Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 09:59 AM EDT

PDB ID	:	6YSQ
Title	:	The hC4Nb8 complement inhibitory nanobody in complex with C4b
Authors	:	Zarantonello, A.; Laursen, N.S.; Andersen, G.R.
Deposited on	:	2020-04-23
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 (i)) were used in the production of this report:

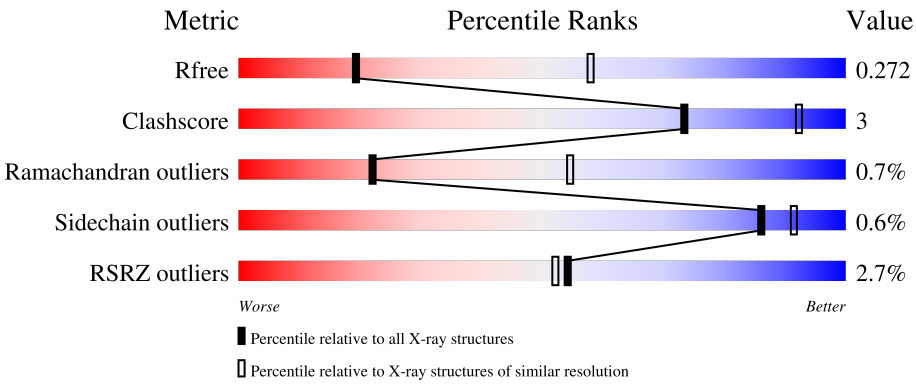
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.30 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	656	2%, 91%, 8%
1	B	656	88%, 11%
2	C	690	2%, 82%, 10%, 8%
2	D	690	3%, 83%, 9%, 8%
3	E	291	9%, 83%, 12%, 5%

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Mol	Chain	Length	Quality of chain
3	F	291	4% 87% 9% 5%
4	G	132	83% 11% 6%
4	H	132	% 83% 11% 6%
5	I	3	100%
5	J	3	100%
5	K	3	100%
5	L	3	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26297 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 Complement C4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	651	5012	3185	872	939	16	0	0	0
1	B	651	5012	3185	872	939	16	0	0	0

- Molecule 2 is a protein called Complement C4-A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	633	4884	3089	845	935	15	0	0	0
2	D	635	4899	3099	847	937	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1013	GLU	GLN	variant	UNP P0C0L4
C	1201	SER	THR	variant	UNP P0C0L4
D	1013	GLU	GLN	variant	UNP P0C0L4
D	1201	SER	THR	variant	UNP P0C0L4

- Molecule 3 is a protein called Complement C4 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	277	2211	1390	396	408	17	0	0	0
3	F	277	2211	1390	396	408	17	0	0	0

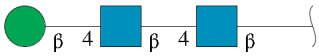
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1735	ASN	GLN	conflict	UNP P0C0L5
E	1737	PHE	TYR	conflict	UNP P0C0L5
F	1735	ASN	GLN	conflict	UNP P0C0L5
F	1737	PHE	TYR	conflict	UNP P0C0L5

- Molecule 4 is a protein called hC4Nb8 nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	124	956	597	168	186	5	0	0	0
4	H	124	956	597	168	186	5	0	0	0

- 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.



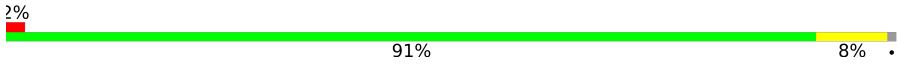
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	3	39	22	2	15	0	0	0
5	J	3	39	22	2	15	0	0	0
5	K	3	39	22	2	15	0	0	0
5	L	3	39	22	2	15	0	0	0

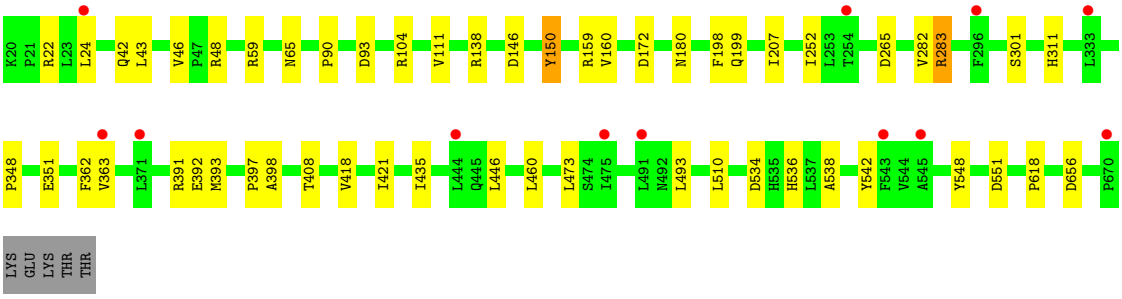
3 Residue-property plots (i)

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: Complement C4 beta chain

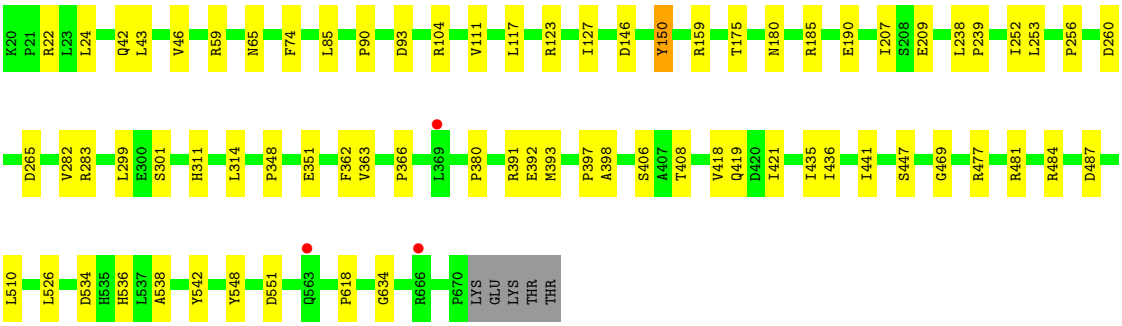
Chain A:





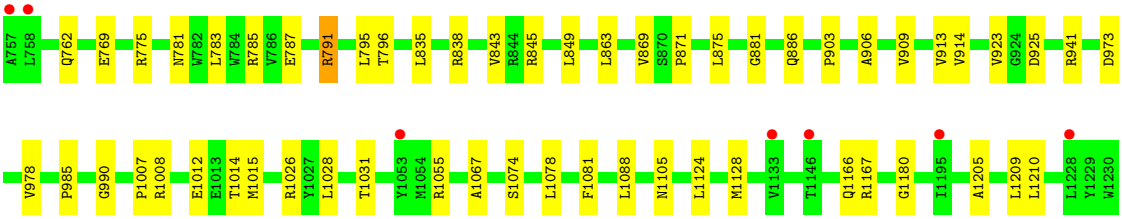
• Molecule 1: Complement C4 beta chain

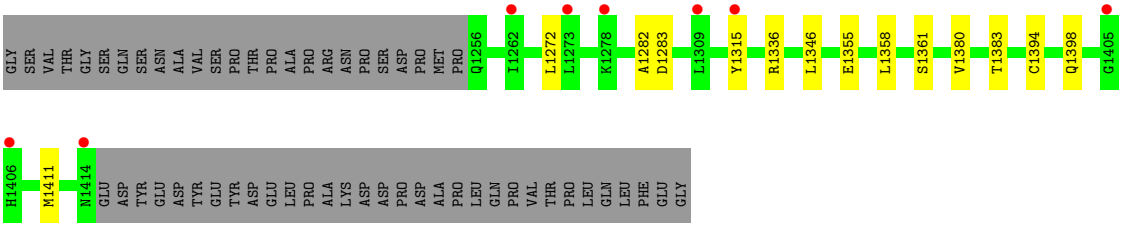
Chain B:



• Molecule 2: Complement C4-A alpha chain

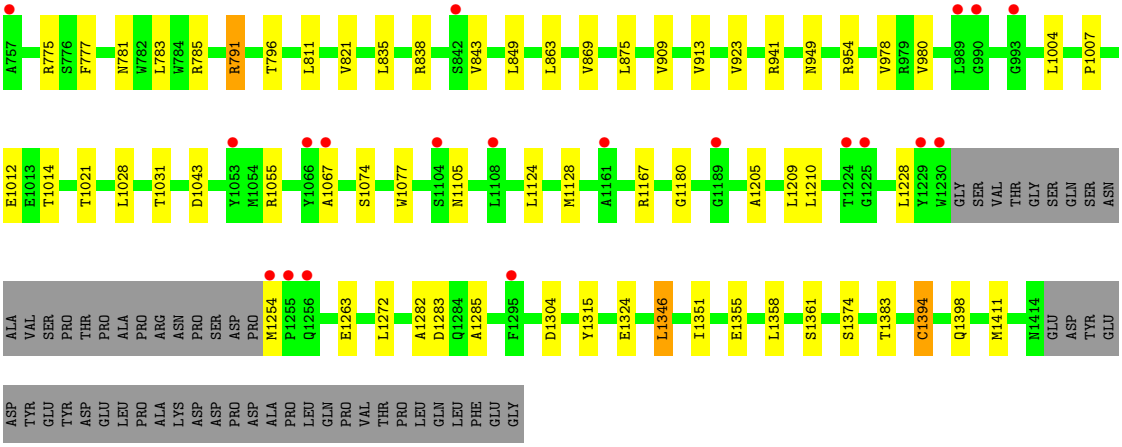
Chain C:





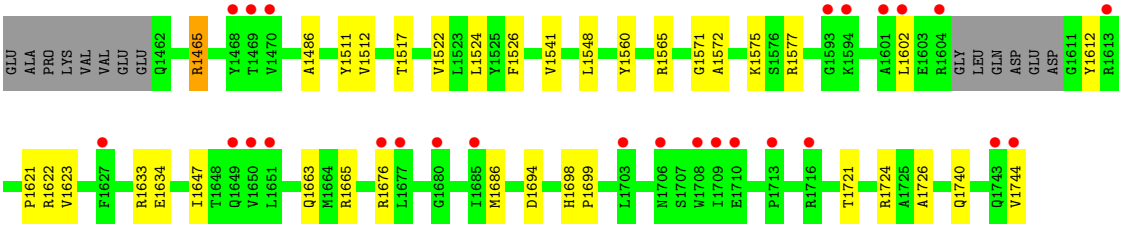
• Molecule 2: Complement C4-A alpha chain

Chain D:



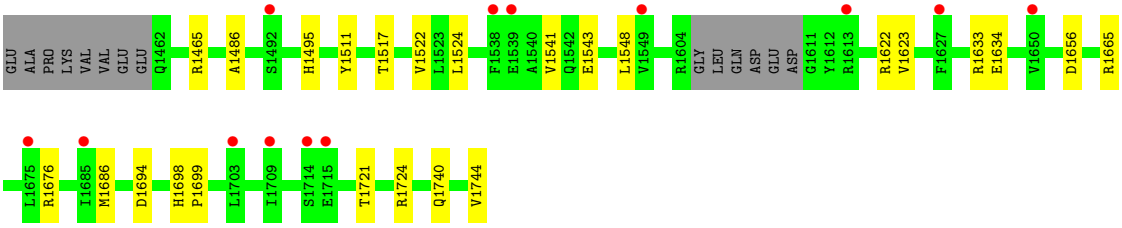
• Molecule 3: Complement C4 gamma chain

Chain E:



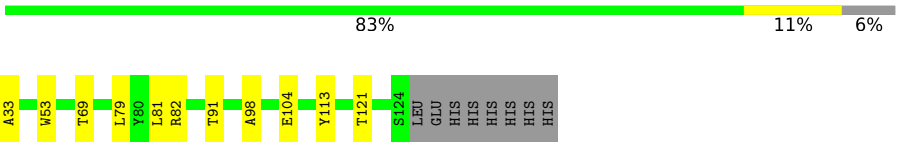
• Molecule 3: Complement C4 gamma chain

Chain F:



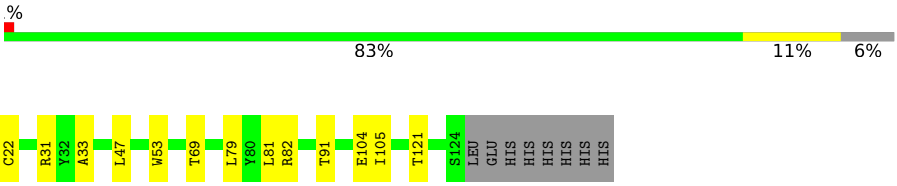
• Molecule 4: hC4Nb8 nanobody

Chain G:



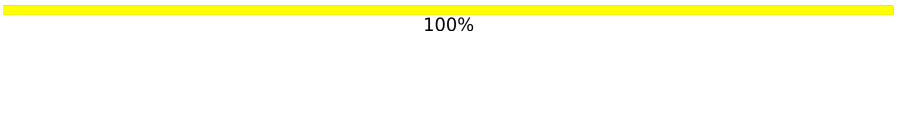
• Molecule 4: hC4Nb8 nanobody

Chain H:



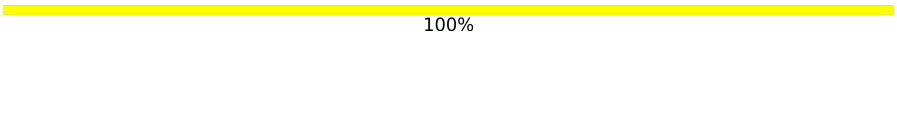
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



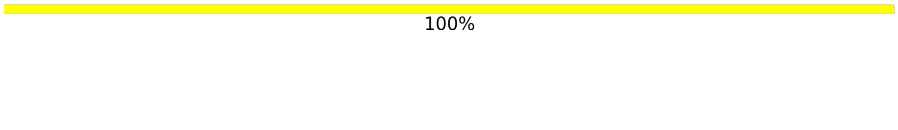
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



