



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2022 – 12:03 AM EDT

PDB ID : 4K63
Title : Structure of an avian influenza H5 hemagglutinin from the influenza virus complexed with avian receptor analog LSTa
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

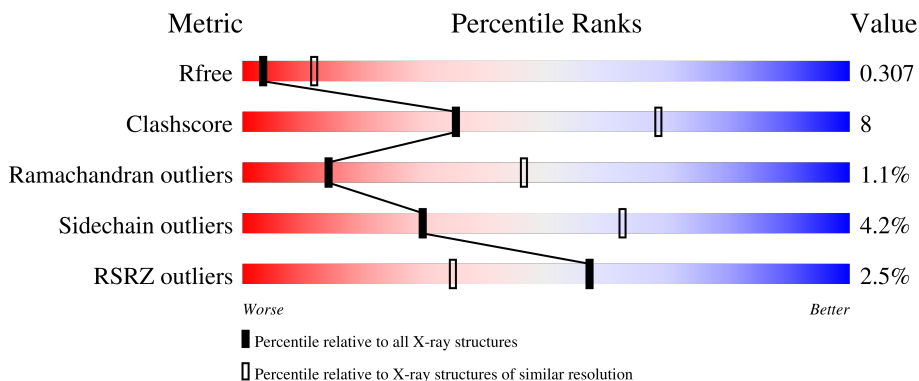
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


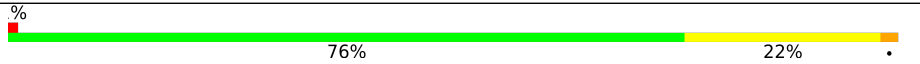
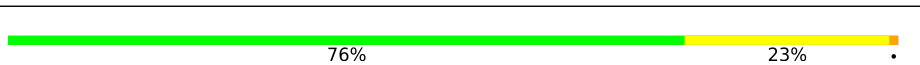

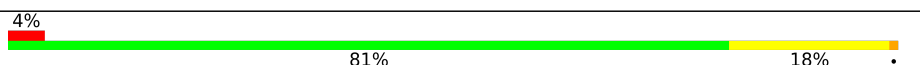
The reported resolution of this entry is 3.10 Å.

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	
1	C	321	
1	E	321	
1	G	321	
2	B	164	

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Mol	Chain	Length	Quality of chain
2	D	164	<p>5% 74% 24%</p>
2	F	164	<p>5% 75% 23%</p>
2	H	164	<p>8% 80% 20%</p>
3	I	3	<p>33% 67%</p>
3	J	3	<p>100%</p>
3	L	3	<p>100%</p>
4	K	2	<p>50% 50%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2541	1605	436	485	15	0	0	0
1	C	321	2541	1605	436	485	15	0	0	0
1	E	321	2541	1605	436	485	15	0	0	0
1	G	321	2541	1605	436	485	15	0	0	0

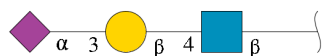
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP A8HWY8
C	4	GLN	-	expression tag	UNP A8HWY8
E	4	GLN	-	expression tag	UNP A8HWY8
G	4	GLN	-	expression tag	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

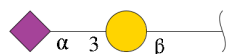
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	164	1328	828	229	263	8	0	0	0
2	D	164	1328	828	229	263	8	0	0	0
2	F	164	1328	828	229	263	8	0	0	0
2	H	164	1328	828	229	263	8	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



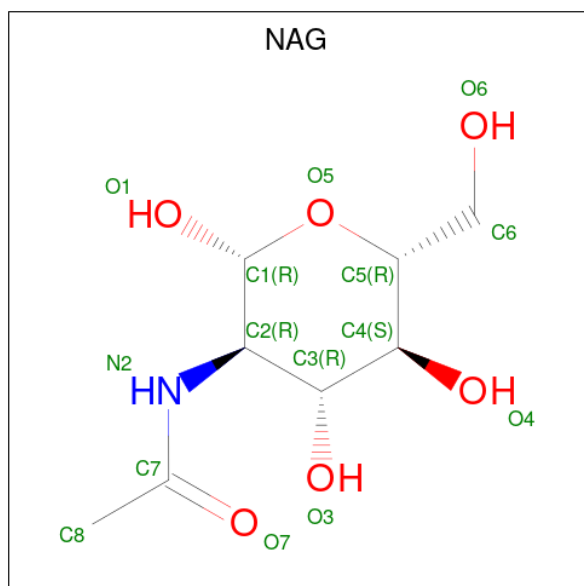
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	3	46	25	2	19	0	0	0
3	J	3	46	25	2	19	0	0	0
3	L	3	46	25	2	19	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	K	2	32	17	1	14	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

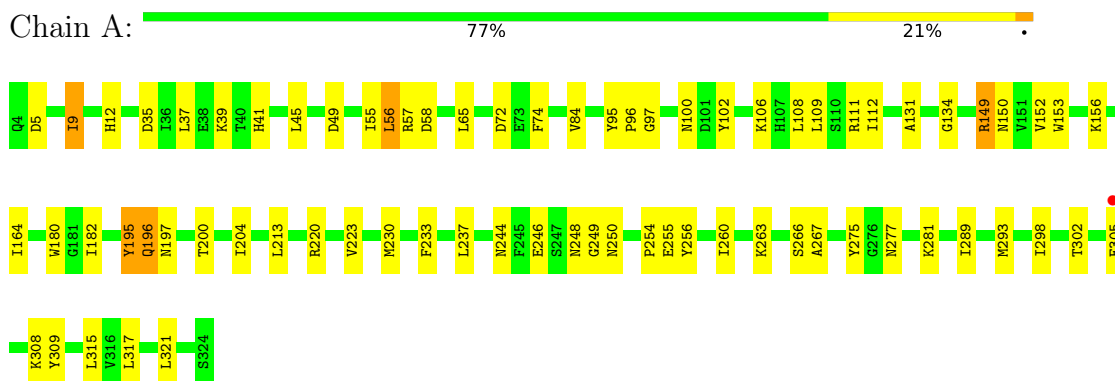


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

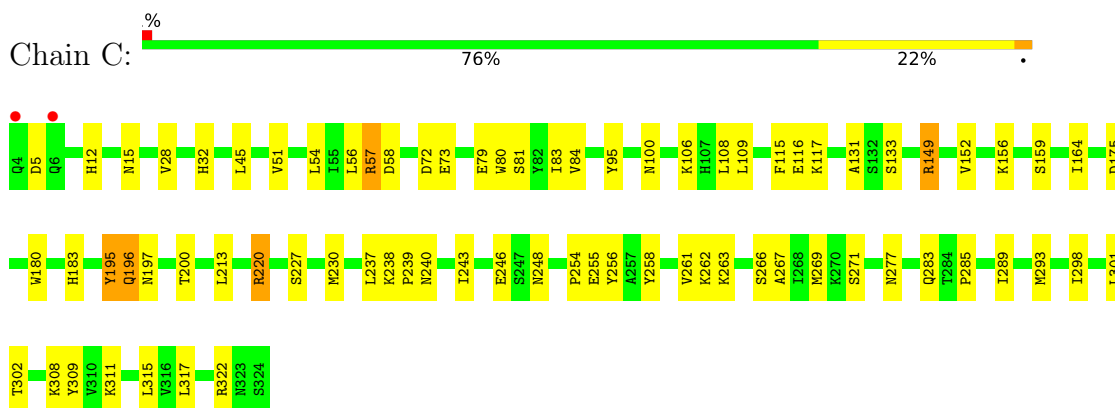
3 Residue-property plots

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

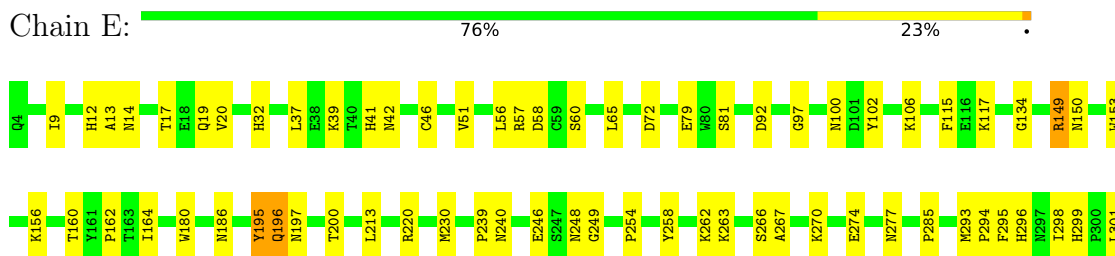
- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin

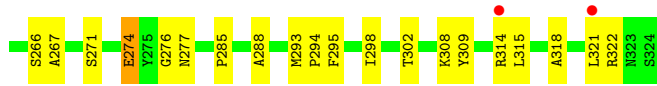
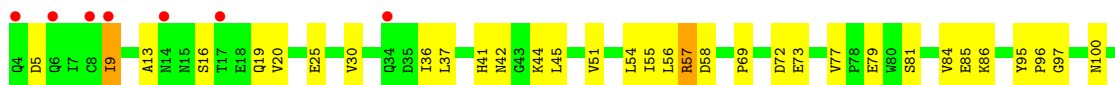
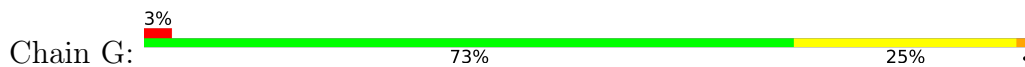


- Molecule 1: Hemagglutinin

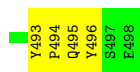
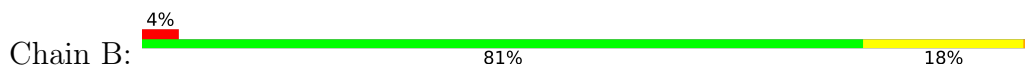




