3:Y:211:VAL:HG23	2.01	0.42
3:S:222:LYS:O	3:S:223:LYS:HD2	2.20	0.42
4:T:118:ILE:HG22	4:T:119:PHE:N	2.33	0.42
3:Y:107:VAL:CB	3:Y:108:GLY:CA	2.84	0.42
3:G:222:LYS:O	3:G:223:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:162:GLU:HB2	4:H:176:LEU:HD11	2.01	0.42
3:O:209:CYS:HB3	3:O:211:VAL:HG23	2.02	0.42
3:K:222:LYS:O	3:K:223:LYS:HD2	2.20	0.42
1:A:207:ARG:NH1	1:A:242:VAL:CG1	2.80	0.42
2:R:52:LEU:HD22	3:S:107:VAL:HG23	2.01	0.42
3:Y:3:GLN:C	3:Y:4:LEU:HD22	2.40	0.42
3:S:214:LYS:HD2	3:S:214:LYS:HA	1.66	0.42
4:L:162:GLU:HB2	4:L:176:LEU:HD11	2.02	0.42
1:I:207:ARG:HG3	1:E:223:VAL:HG22	2.01	0.42
1:A:110:SER:OG	2:J:79:ASP:OD2	2.33	0.41
2:B:123:ARG:HH21	2:B:132:ASP:HB2	1.84	0.41
3:C:110:GLY:HA2	4:D:50:TYR:CE1	2.55	0.41
4:H:107:ILE:C	4:H:107:ILE:HD12	2.40	0.41
3:S:209:CYS:HB3	3:S:211:VAL:HG23	2.01	0.41
1:E:304:ALA:HB2	2:F:61:GLU:HG2	2.01	0.41
2:B:171:PHE:N	2:B:171:PHE:HD1	2.18	0.41
3:C:104:ARG:NH1	3:C:106:GLU:O	2.53	0.41
4:X:107:ILE:C	4:X:107:ILE:HD12	2.41	0.41
3:S:3:GLN:C	3:S:4:LEU:HD22	2.40	0.41
4:T:8:PRO:O	4:T:103:THR:HG23	2.20	0.41
3:O:214:LYS:HD2	3:O:214:LYS:HA	1.69	0.41
1:A:37:THR:HG22	1:A:320:MET:N	2.35	0.41
3:Y:214:LYS:N	3:Y:215:PRO:CD	2.84	0.41
4:T:107:ILE:HD12	4:T:107:ILE:C	2.40	0.41
3:O:222:LYS:O	3:O:223:LYS:HD2	2.20	0.41
1:A:315:LYS:HG3	4:H:28:ARG:HH12	1.85	0.41
1:I:264:LYS:HE3	2:J:63:PHE:CE2	2.55	0.41
4:H:8:PRO:O	4:H:103:THR:HG23	2.20	0.41
3:S:105:VAL:C	3:S:106:GLU:CD	2.79	0.41
1:E:270:SER:HB2	1:E:284:PRO:HA	2.01	0.41
3:C:222:LYS:O	3:C:223:LYS:HD2	2.20	0.41
3:S:214:LYS:N	3:S:215:PRO:CD	2.84	0.41
3:O:4:LEU:HD12	3:O:22:CYS:SG	2.61	0.41
3:K:209:CYS:HB3	3:K:211:VAL:HG23	2.02	0.41
3:Y:104:ARG:NH1	3:Y:106:GLU:O	2.54	0.41
4:P:162:GLU:HB2	4:P:176:LEU:HD11	2.02	0.41
1:I:212:THR:HG21	1:E:216:ASN:HB3	2.02	0.41
1:M:61:GLY:O	1:M:62:ILE:C	2.58	0.41
4:P:8:PRO:O	4:P:103:THR:HG23	2.21	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.36	0.41
3:C:167:TRP:HA	3:C:208:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:61:GLY:O	1:U:62:ILE:C	2.58	0.41
1:M:37:THR:HG22	1:M:320:MET:N	2.36	0.41
2:F:58:LYS:HG3	4:H:53:SER:OG	2.21	0.41
2:J:24:PHE:CD1	2:J:153:ARG:HD3	2.55	0.41
3:C:105:VAL:HG23	3:C:106:GLU:H	1.84	0.41
4:D:107:ILE:C	4:D:107:ILE:HD12	2.41	0.41
3:Y:167:TRP:HA	3:Y:208:ILE:O	2.21	0.41
3:Y:222:LYS:O	3:Y:223:LYS:HD2	2.20	0.41
3:G:209:CYS:HB3	3:G:211:VAL:HG23	2.02	0.41
4:P:107:ILE:C	4:P:107:ILE:HD12	2.41	0.41
3:K:167:TRP:HA	3:K:208:ILE:O	2.21	0.41
3:K:195:VAL:HG12	3:K:197:VAL:HG13	2.03	0.41
1:A:61:GLY:O	1:A:62:ILE:C	2.57	0.41
1:U:216:ASN:HB3	1:Q:212:THR:HG21	2.02	0.41
3:K:104:ARG:NH1	3:K:106:GLU:O	2.54	0.41
3:K:135:PHE:HB3	4:L:122:SER:OG	2.21	0.41
1:Q:132:GLN:HB2	1:Q:133:ASN:HD22	1.86	0.40
3:C:107:VAL:CB	3:C:108:GLY:CA	2.85	0.40
3:O:180:PRO:HG2	4:P:164:VAL:O	2.22	0.40
3:O:195:VAL:HG12	3:O:197:VAL:HG13	2.03	0.40
3:K:4:LEU:HD12	3:K:22:CYS:SG	2.61	0.40
3:Y:105:VAL:C	3:Y:106:GLU:CD	2.79	0.40
3:O:3:GLN:C	3:O:4:LEU:HD22	2.41	0.40
4:L:8:PRO:O	4:L:103:THR:HG23	2.21	0.40
1:U:285:ASN:OD1	7:U:405:NAG:C1	2.68	0.40
2:V:123:ARG:HH21	2:V:132:ASP:HB2	1.85	0.40
1:M:115:SER:HA	1:M:261:ARG:O	2.21	0.40
1:E:318:THR:HG22	2:F:52:LEU:HD12	2.03	0.40
3:C:135:PHE:CE2	4:D:125:GLN:HG3	2.56	0.40
1:I:115:SER:HA	1:I:261:ARG:O	2.22	0.40
3:Y:135:PHE:CE2	4:X:125:GLN:HG3	2.56	0.40
1:E:326:LYS:O	1:E:327:GLN:HB2	2.22	0.40
3:C:135:PHE:HB3	4:D:122:SER:OG	2.22	0.40
4:D:8:PRO:O	4:D:103:THR:HG23	2.21	0.40
4:D:40:LYS:O	4:D:43:GLN:HG2	2.22	0.40
4:X:8:PRO:O	4:X:103:THR:HG23	2.21	0.40
3:G:195:VAL:HG12	3:G:197:VAL:HG13	2.03	0.40
3:O:201:SER:C	3:O:202:LEU:HD12	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:275:ASP:OD1	4:T:188:GLU:OE2[1_445]	1.91	0.29
1:I:275:ASP:OD1	4:H:188:GLU:OE2[1_565]	1.92	0.28

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	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	17	56
1	E	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	17	56
1	I	315/321 (98%)	297 (94%)	16 (5%)	2 (1%)	25	64
1	M	318/321 (99%)	297 (93%)	18 (6%)	3 (1%)	17	56
1	Q	318/321 (99%)	300 (94%)	15 (5%)	3 (1%)	17	56
1	U	318/321 (99%)	296 (93%)	19 (6%)	3 (1%)	17	56
2	B	163/175 (93%)	150 (92%)	13 (8%)	0	100	100
2	F	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	J	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
2	N	161/175 (92%)	150 (93%)	11 (7%)	0	100	100
2	R	164/175 (94%)	151 (92%)	12 (7%)	1 (1%)	25	64
2	V	162/175 (93%)	149 (92%)	13 (8%)	0	100	100
3	C	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	G	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	K	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	3	23
3	O	215/226 (95%)	189 (88%)	16 (7%)	10 (5%)	2	20
3	S	215/226 (95%)	188 (87%)	16 (7%)	11 (5%)	2	19
3	Y	215/226 (95%)	189 (88%)	17 (8%)	9 (4%)	3	23
4	D	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	17	56
4	H	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	211/215 (98%)	200 (95%)	9 (4%)	2 (1%)	17	56
4	P	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56
4	T	211/215 (98%)	201 (95%)	8 (4%)	2 (1%)	17	56
4	X	211/215 (98%)	202 (96%)	7 (3%)	2 (1%)	17	56
All	All	5434/5622 (97%)	5023 (92%)	320 (6%)	91 (2%)	9	42

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	327	GLN
3	C	104	ARG
3	C	105	VAL
3	C	109	SER
3	Y	104	ARG
3	Y	105	VAL
3	Y	109	SER
3	G	104	ARG
3	G	105	VAL
3	G	109	SER
3	S	104	ARG
3	S	105	VAL
3	S	109	SER
3	O	104	ARG
3	O	105	VAL
3	O	109	SER
3	K	104	ARG
3	K	105	VAL
3	K	109	SER
1	A	62	ILE
1	A	137	ASN
1	U	62	ILE
1	U	326	LYS
1	I	62	ILE
1	M	62	ILE
1	M	327	GLN
1	Q	62	ILE
1	E	62	ILE
3	C	106	GLU
3	C	217	ASN
3	Y	100	LYS
3	Y	106	GLU

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Mol	Chain	Res	Type
3	Y	217	ASN
3	G	106	GLU
3	G	217	ASN
3	S	106	GLU
3	O	106	GLU
3	O	217	ASN
3	K	106	GLU
3	K	217	ASN
3	C	16	ALA
3	C	100	LYS
4	D	205	PRO
3	Y	16	ALA
4	X	205	PRO
3	G	16	ALA
3	G	100	LYS
4	H	205	PRO
3	S	16	ALA
3	S	100	LYS
3	S	217	ASN
4	T	205	PRO
3	O	16	ALA
3	O	100	LYS
4	P	205	PRO
3	K	16	ALA
3	K	100	LYS
1	Q	201	ARG
1	Q	327	GLN
3	C	112	ARG
3	Y	112	ARG
3	G	112	ARG
3	S	112	ARG
3	O	112	ARG
3	O	201	SER
3	K	112	ARG
4	L	205	PRO
1	A	201	ARG
1	U	201	ARG
1	I	201	ARG
1	E	201	ARG
3	C	65	GLN
3	Y	65	GLN
3	G	65	GLN

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Mol	Chain	Res	Type
3	G	201	SER
3	S	201	SER
3	K	201	SER
1	M	201	ARG
3	C	201	SER
4	D	9	GLY
4	X	9	GLY
3	S	65	GLN
4	H	9	GLY
4	T	9	GLY
4	P	9	GLY
4	L	9	GLY
2	R	173	ILE
3	C	14	PRO
3	G	2	VAL
3	O	2	VAL
3	S	2	VAL

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	282/283 (100%)	269 (95%)	13 (5%)	27	61
1	E	282/283 (100%)	270 (96%)	12 (4%)	29	62
1	I	279/283 (99%)	271 (97%)	8 (3%)	42	71
1	M	282/283 (100%)	272 (96%)	10 (4%)	36	67
1	Q	282/283 (100%)	268 (95%)	14 (5%)	24	58
1	U	282/283 (100%)	270 (96%)	12 (4%)	29	62
2	B	145/149 (97%)	135 (93%)	10 (7%)	15	47
2	F	143/149 (96%)	133 (93%)	10 (7%)	15	46
2	J	144/149 (97%)	135 (94%)	9 (6%)	18	51
2	N	143/149 (96%)	135 (94%)	8 (6%)	21	54
2	R	145/149 (97%)	133 (92%)	12 (8%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	144/149 (97%)	137 (95%)	7 (5%)	25	59
3	C	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	G	181/187 (97%)	172 (95%)	9 (5%)	24	58
3	K	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	O	181/187 (97%)	171 (94%)	10 (6%)	21	54
3	S	181/187 (97%)	172 (95%)	9 (5%)	24	58
3	Y	181/187 (97%)	172 (95%)	9 (5%)	24	58
4	D	184/186 (99%)	172 (94%)	12 (6%)	17	50
4	H	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	L	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	P	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	T	184/186 (99%)	173 (94%)	11 (6%)	19	52
4	X	184/186 (99%)	172 (94%)	12 (6%)	17	50
All	All	4743/4830 (98%)	4493 (95%)	250 (5%)	22	55

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	27	LYS
1	A	45	SER
1	A	65	THR
1	A	92	LYS
1	A	136	SER
1	A	140	LYS
1	A	145	SER
1	A	160	THR
1	A	207	ARG
1	A	208	ARG
1	A	261	ARG
1	A	315	LYS
1	U	18	HIS
1	U	45	SER
1	U	65	THR
1	U	92	LYS
1	U	136	SER
1	U	145	SER

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Mol	Chain	Res	Type
1	U	160	THR
1	U	189	GLN
1	U	261	ARG
1	U	264	LYS
1	U	299	LYS
1	U	321	ARG
2	V	19	ASP
2	V	57	GLU
2	V	58	LYS
2	V	71	SER
2	V	116	ASN
2	V	128	GLU
2	V	168	ASN
1	I	45	SER
1	I	65	THR
1	I	92	LYS
1	I	136	SER
1	I	145	SER
1	I	160	THR
1	I	238	LYS
1	I	261	ARG
1	M	45	SER
1	M	65	THR
1	M	92	LYS
1	M	145	SER
1	M	160	THR
1	M	188	ASN
1	M	210	GLN
1	M	238	LYS
1	M	261	ARG
1	M	280	GLU
1	Q	9	SER
1	Q	18	HIS
1	Q	45	SER
1	Q	65	THR
1	Q	92	LYS
1	Q	136	SER
1	Q	145	SER
1	Q	160	THR
1	Q	216	ASN
1	Q	222	TRP
1	Q	261	ARG

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Mol	Chain	Res	Type
1	Q	299	LYS
1	Q	310	LYS
1	Q	326	LYS
1	E	9	SER
1	E	18	HIS
1	E	45	SER
1	E	65	THR
1	E	92	LYS
1	E	136	SER
1	E	145	SER
1	E	160	THR
1	E	189	GLN
1	E	208	ARG
1	E	261	ARG
1	E	299	LYS
2	F	10	ILE
2	F	11	GLU
2	F	18	ILE
2	F	19	ASP
2	F	38	LEU
2	F	58	LYS
2	F	71	SER
2	F	116	ASN
2	F	121	LYS
2	F	168	ASN
2	B	9	PHE
2	B	10	ILE
2	B	19	ASP
2	B	57	GLU
2	B	58	LYS
2	B	71	SER
2	B	82	LYS
2	B	116	ASN
2	B	143	LYS
2	B	168	ASN
2	J	9	PHE
2	J	10	ILE
2	J	19	ASP
2	J	58	LYS
2	J	71	SER
2	J	79	ASP
2	J	116	ASN

