Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:29 AM EDT

PDB ID	:	6MEK
Title	:	Crystal structure of Hepatitis C virus envelope glycoprotein E2 core in complex with human antibodies HEPC3 and HEPC46
Authors	:	Flyak, A.I.; Bjorkman, P.J.
Deposited on	:	2018-09-06
Resolution	:	3.10 Å(reported)

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

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

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

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

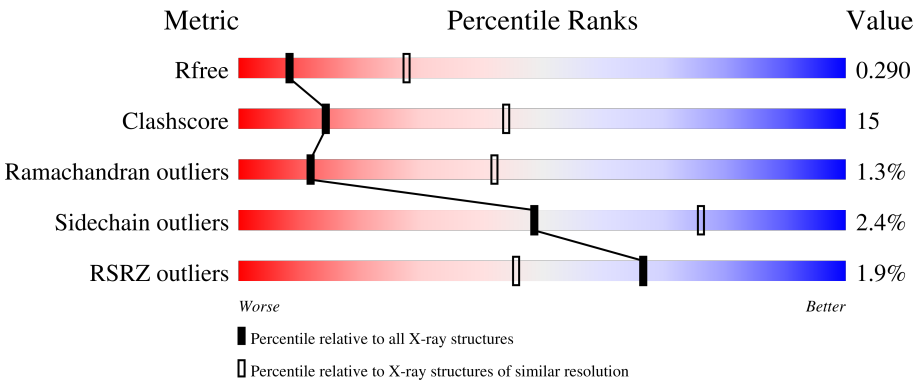
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	235	2%, 42%, 27%, •, 30%
1	C	235	51%, 22%, 28%
2	B	241	2%, 65%, 27%, •, 7%
2	H	241	60%, 30%, •, 8%
3	D	214	%, 64%, 35%, •

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Mol	Chain	Length	Quality of chain
3	L	214	2% 72% 27%
4	E	217	% 67% 22% 8%
4	G	217	8% 65% 31%
5	F	230	70% 20% 9%
5	I	230	56% 37% 7%
6	J	4	25% 75%
7	K	2	100%
7	P	2	100%
8	M	3	33% 67%
8	N	3	100%
8	Q	3	33% 67%
9	O	5	40% 60%

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
6	MAN	J	4	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15747 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 E2 GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1278	814	222	228	14	0	0	0
1	C	170	1317	840	230	233	14	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	ASN	-	expression tag	UNP H2FJ05
A	448	ASP	ASN	engineered mutation	UNP H2FJ05
A	482	GLY	GLN	linker	UNP H2FJ05
A	483	SER	ARG	linker	UNP H2FJ05
A	484	SER	PRO	linker	UNP H2FJ05
A	485	GLY	TYR	linker	UNP H2FJ05
A	576	ASP	ASN	engineered mutation	UNP H2FJ05
C	411	ASN	-	expression tag	UNP H2FJ05
C	448	ASP	ASN	engineered mutation	UNP H2FJ05
C	482	GLY	GLN	linker	UNP H2FJ05
C	483	SER	ARG	linker	UNP H2FJ05
C	484	SER	PRO	linker	UNP H2FJ05
C	485	GLY	TYR	linker	UNP H2FJ05
C	576	ASP	ASN	engineered mutation	UNP H2FJ05

- Molecule 2 is a protein called HEPC3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	224	1674	1053	281	332	8	0	0	0
2	H	222	1661	1046	279	328	8	0	0	0

- Molecule 3 is a protein called HEPC3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	213	1636	1017	281	333	5	0	0	0
3	L	213	1636	1017	281	333	5	0	0	0

- Molecule 4 is a protein called HEPC46 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	200	1467	917	243	303	4	0	0	0
4	G	212	1577	988	264	321	4	0	0	0

- Molecule 5 is a protein called HEPC46 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	210	1581	996	269	309	7	0	0	0
5	I	215	1608	1011	274	316	7	0	0	0

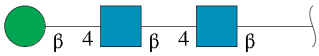
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

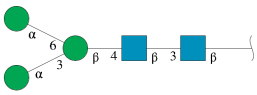
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	K	2	28	16	2	10	0	0	0
7	P	2	28	16	2	10	0	0	0

- Molecule 8 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.



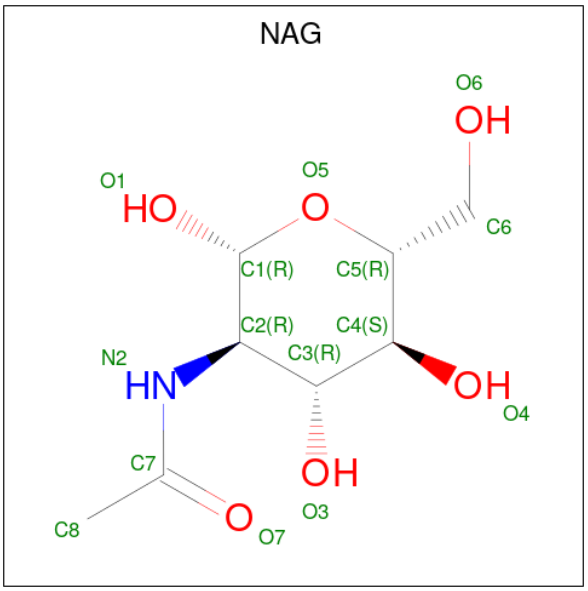
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	M	3	39	22	2	15	0	0	0
8	N	3	39	22	2	15	0	0	0
8	Q	3	39	22	2	15	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



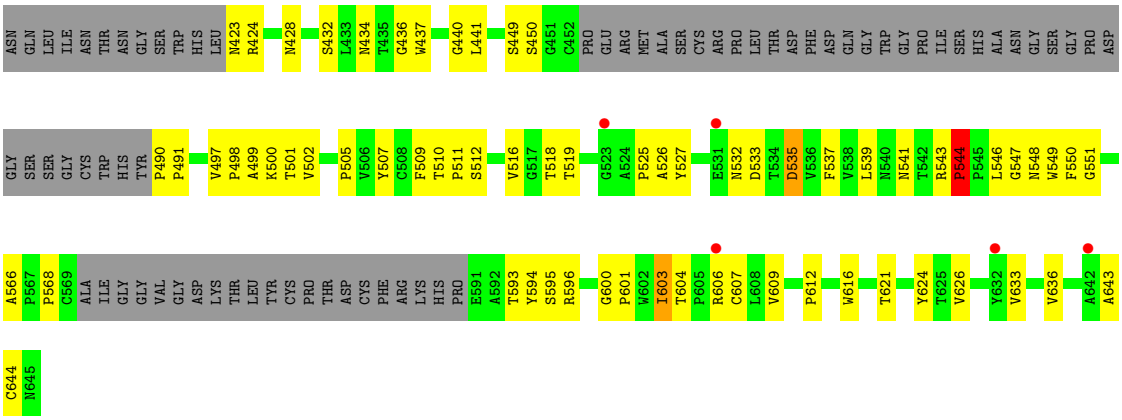
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	14	8	1	5	0	0
			Total	C	N	O		
10	C	1	14	8	1	5	0	0

3 Residue-property plots (i)

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

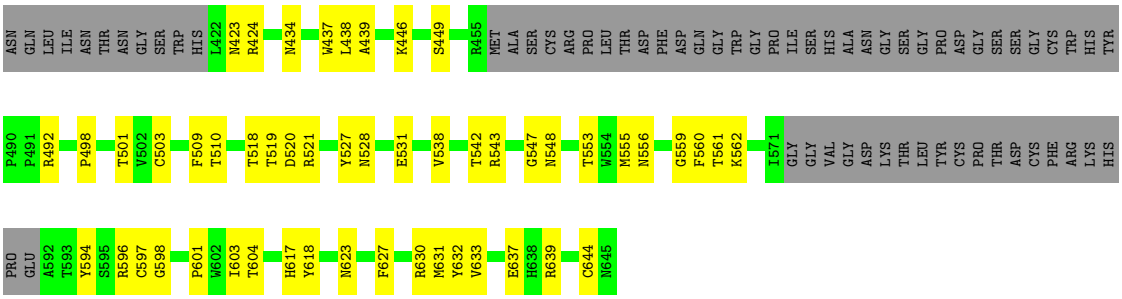
• Molecule 1: E2 GLYCOPROTEIN

Chain A: 2% 42% 27% • 30%



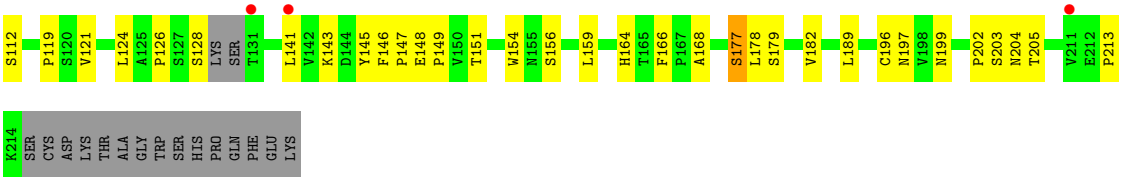
• Molecule 1: E2 GLYCOPROTEIN

Chain C: 51% 22% 28%



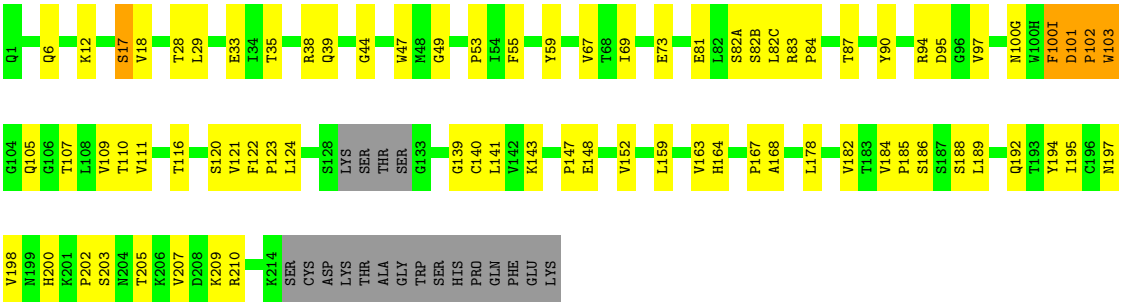
• Molecule 2: HEPC3 Heavy Chain

Chain B: 2% 65% 27% • 7%



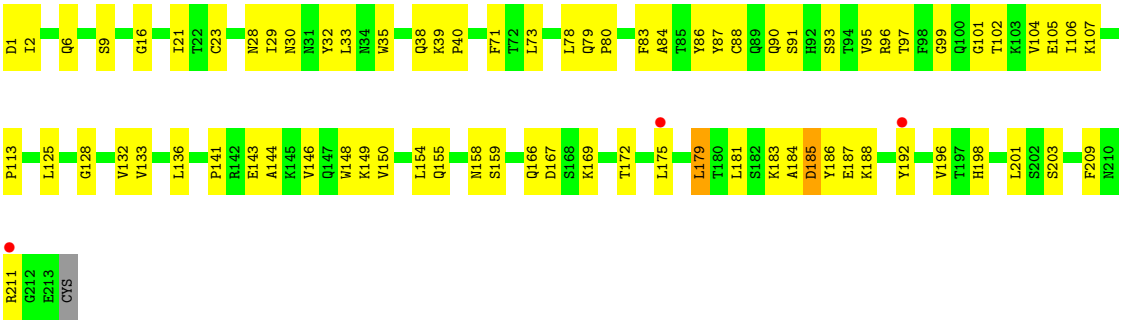
• Molecule 2: HEPC3 Heavy Chain

Chain H:



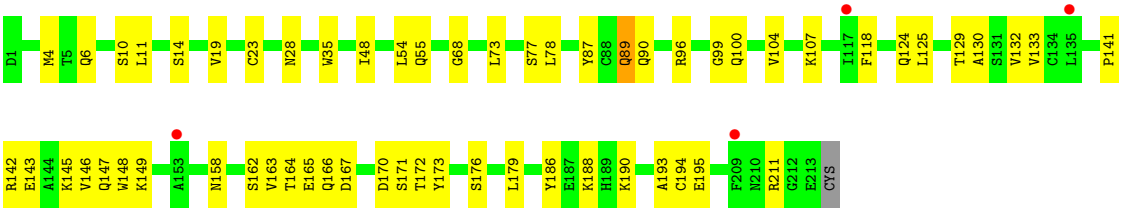
• Molecule 3: HEPC3 Light Chain

Chain D:



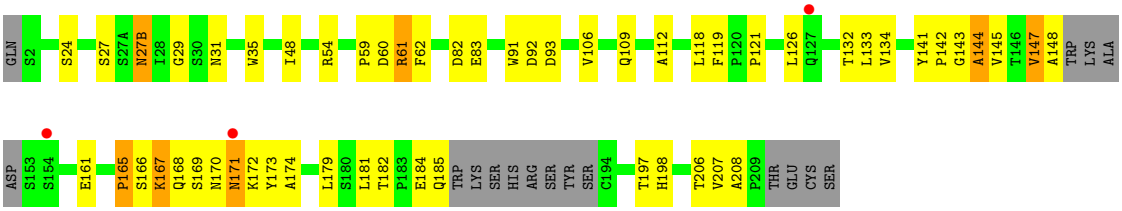
• Molecule 3: HEPC3 Light Chain

Chain L:



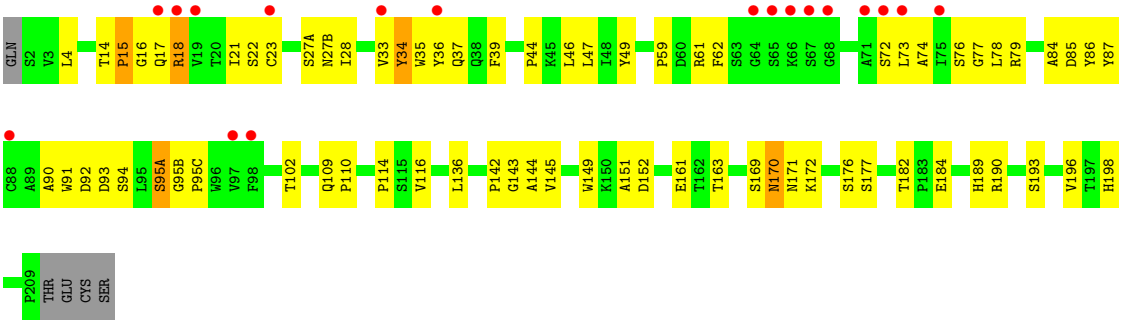
• Molecule 4: HEPC46 Light Chain

Chain E:



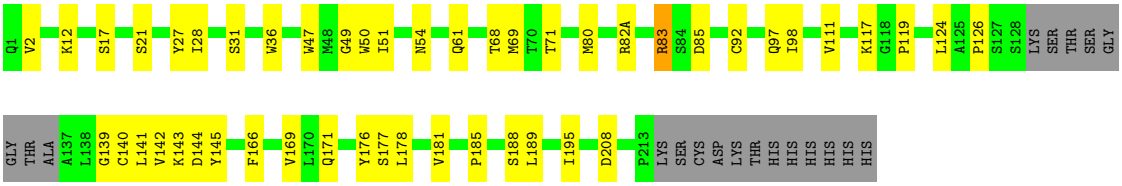
• Molecule 4: HEPC46 Light Chain

Chain G:



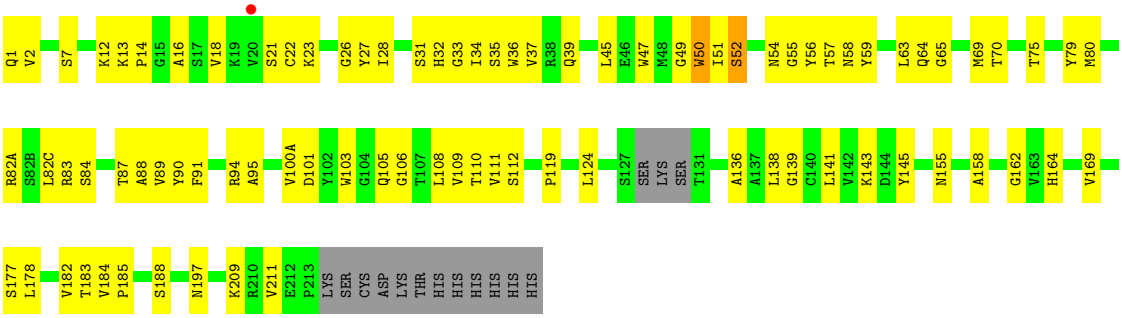
• Molecule 5: HEPC46 Heavy Chain

Chain F:



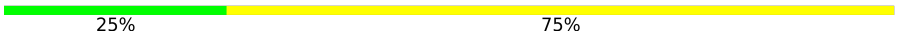
• Molecule 5: HEPC46 Heavy Chain

Chain I:



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

Chain J:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 33% 67%

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 33% 67%

• Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 40% 60%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.40Å 105.59Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.97 – 3.10 76.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (76.97-3.10) 99.9 (76.97-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.223 , 0.290 0.223 , 0.290	Depositor DCC
R_{free} test set	2479 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	77.6	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15747	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% 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: BMA, NAG, 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	0/1323	0.60	0/1812
1	C	0.43	0/1363	0.60	0/1867
2	B	0.44	0/1714	0.60	1/2337 (0.0%)
2	H	0.46	0/1701	0.61	0/2319
3	D	0.44	0/1669	0.62	0/2265
3	L	0.44	0/1669	0.64	1/2265 (0.0%)
4	E	0.41	0/1502	0.64	0/2053
4	G	0.36	0/1620	0.56	0/2216
5	F	0.43	0/1618	0.61	0/2207
5	I	0.43	0/1645	0.64	0/2244
All	All	0.43	0/15824	0.61	2/21585 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	L	0	1
4	E	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	12	LYS	C-N-CA	7.30	139.96	121.70
3	L	23	CYS	CA-CB-SG	-5.25	104.54	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	544	PRO	Peptide
4	E	167	LYS	Peptide
3	L	165	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1278	0	1187	51	0
1	C	1317	0	1233	38	0
2	B	1674	0	1633	48	0
2	H	1661	0	1621	61	0
3	D	1636	0	1589	60	0
3	L	1636	0	1589	41	0
4	E	1467	0	1408	46	0
4	G	1577	0	1509	58	0
5	F	1581	0	1551	29	0
5	I	1608	0	1576	72	0
6	J	50	0	43	1	0
7	K	28	0	25	3	0
7	P	28	0	25	0	0
8	M	39	0	34	0	0
8	N	39	0	34	0	0
8	Q	39	0	34	2	0
9	O	61	0	52	2	0
10	A	14	0	13	1	0
10	C	14	0	13	0	0
All	All	15747	0	15169	478	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 15.