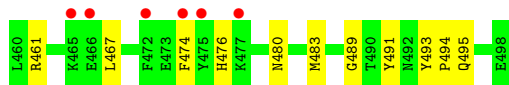
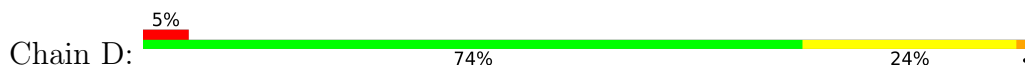
• Molecule 1: Hemagglutinin



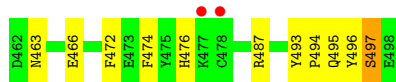
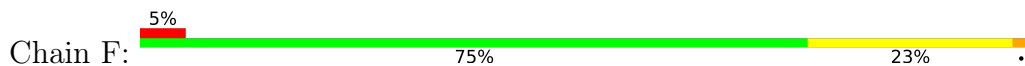
• Molecule 2: Hemagglutinin



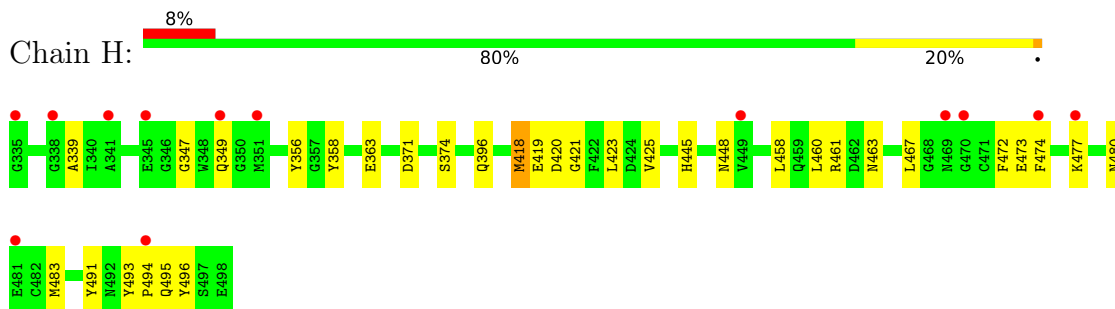
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



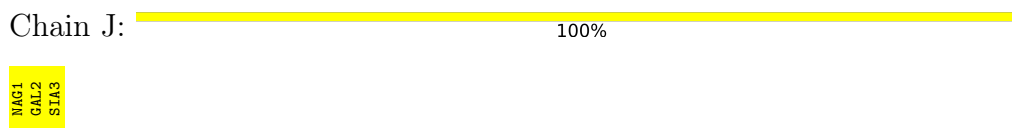
- Molecule 2: Hemagglutinin



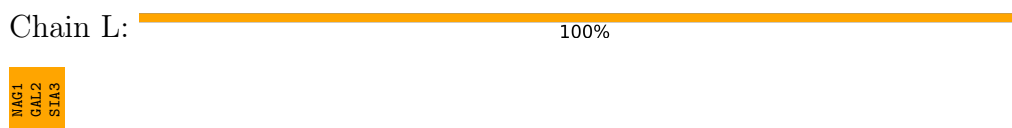
- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.56Å 70.56Å 506.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.49 – 3.10 49.49 – 3.06	Depositor EDS
% Data completeness (in resolution range)	80.8 (49.49-3.10) 80.8 (49.49-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.245 , 0.307 0.246 , 0.307	Depositor DCC
R_{free} test set	2165 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtrriage
Anisotropy	0.390	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 13.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.368 for -h,-k,l 0.099 for h,-h-k,-l 0.085 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.428 for -h,-k,l	Depositor
Outliers	0 of 42807 reflections	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15674	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GAL, SIA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2603	0.50	0/3537
1	C	0.28	0/2603	0.50	0/3537
1	E	0.28	0/2603	0.48	0/3537
1	G	0.27	0/2603	0.48	0/3537
2	B	0.27	0/1355	0.44	0/1823
2	D	0.28	0/1355	0.44	0/1823
2	F	0.28	0/1355	0.46	0/1823
2	H	0.27	0/1355	0.43	0/1823
All	All	0.28	0/15832	0.47	0/21440

