Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 05:53 PM EDT

PDB ID	:	8DF1
Title	:	Chi3l1 bound by antibody C59
Authors	:	Wrapp, D.; McLellan, J.S.
Deposited on	:	2022-06-21
Resolution	:	3.30 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 (1)) were used in the production of this report:

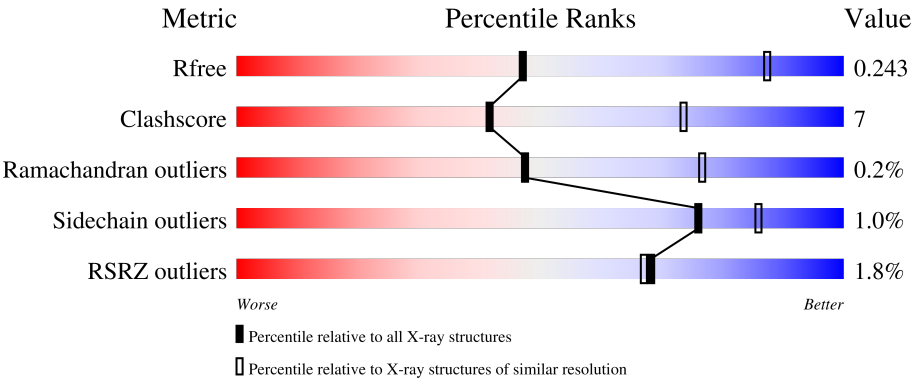
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	362	84% 16%
1	B	362	87% 13%
1	C	362	84% 16%
1	D	362	82% 18%
1	E	362	83% 17%

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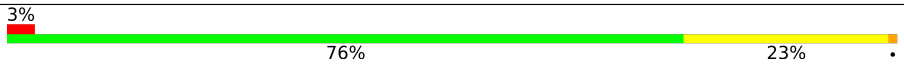
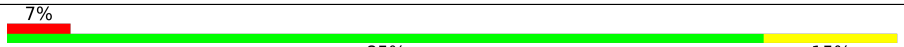
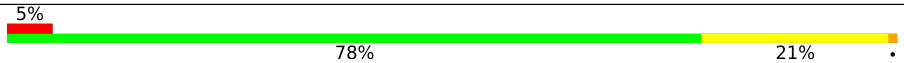
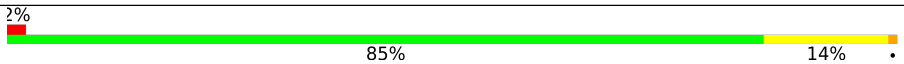
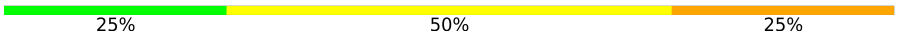
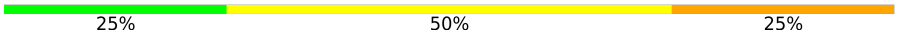
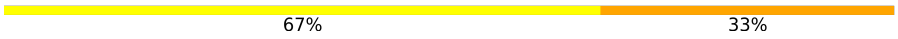
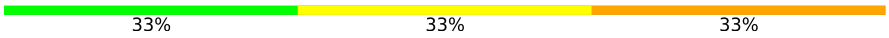
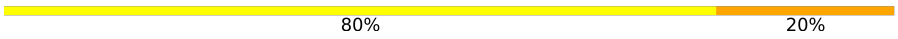
Mol	Chain	Length	Quality of chain
1	F	362	
2	H	223	
2	M	223	
2	O	223	
2	Q	223	
2	S	223	
2	U	223	
3	L	214	
3	N	214	
3	P	214	
3	R	214	
3	T	214	
3	V	214	
4	G	4	
4	W	4	
5	I	3	
5	K	3	
5	X	3	
6	J	5	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36890 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 Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			
1	B	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			
1	C	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			
1	D	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			
1	E	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			
1	F	362	Total	C	N	O	S	0	0	0
			2860	1827	493	529	11			

- Molecule 2 is a protein called C59 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			
2	H	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			
2	O	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			
2	Q	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			
2	S	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			
2	U	223	Total	C	N	O	S	0	0	0
			1647	1042	267	327	11			

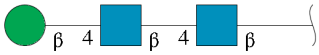
- Molecule 3 is a protein called C59 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	L	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	P	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	R	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	T	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			
3	V	214	Total	C	N	O	S	0	0	0
			1595	999	257	332	7			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	W	4	Total	C	N	O	0	0	0
			50	28	2	20			

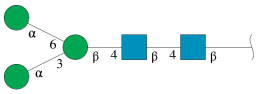
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran

ose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



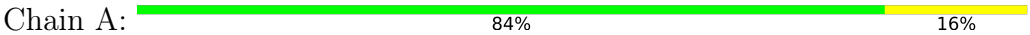
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	5	61	34	2	25	0	0	0

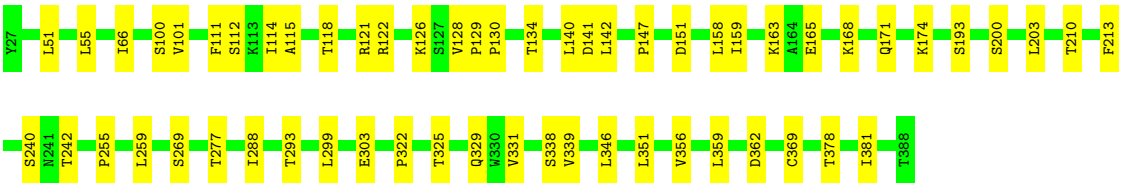
3 Residue-property plots (i)

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: Chitinase-3-like protein 1

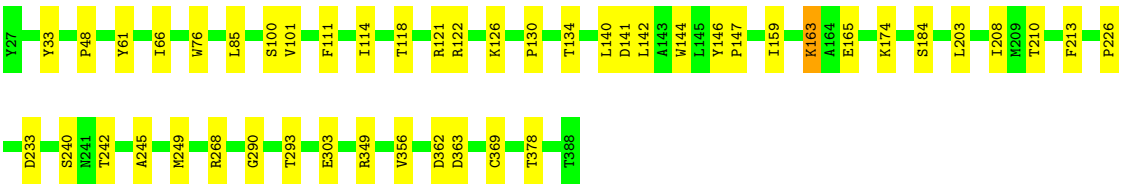
Chain A:





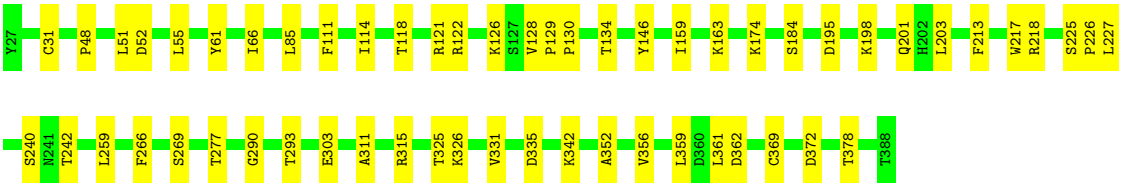
• Molecule 1: Chitinase-3-like protein 1

Chain B:



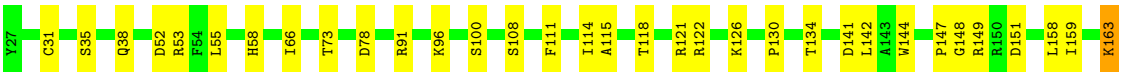
• Molecule 1: Chitinase-3-like protein 1

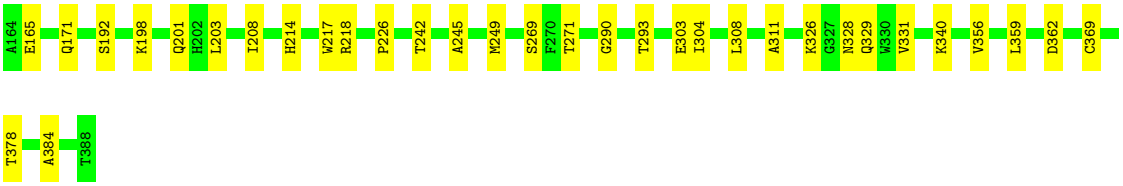
Chain C:



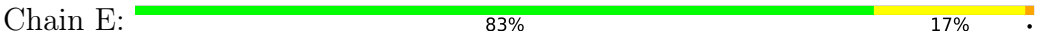
• Molecule 1: Chitinase-3-like protein 1

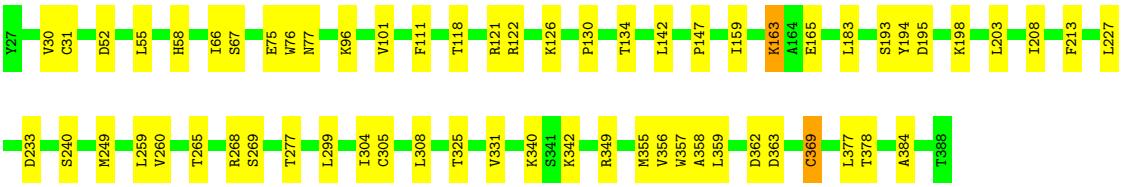
Chain D:



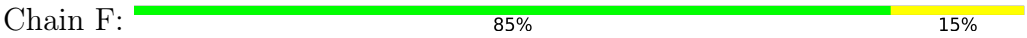


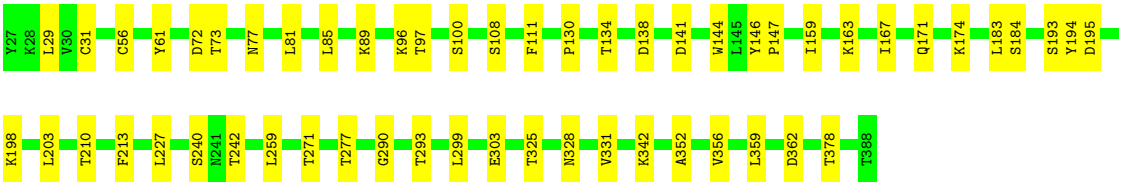
• Molecule 1: Chitinase-3-like protein 1



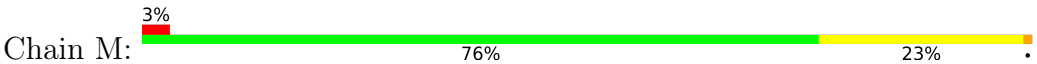


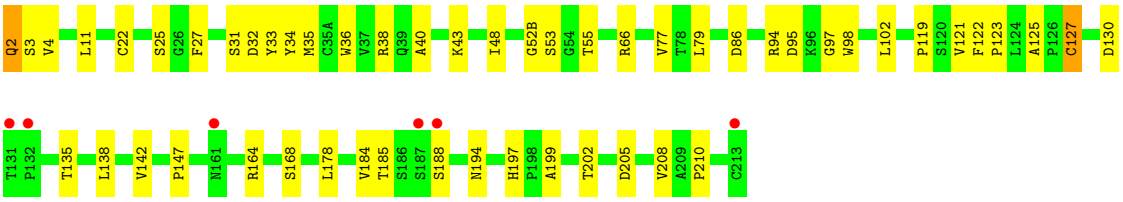
• Molecule 1: Chitinase-3-like protein 1



