Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:42 PM EDT

PDB ID	:	2O26
Title	:	Structure of a class III RTK signaling assembly
Authors	:	Liu, H.; Chen, X.; Focia, P.J.; He, X.
Deposited on	:	2006-11-29
Resolution	:	2.50 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 following versions of software and data (see references (i)) were used in the production of this report:

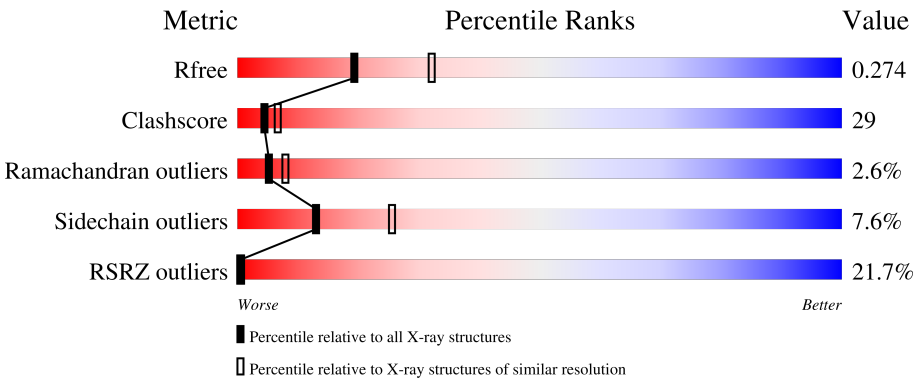
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	145	9% 62% 30% 7%
1	B	145	19% 55% 33% 7%
1	E	145	15% 54% 36% 6%
1	F	145	21% 59% 30% 7%
2	U	290	21% 49% 39% 6% 5%

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Mol	Chain	Length	Quality of chain
2	W	290	33% 56% 33% 6% 5%
2	X	290	18% 47% 40% 8% 5%
2	Y	290	20% 53% 36% 6% 5%
3	C	3	33% 33% 33%
3	G	3	67% 33%
3	I	3	100%
3	K	3	100%
4	D	3	33% 67%
4	H	3	33% 33% 33%
4	J	3	33% 67%
4	L	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	L	1	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15104 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 Kit ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	144	1140	722	189	220	9	0	0	0
			Total	C	N	O	S			
1	B	139	1090	692	174	215	9	0	0	0
			Total	C	N	O	S			
1	E	139	1090	692	174	215	9	0	0	0
			Total	C	N	O	S			
1	F	139	1090	692	174	215	9	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	HIS	-	expression tag	UNP P20826
A	143	HIS	-	expression tag	UNP P20826
A	144	HIS	-	expression tag	UNP P20826
A	145	HIS	-	expression tag	UNP P20826
A	146	HIS	-	expression tag	UNP P20826
A	147	HIS	-	expression tag	UNP P20826
B	142	HIS	-	expression tag	UNP P20826
B	143	HIS	-	expression tag	UNP P20826
B	144	HIS	-	expression tag	UNP P20826
B	145	HIS	-	expression tag	UNP P20826
B	146	HIS	-	expression tag	UNP P20826
B	147	HIS	-	expression tag	UNP P20826
E	142	HIS	-	expression tag	UNP P20826
E	143	HIS	-	expression tag	UNP P20826
E	144	HIS	-	expression tag	UNP P20826
E	145	HIS	-	expression tag	UNP P20826
E	146	HIS	-	expression tag	UNP P20826
E	147	HIS	-	expression tag	UNP P20826
F	142	HIS	-	expression tag	UNP P20826
F	143	HIS	-	expression tag	UNP P20826
F	144	HIS	-	expression tag	UNP P20826

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Chain	Residue	Modelled	Actual	Comment	Reference
F	145	HIS	-	expression tag	UNP P20826
F	146	HIS	-	expression tag	UNP P20826
F	147	HIS	-	expression tag	UNP P20826

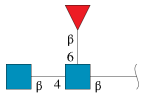
- Molecule 2 is a protein called Mast/stem cell growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	275	2164	1369	372	411	12	0	0	0
2	Y	275	2164	1369	372	411	12	0	0	0
2	U	275	2164	1369	372	411	12	0	0	0
2	W	275	2164	1369	372	411	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	146	GLN	ASN	engineered mutation	UNP P05532
W	146	GLN	ASN	engineered mutation	UNP P05532
X	146	GLN	ASN	engineered mutation	UNP P05532
Y	146	GLN	ASN	engineered mutation	UNP P05532

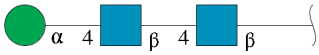
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0
3	G	3	38	22	2	14	0	0	0
3	I	3	38	22	2	14	0	0	0
3	K	3	38	22	2	14	0	0	0

- Molecule 4 is an oligosaccharide called alpha-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			
4	D	3	39	22	2	15	0	0	0
4	H	3	39	22	2	15	0	0	0
4	J	3	39	22	2	15	0	0	0
4	L	3	39	22	2	15	0	0	0

- Molecule 5 is water.

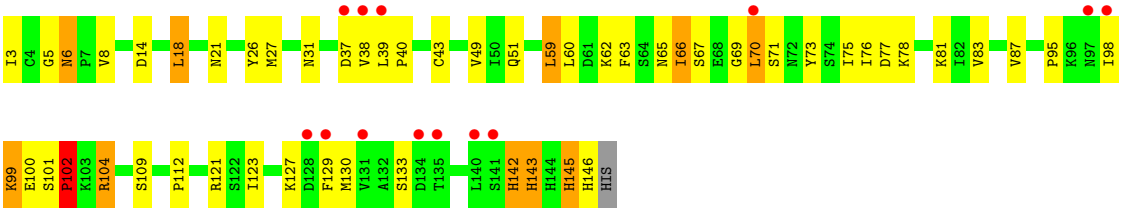
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	171	171	171	0	0
5	B	144	144	144	0	0
5	E	152	152	152	0	0
5	F	143	143	143	0	0
5	X	273	273	273	0	0
5	Y	310	310	310	0	0
5	U	270	270	270	0	0
5	W	267	267	267	0	0

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.

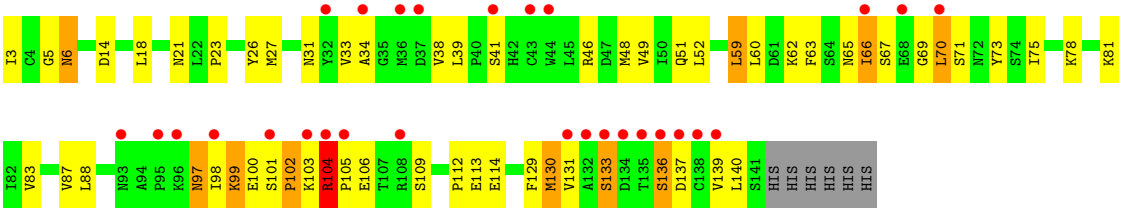
• Molecule 1: Kit ligand

Chain A:



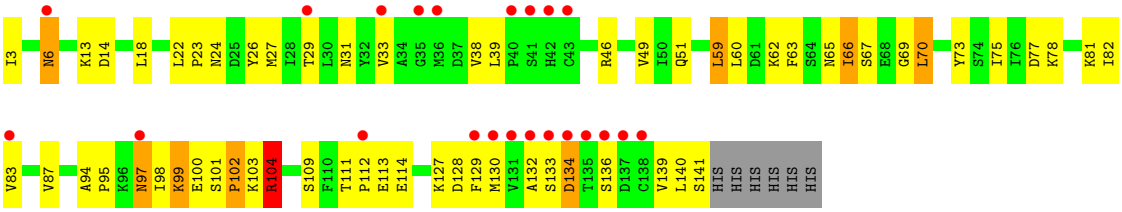
• Molecule 1: Kit ligand

Chain B:



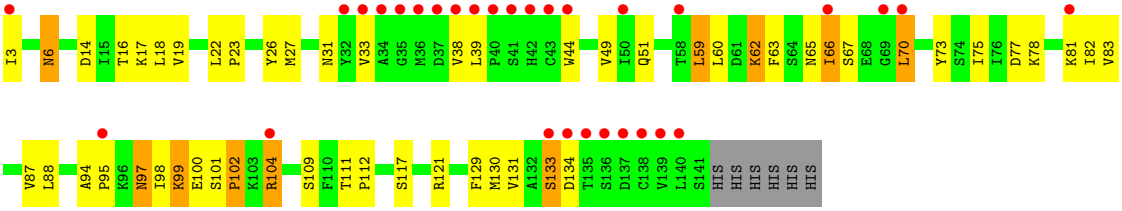
• Molecule 1: Kit ligand

Chain E:



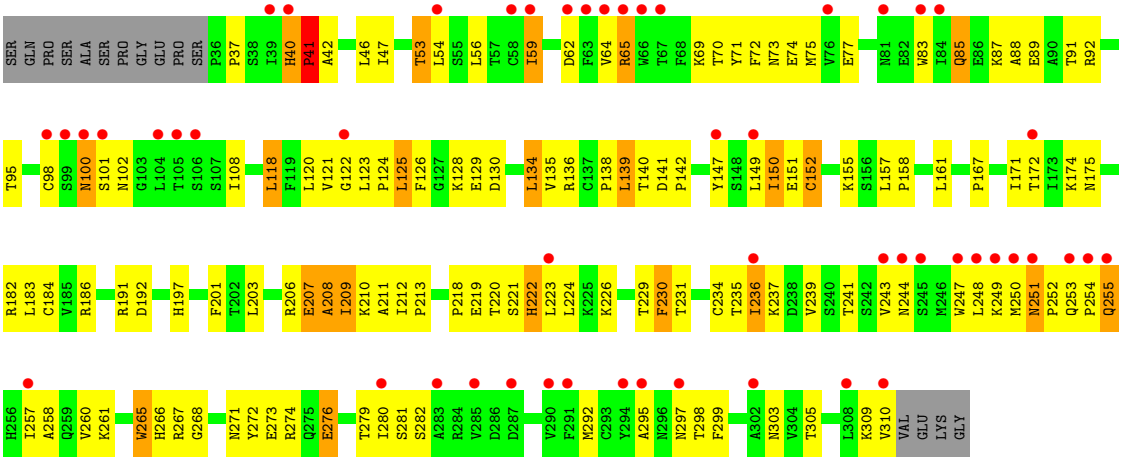
• Molecule 1: Kit ligand

Chain F:



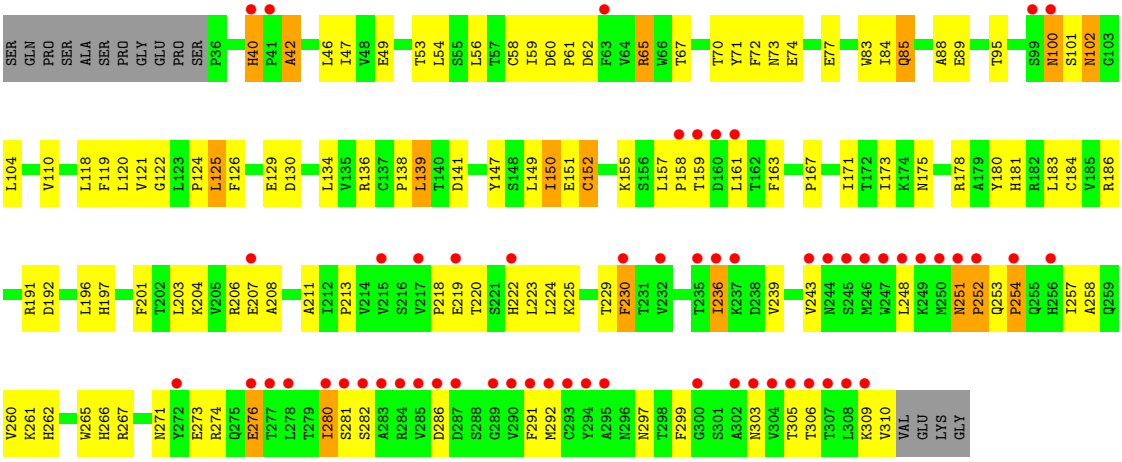
• Molecule 2: Mast/stem cell growth factor receptor

Chain X:



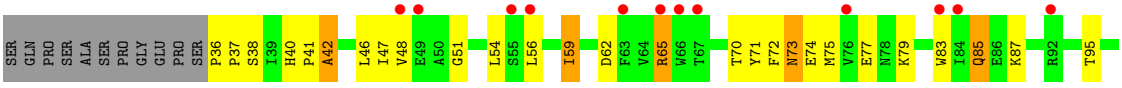
• Molecule 2: Mast/stem cell growth factor receptor

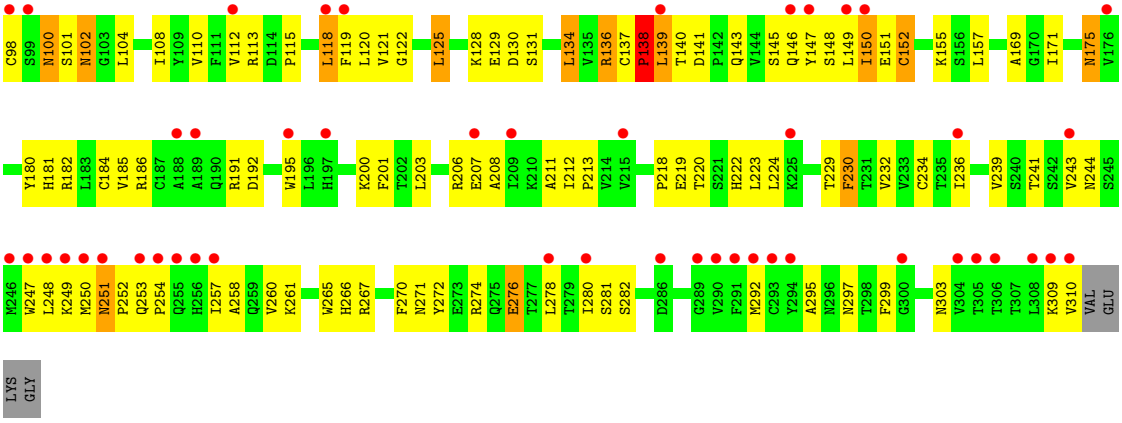
Chain Y:



• Molecule 2: Mast/stem cell growth factor receptor

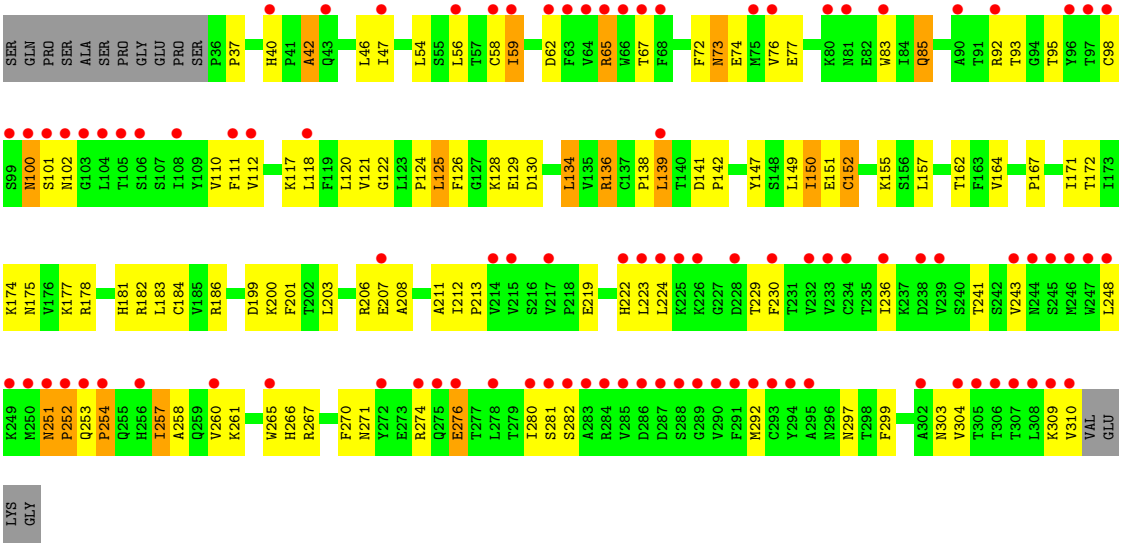
Chain U:





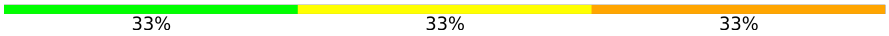
• Molecule 2: Mast/stem cell growth factor receptor

Chain W:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

NAG1 NAG2 FUL3

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

NAG1 NAG2 FUL3

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

Chain D: 33% 67%

NAG1 NAG2 MAN3

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

Chain H: 33% 33% 33%

NAG1 NAG2 MAN3

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

Chain J: 33% 67%

NAG1 NAG2 MAN3

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

Chain L: 67% 33%

NAG1 NAG2 MAN3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.85Å 200.15Å 82.02Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	19.93 – 2.50 48.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.93-2.50) 96.8 (48.46-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.270 0.242 , 0.274	Depositor DCC
R_{free} test set	4160 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	65.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 87.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: NAG, FUL, MAN