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2541	0	2478	50	0
1	C	2541	0	2479	46	0
1	E	2541	0	2478	40	0
1	G	2541	0	2479	52	0
2	B	1328	0	1231	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1328	0	1231	31	0
2	F	1328	0	1231	25	0
2	H	1328	0	1231	23	0
3	I	46	0	40	2	0
3	J	46	0	40	0	0
3	L	46	0	40	3	0
4	K	32	0	28	1	0
5	A	14	0	13	0	0
5	E	14	0	13	0	0
All	All	15674	0	15012	250	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 8.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.60	0.82
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.63	0.80
1:G:309:TYR:HD2	2:H:423:LEU:HD11	1.48	0.77
2:D:476:HIS:HE2	2:D:491:TYR:HH	1.35	0.74
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.72	0.72
1:E:72:ASP:OD1	1:E:149:ARG:NH1	2.24	0.69
1:G:72:ASP:OD1	1:G:149:ARG:NH1	2.25	0.69
1:G:197:ASN:ND2	1:G:248:ASN:O	2.24	0.69
2:B:406:ASN:OD1	2:B:409:ARG:NH2	2.26	0.69
1:A:72:ASP:OD1	1:A:149:ARG:NH1	2.25	0.69
1:C:309:TYR:HD2	2:D:423:LEU:HD11	1.56	0.69
1:G:86:LYS:NZ	1:G:274:GLU:OE2	2.27	0.68
1:C:72:ASP:OD1	1:C:149:ARG:NH1	2.25	0.68
1:G:45:LEU:HD13	1:G:84:VAL:HG21	1.77	0.67
1:G:106:LYS:HA	1:G:109:LEU:HD12	1.77	0.67
1:C:197:ASN:ND2	1:C:248:ASN:O	2.24	0.66
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.27	0.66
1:A:309:TYR:HD2	2:B:423:LEU:HD11	1.60	0.66
2:D:493:TYR:O	2:D:495:GLN:N	2.29	0.66
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.78	0.64
1:C:180:TRP:HB3	1:C:254:PRO:HG3	1.80	0.63
1:A:106:LYS:HA	1:A:109:LEU:HD12	1.80	0.63
1:E:180:TRP:HB3	1:E:254:PRO:HG3	1.81	0.63
1:C:28:VAL:HG13	1:C:322:ARG:HE	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:309:TYR:HD2	2:F:423:LEU:HD11	1.66	0.60
2:B:376:GLN:NE2	2:B:380:ASP:OD1	2.34	0.60
2:F:360:HIS:CD2	2:F:487:ARG:HH12	2.19	0.60
2:H:493:TYR:O	2:H:495:GLN:N	2.34	0.60
2:D:362:ASN:ND2	2:D:480:ASN:OD1	2.34	0.60
2:D:409:ARG:NH1	2:D:412:GLU:OE2	2.34	0.59
1:E:32:HIS:CE1	2:F:355:TRP:HE1	2.20	0.59
1:A:35:ASP:OD2	1:A:39:LYS:NZ	2.36	0.59
1:G:309:TYR:CD2	2:H:423:LEU:HD11	2.35	0.58
1:C:15:ASN:OD1	2:D:349:GLN:NE2	2.36	0.58
1:G:25:GLU:OE1	1:G:322:ARG:NH2	2.32	0.57
1:E:117:LYS:HD3	1:E:258:TYR:CZ	2.39	0.57
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.85	0.57
1:C:32:HIS:CE1	2:D:355:TRP:HE1	2.22	0.57
2:D:339:ALA:HA	2:D:343:PHE:CE2	2.40	0.57
1:E:197:ASN:ND2	1:E:248:ASN:O	2.34	0.56
1:A:164:ILE:O	1:A:246:GLU:HA	2.05	0.56
1:C:266:SER:OG	1:C:267:ALA:N	2.37	0.56
1:G:16:SER:OG	1:G:30:VAL:O	2.23	0.56
1:G:9:ILE:HD11	2:H:358:TYR:HD2	1.70	0.56
2:H:371:ASP:OD1	2:H:374:SER:OG	2.18	0.56
1:G:85:GLU:OE2	1:G:106:LYS:NZ	2.33	0.56
1:A:309:TYR:CD2	2:B:423:LEU:HD11	2.40	0.56
1:E:315:LEU:HD22	2:F:434:VAL:HG21	1.88	0.55
1:C:106:LYS:HA	1:C:109:LEU:HD12	1.87	0.55
1:A:45:LEU:HD13	1:A:84:VAL:HG21	1.88	0.55
1:C:308:LYS:HD3	2:D:396:GLN:HB2	1.88	0.55
1:A:55:ILE:HG12	1:A:84:VAL:HB	1.89	0.55
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.89	0.55
1:G:308:LYS:HD3	2:H:396:GLN:HB2	1.89	0.55
1:E:266:SER:OG	1:E:267:ALA:N	2.38	0.55
1:G:44:LYS:HD3	1:G:276:GLY:HA3	1.89	0.55
2:F:376:GLN:NE2	2:F:380:ASP:OD1	2.40	0.55
1:E:42:ASN:ND2	1:E:46:CYS:SG	2.78	0.54
1:E:160:THR:HG22	1:E:162:PRO:HD3	1.88	0.54
1:E:14:ASN:OD1	1:E:323:ASN:ND2	2.40	0.54
1:C:45:LEU:HD13	1:C:84:VAL:HG21	1.88	0.54
2:D:339:ALA:HA	2:D:343:PHE:HE2	1.72	0.54
1:E:37:LEU:O	1:E:39:LYS:NZ	2.39	0.54
1:G:164:ILE:O	1:G:246:GLU:HA	2.08	0.54
1:A:102:TYR:CE2	1:A:106:LYS:HE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:VAL:HG21	1:E:318:ALA:HB2	1.89	0.54
2:D:476:HIS:NE2	2:D:491:TYR:OH	2.28	0.54
1:G:41:HIS:HB3	1:G:298:ILE:HD13	1.88	0.54
1:G:37:LEU:HB2	1:G:315:LEU:HB2	1.91	0.53
1:A:95:TYR:CD2	1:A:230:MET:HG2	2.43	0.53
2:F:421:GLY:O	2:F:425:VAL:HG13	2.08	0.53
1:G:112:ILE:HD13	1:G:260:ILE:HG12	1.90	0.53
2:F:384:ASN:O	2:F:388:SER:OG	2.23	0.53
2:H:421:GLY:O	2:H:425:VAL:HG13	2.08	0.52
2:F:466:GLU:HG2	2:F:472:PHE:HE2	1.74	0.52
1:A:309:TYR:HE2	2:B:423:LEU:HD21	1.74	0.52
1:A:197:ASN:HD22	1:A:248:ASN:HB2	1.74	0.52
1:E:79:GLU:OE2	1:E:262:LYS:NZ	2.34	0.52
1:G:96:PRO:HB3	1:G:223:VAL:HB	1.91	0.52
1:C:237:LEU:HD11	1:C:243:ILE:HB	1.92	0.51
1:A:266:SER:OG	1:A:267:ALA:N	2.44	0.51
1:C:57:ARG:NE	1:C:73:GLU:OE2	2.40	0.51
1:G:271:SER:OG	1:G:285:PRO:O	2.19	0.51
2:H:358:TYR:OH	2:H:371:ASP:OD2	2.26	0.51
1:G:54:LEU:HD22	1:G:77:VAL:HG11	1.93	0.50
2:B:493:TYR:O	2:B:495:GLN:N	2.44	0.50
1:C:309:TYR:CD2	2:D:423:LEU:HD11	2.43	0.50
1:E:195:TYR:O	1:E:197:ASN:N	2.45	0.50
1:G:266:SER:OG	1:G:267:ALA:N	2.45	0.50
1:C:315:LEU:HD22	2:D:434:VAL:HG21	1.93	0.50
1:A:9:ILE:HD11	2:B:456:VAL:HG21	1.93	0.50
2:D:474:PHE:HB3	2:D:476:HIS:O	2.10	0.50
2:F:493:TYR:O	2:F:495:GLN:N	2.45	0.50
1:G:117:LYS:HD3	1:G:258:TYR:CZ	2.47	0.50
2:B:436:MET:O	2:B:440:ARG:HG2	2.11	0.49
2:D:421:GLY:O	2:D:425:VAL:HG13	2.12	0.49
1:C:51:VAL:HG13	1:C:81:SER:HB3	1.94	0.49
1:E:186:ASN:OD1	1:E:186:ASN:N	2.46	0.49
1:G:309:TYR:CE2	2:H:423:LEU:HD21	2.48	0.49
2:H:460:LEU:HD12	2:H:472:PHE:HD1	1.77	0.49
1:C:54:LEU:HD23	1:C:83:ILE:HG12	1.93	0.49
1:C:289:ILE:HD11	1:C:298:ILE:HD12	1.93	0.49
1:A:315:LEU:HD22	2:B:434:VAL:HG21	1.94	0.49
1:C:12:HIS:ND1	2:D:351:MET:O	2.44	0.49
1:G:79:GLU:OE2	1:G:262:LYS:NZ	2.34	0.49
1:A:65:LEU:O	1:A:150:ASN:ND2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ILE:O	1:C:246:GLU:HA	2.13	0.49
1:E:51:VAL:HG13	1:E:81:SER:HB3	1.93	0.49
1:E:308:LYS:HD3	2:F:396:GLN:HB2	1.95	0.49
1:C:117:LYS:HD3	1:C:258:TYR:CZ	2.47	0.49
1:C:95:TYR:CD2	1:C:230:MET:HG2	2.48	0.48
2:D:456:VAL:HA	2:D:459:GLN:HE21	1.78	0.48
2:D:376:GLN:NE2	2:D:380:ASP:OD1	2.47	0.48
2:F:436:MET:O	2:F:440:ARG:HG2	2.14	0.48
1:G:195:TYR:O	1:G:197:ASN:N	2.47	0.48
2:F:463:ASN:HA	2:F:497:SER:OG	2.14	0.48
2:B:371:ASP:OD1	2:B:374:SER:OG	2.21	0.48
1:G:131:ALA:HB1	1:G:152:VAL:HG21	1.96	0.48
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.94	0.47
1:E:65:LEU:O	1:E:150:ASN:ND2	2.43	0.47
1:A:308:LYS:HD3	2:B:396:GLN:HB2	1.97	0.47
1:C:12:HIS:N	2:D:355:TRP:O	2.47	0.47
2:D:358:TYR:OH	2:D:455:LYS:NZ	2.40	0.47
1:E:270:LYS:HE2	2:F:403:GLU:OE2	2.15	0.47
1:A:55:ILE:HD12	1:A:275:TYR:HB2	1.96	0.47
1:A:96:PRO:HB3	1:A:223:VAL:HB	1.97	0.47
1:C:80:TRP:HH2	1:C:115:PHE:CD1	2.33	0.47
1:G:5:ASP:O	2:H:474:PHE:HB2	2.15	0.47
1:G:309:TYR:HE2	2:H:423:LEU:HD21	1.79	0.47
1:A:131:ALA:HB1	1:A:152:VAL:HG21	1.96	0.47
2:F:355:TRP:CZ3	2:F:379:ILE:HG12	2.50	0.47
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.96	0.46
3:L:1:NAG:H62	3:L:2:GAL:O2	2.14	0.46
1:G:42:ASN:ND2	1:G:288:ALA:HB3	2.30	0.46
1:A:102:TYR:CZ	1:A:106:LYS:HE3	2.50	0.46
1:G:308:LYS:HD3	2:H:396:GLN:CB	2.44	0.46
1:A:281:LYS:O	1:A:305:GLU:N	2.44	0.46
2:H:418:MET:HG3	2:H:419:GLU:N	2.30	0.46
1:G:20:VAL:HG11	1:G:318:ALA:HB2	1.98	0.46
1:C:72:ASP:OD2	1:C:149:ARG:HD2	2.16	0.46
1:E:200:THR:HG21	1:E:249:GLY:HA3	1.98	0.46
1:E:97:GLY:HA3	1:E:230:MET:O	2.15	0.45
1:G:255:GLU:HG2	1:G:256:TYR:CD2	2.51	0.45
1:C:175:ASP:OD1	1:C:238:LYS:HD3	2.16	0.45
1:E:115:PHE:CD2	1:E:258:TYR:HB3	2.51	0.45
1:G:294:PRO:HG2	1:G:295:PHE:HD2	1.82	0.45
1:C:131:ALA:HB1	1:C:152:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:ILE:O	1:E:246:GLU:HA	2.17	0.45
1:G:69:PRO:HB3	1:G:141:TYR:HB2	1.98	0.45
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.99	0.45
2:B:421:GLY:O	2:B:425:VAL:HG13	2.17	0.45
1:E:285:PRO:HD3	1:E:301:LEU:O	2.16	0.45
1:E:309:TYR:CD2	2:F:423:LEU:HD11	2.48	0.45
1:A:255:GLU:HG2	1:A:256:TYR:CD2	2.51	0.45
2:B:418:MET:HG3	2:B:419:GLU:N	2.32	0.45
2:D:338:GLY:O	2:D:342:GLY:HA3	2.16	0.45
1:A:95:TYR:HH	3:I:3:SIA:HO8	1.65	0.45
1:C:195:TYR:O	1:C:197:ASN:N	2.50	0.45
3:I:2:GAL:H3	3:I:3:SIA:H32	1.52	0.45
1:A:49:ASP:OD1	1:A:281:LYS:HG2	2.17	0.45
1:C:159:SER:C	1:C:196:GLN:HG3	2.36	0.45
1:G:13:ALA:HB2	2:H:347:GLY:HA3	1.98	0.45
3:L:1:NAG:HO1	3:L:1:NAG:C7	2.30	0.45
1:A:5:ASP:OD1	2:B:478:CYS:N	2.41	0.45
1:A:5:ASP:OD2	1:A:5:ASP:N	2.50	0.45
1:C:317:LEU:HD13	2:D:434:VAL:HG22	1.98	0.45
2:H:463:ASN:ND2	2:H:491:TYR:OH	2.47	0.45
1:A:195:TYR:O	1:A:197:ASN:N	2.50	0.44
1:G:255:GLU:HG2	1:G:256:TYR:CE2	2.52	0.44
1:G:36:ILE:O	1:G:295:PHE:HB2	2.17	0.44
2:H:363:GLU:OE2	2:H:477:LYS:HD3	2.17	0.44
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.81	0.44
2:F:338:GLY:O	2:F:342:GLY:HA3	2.17	0.44
1:G:19:GLN:O	1:G:314:ARG:NH2	2.42	0.44
1:G:72:ASP:OD2	1:G:149:ARG:HD2	2.16	0.44
1:G:51:VAL:HG13	1:G:81:SER:HB3	2.00	0.44
2:F:474:PHE:HB3	2:F:476:HIS:O	2.18	0.44
1:G:321:LEU:HB3	2:H:445:HIS:CG	2.52	0.44
2:H:356:TYR:OH	2:H:448:ASN:ND2	2.50	0.44
1:A:204:ILE:HA	1:A:244:ASN:O	2.17	0.44
1:A:309:TYR:CE2	2:B:423:LEU:HD21	2.52	0.44
1:G:200:THR:HG21	1:G:249:GLY:HA3	1.99	0.44
1:A:112:ILE:HD13	1:A:260:ILE:HG12	2.00	0.44
2:D:436:MET:O	2:D:440:ARG:HG2	2.18	0.44
2:H:467:LEU:HD13	2:H:473:GLU:HB2	2.00	0.44
1:A:12:HIS:ND1	2:B:351:MET:O	2.50	0.43
1:G:115:PHE:HB3	1:G:258:TYR:HB3	2.00	0.43
1:C:79:GLU:OE2	1:C:262:LYS:NZ	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:PRO:C	1:E:295:PHE:HD1	2.22	0.43
1:C:220:ARG:HD2	1:C:227:SER:O	2.18	0.43
1:C:255:GLU:HG2	1:C:256:TYR:CD2	2.53	0.43
1:C:269:MET:HE3	1:C:283:GLN:HG3	2.00	0.43
2:F:418:MET:HG3	2:F:419:GLU:N	2.33	0.43
2:B:485:SER:O	2:B:490:THR:N	2.51	0.43
1:G:144:SER:HA	1:G:145:PRO:HD3	1.91	0.43
2:D:459:GLN:OE1	2:D:489:GLY:HA2	2.19	0.43
1:C:239:PRO:O	1:C:240:ASN:HB2	2.18	0.43
1:A:200:THR:OG1	1:A:250:ASN:OD1	2.18	0.43
1:G:97:GLY:HA3	1:G:230:MET:O	2.18	0.43
1:G:57:ARG:NE	1:G:73:GLU:OE2	2.49	0.42
2:D:418:MET:HG3	2:D:419:GLU:N	2.34	0.42
1:E:12:HIS:HB2	2:F:355:TRP:HA	2.01	0.42
1:G:185:PRO:HD2	1:G:217:ILE:HG13	2.01	0.42
1:E:41:HIS:HB3	1:E:298:ILE:HD13	2.01	0.42
1:A:37:LEU:O	1:A:39:LYS:NZ	2.52	0.42
1:C:308:LYS:HD3	2:D:396:GLN:CB	2.50	0.42
1:G:55:ILE:HG12	1:G:84:VAL:HB	2.00	0.42
1:A:200:THR:HG21	1:A:249:GLY:HA3	2.01	0.42
2:H:467:LEU:CD1	2:H:473:GLU:HB2	2.50	0.42
1:C:271:SER:OG	1:C:285:PRO:O	2.30	0.42
1:C:311:LYS:HE3	2:D:423:LEU:HD23	2.00	0.42
2:B:339:ALA:HB3	2:B:446:ASP:OD2	2.20	0.42
1:A:12:HIS:O	1:A:321:LEU:HD11	2.20	0.42
1:E:239:PRO:O	1:E:240:ASN:HB2	2.20	0.42
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.55	0.42
1:C:200:THR:HA	1:C:248:ASN:OD1	2.20	0.41
2:D:423:LEU:HD12	2:D:423:LEU:HA	1.87	0.41
1:E:72:ASP:OD2	1:E:149:ARG:HD2	2.20	0.41
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.83	0.41
1:A:197:ASN:ND2	1:A:248:ASN:HB2	2.34	0.41
1:C:115:PHE:HB3	1:C:258:TYR:HB3	2.02	0.41
2:F:339:ALA:HA	2:F:343:PHE:CE2	2.55	0.41
2:F:423:LEU:HD12	2:F:423:LEU:HA	1.91	0.41
1:C:5:ASP:N	1:C:5:ASP:OD2	2.53	0.41
2:D:337:PHE:CE1	2:D:447:SER:HB2	2.56	0.41
2:F:450:LYS:HE3	2:F:454:ASP:OD2	2.21	0.41
1:G:13:ALA:O	2:H:349:GLN:HA	2.20	0.41
1:A:56:LEU:HA	1:A:74:PHE:CZ	2.56	0.41
1:E:60:SER:OG	1:E:92:ASP:OD2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:GAL:H3	3:L:3:SIA:H32	1.63	0.41
1:A:289:ILE:HD11	1:A:298:ILE:HD12	2.02	0.41
1:C:116:GLU:HG2	1:C:261:VAL:HG11	2.02	0.41
1:E:13:ALA:HB2	2:F:347:GLY:HA3	2.02	0.41
1:E:321:LEU:HB3	2:F:445:HIS:CG	2.56	0.41
2:F:336:LEU:HD22	2:F:443:ASP:OD2	2.21	0.41
1:A:72:ASP:OD2	1:A:149:ARG:HD2	2.21	0.41
1:A:182:ILE:HG22	1:A:233:PHE:HE2	1.86	0.41
1:E:102:TYR:CE2	1:E:106:LYS:HE3	2.56	0.41
1:E:296:HIS:HD2	1:E:307:PRO:HB2	1.86	0.41
1:C:285:PRO:HD3	1:C:301:LEU:O	2.20	0.40
2:D:384:ASN:O	2:D:388:SER:OG	2.30	0.40
1:E:285:PRO:HG2	1:E:299:HIS:CE1	2.55	0.40
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.87	0.40
2:D:480:ASN:O	2:D:483:MET:HB2	2.21	0.40
4:K:1:GAL:H3	4:K:2:SIA:H32	1.70	0.40
1:A:317:LEU:HD13	2:B:434:VAL:HG22	2.03	0.40
1:A:97:GLY:HA3	1:A:230:MET:O	2.22	0.40
1:A:255:GLU:HG2	1:A:256:TYR:CE2	2.57	0.40
1:E:17:THR:O	1:E:19:GLN:HG3	2.22	0.40
2:H:480:ASN:O	2:H:483:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	319/321 (99%)	300 (94%)	17 (5%)	2 (1%)	25 59
1	C	319/321 (99%)	299 (94%)	18 (6%)	2 (1%)	25 59
1	E	319/321 (99%)	303 (95%)	14 (4%)	2 (1%)	25 59
1	G	319/321 (99%)	301 (94%)	16 (5%)	2 (1%)	25 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	8	33
2	D	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	8	33
2	F	162/164 (99%)	144 (89%)	14 (9%)	4 (2%)	5	27
2	H	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	8	33
All	All	1924/1940 (99%)	1779 (92%)	124 (6%)	21 (1%)	14	46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	C	196	GLN
1	E	196	GLN
1	G	196	GLN
2	B	461	ARG
2	B	494	PRO
2	D	494	PRO
2	F	461	ARG
2	F	494	PRO
2	H	494	PRO
2	B	339	ALA
2	D	461	ARG
1	E	57	ARG
1	G	57	ARG
2	H	461	ARG
1	A	57	ARG
1	C	57	ARG
2	D	339	ALA
2	F	339	ALA
2	H	339	ALA
2	F	497	SER