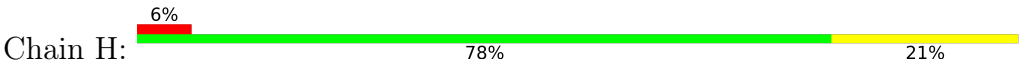


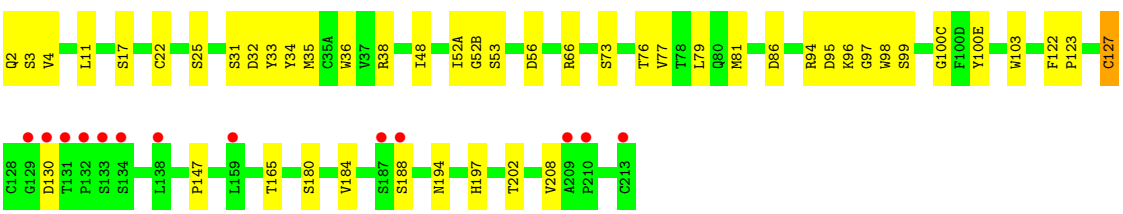
• Molecule 2: C59 Fab Heavy chain



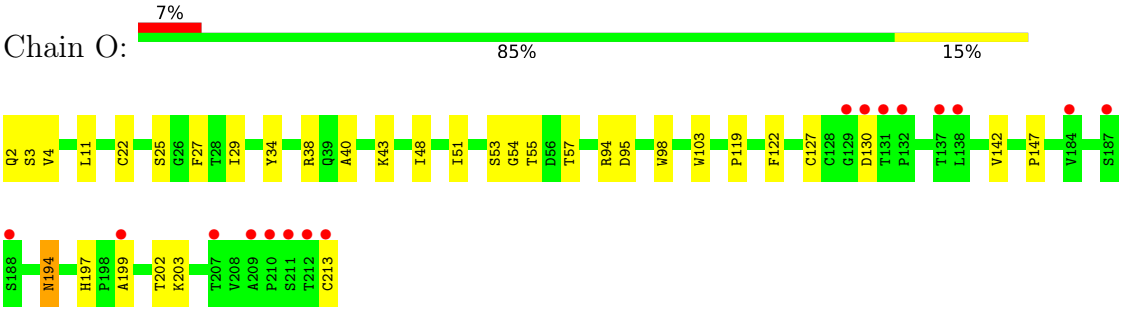


• Molecule 2: C59 Fab Heavy chain

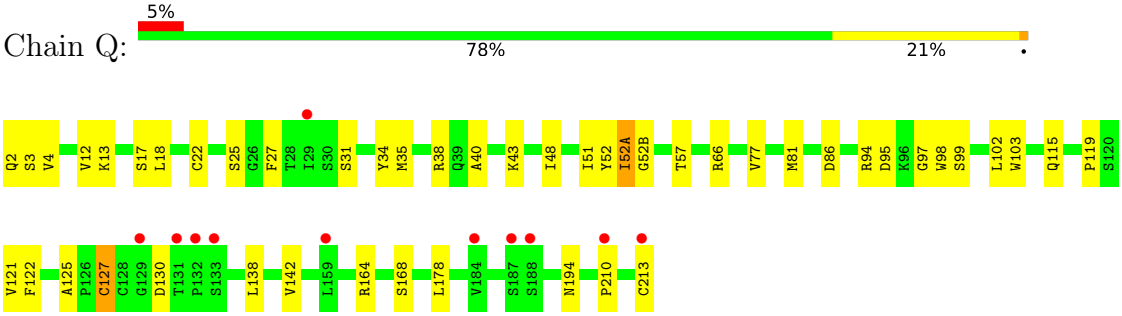




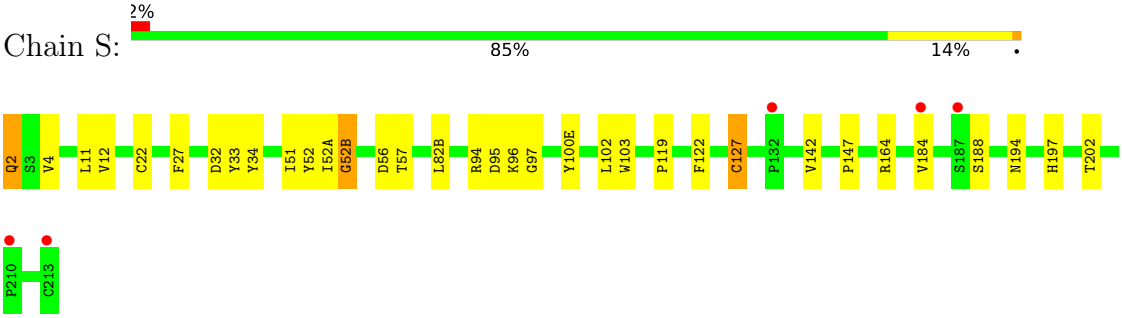
• Molecule 2: C59 Fab Heavy chain



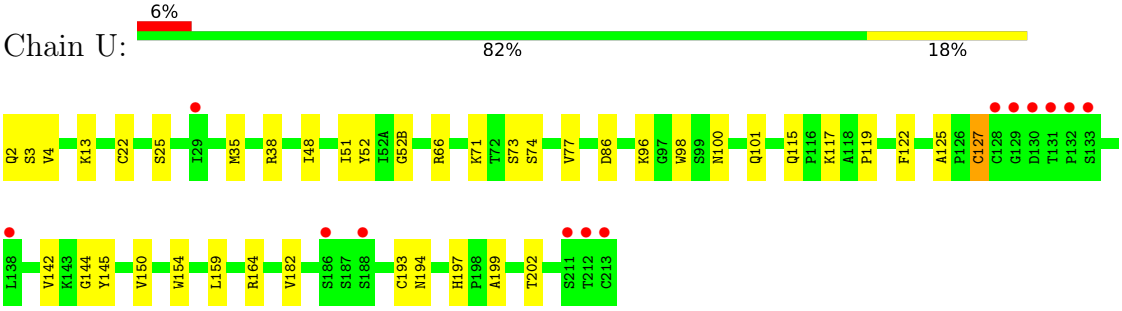
• Molecule 2: C59 Fab Heavy chain



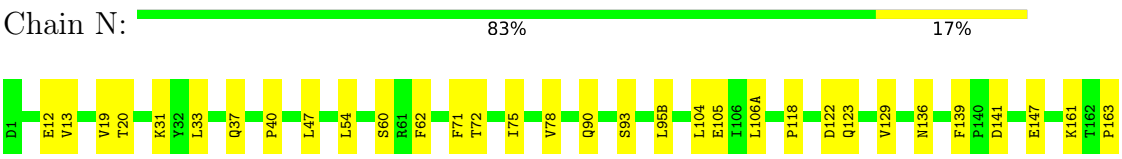
• Molecule 2: C59 Fab Heavy chain



• Molecule 2: C59 Fab Heavy chain

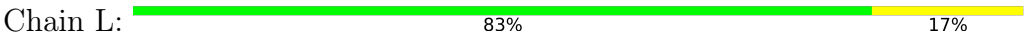


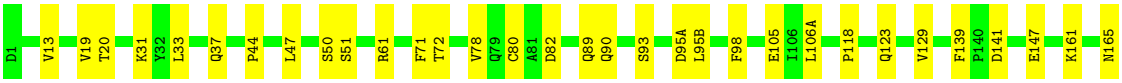
• Molecule 3: C59 Fab Light chain



• Molecule 3: C59 Fab Light chain

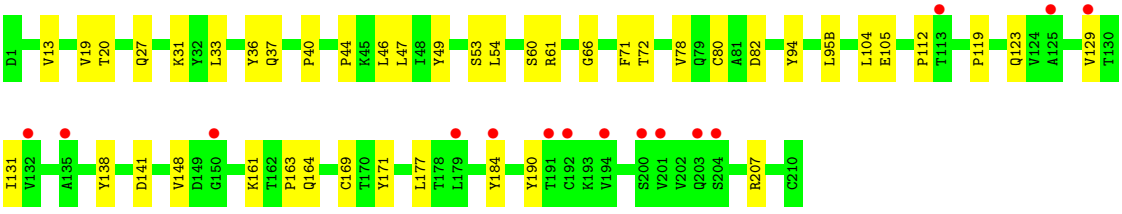
Chain L:





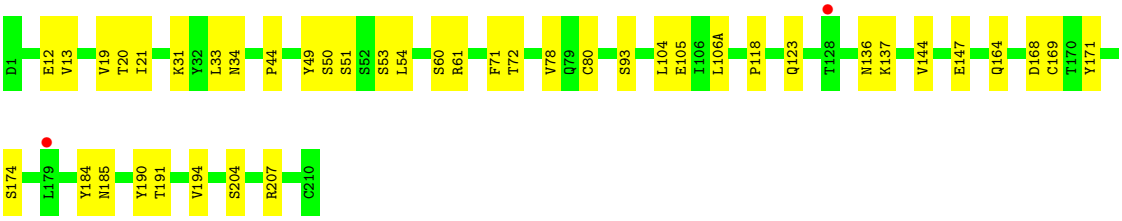
• Molecule 3: C59 Fab Light chain

Chain P:



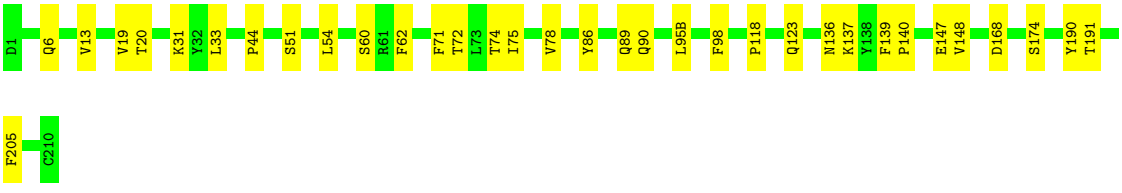
• Molecule 3: C59 Fab Light chain

Chain R:



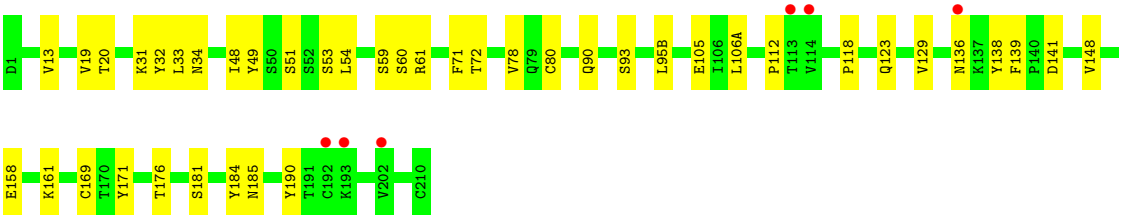
• Molecule 3: C59 Fab Light chain

Chain T:



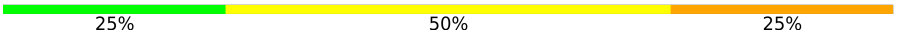
• Molecule 3: C59 Fab Light chain

Chain V:



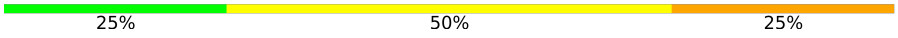
• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

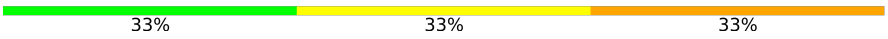
Chain I:

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

Chain K:

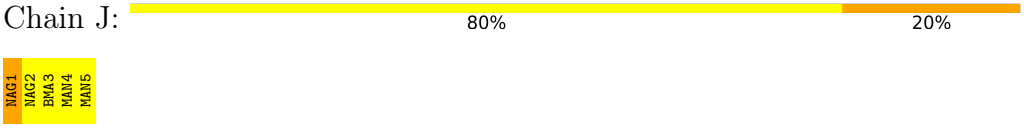
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.10Å 172.92Å 404.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.29 – 3.30 87.29 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.29-3.30) 99.9 (87.29-3.30)	Depositor EDS
R_{merge}	0.80	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.206 , 0.243 0.205 , 0.243	Depositor DCC
R_{free} test set	5499 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36890	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.46% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/2936	0.65	0/3978
1	B	0.40	0/2936	0.63	0/3978
1	C	0.41	0/2936	0.64	0/3978
1	D	0.42	0/2936	0.66	0/3978
1	E	0.41	0/2936	0.65	0/3978
1	F	0.43	0/2936	0.65	0/3978
2	H	0.36	0/1684	0.59	0/2311
2	M	0.37	0/1684	0.62	0/2311
2	O	0.35	0/1684	0.59	0/2311
2	Q	0.36	0/1684	0.60	0/2311
2	S	0.37	0/1684	0.59	0/2311
2	U	0.38	0/1684	0.61	0/2311
3	L	0.37	0/1629	0.59	0/2231
3	N	0.41	0/1629	0.60	0/2231
3	P	0.36	0/1629	0.58	0/2231
3	R	0.37	0/1629	0.58	0/2231
3	T	0.36	0/1629	0.58	0/2231
3	V	0.38	0/1629	0.59	0/2231
All	All	0.39	0/37494	0.62	0/51120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2860	0	2781	36	0
1	B	2860	0	2781	31	2
1	C	2860	0	2781	37	0
1	D	2860	0	2781	42	0
1	E	2860	0	2781	40	2
1	F	2860	0	2781	34	0
2	H	1647	0	1597	30	0
2	M	1647	0	1597	36	0
2	O	1647	0	1597	22	0
2	Q	1647	0	1597	30	0
2	S	1647	0	1597	21	0
2	U	1647	0	1597	25	0
3	L	1595	0	1532	25	0
3	N	1595	0	1532	26	0
3	P	1595	0	1532	31	0
3	R	1595	0	1532	35	0
3	T	1595	0	1532	26	0
3	V	1595	0	1532	34	0
4	G	50	0	43	1	0
4	W	50	0	43	1	0
5	I	39	0	34	1	0
5	K	39	0	34	1	0
5	X	39	0	34	4	0
6	J	61	0	52	1	0
All	All	36890	0	35700	507	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 7.

