



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 AM UTC

PDB ID : 4K63 / pdb_00004k63
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

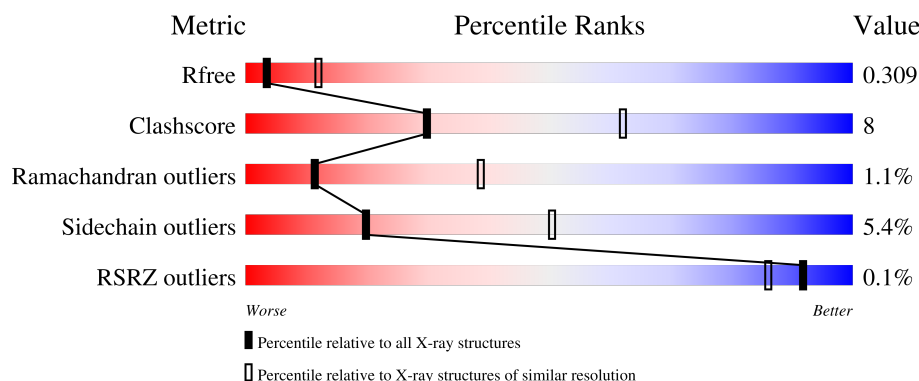
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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	 74% 24% .
1	C	321	 74% 24% .
1	E	321	 75% 24% .
1	G	321	 71% 27% .
2	B	164	 80% 18% .

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Mol	Chain	Length	Quality of chain
2	D	164	 70% 26% .
2	F	164	 76% 21% .
2	H	164	 79% 19% .
3	I	3	 33% 67%
3	J	3	 100%
3	L	3	 100%
4	K	2	 50% 50%

2 Entry composition

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
1	A	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2541	1605	436	485	15			

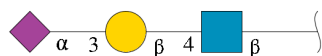
There are 4 discrepancies between the modelled and reference sequences:

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.

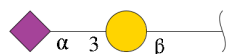
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	D	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	F	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	H	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			

- 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.



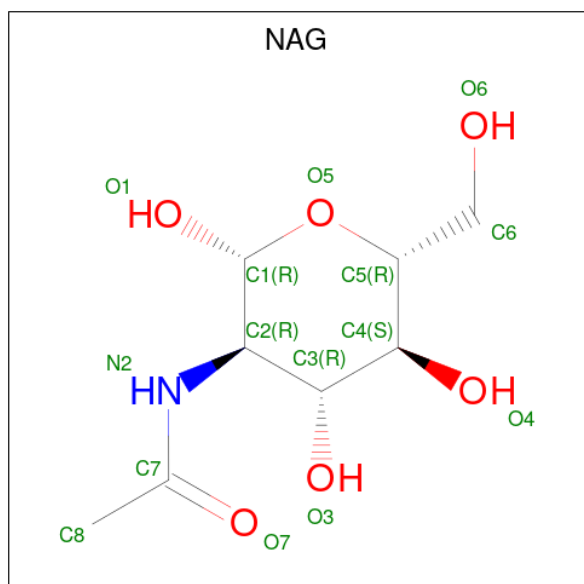
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	J	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	L	3	Total	C	N	O	0	0	0
			46	25	2	19			

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

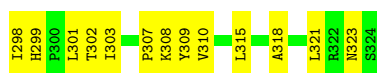


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	2	Total	C	N	O	0	0	0
			32	17	1	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