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	0.40	0/1164	0.70	1/1579 (0.1%)
1	B	0.48	1/1109 (0.1%)	0.67	0/1504
1	E	0.40	0/1109	0.64	1/1504 (0.1%)
1	F	0.41	0/1109	0.65	1/1504 (0.1%)
2	U	0.38	0/2214	0.72	1/3011 (0.0%)
2	W	0.35	0/2214	0.64	0/3011
2	X	0.37	0/2214	0.69	2/3011 (0.1%)
2	Y	0.36	0/2214	0.65	0/3011
All	All	0.39	1/13347 (0.0%)	0.67	6/18135 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	SER	CA-CB	7.77	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	138	PRO	CA-N-CD	-14.78	90.81	111.50
2	X	41	PRO	CA-N-CD	-12.45	94.08	111.50
1	A	102	PRO	CA-N-CD	-8.86	99.09	111.50
1	F	134	ASP	C-N-CA	-5.22	108.64	121.70
2	X	208	ALA	N-CA-C	-5.22	96.92	111.00
1	E	134	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1140	0	1121	62	0
1	B	1090	0	1086	68	0
1	E	1090	0	1086	65	0
1	F	1090	0	1086	54	0
2	U	2164	0	2140	139	0
2	W	2164	0	2140	118	0
2	X	2164	0	2140	145	0
2	Y	2164	0	2140	125	0
3	C	38	0	34	1	0
3	G	38	0	34	2	0
3	I	38	0	34	3	0
3	K	38	0	34	0	0
4	D	39	0	34	1	0
4	H	39	0	34	1	0
4	J	39	0	34	0	0
4	L	39	0	34	3	0
5	A	171	0	0	24	0
5	B	144	0	0	32	0
5	E	152	0	0	24	0
5	F	143	0	0	23	0
5	U	270	0	0	37	0
5	W	267	0	0	35	0
5	X	273	0	0	50	0
5	Y	310	0	0	46	0
All	All	15104	0	13211	762	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (762) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:184:CYS:HB2	5:W:321:HOH:O	1.50	1.08
2:U:251:ASN:HB2	2:U:252:PRO:HD3	1.36	1.06
2:Y:251:ASN:HB2	2:Y:252:PRO:HD3	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:251:ASN:HB2	2:W:252:PRO:HD3	1.37	1.06
2:X:251:ASN:HB2	2:X:252:PRO:HD3	1.35	1.03
1:B:48:MET:HB3	5:B:195:HOH:O	1.59	1.02
2:W:150:ILE:HD12	2:W:151:GLU:H	1.22	1.00
2:X:150:ILE:HD12	2:X:151:GLU:H	1.24	1.00
2:U:150:ILE:HD12	2:U:151:GLU:H	1.31	0.96
1:A:66:ILE:HG23	1:A:67:SER:H	1.31	0.96
1:F:19:VAL:HA	5:F:233:HOH:O	1.65	0.96
2:X:219:GLU:HB2	2:X:222:HIS:CE1	2.01	0.96
1:F:66:ILE:HG23	1:F:67:SER:H	1.30	0.95
2:U:200:LYS:HB3	5:U:331:HOH:O	1.66	0.94
2:U:184:CYS:HB2	5:U:331:HOH:O	1.65	0.94
1:A:8:VAL:HB	5:A:162:HOH:O	1.66	0.93
1:E:66:ILE:HG23	1:E:67:SER:H	1.32	0.93
1:A:76:ILE:HG13	5:A:261:HOH:O	1.67	0.92
2:X:53:THR:HG23	5:X:390:HOH:O	1.67	0.92
2:Y:150:ILE:HD12	2:Y:151:GLU:H	1.33	0.92
2:W:229:THR:HG22	2:W:281:SER:HA	1.53	0.91
1:B:66:ILE:HG23	1:B:67:SER:H	1.33	0.90
2:Y:229:THR:HG22	2:Y:281:SER:HA	1.54	0.90
2:U:146:GLN:OE1	2:U:195:TRP:CZ2	2.27	0.88
2:X:229:THR:HG22	2:X:281:SER:HA	1.56	0.87
2:U:110:VAL:HG21	5:U:415:HOH:O	1.73	0.87
2:W:200:LYS:HB3	5:W:321:HOH:O	1.75	0.87
2:U:229:THR:HG22	2:U:281:SER:HA	1.58	0.86
2:X:236:ILE:N	2:X:236:ILE:HD12	1.91	0.85
2:W:150:ILE:HD12	2:W:151:GLU:N	1.91	0.84
2:Y:150:ILE:HG21	5:Y:624:HOH:O	1.78	0.83
2:X:125:LEU:HD21	2:X:135:VAL:HA	1.58	0.83
2:Y:56:LEU:HG	5:Y:368:HOH:O	1.78	0.83
2:U:150:ILE:HD12	2:U:151:GLU:N	1.94	0.81
1:A:75:ILE:HB	5:A:261:HOH:O	1.81	0.81
2:X:276:GLU:HB2	5:X:511:HOH:O	1.82	0.80
1:F:22:LEU:HB2	5:F:233:HOH:O	1.80	0.80
2:W:157:LEU:HG	5:W:474:HOH:O	1.82	0.79
2:X:41:PRO:HD2	5:X:498:HOH:O	1.83	0.79
1:E:14:ASP:HB3	1:E:75:ILE:HD12	1.64	0.79
1:A:14:ASP:HB3	1:A:75:ILE:HD12	1.65	0.79
2:X:207:GLU:H	2:X:207:GLU:CD	1.87	0.78
2:U:138:PRO:HD3	2:U:169:ALA:O	1.82	0.78
2:X:310:VAL:HG12	5:X:397:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:HB3	1:B:75:ILE:HD12	1.65	0.78
2:X:150:ILE:HD12	2:X:151:GLU:N	2.00	0.77
1:F:14:ASP:HB3	1:F:75:ILE:HD12	1.66	0.77
2:U:260:VAL:HG11	2:U:276:GLU:HG3	1.66	0.77
1:A:76:ILE:HG22	5:A:199:HOH:O	1.84	0.77
1:E:99:LYS:HB3	2:U:77:GLU:HB3	1.66	0.76
2:W:260:VAL:HG11	2:W:276:GLU:HG3	1.67	0.76
1:A:6:ASN:HD22	1:A:6:ASN:N	1.83	0.76
1:F:130:MET:HE1	5:F:165:HOH:O	1.85	0.75
2:Y:125:LEU:HD13	2:Y:203:LEU:HB2	1.68	0.75
1:F:33:VAL:HB	5:F:273:HOH:O	1.86	0.74
2:Y:260:VAL:HG11	2:Y:276:GLU:HG3	1.69	0.74
2:U:185:VAL:HG12	5:U:574:HOH:O	1.86	0.74
2:W:174:LYS:HE2	5:W:417:HOH:O	1.87	0.74
2:W:172:THR:HB	5:W:417:HOH:O	1.86	0.74
1:E:97:ASN:OD1	2:U:75:MET:HG2	1.88	0.74
2:X:219:GLU:CB	2:X:222:HIS:CE1	2.71	0.73
2:U:125:LEU:HD13	2:U:203:LEU:HB2	1.71	0.73
2:X:260:VAL:HG11	2:X:276:GLU:HG3	1.71	0.72
1:E:6:ASN:N	1:E:6:ASN:HD22	1.87	0.72
2:Y:213:PRO:HB3	5:Y:383:HOH:O	1.89	0.72
2:Y:121:VAL:HG12	2:Y:122:GLY:N	2.04	0.72
2:W:206:ARG:HA	5:W:493:HOH:O	1.89	0.72
1:B:6:ASN:N	1:B:6:ASN:HD22	1.87	0.72
1:A:66:ILE:HG23	1:A:67:SER:N	2.05	0.72
1:F:66:ILE:HG23	1:F:67:SER:N	2.04	0.72
2:Y:236:ILE:HD12	2:Y:236:ILE:N	2.05	0.72
2:W:236:ILE:HD12	2:W:236:ILE:N	2.05	0.72
2:Y:121:VAL:HG12	2:Y:122:GLY:H	1.54	0.71
2:X:139:LEU:HB3	5:X:455:HOH:O	1.90	0.71
2:Y:70:THR:HG21	5:Y:340:HOH:O	1.90	0.70
1:B:139:VAL:HG12	1:B:140:LEU:H	1.56	0.70
1:E:23:PRO:HD3	5:E:182:HOH:O	1.91	0.70
2:U:261:LYS:HE2	2:U:261:LYS:HA	1.73	0.70
2:U:54:LEU:HD21	5:U:415:HOH:O	1.91	0.70
2:Y:40:HIS:O	2:Y:42:ALA:N	2.25	0.70
2:U:236:ILE:N	2:U:236:ILE:HD12	2.06	0.70
1:F:78:LYS:HE3	2:W:266:HIS:O	1.92	0.70
2:Y:150:ILE:HD12	2:Y:151:GLU:N	2.06	0.70
2:Y:183:LEU:HD21	5:Y:350:HOH:O	1.91	0.70
2:U:207:GLU:CD	2:U:207:GLU:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLY:C	1:A:6:ASN:HD22	1.97	0.69
1:E:66:ILE:HG23	1:E:67:SER:N	2.08	0.69
2:U:102:ASN:HB3	5:U:360:HOH:O	1.93	0.69
2:W:93:THR:HA	5:W:539:HOH:O	1.93	0.69
2:Y:261:LYS:HE2	2:Y:261:LYS:HA	1.74	0.69
2:X:292:MET:HE2	5:X:497:HOH:O	1.94	0.68
2:U:125:LEU:HB3	2:U:203:LEU:HA	1.76	0.68
2:X:142:PRO:HD2	5:X:501:HOH:O	1.93	0.68
2:W:136:ARG:HD3	5:W:381:HOH:O	1.94	0.68
2:U:243:VAL:HB	5:U:363:HOH:O	1.94	0.68
2:X:118:LEU:HD22	5:X:455:HOH:O	1.93	0.67
2:W:125:LEU:HD13	2:W:203:LEU:HB2	1.75	0.67
2:U:79:LYS:HE2	5:U:494:HOH:O	1.94	0.67
2:W:139:LEU:HD23	2:W:139:LEU:H	1.58	0.67
2:U:220:THR:HG23	5:U:481:HOH:O	1.94	0.67
1:E:99:LYS:HB3	2:U:77:GLU:CB	2.25	0.67
1:E:113:GLU:HB2	5:E:211:HOH:O	1.94	0.67
1:F:17:LYS:HD2	5:F:248:HOH:O	1.95	0.66
2:Y:139:LEU:HD23	2:Y:139:LEU:H	1.60	0.66
2:Y:139:LEU:HD23	2:Y:139:LEU:N	2.10	0.66
2:U:134:LEU:HD13	2:U:136:ARG:HG2	1.77	0.66
2:X:141:ASP:HB2	5:X:319:HOH:O	1.95	0.66
2:U:37:PRO:HB3	2:U:98:CYS:SG	2.36	0.66
2:W:139:LEU:HD23	2:W:139:LEU:N	2.10	0.66
1:B:106:GLU:HA	5:B:227:HOH:O	1.95	0.66
2:U:278:LEU:HD23	5:U:386:HOH:O	1.95	0.66
2:U:56:LEU:HD21	5:U:415:HOH:O	1.96	0.66
2:W:261:LYS:HE2	2:W:261:LYS:HA	1.77	0.66
2:X:236:ILE:N	2:X:236:ILE:CD1	2.59	0.66
1:B:5:GLY:C	1:B:6:ASN:HD22	1.99	0.66
5:U:543:HOH:O	3:I:2:NAG:H61	1.95	0.66
1:B:66:ILE:HG23	1:B:67:SER:N	2.09	0.66
2:Y:196:LEU:HG	5:Y:617:HOH:O	1.97	0.65
2:U:206:ARG:HG3	5:U:375:HOH:O	1.95	0.65
2:Y:207:GLU:CD	2:Y:207:GLU:H	1.98	0.65
2:U:40:HIS:O	2:U:42:ALA:N	2.29	0.65
2:X:261:LYS:HA	2:X:261:LYS:HE2	1.79	0.65
1:E:99:LYS:HD3	2:U:77:GLU:OE1	1.96	0.65
2:U:230:PHE:HB2	5:U:351:HOH:O	1.96	0.65
1:A:69:GLY:HA3	5:B:261:HOH:O	1.95	0.64
1:E:63:PHE:HE2	5:F:154:HOH:O	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:54:LEU:HD11	5:Y:560:HOH:O	1.95	0.64
2:Y:292:MET:HE2	5:Y:407:HOH:O	1.97	0.64
2:U:129:GLU:HB3	2:U:208:ALA:HB2	1.79	0.64
2:W:257:ILE:HD12	2:W:258:ALA:H	1.62	0.64
5:B:155:HOH:O	2:Y:74:GLU:HA	1.97	0.64
2:Y:40:HIS:HA	5:Y:315:HOH:O	1.97	0.64
2:Y:251:ASN:CB	2:Y:252:PRO:HD3	2.20	0.64
1:A:66:ILE:C	1:A:66:ILE:HD12	2.18	0.64
2:X:40:HIS:O	2:X:42:ALA:N	2.30	0.64
2:Y:110:VAL:HG21	5:Y:560:HOH:O	1.98	0.64
2:Y:157:LEU:HG	5:Y:350:HOH:O	1.95	0.64
2:W:151:GLU:HG2	2:W:155:LYS:HB2	1.80	0.64
1:B:66:ILE:HD12	1:B:66:ILE:C	2.19	0.64
1:B:99:LYS:HD3	2:Y:77:GLU:OE1	1.98	0.64
1:E:66:ILE:C	1:E:66:ILE:HD12	2.18	0.64
2:Y:163:PHE:HB3	5:Y:486:HOH:O	1.97	0.64
2:U:131:SER:HB2	5:U:330:HOH:O	1.98	0.64
2:X:139:LEU:N	2:X:139:LEU:HD23	2.12	0.64
2:U:41:PRO:HD3	5:U:476:HOH:O	1.97	0.64
2:W:62:ASP:HB2	2:W:100:ASN:HD21	1.63	0.64
2:X:139:LEU:HD23	2:X:139:LEU:H	1.62	0.63
2:Y:46:LEU:C	2:Y:46:LEU:HD23	2.17	0.63
2:U:36:PRO:HG2	5:U:484:HOH:O	1.96	0.63
2:Y:151:GLU:HG2	2:Y:155:LYS:HB2	1.79	0.63
2:W:251:ASN:CB	2:W:252:PRO:HD3	2.23	0.63
1:E:82:ILE:HA	5:E:154:HOH:O	1.99	0.63
1:F:66:ILE:C	1:F:66:ILE:HD12	2.18	0.63
2:W:124:PRO:HB2	2:W:126:PHE:CE1	2.33	0.63
2:Y:151:GLU:N	2:Y:157:LEU:HD11	2.14	0.63
2:X:151:GLU:N	2:X:157:LEU:HD11	2.14	0.63
2:X:221:SER:C	2:X:222:HIS:ND1	2.52	0.63
2:U:253:GLN:HG2	2:U:254:PRO:HD2	1.81	0.63
1:A:130:MET:HG3	5:A:308:HOH:O	1.98	0.63
1:E:6:ASN:N	1:E:6:ASN:ND2	2.46	0.63
1:B:81:LYS:HB3	5:B:148:HOH:O	1.99	0.62
1:E:33:VAL:HG13	5:E:236:HOH:O	1.99	0.62
1:E:132:ALA:HB1	5:E:215:HOH:O	1.98	0.62
2:X:253:GLN:HG2	2:X:254:PRO:HD2	1.80	0.62
2:U:139:LEU:N	2:U:139:LEU:HD23	2.14	0.62
2:Y:305:THR:HG23	5:Y:407:HOH:O	1.99	0.62
3:I:2:NAG:H3	3:I:2:NAG:H82	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:250:MET:HB3	5:X:471:HOH:O	1.99	0.62
1:A:98:ILE:HG12	5:A:215:HOH:O	1.98	0.62
1:A:121:ARG:HD2	5:A:193:HOH:O	2.00	0.62
1:E:13:LYS:HE2	5:E:272:HOH:O	1.98	0.62
2:X:62:ASP:HB2	2:X:100:ASN:HD21	1.65	0.62
2:W:40:HIS:O	2:W:42:ALA:N	2.32	0.61
2:W:243:VAL:HB	5:W:458:HOH:O	2.00	0.61
2:W:120:LEU:HB2	2:W:138:PRO:HG2	1.80	0.61
1:A:143:HIS:C	1:A:145:HIS:H	2.04	0.61
1:F:117:SER:HA	5:F:261:HOH:O	1.99	0.61
2:U:151:GLU:N	2:U:157:LEU:HD11	2.15	0.61
1:A:37:ASP:HA	5:A:240:HOH:O	2.00	0.61
2:X:244:ASN:HB2	5:X:583:HOH:O	1.99	0.61
2:W:253:GLN:HG2	2:W:254:PRO:HD2	1.82	0.61
1:B:98:ILE:HD12	5:B:192:HOH:O	2.01	0.61
2:X:209:ILE:HG21	2:X:298:THR:OG1	2.00	0.61
2:X:140:THR:HA	5:X:371:HOH:O	2.01	0.61
2:U:121:VAL:HG12	2:U:122:GLY:N	2.15	0.61
1:B:66:ILE:HD13	5:B:200:HOH:O	1.99	0.61
1:B:103:LYS:HD3	5:B:265:HOH:O	2.00	0.61
2:U:100:ASN:HB3	5:U:360:HOH:O	2.01	0.61
1:E:127:LYS:HB3	5:E:188:HOH:O	2.00	0.61
2:W:98:CYS:HA	5:W:434:HOH:O	1.99	0.61
5:A:200:HOH:O	1:B:71:SER:HB2	2.01	0.60
2:Y:243:VAL:HG23	2:Y:274:ARG:HH21	1.66	0.60
1:A:21:ASN:ND2	1:B:21:ASN:ND2	2.49	0.60
2:X:62:ASP:HB3	2:X:101:SER:HB3	1.83	0.60
2:X:151:GLU:HG2	2:X:155:LYS:HB2	1.83	0.60
2:Y:102:ASN:HB2	5:Y:452:HOH:O	2.01	0.60
2:U:151:GLU:HG2	2:U:155:LYS:HB2	1.82	0.60
2:W:112:VAL:HG23	5:W:539:HOH:O	2.02	0.60
2:W:257:ILE:HD12	2:W:258:ALA:N	2.15	0.60
1:A:21:ASN:HD21	1:B:21:ASN:ND2	2.00	0.60
2:U:232:VAL:HB	5:U:386:HOH:O	2.00	0.60
2:W:117:LYS:HE2	2:W:120:LEU:HD23	1.82	0.60
2:X:251:ASN:CB	2:X:252:PRO:HD3	2.21	0.60
4:L:1:NAG:O3	4:L:2:NAG:H2	2.01	0.60
1:B:48:MET:HE2	5:B:157:HOH:O	2.01	0.60
2:U:251:ASN:CB	2:U:252:PRO:HD3	2.22	0.60
2:X:243:VAL:HG23	2:X:274:ARG:HH21	1.67	0.60
2:Y:273:GLU:HG2	5:Y:561:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:243:VAL:HG23	2:U:274:ARG:HH21	1.66	0.60
2:W:59:ILE:N	2:W:59:ILE:HD13	2.17	0.59
2:W:124:PRO:HB2	2:W:126:PHE:HE1	1.66	0.59
2:W:138:PRO:HD3	5:W:569:HOH:O	2.00	0.59
2:W:292:MET:HE2	2:W:303:ASN:HD22	1.67	0.59
2:Y:223:LEU:HD13	2:Y:309:LYS:HG3	1.84	0.59
2:U:145:SER:HA	5:U:435:HOH:O	2.01	0.59
1:A:143:HIS:H	1:A:143:HIS:CD2	2.20	0.59
1:E:139:VAL:HG12	1:E:141:SER:H	1.66	0.59
2:W:149:LEU:HG	2:W:171:ILE:HG21	1.85	0.59
2:W:243:VAL:HG23	2:W:274:ARG:HH21	1.67	0.59
1:B:114:GLU:HA	5:B:255:HOH:O	2.03	0.59
2:W:62:ASP:HB3	2:W:101:SER:HB3	1.84	0.59
1:A:98:ILE:HG22	1:A:99:LYS:HG2	1.85	0.59
2:X:249:LYS:HE3	5:X:405:HOH:O	2.00	0.59
2:W:292:MET:CE	2:W:303:ASN:HD22	2.15	0.59
1:B:129:PHE:HA	5:B:173:HOH:O	2.02	0.59
2:Y:253:GLN:HG2	2:Y:254:PRO:HD2	1.85	0.59
2:U:258:ALA:HA	5:U:400:HOH:O	2.02	0.59
1:F:112:PRO:HB3	5:F:233:HOH:O	2.02	0.59
2:X:129:GLU:HB3	2:X:208:ALA:HB2	1.85	0.58
1:E:46:ARG:HB3	5:E:276:HOH:O	2.04	0.58
2:Y:46:LEU:HD23	2:Y:47:ILE:N	2.18	0.58
2:U:143:GLN:HA	5:U:559:HOH:O	2.03	0.58
2:X:219:GLU:OE2	2:X:222:HIS:CG	2.57	0.58
2:X:100:ASN:HD22	2:X:101:SER:H	1.52	0.58
2:Y:62:ASP:HB2	2:Y:100:ASN:HD21	1.68	0.58
1:F:98:ILE:HG22	1:F:99:LYS:HG2	1.85	0.58
2:Y:62:ASP:HB3	2:Y:101:SER:HB3	1.85	0.58
2:U:129:GLU:HB3	2:U:208:ALA:CB	2.34	0.58
1:B:98:ILE:HG22	1:B:99:LYS:HG2	1.85	0.58
2:U:224:LEU:O	2:U:310:VAL:HG22	2.04	0.58
1:F:133:SER:HB2	5:F:245:HOH:O	2.04	0.58
2:Y:178:ARG:HH12	2:Y:239:VAL:HG11	1.69	0.58
2:W:117:LYS:HE2	2:W:120:LEU:CD2	2.33	0.58
2:W:251:ASN:HB2	2:W:252:PRO:CD	2.24	0.58
2:Y:84:ILE:HG12	5:Y:606:HOH:O	2.03	0.57
1:B:78:LYS:HE3	2:Y:266:HIS:O	2.04	0.57
2:Y:223:LEU:N	2:Y:223:LEU:HD23	2.19	0.57
1:A:123:ILE:HD12	5:A:162:HOH:O	2.03	0.57
2:W:76:VAL:HG11	5:W:387:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:151:GLU:N	2:W:157:LEU:HD11	2.18	0.57
2:X:46:LEU:C	2:X:46:LEU:HD23	2.25	0.57
2:U:46:LEU:HD23	2:U:46:LEU:C	2.25	0.57
2:X:253:GLN:HA	5:X:383:HOH:O	2.04	0.57
1:E:98:ILE:HG22	1:E:99:LYS:HG2	1.86	0.57
2:X:223:LEU:HD13	2:X:309:LYS:HG3	1.85	0.57
2:U:223:LEU:N	2:U:223:LEU:HD23	2.19	0.57
2:W:164:VAL:HB	5:W:417:HOH:O	2.03	0.57
2:U:54:LEU:HD11	5:U:415:HOH:O	2.04	0.57
2:W:46:LEU:C	2:W:46:LEU:HD23	2.24	0.57
2:W:174:LYS:HD2	5:W:570:HOH:O	2.03	0.57
2:X:223:LEU:HD23	2:X:223:LEU:N	2.18	0.57
2:Y:251:ASN:HB2	2:Y:252:PRO:CD	2.22	0.57
2:Y:59:ILE:N	2:Y:59:ILE:HD13	2.19	0.57
2:Y:149:LEU:HG	2:Y:171:ILE:HG21	1.86	0.57
2:W:128:LYS:HE2	5:W:469:HOH:O	2.05	0.57
2:X:183:LEU:HD12	5:X:350:HOH:O	2.03	0.57
2:Y:257:ILE:HD12	2:Y:258:ALA:H	1.70	0.57
2:W:46:LEU:HD23	2:W:47:ILE:N	2.20	0.56
2:W:211:ALA:HA	5:W:385:HOH:O	2.04	0.56
1:F:94:ALA:HB1	5:F:267:HOH:O	2.04	0.56
2:X:251:ASN:HB2	2:X:252:PRO:CD	2.23	0.56
1:F:22:LEU:HD12	5:F:233:HOH:O	2.05	0.56
2:W:224:LEU:O	2:W:310:VAL:HG22	2.05	0.56
2:W:229:THR:CG2	2:W:281:SER:HA	2.30	0.56
1:A:99:LYS:HD3	5:X:391:HOH:O	2.04	0.56
1:E:99:LYS:N	2:U:75:MET:O	2.37	0.56
2:Y:121:VAL:CG1	2:Y:122:GLY:H	2.19	0.56
1:E:97:ASN:HB3	1:E:100:GLU:OE1	2.05	0.56
1:A:67:SER:HB2	5:A:253:HOH:O	2.06	0.56
2:U:118:LEU:HD13	2:U:119:PHE:CE1	2.41	0.56
2:W:292:MET:HE2	5:W:422:HOH:O	2.05	0.56
1:E:78:LYS:HE3	2:U:266:HIS:O	2.06	0.56
2:Y:224:LEU:O	2:Y:310:VAL:HG22	2.06	0.56
2:U:62:ASP:HB2	2:U:100:ASN:HD21	1.70	0.56
2:W:223:LEU:N	2:W:223:LEU:HD23	2.21	0.56
5:Y:384:HOH:O	3:G:1:NAG:H61	2.05	0.55
2:W:223:LEU:HD13	2:W:309:LYS:HG3	1.88	0.55
2:Y:88:ALA:HA	5:Y:330:HOH:O	2.06	0.55
2:U:100:ASN:HD22	2:U:101:SER:H	1.53	0.55
1:B:97:ASN:HB3	1:B:100:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:SER:HB3	5:E:258:HOH:O	2.06	0.55
1:B:33:VAL:HG12	5:B:196:HOH:O	2.06	0.55
1:B:105:PRO:HD2	5:B:201:HOH:O	2.06	0.55
2:U:292:MET:CE	2:U:303:ASN:HD22	2.20	0.55
2:U:46:LEU:HD23	2:U:47:ILE:N	2.22	0.55
2:X:229:THR:CG2	2:X:281:SER:HA	2.33	0.55
2:Y:100:ASN:HD22	2:Y:101:SER:H	1.54	0.55
2:W:83:TRP:HE1	2:W:85:GLN:HE22	1.55	0.55
1:E:22:LEU:HA	5:E:182:HOH:O	2.07	0.55
5:X:582:HOH:O	4:D:2:NAG:H83	2.06	0.55
2:W:213:PRO:HG3	2:W:297:ASN:ND2	2.21	0.55
1:F:97:ASN:HB3	1:F:100:GLU:OE1	2.07	0.55
2:U:139:LEU:HD23	2:U:139:LEU:H	1.72	0.55
1:F:82:ILE:HA	5:F:204:HOH:O	2.05	0.55
2:U:223:LEU:HD13	2:U:309:LYS:HG3	1.88	0.55
2:X:139:LEU:HD12	2:X:141:ASP:O	2.07	0.54
2:U:62:ASP:HB3	2:U:101:SER:HB3	1.90	0.54
2:U:251:ASN:HB2	2:U:252:PRO:CD	2.23	0.54
2:X:229:THR:HG22	2:X:282:SER:H	1.73	0.54
2:X:280:ILE:HA	5:X:481:HOH:O	2.07	0.54
2:Y:159:THR:HA	5:Y:458:HOH:O	2.07	0.54
2:W:100:ASN:HD22	2:W:101:SER:H	1.55	0.54
1:A:78:LYS:HE3	2:X:266:HIS:O	2.07	0.54
2:U:150:ILE:HG21	5:U:521:HOH:O	2.07	0.54
2:X:236:ILE:CD1	5:X:511:HOH:O	2.56	0.54
2:X:261:LYS:HG3	5:X:495:HOH:O	2.06	0.54
1:A:26:TYR:O	1:A:112:PRO:HD3	2.07	0.54
2:W:207:GLU:CD	2:W:207:GLU:H	2.11	0.54
1:B:137:ASP:HB3	5:B:203:HOH:O	2.08	0.53
1:B:98:ILE:HG23	5:Y:455:HOH:O	2.06	0.53
2:X:292:MET:HE2	2:X:303:ASN:HD22	1.73	0.53
2:X:292:MET:CE	2:X:303:ASN:HD22	2.21	0.53
2:U:222:HIS:HD2	5:U:561:HOH:O	1.90	0.53
2:W:150:ILE:HD11	5:W:516:HOH:O	2.07	0.53
2:W:236:ILE:N	2:W:236:ILE:CD1	2.71	0.53
5:W:376:HOH:O	4:L:3:MAN:H3	2.08	0.53
2:X:276:GLU:OE1	2:X:276:GLU:HA	2.09	0.53
1:A:21:ASN:ND2	1:B:21:ASN:HD21	2.06	0.53
2:X:87:LYS:HD3	5:X:362:HOH:O	2.09	0.53
2:X:226:LYS:HB3	5:X:397:HOH:O	2.07	0.53
2:Y:225:LYS:HB2	5:Y:355:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:222:HIS:ND1	2:X:222:HIS:N	2.57	0.53
2:Y:54:LEU:HD11	2:Y:56:LEU:HD21	1.90	0.53
2:Y:236:ILE:N	2:Y:236:ILE:CD1	2.72	0.53
4:H:2:NAG:H82	4:H:2:NAG:H3	1.90	0.53
2:Y:229:THR:HG22	2:Y:282:SER:H	1.74	0.53
2:X:254:PRO:HD3	5:X:383:HOH:O	2.09	0.53
2:Y:211:ALA:HA	5:Y:562:HOH:O	2.09	0.53
2:X:257:ILE:HD12	2:X:258:ALA:H	1.74	0.53
2:X:92:ARG:HG3	5:X:367:HOH:O	2.08	0.53
1:B:69:GLY:HA3	5:B:225:HOH:O	2.08	0.52
1:B:103:LYS:HA	5:B:265:HOH:O	2.08	0.52
2:Y:130:ASP:HA	5:Y:548:HOH:O	2.08	0.52
2:Y:229:THR:CG2	2:Y:281:SER:HA	2.33	0.52
1:A:27:MET:HB3	1:A:109:SER:HB2	1.90	0.52
2:X:209:ILE:HG23	2:X:209:ILE:O	2.10	0.52
2:Y:173:ILE:HA	5:Y:486:HOH:O	2.09	0.52
1:A:133:SER:HB3	5:A:213:HOH:O	2.08	0.52
1:E:140:LEU:HB2	5:E:270:HOH:O	2.09	0.52
2:Y:276:GLU:OE1	2:Y:276:GLU:HA	2.09	0.52
1:F:23:PRO:HD3	5:F:154:HOH:O	2.10	0.52
2:X:46:LEU:HD23	2:X:47:ILE:N	2.24	0.52
2:X:220:THR:HA	5:X:543:HOH:O	2.10	0.52
1:E:26:TYR:O	1:E:112:PRO:HD3	2.09	0.52
2:X:303:ASN:HB2	5:X:497:HOH:O	2.09	0.52
1:B:26:TYR:O	1:B:112:PRO:HD3	2.10	0.52
2:X:254:PRO:HB3	5:X:471:HOH:O	2.10	0.52
2:Y:180:TYR:O	2:Y:181:HIS:C	2.47	0.52
1:F:27:MET:HB3	1:F:109:SER:HB2	1.91	0.52
2:X:83:TRP:HE1	2:X:85:GLN:HE22	1.58	0.52
1:A:95:PRO:HG2	5:A:178:HOH:O	2.08	0.52
1:E:27:MET:HB3	1:E:109:SER:HB2	1.91	0.52
2:X:211:ALA:HB1	5:X:404:HOH:O	2.08	0.52
2:Y:121:VAL:CG1	2:Y:122:GLY:N	2.71	0.52
2:Y:158:PRO:HD3	5:Y:325:HOH:O	2.10	0.52
2:U:121:VAL:CG1	2:U:122:GLY:N	2.73	0.51
2:X:174:LYS:HG2	5:X:410:HOH:O	2.10	0.51
2:Y:139:LEU:HB3	5:Y:341:HOH:O	2.09	0.51
2:U:65:ARG:NH1	2:U:77:GLU:OE2	2.44	0.51
5:A:202:HOH:O	1:B:66:ILE:HG21	2.10	0.51
2:X:54:LEU:HD11	2:X:56:LEU:HD21	1.92	0.51