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Mol	Chain	Res	Type
2	J	124	ARG
2	J	168	ASN
2	N	10	ILE
2	N	46	ASP
2	N	71	SER
2	N	72	GLU
2	N	116	ASN
2	N	124	ARG
2	N	168	ASN
2	N	169	ASN
2	R	10	ILE
2	R	19	ASP
2	R	39	LYS
2	R	46	ASP
2	R	58	LYS
2	R	71	SER
2	R	116	ASN
2	R	123	ARG
2	R	143	LYS
2	R	150	GLU
2	R	168	ASN
2	R	173	ILE
3	C	4	LEU
3	C	89	ASP
3	C	93	THR
3	C	106	GLU
3	C	137	LEU
3	C	153	CYS
3	C	190	SER
3	C	206	THR
3	C	214	LYS
3	C	222	LYS
4	D	5	THR
4	D	17	GLU
4	D	22	SER
4	D	32	THR
4	D	47	ARG
4	D	75	THR
4	D	97	TRP
4	D	122	SER
4	D	160	SER
4	D	165	THR

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Mol	Chain	Res	Type
4	D	178	SER
4	D	183	SER
3	Y	89	ASP
3	Y	93	THR
3	Y	106	GLU
3	Y	137	LEU
3	Y	153	CYS
3	Y	190	SER
3	Y	206	THR
3	Y	214	LYS
3	Y	222	LYS
4	X	5	THR
4	X	17	GLU
4	X	22	SER
4	X	32	THR
4	X	47	ARG
4	X	75	THR
4	X	97	TRP
4	X	122	SER
4	X	160	SER
4	X	165	THR
4	X	178	SER
4	X	183	SER
3	G	89	ASP
3	G	93	THR
3	G	106	GLU
3	G	137	LEU
3	G	153	CYS
3	G	190	SER
3	G	206	THR
3	G	214	LYS
3	G	222	LYS
4	H	5	THR
4	H	17	GLU
4	H	22	SER
4	H	32	THR
4	H	47	ARG
4	H	75	THR
4	H	97	TRP
4	H	122	SER
4	H	160	SER
4	H	178	SER

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Mol	Chain	Res	Type
4	H	183	SER
3	S	89	ASP
3	S	93	THR
3	S	106	GLU
3	S	137	LEU
3	S	153	CYS
3	S	190	SER
3	S	206	THR
3	S	214	LYS
3	S	222	LYS
4	T	5	THR
4	T	17	GLU
4	T	22	SER
4	T	32	THR
4	T	47	ARG
4	T	75	THR
4	T	97	TRP
4	T	122	SER
4	T	160	SER
4	T	178	SER
4	T	183	SER
3	O	28	SER
3	O	89	ASP
3	O	93	THR
3	O	106	GLU
3	O	137	LEU
3	O	153	CYS
3	O	190	SER
3	O	206	THR
3	O	214	LYS
3	O	222	LYS
4	P	5	THR
4	P	17	GLU
4	P	22	SER
4	P	32	THR
4	P	47	ARG
4	P	75	THR
4	P	97	TRP
4	P	122	SER
4	P	160	SER
4	P	178	SER
4	P	183	SER

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Mol	Chain	Res	Type
3	K	89	ASP
3	K	93	THR
3	K	105	VAL
3	K	106	GLU
3	K	137	LEU
3	K	153	CYS
3	K	190	SER
3	K	206	THR
3	K	214	LYS
3	K	222	LYS
4	L	5	THR
4	L	17	GLU
4	L	22	SER
4	L	32	THR
4	L	47	ARG
4	L	75	THR
4	L	97	TRP
4	L	122	SER
4	L	160	SER
4	L	178	SER
4	L	183	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	80	GLN
1	A	216	ASN
1	U	216	ASN
2	V	53	ASN
2	V	159	HIS
1	M	33	GLN
1	M	210	GLN
1	Q	33	GLN
1	Q	133	ASN
1	Q	137	ASN
1	E	133	ASN
2	F	53	ASN
2	F	60	ASN
2	F	159	HIS
2	B	53	ASN
2	B	78	GLN

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Mol	Chain	Res	Type
2	N	60	ASN
2	N	159	HIS
2	R	53	ASN
2	R	159	HIS
3	C	113	HIS
3	C	210	ASN
4	D	43	GLN
4	D	139	ASN
4	D	148	GLN
4	D	161	GLN
3	Y	113	HIS
3	Y	210	ASN
4	X	27	HIS
4	X	43	GLN
4	X	139	ASN
4	X	148	GLN
4	X	161	GLN
3	G	113	HIS
3	G	210	ASN
4	H	43	GLN
4	H	54	ASN
4	H	139	ASN
4	H	148	GLN
3	S	113	HIS
3	S	210	ASN
4	T	43	GLN
4	T	139	ASN
4	T	148	GLN
3	O	113	HIS
3	O	210	ASN
4	P	27	HIS
4	P	43	GLN
4	P	139	ASN
4	P	148	GLN
3	K	113	HIS
3	K	210	ASN
4	L	43	GLN
4	L	139	ASN
4	L	148	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)

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	a	1	6,1	14,14,15	0.97	1 (7%)	17,19,21	2.29	8 (47%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.12	3 (17%)
6	NAG	a	2	6	14,14,15	0.82	1 (7%)	17,19,21	2.26	7 (41%)
5	NAG	e	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.74	6 (35%)
5	NAG	g	1	5,1	14,14,15	0.71	0	17,19,21	1.49	3 (17%)
6	NAG	Z	2	6	14,14,15	0.74	0	17,19,21	1.91	3 (17%)
5	NAG	c	2	5	14,14,15	0.81	1 (7%)	17,19,21	3.79	10 (58%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.54	7 (41%)
7	NAG	V	201	2	14,14,15	0.99	1 (7%)	17,19,21	2.64	7 (41%)
6	NAG	Z	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	2.68	6 (35%)
7	NAG	A	409	1	14,14,15	1.05	1 (7%)	17,19,21	3.28	8 (47%)
6	NAG	f	1	6,1	14,14,15	1.08	1 (7%)	17,19,21	2.97	7 (41%)
5	NAG	b	1	5,1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
5	NAG	c	1	5,1	14,14,15	0.79	0	17,19,21	3.93	9 (52%)
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.90	9 (52%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	8 (47%)
7	NAG	M	405	1	14,14,15	1.03	1 (7%)	17,19,21	1.31	2 (11%)
5	NAG	d	1	5,1	14,14,15	0.55	0	17,19,21	2.17	4 (23%)
5	NAG	W	1	5,1	14,14,15	0.68	0	17,19,21	1.66	4 (23%)
6	NAG	f	2	6	14,14,15	0.85	0	17,19,21	1.75	5 (29%)
7	NAG	I	405	1	14,14,15	1.58	2 (14%)	17,19,21	3.21	10 (58%)
7	NAG	Q	407	1	14,14,15	1.42	2 (14%)	17,19,21	3.34	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	g	2	5	14,14,15	0.78	0	17,19,21	3.23	10 (58%)
7	NAG	F	201	-	14,14,15	0.96	0	17,19,21	2.29	5 (29%)
5	NAG	W	2	5	14,14,15	0.68	0	17,19,21	2.58	7 (41%)

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
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	4/6/23/26	0/1/1/1
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.30	1.58	1.52
6	f	1	NAG	C1-C2	3.45	1.57	1.52
7	Q	407	NAG	C4-C5	3.19	1.59	1.53
7	M	405	NAG	C1-C2	2.92	1.56	1.52
7	U	405	NAG	C3-C2	2.85	1.58	1.52
7	V	201	NAG	C1-C2	2.66	1.56	1.52
7	I	405	NAG	C3-C2	2.44	1.57	1.52
5	c	2	NAG	C3-C2	2.37	1.57	1.52
7	Q	407	NAG	C3-C2	2.37	1.57	1.52
7	A	409	NAG	C3-C2	2.33	1.57	1.52
6	a	2	NAG	C1-C2	2.33	1.55	1.52
7	U	405	NAG	C4-C5	2.27	1.57	1.53
6	Z	1	NAG	C1-C2	2.18	1.55	1.52
5	e	1	NAG	O5-C1	-2.16	1.40	1.43
6	a	1	NAG	C1-C2	2.10	1.55	1.52

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C1-O5-C5	12.12	128.61	112.19
5	c	2	NAG	C1-O5-C5	8.98	124.36	112.19
6	Z	1	NAG	C1-O5-C5	8.09	123.15	112.19
7	I	405	NAG	O5-C1-C2	-7.98	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.85	122.83	112.19
5	d	2	NAG	C1-O5-C5	7.07	121.78	112.19
5	c	2	NAG	C4-C3-C2	6.95	121.21	111.02
6	f	1	NAG	C1-O5-C5	6.95	121.60	112.19
7	Q	407	NAG	C1-O5-C5	6.90	121.54	112.19
5	d	1	NAG	C1-O5-C5	6.89	121.52	112.19
7	V	201	NAG	C1-O5-C5	6.85	121.47	112.19
6	a	2	NAG	C1-O5-C5	6.37	120.82	112.19
5	g	2	NAG	C1-O5-C5	6.26	120.68	112.19
6	f	1	NAG	C3-C4-C5	5.98	120.91	110.24
6	a	1	NAG	C1-O5-C5	5.82	120.08	112.19
7	Q	407	NAG	O4-C4-C5	5.63	123.28	109.30
7	F	201	NAG	C4-C3-C2	5.29	118.76	111.02
5	e	2	NAG	O3-C3-C4	-5.27	98.17	110.35
5	c	1	NAG	O5-C5-C6	5.17	115.31	107.20
6	Z	2	NAG	O5-C5-C6	5.15	115.27	107.20
7	A	409	NAG	O4-C4-C5	5.14	122.06	109.30
7	U	405	NAG	O3-C3-C4	-5.14	98.47	110.35
7	A	409	NAG	O3-C3-C4	-5.13	98.49	110.35
5	e	2	NAG	C4-C3-C2	5.12	118.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	W	2	NAG	O3-C3-C4	-5.04	98.70	110.35
5	c	2	NAG	O3-C3-C4	-5.02	98.73	110.35
5	b	2	NAG	O3-C3-C4	-4.98	98.85	110.35
7	U	405	NAG	O7-C7-C8	-4.88	113.00	122.06
7	Q	407	NAG	O3-C3-C2	4.85	119.50	109.47
5	g	2	NAG	O3-C3-C4	-4.81	99.23	110.35
7	Q	407	NAG	C2-N2-C7	4.67	129.56	122.90
5	W	2	NAG	C1-O5-C5	4.66	118.50	112.19
5	g	2	NAG	C1-C2-N2	4.65	118.43	110.49
6	f	1	NAG	O5-C1-C2	4.57	118.50	111.29
5	c	1	NAG	O4-C4-C3	4.54	120.85	110.35
5	g	2	NAG	O4-C4-C5	4.49	120.45	109.30
7	I	405	NAG	O3-C3-C2	4.47	118.71	109.47
5	g	2	NAG	C4-C3-C2	4.45	117.53	111.02
5	c	2	NAG	C3-C4-C5	-4.42	102.35	110.24
5	b	1	NAG	C1-O5-C5	4.38	118.12	112.19
6	f	2	NAG	C1-O5-C5	4.35	118.08	112.19
5	c	1	NAG	C2-N2-C7	4.34	129.09	122.90
5	b	2	NAG	O4-C4-C5	4.34	120.06	109.30
5	W	2	NAG	C4-C3-C2	4.26	117.26	111.02
7	U	405	NAG	C2-N2-C7	4.23	128.93	122.90
5	c	2	NAG	O5-C1-C2	-4.19	104.67	111.29
6	Z	2	NAG	C1-O5-C5	4.09	117.73	112.19
7	A	409	NAG	O7-C7-N2	4.09	129.47	121.95
6	Z	1	NAG	O5-C5-C4	4.04	120.67	110.83
7	I	405	NAG	C6-C5-C4	4.01	122.40	113.00
5	W	2	NAG	O4-C4-C5	4.00	119.24	109.30
5	c	1	NAG	O7-C7-N2	3.95	129.22	121.95
7	U	405	NAG	O4-C4-C5	3.93	119.06	109.30
7	U	405	NAG	C1-C2-N2	-3.91	103.81	110.49
5	d	2	NAG	O5-C1-C2	-3.91	105.12	111.29
7	A	409	NAG	C2-N2-C7	3.90	128.46	122.90
7	F	201	NAG	O5-C5-C6	3.90	113.31	107.20
5	W	2	NAG	C1-C2-N2	3.86	117.08	110.49
7	Q	407	NAG	O7-C7-C8	-3.83	114.94	122.06
7	V	201	NAG	C1-C2-N2	3.83	117.03	110.49
6	f	1	NAG	O3-C3-C4	3.61	118.69	110.35
5	g	2	NAG	O7-C7-C8	-3.56	115.44	122.06
5	e	1	NAG	O5-C1-C2	-3.56	105.66	111.29
7	Q	407	NAG	C6-C5-C4	3.52	121.24	113.00
6	a	2	NAG	O5-C1-C2	3.50	116.81	111.29
5	c	2	NAG	O4-C4-C5	3.46	117.88	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	405	NAG	C1-C2-N2	3.43	116.35	110.49
5	W	1	NAG	C1-O5-C5	3.43	116.84	112.19
5	b	1	NAG	C4-C3-C2	3.43	116.04	111.02
7	F	201	NAG	O7-C7-C8	-3.42	115.70	122.06
5	b	2	NAG	C4-C3-C2	3.39	115.99	111.02
7	U	405	NAG	O3-C3-C2	3.39	116.48	109.47
7	Q	407	NAG	O7-C7-N2	3.38	128.16	121.95
5	g	2	NAG	O5-C5-C6	-3.35	101.96	107.20
7	U	405	NAG	O7-C7-N2	3.34	128.10	121.95
6	a	2	NAG	O5-C5-C6	3.34	112.43	107.20
5	e	2	NAG	O4-C4-C5	3.33	117.56	109.30
7	I	405	NAG	O7-C7-C8	-3.31	115.92	122.06
7	I	405	NAG	C4-C3-C2	-3.30	106.18	111.02
5	d	1	NAG	O3-C3-C2	-3.29	102.65	109.47
5	d	2	NAG	C3-C4-C5	-3.28	104.39	110.24
7	A	409	NAG	O3-C3-C2	3.25	116.20	109.47
7	V	201	NAG	O5-C1-C2	3.25	116.42	111.29
5	g	2	NAG	C3-C4-C5	-3.24	104.47	110.24
5	c	2	NAG	O5-C5-C4	3.10	118.37	110.83
5	g	1	NAG	O5-C1-C2	-3.09	106.41	111.29
7	V	201	NAG	C2-N2-C7	3.03	127.22	122.90
6	Z	2	NAG	C4-C3-C2	3.02	115.45	111.02
5	g	2	NAG	O7-C7-N2	3.00	127.47	121.95
5	W	1	NAG	C4-C3-C2	2.99	115.41	111.02
7	V	201	NAG	O4-C4-C3	2.99	117.25	110.35
6	f	1	NAG	O5-C5-C6	2.98	111.87	107.20
7	F	201	NAG	C1-O5-C5	2.89	116.10	112.19
7	I	405	NAG	C3-C4-C5	-2.88	105.10	110.24
6	Z	1	NAG	C2-N2-C7	-2.87	118.82	122.90
5	W	2	NAG	O7-C7-C8	-2.85	116.77	122.06
5	c	2	NAG	C6-C5-C4	-2.84	106.36	113.00
6	a	1	NAG	O4-C4-C5	2.83	116.33	109.30
5	d	2	NAG	O3-C3-C4	-2.83	103.80	110.35
7	V	201	NAG	O5-C5-C6	2.82	111.62	107.20
6	a	1	NAG	O5-C5-C4	-2.81	104.00	110.83
6	f	2	NAG	C1-C2-N2	-2.80	105.71	110.49
6	a	1	NAG	C3-C4-C5	-2.78	105.28	110.24
7	A	409	NAG	O7-C7-C8	-2.76	116.93	122.06
7	I	405	NAG	O5-C5-C6	-2.74	102.92	107.20
7	I	405	NAG	O4-C4-C5	2.66	115.91	109.30
5	d	2	NAG	O4-C4-C5	2.63	115.82	109.30
7	F	201	NAG	C2-N2-C7	2.61	126.62	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	405	NAG	O5-C5-C4	-2.60	104.50	110.83
5	e	1	NAG	C4-C3-C2	2.58	114.80	111.02
6	f	1	NAG	C1-C2-N2	2.57	114.88	110.49
5	g	2	NAG	O5-C5-C4	2.55	117.03	110.83
7	M	405	NAG	O3-C3-C2	2.53	114.70	109.47
7	V	201	NAG	O7-C7-C8	-2.51	117.39	122.06
6	Z	1	NAG	C6-C5-C4	-2.50	107.15	113.00
6	f	1	NAG	O4-C4-C5	-2.47	103.15	109.30
7	U	405	NAG	C4-C3-C2	2.46	114.63	111.02
5	c	1	NAG	O7-C7-C8	-2.46	117.49	122.06
5	c	1	NAG	O3-C3-C2	-2.45	104.40	109.47
6	Z	1	NAG	O4-C4-C5	2.43	115.33	109.30
5	g	1	NAG	C1-O5-C5	-2.41	108.93	112.19
6	f	2	NAG	O5-C1-C2	2.41	115.09	111.29
5	c	2	NAG	C1-C2-N2	2.39	114.57	110.49
6	a	1	NAG	O7-C7-C8	-2.39	117.63	122.06
6	Z	1	NAG	C1-C2-N2	2.37	114.54	110.49
7	Q	407	NAG	O3-C3-C4	-2.36	104.88	110.35
7	A	409	NAG	C4-C3-C2	2.36	114.48	111.02
5	e	1	NAG	C1-O5-C5	-2.35	109.01	112.19
5	e	1	NAG	O7-C7-C8	-2.34	117.71	122.06
5	b	1	NAG	C3-C4-C5	2.33	114.39	110.24
6	a	1	NAG	O5-C1-C2	-2.32	107.63	111.29
5	c	1	NAG	O5-C5-C4	2.30	116.43	110.83
5	W	1	NAG	O3-C3-C4	-2.30	105.03	110.35
7	M	405	NAG	O4-C4-C5	2.29	114.97	109.30
5	e	1	NAG	O3-C3-C4	-2.24	105.16	110.35
6	f	2	NAG	O3-C3-C4	2.24	115.53	110.35
6	a	2	NAG	C1-C2-N2	2.24	114.31	110.49
5	b	1	NAG	C1-C2-N2	-2.23	106.68	110.49
6	a	2	NAG	C2-N2-C7	2.22	126.06	122.90
5	e	1	NAG	O5-C5-C6	2.20	110.65	107.20
5	e	2	NAG	C1-C2-N2	2.19	114.23	110.49
6	a	2	NAG	O7-C7-C8	-2.18	118.02	122.06
5	g	1	NAG	C6-C5-C4	2.17	118.09	113.00
5	e	2	NAG	O7-C7-C8	-2.17	118.03	122.06
5	e	2	NAG	C3-C4-C5	-2.16	106.38	110.24
5	c	2	NAG	O7-C7-C8	-2.16	118.05	122.06
5	d	2	NAG	C2-N2-C7	-2.14	119.85	122.90
6	f	2	NAG	O7-C7-N2	2.14	125.88	121.95
6	a	1	NAG	O3-C3-C2	2.12	113.85	109.47
5	W	2	NAG	O7-C7-N2	2.12	125.85	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	O3-C3-C4	-2.11	105.47	110.35
5	d	1	NAG	C8-C7-N2	-2.07	112.59	116.10
6	a	2	NAG	O7-C7-N2	2.06	125.75	121.95
7	Q	407	NAG	C4-C3-C2	2.06	114.04	111.02
5	e	2	NAG	C6-C5-C4	-2.05	108.19	113.00
6	a	1	NAG	C6-C5-C4	2.05	117.80	113.00
5	e	2	NAG	O5-C1-C2	-2.05	108.05	111.29
7	U	405	NAG	O5-C5-C4	2.05	115.81	110.83
5	W	1	NAG	C3-C4-C5	2.03	113.87	110.24
5	d	1	NAG	O5-C5-C4	2.01	115.71	110.83
5	d	2	NAG	O3-C3-C2	2.01	113.62	109.47