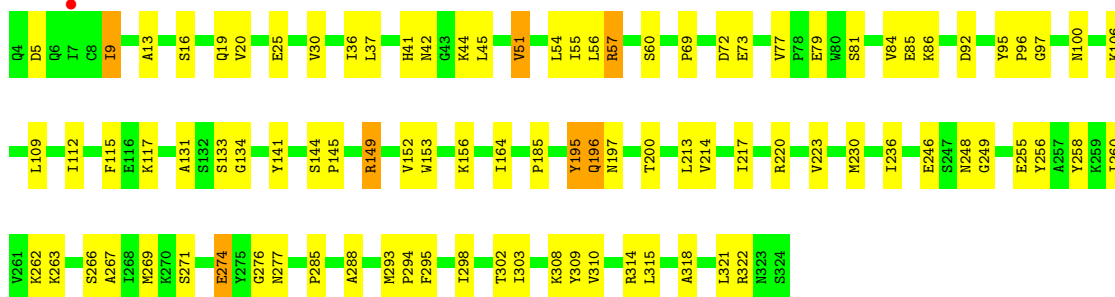


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		



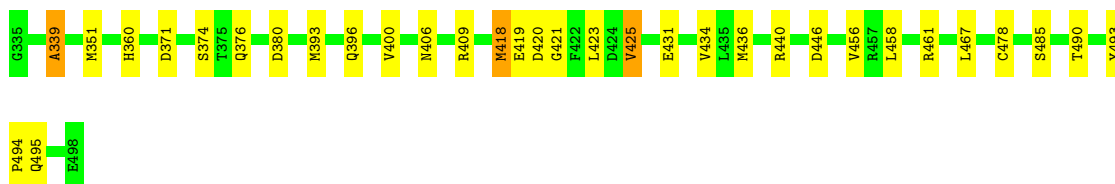
• Molecule 1: Hemagglutinin

Chain G: 71% 27%



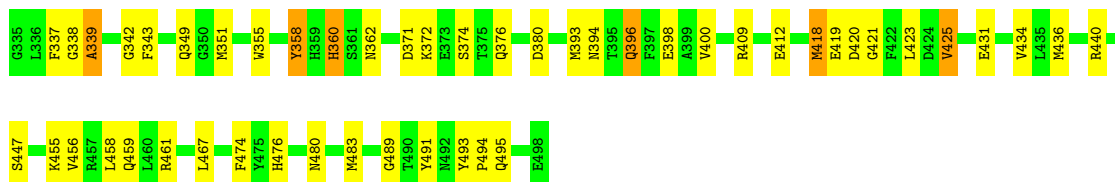
• Molecule 2: Hemagglutinin

Chain B: 80% 18%



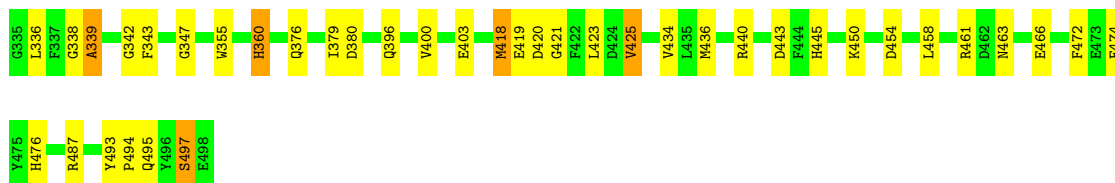
• Molecule 2: Hemagglutinin

Chain D: 70% 26%



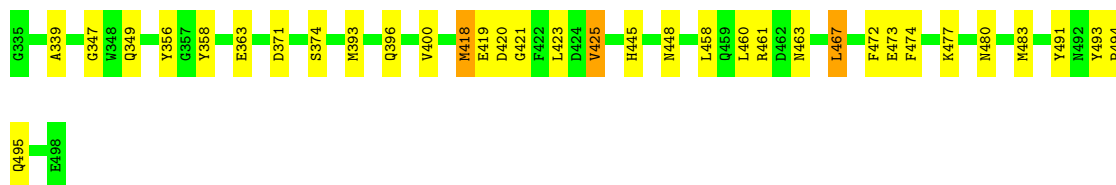
• Molecule 2: Hemagglutinin

Chain F: 76% 21%



• Molecule 2: Hemagglutinin

Chain H:  79% 19% .

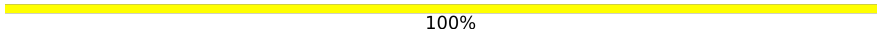


- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



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

Chain J:  100%



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

Chain L:  100%



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

Chain K:  50% 50%



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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	80.8 (49.49-3.10) 81.8 (49.49-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.245 , 0.307 0.248 , 0.309	Depositor DCC
R_{free} test set	2165 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.368 for -h,-k,l 0.099 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
Reported twinning fraction	0.428 for -h,-k,l	Depositor
Outliers	0 of 42807 reflections	Xtriage
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