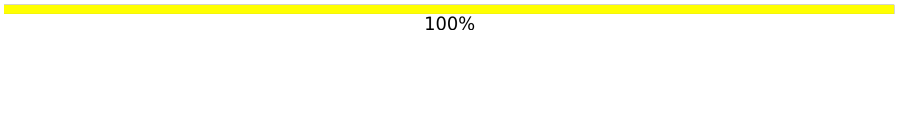
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.20Å 89.51Å 231.20Å 90.00° 97.55° 90.00°	Depositor
Resolution (Å)	48.26 – 3.30 49.87 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.26-3.30) 96.7 (49.87-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549, PHENIX 1.16_3549	Depositor
R, R_{free}	0.221 , 0.272 0.221 , 0.272	Depositor DCC
R_{free} test set	1566 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	149.7	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 110.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26297	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3167e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.31	0/5128	0.58	1/6961 (0.0%)
1	B	0.31	0/5128	0.59	1/6961 (0.0%)
2	C	0.30	0/4983	0.59	0/6776
2	D	0.30	0/4999	0.58	0/6798
3	E	0.30	0/2257	0.61	0/3046
3	F	0.31	0/2257	0.63	0/3046
4	G	0.30	0/976	0.59	1/1319 (0.1%)
4	H	0.29	0/976	0.57	0/1319
All	All	0.30	0/26704	0.59	3/36226 (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
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	TYR	CA-CB-CG	5.36	123.59	113.40
1	B	150	TYR	CA-CB-CG	5.24	123.35	113.40
4	G	1	GLN	C-N-CA	5.24	134.80	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1346	LEU	Peptide
2	D	1346	LEU	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	5012	0	5025	30	0
1	B	5012	0	5025	40	0
2	C	4884	0	4849	38	0
2	D	4899	0	4865	38	0
3	E	2211	0	2159	15	0
3	F	2211	0	2159	12	0
4	G	956	0	915	8	0
4	H	956	0	915	10	0
5	I	39	0	34	0	0
5	J	39	0	34	0	0
5	K	39	0	34	0	0
5	L	39	0	34	0	0
All	All	26297	0	26048	171	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 3.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1012:GLU:OE2	2:C:1124:LEU:N	2.25	0.66
2:C:796:THR:N	4:G:104:GLU:OE2	2.27	0.66
2:D:1012:GLU:OE2	2:D:1124:LEU:N	2.24	0.65
1:B:209:GLU:OE2	2:D:941:ARG:NH1	2.30	0.64
1:A:59:ARG:HE	1:A:111:VAL:HG21	1.64	0.63
2:C:1007:PRO:HB3	2:C:1014:THR:HG23	1.81	0.62
1:A:265:ASP:OD1	1:A:311:HIS:ND1	2.26	0.62
1:B:265:ASP:OD1	1:B:311:HIS:ND1	2.23	0.61
1:B:59:ARG:HE	1:B:111:VAL:HG21	1.65	0.60
1:A:159:ARG:HG2	1:A:199:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HH21	1:B:551:ASP:HB3	1.67	0.59
3:F:1486:ALA:HB3	3:F:1524:LEU:HB2	1.84	0.58
3:F:1740:GLN:NE2	3:F:1744:VAL:OXT	2.36	0.58
1:A:146:ASP:OD1	2:C:781:ASN:ND2	2.37	0.58
4:H:22:CYS:HB3	4:H:79:LEU:HB3	1.86	0.58
1:A:22:ARG:HH21	1:A:551:ASP:HB3	1.68	0.57
3:E:1486:ALA:HB3	3:E:1524:LEU:HB2	1.84	0.57
1:B:146:ASP:OD1	2:D:781:ASN:ND2	2.37	0.57
2:D:811:LEU:HG	2:D:821:VAL:HG12	1.87	0.57
1:B:406:SER:HB3	1:B:447:SER:HB2	1.86	0.57
3:E:1740:GLN:NE2	3:E:1744:VAL:OXT	2.38	0.57
1:B:534:ASP:OD2	1:B:536:HIS:ND1	2.35	0.56
2:C:1272:LEU:HD22	2:C:1282:ALA:HB2	1.87	0.56
1:A:146:ASP:O	2:C:781:ASN:ND2	2.39	0.56
2:D:1272:LEU:HD22	2:D:1282:ALA:HB2	1.87	0.55
3:E:1694:ASP:OD1	3:E:1698:HIS:N	2.39	0.55
2:D:775:ARG:NH2	2:D:835:LEU:O	2.39	0.55
2:D:1014:THR:OG1	2:D:1055:ARG:NH2	2.40	0.55
2:C:978:VAL:HB	2:C:1358:LEU:HD22	1.87	0.55
3:F:1694:ASP:OD1	3:F:1698:HIS:N	2.39	0.55
4:G:22:CYS:HB3	4:G:79:LEU:HB3	1.88	0.55
2:D:1007:PRO:HB3	2:D:1014:THR:HG23	1.89	0.55
4:H:33:ALA:HB2	4:H:53:TRP:HD1	1.72	0.55
2:D:777:PHE:HB2	4:H:31:ARG:HH22	1.72	0.54
2:D:1180:GLY:HA3	2:D:1209:LEU:HD23	1.88	0.54
1:B:299:LEU:HD23	1:B:314:LEU:HD11	1.89	0.54
2:D:978:VAL:HB	2:D:1358:LEU:HD22	1.89	0.54
4:H:47:LEU:HD11	4:H:105:ILE:HG22	1.90	0.54
3:F:1633:ARG:NH1	3:F:1634:GLU:O	2.41	0.53
1:B:282:VAL:HB	1:B:301:SER:HB3	1.91	0.53
1:A:351:GLU:OE2	2:C:838:ARG:NH2	2.39	0.52
1:B:146:ASP:O	2:D:781:ASN:ND2	2.42	0.52
2:C:785:ARG:HH12	4:G:104:GLU:HB2	1.75	0.52
1:B:180:ASN:ND2	2:D:1355:GLU:OE1	2.42	0.52
4:H:20:LEU:HD12	4:H:81:LEU:HD23	1.91	0.52
2:C:1394:CYS:O	2:C:1398:GLN:NE2	2.42	0.52
2:D:1394:CYS:O	2:D:1398:GLN:NE2	2.43	0.52
2:D:1205:ALA:HB3	2:D:1210:LEU:HD12	1.92	0.51
3:E:1517:THR:HG22	3:E:1522:VAL:HA	1.91	0.51
3:E:1633:ARG:NH1	3:E:1634:GLU:O	2.43	0.51
1:A:180:ASN:ND2	2:C:1355:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:33:ALA:HB2	4:G:53:TRP:HD1	1.75	0.51
4:H:69:THR:HB	4:H:82:ARG:HB3	1.93	0.51
1:B:421:ILE:HD12	1:B:435:ILE:HG22	1.91	0.51
1:A:282:VAL:HB	1:A:301:SER:HB3	1.94	0.50
2:C:843:VAL:HG21	2:C:849:LEU:HD22	1.94	0.50
4:G:20:LEU:HD12	4:G:81:LEU:HD23	1.93	0.50
4:G:69:THR:HB	4:G:82:ARG:HB3	1.93	0.50
1:A:59:ARG:NH1	1:A:65:ASN:OD1	2.43	0.50
2:C:1008:ARG:O	2:C:1055:ARG:NH1	2.44	0.50
3:E:1512:VAL:HG22	3:E:1526:PHE:HE1	1.77	0.50
3:F:1517:THR:HG22	3:F:1522:VAL:HA	1.94	0.50
1:A:421:ILE:HD12	1:A:435:ILE:HG22	1.94	0.49
1:A:510:LEU:HB2	1:A:542:TYR:HB2	1.94	0.49
2:D:863:LEU:HD13	2:D:923:VAL:HG21	1.94	0.49
3:F:1623:VAL:HG11	3:F:1686:MET:HB3	1.94	0.49
2:C:775:ARG:NH2	2:C:835:LEU:O	2.41	0.49
3:E:1665:ARG:HH12	3:E:1699:PRO:HD2	1.76	0.49
2:C:1014:THR:OG1	2:C:1055:ARG:NH2	2.45	0.49
1:B:252:ILE:HG13	1:B:260:ASP:HB2	1.93	0.49
2:C:769:GLU:HG3	2:C:914:VAL:HG11	1.94	0.49
2:D:1077:TRP:HZ3	2:D:1128:MET:HE3	1.77	0.49