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C3-C2-N2-C7
7	Q	407	NAG	C3-C2-N2-C7
6	Z	2	NAG	O5-C5-C6-O6
7	U	405	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
7	A	409	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
7	V	201	NAG	O5-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
7	U	405	NAG	C4-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
7	F	201	NAG	O5-C5-C6-O6
7	V	201	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
7	F	201	NAG	C4-C5-C6-O6
7	A	409	NAG	C4-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
7	Q	407	NAG	O5-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	W	2	NAG	O5-C5-C6-O6
6	f	2	NAG	C1-C2-N2-C7
5	g	2	NAG	O5-C5-C6-O6
7	Q	407	NAG	C4-C5-C6-O6
7	A	409	NAG	C1-C2-N2-C7
7	Q	407	NAG	C1-C2-N2-C7
7	M	405	NAG	C3-C2-N2-C7
6	a	2	NAG	C4-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
7	M	405	NAG	C4-C5-C6-O6
7	M	405	NAG	C1-C2-N2-C7
5	d	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C3-C2-N2-C7
6	f	2	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0
7	U	405	NAG	5	0
7	I	405	NAG	2	0

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
5	NAG	W	1	5,1	14,14,15	0.68	0	17,19,21	1.66	4 (23%)
5	NAG	W	2	5	14,14,15	0.68	0	17,19,21	2.58	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	BMA	W	3	5	11,11,12	1.10	0	15,15,17	3.35	8 (53%)
5	MAN	W	4	5	11,11,12	0.78	0	15,15,17	2.82	4 (26%)
6	NAG	Z	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	2.68	6 (35%)
6	NAG	Z	2	6	14,14,15	0.74	0	17,19,21	1.91	3 (17%)
6	NAG	a	1	6,1	14,14,15	0.97	1 (7%)	17,19,21	2.29	8 (47%)
6	NAG	a	2	6	14,14,15	0.82	1 (7%)	17,19,21	2.26	7 (41%)
5	NAG	b	1	5,1	14,14,15	0.73	0	17,19,21	1.76	4 (23%)
5	NAG	b	2	5	14,14,15	0.56	0	17,19,21	2.12	3 (17%)
5	BMA	b	3	5	11,11,12	1.02	0	15,15,17	2.95	6 (40%)
5	MAN	b	4	5	11,11,12	0.82	0	15,15,17	2.91	6 (40%)
5	NAG	c	1	5,1	14,14,15	0.79	0	17,19,21	3.93	9 (52%)
5	NAG	c	2	5	14,14,15	0.81	1 (7%)	17,19,21	3.79	10 (58%)
5	BMA	c	3	5	11,11,12	0.98	0	15,15,17	3.76	9 (60%)
5	MAN	c	4	5	11,11,12	1.23	2 (18%)	15,15,17	2.82	5 (33%)
5	NAG	d	1	5,1	14,14,15	0.55	0	17,19,21	2.17	4 (23%)
5	NAG	d	2	5	14,14,15	0.69	0	17,19,21	2.54	7 (41%)
5	BMA	d	3	5	11,11,12	0.54	0	15,15,17	2.78	6 (40%)
5	MAN	d	4	5	11,11,12	0.77	1 (9%)	15,15,17	1.87	6 (40%)
5	NAG	e	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	1.74	6 (35%)
5	NAG	e	2	5	14,14,15	0.56	0	17,19,21	2.44	8 (47%)
5	BMA	e	3	5	11,11,12	1.19	1 (9%)	15,15,17	2.78	6 (40%)
5	MAN	e	4	5	11,11,12	1.05	1 (9%)	15,15,17	2.37	6 (40%)
6	NAG	f	1	6,1	14,14,15	1.08	1 (7%)	17,19,21	2.97	7 (41%)
6	NAG	f	2	6	14,14,15	0.85	0	17,19,21	1.75	5 (29%)
5	NAG	g	1	5,1	14,14,15	0.71	0	17,19,21	1.49	3 (17%)
5	NAG	g	2	5	14,14,15	0.78	0	17,19,21	3.23	10 (58%)
5	BMA	g	3	5	11,11,12	1.23	1 (9%)	15,15,17	3.25	6 (40%)
5	MAN	g	4	5	11,11,12	0.72	0	15,15,17	2.45	5 (33%)

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	W	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	4/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	2/2/19/22	0/1/1/1
5	MAN	d	4	5	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	BMA	e	3	5	-	2/2/19/22	0/1/1/1
5	MAN	e	4	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	4/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
5	BMA	g	3	5	-	2/2/19/22	0/1/1/1
5	MAN	g	4	5	1/1/4/5	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	1	NAG	C1-C2	3.45	1.57	1.52
5	e	3	BMA	C2-C3	2.57	1.56	1.52
5	e	4	MAN	C1-C2	2.47	1.57	1.52
5	c	4	MAN	C2-C3	2.45	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2	NAG	C3-C2	2.37	1.57	1.52
5	g	3	BMA	C2-C3	2.36	1.56	1.52
6	a	2	NAG	C1-C2	2.33	1.55	1.52
5	c	4	MAN	O5-C1	-2.22	1.40	1.43
6	Z	1	NAG	C1-C2	2.18	1.55	1.52
5	e	1	NAG	O5-C1	-2.16	1.40	1.43
6	a	1	NAG	C1-C2	2.10	1.55	1.52
5	d	4	MAN	O5-C1	-2.01	1.40	1.43