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	288/288 (100%)	275 (96%)	13 (4%)	27	60
1	C	288/288 (100%)	276 (96%)	12 (4%)	30	62
1	E	288/288 (100%)	275 (96%)	13 (4%)	27	60
1	G	288/288 (100%)	275 (96%)	13 (4%)	27	60
2	B	140/140 (100%)	134 (96%)	6 (4%)	29	62
2	D	140/140 (100%)	134 (96%)	6 (4%)	29	62
2	F	140/140 (100%)	135 (96%)	5 (4%)	35	67
2	H	140/140 (100%)	136 (97%)	4 (3%)	42	72
All	All	1712/1712 (100%)	1640 (96%)	72 (4%)	30	62

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	56	LEU
1	A	58	ASP
1	A	100	ASN
1	A	111	ARG
1	A	149	ARG
1	A	195	TYR
1	A	213	LEU
1	A	220	ARG
1	A	263	LYS
1	A	277	ASN
1	A	293	MET
1	A	302	THR
2	B	360	HIS
2	B	418	MET
2	B	420	ASP
2	B	458	LEU
2	B	467	LEU
2	B	496	TYR
1	C	56	LEU
1	C	58	ASP
1	C	100	ASN
1	C	133	SER
1	C	149	ARG
1	C	195	TYR
1	C	213	LEU
1	C	220	ARG

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Mol	Chain	Res	Type
1	C	263	LYS
1	C	277	ASN
1	C	293	MET
1	C	302	THR
2	D	358	TYR
2	D	360	HIS
2	D	418	MET
2	D	420	ASP
2	D	458	LEU
2	D	467	LEU
1	E	9	ILE
1	E	56	LEU
1	E	58	ASP
1	E	100	ASN
1	E	149	ARG
1	E	195	TYR
1	E	213	LEU
1	E	220	ARG
1	E	263	LYS
1	E	274	GLU
1	E	277	ASN
1	E	293	MET
1	E	302	THR
2	F	360	HIS
2	F	418	MET
2	F	420	ASP
2	F	458	LEU
2	F	496	TYR
1	G	9	ILE
1	G	56	LEU
1	G	58	ASP
1	G	100	ASN
1	G	149	ARG
1	G	195	TYR
1	G	213	LEU
1	G	220	ARG
1	G	263	LYS
1	G	274	GLU
1	G	277	ASN
1	G	293	MET
1	G	302	THR
2	H	418	MET

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Mol	Chain	Res	Type
2	H	420	ASP
2	H	458	LEU
2	H	496	TYR

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	211	GLN
2	D	448	ASN
2	F	448	ASN
2	H	448	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