Xtriage'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: SIA, NAG, GAL

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	0.34	0/2603	0.80	1/3537 (0.0%)
1	C	0.34	0/2603	0.79	2/3537 (0.1%)
1	E	0.33	0/2603	0.77	0/3537
1	G	0.33	0/2603	0.78	0/3537
2	B	0.31	0/1355	0.74	0/1823
2	D	0.32	0/1355	0.77	3/1823 (0.2%)
2	F	0.32	0/1355	0.75	0/1823
2	H	0.31	0/1355	0.73	0/1823
All	All	0.33	0/15832	0.77	6/21440 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	GLY	N-CA-C	-5.47	105.28	112.82
2	D	394	ASN	N-CA-C	-5.44	106.81	113.50
1	C	276	GLY	N-CA-C	-5.38	104.46	113.02
1	C	14	ASN	N-CA-C	5.38	115.23	108.45
2	D	372	LYS	N-CA-C	5.26	116.71	110.97
2	D	396	GLN	CA-C-O	5.15	120.93	117.94

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	52	0
1	C	2541	0	2479	48	0
1	E	2541	0	2478	41	0
1	G	2541	0	2479	54	0
2	B	1328	0	1231	21	0
2	D	1328	0	1231	34	0
2	F	1328	0	1231	24	0
2	H	1328	0	1231	24	0
3	I	46	0	40	1	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	260	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 (260) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:35:ASP:OD2	1:A:39:LYS:NZ	2.36	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: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
1:C:266:SER:OG	1:C:267:ALA:N	2.37	0.56
2:H:371:ASP:OD1	2:H:374:SER:OG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ASN:OD1	1:E:323:ASN:ND2	2.40	0.54
1:G:85:GLU:OE2	1:G:106:LYS:NZ	2.33	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
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:85:GLU:OE2	1:A:270:LYS:NZ	2.40	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: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
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:E:269:MET:HE3	1:E:303:ILE:HG22	1.93	0.49
1:C:51:VAL:HG13	1:C:81:SER:HB3	1.94	0.49
1:C:159:SER:C	1:C:196:GLN:HG3	2.36	0.49
1:E:186:ASN:OD1	1:E:186:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:269:MET:HE3	1:G:303:ILE:HG22	1.94	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:C:312:SER:OG	2:D:431:GLU:OE2	2.27	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
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
1:C:79:GLU:OE2	1:C:262:LYS:NZ	2.37	0.48
1:E:294:PRO:C	1:E:295:PHE:HD1	2.22	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
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:C:271:SER:OG	1:C:285:PRO:O	2.30	0.46
1:A:102:TYR:CZ	1:A:106:LYS:HE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:269:MET:HE3	1:A:303:ILE:HG22	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:60:SER:OG	1:G:92:ASP:OD2	2.31	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
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
2:D:358:TYR:OH	2:D:455:LYS:NZ	2.40	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: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: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: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:E:60:SER:OG	1:E:92:ASP:OD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:H:358:TYR:OH	2:H:371:ASP:OD2	2.26	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
2:D:360:HIS:HD1	2:D:360:HIS:C	2.26	0.42
1:G:57:ARG:NE	1:G:73:GLU:OE2	2.49	0.42
1:C:60:SER:OG	1:C:92:ASP:OD2	2.32	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:5:ASP:OD2	1:A:5:ASP:N	2.50	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: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:C:269:MET:HE3	1:C:303:ILE:HG22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:393:MET:HE2	2:D:393:MET:HB3	1.93	0.41
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
2:B:393:MET:HE2	2:B:393:MET:HB3	1.95	0.41
1:C:116:GLU:HG2	1:C:261:VAL:HG11	2.02	0.41
2:D:371:ASP:OD1	2:D:374:SER:OG	2.26	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:E:239:PRO:O	1:E:240:ASN:HB2	2.20	0.40
1:C:285:PRO:HD3	1:C:301:LEU:O	2.20	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
2:H:393:MET:HE2	2:H:393:MET:HB3	1.99	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:A:312:SER:OG	2:B:431:GLU:OE2	2.39	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

5.3.1 Protein backbone

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%)	21	52
1	C	319/321 (99%)	299 (94%)	18 (6%)	2 (1%)	21	52
1	E	319/321 (99%)	303 (95%)	14 (4%)	2 (1%)	21	52
1	G	319/321 (99%)	301 (94%)	16 (5%)	2 (1%)	21	52
2	B	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	6	27
2	D	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	6	27
2	F	162/164 (99%)	144 (89%)	14 (9%)	4 (2%)	4	21
2	H	162/164 (99%)	144 (89%)	15 (9%)	3 (2%)	6	27
All	All	1924/1940 (99%)	1779 (92%)	124 (6%)	21 (1%)	11	39