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C1-O5-C5	12.12	128.61	112.19
5	c	3	BMA	C1-O5-C5	9.86	125.55	112.19
5	c	2	NAG	C1-O5-C5	8.98	124.36	112.19
5	g	3	BMA	C1-C2-C3	8.74	120.41	109.67
5	c	4	MAN	C1-O5-C5	-8.32	100.91	112.19
6	Z	1	NAG	C1-O5-C5	8.09	123.15	112.19
5	W	4	MAN	C1-C2-C3	-7.81	100.07	109.67
5	b	3	BMA	C1-C2-C3	7.74	119.18	109.67
5	W	3	BMA	C1-O5-C5	7.72	122.65	112.19
5	g	4	MAN	O5-C5-C6	7.39	118.79	107.20
5	d	2	NAG	C1-O5-C5	7.07	121.78	112.19
5	c	2	NAG	C4-C3-C2	6.95	121.21	111.02
6	f	1	NAG	C1-O5-C5	6.95	121.60	112.19
5	d	1	NAG	C1-O5-C5	6.89	121.52	112.19
5	b	4	MAN	O5-C5-C6	6.73	117.75	107.20
6	a	2	NAG	C1-O5-C5	6.37	120.82	112.19
5	g	2	NAG	C1-O5-C5	6.26	120.68	112.19
6	f	1	NAG	C3-C4-C5	5.98	120.91	110.24
5	e	3	BMA	C1-C2-C3	5.96	116.99	109.67
5	W	4	MAN	O5-C1-C2	5.90	119.88	110.77
5	d	3	BMA	C1-O5-C5	5.89	120.17	112.19
6	a	1	NAG	C1-O5-C5	5.82	120.08	112.19
5	g	3	BMA	C1-O5-C5	5.75	119.98	112.19
5	e	4	MAN	O5-C1-C2	5.63	119.46	110.77
5	c	3	BMA	C1-C2-C3	5.55	116.49	109.67
5	e	2	NAG	O3-C3-C4	-5.27	98.17	110.35
5	d	3	BMA	O3-C3-C4	-5.23	98.26	110.35
5	c	1	NAG	O5-C5-C6	5.17	115.31	107.20
6	Z	2	NAG	O5-C5-C6	5.15	115.27	107.20
5	e	2	NAG	C4-C3-C2	5.12	118.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	b	4	MAN	C1-C2-C3	-5.08	103.42	109.67
5	W	2	NAG	O3-C3-C4	-5.04	98.70	110.35
5	c	2	NAG	O3-C3-C4	-5.02	98.73	110.35
5	b	2	NAG	O3-C3-C4	-4.98	98.85	110.35
5	g	2	NAG	O3-C3-C4	-4.81	99.23	110.35
5	W	2	NAG	C1-O5-C5	4.66	118.50	112.19
5	g	2	NAG	C1-C2-N2	4.65	118.43	110.49
5	W	3	BMA	O5-C1-C2	4.64	117.94	110.77
5	c	3	BMA	C3-C4-C5	4.64	118.51	110.24
5	c	3	BMA	O3-C3-C4	-4.58	99.77	110.35
6	f	1	NAG	O5-C1-C2	4.57	118.50	111.29
5	c	1	NAG	O4-C4-C3	4.54	120.85	110.35
5	g	2	NAG	O4-C4-C5	4.49	120.45	109.30
5	g	2	NAG	C4-C3-C2	4.45	117.53	111.02
5	c	2	NAG	C3-C4-C5	-4.42	102.35	110.24
5	b	1	NAG	C1-O5-C5	4.38	118.12	112.19
5	e	3	BMA	C1-O5-C5	4.37	118.11	112.19
6	f	2	NAG	C1-O5-C5	4.35	118.08	112.19
5	c	1	NAG	C2-N2-C7	4.34	129.09	122.90
5	b	2	NAG	O4-C4-C5	4.34	120.06	109.30
5	g	3	BMA	C3-C4-C5	4.26	117.84	110.24
5	W	2	NAG	C4-C3-C2	4.26	117.26	111.02
5	c	2	NAG	O5-C1-C2	-4.19	104.67	111.29
5	b	3	BMA	O3-C3-C2	-4.13	102.08	109.99
5	b	3	BMA	C1-O5-C5	4.11	117.76	112.19
6	Z	2	NAG	C1-O5-C5	4.09	117.73	112.19
6	Z	1	NAG	O5-C5-C4	4.04	120.67	110.83
5	b	4	MAN	O5-C1-C2	4.03	116.99	110.77
5	W	3	BMA	C1-C2-C3	4.03	114.62	109.67
5	W	2	NAG	O4-C4-C5	4.00	119.24	109.30
5	c	1	NAG	O7-C7-N2	3.95	129.22	121.95
5	d	3	BMA	C3-C4-C5	3.93	117.26	110.24
5	d	2	NAG	O5-C1-C2	-3.91	105.12	111.29
5	W	2	NAG	C1-C2-N2	3.86	117.08	110.49
5	W	3	BMA	O3-C3-C4	-3.84	101.47	110.35
5	e	3	BMA	C2-C3-C4	3.80	117.48	110.89
5	e	3	BMA	C3-C4-C5	3.80	117.02	110.24
5	W	3	BMA	C3-C4-C5	3.76	116.94	110.24
5	d	3	BMA	C1-C2-C3	3.74	114.26	109.67
5	d	4	MAN	C1-O5-C5	-3.67	107.22	112.19
5	c	4	MAN	O5-C1-C2	3.63	116.38	110.77
6	f	1	NAG	O3-C3-C4	3.61	118.69	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	g	2	NAG	O7-C7-C8	-3.56	115.44	122.06
5	e	1	NAG	O5-C1-C2	-3.56	105.66	111.29
5	W	3	BMA	C2-C3-C4	3.54	117.02	110.89
6	a	2	NAG	O5-C1-C2	3.50	116.81	111.29
5	e	4	MAN	C2-C3-C4	3.50	116.94	110.89
5	c	2	NAG	O4-C4-C5	3.46	117.88	109.30
5	W	1	NAG	C1-O5-C5	3.43	116.84	112.19
5	b	1	NAG	C4-C3-C2	3.43	116.04	111.02
5	b	3	BMA	O3-C3-C4	3.42	118.25	110.35
5	b	2	NAG	C4-C3-C2	3.39	115.99	111.02
5	b	3	BMA	C3-C4-C5	3.38	116.27	110.24
5	b	4	MAN	O3-C3-C4	3.37	118.14	110.35
5	c	3	BMA	O4-C4-C3	-3.36	102.59	110.35
5	g	2	NAG	O5-C5-C6	-3.35	101.96	107.20
6	a	2	NAG	O5-C5-C6	3.34	112.43	107.20
5	e	2	NAG	O4-C4-C5	3.33	117.56	109.30
5	W	4	MAN	C1-O5-C5	-3.29	107.73	112.19
5	c	4	MAN	C3-C4-C5	3.29	116.11	110.24
5	d	1	NAG	O3-C3-C2	-3.29	102.65	109.47
5	d	2	NAG	C3-C4-C5	-3.28	104.39	110.24
5	d	4	MAN	C3-C4-C5	3.25	116.03	110.24
5	g	2	NAG	C3-C4-C5	-3.24	104.47	110.24
5	b	4	MAN	O2-C2-C1	3.23	115.75	109.15
5	e	4	MAN	C3-C4-C5	3.12	115.81	110.24
5	W	3	BMA	O4-C4-C3	-3.11	103.16	110.35
5	c	2	NAG	O5-C5-C4	3.10	118.37	110.83
5	g	1	NAG	O5-C1-C2	-3.09	106.41	111.29
5	e	3	BMA	O3-C3-C4	-3.03	103.34	110.35
6	Z	2	NAG	C4-C3-C2	3.02	115.45	111.02
5	g	2	NAG	O7-C7-N2	3.00	127.47	121.95
5	W	1	NAG	C4-C3-C2	2.99	115.41	111.02
6	f	1	NAG	O5-C5-C6	2.98	111.87	107.20
5	e	4	MAN	O5-C5-C6	2.95	111.82	107.20
5	d	4	MAN	O5-C1-C2	2.93	115.29	110.77
5	g	4	MAN	O5-C1-C2	2.92	115.28	110.77
5	e	4	MAN	C1-C2-C3	2.91	113.24	109.67
5	c	3	BMA	O2-C2-C3	-2.87	104.38	110.14
6	Z	1	NAG	C2-N2-C7	-2.87	118.82	122.90
5	W	2	NAG	O7-C7-C8	-2.85	116.77	122.06
5	c	2	NAG	C6-C5-C4	-2.84	106.36	113.00
6	a	1	NAG	O4-C4-C5	2.83	116.33	109.30
5	d	2	NAG	O3-C3-C4	-2.83	103.80	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	a	1	NAG	O5-C5-C4	-2.81	104.00	110.83
5	g	3	BMA	C2-C3-C4	2.80	115.74	110.89
6	f	2	NAG	C1-C2-N2	-2.80	105.71	110.49
6	a	1	NAG	C3-C4-C5	-2.78	105.28	110.24
5	e	3	BMA	O5-C5-C6	2.73	111.49	107.20
5	c	3	BMA	O5-C1-C2	2.70	114.94	110.77
5	g	3	BMA	O3-C3-C4	-2.70	104.11	110.35
5	g	4	MAN	O2-C2-C3	-2.65	104.82	110.14
5	d	2	NAG	O4-C4-C5	2.63	115.82	109.30
5	e	1	NAG	C4-C3-C2	2.58	114.80	111.02
6	f	1	NAG	C1-C2-N2	2.57	114.88	110.49
5	g	2	NAG	O5-C5-C4	2.55	117.03	110.83
5	d	4	MAN	O5-C5-C6	2.55	111.19	107.20
6	Z	1	NAG	C6-C5-C4	-2.50	107.15	113.00
6	f	1	NAG	O4-C4-C5	-2.47	103.15	109.30
5	c	1	NAG	O7-C7-C8	-2.46	117.49	122.06
5	b	4	MAN	C1-O5-C5	-2.46	108.86	112.19
5	c	1	NAG	O3-C3-C2	-2.45	104.40	109.47
6	Z	1	NAG	O4-C4-C5	2.43	115.33	109.30
5	g	1	NAG	C1-O5-C5	-2.41	108.93	112.19
6	f	2	NAG	O5-C1-C2	2.41	115.09	111.29
5	c	2	NAG	C1-C2-N2	2.39	114.57	110.49
6	a	1	NAG	O7-C7-C8	-2.39	117.63	122.06
5	d	3	BMA	O4-C4-C3	-2.37	104.86	110.35
6	Z	1	NAG	C1-C2-N2	2.37	114.54	110.49
5	e	1	NAG	C1-O5-C5	-2.35	109.01	112.19
5	e	1	NAG	O7-C7-C8	-2.34	117.71	122.06
5	b	1	NAG	C3-C4-C5	2.33	114.39	110.24
5	b	3	BMA	O5-C1-C2	2.32	114.36	110.77
6	a	1	NAG	O5-C1-C2	-2.32	107.63	111.29
5	c	1	NAG	O5-C5-C4	2.30	116.43	110.83
5	W	1	NAG	O3-C3-C4	-2.30	105.03	110.35
5	e	1	NAG	O3-C3-C4	-2.24	105.16	110.35
6	f	2	NAG	O3-C3-C4	2.24	115.53	110.35
6	a	2	NAG	C1-C2-N2	2.24	114.31	110.49
5	b	1	NAG	C1-C2-N2	-2.23	106.68	110.49
6	a	2	NAG	C2-N2-C7	2.22	126.06	122.90
5	c	3	BMA	O6-C6-C5	2.21	118.89	111.29
5	c	3	BMA	O4-C4-C5	2.20	114.76	109.30
5	e	1	NAG	O5-C5-C6	2.20	110.65	107.20
5	c	4	MAN	O3-C3-C2	2.19	114.19	109.99
5	e	2	NAG	C1-C2-N2	2.19	114.23	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	4	MAN	C1-C2-C3	2.18	112.35	109.67
6	a	2	NAG	O7-C7-C8	-2.18	118.02	122.06
5	g	1	NAG	C6-C5-C4	2.17	118.09	113.00
5	e	2	NAG	O7-C7-C8	-2.17	118.03	122.06
5	e	2	NAG	C3-C4-C5	-2.16	106.38	110.24
5	c	2	NAG	O7-C7-C8	-2.16	118.05	122.06
5	W	3	BMA	O6-C6-C5	2.16	118.69	111.29
5	d	2	NAG	C2-N2-C7	-2.14	119.85	122.90
6	f	2	NAG	O7-C7-N2	2.14	125.88	121.95
6	a	1	NAG	O3-C3-C2	2.12	113.85	109.47
5	W	2	NAG	O7-C7-N2	2.12	125.85	121.95
5	g	3	BMA	O2-C2-C1	-2.11	104.83	109.15
5	c	1	NAG	O3-C3-C4	-2.11	105.47	110.35
5	d	1	NAG	C8-C7-N2	-2.07	112.59	116.10
6	a	2	NAG	O7-C7-N2	2.06	125.75	121.95
5	e	2	NAG	C6-C5-C4	-2.05	108.19	113.00
5	d	4	MAN	C6-C5-C4	-2.05	108.19	113.00
5	g	4	MAN	O6-C6-C5	2.05	118.33	111.29
6	a	1	NAG	C6-C5-C4	2.05	117.80	113.00
5	e	2	NAG	O5-C1-C2	-2.05	108.05	111.29
5	W	1	NAG	C3-C4-C5	2.03	113.87	110.24
5	e	4	MAN	O2-C2-C1	2.02	113.29	109.15
5	g	4	MAN	O2-C2-C1	2.02	113.28	109.15
5	d	3	BMA	O5-C5-C4	-2.02	105.92	110.83
5	d	4	MAN	O6-C6-C5	-2.01	104.39	111.29
5	W	4	MAN	O3-C3-C4	2.01	114.99	110.35
5	d	1	NAG	O5-C5-C4	2.01	115.71	110.83
5	d	2	NAG	O3-C3-C2	2.01	113.62	109.47

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	W	4	MAN	C1
5	b	4	MAN	C1
5	c	4	MAN	C1
5	d	4	MAN	C1
5	e	4	MAN	C1
5	g	4	MAN	C1

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	W	4	MAN	C4-C5-C6-O6
5	g	4	MAN	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	g	3	BMA	C4-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	e	4	MAN	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	e	3	BMA	C4-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
5	b	3	BMA	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	c	4	MAN	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
5	e	4	MAN	C4-C5-C6-O6
5	g	4	MAN	C4-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
5	g	3	BMA	O5-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6
5	c	3	BMA	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
5	d	3	BMA	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
6	f	2	NAG	C1-C2-N2-C7
5	c	4	MAN	C4-C5-C6-O6
5	d	4	MAN	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	f	1	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C1-C2-N2-C7
5	W	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C3-C2-N2-C7
6	f	2	NAG	C3-C2-N2-C7

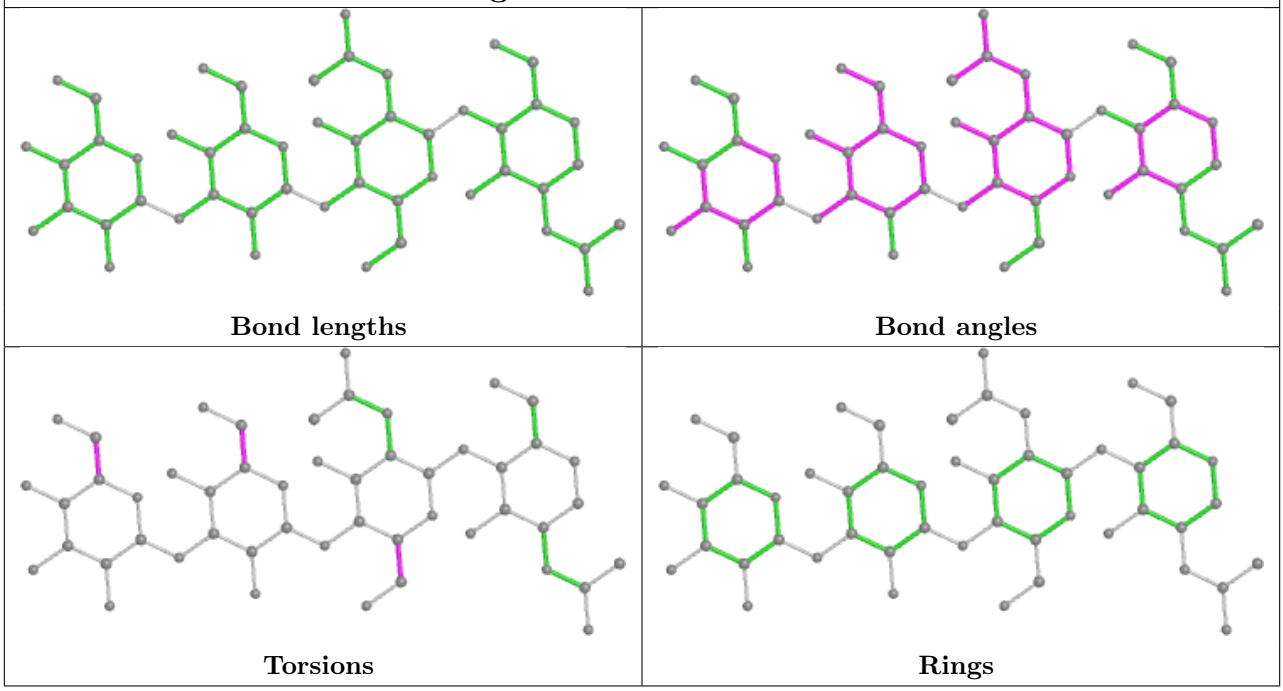
There are no ring outliers.

1 monomer is involved in 1 short contact:

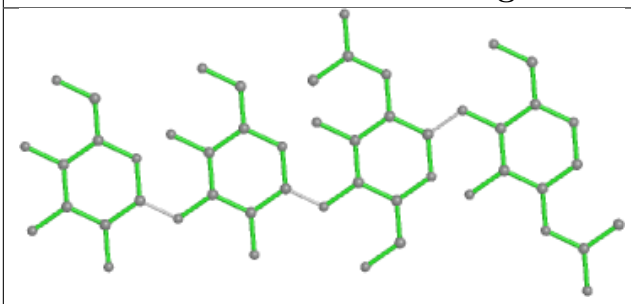
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0