All (507) 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)
3:L:13:VAL:HG21	3:L:19:VAL:HG22	1.46	0.98
3:N:13:VAL:HG21	3:N:19:VAL:HG22	1.55	0.89
3:T:13:VAL:HG21	3:T:19:VAL:HG22	1.57	0.87
2:M:164:ARG:NH2	3:N:136:ASN:OD1	2.08	0.86
3:P:13:VAL:HG21	3:P:19:VAL:HG22	1.56	0.86
3:V:13:VAL:HG21	3:V:19:VAL:HG22	1.56	0.85
3:R:13:VAL:HG21	3:R:19:VAL:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:38:ARG:HB3	2:U:48:ILE:HD11	1.66	0.77
1:D:159:ILE:HD12	1:D:203:LEU:HD21	1.70	0.73
1:F:147:PRO:HG2	1:F:193:SER:HB3	1.73	0.71
1:A:213:PHE:HB3	1:A:240:SER:HB3	1.74	0.70
3:V:105:GLU:OE2	3:V:171:TYR:OH	2.08	0.69
1:A:147:PRO:HB2	1:A:193:SER:HB3	1.74	0.69
5:X:1:NAG:H3	5:X:1:NAG:H83	1.74	0.69
3:L:90:GLN:HE21	3:L:95(B):LEU:HD11	1.58	0.69
2:S:33:TYR:CZ	2:S:52(A):ILE:HG13	2.28	0.69
1:D:362:ASP:OD2	1:D:378:THR:HG23	1.93	0.68
3:P:119:PRO:HD3	3:P:131:ILE:HG22	1.76	0.68
1:B:118:THR:HG22	1:B:121:ARG:HH22	1.59	0.68
3:P:20:THR:HG23	3:P:72:THR:HG23	1.75	0.68
2:M:94:ARG:HD3	2:M:102:LEU:HD12	1.76	0.67
1:F:293:THR:HG23	1:F:303:GLU:OE2	1.93	0.67
1:A:130:PRO:O	1:A:134:THR:HG23	1.94	0.67
3:P:131:ILE:HD11	3:P:177:LEU:HD23	1.76	0.67
1:E:134:THR:HG22	3:T:31:LYS:HG2	1.77	0.67
1:C:293:THR:HG23	1:C:303:GLU:OE2	1.95	0.66
1:B:362:ASP:OD2	1:B:378:THR:HG23	1.94	0.66
1:B:293:THR:HG23	1:B:303:GLU:OE2	1.96	0.66
2:O:213:CYS:O	3:R:207:ARG:NH1	2.29	0.66
2:Q:95:ASP:HB3	2:Q:97:GLY:H	1.60	0.66
1:A:159:ILE:HD12	1:A:203:LEU:HD21	1.78	0.65
2:M:38:ARG:HB3	2:M:48:ILE:HD11	1.79	0.65
1:C:290:GLY:HA3	1:C:303:GLU:OE1	1.97	0.65
2:U:3:SER:HB3	2:U:25:SER:HB2	1.79	0.65
1:F:159:ILE:HD12	1:F:203:LEU:HD21	1.79	0.65
2:O:197:HIS:HB3	2:O:202:THR:HB	1.77	0.65
3:L:20:THR:HG23	3:L:72:THR:HG23	1.79	0.64
3:V:13:VAL:HG11	3:V:78:VAL:HG21	1.80	0.64
1:C:266:PHE:HB3	1:C:361:LEU:HD13	1.78	0.64
2:O:213:CYS:HB2	3:R:185:ASN:HB3	1.79	0.64
3:V:20:THR:HG23	3:V:72:THR:HG23	1.79	0.64
2:H:3:SER:HB3	2:H:25:SER:HB2	1.80	0.63
3:P:37:GLN:HB2	3:P:47:LEU:HD11	1.80	0.63
1:A:210:THR:HB	1:A:242:THR:HG22	1.80	0.63
2:M:168:SER:HB3	2:M:178:LEU:HD23	1.79	0.63
3:P:207:ARG:NH1	2:Q:213:CYS:O	2.32	0.63
1:D:214:HIS:CE1	1:D:218:ARG:HD3	2.34	0.62
2:Q:121:VAL:HG22	2:Q:142:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:THR:HB	1:C:325:THR:HG21	1.81	0.62
2:S:52:TYR:CE2	2:S:52(B):GLY:HA3	2.35	0.62
2:M:121:VAL:HG22	2:M:142:VAL:HG22	1.81	0.62
5:K:1:NAG:H83	5:K:1:NAG:H3	1.81	0.61
3:N:20:THR:HG23	3:N:72:THR:HG23	1.82	0.61
1:B:130:PRO:O	1:B:134:THR:HG23	1.99	0.61
1:D:130:PRO:O	1:D:134:THR:HG23	2.00	0.60
2:M:34:TYR:HB2	2:M:95:ASP:OD2	2.01	0.60
2:Q:52:TYR:CE2	2:Q:52(B):GLY:HA3	2.36	0.60
1:C:362:ASP:OD2	1:C:378:THR:HG23	2.02	0.60
1:C:159:ILE:HD12	1:C:203:LEU:HD21	1.83	0.60
1:B:159:ILE:HD12	1:B:203:LEU:HD21	1.83	0.60
1:D:142:LEU:HD12	1:D:159:ILE:HD13	1.83	0.60
3:V:90:GLN:HE21	3:V:95(B):LEU:HD11	1.67	0.60
1:A:293:THR:HG23	1:A:303:GLU:OE2	2.02	0.59
2:U:66:ARG:HH22	2:U:86:ASP:CG	2.05	0.59
1:B:213:PHE:HB3	1:B:240:SER:HB3	1.83	0.59
3:L:90:GLN:NE2	3:L:95(B):LEU:HD11	2.17	0.59
3:R:20:THR:HG23	3:R:72:THR:HG23	1.84	0.59
1:E:195:ASP:OD2	1:E:198:LYS:HD3	2.03	0.59
2:O:53:SER:O	2:O:55:THR:N	2.36	0.59
2:U:66:ARG:NH2	2:U:86:ASP:OD2	2.35	0.59
1:E:134:THR:HA	3:T:31:LYS:HE2	1.85	0.59
2:O:197:HIS:CE1	2:O:199:ALA:HB3	2.38	0.59
1:C:195:ASP:OD2	1:C:198:LYS:HD3	2.02	0.59
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.84	0.59
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.84	0.59
2:S:95:ASP:HB3	2:S:97:GLY:H	1.68	0.59
2:Q:38:ARG:HB3	2:Q:48:ILE:HD11	1.85	0.58
2:U:13:LYS:NZ	2:U:115:GLN:OE1	2.24	0.58
1:C:130:PRO:O	1:C:134:THR:HG23	2.03	0.58
2:Q:34:TYR:H	2:Q:95:ASP:HB2	1.68	0.58
1:E:362:ASP:OD2	1:E:378:THR:HG23	2.03	0.58
2:M:53:SER:O	2:M:55:THR:N	2.32	0.58
1:D:217:TRP:CZ3	1:D:218:ARG:HG2	2.39	0.58
1:F:210:THR:HB	1:F:242:THR:HG22	1.85	0.58
1:A:134:THR:HA	3:L:31:LYS:HE2	1.84	0.58
1:C:213:PHE:HB3	1:C:240:SER:HB3	1.84	0.58
4:G:1:NAG:H3	4:G:1:NAG:H83	1.86	0.58
2:Q:127:CYS:HB3	3:R:118:PRO:HG2	1.86	0.58
1:B:174:LYS:HG2	2:M:98:TRP:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:HA3	1:B:303:GLU:OE1	2.04	0.57
2:U:164:ARG:NH2	3:V:136:ASN:OD1	2.37	0.57
1:F:213:PHE:HB3	1:F:240:SER:HB3	1.86	0.57
2:O:27:PHE:CE2	2:O:94:ARG:HD2	2.40	0.57
3:N:147:GLU:HB2	3:N:191:THR:HB	1.86	0.57
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.85	0.57
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.31	0.57
2:U:4:VAL:HG13	2:U:22:CYS:SG	2.45	0.57
1:D:293:THR:HG23	1:D:303:GLU:OE2	2.05	0.57
1:E:122:ARG:NH2	1:E:126:LYS:HD3	2.20	0.57
1:A:134:THR:HG22	3:L:31:LYS:HG2	1.86	0.56
1:A:118:THR:HG22	1:A:121:ARG:HH22	1.70	0.56
1:F:134:THR:HG22	3:V:31:LYS:HG2	1.87	0.56
1:A:171:GLN:OE1	3:L:93:SER:HB2	2.05	0.56
3:L:13:VAL:HG11	3:L:78:VAL:HG21	1.87	0.56
2:O:34:TYR:HB2	2:O:95:ASP:OD2	2.05	0.56
3:N:54:LEU:HD11	3:N:60:SER:HA	1.88	0.56
3:T:54:LEU:HD11	3:T:60:SER:HA	1.88	0.56
2:M:127:CYS:HB3	3:N:118:PRO:HG2	1.88	0.56
1:D:118:THR:HG22	1:D:121:ARG:HH22	1.71	0.56
1:B:122:ARG:NH1	1:B:126:LYS:HD3	2.21	0.56
1:C:122:ARG:NH2	1:C:126:LYS:HD3	2.21	0.56
3:P:61:ARG:NH1	3:P:82:ASP:OD2	2.32	0.55
3:T:20:THR:HG23	3:T:72:THR:HG23	1.88	0.55
1:D:35:SER:O	1:D:38:GLN:HG2	2.06	0.55
1:F:277:THR:HB	1:F:325:THR:HG21	1.88	0.55
2:Q:122:PHE:CD2	3:R:123:GLN:HG3	2.42	0.55
1:B:174:LYS:HG2	2:M:98:TRP:CG	2.41	0.55
1:C:227:LEU:HD13	1:C:342:LYS:HG2	1.87	0.55
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.40	0.55
2:Q:51:ILE:HG13	2:Q:57:THR:HG22	1.89	0.55
5:I:1:NAG:H83	5:I:1:NAG:H3	1.87	0.55
3:L:105:GLU:OE2	3:L:171:TYR:OH	2.25	0.55
1:A:142:LEU:HD12	1:A:159:ILE:HD13	1.89	0.54
1:D:328:ASN:OD1	1:D:329:GLN:NE2	2.37	0.54
1:B:118:THR:HG22	1:B:121:ARG:NH2	2.22	0.54
1:F:227:LEU:HD13	1:F:342:LYS:HG2	1.90	0.54
2:O:4:VAL:HG13	2:O:22:CYS:SG	2.47	0.54
1:B:208:ILE:HB	1:B:249:MET:HE1	1.89	0.54
2:Q:13:LYS:NZ	2:Q:115:GLN:OE1	2.33	0.54
3:V:80:CYS:SG	3:V:169:CYS:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:123:PRO:HB3	2:M:208:VAL:HG22	1.90	0.54
2:Q:3:SER:HB3	2:Q:25:SER:HB2	1.90	0.54
3:R:184:TYR:O	3:R:190:TYR:OH	2.24	0.54
1:D:134:THR:HG21	3:R:31:LYS:H	1.73	0.54
2:H:31:SER:HB2	2:H:52(B):GLY:HA2	1.89	0.54
2:M:184:VAL:HB	2:M:188:SER:HB2	1.90	0.54
1:E:183:LEU:HD22	1:E:194:TYR:CZ	2.43	0.53
2:U:117:LYS:HE3	2:U:144:GLY:O	2.08	0.53
1:B:61:TYR:HD2	1:B:85:LEU:HD12	1.72	0.53
1:C:134:THR:HG22	3:P:31:LYS:HG2	1.90	0.53
2:S:34:TYR:H	2:S:95:ASP:HB2	1.72	0.53
2:U:197:HIS:HB3	2:U:202:THR:HB	1.89	0.53
2:S:27:PHE:CE2	2:S:94:ARG:HD3	2.43	0.53
1:C:118:THR:HG22	1:C:121:ARG:HH22	1.73	0.53
1:C:134:THR:HA	3:P:31:LYS:HE2	1.90	0.53
1:C:225:SER:OG	1:C:342:LYS:NZ	2.39	0.53
1:C:55:LEU:HD21	1:C:378:THR:OG1	2.09	0.53
3:N:105:GLU:OE2	3:N:171:TYR:OH	2.26	0.53
2:O:40:ALA:HB3	2:O:43:LYS:HE2	1.90	0.53
1:A:277:THR:HB	1:A:325:THR:HG21	1.91	0.53
1:E:213:PHE:HB3	1:E:240:SER:HB3	1.90	0.53
2:M:119:PRO:HB2	2:M:142:VAL:HG13	1.90	0.52
3:P:33:LEU:HD22	3:P:71:PHE:CG	2.44	0.52
2:Q:119:PRO:HB2	2:Q:142:VAL:HG13	1.91	0.52
2:Q:138:LEU:HD11	2:Q:210:PRO:HA	1.89	0.52
1:A:356:VAL:HG11	1:A:378:THR:HG22	1.92	0.52
3:P:112:PRO:HB3	3:P:138:TYR:HB3	1.91	0.52
2:S:96:LYS:HD2	2:S:100(E):TYR:OH	2.10	0.52
3:P:94:TYR:HA	3:P:95(B):LEU:HD12	1.91	0.52
3:V:31:LYS:O	3:V:51:SER:N	2.43	0.52
1:F:31:CYS:HB3	1:F:359:LEU:HG	1.92	0.52
2:U:154:TRP:CZ3	2:U:193:CYS:HB3	2.44	0.52
2:M:3:SER:HB3	2:M:25:SER:HB2	1.91	0.52
1:B:134:THR:HA	3:N:31:LYS:HE2	1.92	0.52
2:Q:94:ARG:HE	2:Q:102:LEU:HD12	1.75	0.52
1:E:130:PRO:O	1:E:134:THR:HG23	2.10	0.52
2:M:194:ASN:ND2	2:M:205:ASP:OD1	2.43	0.52
2:H:103:TRP:CE3	3:L:44:PRO:HD2	2.45	0.52
5:X:1:NAG:H3	5:X:1:NAG:C8	2.38	0.51
1:D:290:GLY:HA3	1:D:303:GLU:OE1	2.11	0.51
2:Q:103:TRP:CE3	3:R:44:PRO:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:TRP:CZ2	1:E:77:ASN:ND2	2.79	0.51
2:U:154:TRP:HB3	2:U:159:LEU:HD23	1.93	0.51
1:B:134:THR:HG22	3:N:31:LYS:HG2	1.93	0.51
1:F:130:PRO:O	1:F:134:THR:HG23	2.11	0.51
1:F:362:ASP:OD2	1:F:378:THR:HG23	2.10	0.51
2:M:4:VAL:HG13	2:M:22:CYS:SG	2.51	0.51
1:C:356:VAL:HG11	1:C:378:THR:HG22	1.91	0.51
3:P:33:LEU:HD22	3:P:71:PHE:CB	2.41	0.51
2:H:127:CYS:HB3	3:L:118:PRO:HG2	1.93	0.51
3:T:33:LEU:HD22	3:T:71:PHE:CB	2.41	0.51
1:A:66:ILE:HG21	1:A:114:ILE:HD13	1.92	0.51
2:M:66:ARG:NH2	2:M:86:ASP:OD2	2.44	0.51
2:S:4:VAL:HG13	2:S:22:CYS:SG	2.51	0.51
1:E:340:LYS:HD3	1:E:384:ALA:HB2	1.93	0.51
2:M:122:PHE:CD2	3:N:123:GLN:HG3	2.46	0.51
2:H:96:LYS:HD2	2:H:100(E):TYR:HE1	1.76	0.51
3:P:80:CYS:SG	3:P:169:CYS:N	2.83	0.50
2:Q:40:ALA:HB3	2:Q:43:LYS:HE2	1.93	0.50
2:Q:168:SER:HB3	2:Q:178:LEU:HD23	1.92	0.50
2:S:12:VAL:HG21	2:S:82(B):LEU:HD13	1.94	0.50
2:U:96:LYS:HE3	2:U:101:GLN:OE1	2.11	0.50
1:E:147:PRO:HB2	1:E:193:SER:HB3	1.92	0.50
2:M:95:ASP:HB3	2:M:97:GLY:H	1.76	0.50
1:E:67:SER:HA	4:W:1:NAG:H62	1.93	0.50
1:F:290:GLY:HA3	1:F:303:GLU:OE1	2.11	0.50
2:O:213:CYS:HB2	3:R:185:ASN:O	2.11	0.50
3:R:12:GLU:CD	3:R:106(A):LEU:HD21	2.32	0.50
2:S:164:ARG:NH2	3:T:136:ASN:OD1	2.35	0.50
6:J:1:NAG:H3	6:J:1:NAG:H83	1.93	0.50
1:D:134:THR:HA	3:R:31:LYS:HE2	1.93	0.50
1:E:55:LEU:HD21	1:E:378:THR:OG1	2.12	0.50
3:P:141:ASP:OD2	3:P:161:LYS:NZ	2.45	0.50
3:R:54:LEU:HD11	3:R:60:SER:HA	1.94	0.50
3:R:12:GLU:HG2	3:R:105:GLU:HB3	1.93	0.50
3:T:147:GLU:HB2	3:T:191:THR:HB	1.94	0.50
1:D:134:THR:HG22	3:R:31:LYS:HG2	1.92	0.50
3:T:89:GLN:HB2	3:T:98:PHE:CD1	2.47	0.50
1:C:217:TRP:CZ3	1:C:218:ARG:HG2	2.47	0.50
1:E:118:THR:HG22	1:E:121:ARG:HH22	1.77	0.50
3:T:90:GLN:NE2	3:T:95(B):LEU:HD11	2.27	0.49
1:A:51:LEU:HD22	1:A:359:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:VAL:HG13	2:H:22:CYS:SG	2.52	0.49
1:E:58:HIS:HA	1:E:96:LYS:O	2.12	0.49
3:N:12:GLU:HG2	3:N:105:GLU:HB3	1.94	0.49
3:P:105:GLU:OE2	3:P:171:TYR:OH	2.30	0.49
3:V:90:GLN:NE2	3:V:95(B):LEU:HD11	2.26	0.49
1:A:362:ASP:OD2	1:A:378:THR:HG23	2.12	0.49
3:L:89:GLN:HB2	3:L:98:PHE:CD1	2.48	0.49
3:R:147:GLU:HB2	3:R:191:THR:HB	1.94	0.49
2:M:35:MET:HG2	2:M:77:VAL:HG21	1.95	0.49
2:O:29:ILE:O	2:O:29:ILE:HD12	2.12	0.49
1:D:122:ARG:NH2	1:D:126:LYS:HD3	2.28	0.49
1:F:61:TYR:HD2	1:F:85:LEU:HD12	1.76	0.49
2:M:31:SER:HB2	2:M:52(B):GLY:HA2	1.95	0.49
2:O:51:ILE:HG13	2:O:57:THR:HG22	1.93	0.49
3:P:54:LEU:HD11	3:P:60:SER:HA	1.95	0.49
2:Q:17:SER:HB2	2:Q:81:MET:O	2.13	0.49
1:E:277:THR:HB	1:E:325:THR:HG21	1.94	0.48
1:C:134:THR:HG21	3:P:31:LYS:H	1.79	0.48
3:V:141:ASP:OD2	3:V:161:LYS:NZ	2.43	0.48
1:C:126:LYS:HD2	3:P:27:GLN:OE1	2.13	0.48
3:V:106(A):LEU:HA	3:V:139:PHE:CZ	2.48	0.48
1:C:311:ALA:HB2	1:C:326:LYS:HB2	1.95	0.48
3:N:13:VAL:HG11	3:N:78:VAL:HG21	1.95	0.48
3:V:49:TYR:O	3:V:53:SER:HB2	2.12	0.48
1:F:134:THR:HG21	3:V:31:LYS:H	1.78	0.48
2:Q:130:ASP:N	2:Q:130:ASP:OD1	2.46	0.48
3:R:144:VAL:HG22	3:R:194:VAL:HG22	1.94	0.48
2:S:11:LEU:HB2	2:S:147:PRO:HG3	1.94	0.48
1:A:346:LEU:HB2	1:A:351:LEU:HD12	1.95	0.48
1:E:299:LEU:HD12	1:E:331:VAL:HG21	1.95	0.48
3:N:190:TYR:HB2	3:N:205:PHE:CE1	2.49	0.48
3:T:137:LYS:NZ	3:T:168:ASP:OD2	2.33	0.48
2:M:168:SER:HA	2:M:178:LEU:HB3	1.95	0.48
2:H:35:MET:HG2	2:H:77:VAL:HG21	1.96	0.48
1:D:66:ILE:HG21	1:D:114:ILE:HD13	1.95	0.48
1:D:304:ILE:O	1:D:308:LEU:HG	2.14	0.48
2:U:127:CYS:HB3	3:V:118:PRO:HG2	1.96	0.48
1:A:174:LYS:HG2	2:H:98:TRP:CD1	2.49	0.47
1:D:149:ARG:HA	1:D:192:SER:O	2.13	0.47
2:H:197:HIS:HB3	2:H:202:THR:HB	1.95	0.47
2:O:38:ARG:HB3	2:O:48:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:139:PHE:CD1	3:T:140:PRO:HA	2.49	0.47
1:C:61:TYR:HD2	1:C:85:LEU:HD12	1.79	0.47
2:O:3:SER:HB3	2:O:25:SER:HB2	1.95	0.47
1:A:118:THR:HG22	1:A:121:ARG:NH2	2.29	0.47
1:D:58:HIS:HA	1:D:96:LYS:O	2.14	0.47
1:E:134:THR:HG21	3:T:31:LYS:H	1.80	0.47
3:V:59:SER:OG	3:V:61:ARG:HG3	2.15	0.47
3:V:148:VAL:HG22	3:V:190:TYR:HD1	1.79	0.47
2:H:96:LYS:HD2	2:H:100(E):TYR:CE1	2.49	0.47
3:L:80:CYS:SG	3:L:169:CYS:N	2.87	0.47
1:B:208:ILE:HD11	1:B:245:ALA:HB1	1.96	0.47
1:F:174:LYS:HG2	2:U:98:TRP:CG	2.49	0.47
2:Q:35:MET:HG2	2:Q:77:VAL:HG21	1.96	0.47
3:R:49:TYR:O	3:R:53:SER:HB2	2.15	0.47
1:C:146:TYR:CE1	1:C:184:SER:HB2	2.50	0.47
1:E:76:TRP:CE2	1:E:77:ASN:ND2	2.82	0.47
1:E:356:VAL:HG11	1:E:378:THR:HG22	1.96	0.47
1:F:77:ASN:HB2	1:F:81:LEU:HD13	1.97	0.47
2:O:103:TRP:CE3	3:P:44:PRO:HD2	2.50	0.47
3:T:62:PHE:CD1	3:T:75:ILE:HG12	2.50	0.47
1:E:269:SER:HB3	1:E:331:VAL:HG22	1.97	0.47
2:M:11:LEU:HB2	2:M:147:PRO:HG3	1.96	0.47
2:S:33:TYR:CE2	2:S:52(A):ILE:HG13	2.50	0.47
1:B:142:LEU:HD12	1:B:159:ILE:HD13	1.97	0.46
1:E:30:VAL:O	1:E:355:MET:HA	2.15	0.46
1:E:159:ILE:HD12	1:E:203:LEU:HD21	1.97	0.46
2:H:33:TYR:CE2	2:H:52(A):ILE:HG13	2.48	0.46
3:L:106(A):LEU:HA	3:L:139:PHE:CZ	2.50	0.46
3:P:66:GLY:HA3	3:P:71:PHE:HA	1.97	0.46
5:X:1:NAG:H83	5:X:1:NAG:C3	2.44	0.46
1:F:171:GLN:OE1	3:V:93:SER:HB2	2.15	0.46
3:V:33:LEU:HG	3:V:34:ASN:N	2.30	0.46
1:A:55:LEU:HD21	1:A:378:THR:OG1	2.15	0.46
1:C:315:ARG:NH1	1:C:335:ASP:OD2	2.40	0.46
1:B:210:THR:HB	1:B:242:THR:HG22	1.97	0.46
1:F:259:LEU:HD23	1:F:259:LEU:HA	1.71	0.46
3:N:90:GLN:NE2	3:N:95(B):LEU:HD11	2.31	0.46
3:N:129:VAL:HG21	3:N:184:TYR:HB2	1.96	0.46
1:C:52:ASP:HB3	1:C:55:LEU:HB2	1.97	0.46
1:F:134:THR:CG2	3:V:31:LYS:H	2.28	0.46
3:P:13:VAL:HG11	3:P:78:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:181:SER:O	3:V:185:ASN:ND2	2.49	0.46
1:B:134:THR:HG21	3:N:31:LYS:H	1.81	0.46
1:E:208:ILE:HD12	1:E:249:MET:HE2	1.97	0.45
1:F:299:LEU:HD12	1:F:331:VAL:HG21	1.98	0.45
1:A:269:SER:HB3	1:A:331:VAL:HG22	1.98	0.45
1:B:33:TYR:CE2	1:B:48:PRO:HG3	2.51	0.45
1:D:226:PRO:O	1:D:242:THR:HG23	2.16	0.45
2:S:51:ILE:HG13	2:S:57:THR:HG22	1.97	0.45
3:N:141:ASP:OD2	3:N:161:LYS:NZ	2.42	0.45
1:C:198:LYS:O	1:C:201:GLN:HG2	2.16	0.45
1:A:112:SER:HB2	1:A:151:ASP:OD2	2.17	0.45
1:C:174:LYS:HG2	2:O:98:TRP:CD1	2.51	0.45
1:D:340:LYS:HD3	1:D:384:ALA:HB2	1.98	0.45
1:A:259:LEU:HA	1:A:259:LEU:HD23	1.68	0.45
1:F:29:LEU:O	1:F:56:CYS:HB3	2.17	0.45
1:F:96:LYS:HA	1:F:138:ASP:OD2	2.17	0.45
2:M:22:CYS:HB3	2:M:77:VAL:HG22	1.99	0.45
2:H:31:SER:O	2:H:33:TYR:N	2.50	0.45
2:S:127:CYS:HB3	3:T:118:PRO:HG2	1.99	0.45
1:F:163:LYS:O	1:F:167:ILE:HG13	2.17	0.45
2:O:194:ASN:HB3	2:O:203:LYS:HE3	1.99	0.45
1:F:146:TYR:CE1	1:F:184:SER:HB2	2.52	0.45
1:F:183:LEU:HB3	1:F:194:TYR:CE2	2.52	0.45
2:M:122:PHE:CE2	3:N:123:GLN:HG3	2.52	0.44
2:O:119:PRO:HB2	2:O:142:VAL:HG13	1.99	0.44
3:P:129:VAL:HG21	3:P:184:TYR:HB2	1.99	0.44
1:D:271:THR:HG23	1:D:328:ASN:OD1	2.17	0.44
3:L:147:GLU:HB2	3:L:191:THR:HB	1.98	0.44
2:Q:4:VAL:HG13	2:Q:22:CYS:SG	2.57	0.44
2:H:123:PRO:HB3	2:H:208:VAL:HG22	1.99	0.44
3:P:40:PRO:HG2	3:P:163:PRO:HB3	1.98	0.44
2:Q:27:PHE:CE2	2:Q:94:ARG:HD3	2.52	0.44
2:S:103:TRP:CE3	3:T:44:PRO:HD2	2.53	0.44
2:S:122:PHE:CD2	3:T:123:GLN:HG3	2.53	0.44
2:U:100:ASN:O	3:V:32:TYR:OH	2.23	0.44
1:D:148:GLY:H	1:D:151:ASP:HB2	1.81	0.44
2:H:73:SER:HB3	2:H:76:THR:OG1	2.18	0.44
2:H:165:THR:HG23	2:H:180:SER:HB2	1.99	0.44
3:R:34:ASN:OD1	3:R:49:TYR:HA	2.17	0.44
1:B:101:VAL:HG23	1:B:140:LEU:HD11	1.98	0.44
1:E:75:GLU:HG3	1:E:76:TRP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:THR:HG22	1:E:377:LEU:HD12	1.99	0.44
2:O:130:ASP:N	2:O:130:ASP:OD1	2.50	0.44
1:A:101:VAL:HG23	1:A:140:LEU:HD11	1.99	0.44
1:F:271:THR:HG23	1:F:328:ASN:OD1	2.18	0.44
3:P:36:TYR:CD1	3:P:46:LEU:HA	2.52	0.44
3:P:49:TYR:O	3:P:53:SER:HB2	2.17	0.44
1:D:134:THR:CG2	3:R:31:LYS:H	2.31	0.44
2:O:11:LEU:HB2	2:O:147:PRO:HG3	2.00	0.44
3:P:148:VAL:HG22	3:P:190:TYR:CD1	2.53	0.44
3:R:13:VAL:HG11	3:R:78:VAL:HG21	2.00	0.44
1:A:322:PRO:HD3	1:A:338:SER:HB3	1.99	0.44
3:N:106(A):LEU:HA	3:N:139:PHE:CZ	2.53	0.44
3:T:6:GLN:NE2	3:T:86:TYR:O	2.51	0.44
1:C:269:SER:HB3	1:C:331:VAL:HG22	1.98	0.44
1:D:100:SER:HA	1:D:141:ASP:O	2.18	0.44
1:D:144:TRP:O	1:D:147:PRO:HD3	2.18	0.44
2:H:130:ASP:OD1	2:H:130:ASP:N	2.50	0.44
3:R:137:LYS:NZ	3:R:168:ASP:OD2	2.36	0.44
1:A:200:SER:HB3	1:A:255:PRO:HD3	2.00	0.43
1:B:66:ILE:HG21	1:B:114:ILE:HD13	2.00	0.43
2:U:145:TYR:CE2	2:U:150:VAL:HG13	2.53	0.43
1:B:33:TYR:OH	1:B:48:PRO:HD3	2.18	0.43
1:D:55:LEU:HD21	1:D:378:THR:OG1	2.18	0.43
2:M:2:PCA:HB3	2:M:102:LEU:HD11	1.99	0.43
3:P:148:VAL:HG22	3:P:190:TYR:HD1	1.83	0.43
3:R:104:LEU:HD23	3:R:104:LEU:HA	1.91	0.43
2:U:197:HIS:CE1	2:U:199:ALA:HB3	2.53	0.43
1:E:362:ASP:OD1	1:E:363:ASP:N	2.50	0.43
1:D:311:ALA:HB2	1:D:326:LYS:HB2	2.00	0.43
2:M:125:ALA:O	3:N:118:PRO:HD2	2.17	0.43
2:M:135:THR:OG1	2:M:185:THR:HG22	2.18	0.43
3:N:40:PRO:HG2	3:N:163:PRO:HB3	1.98	0.43
2:S:119:PRO:HB2	2:S:142:VAL:HG13	1.99	0.43
2:M:197:HIS:CE1	2:M:199:ALA:HB3	2.53	0.43
2:M:197:HIS:HB3	2:M:202:THR:HB	1.99	0.43
3:L:141:ASP:OD2	3:L:161:LYS:NZ	2.39	0.43
1:B:146:TYR:CE1	1:B:184:SER:HB2	2.54	0.43
1:C:31:CYS:HB3	1:C:359:LEU:HG	2.01	0.43
1:E:76:TRP:CE2	3:R:61:ARG:HG2	2.53	0.43
2:S:197:HIS:HB3	2:S:202:THR:HB	2.01	0.43
3:V:129:VAL:HG21	3:V:184:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:HD3	3:L:95(A):ASP:OD2	2.19	0.43
1:B:163:LYS:HA	1:B:163:LYS:HD3	1.91	0.43
2:M:31:SER:O	2:M:33:TYR:N	2.52	0.43
2:H:36:TRP:CE2	2:H:79:LEU:HB2	2.54	0.43
2:U:35:MET:HG2	2:U:77:VAL:HG21	2.01	0.43
1:B:226:PRO:O	1:B:242:THR:HG23	2.18	0.43
1:C:55:LEU:HD21	1:C:378:THR:HG1	1.84	0.43
1:D:31:CYS:HB3	1:D:359:LEU:HG	2.01	0.43
1:E:208:ILE:HG22	1:E:260:VAL:O	2.18	0.43
1:F:72:ASP:OD1	1:F:73:THR:N	2.51	0.43
3:R:33:LEU:HD22	3:R:71:PHE:CB	2.49	0.43
2:U:122:PHE:CD2	3:V:123:GLN:HG3	2.54	0.43
1:A:288:ILE:HG12	1:A:329:GLN:NE2	2.33	0.43
1:C:48:PRO:O	1:C:51:LEU:HG	2.19	0.43
1:C:128:VAL:HB	1:C:129:PRO:HD3	2.01	0.43
1:C:226:PRO:O	1:C:242:THR:HG23	2.18	0.43
5:X:1:NAG:C8	5:X:1:NAG:C3	2.97	0.43
1:B:356:VAL:HG11	1:B:378:THR:HG22	2.00	0.42
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.22	0.42
3:T:13:VAL:HG11	3:T:78:VAL:HG21	2.01	0.42
1:C:259:LEU:O	1:C:352:ALA:HB3	2.19	0.42
2:S:94:ARG:HG2	2:S:95:ASP:O	2.19	0.42
3:V:54:LEU:HD23	3:V:54:LEU:HA	1.91	0.42
1:B:100:SER:HA	1:B:141:ASP:O	2.19	0.42
3:N:33:LEU:HD22	3:N:71:PHE:CB	2.49	0.42
3:R:54:LEU:HD23	3:R:54:LEU:HA	1.79	0.42
3:T:62:PHE:HD1	3:T:75:ILE:HG12	1.83	0.42
3:T:139:PHE:CG	3:T:140:PRO:HA	2.54	0.42
2:U:125:ALA:O	3:V:118:PRO:HD2	2.19	0.42
1:C:159:ILE:CD1	1:C:203:LEU:HD21	2.49	0.42
1:D:53:ARG:CZ	1:D:91:ARG:HD2	2.49	0.42
1:D:198:LYS:O	1:D:201:GLN:HG2	2.19	0.42
1:D:269:SER:HB3	1:D:331:VAL:HG22	2.01	0.42
2:O:122:PHE:CD2	3:P:123:GLN:HG3	2.55	0.42
2:Q:12:VAL:HG11	2:Q:18:LEU:HB2	2.02	0.42
2:Q:125:ALA:O	3:R:118:PRO:HD2	2.19	0.42
2:U:51:ILE:HD13	2:U:71:LYS:HG3	2.01	0.42
3:V:158:GLU:HB3	3:V:176:THR:OG1	2.20	0.42
1:D:208:ILE:HD11	1:D:245:ALA:HB1	2.01	0.42
1:E:31:CYS:HB3	1:E:359:LEU:HG	2.02	0.42
1:F:89:LYS:HD2	1:F:97:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:31:LYS:O	3:R:51:SER:N	2.53	0.42
1:B:363:ASP:OD2	1:B:369:CYS:HB2	2.20	0.42
1:C:66:ILE:HG21	1:C:114:ILE:HD13	2.02	0.42
1:F:183:LEU:HD22	1:F:194:TYR:CZ	2.55	0.42
2:H:122:PHE:CD2	3:L:123:GLN:HG3	2.55	0.42
1:A:100:SER:HA	1:A:141:ASP:O	2.19	0.42
1:E:259:LEU:HD23	1:E:259:LEU:HA	1.81	0.42
1:F:108:SER:HA	1:F:144:TRP:HE1	1.85	0.42
3:T:190:TYR:HB2	3:T:205:PHE:CE1	2.54	0.42
2:U:73:SER:OG	2:U:74:SER:N	2.53	0.42
1:F:100:SER:HA	1:F:141:ASP:O	2.19	0.41
2:H:17:SER:HB2	2:H:81:MET:O	2.20	0.41
3:L:129:VAL:HG21	3:L:184:TYR:HB2	2.02	0.41
3:P:104:LEU:HA	3:P:104:LEU:HD23	1.74	0.41
2:Q:31:SER:OG	2:Q:52(A):ILE:O	2.34	0.41
3:V:184:TYR:O	3:V:190:TYR:OH	2.38	0.41
1:A:339:VAL:CG1	1:A:381:ILE:HG13	2.50	0.41
1:D:171:GLN:OE1	3:R:93:SER:HB2	2.20	0.41
1:E:304:ILE:O	1:E:308:LEU:HG	2.20	0.41
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.55	0.41
3:T:19:VAL:O	3:T:74:THR:HA	2.20	0.41
1:B:144:TRP:O	1:B:147:PRO:HD3	2.19	0.41
1:D:73:THR:OG1	1:D:78:ASP:HB2	2.21	0.41
2:H:184:VAL:HB	2:H:188:SER:HB2	2.02	0.41
2:Q:164:ARG:NH2	3:R:136:ASN:OD1	2.43	0.41
3:R:80:CYS:SG	3:R:169:CYS:N	2.94	0.41
3:V:33:LEU:HD22	3:V:71:PHE:CB	2.50	0.41
3:V:148:VAL:HG22	3:V:190:TYR:CD1	2.54	0.41
1:A:122:ARG:NH2	1:A:126:LYS:HD3	2.35	0.41
2:M:40:ALA:HB3	2:M:43:LYS:HE2	2.00	0.41
3:L:33:LEU:HD22	3:L:71:PHE:CB	2.51	0.41
2:Q:66:ARG:NH2	2:Q:86:ASP:OD2	2.53	0.41
1:D:163:LYS:HA	1:D:163:LYS:HD3	1.89	0.41
1:D:356:VAL:HG11	1:D:378:THR:HG22	2.03	0.41
1:E:357:TRP:HA	1:E:358:ALA:HA	1.87	0.41
3:N:122:ASP:OD1	3:N:122:ASP:N	2.52	0.41
2:O:213:CYS:CB	3:R:185:ASN:HB3	2.50	0.41
2:S:2:PCA:C	2:S:102:LEU:HD11	2.41	0.41
2:S:184:VAL:HB	2:S:188:SER:HB2	2.02	0.41
3:T:31:LYS:O	3:T:51:SER:N	2.54	0.41
1:D:52:ASP:HB3	1:D:55:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HD12	1:D:249:MET:HE2	2.03	0.41
1:E:52:ASP:HB3	1:E:55:LEU:HB2	2.03	0.41
1:A:115:ALA:HB2	1:A:158:LEU:HD12	2.02	0.41
1:A:128:VAL:HB	1:A:129:PRO:HD3	2.03	0.41
1:E:134:THR:CG2	3:T:31:LYS:H	2.33	0.41
2:Q:122:PHE:CE2	3:R:123:GLN:HG3	2.56	0.41
1:E:66:ILE:HD11	1:E:101:VAL:HG11	2.03	0.41
3:N:104:LEU:HD23	3:N:104:LEU:HA	1.78	0.41
2:H:11:LEU:HB2	2:H:147:PRO:HG3	2.02	0.41
2:H:36:TRP:O	2:H:48:ILE:HB	2.20	0.41
3:P:164:GLN:HG2	3:P:171:TYR:CE1	2.56	0.41
2:U:52:TYR:CE2	2:U:52(B):GLY:HA3	2.56	0.41
1:D:118:THR:HG22	1:D:121:ARG:NH2	2.34	0.41
2:M:66:ARG:HH22	2:M:86:ASP:CG	2.24	0.41
3:L:31:LYS:O	3:L:51:SER:N	2.54	0.41
2:Q:52:TYR:C	2:Q:52(B):GLY:H	2.25	0.41
3:R:164:GLN:HG2	3:R:171:TYR:CE1	2.55	0.41
3:V:112:PRO:HB3	3:V:138:TYR:HB3	2.03	0.41
1:F:356:VAL:HG11	1:F:378:THR:HG22	2.04	0.41
2:M:36:TRP:CE2	2:M:79:LEU:HB2	2.56	0.41
2:H:53:SER:HB2	2:H:56:ASP:OD1	2.21	0.41
2:Q:98:TRP:CG	2:Q:99:SER:N	2.89	0.41
3:V:48:ILE:HA	3:V:53:SER:O	2.21	0.41
1:A:101:VAL:CG2	1:A:140:LEU:HD11	2.51	0.40
1:E:142:LEU:HD12	1:E:159:ILE:HD13	2.02	0.40
1:E:227:LEU:HD13	1:E:342:LYS:HG2	2.02	0.40
2:H:34:TYR:HB2	2:H:95:ASP:OD2	2.20	0.40
1:A:299:LEU:HD12	1:A:331:VAL:HG21	2.03	0.40
1:C:259:LEU:HA	1:C:259:LEU:HD23	1.70	0.40
1:D:115:ALA:HB2	1:D:158:LEU:HD12	2.03	0.40
1:E:163:LYS:HA	1:E:163:LYS:HD3	1.86	0.40
1:F:259:LEU:O	1:F:352:ALA:HB3	2.20	0.40
2:M:130:ASP:N	2:M:130:ASP:OD1	2.53	0.40
2:M:138:LEU:HD21	2:M:210:PRO:HA	2.03	0.40
3:T:148:VAL:HG22	3:T:190:TYR:CD1	2.56	0.40
1:B:76:TRP:HH2	3:V:60:SER:HB2	1.87	0.40
1:D:108:SER:HB2	1:D:144:TRP:HE1	1.85	0.40
1:F:195:ASP:OD2	1:F:198:LYS:HD3	2.22	0.40
3:N:62:PHE:CD1	3:N:75:ILE:HG12	2.57	0.40
2:H:95:ASP:HB3	2:H:97:GLY:H	1.87	0.40
2:H:99:SER:HB3	2:H:100(C):GLY:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:165:ASN:HB3	3:L:168:ASP:OD1	2.20	0.40
2:U:119:PRO:HB2	2:U:142:VAL:HG13	2.04	0.40
1:A:174:LYS:HG2	2:H:98:TRP:CG	2.57	0.40
3:R:21:ILE:HD13	3:R:21:ILE:HG21	1.76	0.40
2:S:34:TYR:HB2	2:S:95:ASP:OD2	2.22	0.40
2:U:159:LEU:HD21	2:U:182:VAL:HG21	2.03	0.40
3:V:33:LEU:HD22	3:V:71:PHE:CG	2.56	0.40
1:E:305:CYS:CB	1:E:369:CYS:HA	2.52	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:B:349:ARG:NH2	1:E:233:ASP:OD2[1_655]	2.01	0.19
1:B:233:ASP:OD2	1:E:349:ARG:NH2[1_655]	2.14	0.06