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

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Mol	Chain	Res	Type
2	D	339	ALA
2	F	339	ALA
2	H	339	ALA
2	F	497	SER

5.3.2 Protein sidechains ⓘ

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%)	272 (94%)	16 (6%)	19	49
1	C	288/288 (100%)	274 (95%)	14 (5%)	22	53
1	E	288/288 (100%)	271 (94%)	17 (6%)	18	48
1	G	288/288 (100%)	271 (94%)	17 (6%)	18	48
2	B	140/140 (100%)	133 (95%)	7 (5%)	22	53
2	D	140/140 (100%)	131 (94%)	9 (6%)	16	44
2	F	140/140 (100%)	134 (96%)	6 (4%)	26	57
2	H	140/140 (100%)	134 (96%)	6 (4%)	26	57
All	All	1712/1712 (100%)	1620 (95%)	92 (5%)	20	50

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	51	VAL
1	A	56	LEU
1	A	100	ASN
1	A	149	ARG
1	A	195	TYR
1	A	213	LEU
1	A	214	VAL
1	A	220	ARG
1	A	236	ILE
1	A	263	LYS

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Mol	Chain	Res	Type
1	A	274	GLU
1	A	277	ASN
1	A	293	MET
1	A	302	THR
1	A	310	VAL
2	B	360	HIS
2	B	400	VAL
2	B	418	MET
2	B	420	ASP
2	B	425	VAL
2	B	458	LEU
2	B	467	LEU
1	C	51	VAL
1	C	56	LEU
1	C	100	ASN
1	C	133	SER
1	C	149	ARG
1	C	195	TYR
1	C	213	LEU
1	C	214	VAL
1	C	220	ARG
1	C	263	LYS
1	C	277	ASN
1	C	293	MET
1	C	302	THR
1	C	310	VAL
2	D	358	TYR
2	D	360	HIS
2	D	398	GLU
2	D	400	VAL
2	D	418	MET
2	D	420	ASP
2	D	425	VAL
2	D	458	LEU
2	D	467	LEU
1	E	9	ILE
1	E	51	VAL
1	E	56	LEU
1	E	100	ASN
1	E	133	SER
1	E	144	SER
1	E	149	ARG

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Mol	Chain	Res	Type
1	E	195	TYR
1	E	213	LEU
1	E	214	VAL
1	E	220	ARG
1	E	263	LYS
1	E	274	GLU
1	E	277	ASN
1	E	293	MET
1	E	302	THR
1	E	310	VAL
2	F	360	HIS
2	F	400	VAL
2	F	418	MET
2	F	420	ASP
2	F	425	VAL
2	F	458	LEU
1	G	9	ILE
1	G	51	VAL
1	G	56	LEU
1	G	100	ASN
1	G	133	SER
1	G	149	ARG
1	G	195	TYR
1	G	213	LEU
1	G	214	VAL
1	G	220	ARG
1	G	236	ILE
1	G	263	LYS
1	G	274	GLU
1	G	277	ASN
1	G	293	MET
1	G	302	THR
1	G	310	VAL
2	H	400	VAL
2	H	418	MET
2	H	420	ASP
2	H	425	VAL
2	H	458	LEU
2	H	467	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	172	ASN
1	A	197	ASN
1	A	210	ASN
1	A	211	GLN
1	C	277	ASN
2	D	396	GLN
2	D	448	ASN
1	E	113	ASN
1	E	226	GLN
2	F	448	ASN
1	G	226	GLN
2	H	448	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.83	1 (4%)
3	GAL	I	2	3	11,11,12	0.71	0	15,15,17	1.51	3 (20%)
3	SIA	I	3	3	20,20,21	4.05	7 (35%)	21,28,31	4.15	6 (28%)
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	0.63	0	15,15,17	1.45	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	4.03	7 (35%)	21,28,31	4.09	7 (33%)
4	GAL	K	1	4	12,12,12	0.55	0	17,17,17	0.63	0
4	SIA	K	2	4	20,20,21	3.75	5 (25%)	21,28,31	1.89	4 (19%)
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	0.62	0	15,15,17	1.18	2 (13%)
3	SIA	L	3	3	20,20,21	4.06	7 (35%)	21,28,31	4.32	7 (33%)