2:W:151:GLU:HG2	2:W:155:LYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:N	1:A:6:ASN:ND2	2.55	0.51
1:B:27:MET:HB3	1:B:109:SER:HB2	1.93	0.51
2:X:149:LEU:HG	2:X:171:ILE:HG21	1.91	0.51
2:W:276:GLU:OE1	2:W:276:GLU:HA	2.11	0.51
1:E:14:ASP:CB	1:E:75:ILE:HD12	2.38	0.51
2:W:151:GLU:CG	2:W:155:LYS:H	2.23	0.51
2:U:212:ILE:H	2:U:212:ILE:HD12	1.76	0.51
2:W:111:PHE:CG	2:W:142:PRO:HD3	2.46	0.51
2:Y:70:THR:HG22	2:Y:71:TYR:N	2.25	0.51
2:Y:83:TRP:HE1	2:Y:85:GLN:HE22	1.58	0.51
2:Y:139:LEU:HD13	5:Y:341:HOH:O	2.11	0.51
1:A:18:LEU:HG	5:A:261:HOH:O	2.11	0.51
2:W:54:LEU:HD11	2:W:56:LEU:HD21	1.93	0.51
1:E:103:LYS:HB3	5:E:168:HOH:O	2.10	0.51
1:F:66:ILE:CG2	1:F:67:SER:H	2.13	0.51
2:X:56:LEU:N	2:X:56:LEU:HD22	2.26	0.51
2:X:235:THR:C	2:X:236:ILE:HD12	2.31	0.51
2:Y:118:LEU:HD12	2:Y:119:PHE:CE1	2.46	0.50
1:A:70:LEU:HD22	1:A:75:ILE:HD11	1.93	0.50
1:A:71:SER:HB2	5:A:211:HOH:O	2.10	0.50
2:X:224:LEU:O	2:X:310:VAL:HG22	2.10	0.50
2:U:37:PRO:CB	2:U:98:CYS:SG	3.00	0.50
1:F:14:ASP:CB	1:F:75:ILE:HD12	2.38	0.50
2:U:276:GLU:HA	2:U:276:GLU:OE1	2.11	0.50
1:B:59:LEU:HD22	1:B:63:PHE:HE1	1.76	0.50
1:B:113:GLU:HB2	5:B:213:HOH:O	2.11	0.50
2:U:229:THR:CG2	2:U:281:SER:HA	2.35	0.50
2:U:236:ILE:N	2:U:236:ILE:CD1	2.72	0.50
2:W:134:LEU:HD13	2:W:136:ARG:HG2	1.93	0.50
2:U:149:LEU:HG	2:U:171:ILE:HG21	1.94	0.50
2:U:250:MET:HB3	5:U:324:HOH:O	2.11	0.50
2:W:67:THR:HG21	5:W:366:HOH:O	2.11	0.50
1:F:26:TYR:O	1:F:112:PRO:HD3	2.12	0.50
1:F:67:SER:HB2	5:F:175:HOH:O	2.12	0.50
2:X:212:ILE:HD12	2:X:212:ILE:N	2.26	0.50
2:X:292:MET:HG3	5:X:497:HOH:O	2.11	0.50
2:X:77:GLU:HB3	5:X:391:HOH:O	2.11	0.50
2:X:118:LEU:HD13	5:X:455:HOH:O	2.11	0.50
2:X:248:LEU:N	2:X:248:LEU:HD22	2.27	0.50
2:U:46:LEU:HD22	2:U:110:VAL:HG13	1.94	0.50
2:U:139:LEU:HD12	2:U:141:ASP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:191:ARG:O	2:U:192:ASP:HB2	2.12	0.50
1:E:70:LEU:HD22	1:E:75:ILE:HD11	1.95	0.49
2:X:273:GLU:HB2	5:X:411:HOH:O	2.11	0.49
2:U:146:GLN:OE1	2:U:195:TRP:HZ2	1.91	0.49
2:W:121:VAL:HG12	2:W:122:GLY:N	2.27	0.49
2:W:130:ASP:HA	5:W:351:HOH:O	2.10	0.49
1:A:142:HIS:ND1	1:A:142:HIS:N	2.58	0.49
1:E:98:ILE:HG12	5:E:180:HOH:O	2.13	0.49
2:X:253:GLN:HG2	2:X:254:PRO:CD	2.43	0.49
2:U:72:PHE:O	2:U:74:GLU:HG3	2.12	0.49
2:U:151:GLU:HG2	2:U:155:LYS:CB	2.43	0.49
2:U:297:ASN:HB3	2:U:299:PHE:H	1.77	0.49
2:W:65:ARG:NH1	2:W:77:GLU:OE2	2.45	0.49
1:E:29:THR:HB	5:E:217:HOH:O	2.11	0.49
5:Y:566:HOH:O	3:G:1:NAG:H81	2.11	0.49
2:U:38:SER:HB2	5:U:579:HOH:O	2.12	0.49
2:U:118:LEU:O	2:U:118:LEU:HD23	2.12	0.49
2:W:40:HIS:HA	5:W:315:HOH:O	2.13	0.49
2:U:180:TYR:O	2:U:181:HIS:C	2.49	0.49
2:W:304:VAL:HA	5:W:423:HOH:O	2.10	0.49
2:X:59:ILE:N	2:X:59:ILE:CD1	2.75	0.49
2:X:128:LYS:HE2	5:X:499:HOH:O	2.13	0.49
2:X:151:GLU:HG2	2:X:155:LYS:CB	2.42	0.49
2:W:219:GLU:OE2	2:W:222:HIS:HB3	2.13	0.49
1:E:59:LEU:HD22	1:E:63:PHE:HE1	1.77	0.49
1:F:70:LEU:HD22	1:F:75:ILE:HD11	1.95	0.49
2:Y:151:GLU:HG2	2:Y:155:LYS:CB	2.43	0.49
2:Y:219:GLU:OE2	2:Y:222:HIS:HB3	2.12	0.49
2:U:70:THR:HG22	2:U:71:TYR:N	2.28	0.49
2:W:151:GLU:HG2	2:W:155:LYS:CB	2.41	0.49
2:U:211:ALA:HA	5:U:418:HOH:O	2.12	0.49
1:B:66:ILE:CG2	1:B:67:SER:H	2.16	0.48
2:Y:257:ILE:HD12	2:Y:258:ALA:N	2.27	0.48
2:W:175:ASN:HB3	5:W:351:HOH:O	2.13	0.48
2:X:209:ILE:CG2	2:X:298:THR:OG1	2.61	0.48
2:U:229:THR:HG22	2:U:282:SER:H	1.77	0.48
2:X:65:ARG:NH1	2:X:77:GLU:OE2	2.46	0.48
2:U:212:ILE:HD12	2:U:212:ILE:N	2.28	0.48
2:Y:65:ARG:NH1	2:Y:77:GLU:OE2	2.47	0.48
2:Y:213:PRO:HG3	2:Y:297:ASN:ND2	2.28	0.48
2:W:292:MET:SD	4:L:1:NAG:H83	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:64:VAL:HG21	5:X:502:HOH:O	2.12	0.48
2:Y:152:CYS:HB2	2:Y:186:ARG:HG3	1.95	0.48
2:U:230:PHE:HE2	2:U:280:ILE:HG13	1.78	0.48
1:A:59:LEU:HD22	1:A:63:PHE:HE1	1.79	0.48
1:A:66:ILE:CG2	1:A:67:SER:H	2.13	0.48
1:E:66:ILE:CG2	1:E:67:SER:H	2.16	0.48
2:Y:129:GLU:HB3	2:Y:208:ALA:HB2	1.95	0.48
2:W:178:ARG:NH2	2:W:208:ALA:O	2.47	0.48
1:B:48:MET:HG3	5:B:157:HOH:O	2.14	0.48
2:U:219:GLU:OE2	2:U:222:HIS:HB3	2.12	0.48
2:W:162:THR:HA	5:W:532:HOH:O	2.13	0.48
2:W:248:LEU:HD22	2:W:248:LEU:N	2.29	0.48
2:W:260:VAL:HG21	5:W:499:HOH:O	2.14	0.48
1:A:66:ILE:C	1:A:66:ILE:CD1	2.82	0.48
1:B:6:ASN:N	1:B:6:ASN:ND2	2.59	0.48
2:U:54:LEU:HD11	2:U:56:LEU:HD21	1.95	0.48
2:U:257:ILE:HD12	2:U:258:ALA:H	1.79	0.48
2:W:229:THR:HG22	2:W:282:SER:H	1.77	0.48
1:B:41:SER:HB3	5:B:246:HOH:O	2.14	0.48
1:B:136:SER:HB3	5:B:266:HOH:O	2.12	0.48
2:X:243:VAL:O	2:X:274:ARG:NH2	2.47	0.48
2:Y:89:GLU:HB2	5:Y:550:HOH:O	2.13	0.48
2:Y:248:LEU:HD22	2:Y:248:LEU:N	2.29	0.48
2:U:248:LEU:N	2:U:248:LEU:HD22	2.28	0.48
2:W:139:LEU:HD12	2:W:141:ASP:O	2.14	0.48
1:B:66:ILE:C	1:B:66:ILE:CD1	2.82	0.48
2:X:120:LEU:HB2	2:X:138:PRO:HG2	1.94	0.48
2:Y:222:HIS:HD2	5:Y:517:HOH:O	1.96	0.48
2:W:252:PRO:HG3	5:W:563:HOH:O	2.12	0.48
2:W:267:ARG:HB2	2:W:271:ASN:ND2	2.28	0.48
1:B:48:MET:HE2	5:B:195:HOH:O	2.13	0.47
1:F:59:LEU:HD22	1:F:63:PHE:HE1	1.77	0.47
1:B:70:LEU:HD22	1:B:75:ILE:HD11	1.97	0.47
2:X:59:ILE:N	2:X:59:ILE:HD13	2.29	0.47
2:X:213:PRO:HG3	2:X:297:ASN:ND2	2.28	0.47
2:X:267:ARG:HB2	2:X:271:ASN:ND2	2.29	0.47
2:W:183:LEU:HD11	5:W:474:HOH:O	2.13	0.47
1:F:66:ILE:C	1:F:66:ILE:CD1	2.82	0.47
2:X:268:GLY:HA3	5:X:552:HOH:O	2.14	0.47
2:Y:286:ASP:HB2	5:Y:518:HOH:O	2.13	0.47
1:A:14:ASP:CB	1:A:75:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HB2	5:B:271:HOH:O	2.15	0.47
1:F:70:LEU:HD22	1:F:75:ILE:CD1	2.45	0.47
2:Y:292:MET:CE	2:Y:303:ASN:HD22	2.27	0.47
2:U:253:GLN:HG2	2:U:254:PRO:CD	2.43	0.47
1:A:70:LEU:HD22	1:A:75:ILE:CD1	2.45	0.47
1:A:98:ILE:HD13	5:X:544:HOH:O	2.14	0.47
1:E:66:ILE:C	1:E:66:ILE:CD1	2.82	0.47
2:X:70:THR:HG22	2:X:71:TYR:N	2.30	0.47
2:X:297:ASN:HB3	2:X:299:PHE:H	1.78	0.47
2:U:138:PRO:CD	2:U:169:ALA:O	2.58	0.47
2:W:72:PHE:O	2:W:74:GLU:N	2.48	0.47
1:E:49:VAL:HG12	1:E:87:VAL:CG2	2.45	0.47
1:F:49:VAL:HG12	1:F:87:VAL:CG2	2.45	0.47
2:Y:85:GLN:HG3	5:Y:454:HOH:O	2.15	0.47
2:U:59:ILE:CD1	2:U:59:ILE:N	2.78	0.47
2:W:253:GLN:HG2	2:W:254:PRO:CD	2.44	0.47
1:F:129:PHE:HD2	1:F:130:MET:HE3	1.80	0.47
2:Y:262:HIS:HA	5:Y:441:HOH:O	2.14	0.47
2:U:72:PHE:O	2:U:74:GLU:N	2.48	0.47
1:E:24:ASN:ND2	1:F:62:LYS:HA	2.30	0.47
2:Y:125:LEU:HB3	2:Y:203:LEU:HA	1.97	0.47
3:C:1:NAG:H61	3:C:2:NAG:O5	2.15	0.47
2:X:209:ILE:HD12	2:X:299:PHE:HB2	1.96	0.46
2:Y:120:LEU:HB2	2:Y:138:PRO:HG2	1.97	0.46
2:W:152:CYS:HB2	2:W:186:ARG:HG3	1.96	0.46
2:U:249:LYS:HD2	5:U:570:HOH:O	2.14	0.46
2:U:87:LYS:HG3	5:U:525:HOH:O	2.14	0.46
1:B:88:LEU:HD13	2:Y:206:ARG:HD3	1.96	0.46
1:E:70:LEU:HD22	1:E:75:ILE:CD1	2.46	0.46
2:X:69:LYS:HB3	5:X:574:HOH:O	2.16	0.46
2:X:139:LEU:HD22	2:X:147:TYR:CE1	2.51	0.46
2:Y:150:ILE:HD11	5:Y:588:HOH:O	2.15	0.46
2:Y:297:ASN:HB3	2:Y:299:PHE:H	1.81	0.46
2:U:115:PRO:HA	5:U:442:HOH:O	2.16	0.46
2:U:207:GLU:HB3	2:U:270:PHE:CD2	2.50	0.46
2:W:56:LEU:N	2:W:56:LEU:HD22	2.31	0.46
1:F:60:LEU:HD11	1:F:73:TYR:CD1	2.51	0.46
2:Y:129:GLU:O	2:Y:130:ASP:HB2	2.15	0.46
2:Y:197:HIS:CE1	5:Y:624:HOH:O	2.67	0.46
2:U:56:LEU:N	2:U:56:LEU:HD22	2.31	0.46
2:U:139:LEU:HD22	2:U:147:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ASP:CB	1:B:75:ILE:HD12	2.39	0.46
1:B:49:VAL:HG12	1:B:87:VAL:CG2	2.46	0.46
1:F:121:ARG:HD2	5:F:187:HOH:O	2.15	0.46
2:U:213:PRO:HG3	2:U:297:ASN:ND2	2.29	0.46
2:W:111:PHE:CD1	2:W:142:PRO:HD3	2.51	0.46
2:X:72:PHE:O	2:X:74:GLU:N	2.49	0.46
2:X:172:THR:HB	5:X:410:HOH:O	2.15	0.46
2:Y:267:ARG:HB2	2:Y:271:ASN:ND2	2.30	0.46
1:A:49:VAL:HG12	1:A:87:VAL:CG2	2.45	0.46
1:A:60:LEU:HB2	5:A:199:HOH:O	2.16	0.46
1:E:129:PHE:HD2	1:E:130:MET:HE3	1.81	0.46
2:Y:220:THR:HA	5:Y:577:HOH:O	2.16	0.46
2:W:125:LEU:HB3	2:W:203:LEU:HA	1.98	0.46
2:X:91:THR:HG23	5:X:356:HOH:O	2.15	0.46
2:X:209:ILE:HD13	2:X:210:LYS:N	2.31	0.46
2:W:37:PRO:HB3	2:W:98:CYS:SG	2.56	0.46
2:W:151:GLU:HG2	2:W:155:LYS:N	2.31	0.46
1:A:81:LYS:HD2	5:A:151:HOH:O	2.16	0.45
1:E:24:ASN:HD21	1:F:62:LYS:HA	1.80	0.45
2:X:230:PHE:HE2	2:X:280:ILE:HG13	1.82	0.45
2:Y:158:PRO:HB2	2:Y:161:LEU:HB2	1.98	0.45
2:W:199:ASP:HB2	5:W:361:HOH:O	2.16	0.45
1:A:129:PHE:HD2	1:A:130:MET:HE3	1.81	0.45
1:F:88:LEU:HB2	5:F:226:HOH:O	2.16	0.45
1:F:101:SER:N	1:F:102:PRO:HD3	2.31	0.45
5:F:210:HOH:O	2:W:73:ASN:HB3	2.16	0.45
2:X:209:ILE:HD13	2:X:209:ILE:C	2.36	0.45
2:X:305:THR:HG23	5:X:497:HOH:O	2.16	0.45
2:Y:253:GLN:HG2	2:Y:254:PRO:CD	2.46	0.45
2:W:129:GLU:HB3	2:W:208:ALA:HB2	1.98	0.45
1:B:103:LYS:HG3	5:B:182:HOH:O	2.15	0.45
2:Y:56:LEU:N	2:Y:56:LEU:HD22	2.32	0.45
2:Y:139:LEU:HD12	2:Y:141:ASP:O	2.16	0.45
2:W:58:CYS:C	2:W:59:ILE:HD13	2.37	0.45
1:E:101:SER:N	1:E:102:PRO:HD3	2.31	0.45
2:U:119:PHE:CD1	2:U:119:PHE:N	2.84	0.45
2:W:46:LEU:HD22	2:W:110:VAL:HG13	1.99	0.45
1:A:40:PRO:HG2	1:A:43:CYS:SG	2.57	0.45
1:A:142:HIS:HB2	1:A:146:HIS:CE1	2.51	0.45
1:B:70:LEU:HD22	1:B:75:ILE:CD1	2.47	0.45
1:F:131:VAL:HG11	5:F:166:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:209:ILE:HG22	5:X:361:HOH:O	2.15	0.45
2:Y:124:PRO:HB2	2:Y:126:PHE:CE1	2.52	0.45
2:X:257:ILE:HD12	2:X:258:ALA:N	2.30	0.45
1:A:66:ILE:HG23	5:A:253:HOH:O	2.16	0.45
1:B:101:SER:N	1:B:102:PRO:HD3	2.31	0.45
1:E:38:VAL:HG23	1:E:39:LEU:N	2.32	0.45
1:E:97:ASN:ND2	2:U:73:ASN:O	2.49	0.45
2:Y:291:PHE:HD1	5:Y:445:HOH:O	2.00	0.45
1:B:129:PHE:HD2	1:B:130:MET:CE	2.30	0.45
1:E:130:MET:H	1:E:130:MET:HG2	1.60	0.45
1:B:3:ILE:HA	5:B:286:HOH:O	2.18	0.44
1:E:3:ILE:HG22	1:E:3:ILE:O	2.17	0.44
1:E:70:LEU:HA	5:E:226:HOH:O	2.17	0.44
1:F:38:VAL:HG23	1:F:39:LEU:N	2.32	0.44
2:X:88:ALA:HA	5:X:352:HOH:O	2.16	0.44
2:X:129:GLU:O	2:X:130:ASP:HB2	2.17	0.44
2:Y:280:ILE:HA	5:Y:586:HOH:O	2.17	0.44
2:U:254:PRO:HB3	5:U:324:HOH:O	2.16	0.44
1:B:3:ILE:HG22	1:B:3:ILE:O	2.17	0.44
1:B:34:ALA:HB1	5:B:197:HOH:O	2.17	0.44
2:Y:72:PHE:O	2:Y:74:GLU:N	2.50	0.44
1:A:127:LYS:HG2	5:A:153:HOH:O	2.17	0.44
1:F:77:ASP:OD2	2:W:182:ARG:NH2	2.51	0.44
2:X:134:LEU:HD13	2:X:136:ARG:HG2	1.99	0.44
2:X:253:GLN:HB3	2:X:255:GLN:HE22	1.82	0.44
1:B:131:VAL:HG11	5:B:181:HOH:O	2.17	0.44
2:X:152:CYS:HB2	2:X:186:ARG:HG3	1.99	0.44
2:Y:257:ILE:HD11	5:Y:541:HOH:O	2.17	0.44
1:B:6:ASN:ND2	5:B:228:HOH:O	2.49	0.44
1:E:60:LEU:HD11	1:E:73:TYR:CD1	2.52	0.44
1:A:38:VAL:HG23	1:A:39:LEU:N	2.32	0.44
1:B:38:VAL:HG23	1:B:39:LEU:N	2.32	0.44
1:F:31:ASN:HB2	1:F:51:GLN:OE1	2.16	0.44
2:Y:184:CYS:HA	2:Y:201:PHE:O	2.18	0.44
2:U:108:ILE:HG23	2:U:108:ILE:O	2.18	0.44
2:W:212:ILE:N	2:W:212:ILE:HD12	2.32	0.44
2:W:213:PRO:HB3	5:W:393:HOH:O	2.18	0.44
5:F:199:HOH:O	2:W:181:HIS:HE1	2.01	0.44
2:X:151:GLU:HG2	2:X:155:LYS:H	1.81	0.44
2:X:191:ARG:O	2:X:192:ASP:HB2	2.17	0.44
2:Y:139:LEU:HD22	2:Y:147:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:230:PHE:HE1	5:Y:477:HOH:O	2.01	0.44
1:A:3:ILE:O	1:A:3:ILE:HG22	2.18	0.44
1:A:60:LEU:HD11	1:A:73:TYR:CD1	2.53	0.44
1:E:81:LYS:HD3	5:E:165:HOH:O	2.18	0.44
2:X:89:GLU:HB3	5:X:356:HOH:O	2.17	0.44
1:F:3:ILE:O	1:F:3:ILE:HG22	2.18	0.43
1:F:38:VAL:HG21	5:F:176:HOH:O	2.18	0.43
2:X:237:LYS:HB3	5:X:335:HOH:O	2.18	0.43
2:U:128:LYS:HE3	2:U:208:ALA:HA	1.99	0.43
2:U:244:ASN:O	2:U:295:ALA:HA	2.18	0.43
2:U:260:VAL:CG1	2:U:276:GLU:HG3	2.45	0.43
1:B:46:ARG:NH2	5:B:216:HOH:O	2.52	0.43
1:F:6:ASN:O	2:W:241:THR:HB	2.18	0.43
1:F:94:ALA:HA	1:F:95:PRO:HD3	1.87	0.43
2:X:128:LYS:HA	2:X:206:ARG:HB2	2.00	0.43
2:Y:54:LEU:HD13	2:Y:54:LEU:O	2.18	0.43
2:Y:118:LEU:O	2:Y:118:LEU:HD22	2.18	0.43
1:A:77:ASP:HA	5:A:199:HOH:O	2.18	0.43
1:B:31:ASN:HB2	1:B:51:GLN:OE1	2.18	0.43
2:U:192:ASP:N	5:U:425:HOH:O	2.48	0.43
2:X:212:ILE:HD12	2:X:212:ILE:H	1.83	0.43
2:W:206:ARG:HB3	5:W:439:HOH:O	2.18	0.43
1:A:49:VAL:HG12	1:A:87:VAL:HG23	2.01	0.43
1:A:129:PHE:HD2	1:A:130:MET:CE	2.31	0.43
1:E:31:ASN:HB2	1:E:51:GLN:OE1	2.18	0.43
1:F:129:PHE:HD2	1:F:130:MET:CE	2.31	0.43
2:X:237:LYS:HG2	5:X:411:HOH:O	2.17	0.43
2:Y:178:ARG:NH1	2:Y:239:VAL:HG11	2.33	0.43
2:U:234:CYS:HB2	2:U:247:TRP:CZ2	2.54	0.43
1:A:63:PHE:CZ	1:B:23:PRO:HG3	2.53	0.43
1:B:100:GLU:CG	5:B:155:HOH:O	2.66	0.43
1:E:129:PHE:HD2	1:E:130:MET:CE	2.31	0.43
2:Y:46:LEU:C	2:Y:46:LEU:CD2	2.85	0.43
2:W:260:VAL:CG1	2:W:276:GLU:HG3	2.45	0.43
1:E:49:VAL:HG12	1:E:87:VAL:HG23	2.00	0.43
1:E:97:ASN:O	2:U:75:MET:CG	2.67	0.43
2:X:100:ASN:HD22	2:X:101:SER:N	2.17	0.43
2:Y:292:MET:HE2	2:Y:303:ASN:HD22	1.84	0.43
2:U:128:LYS:HA	2:U:206:ARG:HB2	2.01	0.43
2:U:267:ARG:HB2	2:U:271:ASN:ND2	2.33	0.43
5:A:176:HOH:O	2:X:265:TRP:HZ3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:48:VAL:CG1	2:U:112:VAL:HG22	2.49	0.43
2:U:253:GLN:HG3	5:U:581:HOH:O	2.18	0.43
1:E:102:PRO:HA	5:E:239:HOH:O	2.18	0.42
2:X:151:GLU:CG	2:X:155:LYS:H	2.31	0.42
2:Y:58:CYS:C	2:Y:59:ILE:HD13	2.38	0.42
2:Y:243:VAL:O	2:Y:274:ARG:NH2	2.51	0.42
2:U:59:ILE:N	2:U:59:ILE:HD13	2.34	0.42
2:U:184:CYS:HA	2:U:201:PHE:O	2.19	0.42
2:X:174:LYS:HE2	5:X:410:HOH:O	2.19	0.42
2:Y:191:ARG:O	2:Y:192:ASP:HB2	2.18	0.42
2:U:121:VAL:CG1	2:U:122:GLY:H	2.32	0.42
2:W:297:ASN:HB3	2:W:299:PHE:H	1.83	0.42
1:F:49:VAL:HG12	1:F:87:VAL:HG23	1.99	0.42
2:W:177:LYS:HA	5:W:430:HOH:O	2.19	0.42
3:I:2:NAG:H62	3:I:3:FUL:H61	2.00	0.42
2:X:108:ILE:O	2:X:108:ILE:HG23	2.18	0.42
2:X:237:LYS:HD3	5:X:439:HOH:O	2.19	0.42
2:U:182:ARG:O	2:U:182:ARG:HG2	2.20	0.42
2:W:129:GLU:O	2:W:130:ASP:HB2	2.19	0.42
1:B:60:LEU:HD11	1:B:73:TYR:CD1	2.54	0.42
1:F:44:TRP:HB2	5:F:273:HOH:O	2.20	0.42
2:X:151:GLU:HG2	2:X:155:LYS:N	2.34	0.42
2:U:175:ASN:HB3	5:U:384:HOH:O	2.19	0.42
2:W:92:ARG:NH1	5:W:317:HOH:O	2.50	0.42
1:E:94:ALA:HA	1:E:95:PRO:HD3	1.85	0.42
2:Y:40:HIS:HD2	5:Y:401:HOH:O	2.01	0.42
2:U:83:TRP:HE1	2:U:85:GLN:HE22	1.66	0.42
1:E:111:THR:OG1	1:E:114:GLU:CD	2.58	0.42
2:X:207:GLU:HG3	2:X:239:VAL:HG23	2.02	0.42
2:X:231:THR:HG22	2:X:279:THR:OG1	2.20	0.42
1:F:16:THR:HB	5:F:153:HOH:O	2.19	0.42
2:X:209:ILE:HD13	2:X:211:ALA:H	1.85	0.42
2:Y:67:THR:HB	5:Y:585:HOH:O	2.20	0.42
2:U:120:LEU:O	2:U:137:CYS:HA	2.19	0.42
2:U:129:GLU:O	2:U:130:ASP:HB2	2.19	0.42
2:U:152:CYS:HB2	2:U:186:ARG:HG3	2.01	0.42
1:E:46:ARG:HD3	5:E:228:HOH:O	2.20	0.42
2:X:125:LEU:HB3	2:X:203:LEU:HA	2.01	0.42
2:X:158:PRO:HB2	2:X:161:LEU:HB2	2.02	0.42
2:Y:254:PRO:HD3	5:Y:498:HOH:O	2.20	0.42
2:U:241:THR:HG22	2:U:272:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:139:LEU:HD22	2:W:147:TYR:CE1	2.55	0.42
2:W:184:CYS:HA	2:W:201:PHE:O	2.20	0.42
2:U:51:GLY:O	2:U:87:LYS:HA	2.20	0.42
1:E:104:ARG:HA	1:E:104:ARG:NE	2.34	0.41
1:E:112:PRO:HB2	5:E:148:HOH:O	2.20	0.41
1:B:49:VAL:HG12	1:B:87:VAL:HG23	2.02	0.41
1:B:81:LYS:HD2	5:B:148:HOH:O	2.20	0.41
1:B:104:ARG:HA	1:B:105:PRO:HD3	1.90	0.41
1:E:134:ASP:HB2	5:E:201:HOH:O	2.19	0.41
2:X:184:CYS:HA	2:X:201:PHE:O	2.21	0.41
2:X:241:THR:HG22	2:X:272:TYR:CE1	2.55	0.41
1:E:128:ASP:HB3	5:E:243:HOH:O	2.20	0.41
2:X:234:CYS:HB2	2:X:247:TRP:CZ2	2.56	0.41
1:A:6:ASN:OD1	5:A:290:HOH:O	2.22	0.41
2:X:139:LEU:HD21	2:X:167:PRO:HA	2.01	0.41
2:Y:139:LEU:HD21	2:Y:167:PRO:HA	2.02	0.41
2:U:207:GLU:HG3	2:U:239:VAL:O	2.20	0.41
2:W:121:VAL:HG11	2:W:199:ASP:HB2	2.01	0.41
1:A:98:ILE:N	1:A:100:GLU:OE2	2.52	0.41
1:B:66:ILE:CG2	1:B:67:SER:N	2.81	0.41
2:X:37:PRO:HB3	2:X:98:CYS:SG	2.60	0.41
2:Y:53:THR:HG22	5:Y:601:HOH:O	2.19	0.41
2:Y:60:ASP:HA	2:Y:61:PRO:HD3	1.91	0.41
2:W:139:LEU:HD21	2:W:167:PRO:HA	2.02	0.41
1:F:130:MET:H	1:F:130:MET:HG2	1.61	0.41
2:Y:203:LEU:HD12	2:Y:204:LYS:N	2.36	0.41
1:A:77:ASP:OD2	2:X:182:ARG:NH2	2.54	0.41
5:E:162:HOH:O	1:F:66:ILE:HG21	2.20	0.41
2:U:148:SER:HB3	5:U:329:HOH:O	2.20	0.41
1:A:142:HIS:O	1:A:146:HIS:ND1	2.54	0.41
2:X:123:LEU:HA	2:X:124:PRO:HD3	1.91	0.41
2:W:128:LYS:HA	2:W:206:ARG:HB2	2.03	0.41
1:A:31:ASN:HB2	1:A:51:GLN:OE1	2.20	0.41
1:A:127:LYS:HE2	5:A:248:HOH:O	2.21	0.41
1:B:97:ASN:HB2	5:B:155:HOH:O	2.21	0.41
1:E:46:ARG:HD2	5:E:241:HOH:O	2.21	0.41
1:F:6:ASN:ND2	1:F:6:ASN:N	2.69	0.41
1:F:111:THR:HB	5:F:241:HOH:O	2.21	0.41
2:X:244:ASN:O	2:X:295:ALA:HA	2.20	0.41
2:Y:100:ASN:HB3	2:Y:104:LEU:H	1.86	0.41
1:B:52:LEU:CD1	5:B:195:HOH:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:LYS:NZ	5:W:343:HOH:O	2.53	0.41
2:Y:70:THR:HG22	2:Y:71:TYR:H	1.86	0.41
2:U:261:LYS:HE2	2:U:261:LYS:CA	2.47	0.41
1:E:77:ASP:OD2	2:U:182:ARG:NH2	2.54	0.40
2:X:124:PRO:HB2	2:X:126:PHE:HE1	1.86	0.40
2:Y:222:HIS:HE1	5:Y:477:HOH:O	2.03	0.40
2:U:104:LEU:N	5:U:360:HOH:O	2.40	0.40
2:U:113:ARG:HA	2:U:140:THR:O	2.21	0.40
1:E:69:GLY:HA3	5:E:232:HOH:O	2.20	0.40
2:X:75:MET:HE1	5:X:433:HOH:O	2.21	0.40
2:U:257:ILE:HD12	2:U:258:ALA:N	2.35	0.40
2:W:59:ILE:N	2:W:59:ILE:CD1	2.84	0.40
1:A:101:SER:N	1:A:102:PRO:CD	2.84	0.40
1:F:88:LEU:CD1	2:W:206:ARG:HG2	2.51	0.40
2:X:125:LEU:HD22	2:X:125:LEU:HA	1.84	0.40
2:Y:306:THR:HA	5:Y:577:HOH:O	2.20	0.40
2:U:51:GLY:O	2:U:87:LYS:HD2	2.21	0.40
2:U:151:GLU:HG2	2:U:155:LYS:H	1.85	0.40
2:W:207:GLU:HB3	2:W:270:PHE:CD2	2.56	0.40
2:X:121:VAL:HG12	2:X:122:GLY:N	2.37	0.40
2:X:197:HIS:HB2	5:X:322:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	142/145 (98%)	124 (87%)	13 (9%)	5 (4%)	3 4
1	B	137/145 (94%)	122 (89%)	10 (7%)	5 (4%)	3 4
1	E	137/145 (94%)	124 (90%)	9 (7%)	4 (3%)	4 6
1	F	137/145 (94%)	121 (88%)	12 (9%)	4 (3%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U	273/290 (94%)	252 (92%)	15 (6%)	6 (2%)	6	10
2	W	273/290 (94%)	255 (93%)	12 (4%)	6 (2%)	6	10
2	X	273/290 (94%)	253 (93%)	15 (6%)	5 (2%)	8	14
2	Y	273/290 (94%)	249 (91%)	16 (6%)	8 (3%)	4	6
All	All	1645/1740 (94%)	1500 (91%)	102 (6%)	43 (3%)	5	8