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	360/362 (99%)	352 (98%)	8 (2%)	0	100	100
1	B	360/362 (99%)	351 (98%)	9 (2%)	0	100	100
1	C	360/362 (99%)	351 (98%)	9 (2%)	0	100	100
1	D	360/362 (99%)	353 (98%)	7 (2%)	0	100	100
1	E	360/362 (99%)	352 (98%)	8 (2%)	0	100	100
1	F	360/362 (99%)	350 (97%)	10 (3%)	0	100	100
2	H	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	29	61
2	M	221/223 (99%)	210 (95%)	10 (4%)	1 (0%)	29	61
2	O	221/223 (99%)	210 (95%)	10 (4%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Q	221/223 (99%)	209 (95%)	11 (5%)	1 (0%)	29 61
2	S	221/223 (99%)	209 (95%)	10 (4%)	2 (1%)	17 48
2	U	221/223 (99%)	211 (96%)	10 (4%)	0	100 100
3	L	212/214 (99%)	207 (98%)	4 (2%)	1 (0%)	29 61
3	N	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
3	P	212/214 (99%)	206 (97%)	6 (3%)	0	100 100
3	R	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29 61
3	T	212/214 (99%)	206 (97%)	6 (3%)	0	100 100
3	V	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
All	All	4758/4794 (99%)	4603 (97%)	147 (3%)	8 (0%)	47 77