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	-	5/18/34/38	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	-	6/18/34/38	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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	3	SIA	C7-C6	-12.70	1.37	1.52
3	J	3	SIA	C7-C6	-12.42	1.37	1.52
3	I	3	SIA	C7-C6	-12.39	1.37	1.52
4	K	2	SIA	C7-C6	-11.84	1.38	1.52
4	K	2	SIA	C4-C5	-7.91	1.46	1.53
3	I	3	SIA	C4-C5	-7.47	1.46	1.53
3	J	3	SIA	C4-C5	-7.42	1.46	1.53
3	L	3	SIA	C4-C5	-7.24	1.46	1.53
3	J	3	SIA	C3-C2	-5.72	1.43	1.52
4	K	2	SIA	C3-C2	-5.65	1.43	1.52
3	L	3	SIA	C3-C2	-5.52	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	SIA	C3-C2	-5.47	1.43	1.52
3	I	3	SIA	O6-C6	5.39	1.52	1.44
3	J	3	SIA	C3-C4	-5.11	1.43	1.52
4	K	2	SIA	C3-C4	-5.09	1.43	1.52
3	I	3	SIA	C3-C4	-5.00	1.43	1.52
3	L	3	SIA	O6-C6	4.94	1.51	1.44
3	L	3	SIA	C3-C4	-4.89	1.43	1.52
3	J	3	SIA	O6-C6	4.52	1.51	1.44
3	L	3	SIA	C10-N5	3.63	1.46	1.34
3	J	3	SIA	C10-N5	3.58	1.45	1.34
3	I	3	SIA	C10-N5	3.55	1.45	1.34
4	K	2	SIA	O6-C6	2.74	1.48	1.44
3	J	3	SIA	O8-C8	-2.65	1.37	1.43
3	I	3	SIA	O8-C8	-2.64	1.37	1.43
3	L	3	SIA	O8-C8	-2.57	1.37	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	3	SIA	O6-C2-C3	-15.64	89.52	110.56
3	J	3	SIA	O6-C2-C3	-14.80	90.67	110.56
3	I	3	SIA	O6-C2-C3	-14.07	91.64	110.56
3	I	3	SIA	O6-C2-C1	9.98	126.56	107.72
3	L	3	SIA	O6-C2-C1	9.53	125.70	107.72
3	J	3	SIA	O6-C2-C1	8.94	124.60	107.72
4	K	2	SIA	O6-C2-C3	-6.10	102.36	110.56
3	I	3	SIA	O9-C9-C8	4.24	120.06	111.16
3	J	2	GAL	C1-C2-C3	3.82	115.20	109.64
3	I	2	GAL	C1-C2-C3	3.79	115.16	109.64
3	J	1	NAG	C4-C3-C2	3.61	115.66	110.40
3	L	3	SIA	C8-C7-C6	-3.47	106.54	113.05
4	K	2	SIA	O6-C2-C1	3.38	114.09	107.72
3	J	3	SIA	C8-C7-C6	-3.37	106.72	113.05
3	L	3	SIA	O9-C9-C8	3.35	118.19	111.16
4	K	2	SIA	O1B-C1-C2	3.31	121.32	112.71
3	L	3	SIA	O1B-C1-C2	3.25	121.16	112.71
3	J	1	NAG	C3-C4-C5	3.16	115.96	110.23
3	I	3	SIA	C8-C7-C6	-3.13	107.17	113.05
3	I	3	SIA	C11-C10-N5	3.06	121.19	116.12
3	I	3	SIA	O1B-C1-C2	2.90	120.24	112.71
3	L	2	GAL	C1-C2-C3	2.87	113.83	109.64
3	J	3	SIA	C11-C10-N5	2.81	120.78	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	3	SIA	O9-C9-C8	2.79	117.02	111.16
3	J	2	GAL	O3-C3-C2	-2.67	104.59	110.05
3	I	2	GAL	O3-C3-C2	-2.59	104.78	110.05
4	K	2	SIA	O1B-C1-O1A	-2.56	118.27	124.08
3	L	3	SIA	C11-C10-N5	2.54	120.33	116.12
3	L	3	SIA	O1B-C1-O1A	-2.50	118.40	124.08
3	L	2	GAL	O3-C3-C2	-2.48	104.99	110.05
3	J	3	SIA	O1B-C1-C2	2.47	119.12	112.71
3	J	3	SIA	O1B-C1-O1A	-2.43	118.57	124.08
3	I	2	GAL	C1-O5-C5	-2.32	109.08	112.19
3	L	1	NAG	C1-C2-N2	2.28	113.36	110.73
3	J	1	NAG	O5-C5-C4	2.26	113.77	109.70
3	I	1	NAG	C4-C3-C2	2.19	113.59	110.40
3	J	1	NAG	O5-C1-C2	-2.04	107.47	109.52
3	J	1	NAG	O4-C4-C3	-2.02	105.61	110.38
3	L	1	NAG	C4-C3-C2	2.01	113.33	110.40