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	PRO
1	E	102	PRO
1	F	102	PRO
2	X	73	ASN
2	Y	73	ASN
2	W	73	ASN
1	A	70	LEU
1	A	102	PRO
1	B	70	LEU
1	E	70	LEU
1	F	70	LEU
2	Y	42	ALA
2	U	73	ASN
2	U	136	ARG
2	W	42	ALA
2	W	136	ARG
2	X	251	ASN
2	Y	175	ASN
2	Y	251	ASN
2	U	251	ASN
2	W	251	ASN
1	A	99	LYS
1	B	99	LYS
1	E	99	LYS
1	F	99	LYS
2	Y	136	ARG
2	U	42	ALA
1	A	145	HIS
1	B	136	SER
2	X	41	PRO
2	X	175	ASN
1	B	104	ARG

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Mol	Chain	Res	Type
1	F	104	ARG
2	U	175	ASN
2	X	218	PRO
2	U	218	PRO
1	A	104	ARG
1	E	104	ARG
2	Y	218	PRO
2	Y	252	PRO
2	W	254	PRO
2	Y	254	PRO
2	W	252	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	135/136 (99%)	124 (92%)	11 (8%)	11 23
1	B	130/136 (96%)	119 (92%)	11 (8%)	10 21
1	E	130/136 (96%)	120 (92%)	10 (8%)	13 25
1	F	130/136 (96%)	120 (92%)	10 (8%)	13 25
2	U	247/259 (95%)	231 (94%)	16 (6%)	17 33
2	W	247/259 (95%)	230 (93%)	17 (7%)	15 30
2	X	247/259 (95%)	224 (91%)	23 (9%)	9 17
2	Y	247/259 (95%)	230 (93%)	17 (7%)	15 30
All	All	1513/1580 (96%)	1398 (92%)	115 (8%)	13 25