All (478) 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)
4:G:34:TYR:HH	4:G:91:TRP:HE1	1.11	0.97
3:D:150:VAL:HA	3:D:192:TYR:HB3	1.51	0.92
1:A:490:PRO:HB2	1:A:491:PRO:HD3	1.51	0.89
5:I:70:THR:HG23	5:I:79:TYR:HB2	1.54	0.87
1:A:424:ARG:HG2	1:A:518:THR:H	1.40	0.84
2:H:152:VAL:HG22	2:H:198:VAL:HG22	1.61	0.82
5:I:143:LYS:HA	5:I:177:SER:HB3	1.61	0.82
5:F:142:VAL:HG22	5:F:178:LEU:HB2	1.64	0.79
2:B:151:THR:HG23	2:B:199:ASN:HB3	1.64	0.79
4:E:144:ALA:HB2	4:E:165:PRO:HD3	1.64	0.78
4:G:182:THR:HG22	4:G:184:GLU:H	1.48	0.77
4:E:133:LEU:HB3	4:E:179:LEU:HB3	1.66	0.77
3:L:6:GLN:HE21	3:L:99:GLY:HA3	1.48	0.77
2:H:84:PRO:HA	2:H:111:VAL:HG13	1.66	0.77
4:G:33:VAL:HG22	4:G:90:ALA:HB2	1.66	0.76
4:G:17:GLN:H	4:G:78:LEU:HD13	1.50	0.76
3:D:79:GLN:HG3	3:D:80:PRO:HD2	1.67	0.75
1:A:424:ARG:NH1	1:A:518:THR:O	2.20	0.74
4:E:119:PHE:HB2	4:E:134:VAL:HG13	1.70	0.73
2:H:184:VAL:HG21	2:H:194:TYR:OH	1.87	0.73
4:E:167:LYS:O	4:E:171:ASN:HA	1.87	0.73
2:H:83:ARG:O	2:H:111:VAL:HG11	1.87	0.73
10:A:5401:NAG:H82	5:I:28:ILE:HG12	1.71	0.73
5:I:13:LYS:HB2	5:I:14:PRO:HD3	1.71	0.71
2:H:6:GLN:HE21	2:H:107:THR:HG23	1.54	0.70
2:H:184:VAL:HG22	2:H:185:PRO:HD2	1.72	0.70
4:G:116:VAL:HG11	4:G:196:VAL:HG11	1.72	0.69
4:E:145:VAL:HB	4:E:197:THR:O	1.93	0.69
3:D:6:GLN:HE21	3:D:99:GLY:HA3	1.57	0.69
5:I:94:ARG:NH2	5:I:101:ASP:OD2	2.23	0.69
4:G:16:GLY:H	4:G:78:LEU:HB2	1.56	0.68
4:G:170:ASN:HD22	4:G:172:LYS:HE2	1.58	0.68
2:H:116:THR:HG22	2:H:147:PRO:HD3	1.75	0.68
3:D:146:VAL:HG22	3:D:196:VAL:HG22	1.74	0.67
4:G:14:THR:HG22	4:G:15:PRO:HD2	1.76	0.67
3:L:147:GLN:HB2	3:L:195:GLU:HB3	1.74	0.67
2:B:100(D):ARG:HD2	3:D:32:TYR:OH	1.93	0.67
4:E:179:LEU:HG	4:E:181:LEU:HD13	1.76	0.67
2:H:121:VAL:HG11	2:H:207:VAL:HG11	1.76	0.67
1:C:556:ASN:HB3	1:C:560:PHE:H	1.60	0.66
2:B:143:LYS:HA	2:B:177:SER:HB2	1.78	0.66
5:I:16:ALA:HB3	5:I:82(C):LEU:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:PRO:O	2:H:188:SER:OG	2.14	0.65
3:D:132:VAL:HG11	3:D:192:TYR:HE1	1.62	0.65
4:G:16:GLY:HA2	4:G:78:LEU:H	1.61	0.65
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.29	0.65
3:L:11:LEU:HD21	3:L:19:VAL:HG11	1.77	0.65
4:G:161:GLU:HB3	5:I:169:VAL:HG11	1.79	0.65
3:D:6:GLN:HE22	3:D:87:TYR:HA	1.61	0.65
4:G:149:TRP:HE1	4:G:177:SER:HG	1.43	0.64
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.80	0.64
2:H:17:SER:HB2	2:H:82(A):SER:HA	1.80	0.64
1:C:434:ASN:OD1	2:H:94:ARG:NH1	2.31	0.63
3:D:155:GLN:HB3	3:D:158:ASN:ND2	2.13	0.63
1:A:428:ASN:ND2	1:A:500:LYS:HA	2.14	0.63
3:D:32:TYR:HB3	3:D:91:SER:HB3	1.81	0.62
5:I:51:ILE:HG13	5:I:57:THR:HG22	1.81	0.62
1:C:519:THR:HG21	1:C:538:VAL:HG12	1.81	0.62
4:E:142:PRO:HD2	4:E:198:HIS:CE1	2.34	0.62
4:E:35:TRP:HB2	4:E:48:ILE:HB	1.82	0.61
5:I:138:LEU:HD13	5:I:211:VAL:HG21	1.82	0.61
4:G:109:GLN:HG3	4:G:110:PRO:HD2	1.81	0.61
2:H:184:VAL:CG2	2:H:185:PRO:HD2	2.30	0.61
4:E:61:ARG:NH2	4:E:82:ASP:OD1	2.31	0.61
2:B:95:ASP:O	2:B:100(G):ASN:ND2	2.33	0.61
5:F:28:ILE:O	5:F:31:SER:OG	2.18	0.61
3:L:132:VAL:HG13	3:L:179:LEU:HB3	1.82	0.61
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.35	0.61
5:I:155:ASN:HB3	5:I:158:ALA:HB3	1.82	0.61
4:E:145:VAL:HG21	4:E:198:HIS:HA	1.83	0.60
5:I:91:PHE:CD2	5:I:106:GLY:HA2	2.36	0.60
4:E:168:GLN:OE1	4:E:168:GLN:HA	2.01	0.60
2:H:121:VAL:CG1	2:H:207:VAL:HG11	2.32	0.60
4:G:163:THR:HG23	5:I:169:VAL:HG22	1.81	0.60
3:D:149:LYS:HZ2	3:D:154:LEU:HD21	1.67	0.60
7:K:1:NAG:H61	7:K:2:NAG:C7	2.31	0.60
5:I:28:ILE:HB	5:I:31:SER:HB3	1.83	0.60
5:I:33:GLY:O	5:I:95:ALA:N	2.33	0.59
3:L:167:ASP:HB3	3:L:170:ASP:HB3	1.82	0.59
1:C:509:PHE:CE1	1:C:601:PRO:HB3	2.37	0.59
4:E:118:LEU:HD12	4:E:207:VAL:HG12	1.85	0.59
4:G:35:TRP:CZ3	4:G:73:LEU:HB2	2.36	0.59
3:D:132:VAL:HG11	3:D:192:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:GLU:HG3	2:H:53:PRO:HD3	1.84	0.59
1:A:511:PRO:HB3	1:A:594:TYR:CE2	2.37	0.59
5:I:82(C):LEU:HB3	5:I:111:VAL:HG11	1.84	0.59
4:G:34:TYR:HD1	4:G:49:TYR:HA	1.66	0.59
4:G:39:PHE:CE1	4:G:84:ALA:HB2	2.38	0.59
3:D:149:LYS:NZ	3:D:154:LEU:HD21	2.18	0.58
5:F:195:ILE:HD11	5:F:208:ASP:HB3	1.84	0.58
2:B:168:ALA:HA	2:B:178:LEU:HB3	1.85	0.58
4:G:116:VAL:HG11	4:G:196:VAL:CG1	2.33	0.58
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.84	0.58
4:G:114:PRO:HD3	4:G:198:HIS:CD2	2.38	0.58
3:D:155:GLN:HB3	3:D:158:ASN:HD22	1.68	0.58
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.69	0.58
3:L:125:LEU:HD13	3:L:130:ALA:HB2	1.85	0.58
2:H:6:GLN:NE2	2:H:107:THR:HG23	2.18	0.58
5:I:87:THR:HG22	5:I:111:VAL:H	1.69	0.58
1:C:561:THR:OG1	1:C:617:HIS:O	2.14	0.58
3:D:192:TYR:CZ	3:D:209:PHE:HZ	2.23	0.57
2:B:36:TRP:CE2	2:B:80:MET:HB2	2.39	0.57
4:G:47:LEU:HD21	4:G:62:PHE:CD1	2.39	0.57
3:L:145:LYS:HD3	3:L:146:VAL:N	2.19	0.57
2:B:203:SER:O	2:B:205:THR:OG1	2.19	0.57
5:I:13:LYS:HB3	5:I:112:SER:O	2.04	0.57
1:A:490:PRO:HB2	1:A:491:PRO:CD	2.28	0.57
2:H:6:GLN:N	2:H:105:GLN:OE1	2.31	0.57
2:H:200:HIS:ND1	2:H:203:SER:HB3	2.20	0.57
2:B:23:LYS:HG3	2:B:77:THR:HG22	1.87	0.57
5:F:166:PHE:HE1	5:F:181:VAL:HG22	1.70	0.57
2:H:38:ARG:HD3	2:H:90:TYR:CE2	2.40	0.56
2:H:184:VAL:HG21	2:H:194:TYR:CZ	2.39	0.56
5:F:139:GLY:HA3	5:F:181:VAL:HG12	1.87	0.56
5:I:91:PHE:HD2	5:I:106:GLY:HA2	1.70	0.56
2:B:12:LYS:HG3	2:B:18:VAL:HB	1.86	0.56
4:G:151:ALA:HB1	4:G:189:HIS:HD2	1.71	0.56
2:H:101:ASP:HB3	2:H:102:PRO:HD3	1.86	0.56
2:B:72:ASP:OD2	2:B:74:SER:OG	2.23	0.56
9:O:1:NAG:O4	9:O:2:NAG:N2	2.38	0.56
1:A:603:ILE:HG22	1:A:604:THR:H	1.71	0.56
2:B:6:GLN:H	2:B:105:GLN:HE22	1.52	0.56
4:E:181:LEU:HG	4:E:185:GLN:HG3	1.88	0.56
1:A:518:THR:HB	1:A:526:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:132:THR:HA	4:E:179:LEU:O	2.05	0.56
4:E:144:ALA:CB	4:E:165:PRO:HD3	2.33	0.56
3:D:167:ASP:OD1	3:D:169:LYS:HG2	2.06	0.56
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.88	0.56
5:I:18:VAL:HG21	5:I:109:VAL:HG21	1.88	0.56
4:G:35:TRP:CD2	4:G:73:LEU:HD13	2.41	0.55
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.87	0.55
4:G:76:SER:O	4:G:78:LEU:HD12	2.07	0.55
4:G:170:ASN:N	4:G:170:ASN:OD1	2.39	0.55
2:B:128:SER:OG	2:B:189:LEU:HD12	2.06	0.55
3:D:29:ILE:HD11	3:D:90:GLN:HB2	1.87	0.55
1:A:541:ASN:HA	1:A:548:ASN:HD21	1.71	0.55
4:E:169:SER:HB3	4:E:172:LYS:O	2.06	0.55
5:I:143:LYS:HA	5:I:177:SER:CB	2.35	0.55
3:D:39:LYS:HB2	3:D:40:PRO:HD3	1.89	0.54
2:B:203:SER:O	2:B:203:SER:OG	2.24	0.54
3:D:80:PRO:HA	3:D:83:PHE:CE1	2.42	0.54
4:E:91:TRP:CZ2	5:F:97:GLN:HA	2.42	0.54
2:H:12:LYS:O	2:H:111:VAL:HG23	2.07	0.54
4:G:27(B):ASN:OD1	4:G:28:ILE:N	2.36	0.54
5:I:87:THR:HG22	5:I:110:THR:HA	1.88	0.54
3:L:158:ASN:N	3:L:158:ASN:OD1	2.41	0.54
4:G:152:ASP:OD1	4:G:190:ARG:N	2.38	0.54
1:C:509:PHE:CZ	1:C:601:PRO:HB3	2.43	0.54
3:D:141:PRO:HB2	3:D:143:GLU:OE2	2.07	0.54
5:I:83:ARG:O	5:I:111:VAL:HG21	2.06	0.54
5:F:124:LEU:HD21	5:F:141:LEU:HD23	1.89	0.54
1:A:424:ARG:HG2	1:A:518:THR:N	2.18	0.54
1:A:505:PRO:HB2	1:A:507:TYR:CE2	2.43	0.54
4:E:141:TYR:HB3	4:E:142:PRO:HD3	1.90	0.53
3:D:144:ALA:HB2	3:D:198:HIS:CD2	2.43	0.53
3:D:144:ALA:HB2	3:D:198:HIS:HD2	1.73	0.53
4:E:184:GLU:OE1	4:E:184:GLU:N	2.37	0.53
2:H:167:PRO:HG2	3:L:163:VAL:O	2.08	0.53
1:C:594:TYR:CD2	1:C:598:GLY:HA3	2.43	0.53
2:H:122:PHE:CD2	3:L:124:GLN:HB2	2.44	0.53
3:D:93:SER:O	3:D:96:ARG:NH1	2.41	0.53
3:L:89:GLN:HG2	3:L:90:GLN:N	2.24	0.53
4:G:59:PRO:HD2	4:G:62:PHE:HD2	1.74	0.53
3:L:141:PRO:HB2	3:L:143:GLU:OE2	2.09	0.53
4:E:59:PRO:HG2	4:E:62:PHE:CE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:THR:HG22	2:H:29:LEU:HD23	1.91	0.52
5:I:162:GLY:O	5:I:182:VAL:HA	2.08	0.52
3:L:132:VAL:HG22	3:L:148:TRP:HH2	1.73	0.52
5:F:145:TYR:CE2	5:F:176:TYR:HB2	2.45	0.52
3:L:11:LEU:HD22	3:L:104:VAL:HG22	1.91	0.52
1:A:434:ASN:O	2:B:2:VAL:HG23	2.09	0.52
4:E:161:GLU:HB3	5:F:169:VAL:HG21	1.92	0.52
2:H:94:ARG:HB3	2:H:102:PRO:HD2	1.91	0.52
5:F:36:TRP:CE2	5:F:80:MET:HB2	2.44	0.52
3:L:6:GLN:O	3:L:100:GLN:NE2	2.36	0.52
4:E:59:PRO:HG2	4:E:62:PHE:HE1	1.75	0.52
5:I:13:LYS:HB2	5:I:14:PRO:CD	2.37	0.52
3:L:14:SER:OG	3:L:107:LYS:HE3	2.10	0.52
1:A:516:VAL:HG21	1:A:539:LEU:HD11	1.92	0.52
2:H:148:GLU:OE2	2:H:168:ALA:HB3	2.10	0.52
2:B:126:PRO:HD2	2:B:213:PRO:HA	1.90	0.52
1:A:604:THR:CG2	1:A:607:CYS:HB2	2.40	0.51
3:D:6:GLN:NE2	3:D:101:GLY:H	2.08	0.51
5:I:54:ASN:HB2	5:I:56:TYR:H	1.76	0.51
5:F:143:LYS:NZ	5:F:171:GLN:OE1	2.43	0.51
2:H:95:ASP:O	2:H:100(G):ASN:ND2	2.35	0.51
1:A:544:PRO:HD2	1:A:550:PHE:CE1	2.45	0.51
5:I:145:TYR:OH	5:I:178:LEU:HD23	2.11	0.51
1:A:436:GLY:O	2:B:29:LEU:HD21	2.09	0.51
1:A:544:PRO:HD2	1:A:550:PHE:CZ	2.46	0.51
3:D:90:GLN:HG2	3:D:97:THR:OG1	2.11	0.51
3:L:166:GLN:HB2	3:L:171:SER:HA	1.92	0.51
5:F:98:ILE:HD12	5:F:98:ILE:H	1.75	0.51
4:G:87:TYR:CD2	5:I:45:LEU:HD12	2.45	0.51
4:G:36:TYR:OH	5:I:100(A):VAL:HG23	2.11	0.51
1:A:502:VAL:HG11	1:A:537:PHE:CE1	2.46	0.50
5:I:12:LYS:HD2	5:I:13:LYS:H	1.76	0.50
2:H:163:VAL:O	2:H:164:HIS:ND1	2.44	0.50
2:B:121:VAL:HA	2:B:141:LEU:O	2.10	0.50
4:G:21:ILE:O	4:G:72:SER:HB2	2.12	0.50
3:L:28:ASN:ND2	3:L:68:GLY:HA2	2.27	0.50
4:E:167:LYS:HA	4:E:173:TYR:CD2	2.47	0.50
1:A:544:PRO:HA	1:A:547:GLY:H	1.76	0.50
5:F:12:LYS:O	5:F:111:VAL:HA	2.12	0.50
4:G:44:PRO:HD2	5:I:103:TRP:CE3	2.45	0.50
4:G:95(C):PRO:HD3	5:I:58:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLN:HG2	3:D:23:CYS:SG	2.52	0.50
5:F:189:LEU:HD12	5:F:189:LEU:H	1.77	0.50
4:G:170:ASN:ND2	4:G:172:LYS:HE2	2.24	0.50
5:I:59:TYR:CE1	5:I:69:MET:HG3	2.47	0.50
1:C:632:TYR:CE2	1:C:637:GLU:HB3	2.47	0.49
2:H:83:ARG:O	2:H:111:VAL:CG1	2.57	0.49
5:I:36:TRP:CE2	5:I:80:MET:HB2	2.47	0.49
1:A:509:PHE:CE1	1:A:601:PRO:HB3	2.47	0.49
2:B:156:SER:H	2:B:197:ASN:HD21	1.59	0.49
2:B:168:ALA:HB2	2:B:178:LEU:HD23	1.93	0.49
1:A:541:ASN:HB3	1:A:549:TRP:NE1	2.28	0.49
4:E:168:GLN:O	4:E:170:ASN:N	2.44	0.49
2:B:112:SER:HB3	2:B:146:PHE:CZ	2.48	0.49
3:D:125:LEU:HD21	3:D:211:ARG:HH12	1.78	0.49
4:G:4:LEU:HD23	4:G:23:CYS:SG	2.52	0.49
4:G:163:THR:HG1	4:G:176:SER:H	1.57	0.49
2:B:6:GLN:H	2:B:105:GLN:NE2	2.10	0.49
1:C:423:ASN:HB3	1:C:527:TYR:HB3	1.94	0.49
5:F:185:PRO:O	5:F:188:SER:OG	2.21	0.49
1:C:498:PRO:O	1:C:501:THR:HG22	2.12	0.49
5:F:68:THR:OG1	5:F:82(A):ARG:NH2	2.45	0.49
5:F:117:LYS:HE3	5:F:144:ASP:HB3	1.94	0.49
4:G:61:ARG:HD3	4:G:77:GLY:O	2.13	0.49
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.48	0.49
5:I:59:TYR:HE1	5:I:69:MET:HG3	1.78	0.49
1:A:450:SER:HA	6:J:2:NAG:O6	2.12	0.49
3:D:86:TYR:O	3:D:101:GLY:HA2	2.13	0.49
4:G:161:GLU:HB3	5:I:169:VAL:CG1	2.41	0.49
1:C:543:ARG:HH12	1:C:597:CYS:C	2.16	0.48
3:D:186:TYR:O	3:D:188:LYS:N	2.39	0.48
4:G:21:ILE:HD13	4:G:102:THR:HG21	1.93	0.48
2:H:47:TRP:CD1	3:L:96:ARG:HB2	2.48	0.48
2:H:67:VAL:HA	2:H:81:GLU:O	2.13	0.48
5:I:34:ILE:O	5:I:34:ILE:HG13	2.13	0.48
3:L:6:GLN:HE21	3:L:99:GLY:CA	2.23	0.48
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.48	0.48
3:D:38:GLN:O	3:D:84:ALA:HB1	2.12	0.48