There are no chirality outliers.

All (31) 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
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
4	K	2	SIA	C6-C7-C8-O8
3	L	2	GAL	O5-C5-C6-O6
3	J	3	SIA	O7-C7-C8-O8
3	L	3	SIA	O7-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
4	K	1	GAL	O5-C5-C6-O6

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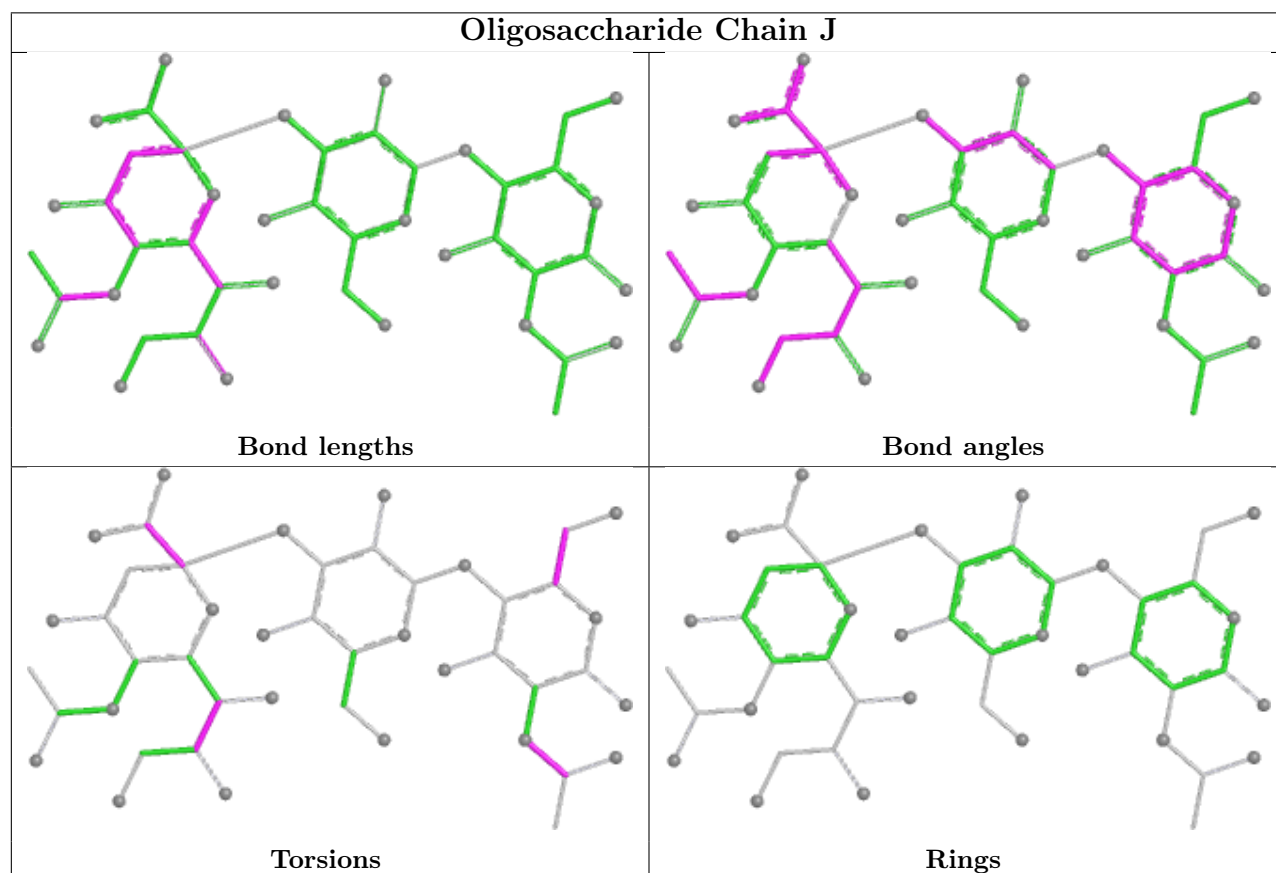
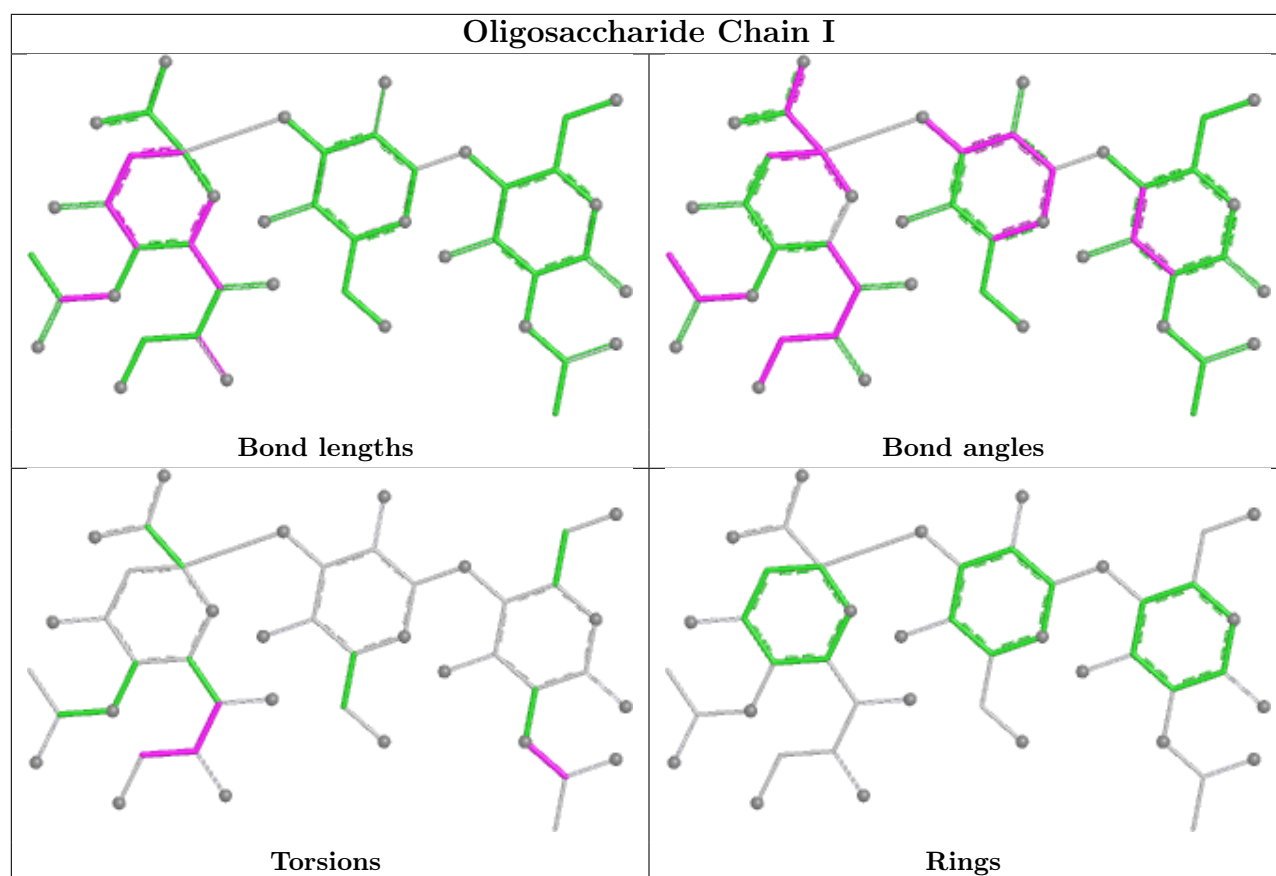
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
3	I	3	SIA	O7-C7-C8-C9
3	I	3	SIA	C6-C7-C8-O8
3	I	3	SIA	O8-C8-C9-O9
4	K	2	SIA	O8-C8-C9-O9
3	I	3	SIA	O7-C7-C8-O8
4	K	2	SIA	C7-C8-C9-O9
3	I	1	NAG	C8-C7-N2-C2
3	J	3	SIA	O1A-C1-C2-O6
3	I	1	NAG	O7-C7-N2-C2