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	18	LEU
1	A	59	LEU
1	A	62	LYS

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Mol	Chain	Res	Type
1	A	65	ASN
1	A	66	ILE
1	A	83	VAL
1	A	102	PRO
1	A	104	ARG
1	A	142	HIS
1	A	143	HIS
1	B	6	ASN
1	B	18	LEU
1	B	59	LEU
1	B	62	LYS
1	B	65	ASN
1	B	66	ILE
1	B	83	VAL
1	B	97	ASN
1	B	104	ARG
1	B	130	MET
1	B	133	SER
1	E	6	ASN
1	E	18	LEU
1	E	59	LEU
1	E	62	LYS
1	E	65	ASN
1	E	66	ILE
1	E	83	VAL
1	E	97	ASN
1	E	104	ARG
1	E	133	SER
1	F	6	ASN
1	F	18	LEU
1	F	59	LEU
1	F	62	LYS
1	F	65	ASN
1	F	66	ILE
1	F	83	VAL
1	F	97	ASN
1	F	104	ARG
1	F	133	SER
2	X	40	HIS
2	X	41	PRO
2	X	53	THR
2	X	59	ILE

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Mol	Chain	Res	Type
2	X	65	ARG
2	X	85	GLN
2	X	95	THR
2	X	100	ASN
2	X	102	ASN
2	X	118	LEU
2	X	125	LEU
2	X	134	LEU
2	X	139	LEU
2	X	150	ILE
2	X	152	CYS
2	X	207	GLU
2	X	209	ILE
2	X	222	HIS
2	X	230	PHE
2	X	236	ILE
2	X	255	GLN
2	X	265	TRP
2	X	276	GLU
2	Y	40	HIS
2	Y	49	GLU
2	Y	65	ARG
2	Y	85	GLN
2	Y	95	THR
2	Y	100	ASN
2	Y	102	ASN
2	Y	125	LEU
2	Y	134	LEU
2	Y	139	LEU
2	Y	150	ILE
2	Y	152	CYS
2	Y	230	PHE
2	Y	236	ILE
2	Y	265	TRP
2	Y	276	GLU
2	Y	280	ILE
2	U	59	ILE
2	U	65	ARG
2	U	85	GLN
2	U	95	THR
2	U	100	ASN
2	U	102	ASN

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Mol	Chain	Res	Type
2	U	118	LEU
2	U	125	LEU
2	U	134	LEU
2	U	138	PRO
2	U	139	LEU
2	U	150	ILE
2	U	152	CYS
2	U	230	PHE
2	U	265	TRP
2	U	276	GLU
2	W	59	ILE
2	W	65	ARG
2	W	85	GLN
2	W	95	THR
2	W	100	ASN
2	W	102	ASN
2	W	118	LEU
2	W	125	LEU
2	W	134	LEU
2	W	139	LEU
2	W	150	ILE
2	W	152	CYS
2	W	230	PHE
2	W	257	ILE
2	W	265	TRP
2	W	276	GLU
2	W	280	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	65	ASN
1	A	120	ASN
1	A	143	HIS
1	B	6	ASN
1	B	21	ASN
1	B	65	ASN
1	B	120	ASN
1	E	6	ASN
1	E	65	ASN
1	E	120	ASN

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Mol	Chain	Res	Type
1	F	65	ASN
1	F	120	ASN
2	X	85	GLN
2	X	100	ASN
2	X	102	ASN
2	X	251	ASN
2	X	255	GLN
2	X	259	GLN
2	X	297	ASN
2	Y	85	GLN
2	Y	100	ASN
2	Y	102	ASN
2	Y	251	ASN
2	Y	259	GLN
2	Y	297	ASN
2	U	85	GLN
2	U	100	ASN
2	U	102	ASN
2	U	251	ASN
2	U	259	GLN
2	U	297	ASN
2	W	85	GLN
2	W	100	ASN
2	W	102	ASN
2	W	251	ASN
2	W	259	GLN
2	W	297	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1	2,3	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
3	NAG	C	2	3	14,14,15	0.56	0	17,19,21	0.65	0
3	FUL	C	3	3	10,10,11	0.46	0	14,14,16	0.51	0
4	NAG	D	1	2,4	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
4	NAG	D	2	4	14,14,15	0.72	0	17,19,21	0.75	0
4	MAN	D	3	4	11,11,12	0.65	0	15,15,17	0.66	0
3	NAG	G	1	2,3	14,14,15	0.73	0	17,19,21	1.16	2 (11%)
3	NAG	G	2	3	14,14,15	0.62	0	17,19,21	0.58	0
3	FUL	G	3	3	10,10,11	0.50	0	14,14,16	0.50	0
4	NAG	H	1	2,4	14,14,15	0.82	0	17,19,21	1.63	2 (11%)
4	NAG	H	2	4	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
4	MAN	H	3	4	11,11,12	0.59	0	15,15,17	0.56	0
3	NAG	I	1	2,3	14,14,15	0.76	0	17,19,21	1.08	1 (5%)
3	NAG	I	2	3	14,14,15	0.58	0	17,19,21	0.71	0
3	FUL	I	3	3	10,10,11	0.52	0	14,14,16	0.61	0
4	NAG	J	1	2,4	14,14,15	0.80	0	17,19,21	1.34	2 (11%)
4	NAG	J	2	4	14,14,15	0.73	0	17,19,21	0.76	0
4	MAN	J	3	4	11,11,12	0.66	0	15,15,17	0.74	1 (6%)
3	NAG	K	1	2,3	14,14,15	0.60	0	17,19,21	0.90	0
3	NAG	K	2	3	14,14,15	0.54	0	17,19,21	0.54	0
3	FUL	K	3	3	10,10,11	0.48	0	14,14,16	0.35	0
4	NAG	L	1	2,4	14,14,15	0.81	0	17,19,21	0.55	0
4	NAG	L	2	4	14,14,15	0.65	0	17,19,21	0.79	0
4	MAN	L	3	4	11,11,12	0.71	0	15,15,17	0.68	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	2,3	-	6/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	FUL	C	3	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	2,4	-	6/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	5/6/23/26	0/1/1/1
3	FUL	G	3	3	-	-	0/1/1/1
4	NAG	H	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	5/6/23/26	0/1/1/1
4	MAN	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	FUL	I	3	3	-	-	0/1/1/1
4	NAG	J	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	MAN	J	3	4	-	1/2/19/22	0/1/1/1
3	NAG	K	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	FUL	K	3	3	-	-	0/1/1/1
4	NAG	L	1	2,4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	0/1/1/1
4	MAN	L	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	NAG	C4-C3-C2	4.95	118.27	111.02
4	J	1	NAG	C4-C3-C2	3.83	116.63	111.02
4	D	1	NAG	C4-C3-C2	3.43	116.05	111.02
4	H	1	NAG	C3-C4-C5	3.10	115.77	110.24
4	J	1	NAG	C3-C4-C5	2.95	115.50	110.24
4	D	1	NAG	C3-C4-C5	2.78	115.20	110.24
3	I	1	NAG	C2-N2-C7	-2.50	119.34	122.90
4	J	3	MAN	C1-C2-C3	2.31	112.50	109.67
4	L	3	MAN	C1-C2-C3	2.25	112.44	109.67
4	H	2	NAG	C4-C3-C2	2.25	114.32	111.02
3	C	1	NAG	C2-N2-C7	-2.25	119.70	122.90
3	G	1	NAG	C6-C5-C4	-2.05	108.19	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C2-N2-C7	-2.04	120.00	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	1	NAG	C1

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C3-C2-N2-C7
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O7-C7-N2-C2
4	L	1	NAG	C3-C2-N2-C7
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	L	3	MAN	O5-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	L	3	MAN	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	J	3	MAN	O5-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
4	D	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C3-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7

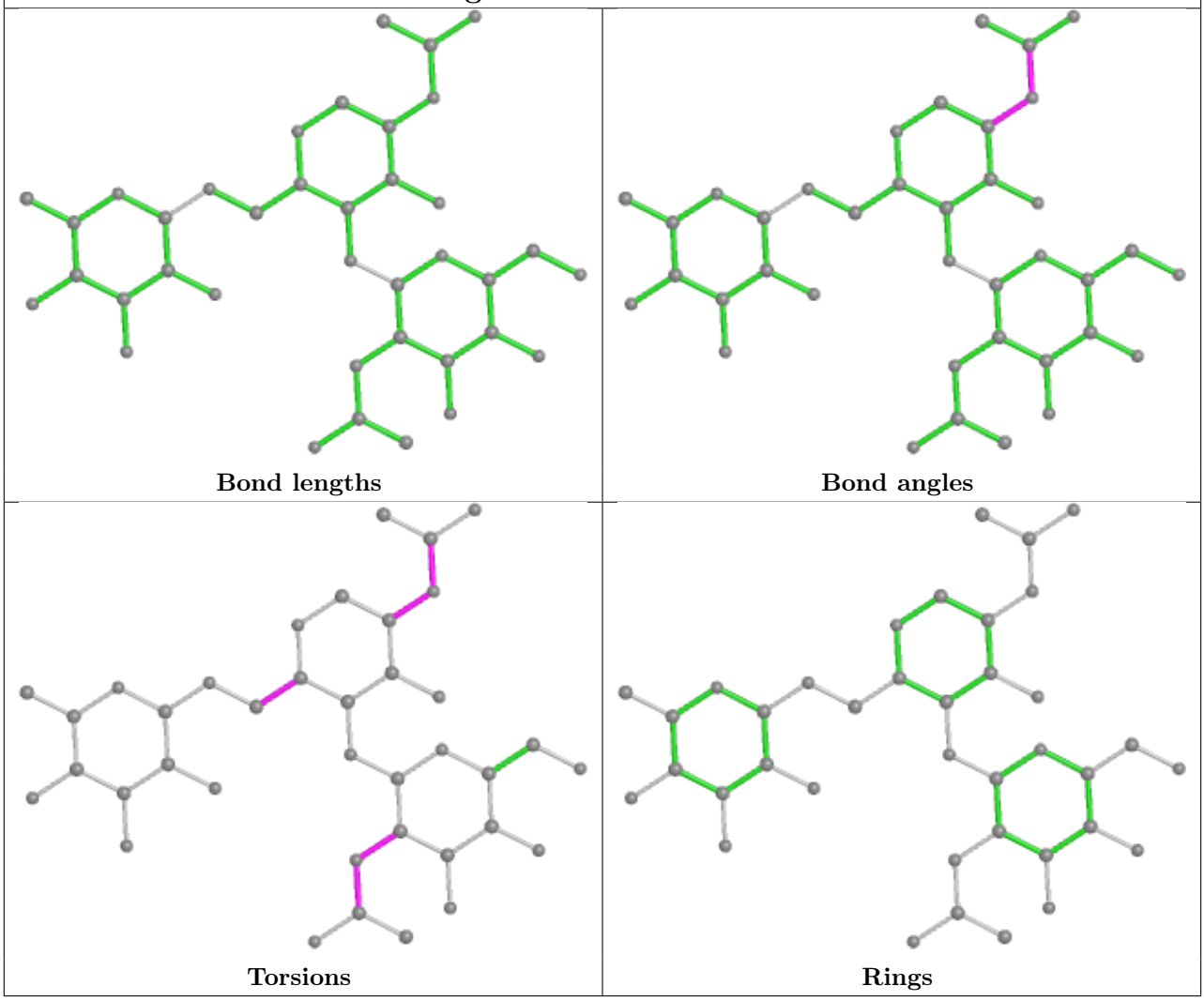
There are no ring outliers.