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

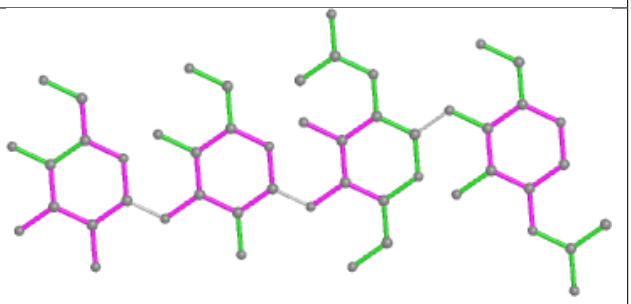
Oligosaccharide Chain W



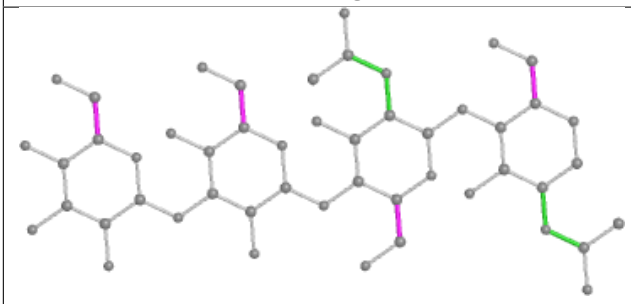
Oligosaccharide Chain b



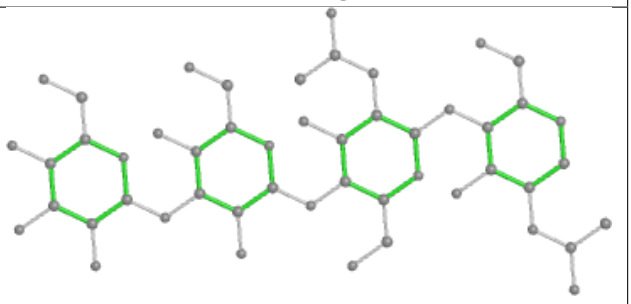
Bond lengths



Bond angles

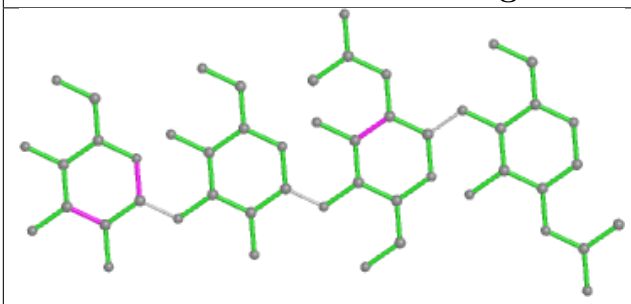


Torsions

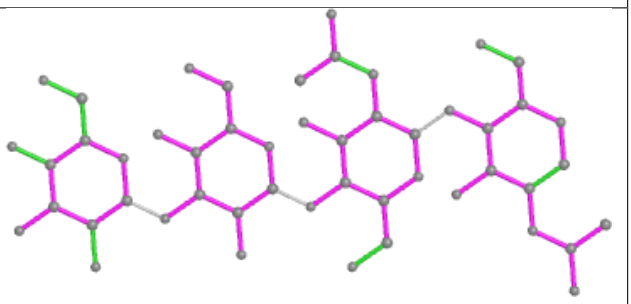


Rings

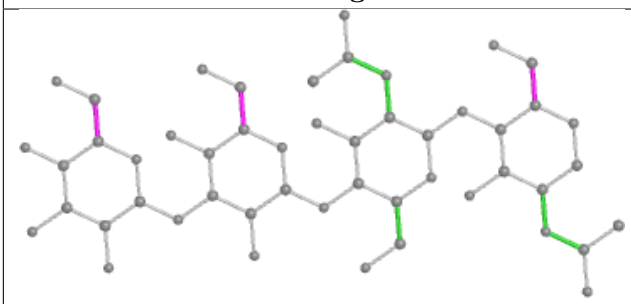
Oligosaccharide Chain c



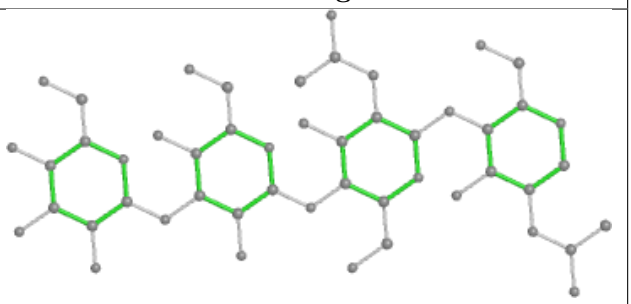
Bond lengths



Bond angles

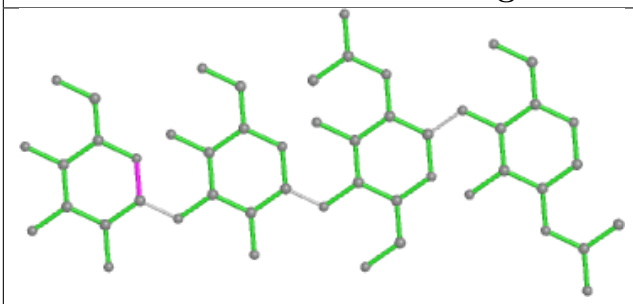


Torsions

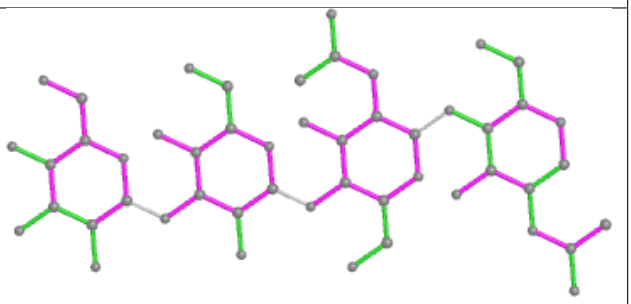


Rings

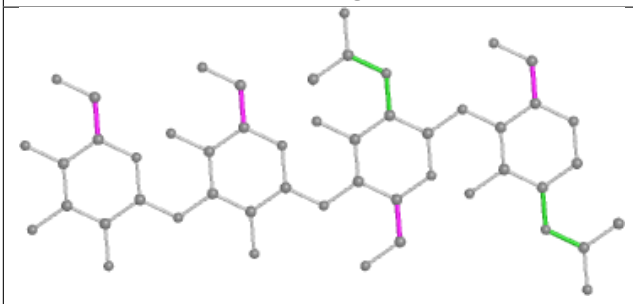
Oligosaccharide Chain d



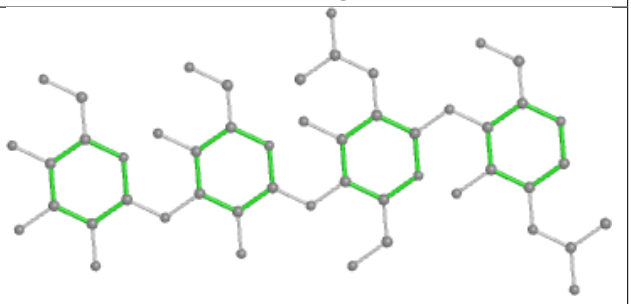
Bond lengths



Bond angles

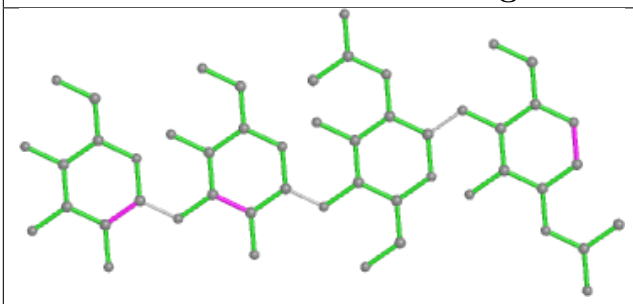


Torsions

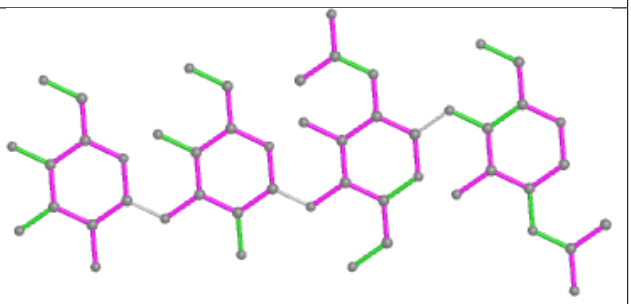


Rings

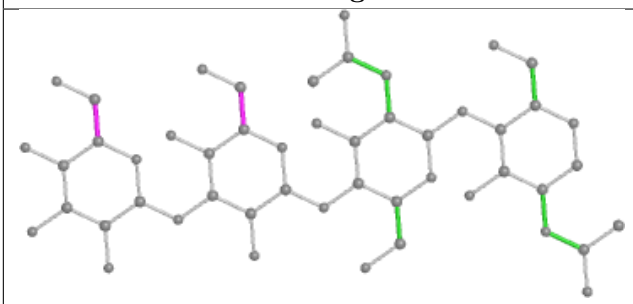
Oligosaccharide Chain e



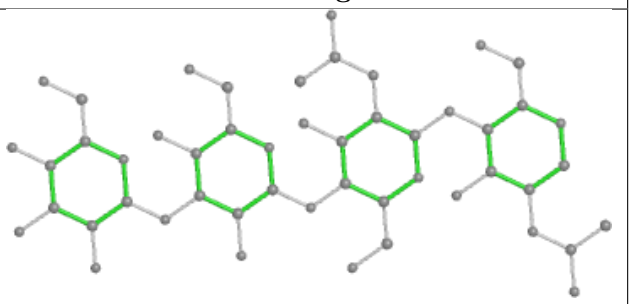
Bond lengths



Bond angles

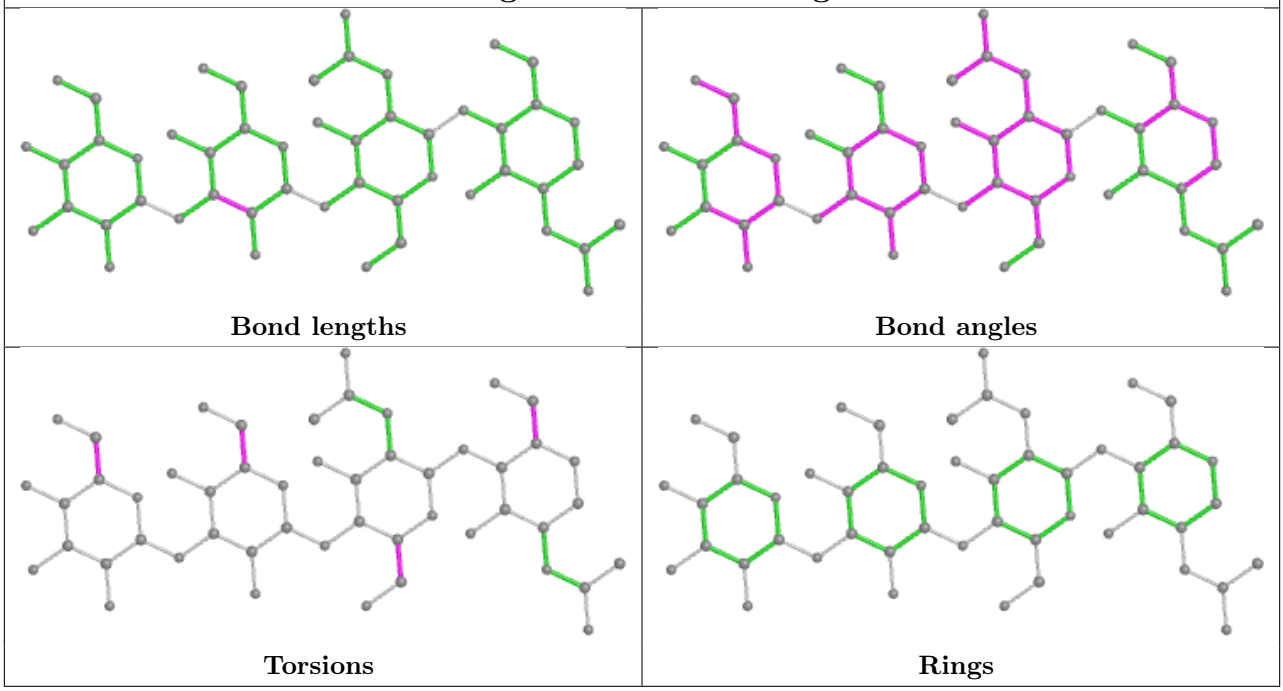


Torsions

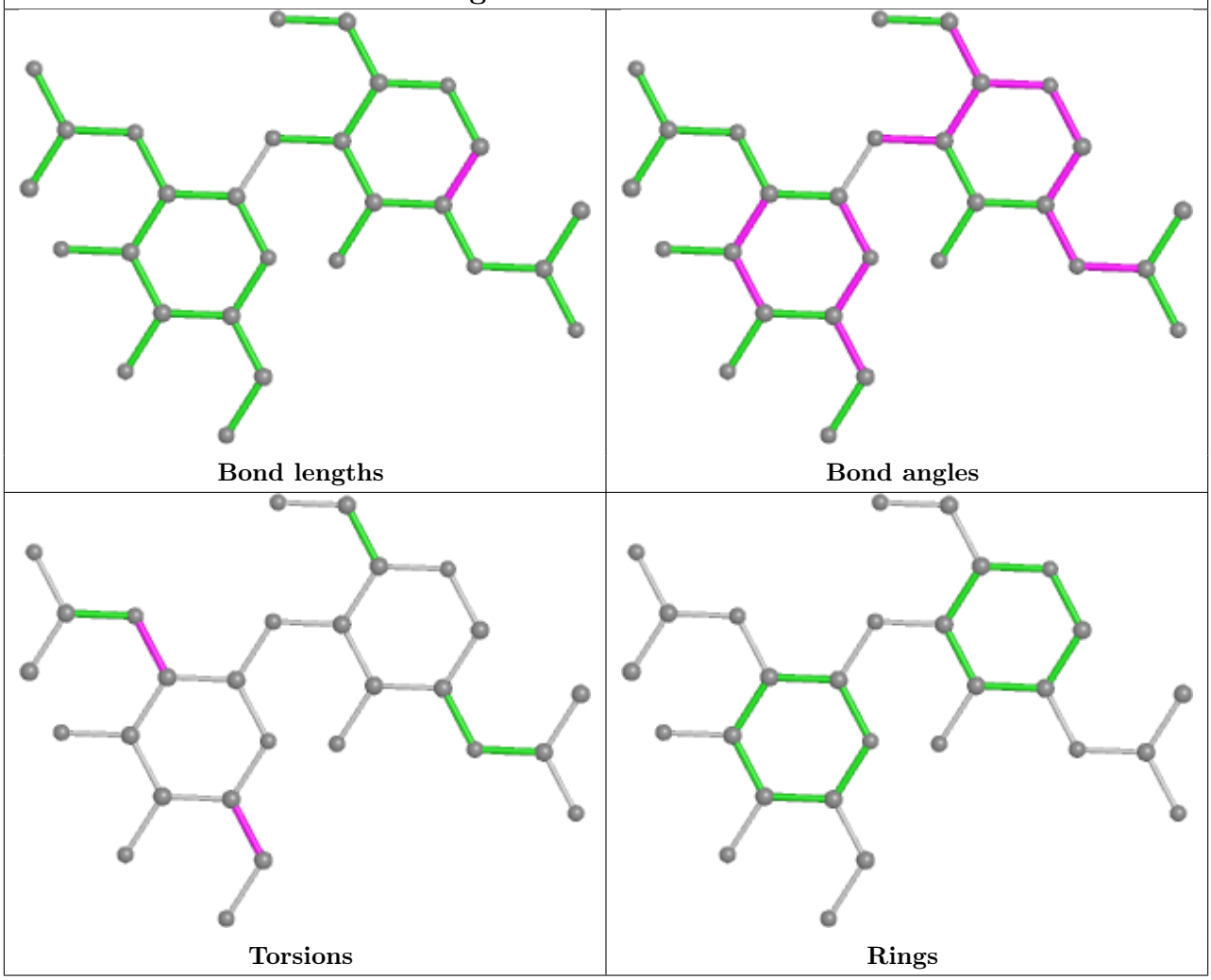


Rings

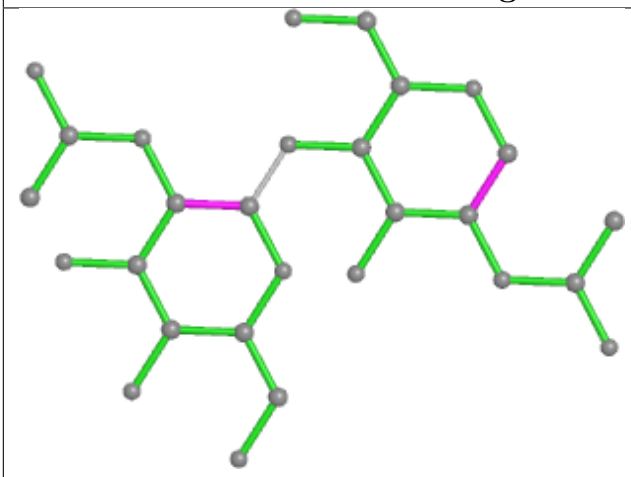
Oligosaccharide Chain g



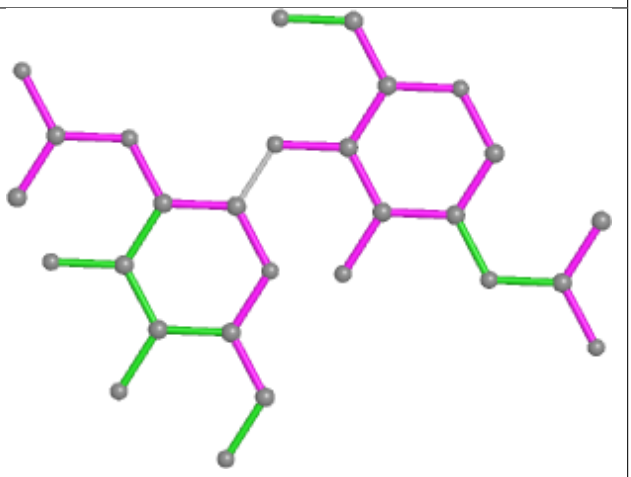
Oligosaccharide Chain Z



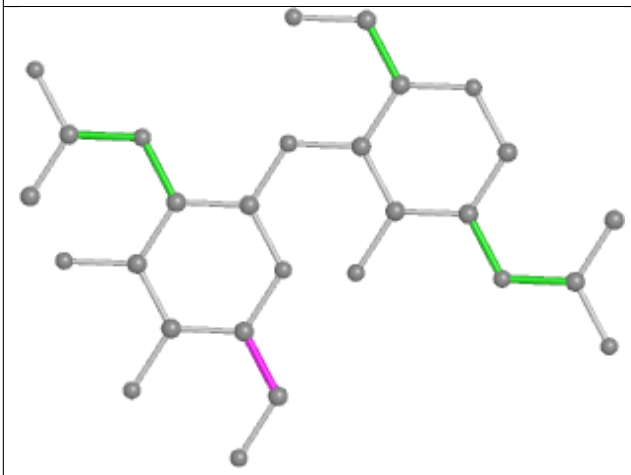
Oligosaccharide Chain a



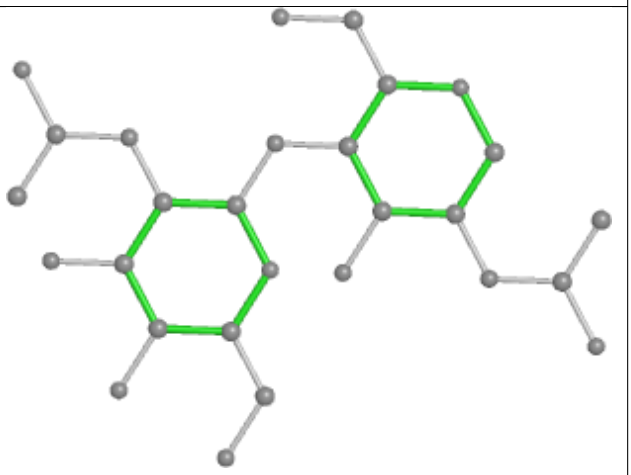
Bond lengths



Bond angles

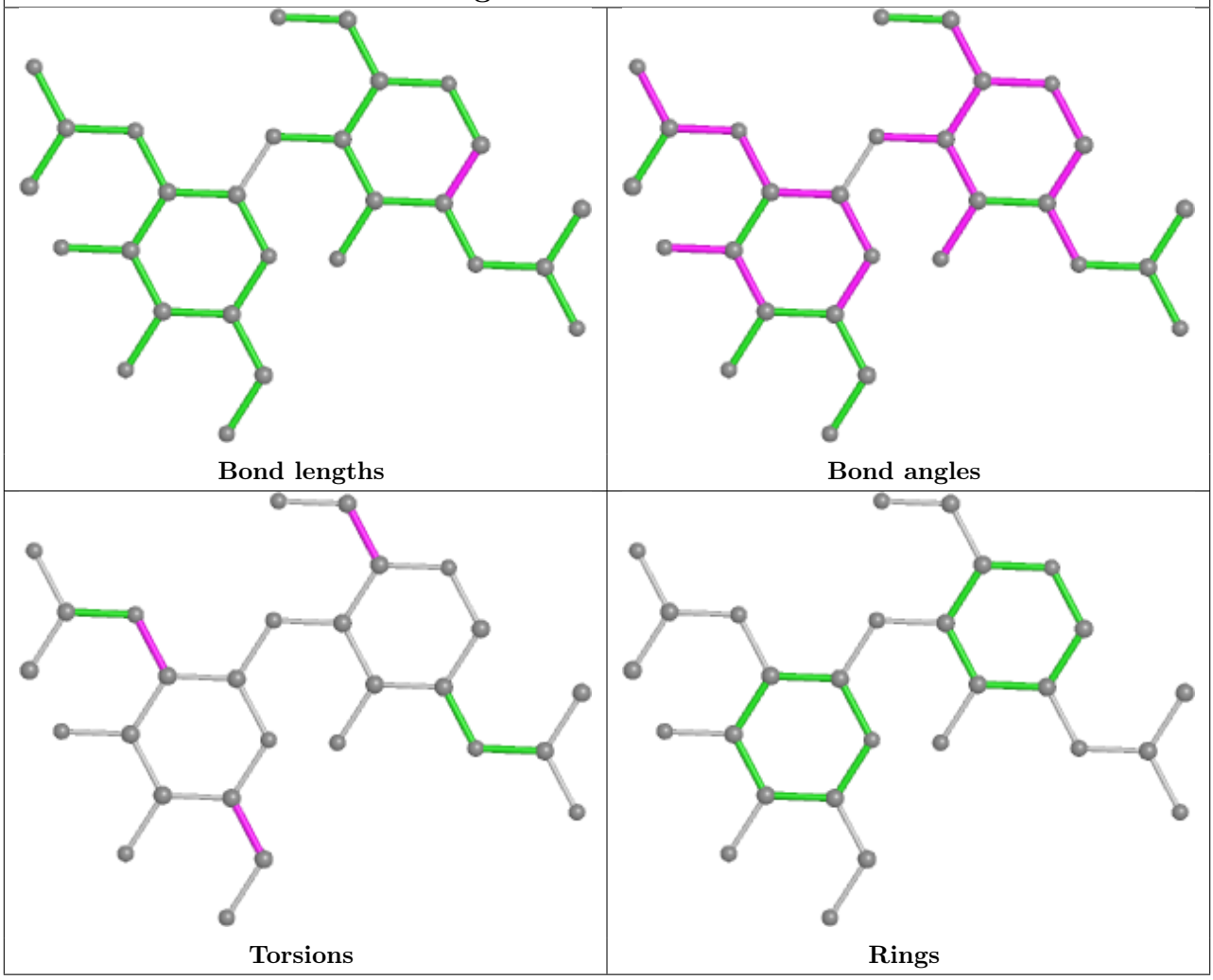


Torsions



Rings

Oligosaccharide Chain f



5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
7	NAG	I	405	1	14,14,15	1.58	2 (14%)	17,19,21	3.21	10 (58%)
7	NAG	Q	407	1	14,14,15	1.42	2 (14%)	17,19,21	3.34	9 (52%)
7	NAG	U	405	-	14,14,15	1.34	2 (14%)	17,19,21	2.90	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	V	201	2	14,14,15	0.99	1 (7%)	17,19,21	2.64	7 (41%)
7	NAG	A	409	1	14,14,15	1.05	1 (7%)	17,19,21	3.28	8 (47%)
7	NAG	F	201	-	14,14,15	0.96	0	17,19,21	2.29	5 (29%)
7	NAG	M	405	1	14,14,15	1.03	1 (7%)	17,19,21	1.31	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	405	1	-	0/6/23/26	0/1/1/1
7	NAG	Q	407	1	-	4/6/23/26	0/1/1/1
7	NAG	U	405	-	-	2/6/23/26	0/1/1/1
7	NAG	V	201	2	-	2/6/23/26	0/1/1/1
7	NAG	A	409	1	-	4/6/23/26	0/1/1/1
7	NAG	F	201	-	-	2/6/23/26	0/1/1/1
7	NAG	M	405	1	-	3/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	405	NAG	C1-C2	4.30	1.58	1.52
7	Q	407	NAG	C4-C5	3.19	1.59	1.53
7	M	405	NAG	C1-C2	2.92	1.56	1.52
7	U	405	NAG	C3-C2	2.85	1.58	1.52
7	V	201	NAG	C1-C2	2.66	1.56	1.52
7	I	405	NAG	C3-C2	2.44	1.57	1.52
7	Q	407	NAG	C3-C2	2.37	1.57	1.52
7	A	409	NAG	C3-C2	2.33	1.57	1.52
7	U	405	NAG	C4-C5	2.27	1.57	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	405	NAG	O5-C1-C2	-7.98	98.68	111.29
7	A	409	NAG	C1-O5-C5	7.85	122.83	112.19
7	Q	407	NAG	C1-O5-C5	6.90	121.54	112.19
7	V	201	NAG	C1-O5-C5	6.85	121.47	112.19
7	Q	407	NAG	O4-C4-C5	5.63	123.28	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	201	NAG	C4-C3-C2	5.29	118.76	111.02
7	A	409	NAG	O4-C4-C5	5.14	122.06	109.30
7	U	405	NAG	O3-C3-C4	-5.14	98.47	110.35
7	A	409	NAG	O3-C3-C4	-5.13	98.49	110.35
7	U	405	NAG	O7-C7-C8	-4.88	113.00	122.06
7	Q	407	NAG	O3-C3-C2	4.85	119.50	109.47
7	Q	407	NAG	C2-N2-C7	4.67	129.56	122.90
7	I	405	NAG	O3-C3-C2	4.47	118.71	109.47
7	U	405	NAG	C2-N2-C7	4.23	128.93	122.90
7	A	409	NAG	O7-C7-N2	4.09	129.47	121.95
7	I	405	NAG	C6-C5-C4	4.01	122.40	113.00
7	U	405	NAG	O4-C4-C5	3.93	119.06	109.30
7	U	405	NAG	C1-C2-N2	-3.91	103.81	110.49
7	A	409	NAG	C2-N2-C7	3.90	128.46	122.90
7	F	201	NAG	O5-C5-C6	3.90	113.31	107.20
7	Q	407	NAG	O7-C7-C8	-3.83	114.94	122.06
7	V	201	NAG	C1-C2-N2	3.83	117.03	110.49
7	Q	407	NAG	C6-C5-C4	3.52	121.24	113.00
7	I	405	NAG	C1-C2-N2	3.43	116.35	110.49
7	F	201	NAG	O7-C7-C8	-3.42	115.70	122.06
7	U	405	NAG	O3-C3-C2	3.39	116.48	109.47
7	Q	407	NAG	O7-C7-N2	3.38	128.16	121.95
7	U	405	NAG	O7-C7-N2	3.34	128.10	121.95
7	I	405	NAG	O7-C7-C8	-3.31	115.92	122.06
7	I	405	NAG	C4-C3-C2	-3.30	106.18	111.02
7	A	409	NAG	O3-C3-C2	3.25	116.20	109.47
7	V	201	NAG	O5-C1-C2	3.25	116.42	111.29
7	V	201	NAG	C2-N2-C7	3.03	127.22	122.90
7	V	201	NAG	O4-C4-C3	2.99	117.25	110.35
7	F	201	NAG	C1-O5-C5	2.89	116.10	112.19
7	I	405	NAG	C3-C4-C5	-2.88	105.10	110.24
7	V	201	NAG	O5-C5-C6	2.82	111.62	107.20
7	A	409	NAG	O7-C7-C8	-2.76	116.93	122.06
7	I	405	NAG	O5-C5-C6	-2.74	102.92	107.20
7	I	405	NAG	O4-C4-C5	2.66	115.91	109.30
7	F	201	NAG	C2-N2-C7	2.61	126.62	122.90
7	I	405	NAG	O5-C5-C4	-2.60	104.50	110.83
7	M	405	NAG	O3-C3-C2	2.53	114.70	109.47