3:L:142:ARG:HB2	3:L:173:TYR:CE2	2.48	0.48
1:C:603:ILE:HG23	1:C:631:MET:HE1	1.95	0.48
3:D:21:ILE:HG23	3:D:102:THR:HG21	1.96	0.48
5:I:23:LYS:NZ	5:I:75:THR:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:ILE:HD12	2:H:210:ARG:HG2	1.95	0.48
7:K:1:NAG:H61	7:K:2:NAG:N2	2.29	0.48
5:F:83:ARG:HG3	5:F:85:ASP:H	1.79	0.48
4:G:27(B):ASN:OD1	4:G:28:ILE:HG13	2.14	0.48
2:H:186:SER:HA	2:H:189:LEU:HD13	1.96	0.48
4:G:59:PRO:HD2	4:G:62:PHE:CD2	2.49	0.48
4:G:169:SER:C	4:G:171:ASN:H	2.17	0.48
4:G:27(A):SER:O	4:G:92:ASP:HA	2.14	0.47
4:E:182:THR:H	4:E:185:GLN:HG2	1.79	0.47
5:I:37:VAL:HG11	5:I:45:LEU:HB3	1.95	0.47
5:I:63:LEU:O	5:I:65:GLY:N	2.46	0.47
3:D:1:ASP:CG	3:D:2:ILE:H	2.17	0.47
1:A:497:VAL:HG23	1:A:537:PHE:HB2	1.95	0.47
4:E:54:ARG:NE	4:E:60:ASP:HA	2.29	0.47
4:E:83:GLU:CG	4:E:106:VAL:H	2.27	0.47
4:E:121:PRO:HB3	4:E:132:THR:H	1.79	0.47
1:A:437:TRP:O	1:A:440:GLY:N	2.47	0.47
5:F:119:PRO:HB3	5:F:145:TYR:HB3	1.96	0.47
2:H:121:VAL:HA	2:H:141:LEU:O	2.15	0.47
5:I:35:SER:HB2	5:I:49:GLY:O	2.15	0.47
1:C:434:ASN:HD21	2:H:102:PRO:HD3	1.79	0.47
2:H:18:VAL:HG11	2:H:109:VAL:HG11	1.97	0.47
5:I:124:LEU:HD11	5:I:141:LEU:HB2	1.96	0.47
2:B:87:THR:HG23	2:B:110:THR:HA	1.96	0.47
3:D:6:GLN:NE2	3:D:88:CYS:H	2.12	0.47
3:D:136:LEU:HB2	3:D:175:LEU:HB3	1.97	0.47
5:I:87:THR:CG2	5:I:111:VAL:H	2.28	0.47
3:D:105:GLU:HB3	3:D:166:GLN:OE1	2.14	0.47
4:E:27:SER:HA	4:E:29:GLY:HA3	1.96	0.47
4:G:35:TRP:CE2	4:G:73:LEU:HD13	2.49	0.47
1:A:606:ARG:O	1:A:644:CYS:HA	2.14	0.46
1:C:438:LEU:HD22	2:H:97:VAL:HG13	1.97	0.46
5:I:94:ARG:O	5:I:100(A):VAL:HA	2.15	0.46
2:B:124:LEU:HD21	3:D:133:VAL:HG11	1.97	0.46
1:C:548:ASN:OD1	1:C:548:ASN:N	2.47	0.46
1:C:446:LYS:HE2	2:H:53:PRO:O	2.16	0.46
1:C:503:CYS:O	1:C:555:MET:HB3	2.16	0.46
3:D:29:ILE:CD1	3:D:90:GLN:HB2	2.46	0.46
2:B:2:VAL:O	2:B:102:PRO:HG3	2.16	0.46
3:L:170:ASP:OD2	3:L:172:THR:OG1	2.33	0.46
1:A:518:THR:HG21	1:A:535:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:PRO:HB2	1:A:527:TYR:HE1	1.81	0.46
2:B:148:GLU:OE2	2:B:149:PRO:HA	2.16	0.46
1:C:492:ARG:HH12	1:C:562:LYS:HD3	1.81	0.46
5:I:12:LYS:CD	5:I:13:LYS:H	2.29	0.46
2:B:30:ASN:HB2	2:B:73:GLU:OE1	2.16	0.46
3:D:83:PHE:CE2	3:D:106:ILE:HG12	2.51	0.46
5:I:7:SER:HB3	5:I:21:SER:OG	2.16	0.45
3:L:35:TRP:HD1	3:L:48:ILE:HB	1.81	0.45
2:H:87:THR:HG23	2:H:110:THR:HA	1.96	0.45
1:C:603:ILE:HG22	1:C:604:THR:HG23	1.98	0.45
3:D:125:LEU:HD12	3:D:183:LYS:HE2	1.99	0.45
3:D:149:LYS:HG2	3:D:154:LEU:HD21	1.98	0.45
5:F:36:TRP:CD2	5:F:80:MET:HB2	2.50	0.45
1:A:546:LEU:O	5:I:52:SER:OG	2.35	0.45
1:C:596:ARG:NH2	4:E:93:ASP:OD2	2.50	0.45
4:G:59:PRO:HB2	4:G:61:ARG:HB3	1.98	0.45
2:H:147:PRO:HD2	2:H:202:PRO:CB	2.47	0.45
5:I:2:VAL:HA	5:I:26:GLY:HA3	1.98	0.45
1:C:542:THR:O	1:C:547:GLY:HA3	2.16	0.45
5:I:35:SER:CB	5:I:50:TRP:HB3	2.45	0.45
5:I:39:GLN:HB3	5:I:89:VAL:HG23	1.99	0.45
3:L:125:LEU:CD1	3:L:130:ALA:HB2	2.47	0.45
1:A:509:PHE:HB3	1:A:511:PRO:O	2.17	0.45
4:E:31:ASN:HB3	4:E:91:TRP:HB2	1.98	0.45
2:H:59:TYR:HE1	2:H:69:ILE:HG13	1.82	0.45
5:I:1:GLN:HG3	5:I:2:VAL:N	2.32	0.45
4:E:118:LEU:HD13	4:E:119:PHE:N	2.31	0.45
5:I:119:PRO:HB3	5:I:145:TYR:HB3	1.97	0.45
3:L:132:VAL:HG22	3:L:148:TRP:CH2	2.52	0.45
3:L:149:LYS:HB2	3:L:193:ALA:HB3	1.98	0.45
2:B:96:GLY:O	2:B:98:ARG:HG3	2.17	0.45
1:C:623:ASN:HD22	8:Q:1:NAG:C7	2.30	0.45
5:I:138:LEU:HD13	5:I:211:VAL:CG2	2.46	0.45
1:C:437:TRP:CE2	1:C:559:GLY:HA3	2.51	0.45
3:D:83:PHE:CZ	3:D:106:ILE:HG12	2.52	0.45
4:E:165:PRO:HB2	4:E:173:TYR:HB3	1.98	0.45
1:A:603:ILE:HG22	1:A:604:THR:N	2.31	0.45
3:D:201:LEU:HD23	3:D:201:LEU:HA	1.73	0.45
3:D:28:ASN:ND2	3:D:30:ASN:OD1	2.50	0.44
1:A:593:THR:HG22	1:A:595:SER:H	1.81	0.44
4:E:165:PRO:HA	4:E:174:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102:PRO:O	2:H:103:TRP:HB2	2.18	0.44
4:E:121:PRO:HG3	4:E:133:LEU:N	2.32	0.44
4:G:37:GLN:HB2	4:G:86:TYR:HE2	1.83	0.44
1:C:630:ARG:HD3	1:C:639:ARG:HG2	2.00	0.44
1:C:631:MET:HE2	1:C:631:MET:HB2	1.71	0.44
4:G:182:THR:HG22	4:G:184:GLU:N	2.24	0.44
2:H:12:LYS:NZ	2:H:18:VAL:HA	2.32	0.44
1:A:626:VAL:HA	1:A:643:ALA:HA	1.99	0.44
5:I:52:SER:HB3	5:I:54:ASN:H	1.82	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.17	0.44
2:B:203:SER:O	2:B:205:THR:N	2.50	0.44
2:B:151:THR:CG2	2:B:199:ASN:HB3	2.43	0.44
5:I:12:LYS:O	5:I:111:VAL:HA	2.17	0.44
2:B:61:GLN:HG3	2:B:64:GLN:OE1	2.17	0.44
1:C:439:ALA:HB3	2:H:29:LEU:HD11	2.00	0.44
5:I:184:VAL:HG13	5:I:185:PRO:HD2	1.99	0.44
2:B:66:ARG:HH22	2:B:86:ASP:CG	2.20	0.43
1:C:519:THR:OG1	1:C:520:ASP:N	2.51	0.43
3:D:90:GLN:NE2	3:D:95:VAL:O	2.50	0.43
1:C:543:ARG:HH12	1:C:598:GLY:N	2.16	0.43
4:E:121:PRO:HB2	4:E:126:LEU:HD11	2.01	0.43
1:A:505:PRO:HB2	1:A:507:TYR:HE2	1.82	0.43
1:A:633:VAL:O	1:A:636:VAL:HG12	2.18	0.43
2:B:159:LEU:HD21	2:B:182:VAL:HG21	1.99	0.43
5:F:61:GLN:OE1	5:F:61:GLN:N	2.31	0.43
2:H:141:LEU:CD2	2:H:143:LYS:HB2	2.48	0.43
1:A:518:THR:HG22	1:A:519:THR:H	1.82	0.43
5:F:36:TRP:CH2	5:F:92:CYS:HB3	2.53	0.43
5:I:55:GLY:O	5:I:57:THR:HG23	2.18	0.43
3:L:190:LYS:HA	3:L:211:ARG:HB2	2.00	0.43
1:A:499:ALA:HA	1:A:502:VAL:HG12	2.01	0.43
2:B:76:SER:O	2:B:76:SER:OG	2.36	0.43
2:B:83:ARG:HB3	2:B:85:GLU:OE1	2.18	0.43
5:F:47:TRP:CH2	5:F:49:GLY:HA2	2.53	0.43
1:C:553:THR:HG21	1:C:618:TYR:CE2	2.54	0.43
3:D:128:GLY:O	3:D:183:LYS:HG3	2.19	0.43
4:E:112:ALA:HB3	4:E:141:TYR:N	2.33	0.43
2:H:35:THR:HG21	2:H:100(I):PHE:CE2	2.54	0.43
1:A:441:LEU:HD12	1:A:616:TRP:CH2	2.54	0.43
2:B:40:ALA:HB3	2:B:43:GLN:HB2	1.99	0.43
3:D:192:TYR:CE2	3:D:209:PHE:HZ	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:206:THR:OG1	4:E:207:VAL:N	2.52	0.43
5:I:209:LYS:HE2	5:I:209:LYS:HB2	1.84	0.43
2:H:101:ASP:OD2	3:L:55:GLN:NE2	2.51	0.43
3:L:125:LEU:HD21	3:L:186:TYR:HE2	1.84	0.43
1:A:544:PRO:HA	1:A:547:GLY:N	2.34	0.43
3:D:159:SER:HB3	3:D:179:LEU:HD12	1.99	0.43
4:G:142:PRO:O	4:G:144:ALA:N	2.46	0.43
2:H:152:VAL:HA	2:H:197:ASN:O	2.19	0.43
3:L:6:GLN:HG3	3:L:100:GLN:OE1	2.19	0.43
3:L:166:GLN:HA	3:L:172:THR:O	2.19	0.42
1:A:621:THR:HA	1:A:624:TYR:CD2	2.54	0.42
2:B:126:PRO:HG2	2:B:213:PRO:HB3	2.00	0.42
3:D:83:PHE:HA	3:D:104:VAL:HG23	2.00	0.42
4:G:109:GLN:HG3	4:G:110:PRO:CD	2.49	0.42
2:H:120:SER:HB3	2:H:122:PHE:CZ	2.54	0.42
9:O:3:BMA:H62	9:O:5:MAN:H2	1.53	0.42
3:D:181:LEU:HB3	3:D:185:ASP:HB2	2.01	0.42
4:E:109:GLN:HB2	4:E:141:TYR:CE1	2.55	0.42
4:G:92:ASP:HB3	4:G:95(B):GLY:HA3	2.00	0.42
5:I:95:ALA:HB2	5:I:100(A):VAL:HG12	2.00	0.42
3:D:149:LYS:HG2	3:D:154:LEU:CD2	2.50	0.42
4:E:54:ARG:HE	4:E:60:ASP:HA	1.84	0.42
5:F:36:TRP:CZ3	5:F:92:CYS:HB3	2.54	0.42
5:F:36:TRP:HB2	5:F:69:MET:CE	2.49	0.42
3:L:164:THR:O	3:L:173:TYR:HD1	2.02	0.42
1:A:532:ASN:O	1:A:535:ASP:HB2	2.20	0.42
2:B:41:PRO:HD3	2:B:88:ALA:HA	2.01	0.42
3:L:147:GLN:O	3:L:194:CYS:HA	2.20	0.42
1:A:497:VAL:CG2	1:A:537:PHE:HB2	2.49	0.42
1:C:556:ASN:CB	1:C:560:PHE:H	2.31	0.42
3:D:148:TRP:CG	3:D:179:LEU:HD13	2.54	0.42
5:I:35:SER:HA	5:I:50:TRP:HA	2.01	0.42
1:A:541:ASN:HD21	1:A:566:ALA:N	2.17	0.42
3:D:167:ASP:N	3:D:172:THR:O	2.48	0.42
4:G:79:ARG:HA	4:G:79:ARG:HD2	1.82	0.42
2:H:124:LEU:HB2	2:H:139:GLY:C	2.40	0.42
3:L:118:PHE:HB2	3:L:133:VAL:HG13	2.00	0.42
1:A:516:VAL:HG23	1:A:537:PHE:HD2	1.85	0.42
4:E:147:VAL:HG23	4:E:148:ALA:N	2.35	0.41
2:H:192:GLN:HG2	2:H:194:TYR:CE2	2.55	0.41
5:I:16:ALA:H	5:I:82(C):LEU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:32:HIS:CG	5:I:94:ARG:HD2	2.55	0.41
1:A:432:SER:OG	7:K:1:NAG:H62	2.20	0.41
1:A:551:GLY:HA3	1:A:600:GLY:HA2	2.02	0.41
2:B:154:TRP:CZ3	2:B:196:CYS:HB3	2.55	0.41
4:E:145:VAL:HG21	4:E:198:HIS:CD2	2.55	0.41
4:G:145:VAL:HG22	4:G:198:HIS:HB2	2.01	0.41
1:C:492:ARG:H	1:C:492:ARG:HG3	1.60	0.41
4:E:166:SER:O	4:E:173:TYR:HA	2.20	0.41
4:G:116:VAL:HA	4:G:136:LEU:O	2.20	0.41
5:I:89:VAL:HG13	5:I:108:LEU:HD23	2.00	0.41
2:H:55:PHE:HZ	2:H:73:GLU:OE2	2.03	0.41
5:I:105:GLN:OE1	5:I:105:GLN:N	2.47	0.41
1:A:498:PRO:O	1:A:501:THR:HB	2.20	0.41
5:I:27:TYR:CE1	5:I:94:ARG:HD3	2.56	0.41
1:C:543:ARG:NH1	1:C:598:GLY:O	2.53	0.41
3:D:125:LEU:HD12	3:D:125:LEU:HA	1.75	0.41
5:F:143:LYS:HA	5:F:177:SER:HB3	2.01	0.41
2:H:203:SER:O	2:H:205:THR:HG23	2.19	0.41
3:L:4:MET:SD	3:L:90:GLN:HB3	2.60	0.41
1:C:633:VAL:O	1:C:633:VAL:HG13	2.21	0.41
1:A:543:ARG:HG3	1:A:550:PHE:CE1	2.55	0.41
3:D:35:TRP:CD2	3:D:73:LEU:HD12	2.55	0.41
4:E:27(B):ASN:ND2	4:E:92:ASP:OD1	2.34	0.41
4:E:143:GLY:O	4:E:145:VAL:N	2.52	0.41
4:G:18:ARG:HE	4:G:74:ALA:HB1	1.85	0.41
5:I:88:ALA:HB3	5:I:90:TYR:CE2	2.56	0.41
5:I:139:GLY:O	5:I:211:VAL:HG11	2.19	0.41
5:I:185:PRO:HD2	5:I:188:SER:OG	2.21	0.41
3:L:4:MET:HE2	3:L:4:MET:HB3	2.00	0.41
1:A:441:LEU:O	1:A:441:LEU:HD23	2.21	0.41
1:A:596:ARG:NH2	4:G:93:ASP:OD1	2.54	0.41
2:B:105:GLN:OE1	2:B:105:GLN:N	2.46	0.41
2:B:141:LEU:HD22	2:B:143:LYS:HB2	2.03	0.41
2:B:164:HIS:HE1	3:D:167:ASP:OD2	2.04	0.41
2:B:166:PHE:HD1	2:B:179:SER:O	2.04	0.41
1:C:424:ARG:O	1:C:518:THR:HG23	2.21	0.41
3:D:16:GLY:N	3:D:78:LEU:O	2.47	0.41
4:G:46:LEU:HD13	5:I:101:ASP:HA	2.02	0.41
4:G:94:SER:OG	4:G:95(A):SER:HB3	2.21	0.41
5:I:12:LYS:O	5:I:111:VAL:HG12	2.21	0.41
1:C:449:SER:OG	8:Q:1:NAG:H3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ASN:O	1:C:531:GLU:HG2	2.21	0.41
3:D:35:TRP:CG	3:D:73:LEU:HD12	2.56	0.41
4:E:145:VAL:HG21	4:E:198:HIS:CB	2.51	0.40
5:F:51:ILE:HD13	5:F:71:THR:HG23	2.03	0.40
4:G:35:TRP:CE3	4:G:73:LEU:HB2	2.55	0.40
3:L:48:ILE:HD13	3:L:54:LEU:HD23	2.02	0.40
1:A:434:ASN:OD1	2:B:94:ARG:NH1	2.48	0.40
1:A:601:PRO:O	1:A:609:VAL:HG23	2.21	0.40
3:L:73:LEU:HD12	3:L:73:LEU:HA	1.80	0.40
2:B:147:PRO:HD2	2:B:202:PRO:HB3	2.03	0.40
3:D:150:VAL:HG12	3:D:155:GLN:HG2	2.03	0.40
4:G:163:THR:CG2	5:I:169:VAL:HG22	2.49	0.40
2:H:39:GLN:HG3	2:H:44:GLY:O	2.21	0.40
2:H:100(I):PHE:CD1	2:H:100(I):PHE:N	2.89	0.40
2:B:101:ASP:HA	2:B:102:PRO:HA	1.81	0.40
2:B:154:TRP:CH2	2:B:196:CYS:HB3	2.56	0.40
1:C:627:PHE:CE2	1:C:644:CYS:HB2	2.56	0.40
1:C:637:GLU:O	1:C:637:GLU:HG3	2.22	0.40
3:D:154:LEU:HA	3:D:154:LEU:HD23	1.81	0.40
5:F:17:SER:HB3	5:F:82(A):ARG:HA	2.03	0.40
4:G:34:TYR:C	4:G:35:TRP:HD1	2.25	0.40
2:H:18:VAL:HG12	2:H:82(C):LEU:HD11	2.03	0.40
5:I:47:TRP:CH2	5:I:49:GLY:HA2	2.56	0.40
5:I:136:ALA:O	5:I:183:THR:HA	2.21	0.40
3:D:84:ALA:O	3:D:104:VAL:HG22	2.20	0.40
5:F:2:VAL:HG13	5:F:27:TYR:CD1	2.57	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	159/235 (68%)	144 (91%)	9 (6%)	6 (4%)	3	19
1	C	164/235 (70%)	148 (90%)	14 (8%)	2 (1%)	13	44
2	B	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	29	64
2	H	218/241 (90%)	206 (94%)	9 (4%)	3 (1%)	11	40
3	D	211/214 (99%)	183 (87%)	25 (12%)	3 (1%)	11	40
3	L	211/214 (99%)	196 (93%)	14 (7%)	1 (0%)	29	64
4	E	194/217 (89%)	156 (80%)	33 (17%)	5 (3%)	5	26
4	G	210/217 (97%)	185 (88%)	22 (10%)	3 (1%)	11	40
5	F	206/230 (90%)	186 (90%)	19 (9%)	1 (0%)	29	64
5	I	211/230 (92%)	195 (92%)	15 (7%)	1 (0%)	29	64
All	All	2004/2274 (88%)	1806 (90%)	172 (9%)	26 (1%)	12	42