1:B:363:VAL:HG11	1:B:393:MET:HG2	1.95	0.49
3:F:1465:ARG:HB3	3:F:1541:VAL:HG12	1.94	0.49
4:G:98:ALA:HB3	4:G:113:TYR:HB2	1.94	0.49
1:A:391:ARG:HA	1:A:397:PRO:HA	1.95	0.48
2:C:787:GLU:HG3	2:C:795:LEU:HD11	1.95	0.48
1:A:199:GLN:H	1:B:256:PRO:HB3	1.77	0.48
2:C:1026:ARG:HH12	2:C:1088:LEU:HD22	1.79	0.48
2:D:785:ARG:HH12	4:H:104:GLU:HB2	1.77	0.48
2:C:775:ARG:NH2	2:C:925:ASP:OD2	2.42	0.47
2:D:843:VAL:HG21	2:D:849:LEU:HD22	1.94	0.47
1:B:185:ARG:HD3	2:D:1351:ILE:HD13	1.96	0.47
2:C:1180:GLY:HA3	2:C:1209:LEU:HD23	1.95	0.47
1:A:408:THR:HG22	1:A:418:VAL:HG22	1.96	0.47
2:C:863:LEU:HD13	2:C:923:VAL:HG21	1.97	0.47
2:C:1067:ALA:HB2	2:C:1074:SER:HA	1.97	0.47
2:D:796:THR:N	4:H:104:GLU:OE2	2.35	0.47
1:B:59:ARG:NH1	1:B:65:ASN:OD1	2.45	0.47
2:C:875:LEU:HG	2:C:909:VAL:HG11	1.98	0.46
3:E:1647:ILE:HD12	3:E:1663:GLN:HB2	1.96	0.46
1:B:22:ARG:HG3	1:B:548:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:869:VAL:HG22	2:C:913:VAL:HG22	1.97	0.46
2:C:973:ASP:OD2	2:C:1336:ARG:NH1	2.48	0.46
2:D:869:VAL:HG22	2:D:913:VAL:HG22	1.97	0.46
1:B:477:ARG:NH2	1:B:481:ARG:O	2.48	0.46
3:F:1495:HIS:ND1	3:F:1543:GLU:OE2	2.49	0.46
1:B:90:PRO:HG2	1:B:93:ASP:HB2	1.96	0.45
2:D:949:ASN:HB3	2:D:954:ARG:HB2	1.98	0.45
2:D:941:ARG:HG3	2:D:1383:THR:HG22	1.98	0.45
3:E:1623:VAL:HG11	3:E:1686:MET:HB3	1.97	0.45
1:B:24:LEU:HB2	1:B:42:GLN:HB3	1.97	0.45
1:B:74:PHE:HB3	1:B:85:LEU:HD11	1.99	0.45
2:D:1067:ALA:HB2	2:D:1074:SER:HA	1.98	0.45
3:E:1721:THR:HG22	3:E:1724:ARG:HH22	1.80	0.45
1:A:160:VAL:HG22	1:A:198:PHE:HB3	1.99	0.45
1:B:175:THR:HG22	1:B:190:GLU:HB3	1.96	0.45
1:B:127:ILE:HG13	2:D:1043:ASP:OD2	2.17	0.45
1:B:392:GLU:HG2	1:B:398:ALA:HB2	1.99	0.45
1:A:24:LEU:HB2	1:A:42:GLN:HB3	1.98	0.45
2:D:1105:ASN:OD1	2:D:1167:ARG:NH2	2.49	0.45
2:D:1263:GLU:HB2	2:D:1304:ASP:HB3	1.98	0.45
1:B:542:TYR:HE2	1:B:634:GLY:HA3	1.82	0.44
3:F:1656:ASP:OD2	3:F:1665:ARG:NH1	2.50	0.44
1:A:22:ARG:HG3	1:A:548:TYR:HE2	1.82	0.44
1:A:43:LEU:HB3	1:A:46:VAL:HG21	1.99	0.44
1:B:380:PRO:HB3	1:B:441:ILE:HG22	2.00	0.44
1:A:22:ARG:HD2	1:A:656:ASP:HB2	1.99	0.44
1:A:534:ASP:OD2	1:A:536:HIS:ND1	2.42	0.44
1:B:351:GLU:OE2	2:D:838:ARG:NH2	2.44	0.44
1:A:363:VAL:HG11	1:A:393:MET:HG2	1.99	0.44
2:C:1105:ASN:OD1	2:C:1167:ARG:NH2	2.50	0.44
2:C:1205:ALA:HB3	2:C:1210:LEU:HD12	2.00	0.43
1:B:43:LEU:HB3	1:B:46:VAL:HG21	1.99	0.43
1:B:391:ARG:HA	1:B:397:PRO:HA	2.00	0.43
2:D:1228:LEU:HD22	2:D:1285:ALA:HB2	2.00	0.43
2:D:1004:LEU:HA	2:D:1021:THR:HG23	2.00	0.43
2:C:1028:LEU:HA	2:C:1031:THR:HG22	2.01	0.43
4:G:91:THR:HG23	4:G:121:THR:HA	2.01	0.43
3:E:1571:GLY:HA3	3:E:1577:ARG:HA	2.01	0.43
1:B:253:LEU:HD21	1:B:366:PRO:HD3	2.00	0.43
2:D:980:VAL:HG13	2:D:1346:LEU:HD12	2.01	0.43
2:C:1015:MET:HB3	2:C:1081:PHE:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ARG:HG2	1:B:487:ASP:OD2	2.19	0.42
2:C:978:VAL:HG23	2:C:1380:VAL:HG22	2.01	0.42
3:E:1602:LEU:HD11	3:E:1726:ALA:HB1	2.02	0.42
1:B:207:ILE:HD13	2:D:1383:THR:HG21	2.01	0.42
1:B:408:THR:HG22	1:B:418:VAL:HG22	2.01	0.42
1:B:252:ILE:HG23	1:B:362:PHE:HA	2.00	0.42
2:C:1078:LEU:HD13	2:C:1128:MET:HE3	2.01	0.42
1:A:446:LEU:HD12	1:A:460:LEU:HD23	2.00	0.42
2:C:1166:GLN:HB2	2:D:1254:MET:HA	2.02	0.42
2:C:1283:ASP:OD1	2:C:1315:TYR:OH	2.37	0.42
1:B:238:LEU:HD12	1:B:239:PRO:HD2	2.01	0.42
1:A:138:ARG:NH1	1:A:172:ASP:OD2	2.42	0.42
2:D:1028:LEU:HA	2:D:1031:THR:HG22	2.02	0.42
1:A:283:ARG:NH1	3:E:1560:TYR:O	2.53	0.42
2:C:871:PRO:HB3	2:C:881:GLY:HA3	2.01	0.42
1:B:117:LEU:HD12	1:B:123:ARG:HD2	2.02	0.42
1:B:510:LEU:HB2	1:B:542:TYR:HB2	2.01	0.41
2:D:875:LEU:HG	2:D:909:VAL:HG11	2.01	0.41
1:B:419:GLN:HE22	1:B:436:ILE:HB	1.85	0.41
1:A:392:GLU:HG2	1:A:398:ALA:HB2	2.02	0.41
4:H:91:THR:HG23	4:H:121:THR:HA	2.02	0.41
1:A:90:PRO:HG2	1:A:93:ASP:HB2	2.01	0.41
2:C:762:GLN:O	2:C:886:GLN:NE2	2.45	0.41
2:C:845:ARG:HH11	2:C:906:ALA:HB2	1.85	0.41
2:D:1283:ASP:OD1	2:D:1315:TYR:OH	2.38	0.41
1:A:207:ILE:H	1:A:207:ILE:HG13	1.72	0.41
1:A:473:LEU:HD11	1:A:493:LEU:HD12	2.02	0.41
2:C:941:ARG:HG2	2:C:1383:THR:HG22	2.03	0.41
3:F:1694:ASP:OD2	3:F:1698:HIS:HB2	2.20	0.41
1:A:252:ILE:HG23	1:A:362:PHE:HA	2.03	0.41
3:E:1572:ALA:HB3	3:E:1575:LYS:HB2	2.04	0.41
1:B:111:VAL:HG13	1:B:127:ILE:HG23	2.03	0.40
3:E:1465:ARG:HB3	3:E:1541:VAL:HG12	2.03	0.40
3:F:1721:THR:HG22	3:F:1724:ARG:HH22	1.87	0.40
2:C:845:ARG:HA	2:C:903:PRO:HG2	2.03	0.40
4:H:20:LEU:HB2	4:H:81:LEU:HB3	2.04	0.40
2:D:1324:GLU:OE2	2:D:1374:SER:HA	2.22	0.40
3:F:1665:ARG:HH12	3:F:1699:PRO:HD2	1.86	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	649/656 (99%)	609 (94%)	36 (6%)	4 (1%)	25	57
1	B	649/656 (99%)	608 (94%)	35 (5%)	6 (1%)	17	48
2	C	629/690 (91%)	573 (91%)	52 (8%)	4 (1%)	25	57
2	D	631/690 (91%)	575 (91%)	53 (8%)	3 (0%)	29	61
3	E	273/291 (94%)	247 (90%)	22 (8%)	4 (2%)	10	38
3	F	273/291 (94%)	246 (90%)	25 (9%)	2 (1%)	22	54
4	G	122/132 (92%)	115 (94%)	6 (5%)	1 (1%)	19	51
4	H	122/132 (92%)	114 (93%)	7 (6%)	1 (1%)	19	51
All	All	3348/3538 (95%)	3087 (92%)	236 (7%)	25 (1%)	22	54