7	V	201	NAG	O7-C7-C8	-2.51	117.39	122.06
7	U	405	NAG	C4-C3-C2	2.46	114.63	111.02
7	Q	407	NAG	O3-C3-C4	-2.36	104.88	110.35
7	A	409	NAG	C4-C3-C2	2.36	114.48	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	405	NAG	O4-C4-C5	2.29	114.97	109.30
7	Q	407	NAG	C4-C3-C2	2.06	114.04	111.02
7	U	405	NAG	O5-C5-C4	2.05	115.81	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	NAG	C3-C2-N2-C7
7	Q	407	NAG	C3-C2-N2-C7
7	U	405	NAG	O5-C5-C6-O6
7	A	409	NAG	O5-C5-C6-O6
7	V	201	NAG	O5-C5-C6-O6
7	U	405	NAG	C4-C5-C6-O6
7	F	201	NAG	O5-C5-C6-O6
7	V	201	NAG	C4-C5-C6-O6
7	F	201	NAG	C4-C5-C6-O6
7	A	409	NAG	C4-C5-C6-O6
7	Q	407	NAG	O5-C5-C6-O6
7	Q	407	NAG	C4-C5-C6-O6
7	A	409	NAG	C1-C2-N2-C7
7	Q	407	NAG	C1-C2-N2-C7
7	M	405	NAG	C3-C2-N2-C7
7	M	405	NAG	C4-C5-C6-O6
7	M	405	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	405	NAG	2	0
7	U	405	NAG	5	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	320/321 (99%)	-0.20	2 (0%)	89	86	68, 103, 128, 172	0
1	E	320/321 (99%)	-0.11	1 (0%)	94	91	57, 99, 124, 184	0
1	I	317/321 (98%)	-0.09	1 (0%)	94	91	57, 93, 117, 143	0
1	M	320/321 (99%)	-0.07	1 (0%)	94	91	60, 94, 118, 199	0
1	Q	320/321 (99%)	-0.14	0	100	100	57, 99, 129, 188	0
1	U	320/321 (99%)	-0.19	2 (0%)	89	86	67, 103, 132, 177	0
2	B	165/175 (94%)	-0.07	1 (0%)	89	86	58, 94, 129, 183	0
2	F	163/175 (93%)	-0.07	0	100	100	66, 104, 139, 175	0
2	J	164/175 (93%)	-0.07	4 (2%)	59	53	63, 104, 138, 178	0
2	N	163/175 (93%)	-0.12	2 (1%)	79	73	64, 102, 135, 163	0
2	R	166/175 (94%)	-0.06	1 (0%)	89	86	64, 103, 141, 185	0
2	V	164/175 (93%)	-0.11	1 (0%)	89	86	59, 94, 129, 171	0
3	C	219/226 (96%)	-0.14	0	100	100	70, 96, 142, 202	0
3	G	219/226 (96%)	-0.07	4 (1%)	68	62	77, 117, 170, 219	0
3	K	219/226 (96%)	0.79	43 (19%)	1	1	100, 175, 253, 286	0
3	O	219/226 (96%)	1.25	54 (24%)	0	0	111, 189, 304, 357	0
3	S	219/226 (96%)	0.01	5 (2%)	60	54	83, 117, 169, 217	0
3	Y	219/226 (96%)	-0.11	1 (0%)	91	88	70, 95, 145, 206	0
4	D	213/215 (99%)	-0.03	0	100	100	69, 96, 127, 156	0
4	H	213/215 (99%)	-0.00	1 (0%)	91	88	75, 115, 164, 197	0
4	L	213/215 (99%)	0.63	31 (14%)	2	3	99, 186, 239, 267	0
4	P	213/215 (99%)	0.87	46 (21%)	0	1	96, 205, 273, 317	0
4	T	213/215 (99%)	0.04	5 (2%)	60	54	76, 115, 170, 216	0
4	X	213/215 (99%)	0.01	3 (1%)	75	69	69, 95, 126, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5494/5622 (97%)	0.07	209 (3%) 40 36	57, 105, 215, 357	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	197	VAL	12.1
3	O	226	PRO	11.3
3	O	167	TRP	10.8
3	O	198	PRO	10.1
4	P	118	ILE	9.1
3	O	192	SER	9.1
4	L	195	CYS	8.9
3	O	196	THR	8.9
3	K	192	SER	8.7
4	L	118	ILE	8.5
3	K	198	PRO	8.3
3	O	151	LEU	8.1
3	K	193	SER	8.0
4	P	119	PHE	6.9
4	L	135	CYS	6.8
3	O	164	THR	6.8
4	P	178	SER	6.7
3	K	194	VAL	6.5
3	O	166	SER	6.5
4	P	136	LEU	6.5
4	P	135	CYS	6.3
4	L	137	LEU	6.3
3	K	152	GLY	6.1
4	P	184	LYS	6.1
3	O	207	TYR	6.1
3	O	193	SER	6.0
3	O	194	VAL	6.0
3	K	191	LEU	5.9
3	K	201	SER	5.9
3	K	151	LEU	5.8
3	O	204	THR	5.7
3	O	208	ILE	5.7
3	K	204	THR	5.4
3	O	104	ARG	5.4
3	K	150	ALA	5.3
2	J	141	TYR	5.2
4	P	116	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
3	O	173	THR	5.2
3	O	150	ALA	5.1
4	L	136	LEU	5.1
4	P	117	PHE	5.1
4	P	134	VAL	5.1
4	L	134	VAL	5.1
4	L	116	VAL	5.1
3	O	168	ASN	5.0
4	P	137	LEU	4.9
4	L	119	PHE	4.9
3	O	174	SER	4.8
4	P	177	SER	4.8
4	P	120	PRO	4.8
3	O	165	VAL	4.6
3	O	225	GLU	4.5
4	P	195	CYS	4.5
4	P	182	LEU	4.3
3	O	178	THR	4.3
4	P	131	ALA	4.2
4	L	117	PHE	4.2
4	L	131	ALA	4.1
3	K	162	PRO	4.0
4	P	147	VAL	4.0
4	P	197	VAL	4.0
4	P	176	LEU	3.9
3	K	148	THR	3.9
4	P	37	TYR	3.9
3	O	125	SER	3.9
4	L	178	SER	3.9
3	K	197	VAL	3.9
3	K	147	GLY	3.9
3	O	199	SER	3.8
3	O	29	PHE	3.8
4	L	149	TRP	3.8
4	P	181	THR	3.7
4	P	161	GLN	3.7
3	O	206	THR	3.7
3	O	195	VAL	3.6
3	O	149	ALA	3.6
4	P	163	SER	3.6
3	O	163	VAL	3.5
3	O	205	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
3	O	179	PHE	3.5
4	P	202	LEU	3.5
4	L	176	LEU	3.4
4	L	177	SER	3.4
4	P	162	GLU	3.4
4	L	184	LYS	3.3
2	N	141	TYR	3.3
4	L	191	LYS	3.3
3	K	104	ARG	3.2
3	O	191	LEU	3.2
3	K	170	GLY	3.2
4	P	115	SER	3.2
3	K	20	VAL	3.2
3	O	169	SER	3.2
4	P	188	GLU	3.2
4	P	49	ILE	3.1
4	P	179	THR	3.1
4	L	206	VAL	3.1
2	J	140	ILE	3.1
2	N	130	ALA	3.1
3	K	166	SER	3.0
3	K	179	PHE	3.0
4	P	63	PHE	3.0
4	P	48	LEU	2.9
3	K	219	LYS	2.9
3	K	226	PRO	2.9
4	P	132	SER	2.9
4	P	79	LEU	2.8
3	O	171	ALA	2.8
4	L	49	ILE	2.8
3	S	193	SER	2.8
3	K	164	THR	2.8
3	O	170	GLY	2.8
4	P	18	ARG	2.8
2	J	171	PHE	2.8
3	O	162	PRO	2.8
4	P	180	LEU	2.8
3	O	210	ASN	2.8