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
4	E	171	ASN
5	I	64	GLN
1	A	544	PRO
4	E	144	ALA
4	G	170	ASN
1	A	449	SER
1	A	568	PRO
1	A	603	ILE
3	D	187	GLU
4	E	165	PRO
2	H	103	TRP
3	D	184	ALA
4	E	208	ALA
5	F	126	PRO
2	H	101	ASP
1	C	521	ARG
3	D	113	PRO
4	G	15	PRO
2	H	102	PRO
3	L	188	LYS
1	A	510	THR
1	C	510	THR
4	E	147	VAL

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Mol	Chain	Res	Type
4	G	143	GLY
1	A	612	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	138/195 (71%)	134 (97%)	4 (3%)	42	72
1	C	142/195 (73%)	142 (100%)	0	100	100
2	B	188/203 (93%)	187 (100%)	1 (0%)	88	94
2	H	186/203 (92%)	182 (98%)	4 (2%)	52	78
3	D	187/188 (100%)	182 (97%)	5 (3%)	44	74
3	L	187/188 (100%)	181 (97%)	6 (3%)	39	69
4	E	165/181 (91%)	162 (98%)	3 (2%)	59	82
4	G	176/181 (97%)	170 (97%)	6 (3%)	37	69
5	F	178/195 (91%)	173 (97%)	5 (3%)	43	73
5	I	180/195 (92%)	173 (96%)	7 (4%)	32	65
All	All	1727/1924 (90%)	1686 (98%)	41 (2%)	49	76

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	ASN
1	A	512	SER
1	A	533	ASP
1	A	535	ASP
2	B	177	SER
3	D	9	SER
3	D	107	LYS
3	D	179	LEU
3	D	185	ASP
3	D	203	SER
4	E	24	SER

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Mol	Chain	Res	Type
4	E	27(B)	ASN
4	E	61	ARG
5	F	21	SER
5	F	50	TRP
5	F	54	ASN
5	F	83	ARG
5	F	140	CYS
4	G	18	ARG
4	G	22	SER
4	G	34	TYR
4	G	85	ASP
4	G	95(A)	SER
4	G	193	SER
2	H	17	SER
2	H	82(B)	SER
2	H	100(I)	PHE
2	H	140	CYS
5	I	22	CYS
5	I	50	TRP
5	I	52	SER
5	I	82(A)	ARG
5	I	84	SER
5	I	164	HIS
5	I	197	ASN
3	L	10	SER
3	L	77	SER
3	L	78	LEU
3	L	89	GLN
3	L	162	SER
3	L	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
3	D	6	GLN
3	D	28	ASN
3	D	30	ASN
3	D	158	ASN
3	L	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
6	NAG	J	1	1,6	14,14,15	0.31	0	17,19,21	0.83	0
6	NAG	J	2	6	14,14,15	0.31	0	17,19,21	0.77	0
6	BMA	J	3	6	11,11,12	1.11	1 (9%)	15,15,17	1.26	1 (6%)
6	MAN	J	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.46	1 (6%)
7	NAG	K	1	1,7	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
7	NAG	K	2	7	14,14,15	0.38	0	17,19,21	1.19	2 (11%)
8	NAG	M	1	1,8	14,14,15	0.27	0	17,19,21	0.76	0
8	NAG	M	2	8	14,14,15	0.54	0	17,19,21	1.09	1 (5%)
8	BMA	M	3	8	11,11,12	1.44	2 (18%)	15,15,17	0.82	0
8	NAG	N	1	1,8	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
8	NAG	N	2	8	14,14,15	0.37	0	17,19,21	1.08	1 (5%)
8	BMA	N	3	8	11,11,12	1.04	1 (9%)	15,15,17	0.72	0
9	NAG	O	1	1,9	14,14,15	0.66	0	17,19,21	1.86	4 (23%)
9	NAG	O	2	9	14,14,15	0.37	0	17,19,21	1.59	4 (23%)
9	BMA	O	3	9	11,11,12	0.88	0	15,15,17	0.80	0
9	MAN	O	4	9	11,11,12	1.01	0	15,15,17	1.21	1 (6%)
9	MAN	O	5	9	11,11,12	1.21	2 (18%)	15,15,17	1.21	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.43	0	17,19,21	1.24	1 (5%)
7	NAG	P	2	7	14,14,15	0.48	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	Q	1	1,8	14,14,15	0.40	0	17,19,21	0.73	0
8	NAG	Q	2	8	14,14,15	0.49	0	17,19,21	0.69	0
8	BMA	Q	3	8	11,11,12	1.24	2 (18%)	15,15,17	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	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
7	NAG	K	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
8	NAG	M	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
8	BMA	M	3	8	-	2/2/19/22	0/1/1/1
8	NAG	N	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	4/6/23/26	0/1/1/1
8	BMA	N	3	8	-	2/2/19/22	0/1/1/1
9	NAG	O	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	O	2	9	-	3/6/23/26	0/1/1/1
9	BMA	O	3	9	-	2/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
9	MAN	O	5	9	-	1/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Q	3	BMA	C2-C3	2.84	1.56	1.52
6	J	3	BMA	C1-C2	2.82	1.58	1.52
6	J	4	MAN	C1-C2	2.46	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	3	BMA	C1-C2	2.46	1.57	1.52
8	N	3	BMA	C1-C2	2.33	1.57	1.52
9	O	5	MAN	C2-C3	2.24	1.55	1.52
8	M	3	BMA	C4-C3	2.23	1.58	1.52
9	O	5	MAN	O5-C5	2.22	1.47	1.43
8	Q	3	BMA	C1-C2	2.06	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	4	MAN	C1-O5-C5	4.64	118.48	112.19
9	O	1	NAG	O3-C3-C2	-4.30	100.58	109.47
9	O	1	NAG	C1-C2-N2	-4.28	103.17	110.49
9	O	5	MAN	C1-O5-C5	3.87	117.44	112.19
7	K	1	NAG	C1-O5-C5	3.78	117.31	112.19
7	K	2	NAG	C2-N2-C7	3.53	127.93	122.90
9	O	4	MAN	C1-O5-C5	3.47	116.90	112.19
7	P	1	NAG	O3-C3-C2	-3.47	102.29	109.47
9	O	2	NAG	C2-N2-C7	2.99	127.16	122.90
9	O	2	NAG	O4-C4-C5	-2.86	102.19	109.30
6	J	3	BMA	C1-C2-C3	2.85	113.17	109.67
8	N	1	NAG	C2-N2-C7	-2.84	118.86	122.90
7	P	2	NAG	O5-C1-C2	-2.65	107.10	111.29
9	O	1	NAG	O3-C3-C4	-2.34	104.95	110.35
9	O	2	NAG	O4-C4-C3	-2.27	105.11	110.35
9	O	1	NAG	O5-C5-C4	-2.18	105.53	110.83
8	M	2	NAG	O4-C4-C5	2.11	114.55	109.30
7	K	2	NAG	O5-C5-C6	2.10	110.50	107.20
8	N	2	NAG	O5-C5-C6	-2.03	104.02	107.20
9	O	2	NAG	C1-O5-C5	-2.03	109.45	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	J	2	NAG	C3-C2-N2-C7
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C3-C2-N2-C7
7	P	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	P	1	NAG	O7-C7-N2-C2
8	Q	1	NAG	C8-C7-N2-C2
8	Q	1	NAG	O7-C7-N2-C2
8	Q	2	NAG	C8-C7-N2-C2
8	Q	2	NAG	O7-C7-N2-C2
9	O	3	BMA	C4-C5-C6-O6
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
9	O	3	BMA	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
8	M	3	BMA	C4-C5-C6-O6
8	N	3	BMA	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
8	M	2	NAG	O5-C5-C6-O6
7	K	1	NAG	C1-C2-N2-C7
8	M	2	NAG	C4-C5-C6-O6
8	N	1	NAG	C8-C7-N2-C2
9	O	5	MAN	O5-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
8	M	3	BMA	O5-C5-C6-O6
9	O	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O5-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
8	N	1	NAG	O7-C7-N2-C2
7	K	2	NAG	O5-C5-C6-O6
9	O	2	NAG	C1-C2-N2-C7
9	O	1	NAG	O7-C7-N2-C2
8	N	2	NAG	C8-C7-N2-C2
8	N	2	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
8	Q	1	NAG	O5-C5-C6-O6
8	N	2	NAG	O7-C7-N2-C2
7	K	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C3-C2-N2-C7
9	O	2	NAG	C3-C2-N2-C7

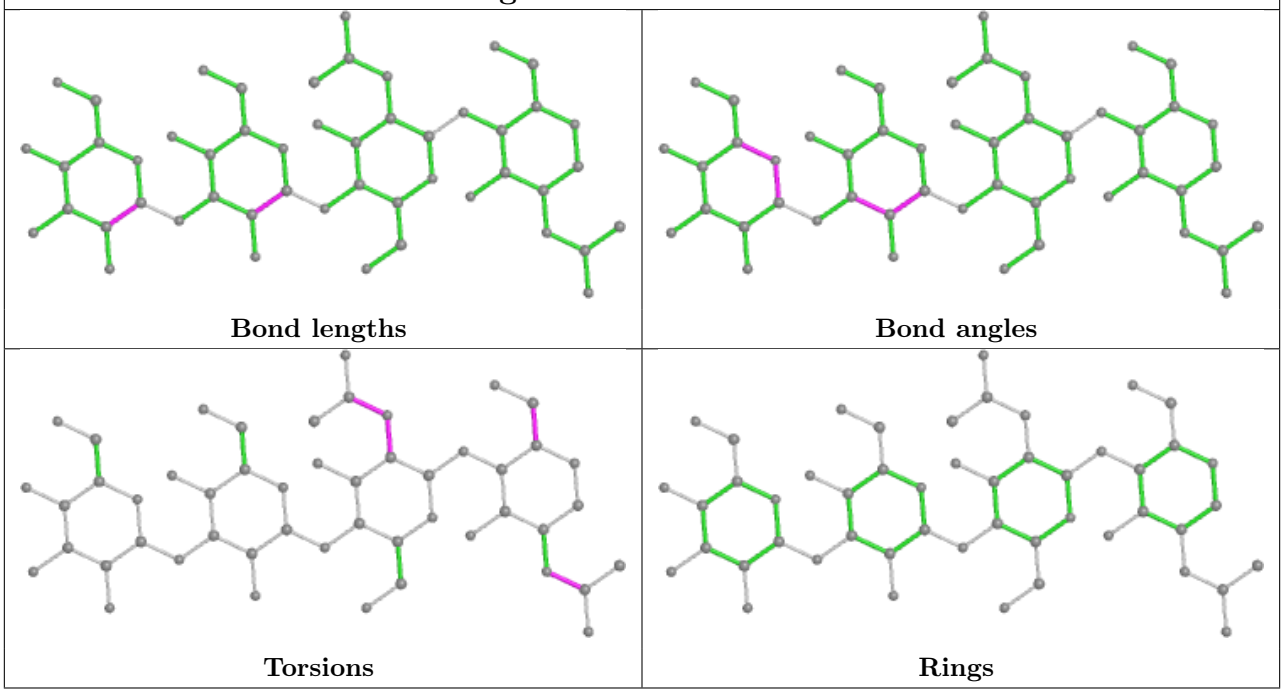
There are no ring outliers.