10 monomers are involved in 11 short contacts:

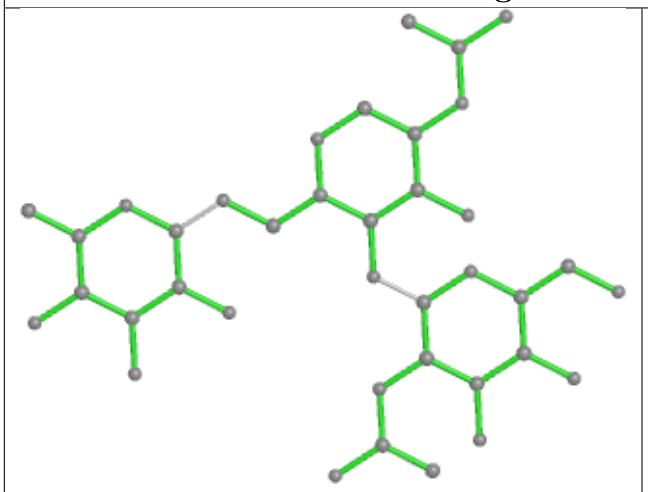
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	FUL	1	0
3	G	1	NAG	2	0
4	D	2	NAG	1	0
4	L	3	MAN	1	0
3	C	1	NAG	1	0
3	C	2	NAG	1	0
3	I	2	NAG	3	0
4	L	1	NAG	2	0
4	L	2	NAG	1	0
4	H	2	NAG	1	0