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	B	104	ARG
4	G	2	VAL
2	C	990	GLY
2	C	1361	SER
3	E	1622	ARG
2	D	1361	SER
4	H	2	VAL
1	A	538	ALA
3	F	1622	ARG
1	A	618	PRO
2	C	985	PRO
3	E	1511	TYR
1	B	538	ALA
1	B	618	PRO
3	F	1511	TYR
2	C	791	ARG

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Mol	Chain	Res	Type
3	E	1612	TYR
1	B	526	LEU
2	D	791	ARG
2	D	1394	CYS
1	B	348	PRO
1	A	348	PRO
3	E	1621	PRO
1	B	469	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	557/562 (99%)	554 (100%)	3 (0%)	88	93
1	B	557/562 (99%)	554 (100%)	3 (0%)	88	93
2	C	525/575 (91%)	522 (99%)	3 (1%)	86	91
2	D	527/575 (92%)	524 (99%)	3 (1%)	86	91
3	E	237/249 (95%)	233 (98%)	4 (2%)	60	78
3	F	237/249 (95%)	235 (99%)	2 (1%)	81	89
4	G	97/105 (92%)	97 (100%)	0	100	100
4	H	97/105 (92%)	97 (100%)	0	100	100
All	All	2834/2982 (95%)	2816 (99%)	18 (1%)	86	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	150	TYR
1	A	283	ARG
2	C	783	LEU
2	C	791	ARG
2	C	1411	MET
3	E	1465	ARG

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Mol	Chain	Res	Type
3	E	1548	LEU
3	E	1565	ARG
3	E	1676	ARG
1	B	150	TYR
1	B	159	ARG
1	B	283	ARG
2	D	783	LEU
2	D	791	ARG
2	D	1411	MET
3	F	1548	LEU
3	F	1676	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	HIS
1	A	629	ASN
3	E	1740	GLN
3	F	1740	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)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	I	1	1,5	14,14,15	0.84	1 (7%)	17,19,21	0.55	0
5	NAG	I	2	5	14,14,15	0.84	2 (14%)	17,19,21	1.27	2 (11%)
5	BMA	I	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.02	1 (6%)
5	NAG	J	1	5,2	14,14,15	0.78	1 (7%)	17,19,21	0.74	1 (5%)
5	NAG	J	2	5	14,14,15	0.73	1 (7%)	17,19,21	0.66	1 (5%)
5	BMA	J	3	5	11,11,12	1.07	0	15,15,17	0.98	1 (6%)
5	NAG	K	1	1,5	14,14,15	0.87	1 (7%)	17,19,21	0.55	0
5	NAG	K	2	5	14,14,15	0.80	0	17,19,21	1.28	2 (11%)
5	BMA	K	3	5	11,11,12	1.08	1 (9%)	15,15,17	1.01	1 (6%)
5	NAG	L	1	5,2	14,14,15	0.78	1 (7%)	17,19,21	0.73	1 (5%)
5	NAG	L	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.65	1 (5%)
5	BMA	L	3	5	11,11,12	1.06	0	15,15,17	0.98	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
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	NAG	J	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	1/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	3/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	NAG	L	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	1/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1	NAG	O5-C1	2.39	1.47	1.43
5	K	1	NAG	O5-C1	2.38	1.47	1.43
5	L	1	NAG	O5-C1	2.35	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	O5-C1	2.28	1.47	1.43
5	J	2	NAG	O5-C1	2.26	1.47	1.43
5	L	2	NAG	O5-C1	2.17	1.47	1.43
5	I	3	BMA	C2-C3	2.09	1.55	1.52
5	K	3	BMA	C2-C3	2.08	1.55	1.52
5	I	2	NAG	O5-C1	2.06	1.47	1.43
5	I	2	NAG	C1-C2	2.01	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	2	NAG	C2-N2-C7	3.95	128.53	122.90
5	I	2	NAG	C2-N2-C7	3.95	128.52	122.90
5	J	1	NAG	C1-O5-C5	2.72	115.88	112.19
5	L	1	NAG	C1-O5-C5	2.69	115.84	112.19
5	L	3	BMA	C1-O5-C5	2.59	115.71	112.19
5	I	3	BMA	C1-O5-C5	2.59	115.69	112.19
5	J	3	BMA	C1-O5-C5	2.58	115.69	112.19
5	K	3	BMA	C1-O5-C5	2.54	115.64	112.19
5	J	2	NAG	C1-O5-C5	2.44	115.50	112.19
5	L	2	NAG	C1-O5-C5	2.41	115.45	112.19
5	I	2	NAG	C1-O5-C5	2.37	115.41	112.19
5	K	2	NAG	C1-O5-C5	2.36	115.39	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6

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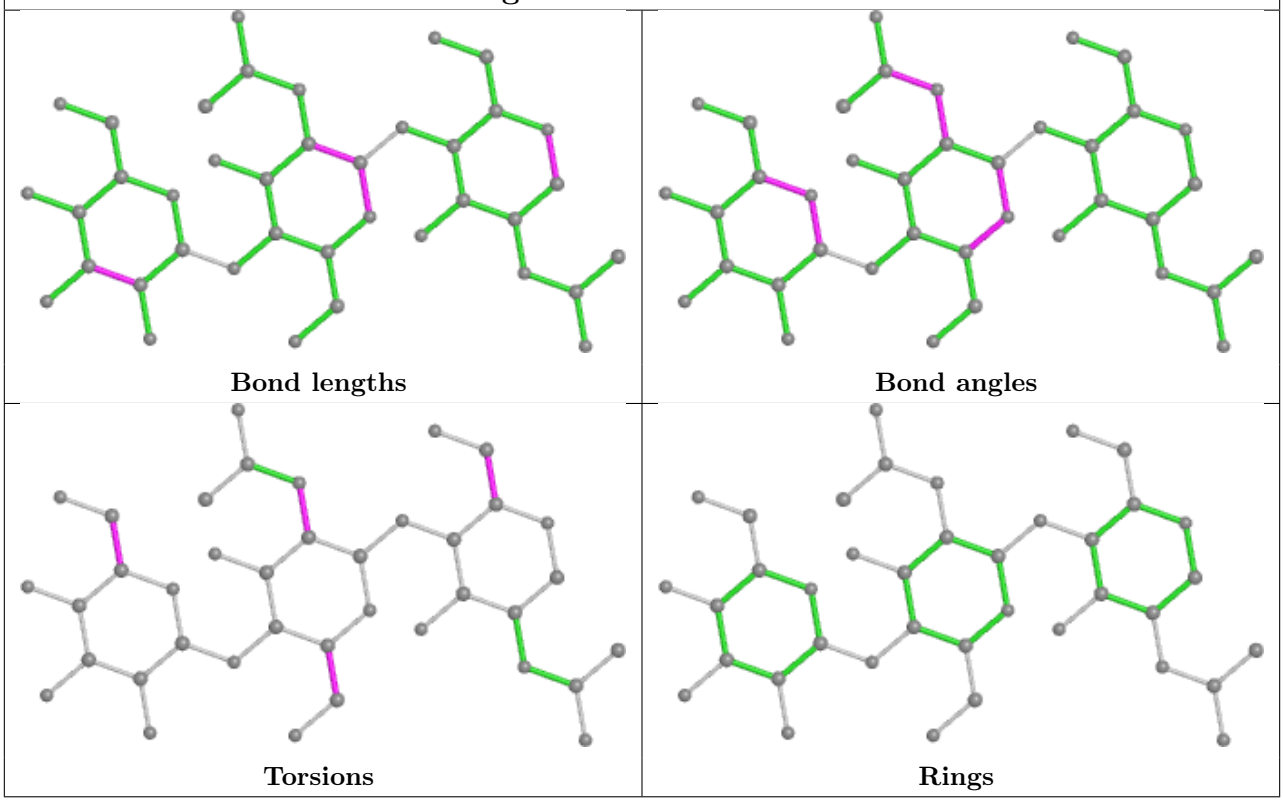
Mol	Chain	Res	Type	Atoms
5	I	3	BMA	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	I	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7

There are no ring outliers.