8 monomers are involved in 8 short contacts:

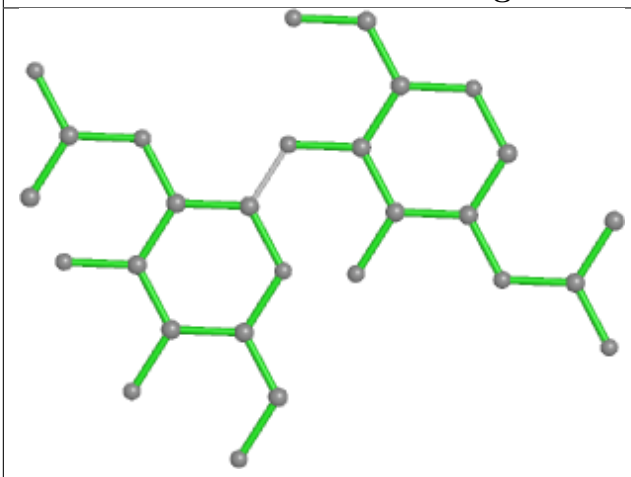
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	O	1	NAG	1	0
9	O	3	BMA	1	0
9	O	2	NAG	1	0
7	K	1	NAG	3	0
6	J	2	NAG	1	0
7	K	2	NAG	2	0
9	O	5	MAN	1	0
8	Q	1	NAG	2	0