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

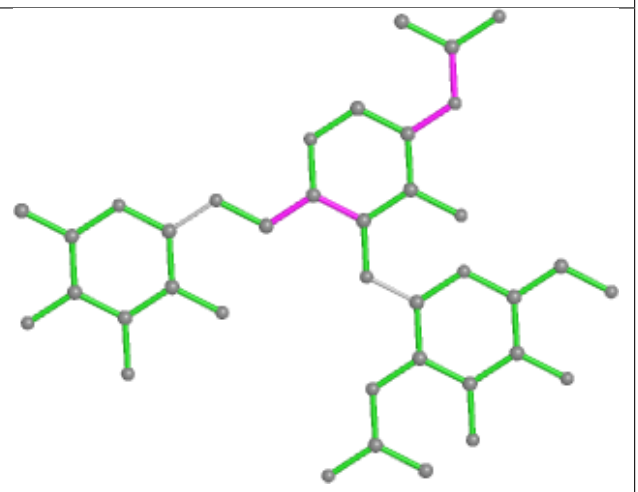
Oligosaccharide Chain C



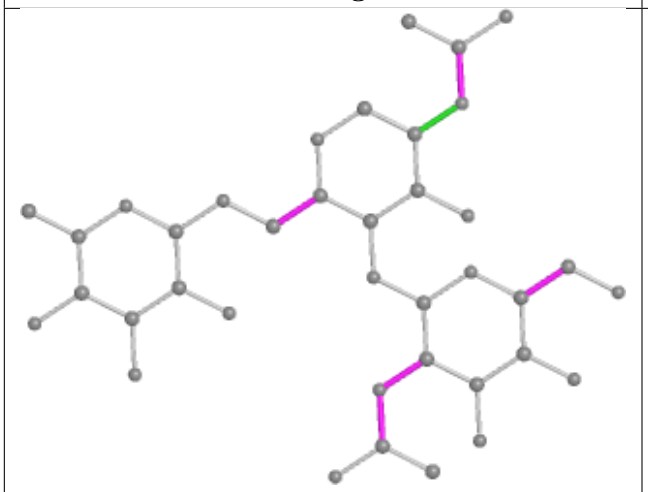
Oligosaccharide Chain G



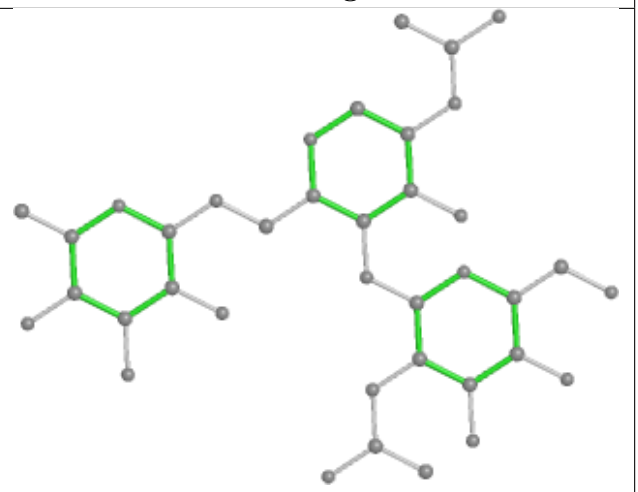
Bond lengths



Bond angles

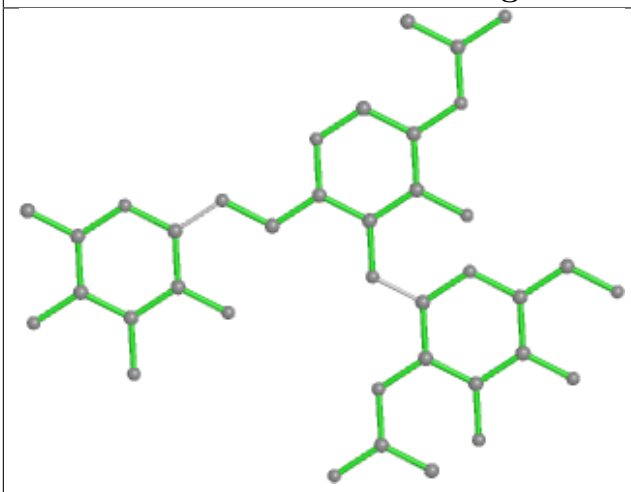


Torsions

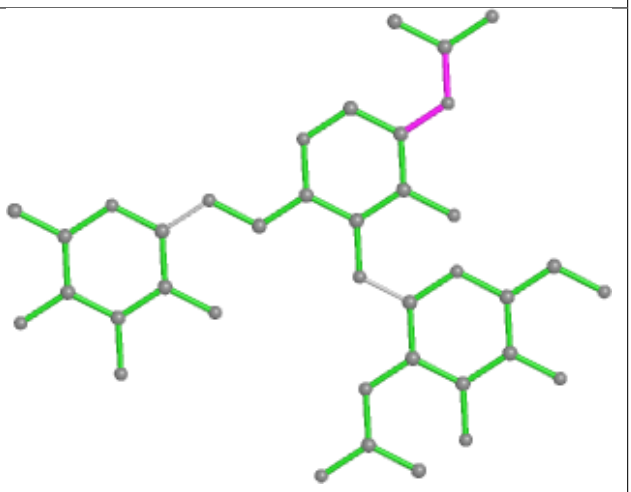


Rings

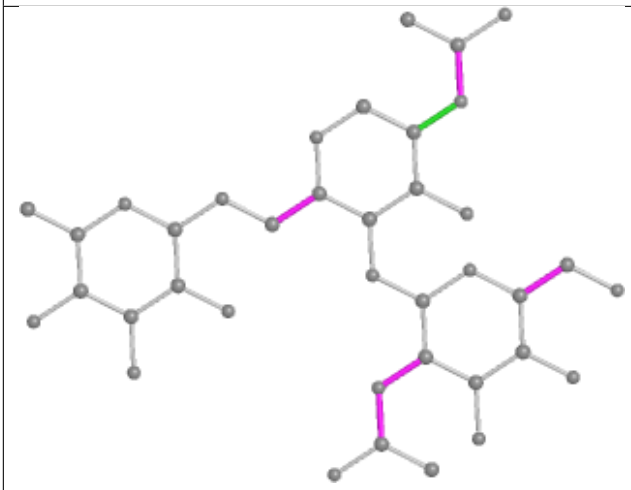
Oligosaccharide Chain I



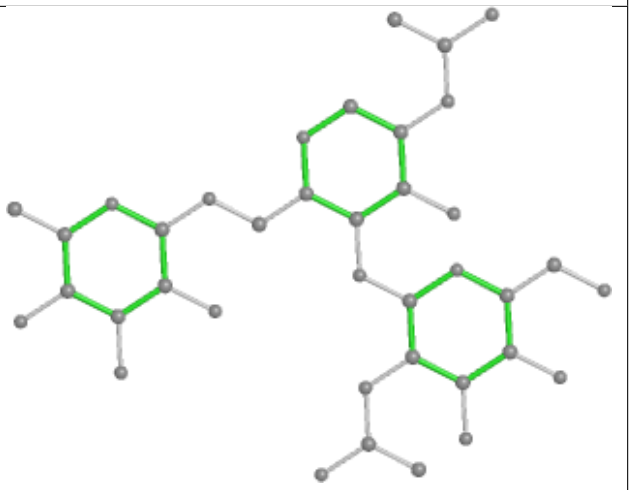
Bond lengths



Bond angles

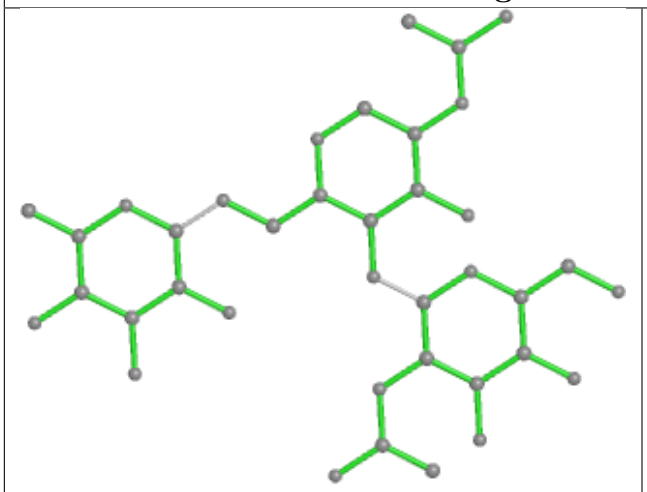


Torsions

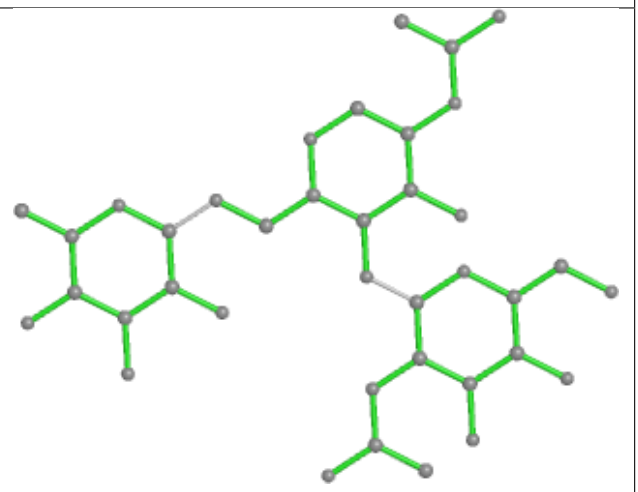


Rings

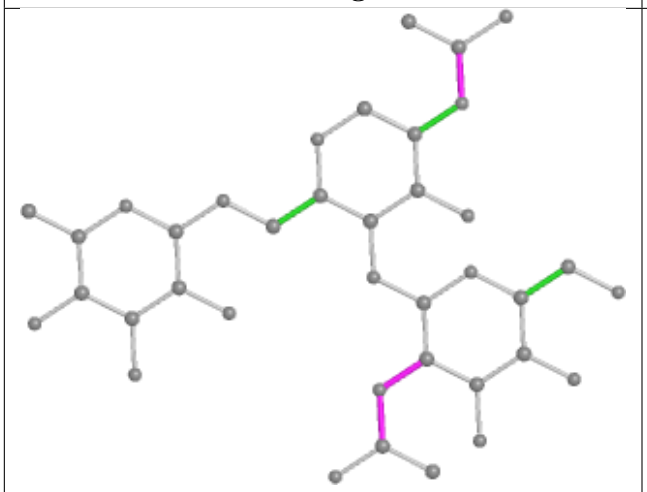
Oligosaccharide Chain K



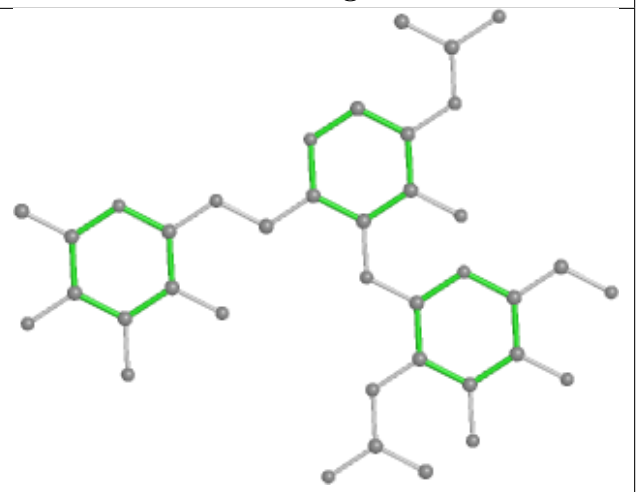
Bond lengths



Bond angles

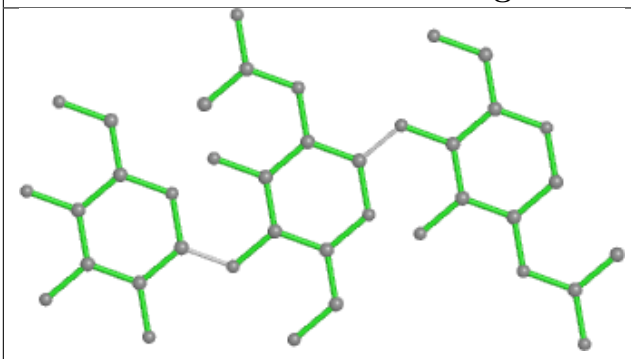


Torsions

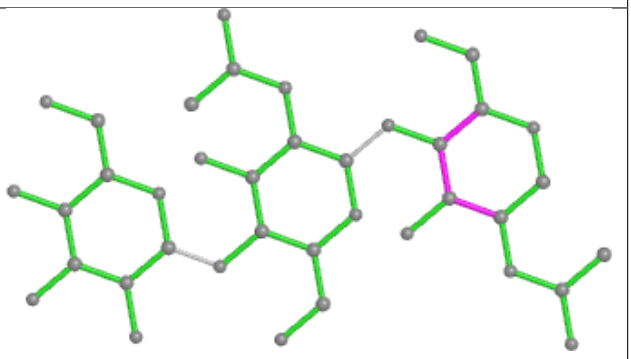


Rings

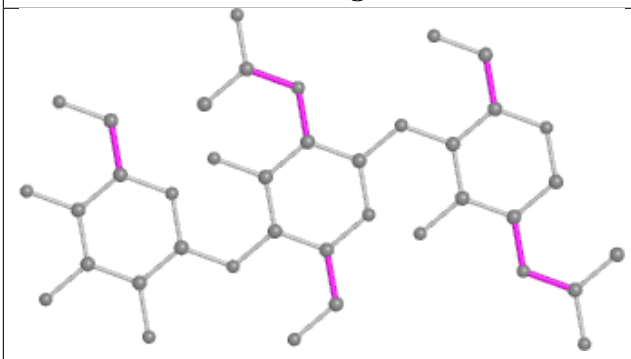
Oligosaccharide Chain D



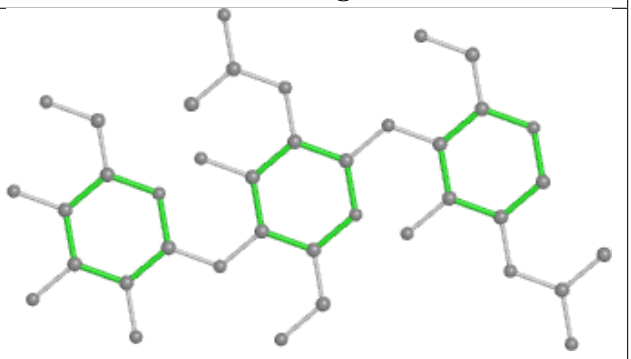
Bond lengths



Bond angles

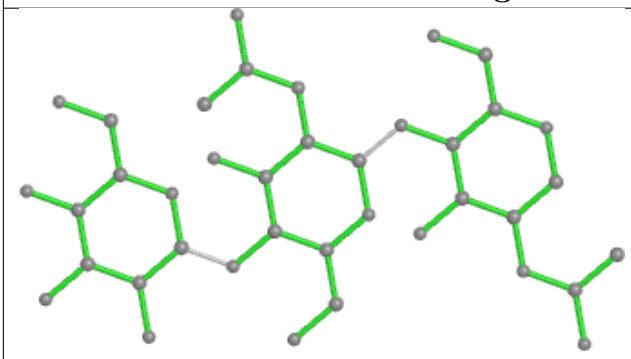


Torsions

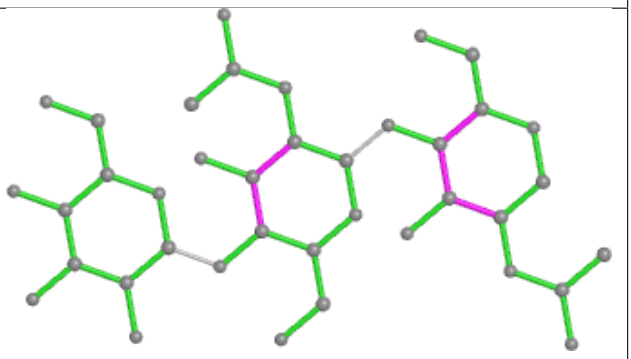


Rings

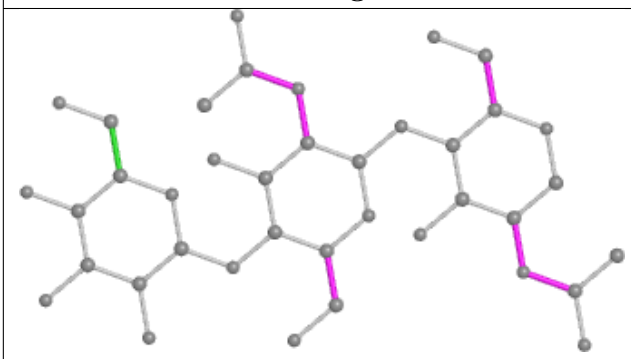
Oligosaccharide Chain H



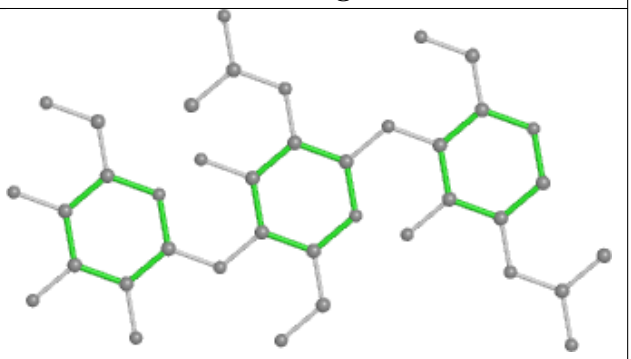
Bond lengths



Bond angles

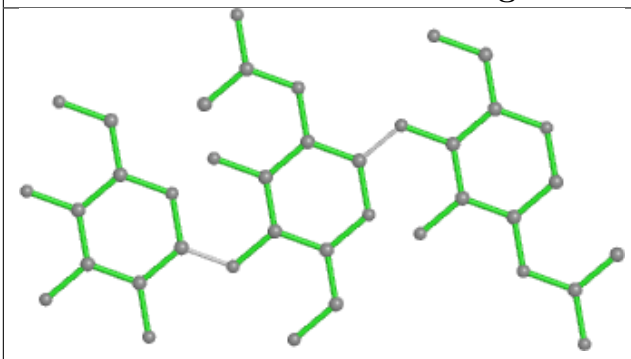


Torsions

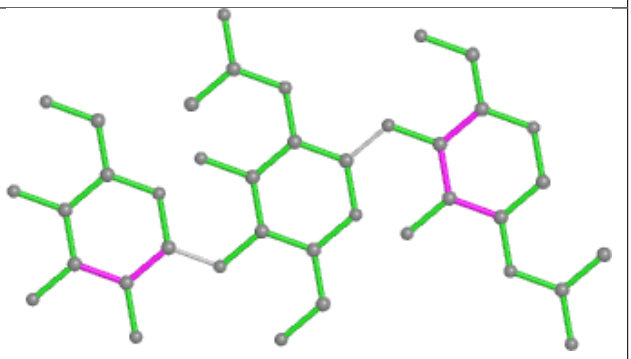


Rings

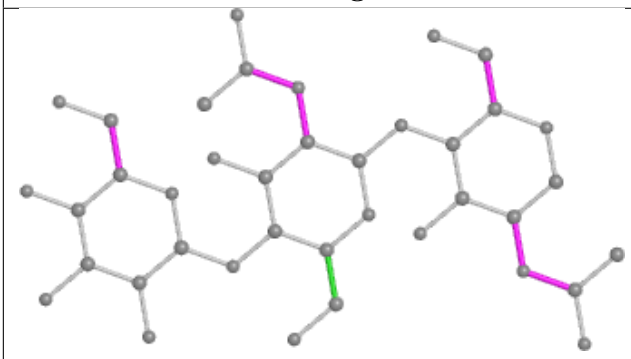
Oligosaccharide Chain J



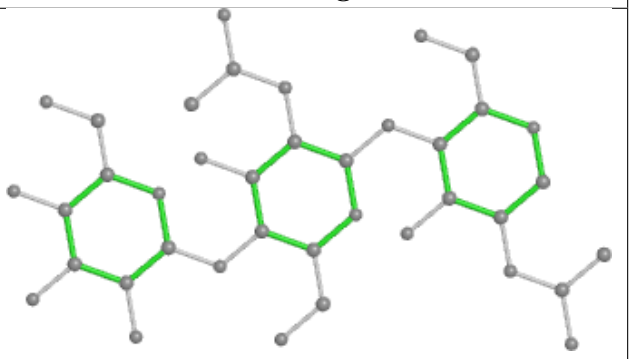
Bond lengths



Bond angles

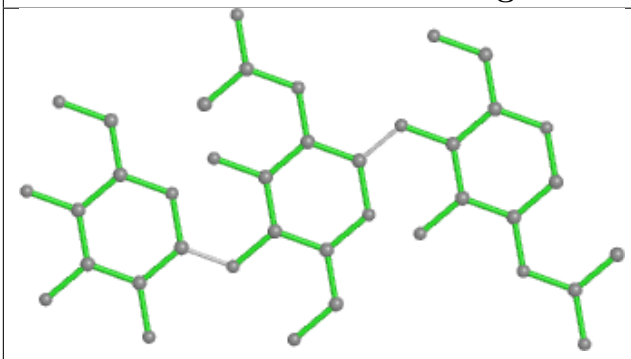


Torsions

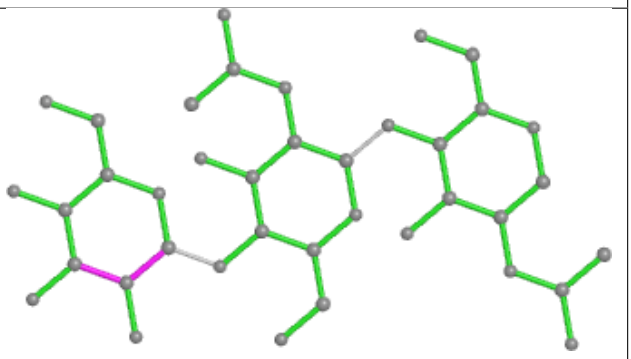


Rings

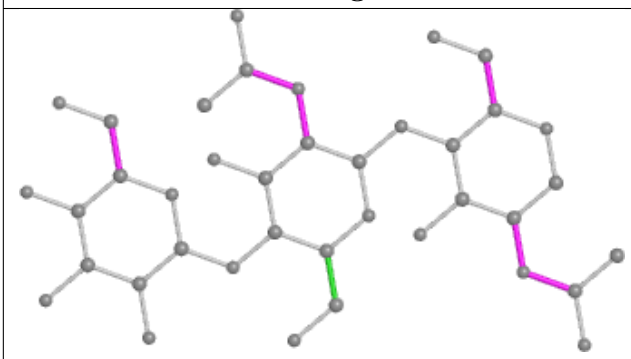
Oligosaccharide Chain L



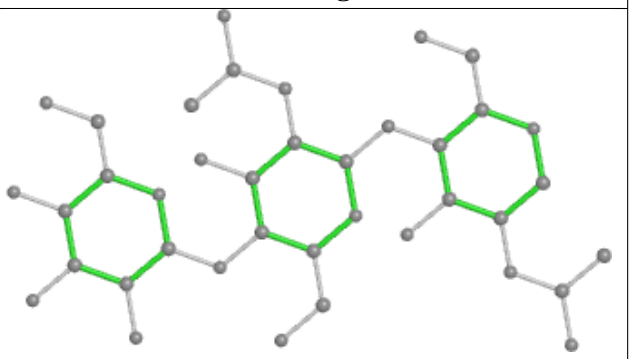
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	144/145 (99%)	0.75	13 (9%)	9	9	42, 68, 170, 188	0
1	B	139/145 (95%)	1.31	28 (20%)	1	0	39, 76, 187, 194	0
1	E	139/145 (95%)	1.50	22 (15%)	2	1	39, 69, 184, 200	0
1	F	139/145 (95%)	1.57	30 (21%)	0	0	45, 86, 185, 197	0
2	U	275/290 (94%)	1.11	60 (21%)	0	0	44, 85, 168, 187	0
2	W	275/290 (94%)	2.12	97 (35%)	0	0	59, 104, 183, 193	0
2	X	275/290 (94%)	1.18	52 (18%)	1	1	49, 90, 162, 189	0
2	Y	275/290 (94%)	1.54	59 (21%)	0	0	46, 81, 180, 191	0
All	All	1661/1740 (95%)	1.42	361 (21%)	0	0	39, 87, 177, 200	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	36	MET	15.0
2	W	224	LEU	13.2
2	Y	247	TRP	13.0
1	B	133	SER	13.0
2	Y	248	LEU	12.7
1	F	34	ALA	12.6
2	W	96	TYR	12.5
2	Y	290	VAL	12.3
2	W	246	MET	11.8
1	E	133	SER	11.5
2	W	247	TRP	11.4
2	X	63	PHE	11.2
1	F	39	LEU	11.1
1	F	35	GLY	10.6
1	E	134	ASP	10.1
2	W	249	LYS	9.8

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Mol	Chain	Res	Type	RSRZ
2	U	290	VAL	9.8
2	Y	232	VAL	9.7
2	Y	249	LYS	9.6
1	B	135	THR	9.5
2	W	280	ILE	9.5
2	X	287	ASP	9.2
2	W	99	SER	9.2
2	Y	293	CYS	9.1
1	F	33	VAL	9.1
2	W	66	TRP	9.1
1	B	132	ALA	8.9
1	B	134	ASP	8.8
2	Y	246	MET	8.8
2	W	291	PHE	8.7
2	X	65	ARG	8.5
2	W	215	VAL	8.4
1	B	36	MET	8.4
2	Y	304	VAL	8.2
2	W	98	CYS	8.2
2	U	291	PHE	8.2
2	W	287	ASP	8.0
2	Y	291	PHE	7.8
2	W	283	ALA	7.8
2	Y	286	ASP	7.8
2	Y	295	ALA	7.7
2	Y	294	TYR	7.6
2	W	248	LEU	7.6
1	F	38	VAL	7.5
1	E	130	MET	7.5
2	X	99	SER	7.4
2	W	308	LEU	7.4
2	W	290	VAL	7.4
2	W	304	VAL	7.3
2	W	236	ILE	7.3
1	F	138	CYS	7.3
2	W	292	MET	7.3
1	E	136	SER	7.3
2	X	66	TRP	7.3
2	U	248	LEU	7.1
2	Y	278	LEU	6.8
2	W	232	VAL	6.8
1	B	131	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	F	134	ASP	6.8
2	W	293	CYS	6.7
2	W	295	ALA	6.7
2	Y	250	MET	6.7
2	X	81	ASN	6.7
1	E	42	HIS	6.6
2	W	234	CYS	6.6
2	X	291	PHE	6.5
1	F	136	SER	6.5
1	F	43	CYS	6.5
2	U	250	MET	6.5
2	W	225	LYS	6.4
2	X	250	MET	6.4
2	U	249	LYS	6.4
2	W	284	ARG	6.4
1	F	41	SER	6.4
2	W	222	HIS	6.3
2	Y	307	THR	6.3
1	F	37	ASP	6.3
2	W	254	PRO	6.3
2	W	67	THR	6.2
2	W	233	VAL	6.2
2	W	100	ASN	6.2
2	X	249	LYS	6.2
2	W	226	LYS	6.2
2	W	288	SER	6.1
2	Y	236	ILE	6.1
1	E	131	VAL	6.0
2	W	286	ASP	6.0
1	F	44	TRP	6.0
2	W	243	VAL	6.0
1	F	42	HIS	6.0
2	Y	302	ALA	6.0
2	X	285	VAL	5.8
2	X	64	VAL	5.8
2	W	245	SER	5.8
2	Y	283	ALA	5.8
1	A	38	VAL	5.8
2	W	63	PHE	5.8
2	Y	305	THR	5.7
2	U	66	TRP	5.7
2	X	58	CYS	5.6

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Mol	Chain	Res	Type	RSRZ
2	W	59	ILE	5.6
2	Y	252	PRO	5.5
1	E	138	CYS	5.5
2	W	274	ARG	5.5
1	E	137	ASP	5.4
1	E	132	ALA	5.4
2	W	310	VAL	5.3
2	Y	292	MET	5.3
1	B	93	ASN	5.2
2	Y	306	THR	5.2
2	X	100	ASN	5.1
2	U	56	LEU	5.1
1	A	134	ASP	5.1
1	E	135	THR	5.1
1	B	32	TYR	5.0
2	W	75	MET	5.0
2	W	294	TYR	5.0
2	X	98	CYS	5.0
1	F	70	LEU	5.0
2	X	104	LEU	5.0
2	W	56	LEU	5.0
2	Y	308	LEU	4.9
1	E	41	SER	4.9
2	W	217	VAL	4.9
2	W	278	LEU	4.9
2	Y	230	PHE	4.9
2	X	254	PRO	4.8
2	W	223	LEU	4.7
2	W	108	ILE	4.7
2	U	255	GLN	4.7
1	B	95	PRO	4.7
2	U	304	VAL	4.7
1	F	140	LEU	4.7
1	B	98	ILE	4.6
2	Y	100	ASN	4.6
2	W	256	HIS	4.5
2	W	214	VAL	4.5
2	X	248	LEU	4.5
2	X	67	THR	4.5
2	W	305	THR	4.5
2	Y	285	VAL	4.4
2	W	285	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
2	Y	219	GLU	4.4
1	B	41	SER	4.4
2	W	230	PHE	4.4
2	W	253	GLN	4.4
2	Y	289	GLY	4.3
2	U	243	VAL	4.3
2	W	102	ASN	4.2
2	W	244	ASN	4.2
2	X	310	VAL	4.2
2	U	251	ASN	4.2
2	Y	245	SER	4.1
1	F	3	ILE	4.1
2	Y	280	ILE	4.1
2	W	101	SER	4.1
2	W	97	THR	4.1
2	U	189	ALA	4.1
2	Y	309	LYS	4.1
2	W	92	ARG	4.1
1	B	66	ILE	4.0
2	W	47	ILE	4.0
2	W	282	SER	4.0
2	U	292	MET	4.0
2	X	294	TYR	3.9
2	Y	256	HIS	3.9
2	X	255	GLN	3.9
2	W	65	ARG	3.9
1	E	97	ASN	3.9
2	X	59	ILE	3.8
2	W	105	THR	3.8
1	B	105	PRO	3.8
1	A	128	ASP	3.8
2	U	83	TRP	3.8
2	Y	217	VAL	3.8
2	X	236	ILE	3.7
2	Y	303	ASN	3.7
2	U	118	LEU	3.7
2	Y	222	HIS	3.7
2	W	309	LYS	3.7
2	U	112	VAL	3.7
2	X	105	THR	3.7
2	X	302	ALA	3.6
1	F	137	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	129	PHE	3.6
2	W	58	CYS	3.6
2	W	281	SER	3.6
2	U	246	MET	3.6
2	Y	254	PRO	3.5
2	W	104	LEU	3.5
2	Y	159	THR	3.5
2	W	289	GLY	3.5
1	B	43	CYS	3.5
1	A	131	VAL	3.5
2	U	256	HIS	3.5
2	W	76	VAL	3.5
2	U	67	THR	3.5
1	E	40	PRO	3.4
1	B	37	ASP	3.4
1	F	40	PRO	3.4
2	W	306	THR	3.4
2	U	309	LYS	3.4
1	F	32	TYR	3.3
2	W	250	MET	3.3
2	Y	40	HIS	3.3
2	W	252	PRO	3.3
2	W	207	GLU	3.3
2	X	283	ALA	3.3
2	X	106	SER	3.3
2	U	48	VAL	3.2
2	U	254	PRO	3.2
1	A	37	ASP	3.2
1	F	135	THR	3.2
1	E	129	PHE	3.2
2	Y	276	GLU	3.2
1	F	104	ARG	3.1
1	A	98	ILE	3.1
2	X	295	ALA	3.1
2	W	118	LEU	3.1
2	Y	237	LYS	3.1
2	X	54	LEU	3.1
1	B	138	CYS	3.1
2	U	76	VAL	3.1
2	Y	158	PRO	3.1
2	Y	287	ASP	3.1
2	U	55	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	44	TRP	3.1
1	B	70	LEU	3.1
2	X	280	ILE	3.0
2	W	111	PHE	3.0
2	W	275	GLN	3.0
1	F	95	PRO	3.0
1	E	35	GLY	3.0
2	Y	300	GLY	3.0
2	W	68	PHE	3.0
2	U	294	TYR	3.0
2	X	251	ASN	3.0
2	X	223	LEU	3.0
2	W	43	GLN	3.0
2	X	290	VAL	2.9
2	W	307	THR	2.9
2	X	247	TRP	2.9
2	Y	282	SER	2.9
1	B	34	ALA	2.9
2	W	251	ASN	2.8
2	U	92	ARG	2.8
2	Y	235	THR	2.8
2	U	147	TYR	2.8
2	U	63	PHE	2.8
1	A	39	LEU	2.8
2	Y	99	SER	2.8
2	X	147	TYR	2.8
2	U	176	VAL	2.8
2	Y	272	TYR	2.8
2	U	280	ILE	2.8
2	W	239	VAL	2.8
2	U	188	ALA	2.8
1	E	43	CYS	2.7
2	U	257	ILE	2.7
1	A	141	SER	2.7
2	X	253	GLN	2.7
2	Y	251	ASN	2.7
2	U	236	ILE	2.7
2	W	40	HIS	2.7
2	W	238	ASP	2.7
1	F	81	LYS	2.6
2	U	305	THR	2.6
2	X	257	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	U	253	GLN	2.6
2	W	276	GLU	2.6
2	Y	41	PRO	2.6
1	B	139	VAL	2.6
1	F	139	VAL	2.6
2	U	247	TRP	2.6
2	W	80	LYS	2.6
1	B	104	ARG	2.6
2	U	225	LYS	2.5
2	Y	160	ASP	2.5
2	W	302	ALA	2.5
2	Y	244	ASN	2.5
2	Y	277	THR	2.5
2	U	149	LEU	2.5
2	W	139	LEU	2.5
2	X	40	HIS	2.5
1	B	101	SER	2.5
2	Y	284	ARG	2.5
2	X	62	ASP	2.5
2	U	278	LEU	2.4
2	U	306	THR	2.4
1	E	6	ASN	2.4
1	B	108	ARG	2.4
2	Y	63	PHE	2.4
1	A	135	THR	2.4
2	W	90	ALA	2.4
1	A	140	LEU	2.4
2	Y	243	VAL	2.4
2	X	39	ILE	2.4
1	E	29	THR	2.4
2	W	106	SER	2.4
1	B	96	LYS	2.4
1	F	133	SER	2.4
2	X	149	LEU	2.4
2	U	215	VAL	2.4
2	X	244	ASN	2.3
1	A	97	ASN	2.3
2	W	228	ASP	2.3
2	Y	215	VAL	2.3
2	U	119	PHE	2.3
2	U	146	GLN	2.3
2	W	260	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	U	197	HIS	2.3
2	U	289	GLY	2.3
2	W	103	GLY	2.3
2	U	139	LEU	2.3
2	U	207	GLU	2.3
2	U	308	LEU	2.3
2	U	65	ARG	2.2
2	X	243	VAL	2.2
2	W	272	TYR	2.2
2	U	293	CYS	2.2
2	U	300	GLY	2.2
2	W	64	VAL	2.2
1	F	50	ILE	2.2
2	Y	161	LEU	2.2
2	X	297	ASN	2.2
2	X	122	GLY	2.2
2	U	84	ILE	2.2
2	U	195	TRP	2.2
1	E	83	VAL	2.2
1	F	58	THR	2.2
1	B	136	SER	2.2
2	U	286	ASP	2.1
2	W	83	TRP	2.1
2	X	101	SER	2.1
2	Y	281	SER	2.1
2	U	49	GLU	2.1
2	Y	207	GLU	2.1
2	X	84	ILE	2.1
2	X	83	TRP	2.1
2	W	265	TRP	2.1
1	B	103	LYS	2.1
1	F	69	GLY	2.1
1	E	33	VAL	2.1
2	X	76	VAL	2.1
2	U	310	VAL	2.1
1	F	66	ILE	2.1
1	B	68	GLU	2.1
1	E	36	MET	2.1
2	X	172	THR	2.1
2	W	112	VAL	2.1
2	W	62	ASP	2.1
2	W	81	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	137	ASP	2.0
2	U	99	SER	2.0
2	X	308	LEU	2.0
2	U	209	ILE	2.0
2	U	98	CYS	2.0
2	X	245	SER	2.0
1	A	70	LEU	2.0
2	U	150	ILE	2.0
1	E	112	PRO	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	L	3	11/12	0.50	0.29	190,196,198,198	0
4	NAG	D	2	14/15	0.67	0.20	183,193,195,196	0
4	NAG	L	2	14/15	0.68	0.31	187,195,198,198	0
3	FUL	K	3	10/11	0.72	0.26	160,171,172,173	0
3	NAG	K	1	14/15	0.73	0.14	145,156,169,178	0
3	NAG	G	2	14/15	0.74	0.18	185,191,194,196	0
4	NAG	J	2	14/15	0.77	0.21	179,186,194,197	0
4	NAG	L	1	14/15	0.77	0.30	164,180,187,190	0
3	NAG	K	2	14/15	0.79	0.17	185,191,194,196	0
4	NAG	H	2	14/15	0.79	0.15	180,190,198,198	0
4	NAG	D	1	14/15	0.80	0.19	112,143,156,171	0
4	MAN	D	3	11/12	0.81	0.12	193,197,198,198	0
3	NAG	G	1	14/15	0.82	0.27	156,169,179,192	0
4	MAN	H	3	11/12	0.82	0.11	161,171,175,177	0
3	FUL	I	3	10/11	0.84	0.31	124,131,139,141	0
3	NAG	I	2	14/15	0.84	0.15	170,189,193,194	0
4	MAN	J	3	11/12	0.84	0.10	191,196,198,198	0
3	FUL	G	3	10/11	0.85	0.44	154,171,175,177	0
4	NAG	J	1	14/15	0.86	0.17	151,162,169,171	0