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	32	ASP
2	H	32	ASP
2	O	54	GLY
2	S	32	ASP
2	Q	52(A)	ILE
3	L	50	SER
3	R	50	SER
2	S	52(B)	GLY

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	302/302 (100%)	298 (99%)	4 (1%)	69 82
1	B	302/302 (100%)	298 (99%)	4 (1%)	69 82
1	C	302/302 (100%)	298 (99%)	4 (1%)	69 82
1	D	302/302 (100%)	298 (99%)	4 (1%)	69 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	302/302 (100%)	297 (98%)	5 (2%)	60 78
1	F	302/302 (100%)	301 (100%)	1 (0%)	92 96
2	H	186/186 (100%)	183 (98%)	3 (2%)	62 79
2	M	186/186 (100%)	184 (99%)	2 (1%)	73 85
2	O	186/186 (100%)	184 (99%)	2 (1%)	73 85
2	Q	186/186 (100%)	184 (99%)	2 (1%)	73 85
2	S	186/186 (100%)	183 (98%)	3 (2%)	62 79
2	U	186/186 (100%)	184 (99%)	2 (1%)	73 85
3	L	182/182 (100%)	182 (100%)	0	100 100
3	N	182/182 (100%)	181 (100%)	1 (0%)	88 93
3	P	182/182 (100%)	182 (100%)	0	100 100
3	R	182/182 (100%)	180 (99%)	2 (1%)	73 85
3	T	182/182 (100%)	181 (100%)	1 (0%)	88 93
3	V	182/182 (100%)	182 (100%)	0	100 100
All	All	4020/4020 (100%)	3980 (99%)	40 (1%)	76 86

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	PHE
1	A	163	LYS
1	A	165	GLU
1	A	369	CYS
1	B	111	PHE
1	B	163	LYS
1	B	165	GLU
1	B	268	ARG
1	C	111	PHE
1	C	163	LYS
1	C	369	CYS
1	C	372	ASP
1	D	111	PHE
1	D	163	LYS
1	D	165	GLU
1	D	369	CYS
1	E	111	PHE
1	E	163	LYS

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Mol	Chain	Res	Type
1	E	165	GLU
1	E	268	ARG
1	E	369	CYS
1	F	111	PHE
2	M	27	PHE
2	M	127	CYS
3	N	93	SER
2	H	94	ARG
2	H	127	CYS
2	H	194	ASN
2	O	127	CYS
2	O	194	ASN
2	Q	127	CYS
2	Q	194	ASN
3	R	174	SER
3	R	204	SER
2	S	56	ASP
2	S	127	CYS
2	S	194	ASN
3	T	174	SER
2	U	127	CYS
2	U	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	38	GLN
3	V	27	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)

6 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	$\#\|Z\| > 2$
2	PCA	H	2	2	7,8,9	1.75	1 (14%)	9,10,12	2.27	5 (55%)
2	PCA	O	2	2	7,8,9	1.83	1 (14%)	9,10,12	2.51	5 (55%)
2	PCA	M	2	2	7,8,9	1.84	1 (14%)	9,10,12	2.67	5 (55%)
2	PCA	Q	2	2	7,8,9	1.78	1 (14%)	9,10,12	1.97	5 (55%)
2	PCA	S	2	2	7,8,9	1.79	1 (14%)	9,10,12	2.43	5 (55%)
2	PCA	U	2	2	7,8,9	1.73	1 (14%)	9,10,12	2.20	5 (55%)

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
2	PCA	H	2	2	-	0/0/11/13	0/1/1/1
2	PCA	O	2	2	-	0/0/11/13	0/1/1/1
2	PCA	M	2	2	-	0/0/11/13	0/1/1/1
2	PCA	Q	2	2	-	0/0/11/13	0/1/1/1
2	PCA	S	2	2	-	0/0/11/13	0/1/1/1
2	PCA	U	2	2	-	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	PCA	CD-N	4.71	1.47	1.34
2	O	2	PCA	CD-N	4.62	1.46	1.34
2	Q	2	PCA	CD-N	4.60	1.46	1.34
2	S	2	PCA	CD-N	4.56	1.46	1.34
2	H	2	PCA	CD-N	4.44	1.46	1.34
2	U	2	PCA	CD-N	4.43	1.46	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	2	PCA	CB-CA-C	-4.44	106.59	112.70
2	M	2	PCA	OE-CD-CG	-3.93	119.91	126.76
2	O	2	PCA	OE-CD-CG	-3.67	120.35	126.76
2	O	2	PCA	CB-CA-C	-3.50	107.89	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	PCA	OE-CD-CG	-3.35	120.92	126.76
2	S	2	PCA	CB-CA-C	-3.33	108.12	112.70
2	U	2	PCA	OE-CD-CG	-3.25	121.09	126.76
2	S	2	PCA	OE-CD-CG	-3.21	121.16	126.76
2	S	2	PCA	CA-N-CD	-3.16	102.77	113.58
2	H	2	PCA	CA-N-CD	-3.09	102.99	113.58
2	O	2	PCA	CA-N-CD	-3.03	103.19	113.58
2	M	2	PCA	CA-N-CD	-3.03	103.20	113.58
2	S	2	PCA	CB-CA-N	3.01	111.94	103.30
2	U	2	PCA	CA-N-CD	-3.00	103.30	113.58
2	Q	2	PCA	OE-CD-CG	-2.96	121.59	126.76
2	O	2	PCA	CG-CD-N	2.92	115.94	108.39
2	H	2	PCA	CB-CA-N	2.88	111.56	103.30
2	M	2	PCA	CG-CD-N	2.81	115.68	108.39
2	U	2	PCA	CB-CA-N	2.76	111.22	103.30
2	H	2	PCA	CG-CD-N	2.74	115.49	108.39
2	S	2	PCA	CG-CD-N	2.71	115.40	108.39
2	Q	2	PCA	CA-N-CD	-2.68	104.41	113.58
2	U	2	PCA	CG-CD-N	2.64	115.22	108.39
2	M	2	PCA	CB-CA-N	2.50	110.47	103.30
2	O	2	PCA	CB-CA-N	2.46	110.35	103.30
2	U	2	PCA	CB-CA-C	-2.41	109.39	112.70
2	Q	2	PCA	CG-CD-N	2.39	114.58	108.39
2	Q	2	PCA	CB-CA-N	2.37	110.11	103.30
2	H	2	PCA	CB-CA-C	-2.26	109.59	112.70
2	Q	2	PCA	CB-CA-C	-2.02	109.93	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	PCA	1	0
2	S	2	PCA	1	0