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

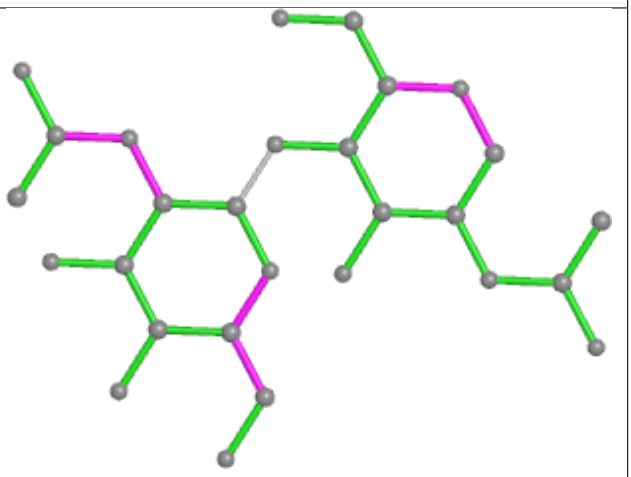
Oligosaccharide Chain J



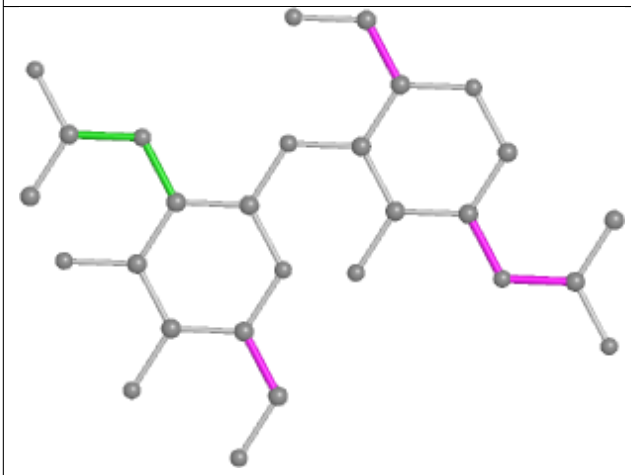
Oligosaccharide Chain K



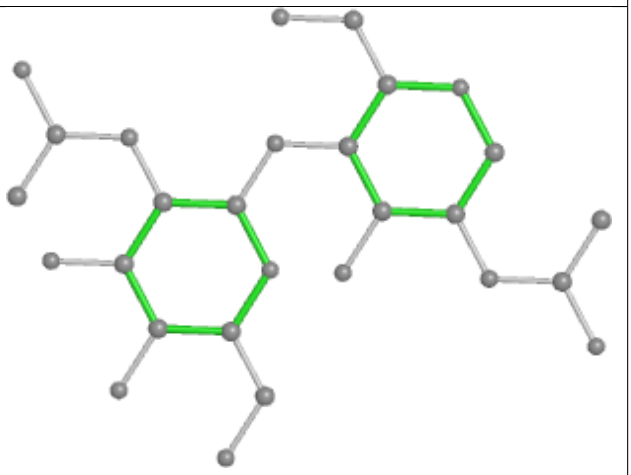
Bond lengths



Bond angles

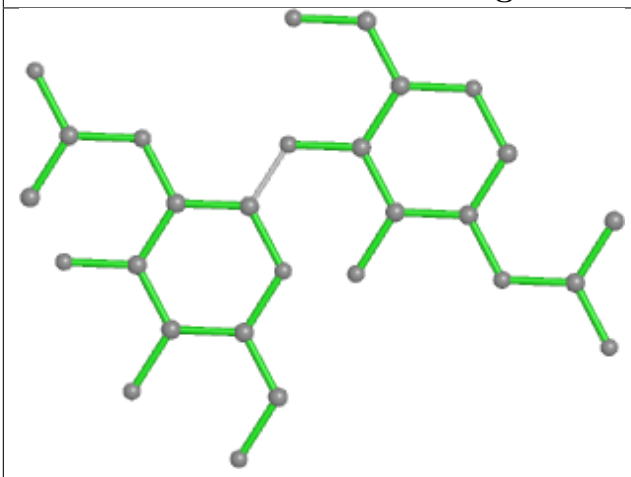


Torsions

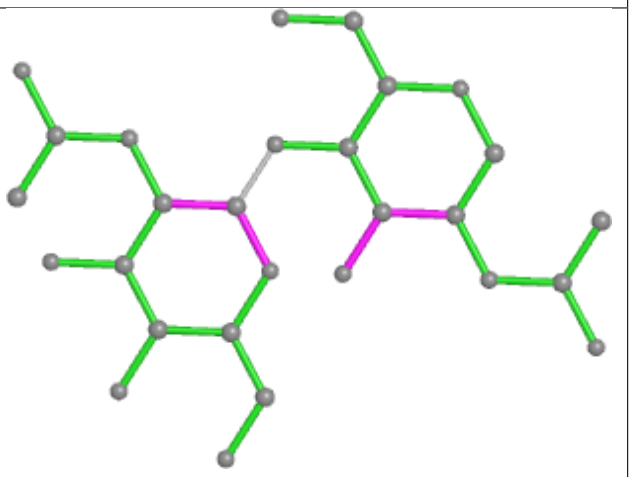


Rings

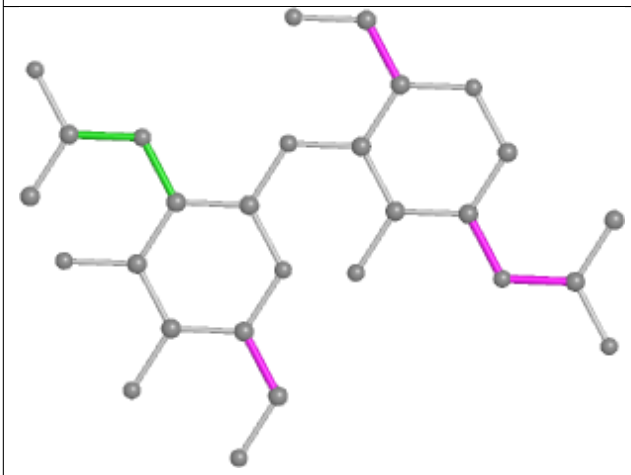
Oligosaccharide Chain P



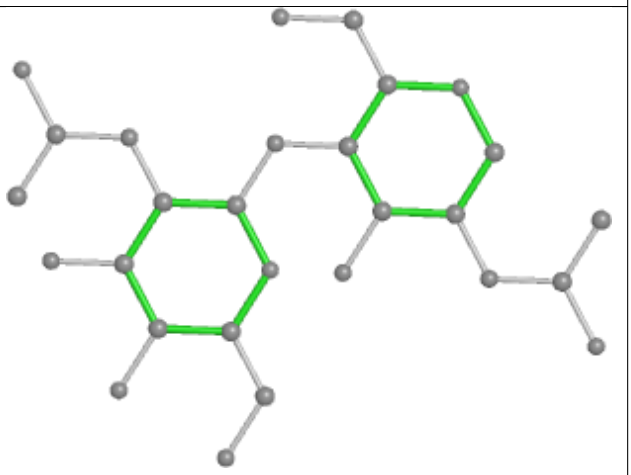
Bond lengths



Bond angles

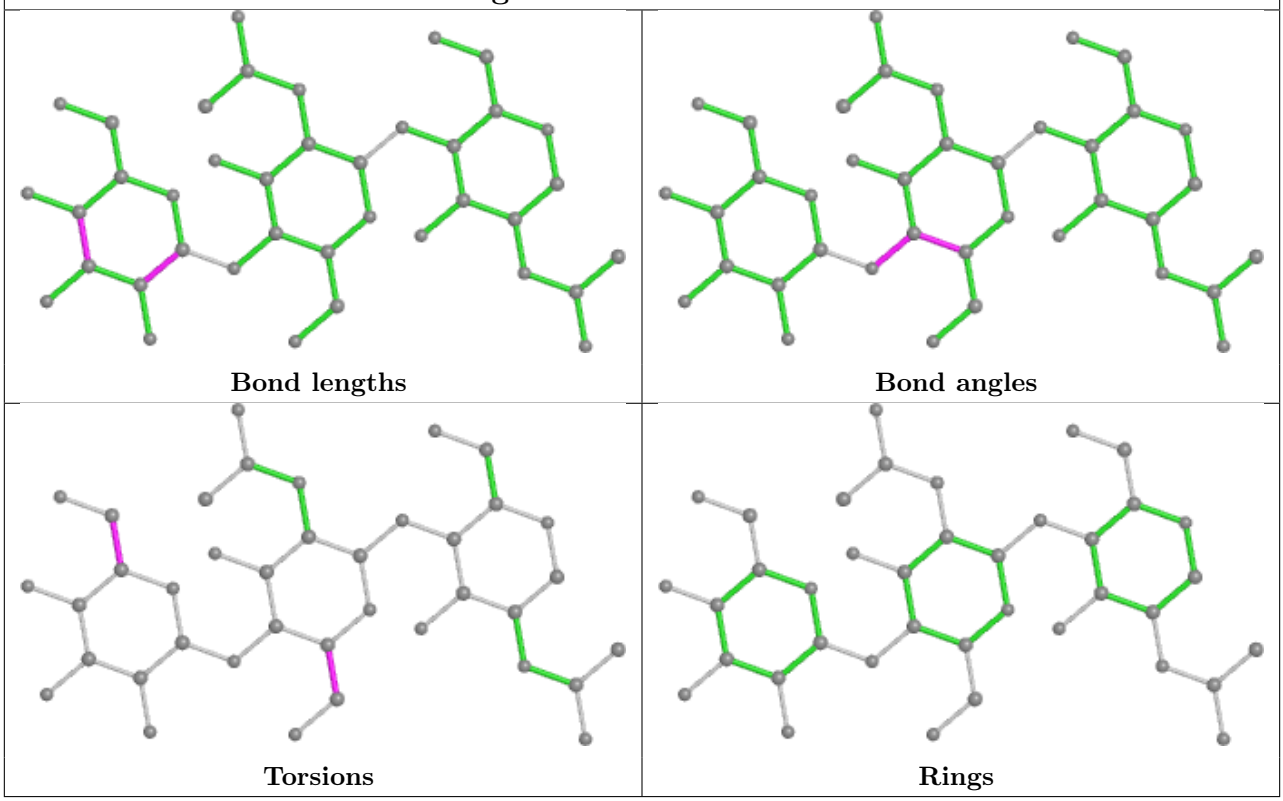


Torsions

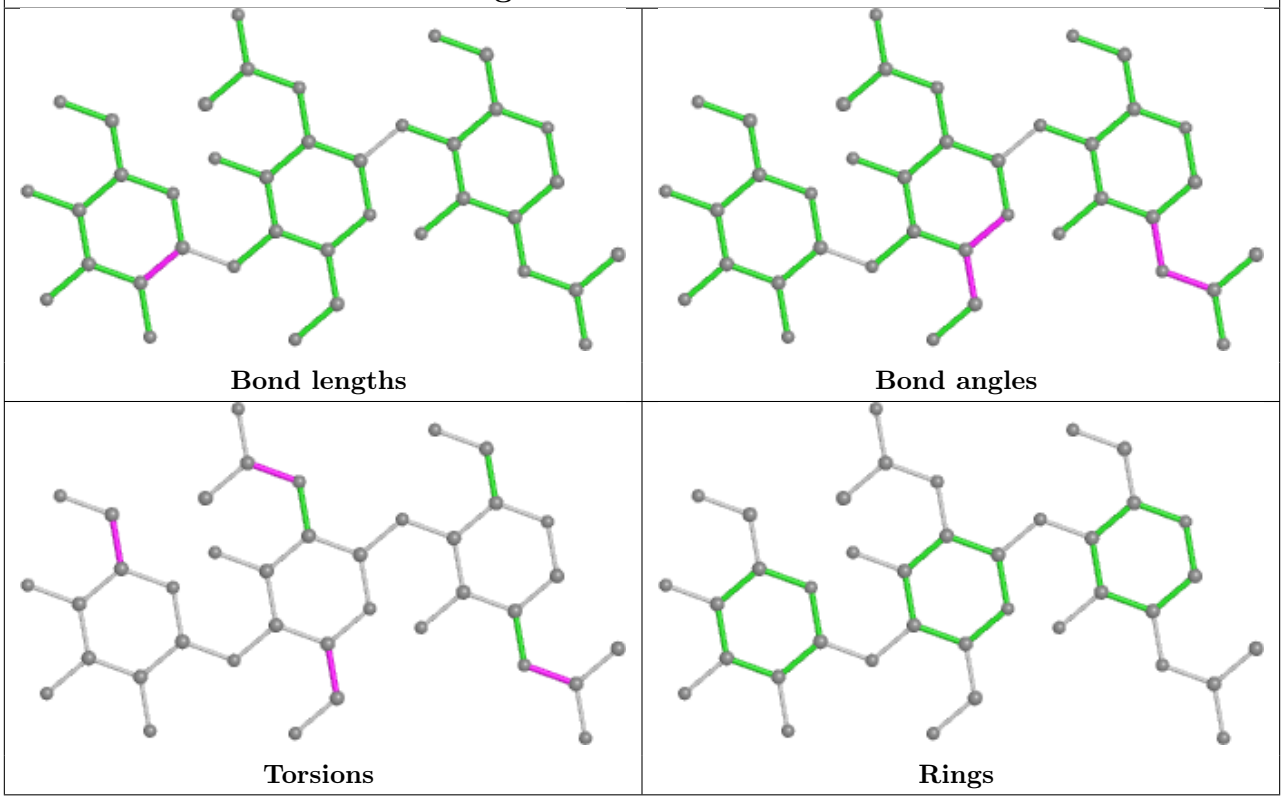


Rings

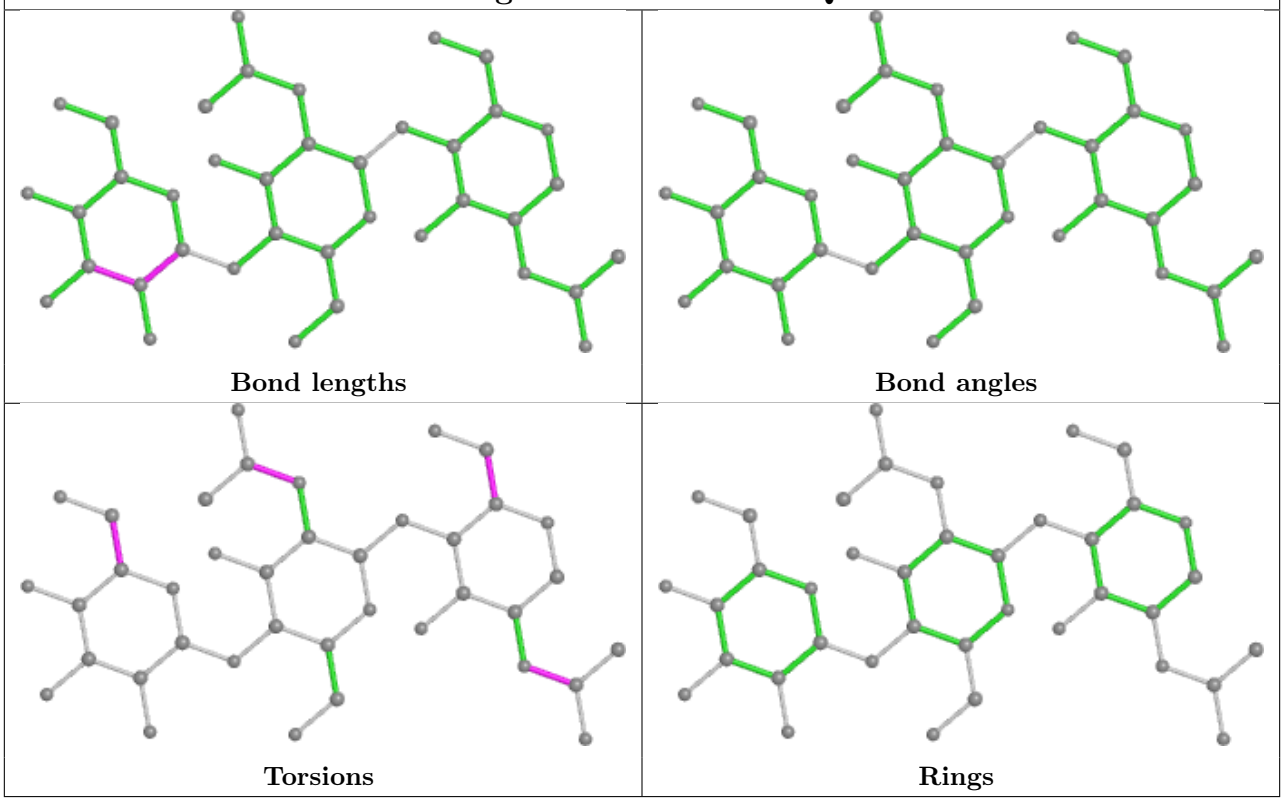
Oligosaccharide Chain M



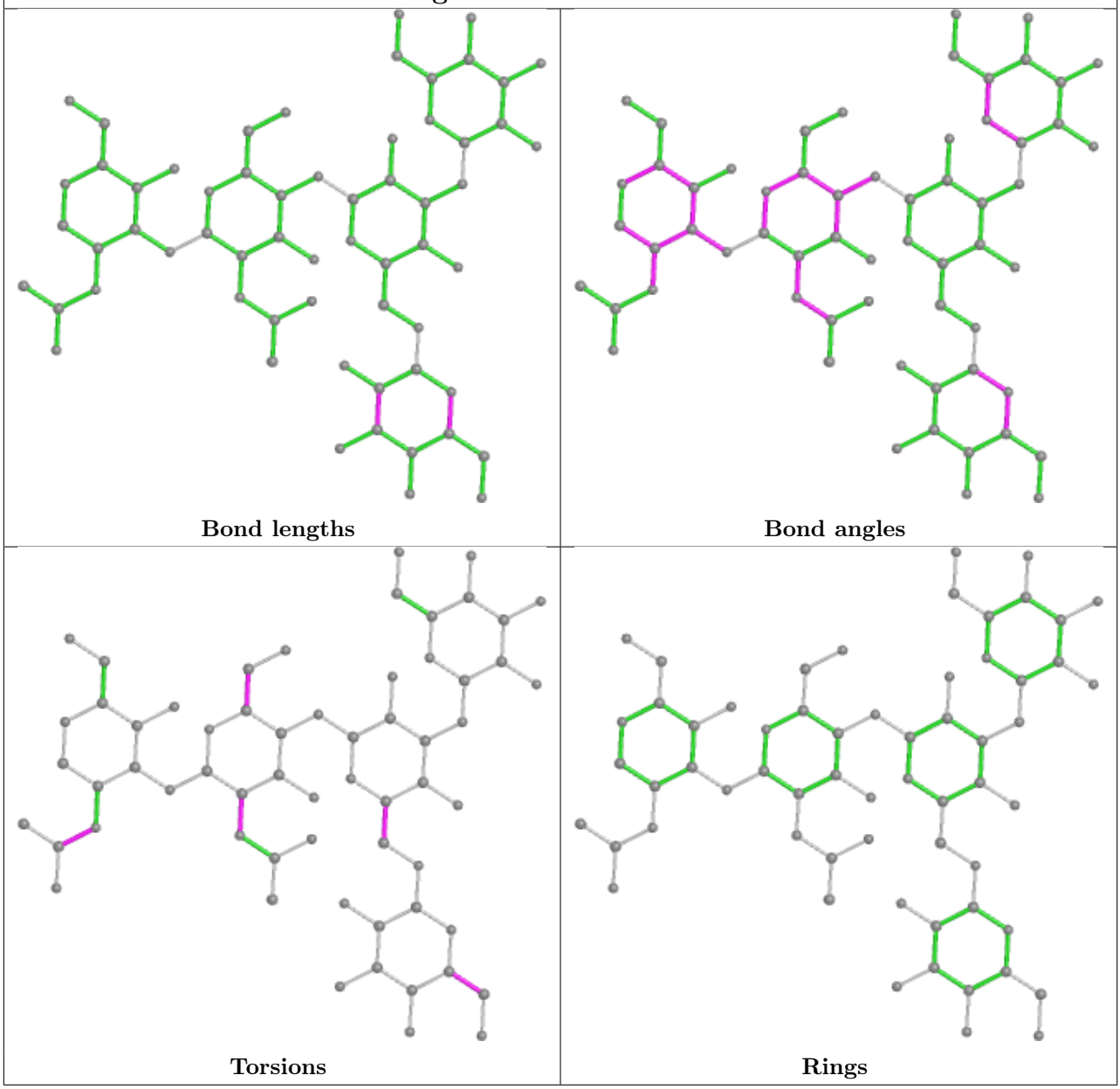
Oligosaccharide Chain N



Oligosaccharide Chain Q



Oligosaccharide Chain O



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	A	5401	1	14,14,15	0.47	0	17,19,21	1.57	3 (17%)
10	NAG	C	4301	1	14,14,15	0.50	0	17,19,21	1.11	1 (5%)

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
10	NAG	A	5401	1	-	1/6/23/26	0/1/1/1
10	NAG	C	4301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	5401	NAG	O5-C1-C2	-3.72	105.42	111.29
10	A	5401	NAG	C2-N2-C7	-3.11	118.47	122.90
10	C	4301	NAG	C2-N2-C7	2.77	126.84	122.90
10	A	5401	NAG	C6-C5-C4	-2.73	106.62	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	4301	NAG	O5-C5-C6-O6
10	C	4301	NAG	C4-C5-C6-O6
10	A	5401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	5401	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	165/235 (70%)	0.25	5 (3%) 50 27	57, 76, 121, 131	0
1	C	170/235 (72%)	-0.05	0 100 100	47, 66, 106, 135	0
2	B	224/241 (92%)	0.18	4 (1%) 68 47	49, 67, 88, 116	0
2	H	222/241 (92%)	-0.14	0 100 100	45, 66, 84, 99	0
3	D	213/214 (99%)	0.07	3 (1%) 75 56	50, 72, 114, 129	0
3	L	213/214 (99%)	-0.07	4 (1%) 66 46	43, 64, 92, 103	0
4	E	200/217 (92%)	0.02	3 (1%) 73 54	44, 74, 134, 140	0
4	G	212/217 (97%)	0.26	18 (8%) 10 4	58, 90, 125, 129	0
5	F	210/230 (91%)	-0.11	0 100 100	45, 67, 116, 128	0
5	I	215/230 (93%)	0.07	1 (0%) 91 81	49, 73, 103, 115	0
All	All	2044/2274 (89%)	0.05	38 (1%) 66 46	43, 71, 120, 140	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	66	LYS	5.4
4	G	65	SER	4.4
4	E	171	ASN	3.6
4	G	23	CYS	3.2
4	G	67	SER	3.2
4	G	71	ALA	3.1
4	G	73	LEU	3.0
3	L	209	PHE	2.9
4	G	36	TYR	2.9
4	G	17	GLN	2.8
4	G	33	VAL	2.7
4	G	75	ILE	2.6
3	L	153	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	G	98	PHE	2.5
4	G	19	VAL	2.5
1	A	531	GLU	2.4
2	B	1	GLN	2.4
1	A	523	GLY	2.4
3	D	211	ARG	2.3
4	E	127	GLN	2.3
4	G	18	ARG	2.3
2	B	131	THR	2.3
2	B	141	LEU	2.3
4	G	64	GLY	2.2
4	E	154	SER	2.2
1	A	642	ALA	2.2
4	G	68	GLY	2.2
4	G	72	SER	2.2
5	I	20	VAL	2.2
2	B	211	VAL	2.2
1	A	632	TYR	2.1
3	L	117	ILE	2.1
3	D	175	LEU	2.1
1	A	606	ARG	2.0
4	G	97	VAL	2.0
3	L	135	LEU	2.0
4	G	88	CYS	2.0
3	D	192	TYR	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
8	BMA	M	3	11/12	0.59	0.23	119,126,130,130	0
6	MAN	J	4	11/12	0.68	0.47	142,149,153,155	0
8	BMA	Q	3	11/12	0.69	0.32	110,119,125,126	0

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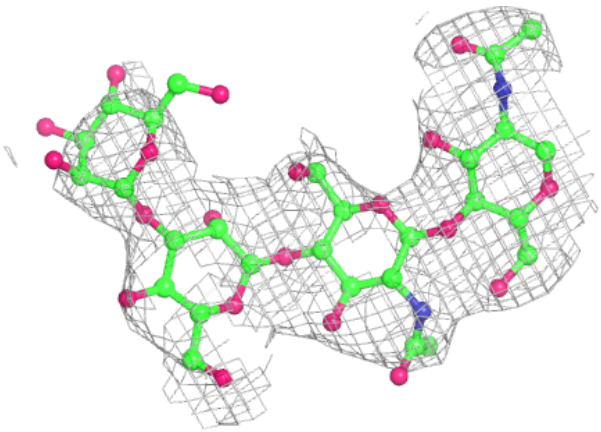
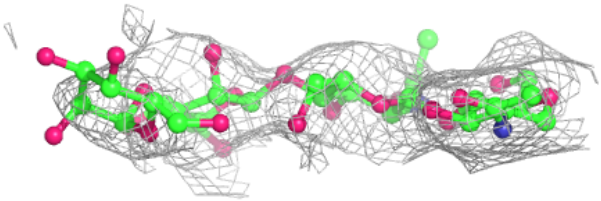
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	K	2	14/15	0.70	0.40	97,117,128,130	0
7	NAG	P	2	14/15	0.70	0.38	121,133,138,138	0
8	BMA	N	3	11/12	0.71	0.36	112,120,131,136	0
6	BMA	J	3	11/12	0.72	0.17	118,137,143,149	0
9	MAN	O	4	11/12	0.72	0.21	114,123,132,134	0
7	NAG	P	1	14/15	0.76	0.21	102,119,127,130	0
9	MAN	O	5	11/12	0.76	0.23	119,129,132,135	0
7	NAG	K	1	14/15	0.79	0.25	90,98,111,113	0
9	BMA	O	3	11/12	0.79	0.14	116,122,131,133	0
6	NAG	J	2	14/15	0.82	0.24	122,128,131,140	0
8	NAG	M	2	14/15	0.84	0.23	86,100,112,114	0
8	NAG	Q	2	14/15	0.85	0.44	103,112,117,117	0
6	NAG	J	1	14/15	0.86	0.18	91,107,116,120	0
9	NAG	O	2	14/15	0.87	0.14	85,91,107,110	0
8	NAG	N	2	14/15	0.89	0.25	88,93,103,112	0
8	NAG	Q	1	14/15	0.90	0.43	77,100,108,112	0
8	NAG	N	1	14/15	0.93	0.17	66,76,83,83	0
9	NAG	O	1	14/15	0.94	0.16	62,74,81,84	0
8	NAG	M	1	14/15	0.96	0.18	73,82,89,89	0