11 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	1	3	15,15,15	0.47	0	21,21,21	0.84	1 (4%)
3	GAL	I	2	3	11,11,12	0.73	0	15,15,17	1.69	4 (26%)
3	SIA	I	3	3	20,20,21	4.04	8 (40%)	24,28,31	4.04	9 (37%)
3	NAG	J	1	3	15,15,15	0.53	0	21,21,21	1.41	5 (23%)
3	GAL	J	2	3	11,11,12	0.65	0	15,15,17	1.62	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	J	3	3	20,20,21	4.02	8 (40%)	24,28,31	4.00	10 (41%)
4	GAL	K	1	4	12,12,12	0.56	0	17,17,17	0.64	0
4	SIA	K	2	4	20,20,21	3.78	7 (35%)	24,28,31	2.46	7 (29%)
3	NAG	L	1	3	15,15,15	0.47	0	21,21,21	1.08	2 (9%)
3	GAL	L	2	3	11,11,12	0.64	0	15,15,17	1.35	2 (13%)
3	SIA	L	3	3	20,20,21	4.05	8 (40%)	24,28,31	4.14	10 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3	-	2/6/26/26	0/1/1/1
3	GAL	I	2	3	-	0/2/19/22	0/1/1/1
3	SIA	I	3	3	-	6/18/34/38	0/1/1/1
3	NAG	J	1	3	-	3/6/26/26	0/1/1/1
3	GAL	J	2	3	-	0/2/19/22	0/1/1/1
3	SIA	J	3	3	-	5/18/34/38	0/1/1/1
4	GAL	K	1	4	-	1/2/22/22	0/1/1/1
4	SIA	K	2	4	-	8/18/34/38	0/1/1/1
3	NAG	L	1	3	-	3/6/26/26	0/1/1/1
3	GAL	L	2	3	-	2/2/19/22	0/1/1/1
3	SIA	L	3	3	-	4/18/34/38	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	3	SIA	C7-C6	-12.41	1.37	1.53
3	J	3	SIA	C7-C6	-12.14	1.37	1.53
3	I	3	SIA	C7-C6	-12.11	1.37	1.53
4	K	2	SIA	C7-C6	-11.58	1.38	1.53
4	K	2	SIA	C4-C5	-8.02	1.46	1.53
3	I	3	SIA	C4-C5	-7.58	1.46	1.53
3	J	3	SIA	C4-C5	-7.52	1.46	1.53
3	L	3	SIA	C4-C5	-7.34	1.46	1.53
3	J	3	SIA	C3-C4	-5.63	1.43	1.52
4	K	2	SIA	C3-C4	-5.62	1.43	1.52
3	I	3	SIA	C3-C4	-5.51	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	3	SIA	C3-C2	-5.50	1.43	1.52
4	K	2	SIA	C3-C2	-5.43	1.43	1.52
3	L	3	SIA	C3-C4	-5.40	1.43	1.52
3	I	3	SIA	O6-C6	5.35	1.52	1.44
3	L	3	SIA	C3-C2	-5.31	1.43	1.52
3	I	3	SIA	C3-C2	-5.26	1.43	1.52
3	L	3	SIA	O6-C6	4.90	1.51	1.44
3	J	3	SIA	O6-C6	4.49	1.51	1.44
3	L	3	SIA	C10-N5	3.40	1.46	1.34
3	J	3	SIA	C10-N5	3.36	1.45	1.34
3	I	3	SIA	C10-N5	3.33	1.45	1.34
4	K	2	SIA	O6-C6	2.72	1.48	1.44
4	K	2	SIA	O6-C2	2.70	1.47	1.43
3	J	3	SIA	O8-C8	-2.63	1.37	1.43
3	I	3	SIA	O8-C8	-2.62	1.37	1.43
3	L	3	SIA	O8-C8	-2.55	1.37	1.43
3	J	3	SIA	C2-C1	2.21	1.54	1.52
3	L	3	SIA	C2-C1	2.19	1.54	1.52
4	K	2	SIA	C2-C1	2.16	1.54	1.52
3	I	3	SIA	O6-C2	2.06	1.46	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3	SIA	O6-C2-C3	-15.21	89.52	110.46
3	J	3	SIA	O6-C2-C3	-14.38	90.67	110.46
3	I	3	SIA	O6-C2-C3	-13.67	91.64	110.46
3	I	3	SIA	O6-C2-C1	9.61	126.56	107.70
3	L	3	SIA	O6-C2-C1	9.18	125.70	107.70
3	J	3	SIA	O6-C2-C1	8.62	124.60	107.70
4	K	2	SIA	C4-C3-C2	6.39	121.27	109.81
3	J	3	SIA	C4-C3-C2	5.96	120.49	109.81
4	K	2	SIA	O6-C2-C3	-5.88	102.36	110.46
3	I	3	SIA	C4-C3-C2	5.83	120.27	109.81
4	K	2	SIA	C6-O6-C2	5.42	122.94	111.34
3	L	3	SIA	C4-C3-C2	5.25	119.22	109.81
3	J	2	GAL	C1-C2-C3	4.50	115.20	109.67
3	I	2	GAL	C1-C2-C3	4.47	115.16	109.67
3	I	3	SIA	O9-C9-C8	4.12	120.06	111.07
3	I	3	SIA	C6-O6-C2	3.74	119.33	111.34
3	J	1	NAG	C4-C3-C2	3.63	115.66	110.34
3	L	3	SIA	C8-C7-C6	-3.43	106.54	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	GAL	C1-C2-C3	3.39	113.83	109.67
3	J	3	SIA	C8-C7-C6	-3.33	106.72	113.03
3	L	3	SIA	O9-C9-C8	3.26	118.19	111.07
4	K	2	SIA	O6-C2-C1	3.26	114.09	107.70
3	J	1	NAG	C3-C4-C5	3.21	115.96	110.24
3	J	3	SIA	C6-O6-C2	3.21	118.20	111.34
3	I	3	SIA	C8-C7-C6	-3.09	107.17	113.03
3	L	3	SIA	C3-C4-C5	3.04	115.14	111.46
3	I	3	SIA	C11-C10-N5	3.01	121.19	116.10
3	J	3	SIA	C3-C4-C5	2.97	115.05	111.46
4	K	2	SIA	O1B-C1-C2	2.90	121.32	113.03
3	L	3	SIA	O1B-C1-C2	2.85	121.16	113.03
3	J	2	GAL	O3-C3-C2	-2.82	104.59	109.99
3	L	3	SIA	C6-O6-C2	2.80	117.32	111.34
3	J	3	SIA	C11-C10-N5	2.77	120.78	116.10
3	J	3	SIA	O9-C9-C8	2.73	117.02	111.07
3	I	2	GAL	O3-C3-C2	-2.72	104.78	109.99
3	L	2	GAL	O3-C3-C2	-2.61	104.99	109.99
4	K	2	SIA	C3-C4-C5	2.58	114.58	111.46
4	K	2	SIA	O1B-C1-O1A	-2.56	118.27	124.09
3	I	3	SIA	O1B-C1-C2	2.53	120.24	113.03
3	L	3	SIA	O1B-C1-O1A	-2.51	118.40	124.09
3	L	3	SIA	C11-C10-N5	2.50	120.33	116.10
3	J	3	SIA	O1B-C1-O1A	-2.43	118.57	124.09
3	I	3	SIA	C3-C4-C5	2.30	114.24	111.46
3	I	2	GAL	C1-O5-C5	-2.30	109.08	112.19
3	L	1	NAG	C1-C2-N2	2.28	113.36	110.73
3	J	1	NAG	O5-C5-C4	2.25	113.77	109.69
3	I	1	NAG	C4-C3-C2	2.22	113.59	110.34
3	J	3	SIA	O1B-C1-C2	2.13	119.12	113.03
3	I	2	GAL	O5-C5-C6	2.06	110.44	107.20
3	J	1	NAG	O4-C4-C3	-2.05	105.61	110.35
3	J	1	NAG	O5-C1-C2	-2.04	107.47	109.52
3	L	1	NAG	C4-C3-C2	2.04	113.33	110.34

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	3	SIA	O7-C7-C8-C9
3	L	1	NAG	C1-C2-N2-C7
3	L	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	L	1	NAG	O7-C7-N2-C2
3	L	3	SIA	C6-C7-C8-C9
3	L	3	SIA	C6-C7-C8-O8
3	L	3	SIA	O7-C7-C8-C9
4	K	2	SIA	C6-C7-C8-C9
4	K	2	SIA	O7-C7-C8-C9
4	K	2	SIA	O7-C7-C8-O8
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	L	2	GAL	O5-C5-C6-O6
3	J	3	SIA	O7-C7-C8-O8
3	L	3	SIA	O7-C7-C8-O8
4	K	2	SIA	C6-C7-C8-O8
3	J	3	SIA	C6-C7-C8-O8
3	I	3	SIA	C6-C7-C8-C9
3	J	3	SIA	C6-C7-C8-C9
3	L	2	GAL	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
4	K	1	GAL	O5-C5-C6-O6
3	I	3	SIA	O7-C7-C8-C9
3	I	3	SIA	C6-C7-C8-O8
3	I	3	SIA	O8-C8-C9-O9
4	K	2	SIA	O8-C8-C9-O9
3	I	3	SIA	O7-C7-C8-O8
4	K	2	SIA	C7-C8-C9-O9
3	I	1	NAG	C8-C7-N2-C2
4	K	2	SIA	O1B-C1-C2-O6
3	J	3	SIA	O1A-C1-C2-O6
3	I	3	SIA	O1A-C1-C2-C3
4	K	2	SIA	O1A-C1-C2-C3
3	I	1	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 6 short contacts:

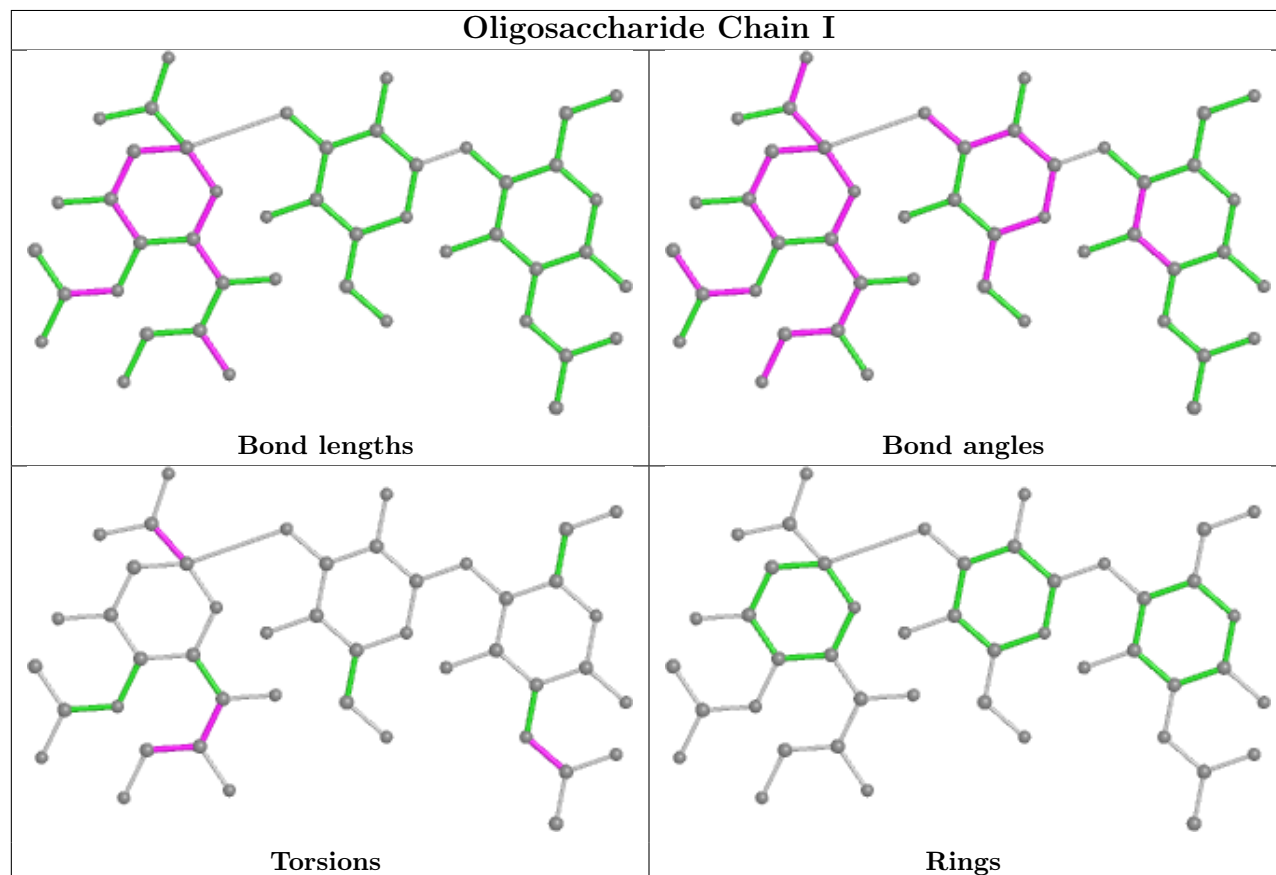
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	GAL	1	0
3	L	2	GAL	2	0
3	L	1	NAG	2	0
3	I	3	SIA	2	0
4	K	2	SIA	1	0
3	I	2	GAL	1	0

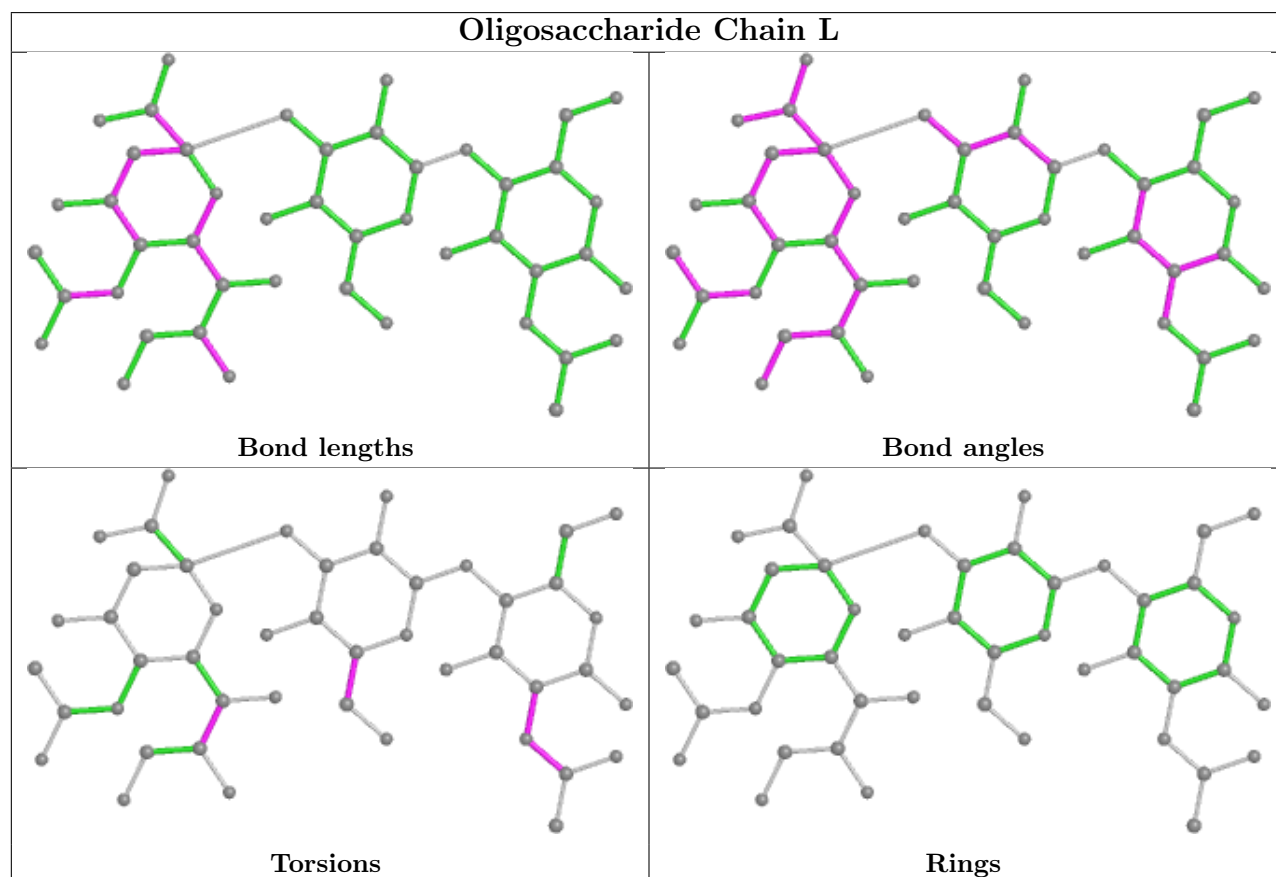
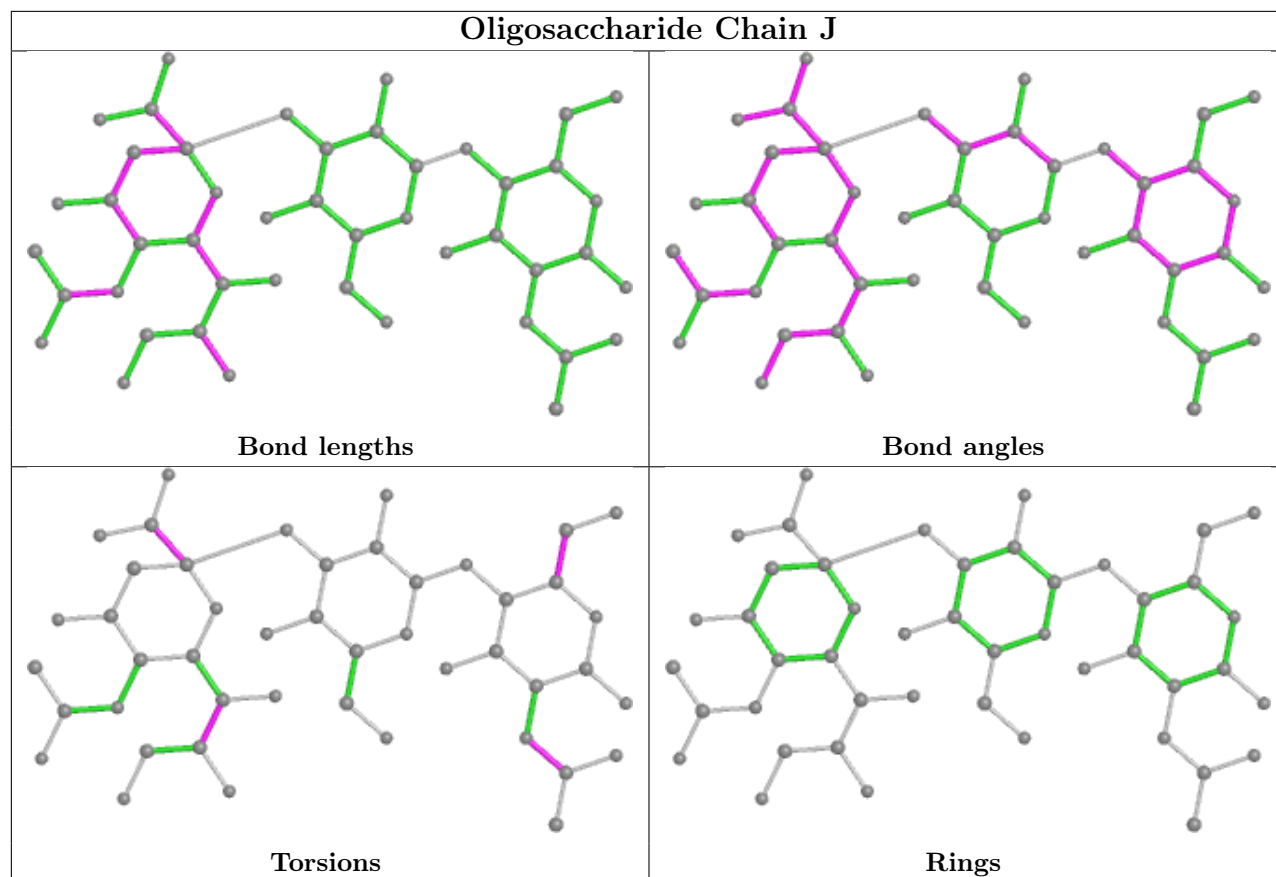
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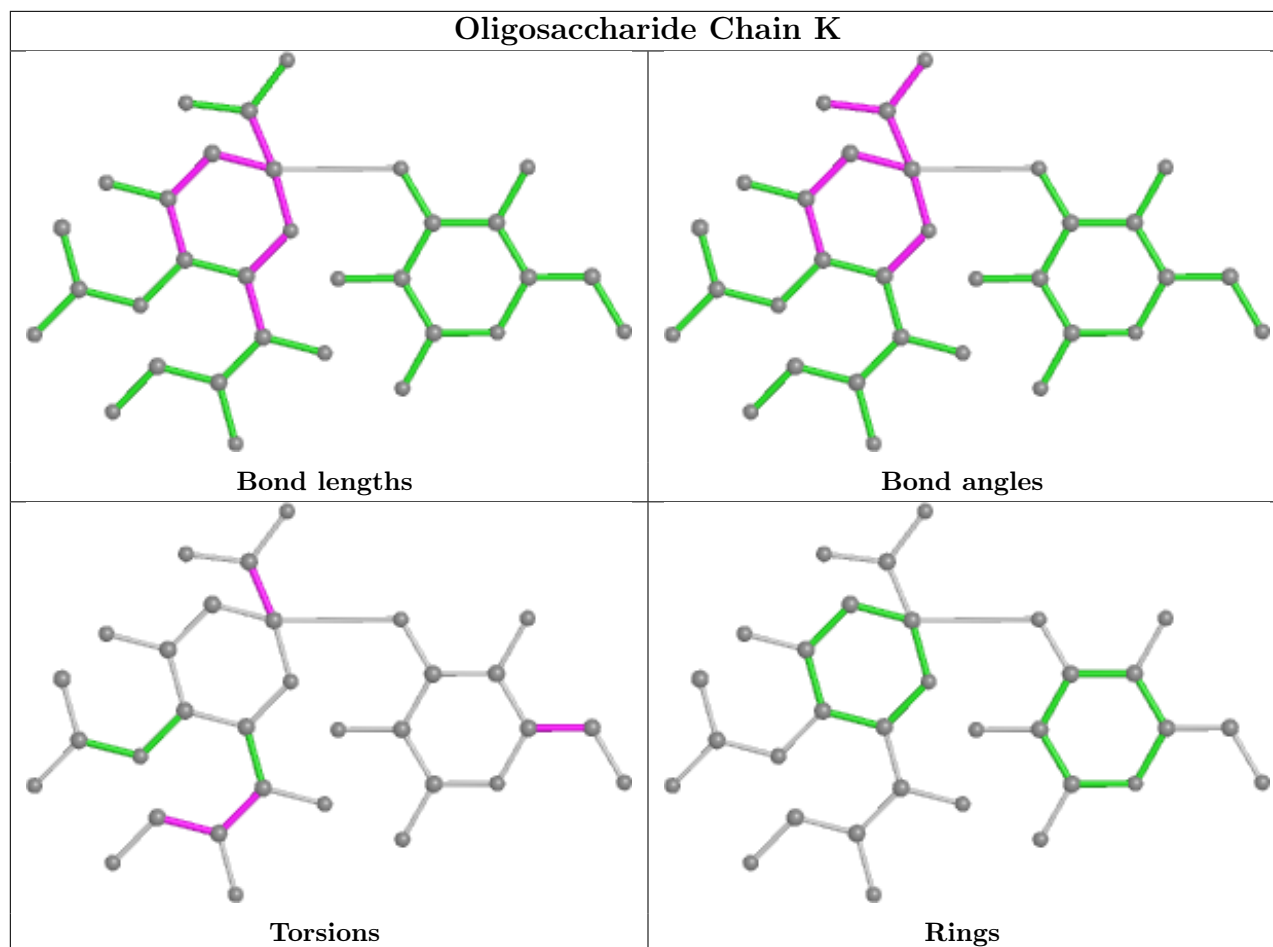
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	3	SIA	1	0