5.5 Carbohydrates (i)

22 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	$\#\|Z\| > 2$
4	NAG	G	1	1,4	14,14,15	0.50	0	17,19,21	1.18	1 (5%)
4	NAG	G	2	4	14,14,15	0.52	0	17,19,21	0.55	0
4	BMA	G	3	4	11,11,12	1.28	1 (9%)	15,15,17	1.03	2 (13%)
4	MAN	G	4	4	11,11,12	1.25	2 (18%)	15,15,17	1.03	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.44	0	17,19,21	1.38	2 (11%)
5	NAG	I	2	5	14,14,15	0.40	0	17,19,21	0.42	0
5	BMA	I	3	5	11,11,12	0.89	0	15,15,17	0.90	0
6	NAG	J	1	1,6	14,14,15	0.37	0	17,19,21	1.33	2 (11%)
6	NAG	J	2	6	14,14,15	0.64	1 (7%)	17,19,21	0.56	0
6	BMA	J	3	6	11,11,12	0.89	0	15,15,17	1.01	1 (6%)
6	MAN	J	4	6	11,11,12	1.37	1 (9%)	15,15,17	1.02	1 (6%)
6	MAN	J	5	6	11,11,12	1.00	0	15,15,17	0.85	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.55	0	17,19,21	1.19	2 (11%)
5	NAG	K	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.40	0
5	BMA	K	3	5	11,11,12	1.06	1 (9%)	15,15,17	0.88	0
4	NAG	W	1	1,4	14,14,15	0.64	1 (7%)	17,19,21	0.55	0
4	NAG	W	2	4	14,14,15	0.35	0	17,19,21	0.41	0
4	BMA	W	3	4	11,11,12	0.98	0	15,15,17	1.05	1 (6%)
4	MAN	W	4	4	11,11,12	1.49	2 (18%)	15,15,17	1.35	2 (13%)
5	NAG	X	1	1,5	14,14,15	0.75	1 (7%)	17,19,21	1.28	1 (5%)
5	NAG	X	2	5	14,14,15	0.46	0	17,19,21	0.50	0
5	BMA	X	3	5	11,11,12	1.16	1 (9%)	15,15,17	0.81	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
4	NAG	G	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
4	MAN	W	4	4	-	2/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	4	MAN	C1-C2	3.17	1.59	1.52
6	J	4	MAN	C2-C3	3.15	1.57	1.52
5	K	2	NAG	O5-C1	-3.05	1.38	1.43
5	X	3	BMA	C2-C3	2.47	1.56	1.52
5	X	1	NAG	C1-C2	-2.46	1.48	1.52
4	G	4	MAN	C4-C5	2.42	1.58	1.53
4	G	4	MAN	C1-C2	2.27	1.57	1.52
4	W	4	MAN	O5-C1	2.27	1.47	1.43
4	W	1	NAG	O5-C1	-2.23	1.40	1.43
5	K	3	BMA	C1-C2	2.19	1.57	1.52
4	G	3	BMA	C1-C2	2.18	1.57	1.52
6	J	2	NAG	O5-C1	-2.12	1.40	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	4	MAN	C1-O5-C5	4.12	117.77	112.19
5	I	1	NAG	C2-N2-C7	3.69	128.16	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	X	1	NAG	C2-N2-C7	3.61	128.05	122.90
4	G	1	NAG	C2-N2-C7	3.59	128.01	122.90
5	K	1	NAG	C2-N2-C7	3.53	127.93	122.90
6	J	1	NAG	C2-N2-C7	3.53	127.93	122.90
5	I	1	NAG	C1-C2-N2	2.88	115.40	110.49
6	J	1	NAG	C1-C2-N2	2.77	115.23	110.49
6	J	4	MAN	C1-O5-C5	2.68	115.82	112.19
4	W	3	BMA	C1-O5-C5	2.67	115.81	112.19
4	G	4	MAN	C1-O5-C5	2.65	115.78	112.19
5	K	1	NAG	C1-C2-N2	2.25	114.33	110.49
4	G	3	BMA	C1-O5-C5	2.24	115.23	112.19
6	J	5	MAN	C1-O5-C5	2.24	115.23	112.19
4	G	3	BMA	O2-C2-C1	2.20	113.65	109.15
6	J	3	BMA	C1-O5-C5	2.15	115.11	112.19
5	X	3	BMA	C1-O5-C5	2.12	115.06	112.19
4	W	4	MAN	C1-C2-C3	2.08	112.23	109.67

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
4	W	4	MAN	O5-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	X	1	NAG	C3-C2-N2-C7
4	W	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C3-C2-N2-C7

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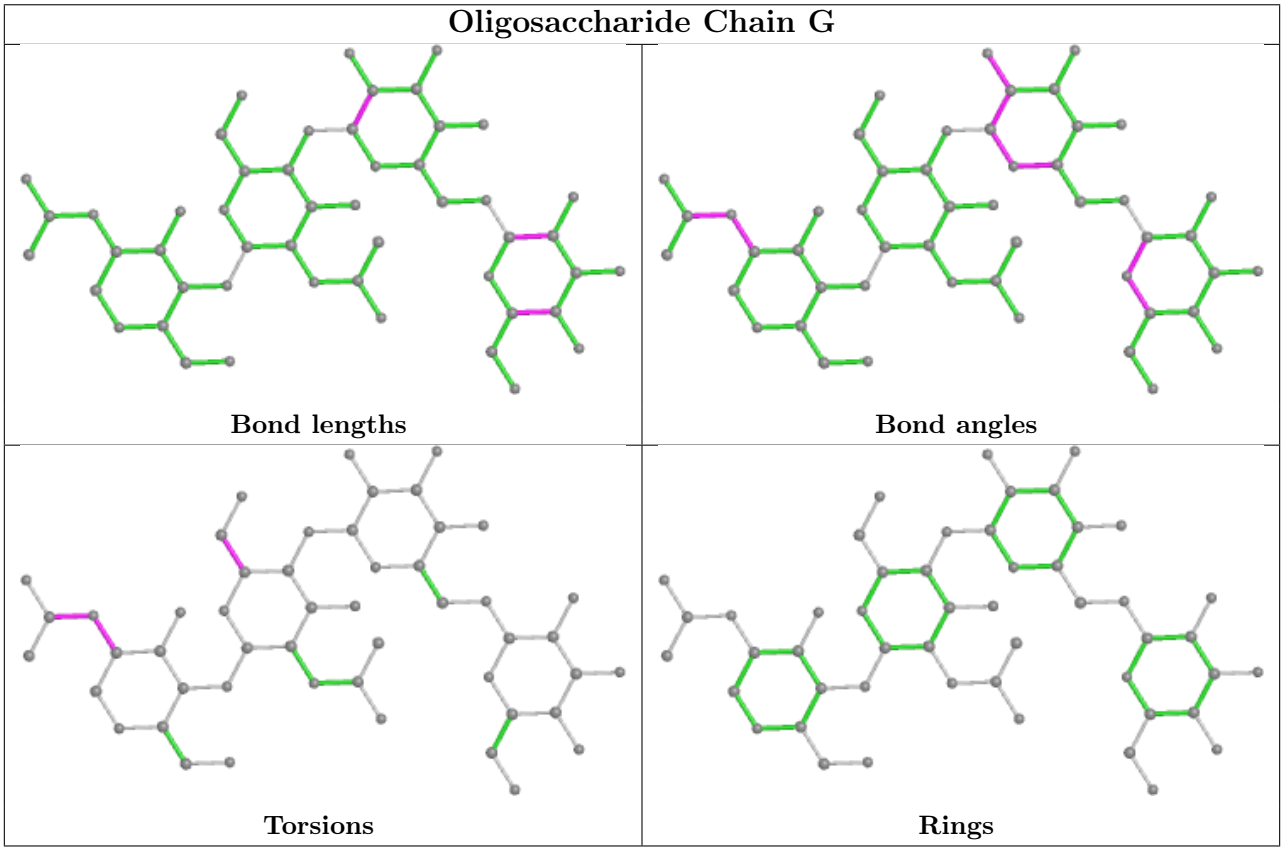
Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
4	W	4	MAN	C4-C5-C6-O6
4	G	1	NAG	C3-C2-N2-C7

There are no ring outliers.

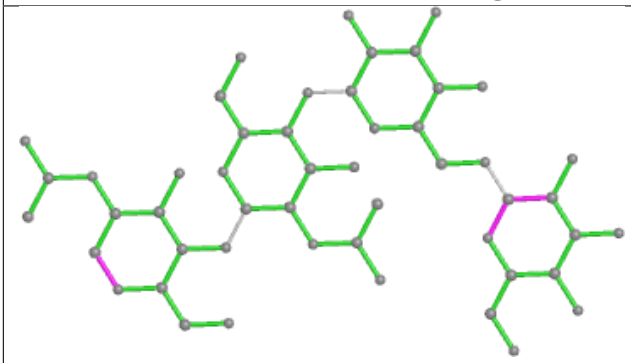
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0
5	X	1	NAG	4	0
5	K	1	NAG	1	0
6	J	1	NAG	1	0
4	W	1	NAG	1	0
4	G	1	NAG	1	0

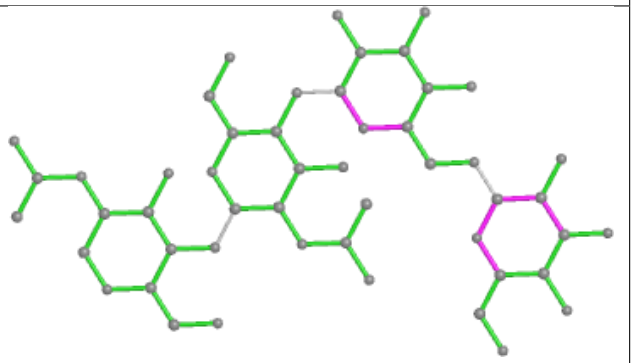
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