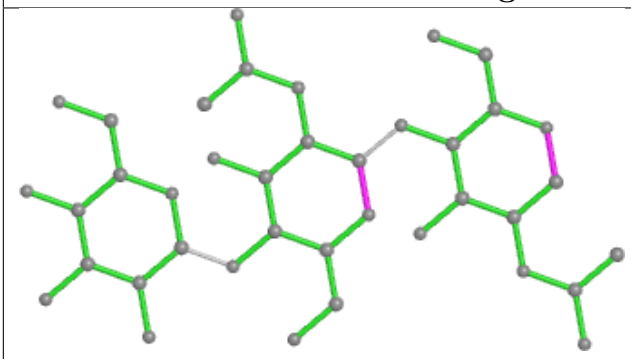
No monomer is involved in short contacts.

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

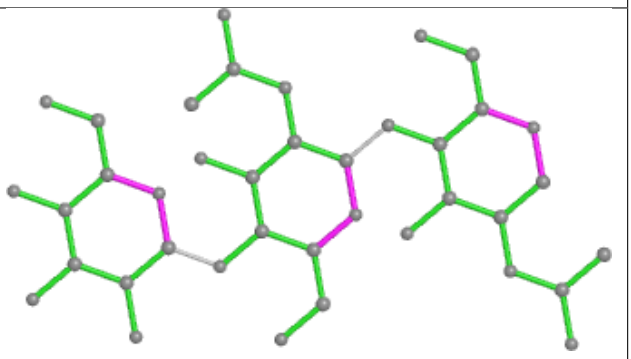
Oligosaccharide Chain I



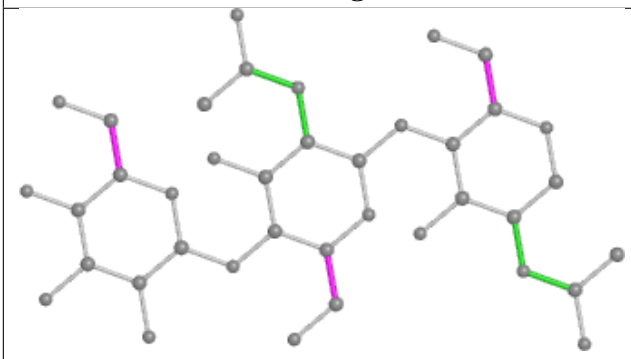
Oligosaccharide Chain J



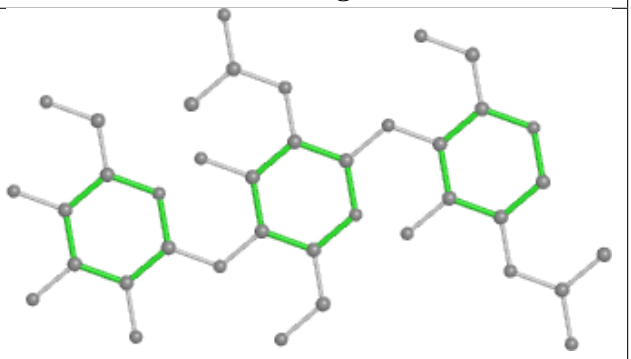
Bond lengths



Bond angles

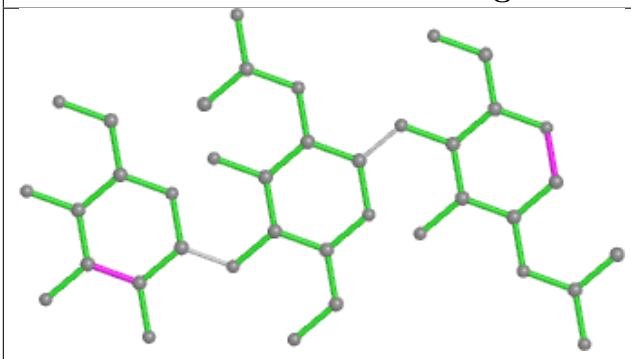


Torsions

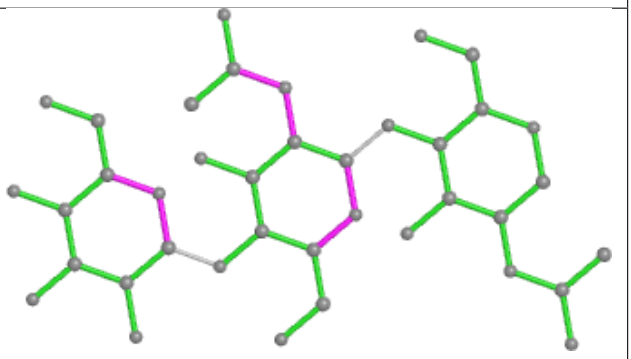


Rings

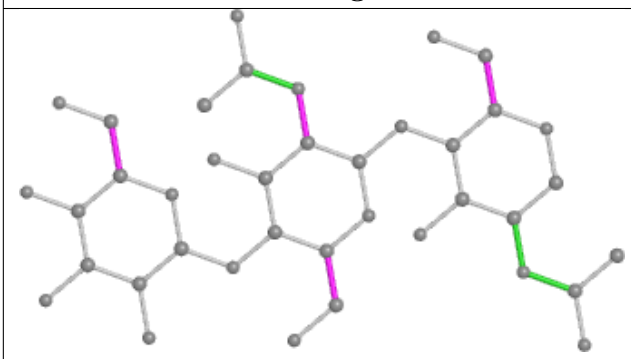
Oligosaccharide Chain K



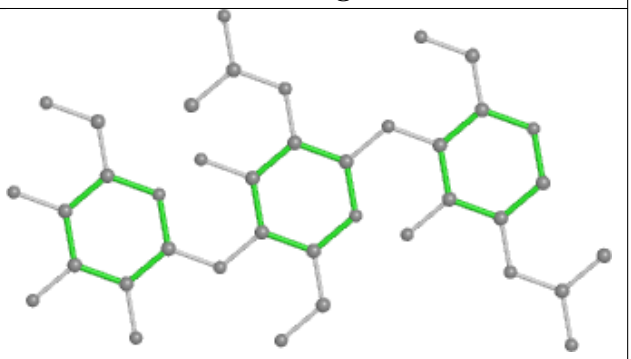
Bond lengths



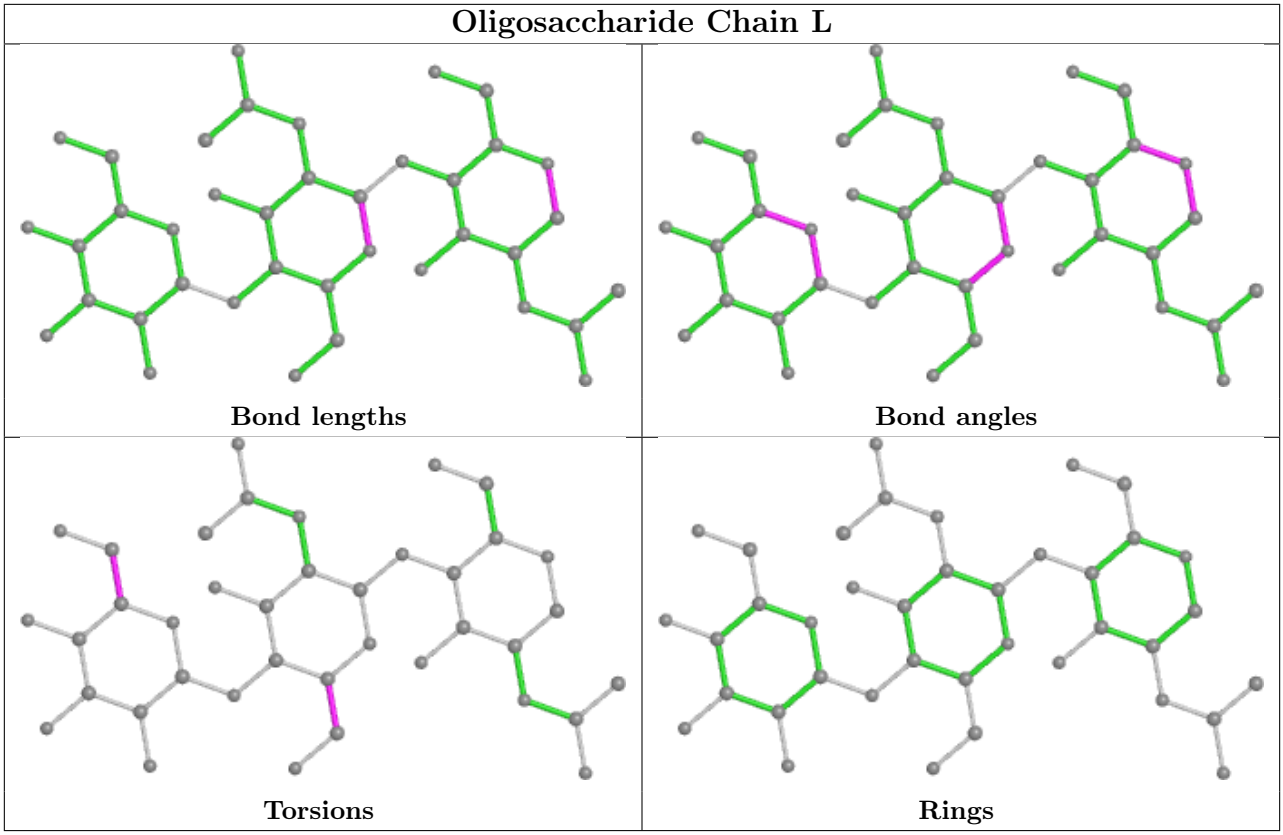
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	651/656 (99%)	-0.02	12 (1%)	68	67	103, 178, 258, 316	0
1	B	651/656 (99%)	-0.18	3 (0%)	91	91	103, 152, 215, 304	0
2	C	633/690 (91%)	0.05	15 (2%)	59	56	108, 203, 287, 343	0
2	D	635/690 (92%)	0.11	20 (3%)	49	48	113, 212, 307, 432	0
3	E	277/291 (95%)	0.23	26 (9%)	8	9	162, 238, 326, 390	0
3	F	277/291 (95%)	-0.06	13 (4%)	31	29	140, 211, 272, 351	0
4	G	124/132 (93%)	-0.17	0	100	100	108, 165, 224, 249	0
4	H	124/132 (93%)	-0.28	1 (0%)	86	86	116, 180, 238, 275	0
All	All	3372/3538 (95%)	-0.01	90 (2%)	54	52	103, 188, 282, 432	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	1744	VAL	6.9
3	E	1708	TRP	5.3
3	E	1713	PRO	5.3
2	C	1405	GLY	5.1
2	D	1254	MET	5.0
2	D	1067	ALA	4.1
1	A	670	PRO	4.1
2	D	757	ALA	4.0
3	E	1468	TYR	3.8
3	E	1743	GLN	3.7
3	E	1703	LEU	3.7
3	E	1650	VAL	3.7
4	H	10	GLY	3.6
3	E	1613	ARG	3.5
2	C	1146	THR	3.4