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







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
5	NAG	E	601	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)
5	NAG	A	601	1	14,14,15	0.47	0	17,19,21	0.91	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
5	NAG	E	601	1	-	4/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C1-O5-C5	2.71	115.86	112.19
5	E	601	NAG	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	601	NAG	C3-C2-N2-C7
5	E	601	NAG	C8-C7-N2-C2
5	E	601	NAG	O7-C7-N2-C2
5	A	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	321/321 (100%)	-0.10	1 (0%) 94 88	3, 37, 92, 128	0
1	C	321/321 (100%)	-0.02	2 (0%) 89 78	8, 41, 106, 167	0
1	E	321/321 (100%)	-0.03	0 100 100	21, 49, 99, 130	0
1	G	321/321 (100%)	0.11	9 (2%) 53 30	23, 54, 117, 179	0
2	B	164/164 (100%)	0.23	6 (3%) 41 21	15, 88, 126, 140	0
2	D	164/164 (100%)	0.31	9 (5%) 25 11	18, 104, 151, 179	0
2	F	164/164 (100%)	0.30	8 (4%) 29 14	34, 98, 139, 153	0
2	H	164/164 (100%)	0.56	13 (7%) 12 5	31, 112, 156, 169	0
All	All	1940/1940 (100%)	0.11	48 (2%) 57 34	3, 59, 133, 179	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	470	GLY	6.0
1	G	9	ILE	5.0
2	F	477	LYS	4.6
1	G	8	CYS	4.3
2	H	335	GLY	4.3
2	B	353	ASP	4.2
2	H	341	ALA	3.9
2	D	472	PHE	3.7
2	H	469	ASN	3.7
1	G	17	THR	3.6
2	H	345	GLU	3.3
2	D	353	ASP	3.3
2	H	494	PRO	3.2
2	F	355	TRP	3.2
2	D	475	TYR	3.2
1	G	34	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	474	PHE	3.0
2	H	481	GLU	3.0
1	G	314	ARG	2.9
1	G	6	GLN	2.9
2	H	338	GLY	2.9
2	F	356	TYR	2.8
2	F	366	SER	2.8
2	F	478	CYS	2.7
2	D	356	TYR	2.6
2	F	360	HIS	2.6
2	D	477	LYS	2.6
2	D	465	LYS	2.5
2	D	474	PHE	2.5
2	B	363	GLU	2.5
1	G	321	LEU	2.5
1	G	14	ASN	2.5
2	D	355	TRP	2.4
2	F	357	GLY	2.4
2	H	349	GLN	2.4
2	B	335	GLY	2.4
2	D	466	GLU	2.3
2	B	367	GLY	2.2
1	G	4	GLN	2.2
2	H	477	LYS	2.2
2	H	351	MET	2.2
1	A	305	GLU	2.2
2	F	349	GLN	2.2
2	B	361	SER	2.1
1	C	6	GLN	2.0
2	B	350	GLY	2.0
2	H	449	VAL	2.0
1	C	4	GLN	2.0

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

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

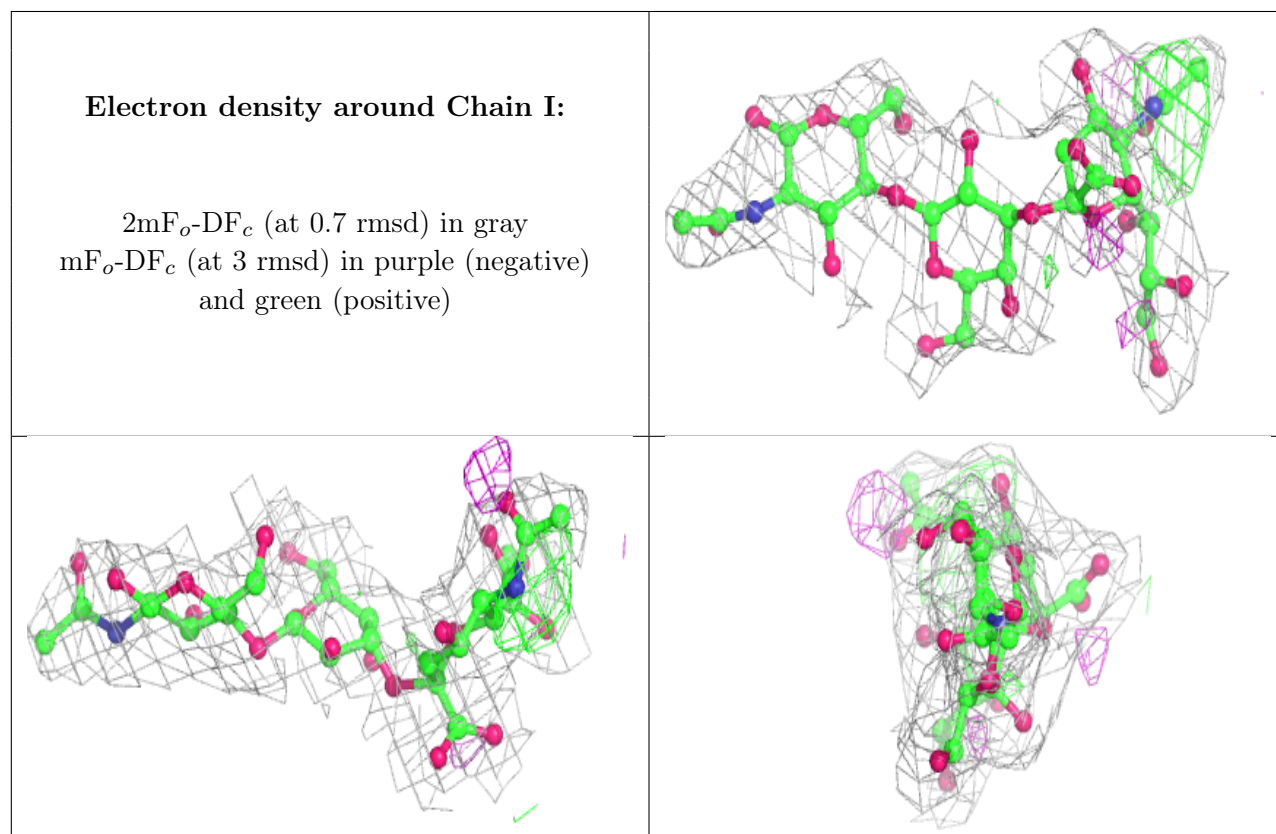
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