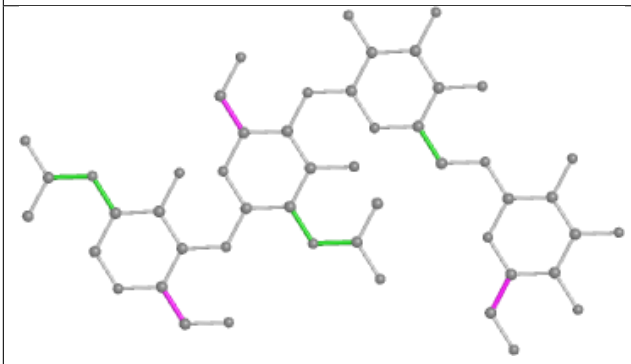
Oligosaccharide Chain W



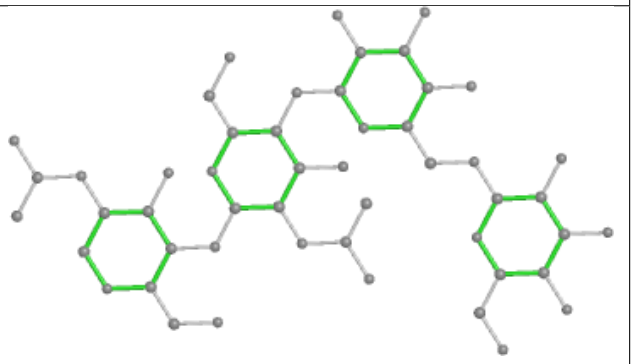
Bond lengths



Bond angles

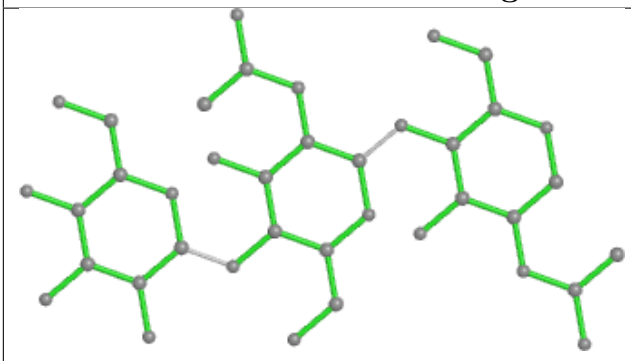


Torsions

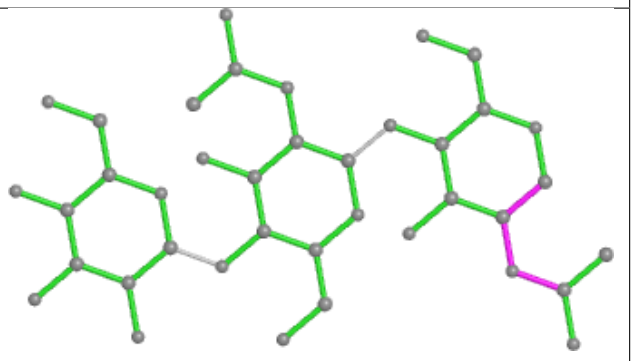


Rings

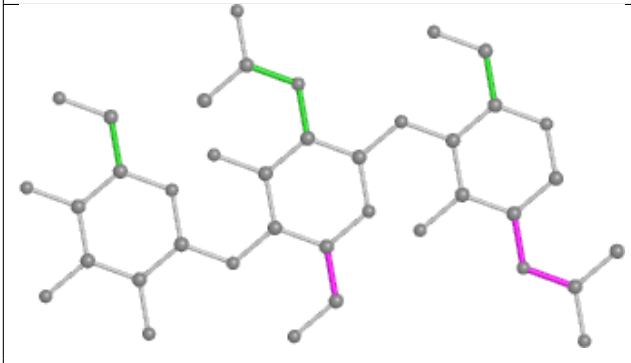
Oligosaccharide Chain I



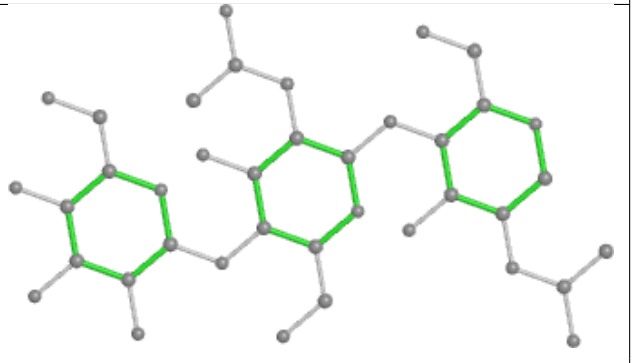
Bond lengths



Bond angles

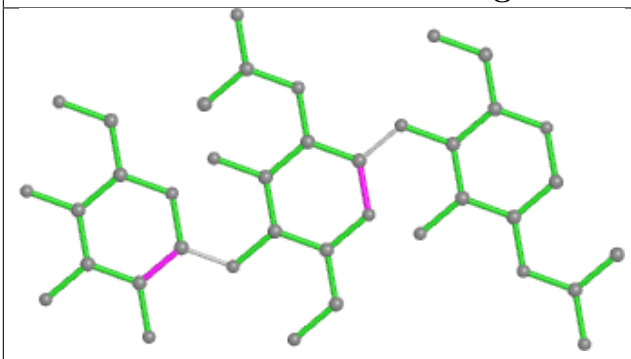


Torsions

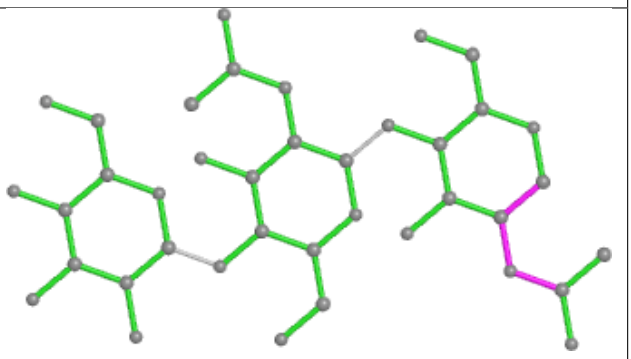


Rings

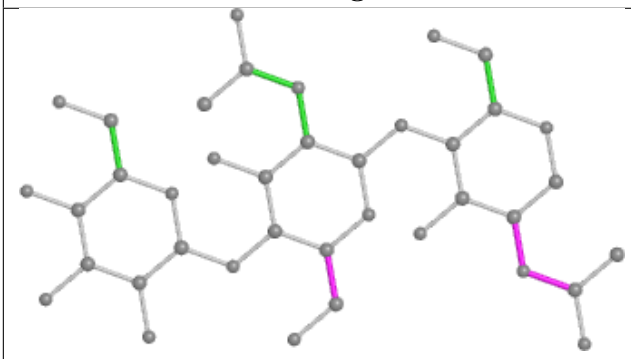
Oligosaccharide Chain K



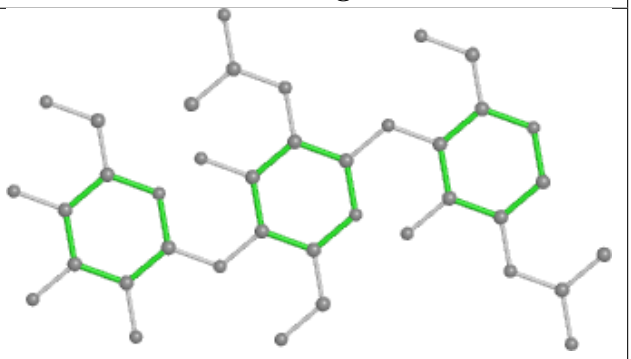
Bond lengths



Bond angles

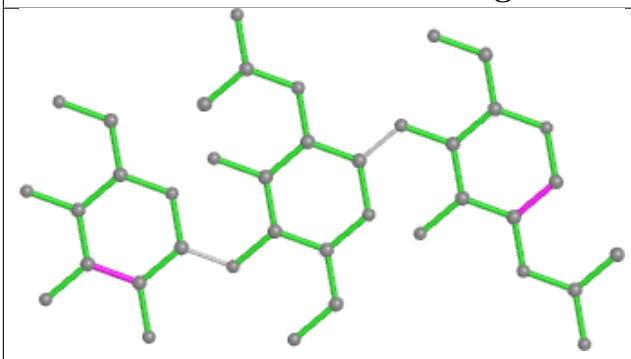


Torsions

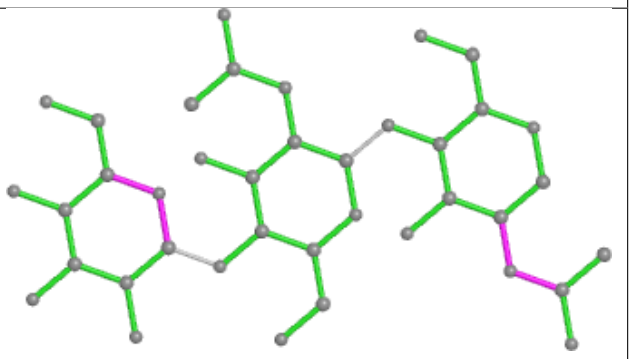


Rings

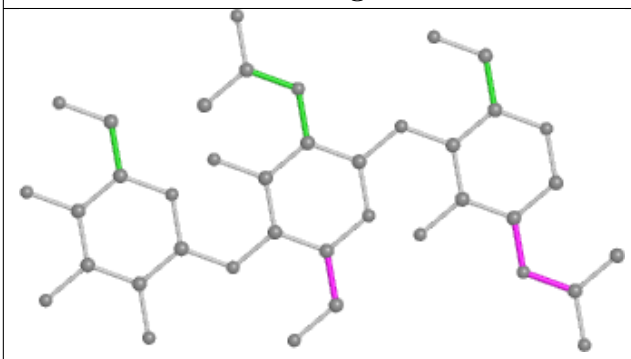
Oligosaccharide Chain X



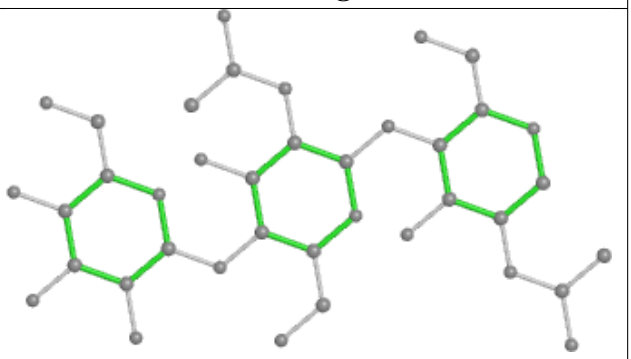
Bond lengths



Bond angles

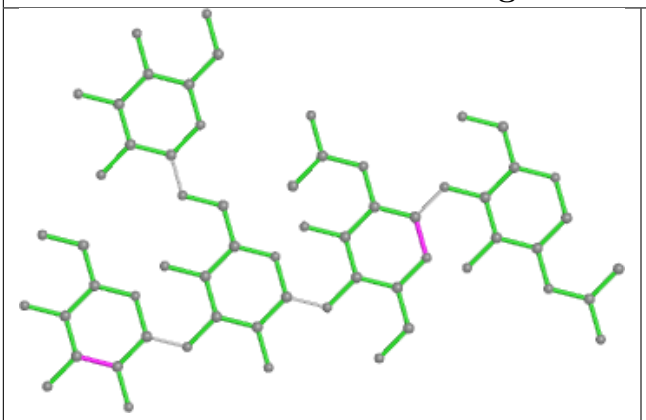


Torsions

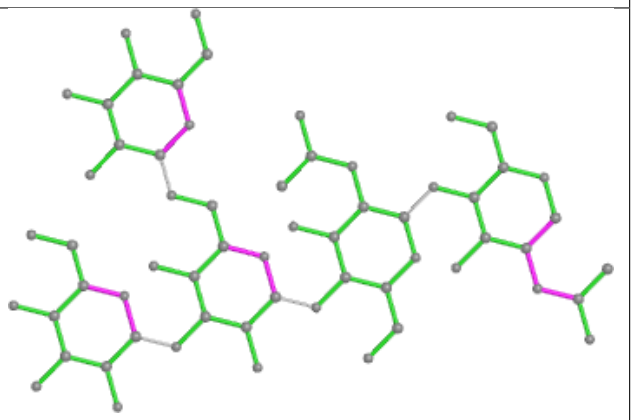


Rings

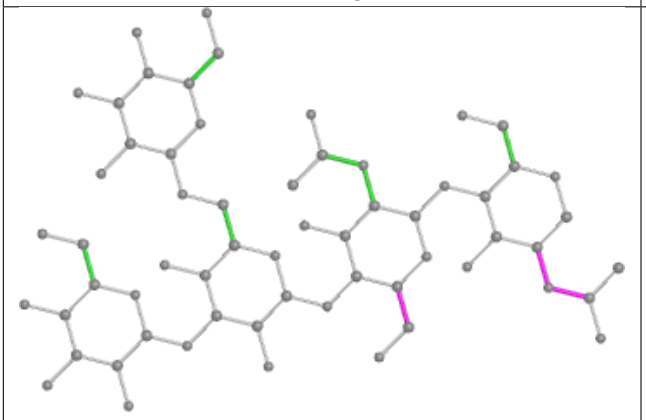
Oligosaccharide Chain J



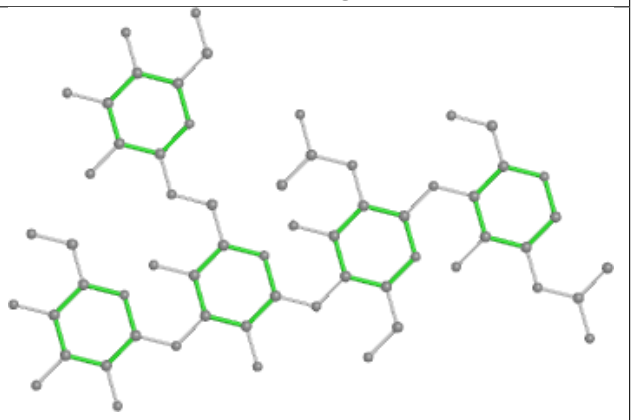
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	362/362 (100%)	-0.25	0 100 100	35, 52, 81, 133	0
1	B	362/362 (100%)	-0.29	0 100 100	35, 53, 82, 133	0
1	C	362/362 (100%)	-0.30	0 100 100	40, 55, 86, 143	0
1	D	362/362 (100%)	-0.24	0 100 100	39, 52, 80, 133	0
1	E	362/362 (100%)	-0.24	0 100 100	39, 55, 84, 124	0
1	F	362/362 (100%)	-0.25	0 100 100	33, 48, 84, 133	0
2	H	222/223 (99%)	0.15	13 (5%) 22 22	42, 76, 159, 211	0
2	M	222/223 (99%)	-0.02	6 (2%) 54 52	37, 66, 132, 187	0
2	O	222/223 (99%)	0.28	16 (7%) 15 15	48, 84, 191, 218	0
2	Q	222/223 (99%)	0.17	11 (4%) 28 27	48, 84, 152, 212	0
2	S	222/223 (99%)	0.08	5 (2%) 60 59	51, 80, 140, 189	0
2	U	222/223 (99%)	0.14	13 (5%) 22 22	43, 69, 178, 235	0
3	L	214/214 (100%)	0.03	0 100 100	37, 69, 150, 178	0
3	N	214/214 (100%)	-0.24	0 100 100	34, 59, 114, 155	0
3	P	214/214 (100%)	0.13	15 (7%) 16 16	44, 79, 181, 233	0
3	R	214/214 (100%)	-0.08	2 (0%) 84 84	43, 69, 144, 163	0
3	T	214/214 (100%)	-0.24	0 100 100	44, 68, 108, 128	0
3	V	214/214 (100%)	0.10	6 (2%) 53 51	39, 75, 165, 199	0
All	All	4788/4794 (99%)	-0.10	87 (1%) 68 67	33, 59, 148, 235	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	213	CYS	11.4
2	Q	213	CYS	5.9
2	O	213	CYS	5.4

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Mol	Chain	Res	Type	RSRZ
2	U	133	SER	4.8
2	U	138	LEU	4.8
2	O	210	PRO	4.7
2	S	132	PRO	4.7
2	H	188	SER	4.5
2	Q	132	PRO	4.2
2	S	213	CYS	4.2
2	O	132	PRO	4.0
2	U	212	THR	3.7
2	U	129	GLY	3.7
3	P	204	SER	3.7
2	H	130	ASP	3.6
3	V	114	VAL	3.6
2	U	188	SER	3.6
2	H	132	PRO	3.5
2	Q	133	SER	3.4
2	U	131	THR	3.3
2	O	138	LEU	3.3
3	P	113	THR	3.3
3	P	203	GLN	3.3
2	O	131	THR	3.2
2	U	132	PRO	3.2
3	P	132	VAL	3.2
2	Q	188	SER	3.1
2	O	129	GLY	3.1
2	H	131	THR	3.0
2	O	130	ASP	3.0
2	O	187	SER	3.0
2	H	129	GLY	3.0
2	Q	29	ILE	2.9
2	U	130	ASP	2.9
3	P	150	GLY	2.8
2	H	210	PRO	2.8
2	H	209	ALA	2.8
3	P	192	CYS	2.8
2	Q	129	GLY	2.8
2	O	188	SER	2.7
3	P	135	ALA	2.7
2	M	187	SER	2.7
2	S	184	VAL	2.7
3	P	191	THR	2.7
2	O	209	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	Q	159	LEU	2.6
3	P	179	LEU	2.6
2	M	213	CYS	2.6
2	O	199	ALA	2.6
2	M	132	PRO	2.6
3	V	193	LYS	2.5
2	Q	210	PRO	2.5
3	P	201	VAL	2.5
2	O	212	THR	2.5
2	O	211	SER	2.5
2	U	128	CYS	2.4
3	P	129	VAL	2.4
2	U	29	ILE	2.4
3	P	125	ALA	2.4
2	M	188	SER	2.4
3	P	194	VAL	2.3
3	V	202	VAL	2.3
2	H	134	SER	2.3
2	H	187	SER	2.3
2	O	184	VAL	2.3
2	Q	187	SER	2.3
2	H	159	LEU	2.3
2	U	186	SER	2.3
3	P	200	SER	2.3
2	S	187	SER	2.2
3	R	179	LEU	2.2
3	V	113	THR	2.2
3	P	184	TYR	2.2
2	Q	131	THR	2.2
2	S	210	PRO	2.2
3	V	136	ASN	2.2
2	O	137	THR	2.2
2	O	207	THR	2.2
2	U	211	SER	2.1
2	M	161	ASN	2.1
2	H	133	SER	2.1
2	M	131	THR	2.1
3	R	128	THR	2.1
2	H	138	LEU	2.1
2	H	213	CYS	2.0
3	V	192	CYS	2.0
2	Q	184	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PCA	Q	2	8/9	0.92	0.20	63,65,69,71	0
2	PCA	S	2	8/9	0.92	0.27	64,69,73,74	0
2	PCA	H	2	8/9	0.93	0.18	62,67,70,72	0
2	PCA	M	2	8/9	0.94	0.20	57,62,64,66	0
2	PCA	O	2	8/9	0.95	0.17	66,68,70,72	0
2	PCA	U	2	8/9	0.95	0.25	63,64,66,67	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	J	3	11/12	0.63	0.17	164,169,177,178	0
6	MAN	J	4	11/12	0.67	0.20	151,159,161,162	0
4	MAN	G	4	11/12	0.69	0.25	114,121,125,126	0
4	BMA	W	3	11/12	0.69	0.21	142,149,154,156	0
4	BMA	G	3	11/12	0.71	0.22	109,117,120,123	0
4	MAN	W	4	11/12	0.73	0.21	122,124,128,131	0
5	BMA	X	3	11/12	0.79	0.20	129,138,143,143	0
5	BMA	K	3	11/12	0.81	0.14	132,134,136,136	0
5	BMA	I	3	11/12	0.81	0.16	99,101,102,102	0
6	MAN	J	5	11/12	0.82	0.14	132,141,145,147	0
5	NAG	K	2	14/15	0.87	0.19	104,108,126,130	0
5	NAG	X	2	14/15	0.88	0.15	84,90,107,116	0
5	NAG	I	2	14/15	0.89	0.17	83,85,100,100	0
4	NAG	W	2	14/15	0.90	0.14	92,102,117,124	0
6	NAG	J	2	14/15	0.91	0.17	87,95,120,129	0
4	NAG	G	2	14/15	0.91	0.15	72,77,95,99	0
5	NAG	X	1	14/15	0.92	0.21	51,55,66,77	0
5	NAG	I	1	14/15	0.93	0.17	49,56,65,75	0
4	NAG	W	1	14/15	0.93	0.15	59,67,77,86	0
4	NAG	G	1	14/15	0.94	0.24	50,54,62,70	0
6	NAG	J	1	14/15	0.94	0.16	60,67,76,84	0