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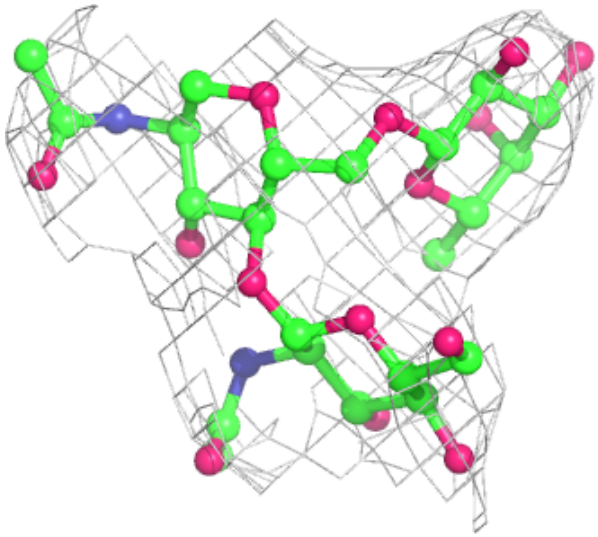
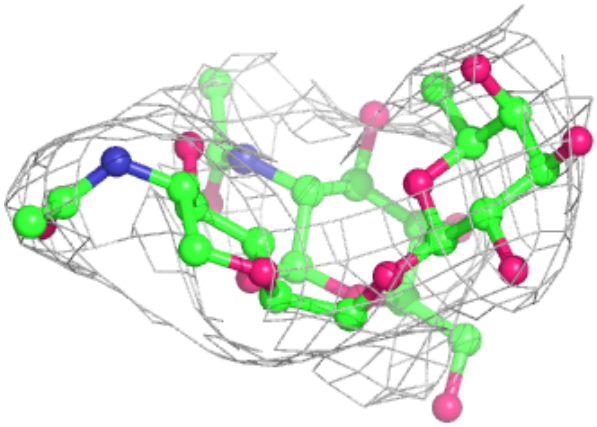
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	H	1	14/15	0.88	0.24	137,150,160,170	0
3	NAG	I	1	14/15	0.91	0.14	97,118,131,148	0
3	NAG	C	2	14/15	0.91	0.14	156,163,170,171	0
3	FUL	C	3	10/11	0.93	0.18	112,119,127,129	0
3	NAG	C	1	14/15	0.93	0.13	111,124,133,143	0

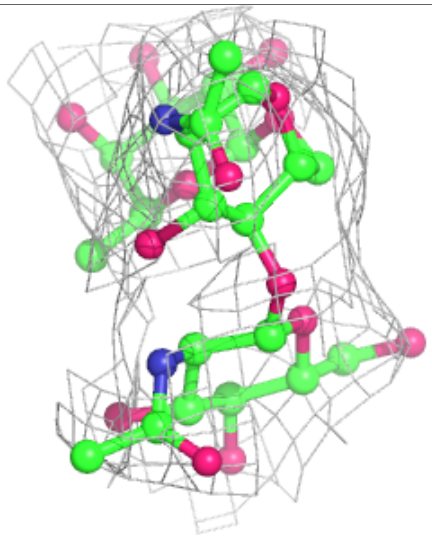
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

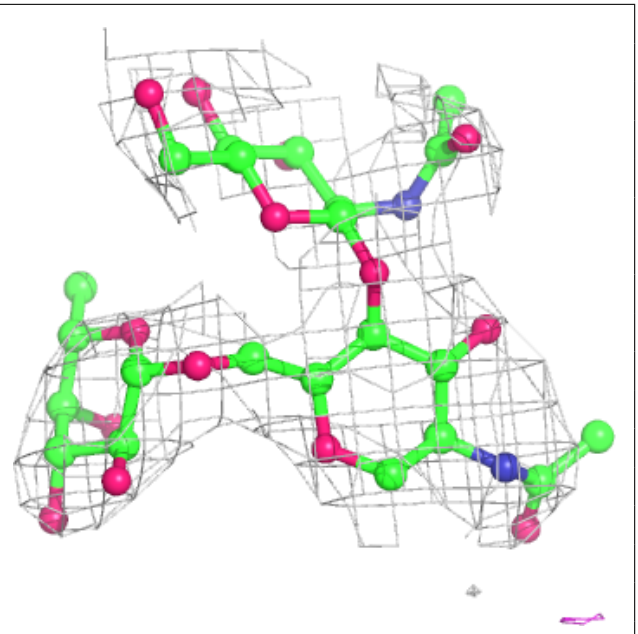


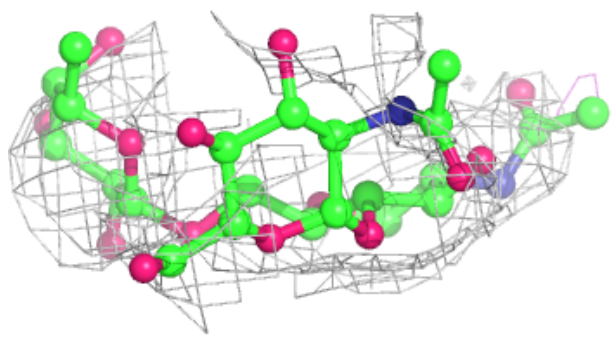


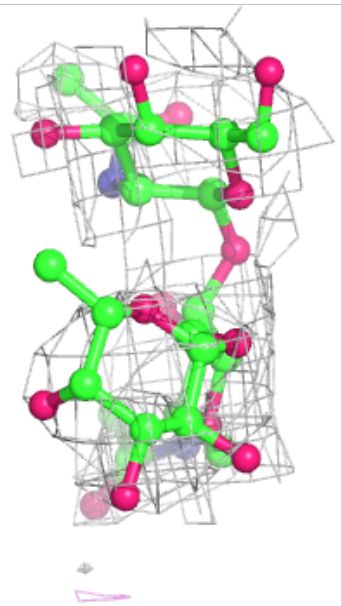


Electron density around Chain G:

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

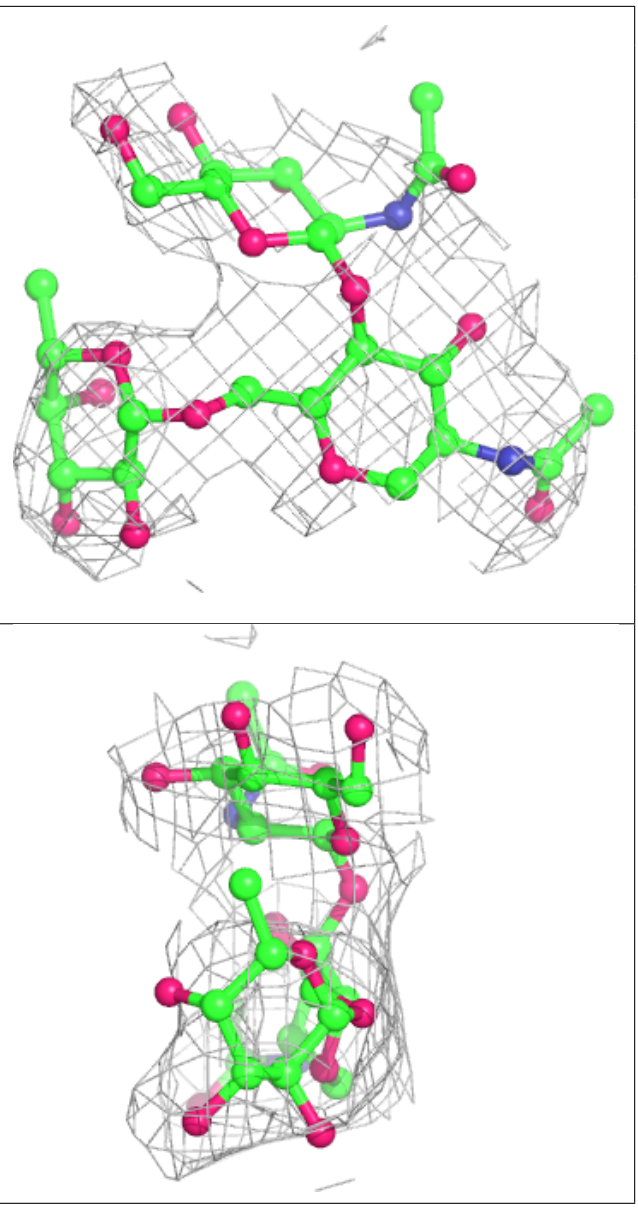






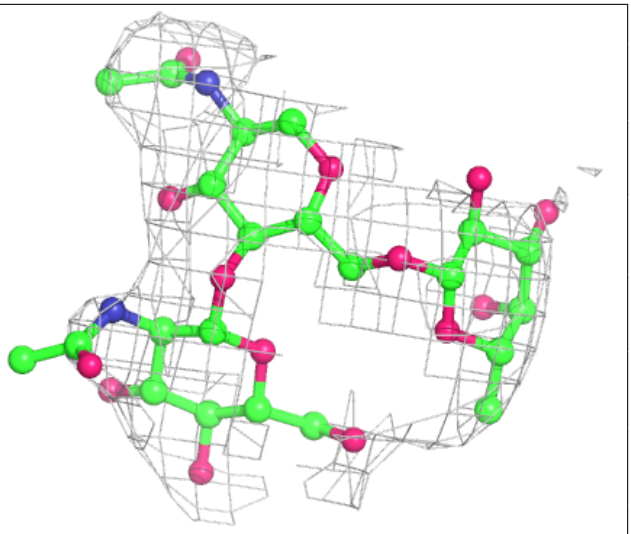
Electron density around Chain I:

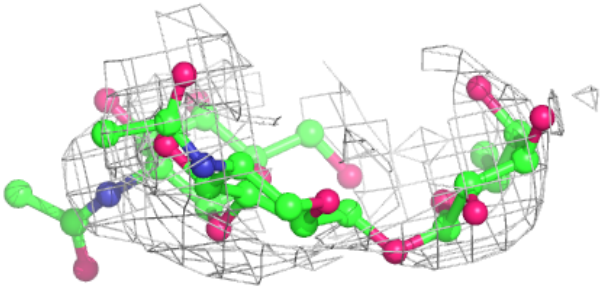
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

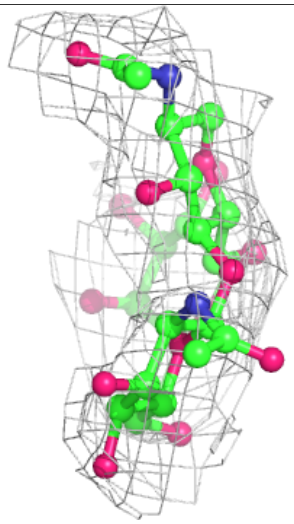


Electron density around Chain K:

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

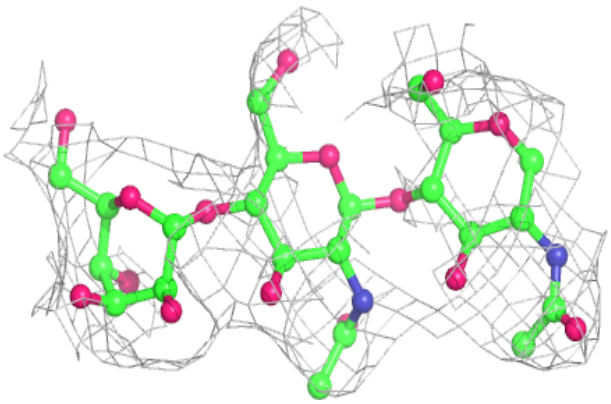


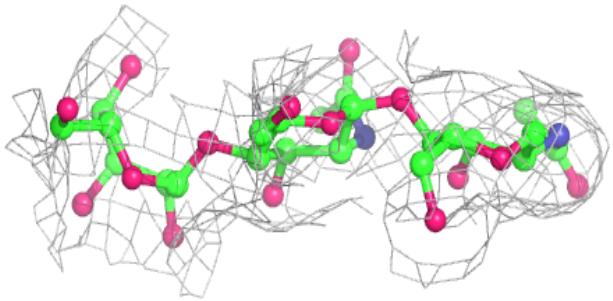


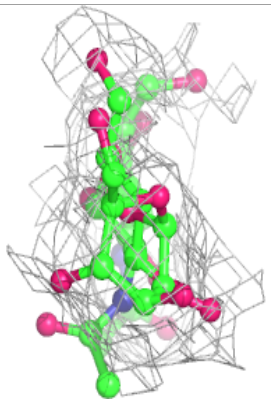


Electron density around Chain D:

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

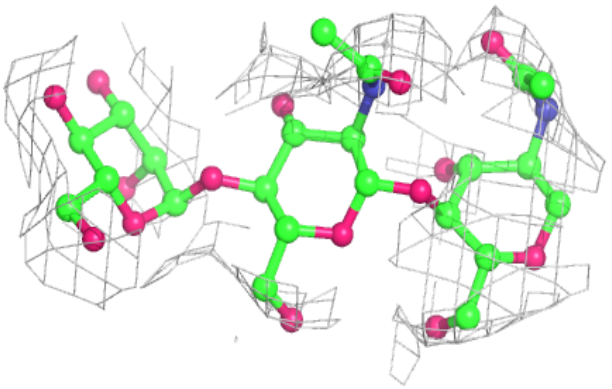


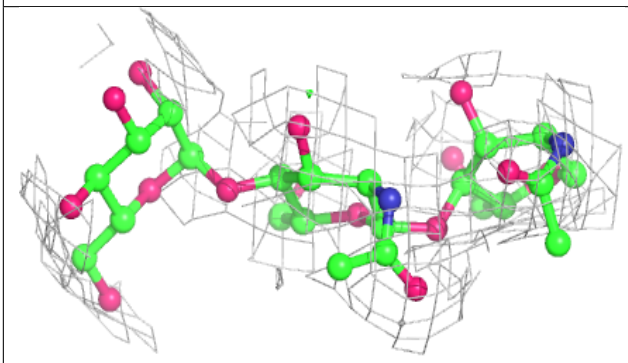


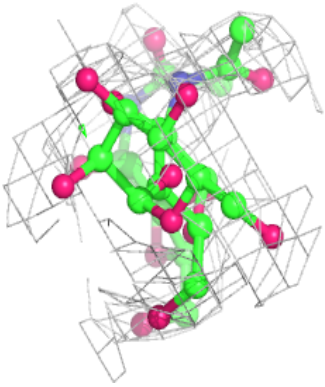


Electron density around Chain H:

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

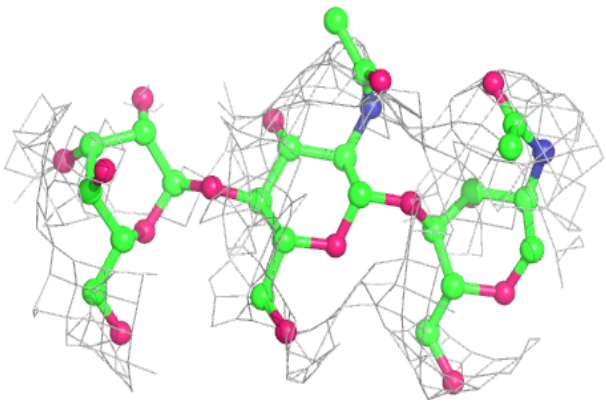


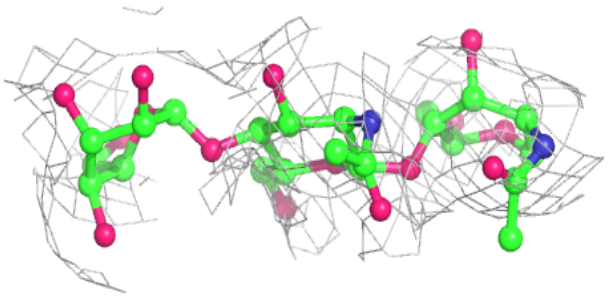


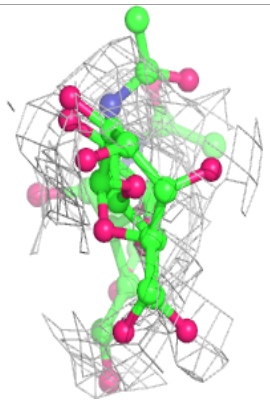


Electron density around Chain J:

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

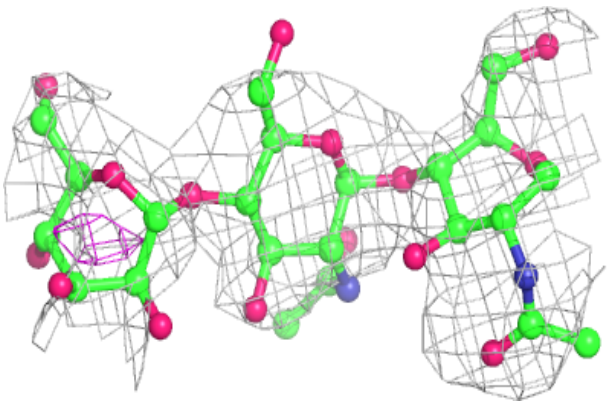


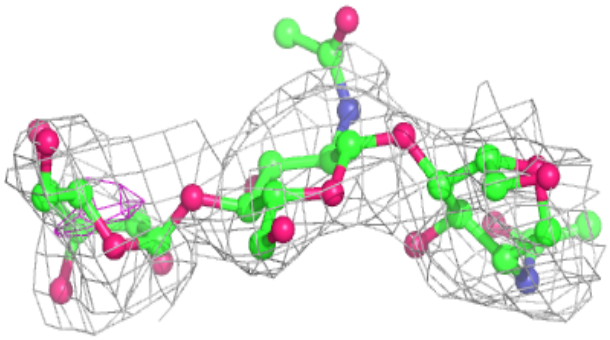


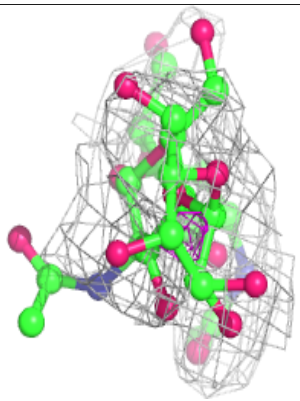


Electron density around Chain L:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.