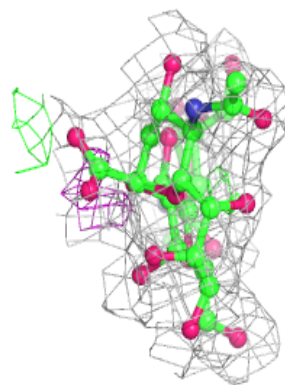
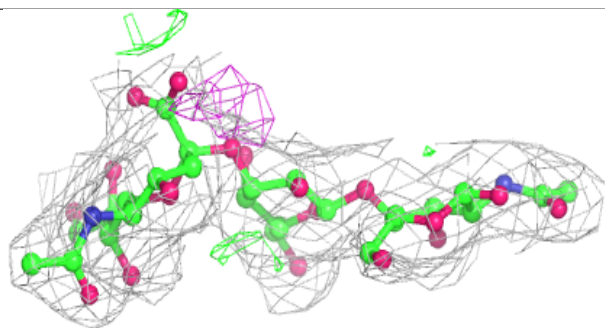
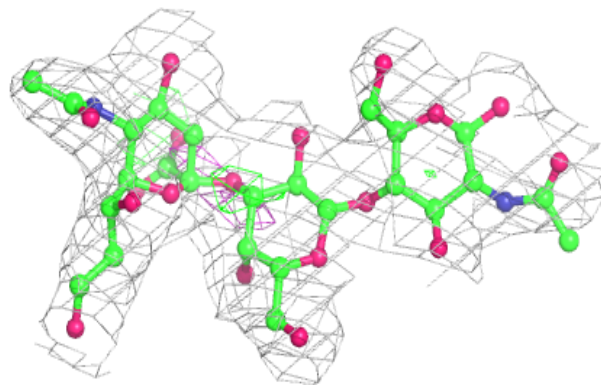
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GAL	K	1	12/12	0.84	0.15	52,60,67,72	0
3	NAG	J	1	15/15	0.85	0.17	57,65,79,83	0
3	NAG	I	1	15/15	0.85	0.16	67,79,91,97	0
3	NAG	L	1	15/15	0.86	0.19	59,73,84,84	0
3	SIA	I	3	20/21	0.89	0.22	19,37,43,44	0
3	GAL	J	2	11/12	0.90	0.14	25,43,49,50	0
3	SIA	L	3	20/21	0.91	0.15	30,42,48,53	0
3	GAL	L	2	11/12	0.91	0.12	44,53,60,65	0
3	GAL	I	2	11/12	0.92	0.15	47,54,61,65	0
3	SIA	J	3	20/21	0.92	0.19	22,26,40,42	0
4	SIA	K	2	20/21	0.92	0.17	22,35,47,50	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.

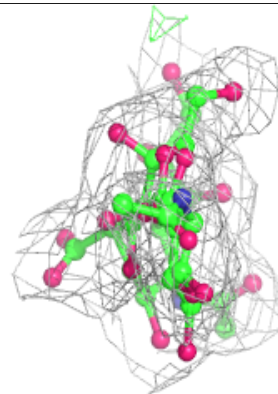
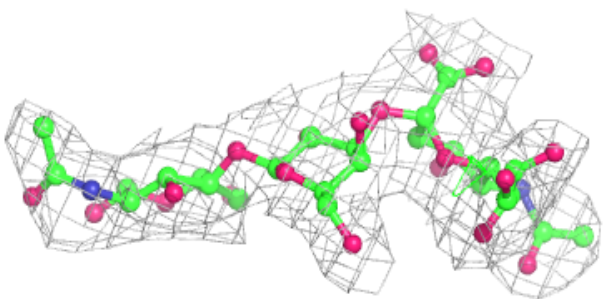
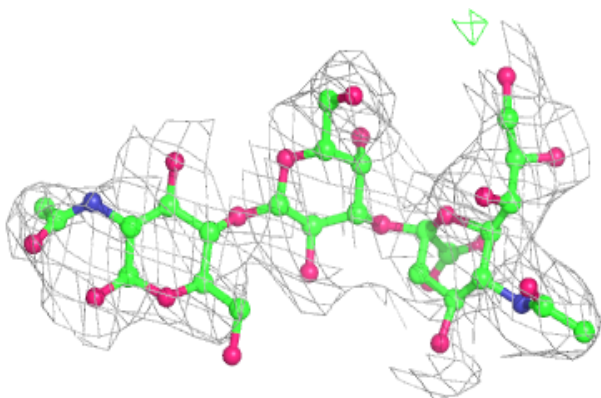


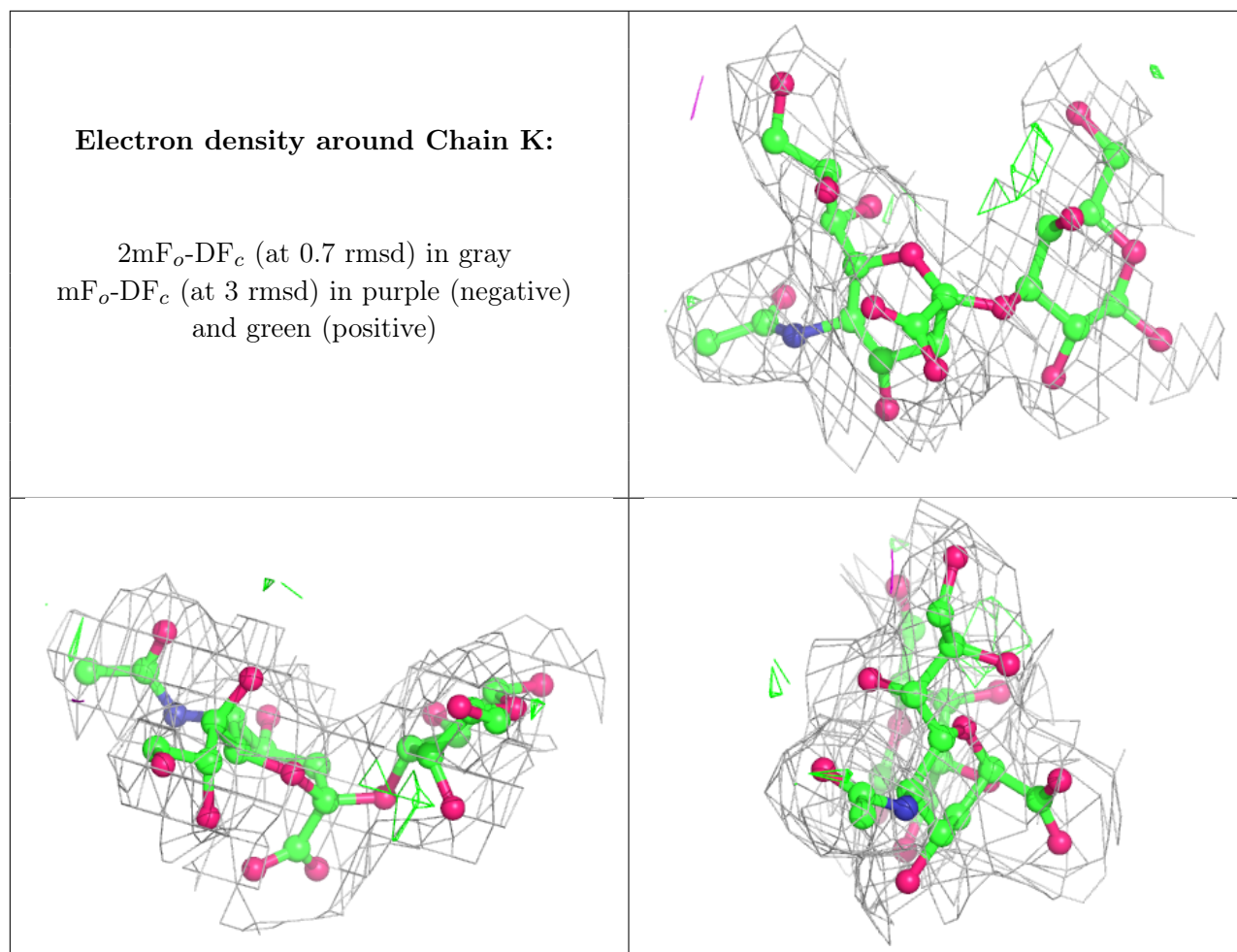
Electron density around Chain J:

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

**Electron density around Chain 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](#)

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	NAG	A	601	14/15	0.88	0.19	31,44,50,51	0
5	NAG	E	601	14/15	0.90	0.15	49,57,69,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.