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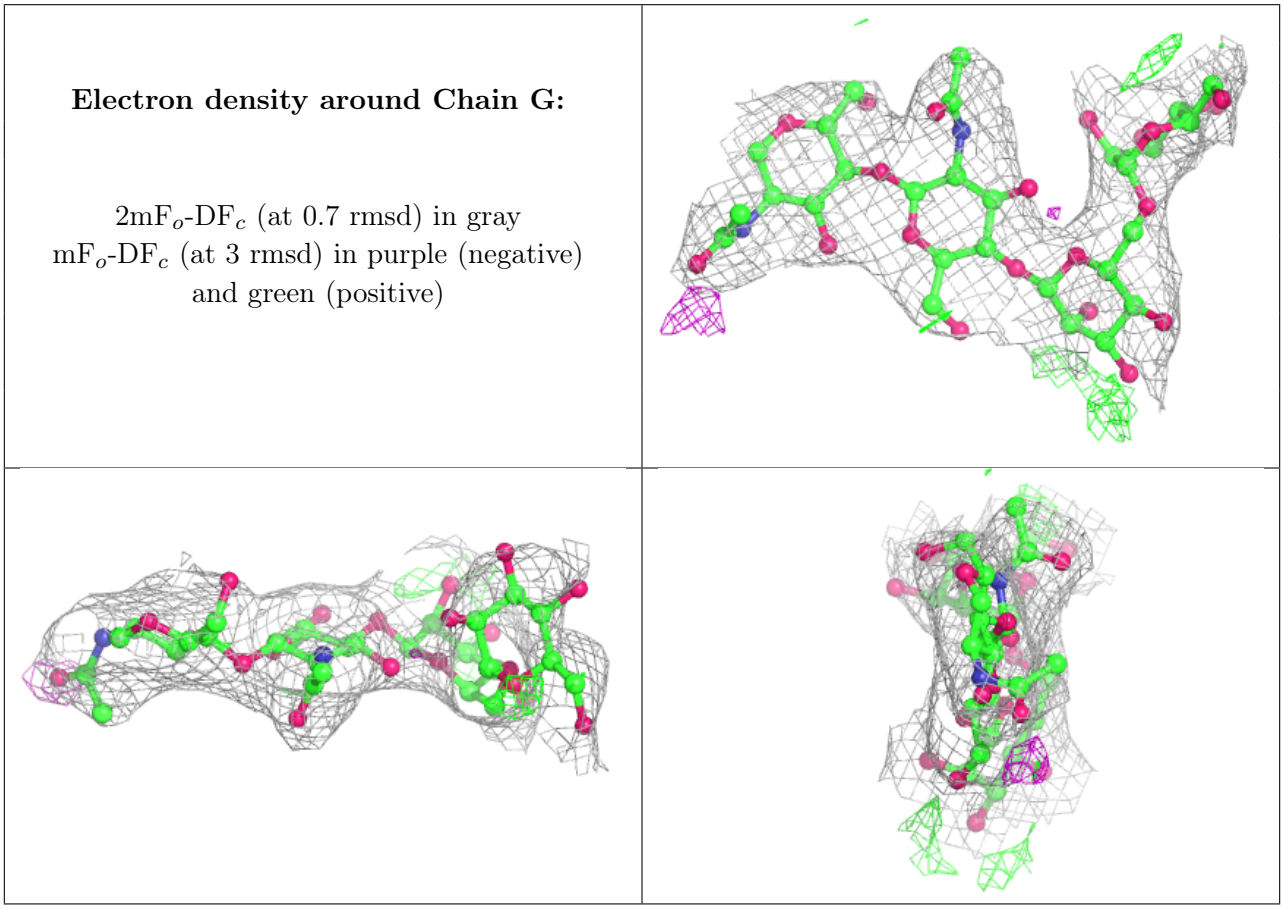
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	K	1	14/15	0.94	0.20	56,61,74,88	0

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.

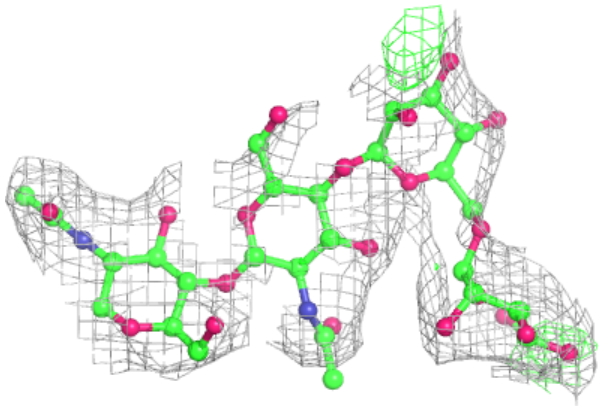
Electron density around Chain G:

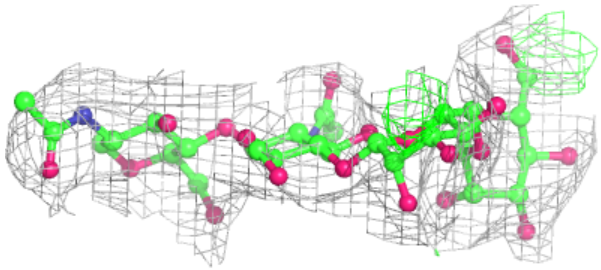
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

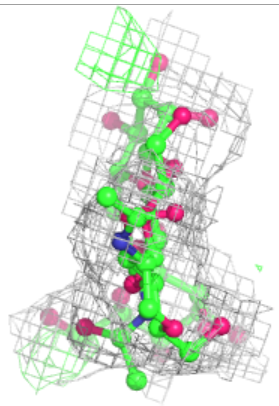


Electron density around Chain W:

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

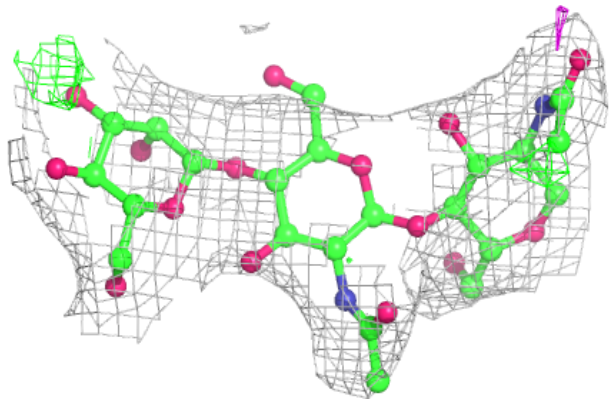


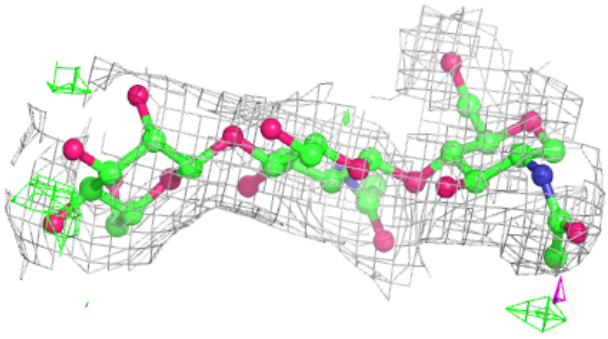


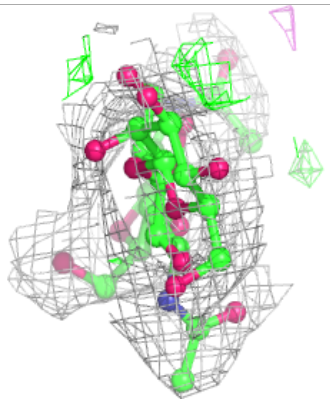


Electron density around Chain I:

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

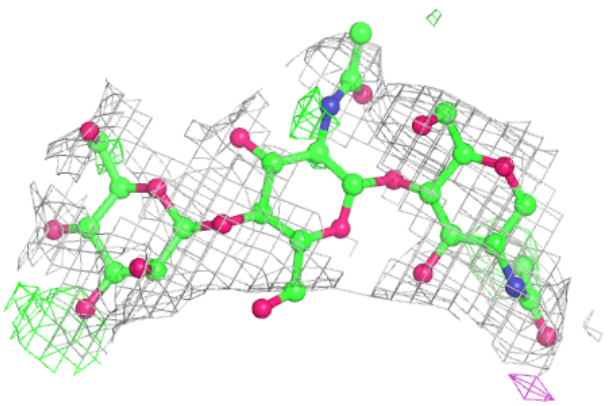


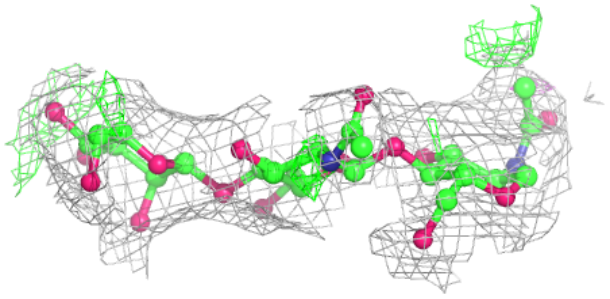


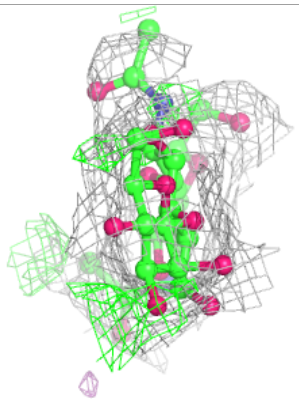


Electron density around Chain K:

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

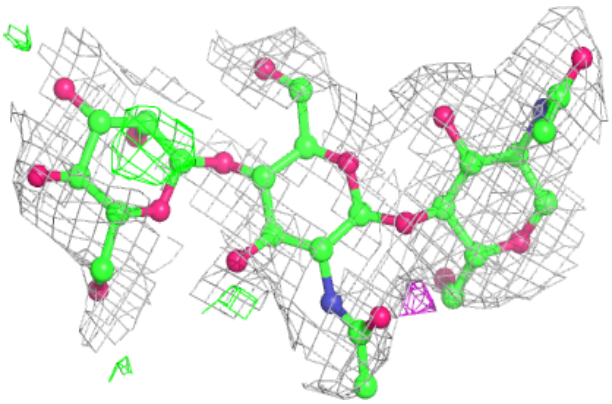


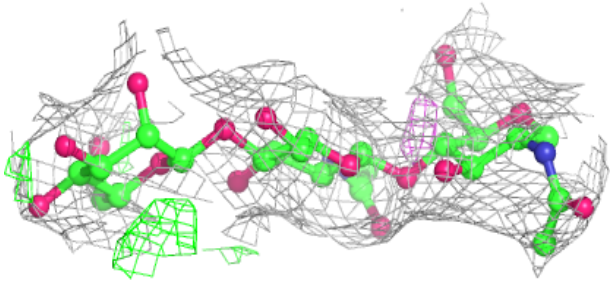


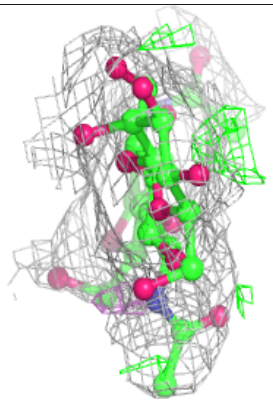


Electron density around Chain X:

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

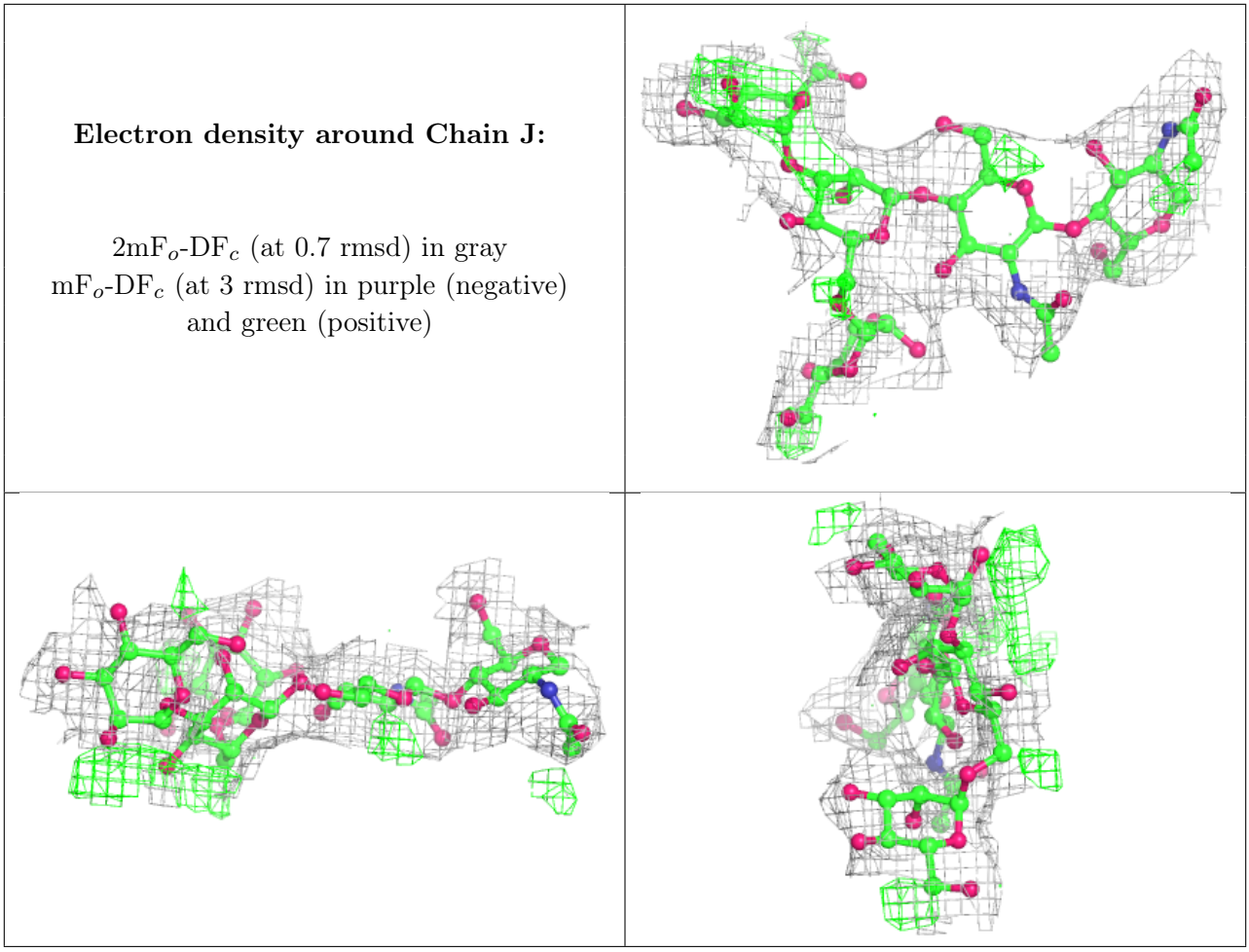






Electron density around Chain J:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.