2	D	1189	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	E	1594	LYS	3.2
2	C	758	LEU	3.2
1	A	254	THR	3.2
1	A	24	LEU	3.1
1	A	475	ILE	3.1
3	E	1685	ILE	3.1
3	F	1650	VAL	3.0
3	F	1538	PHE	3.0
3	F	1539	GLU	3.0
3	E	1676	ARG	3.0
2	D	993	GLY	2.9
1	A	543	PHE	2.9
2	C	1309	LEU	2.9
2	C	1228	LEU	2.9
1	B	666	ARG	2.8
2	D	1256	GLN	2.8
2	C	757	ALA	2.8
2	D	1230	TRP	2.7
3	E	1470	VAL	2.7
2	D	989	LEU	2.7
3	F	1613	ARG	2.6
2	C	1414	ASN	2.6
2	C	1133	VAL	2.6
3	F	1709	ILE	2.6
2	D	1161	ALA	2.5
3	E	1651	LEU	2.5
1	A	491	LEU	2.5
3	F	1714	SER	2.5
3	F	1675	LEU	2.5
3	E	1593	GLY	2.5
3	E	1602	LEU	2.5
3	E	1716	ARG	2.5
3	F	1492	SER	2.5
3	F	1715	GLU	2.4
3	E	1627	PHE	2.4
2	D	990	GLY	2.4
2	D	1255	PRO	2.4
3	E	1601	ALA	2.4
1	A	545	ALA	2.4
2	C	1278	LYS	2.4
2	D	1104	SER	2.4
2	D	1224	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	1315	TYR	2.3
2	C	1273	LEU	2.3
3	F	1703	LEU	2.3
2	C	1262	ILE	2.3
3	E	1706	ASN	2.3
2	D	1108	LEU	2.3
2	C	1053	TYR	2.3
2	C	1195	ILE	2.2
3	F	1627	PHE	2.2
2	D	1229	TYR	2.2
1	B	563	GLN	2.2
3	E	1710	GLU	2.2
2	D	1295	PHE	2.2
1	A	444	LEU	2.2
3	E	1604	ARG	2.2
3	E	1680	GLY	2.2
2	D	1066	TYR	2.2
2	C	1406	HIS	2.2
3	E	1677	LEU	2.2
3	E	1649	GLN	2.1
2	D	1053	TYR	2.1
3	E	1469	THR	2.1
3	E	1709	ILE	2.1
1	A	371	LEU	2.1
1	A	333	LEU	2.1
2	D	1225	GLY	2.1
1	A	363	VAL	2.1
3	F	1549	VAL	2.1
1	B	369	LEU	2.1
1	A	296	PHE	2.0
2	D	842	SER	2.0
3	F	1685	ILE	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,

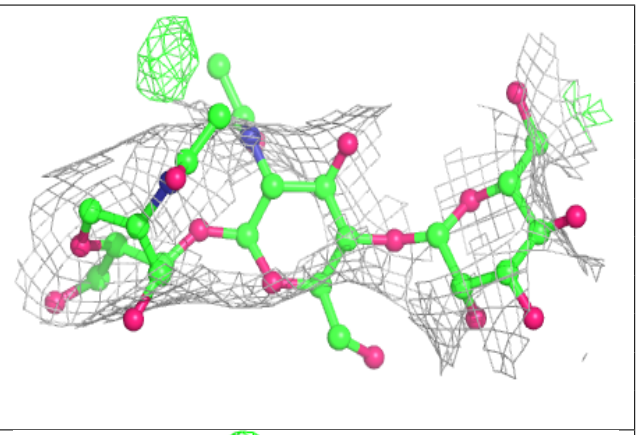
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