3	O	138	ALA	2.8
4	P	209	SER	2.8
3	O	152	GLY	2.8
3	O	172	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	132	SER	2.7
4	L	197	VAL	2.7
3	O	153	CYS	2.7
1	I	9	SER	2.6
3	O	32	TYR	2.6
3	K	160	PRO	2.6
4	T	136	LEU	2.6
3	O	113	HIS	2.6
3	K	190	SER	2.6
2	B	173	ILE	2.6
3	O	177	HIS	2.6
4	L	146	LYS	2.6
3	O	139	PRO	2.6
3	K	90	ASP	2.6
3	K	155	VAL	2.5
3	O	53	ALA	2.5
3	K	29	PHE	2.5
3	K	169	SER	2.5
4	L	41	SER	2.5
4	L	130	THR	2.5
4	L	48	LEU	2.5
4	H	136	LEU	2.5
3	O	27	TYR	2.5
3	O	31	THR	2.5
3	S	194	VAL	2.5
3	O	221	ASP	2.4
4	L	156	GLN	2.4
3	G	1	GLN	2.4
4	L	114	PRO	2.4
3	S	149	ALA	2.4
4	L	147	VAL	2.4
3	G	193	SER	2.4
4	T	177	SER	2.4
1	U	127	TRP	2.3
3	K	165	VAL	2.3
4	T	149	TRP	2.3
3	S	177	HIS	2.3
1	A	251	LEU	2.3
4	P	123	ASP	2.3
4	P	196	GLU	2.3
3	K	205	GLN	2.3
4	P	38	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	189	TYR	2.3
3	K	161	GLU	2.3
4	X	28	ARG	2.3
3	K	195	VAL	2.3
4	P	76	ILE	2.3
3	S	150	ALA	2.3
4	X	195	CYS	2.3
4	P	130	THR	2.3
1	A	245	ILE	2.2
3	G	194	VAL	2.2
4	P	41	SER	2.2
4	T	189	LYS	2.2
3	O	48	VAL	2.2
3	K	178	THR	2.2
4	P	39	GLN	2.2
4	L	211	ASN	2.2
3	O	154	LEU	2.2
4	L	209	SER	2.2
4	T	156	GLN	2.2
2	R	138	PHE	2.1
2	V	61	GLU	2.1
4	L	115	SER	2.1
3	K	153	CYS	2.1
3	K	207	TYR	2.1
3	Y	204	THR	2.1
3	K	114	ASP	2.1
4	P	160	SER	2.1
3	K	139	PRO	2.1
4	L	187	TYR	2.1
3	K	200	SER	2.1
3	K	138	ALA	2.1
3	K	19	LYS	2.1
3	K	214	LYS	2.1
1	E	12	THR	2.1
3	O	161	GLU	2.1
3	K	167	TRP	2.1
4	X	150	LYS	2.0
3	G	170	GLY	2.0
2	J	124	ARG	2.0
1	M	9	SER	2.0
1	U	245	ILE	2.0
4	P	35	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	155	VAL	2.0
4	P	189	LYS	2.0
4	P	148	GLN	2.0
3	O	36	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
6	NAG	f	2	14/15	0.57	0.27	152,179,197,197	0
7	NAG	F	201	14/15	0.58	0.27	155,185,196,198	0
6	NAG	a	1	14/15	0.73	0.20	179,195,202,203	0
7	NAG	V	201	14/15	0.76	0.30	103,112,121,121	0
6	NAG	a	2	14/15	0.83	0.18	151,173,185,190	0
6	NAG	Z	2	14/15	0.83	0.24	147,155,164,165	0
7	NAG	I	405	14/15	0.84	0.21	106,126,133,137	0
5	NAG	W	2	14/15	0.85	0.20	108,122,129,133	0
7	NAG	Q	407	14/15	0.88	0.26	85,101,107,107	0
7	NAG	A	409	14/15	0.88	0.19	89,104,118,124	0
7	NAG	M	405	14/15	0.89	0.24	101,119,136,138	0
7	NAG	U	405	14/15	0.89	0.20	84,97,121,129	0
5	NAG	b	1	14/15	0.90	0.18	120,124,127,128	0
5	NAG	g	1	14/15	0.91	0.19	101,108,117,119	0
5	NAG	g	2	14/15	0.91	0.22	102,121,142,146	0
5	NAG	W	1	14/15	0.91	0.17	105,108,112,113	0
5	NAG	c	1	14/15	0.92	0.16	85,91,92,92	0
6	NAG	Z	1	14/15	0.93	0.20	130,133,144,145	0
5	NAG	e	1	14/15	0.93	0.17	96,104,115,116	0
5	NAG	e	2	14/15	0.93	0.21	107,116,134,136	0
5	NAG	d	1	14/15	0.93	0.16	90,94,96,97	0
5	NAG	b	2	14/15	0.94	0.18	102,125,137,141	0
5	NAG	c	2	14/15	0.94	0.25	101,107,116,121	0
6	NAG	f	1	14/15	0.96	0.18	112,128,138,152	0
5	NAG	d	2	14/15	0.96	0.16	94,104,111,111	0

6.3 Carbohydrates (i)

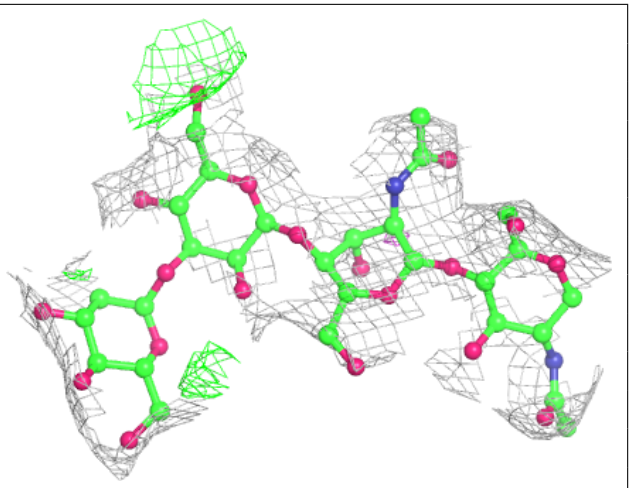
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

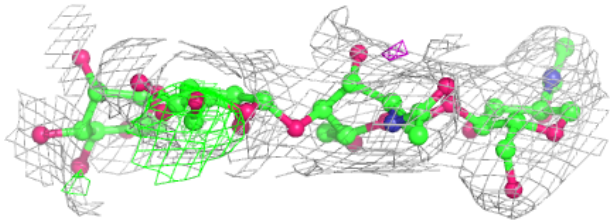
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	f	2	14/15	0.57	0.27	152,179,197,197	0
5	BMA	g	3	11/12	0.66	0.19	116,129,135,137	0
5	BMA	e	3	11/12	0.70	0.19	107,121,124,132	0
5	BMA	W	3	11/12	0.72	0.21	109,123,131,147	0
6	NAG	a	1	14/15	0.73	0.20	179,195,202,203	0
5	MAN	e	4	11/12	0.77	0.36	129,145,149,150	0
5	MAN	b	4	11/12	0.77	0.19	135,149,150,150	0
5	BMA	b	3	11/12	0.80	0.14	114,124,135,146	0
5	MAN	c	4	11/12	0.81	0.18	134,140,148,169	0
5	BMA	c	3	11/12	0.83	0.17	104,110,118,121	0
6	NAG	a	2	14/15	0.83	0.18	151,173,185,190	0
6	NAG	Z	2	14/15	0.83	0.24	147,155,164,165	0
5	MAN	d	4	11/12	0.84	0.20	141,147,157,173	0
5	NAG	W	2	14/15	0.85	0.20	108,122,129,133	0
5	MAN	W	4	11/12	0.85	0.23	147,149,156,160	0
5	NAG	b	1	14/15	0.90	0.18	120,124,127,128	0
5	NAG	g	1	14/15	0.91	0.19	101,108,117,119	0
5	NAG	g	2	14/15	0.91	0.22	102,121,142,146	0
5	NAG	W	1	14/15	0.91	0.17	105,108,112,113	0
5	MAN	g	4	11/12	0.91	0.14	125,138,145,146	0
5	NAG	c	1	14/15	0.92	0.16	85,91,92,92	0
6	NAG	Z	1	14/15	0.93	0.20	130,133,144,145	0
5	NAG	e	1	14/15	0.93	0.17	96,104,115,116	0
5	NAG	e	2	14/15	0.93	0.21	107,116,134,136	0
5	BMA	d	3	11/12	0.93	0.14	106,111,126,130	0
5	NAG	d	1	14/15	0.93	0.16	90,94,96,97	0
5	NAG	b	2	14/15	0.94	0.18	102,125,137,141	0
5	NAG	c	2	14/15	0.94	0.25	101,107,116,121	0
6	NAG	f	1	14/15	0.96	0.18	112,128,138,152	0
5	NAG	d	2	14/15	0.96	0.16	94,104,111,111	0

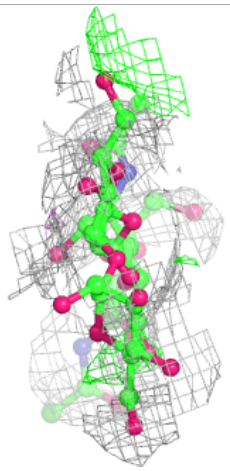
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain W:

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

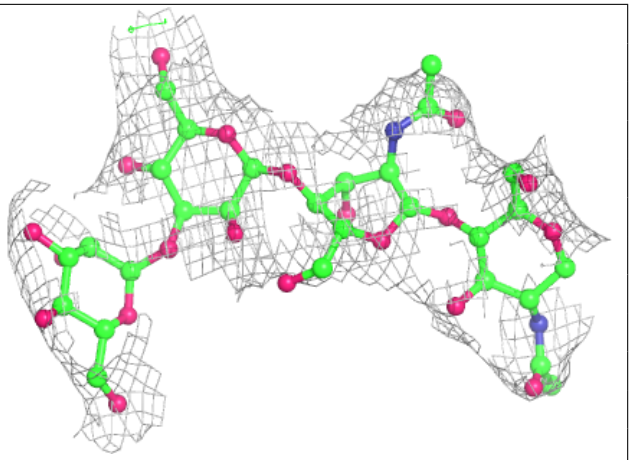


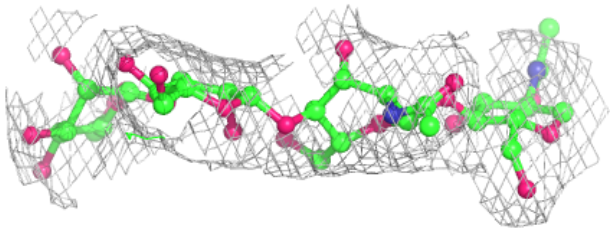


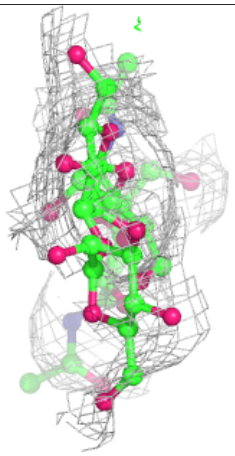


Electron density around Chain b:

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

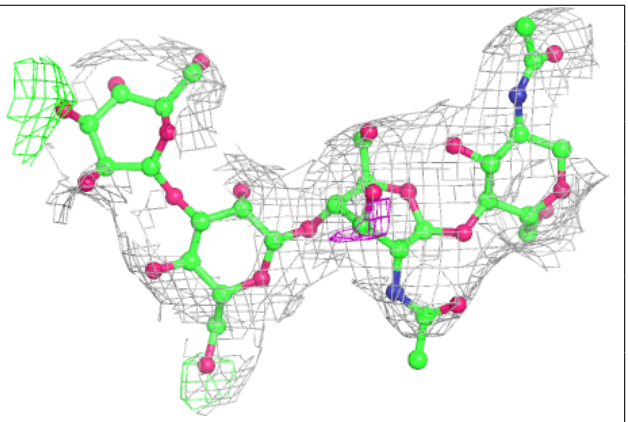


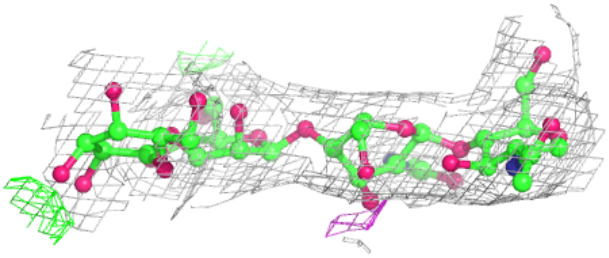


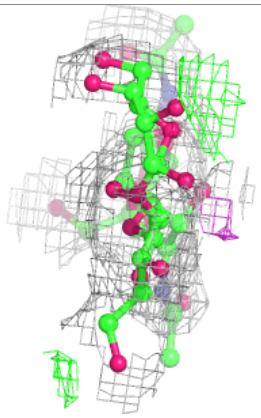


Electron density around Chain c:

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

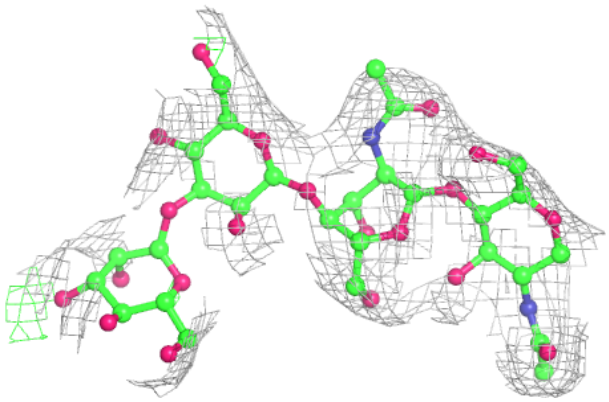


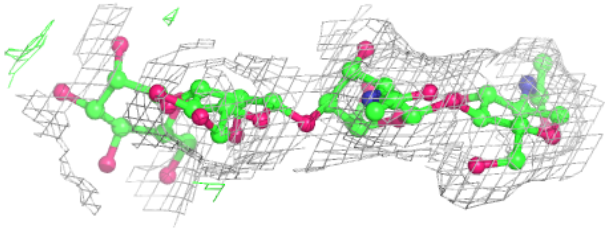


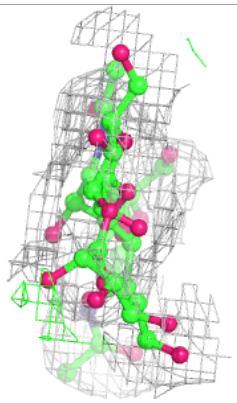


Electron density around Chain d:

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

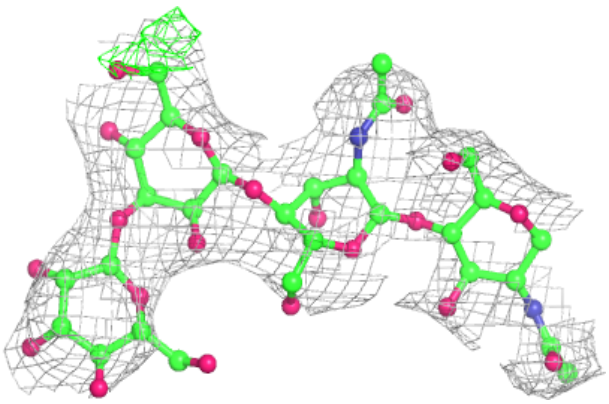


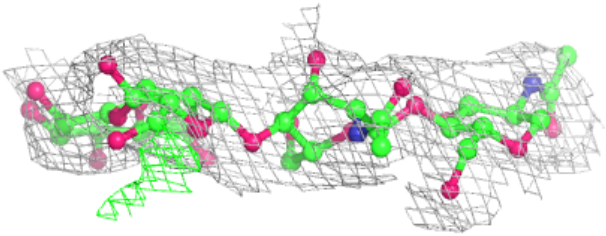


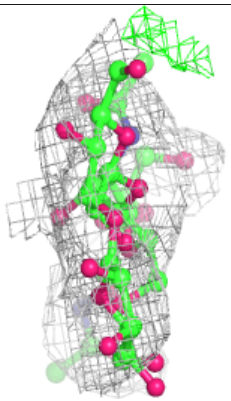


Electron density around Chain e:

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

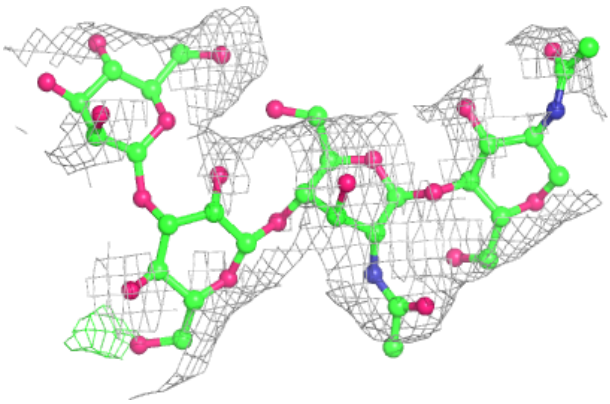


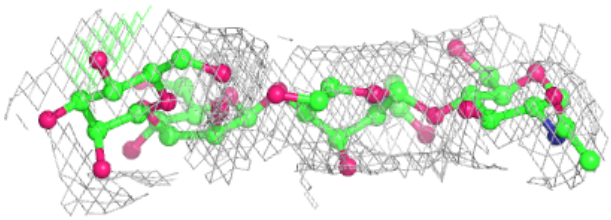


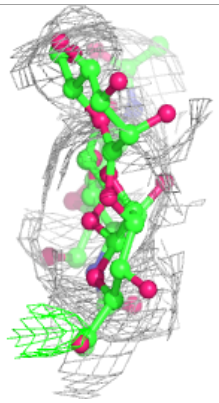


Electron density around Chain g:

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

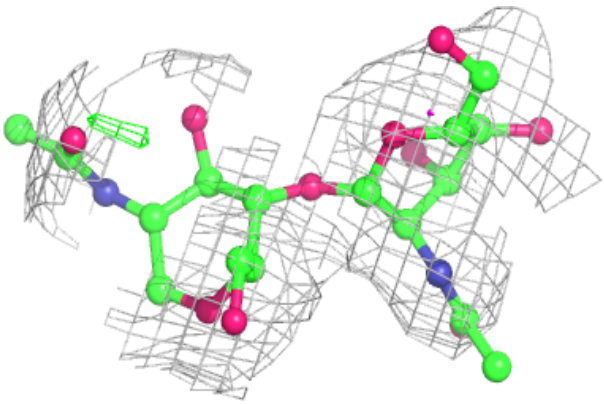


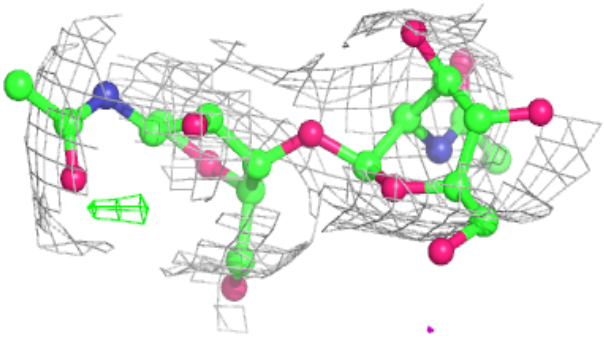


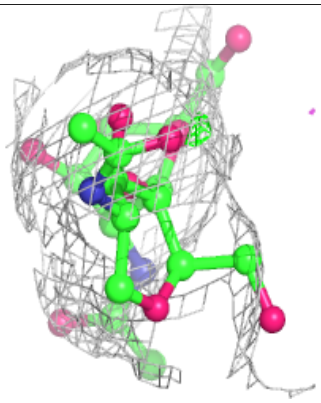


Electron density around Chain Z:

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

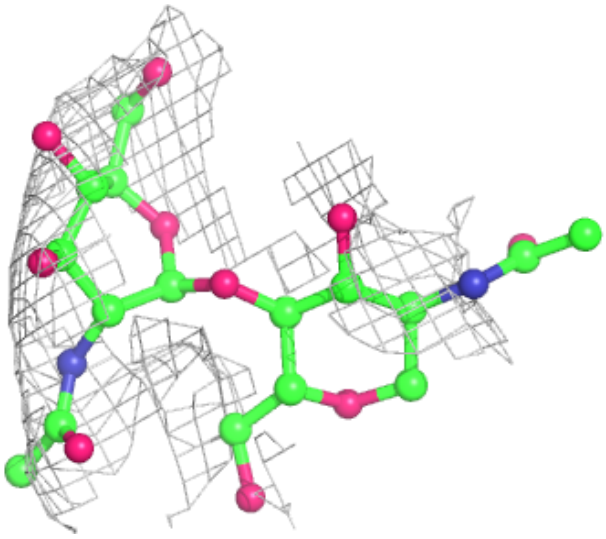


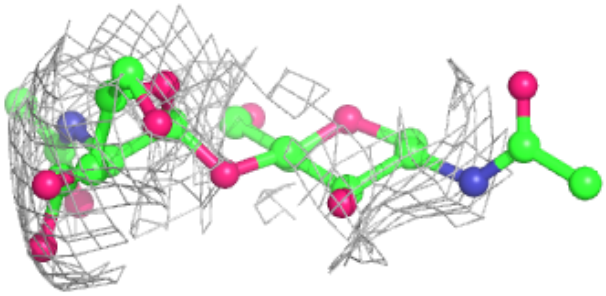


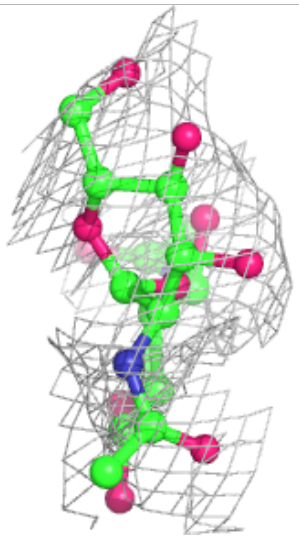


Electron density around Chain a:

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

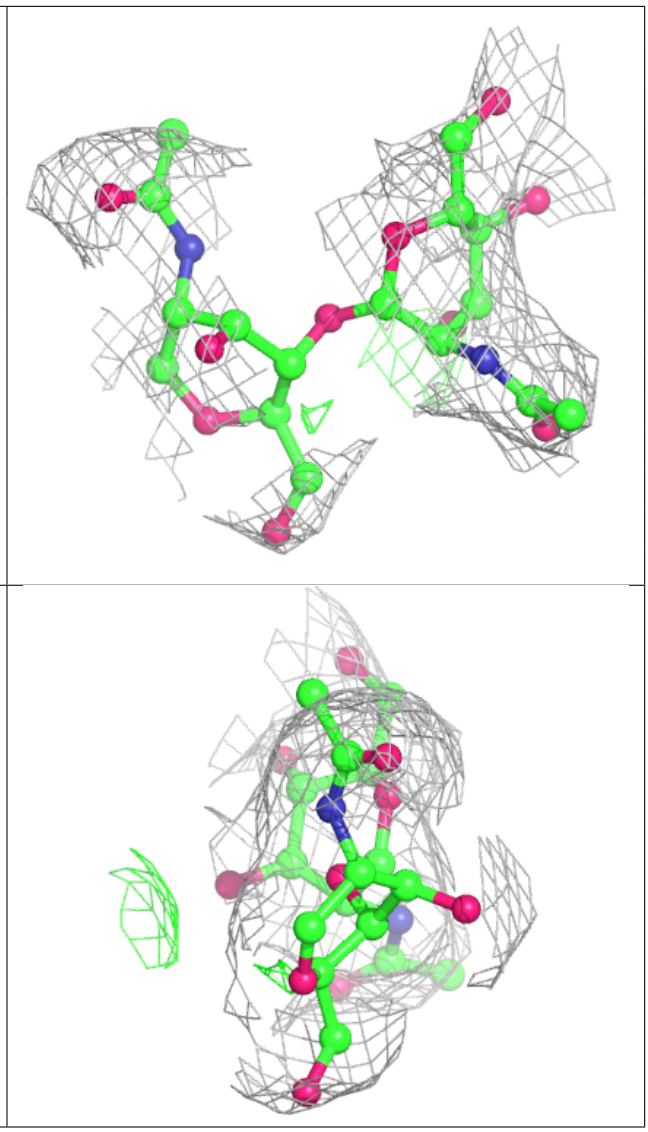






Electron density around Chain f:

$2mF_o$-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
7	NAG	F	201	14/15	0.58	0.27	155,185,196,198	0
7	NAG	V	201	14/15	0.76	0.30	103,112,121,121	0
7	NAG	I	405	14/15	0.84	0.21	106,126,133,137	0
7	NAG	Q	407	14/15	0.88	0.26	85,101,107,107	0
7	NAG	A	409	14/15	0.88	0.19	89,104,118,124	0
7	NAG	U	405	14/15	0.89	0.20	84,97,121,129	0
7	NAG	M	405	14/15	0.89	0.24	101,119,136,138	0

6.5 Other polymers (i)

There are no such residues in this entry.