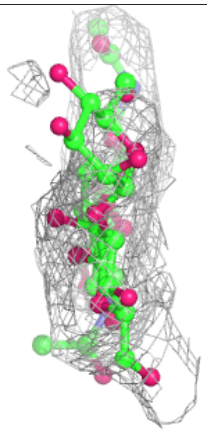
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain J:

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

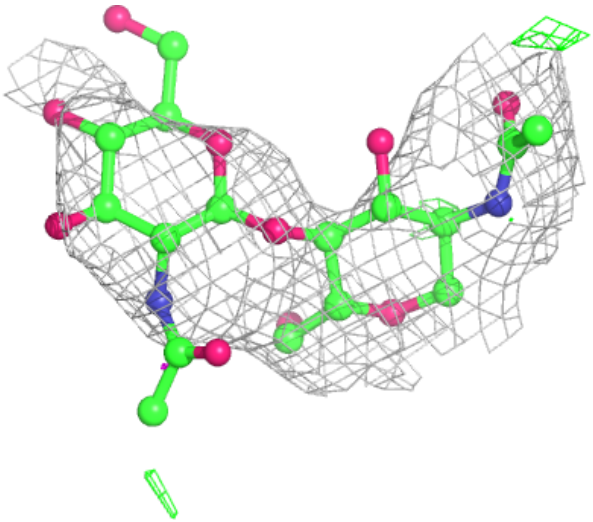


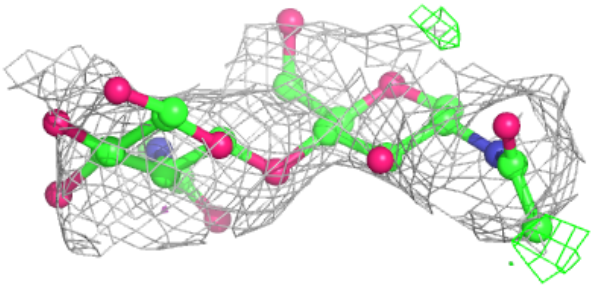


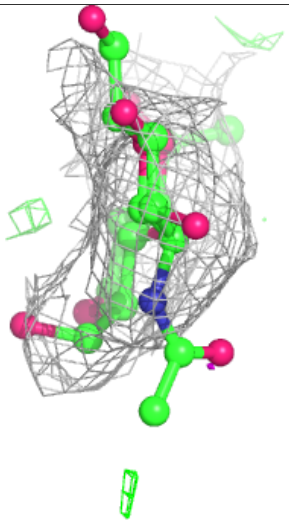


Electron density around Chain K:

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

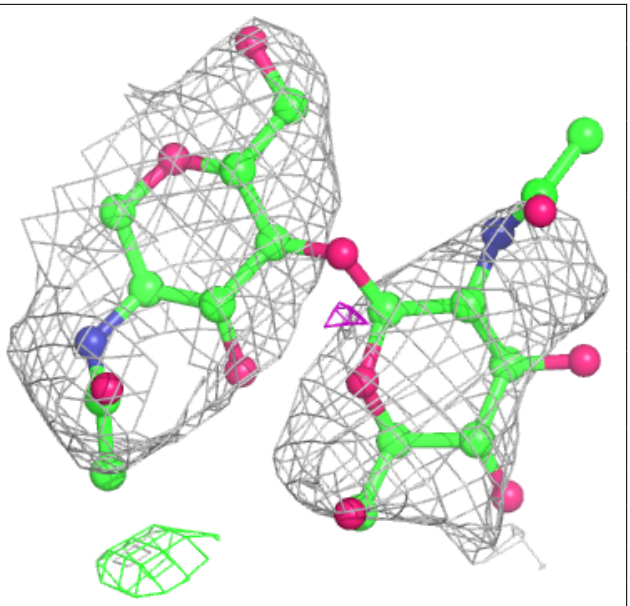


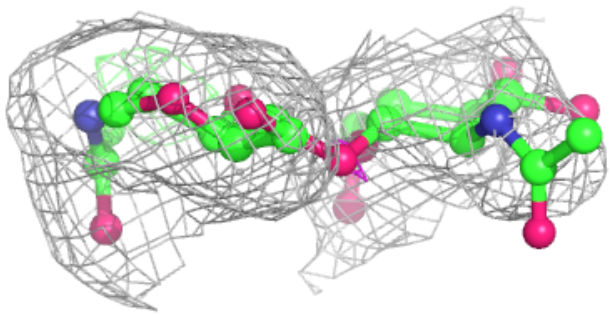


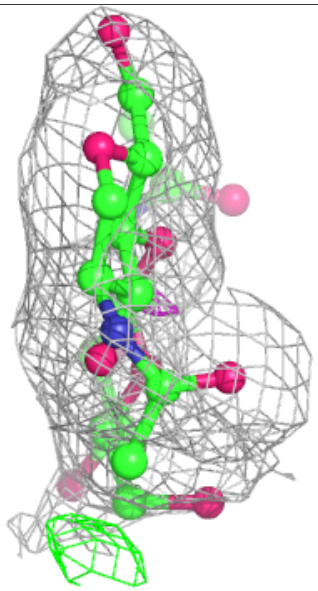


Electron density around Chain P:

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

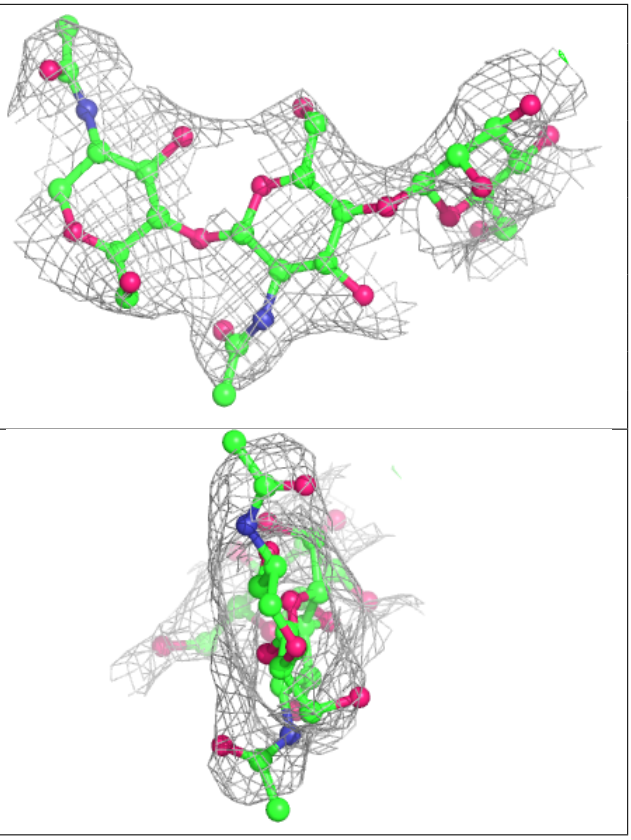


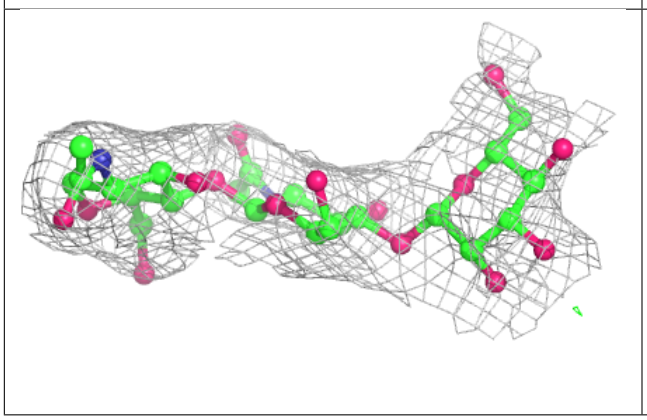




Electron density around Chain M:

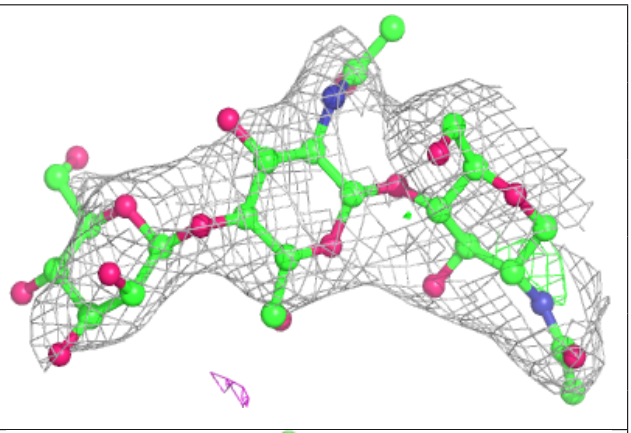
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

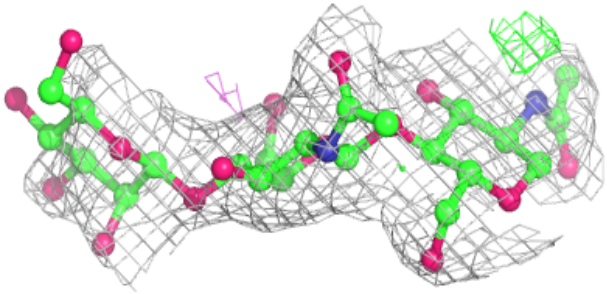


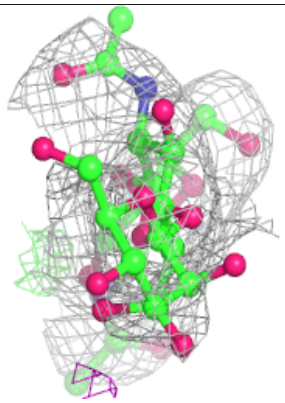


Electron density around Chain N:

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

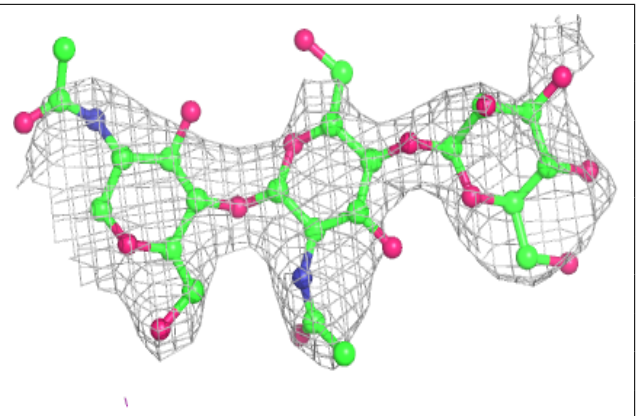


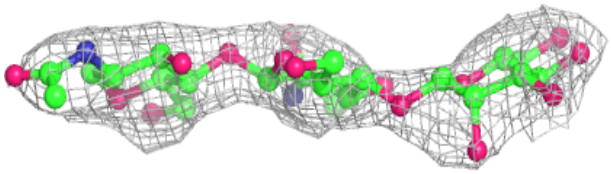


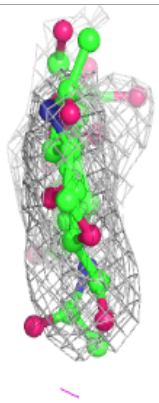


Electron density around Chain Q:

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

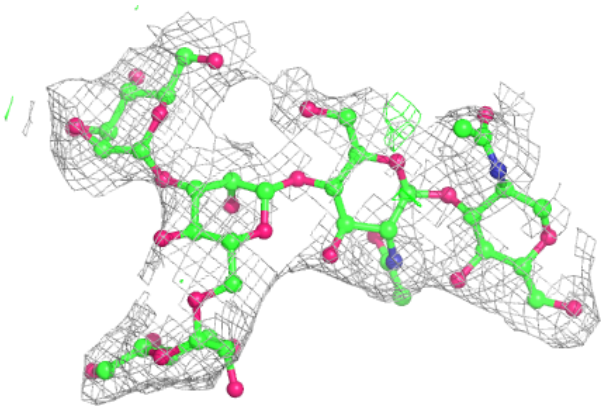


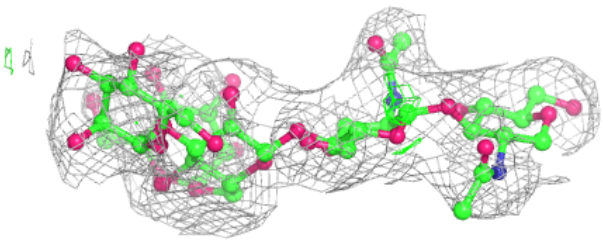


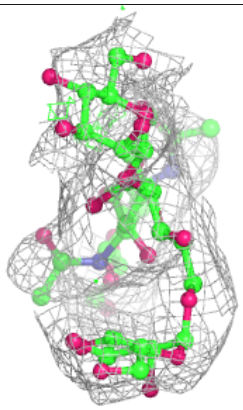


Electron density around Chain O:

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







6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NAG	A	5401	14/15	0.85	0.20	80,89,97,97	0
10	NAG	C	4301	14/15	0.87	0.15	68,90,99,103	0

6.5 Other polymers (i)

There are no such residues in this entry.