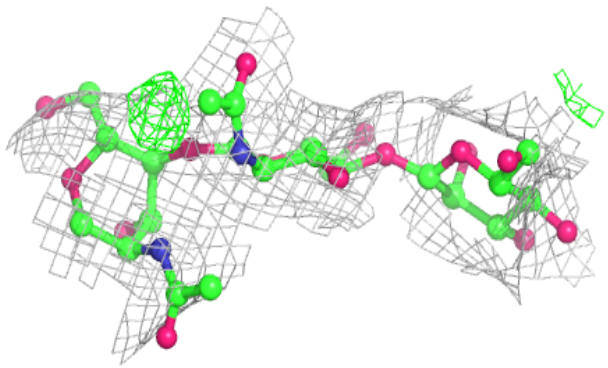
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	K	3	11/12	0.46	0.17	234,292,314,317	0
5	BMA	I	3	11/12	0.53	0.17	254,294,312,319	0
5	NAG	I	2	14/15	0.74	0.24	235,287,305,313	0
5	BMA	L	3	11/12	0.75	0.10	193,249,264,270	0
5	BMA	J	3	11/12	0.76	0.19	246,280,298,298	0
5	NAG	L	2	14/15	0.87	0.17	184,278,295,306	0
5	NAG	K	2	14/15	0.88	0.15	233,272,297,323	0
5	NAG	J	2	14/15	0.88	0.19	212,280,316,335	0
5	NAG	J	1	14/15	0.93	0.10	172,223,251,284	0
5	NAG	L	1	14/15	0.93	0.09	139,186,220,257	0
5	NAG	K	1	14/15	0.94	0.14	135,202,264,268	0
5	NAG	I	1	14/15	0.94	0.17	131,209,264,280	0

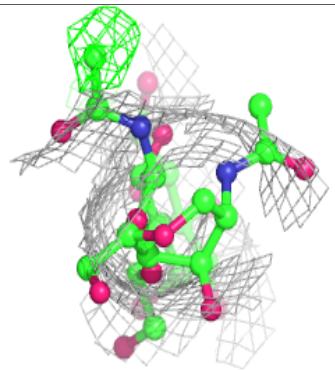
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

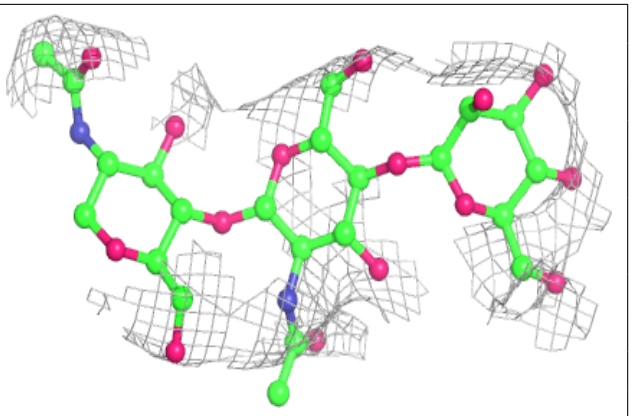


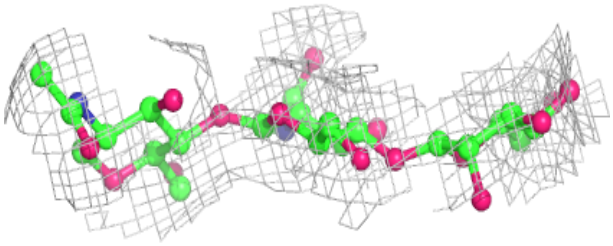


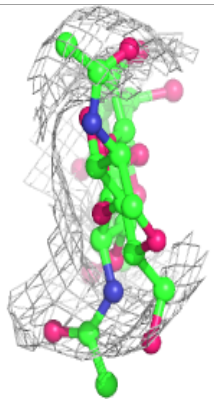


Electron density around Chain J:

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

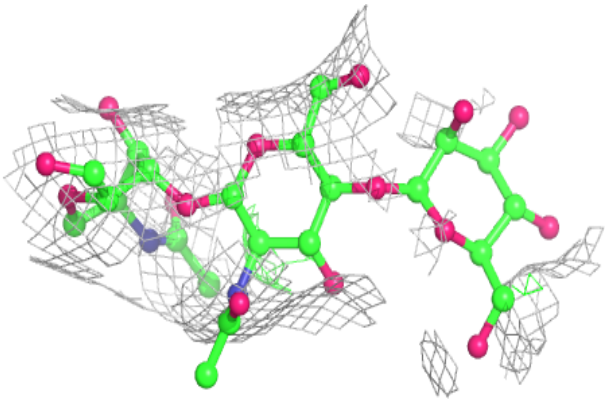


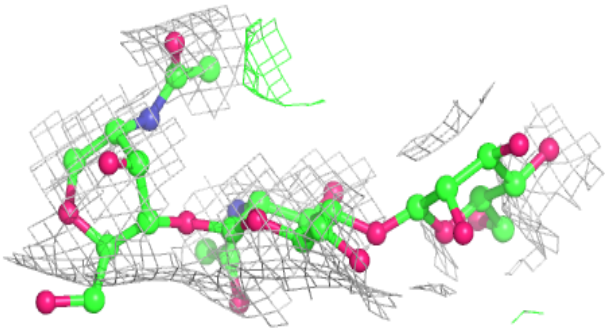


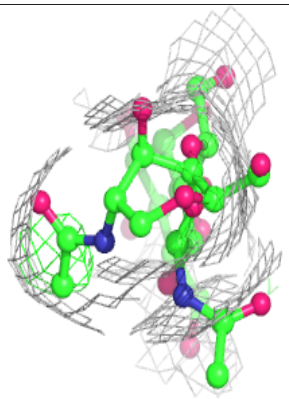


Electron density around Chain K:

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

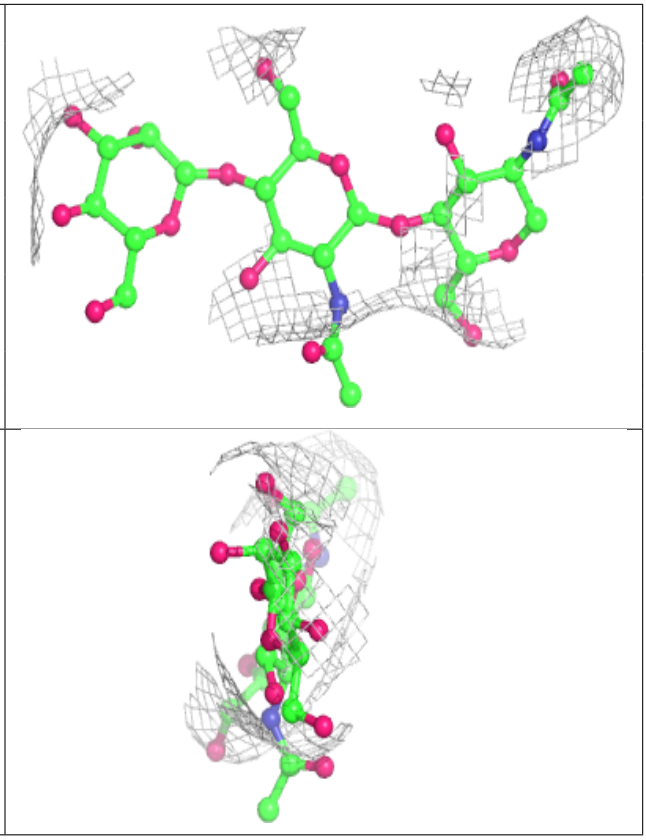






Electron density around Chain L:

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



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.