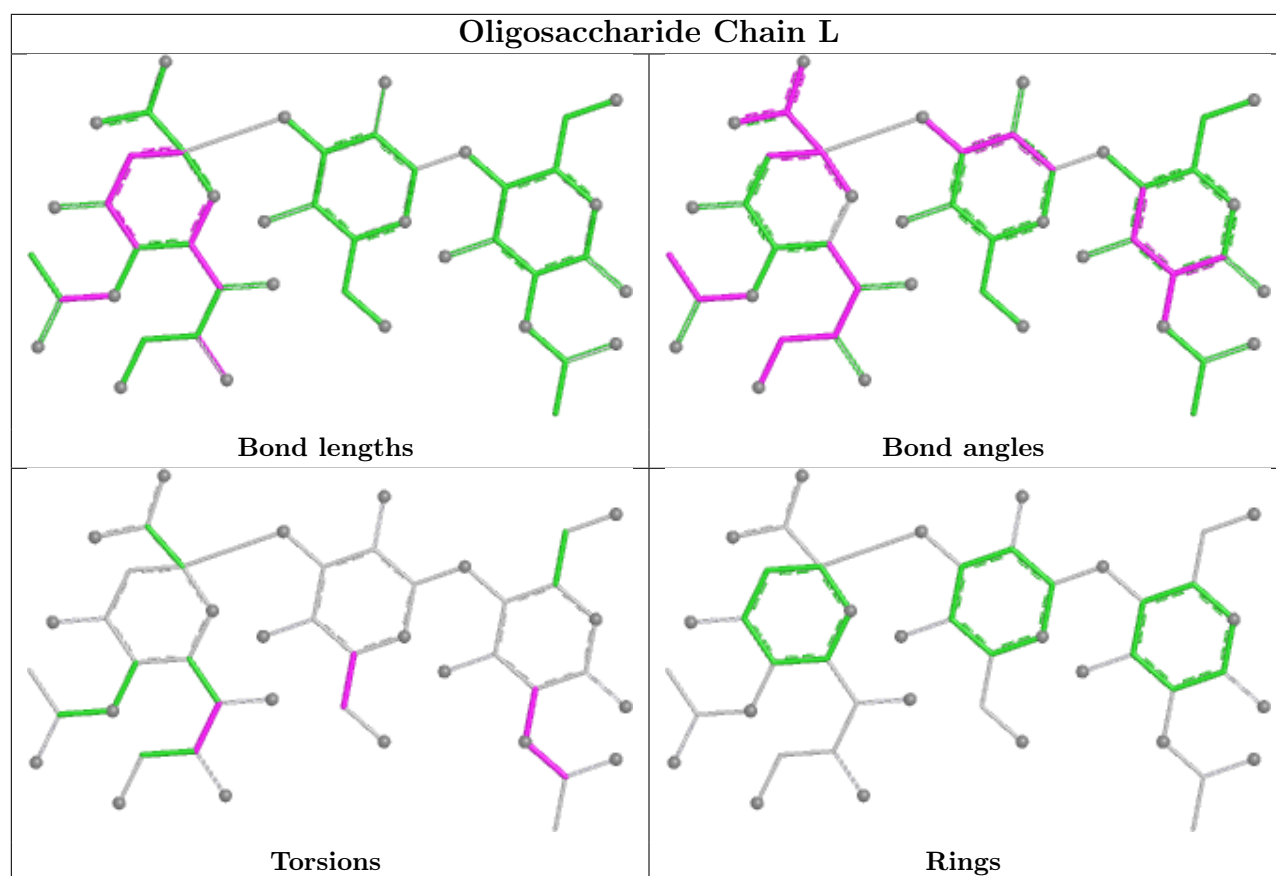
There are no ring outliers.

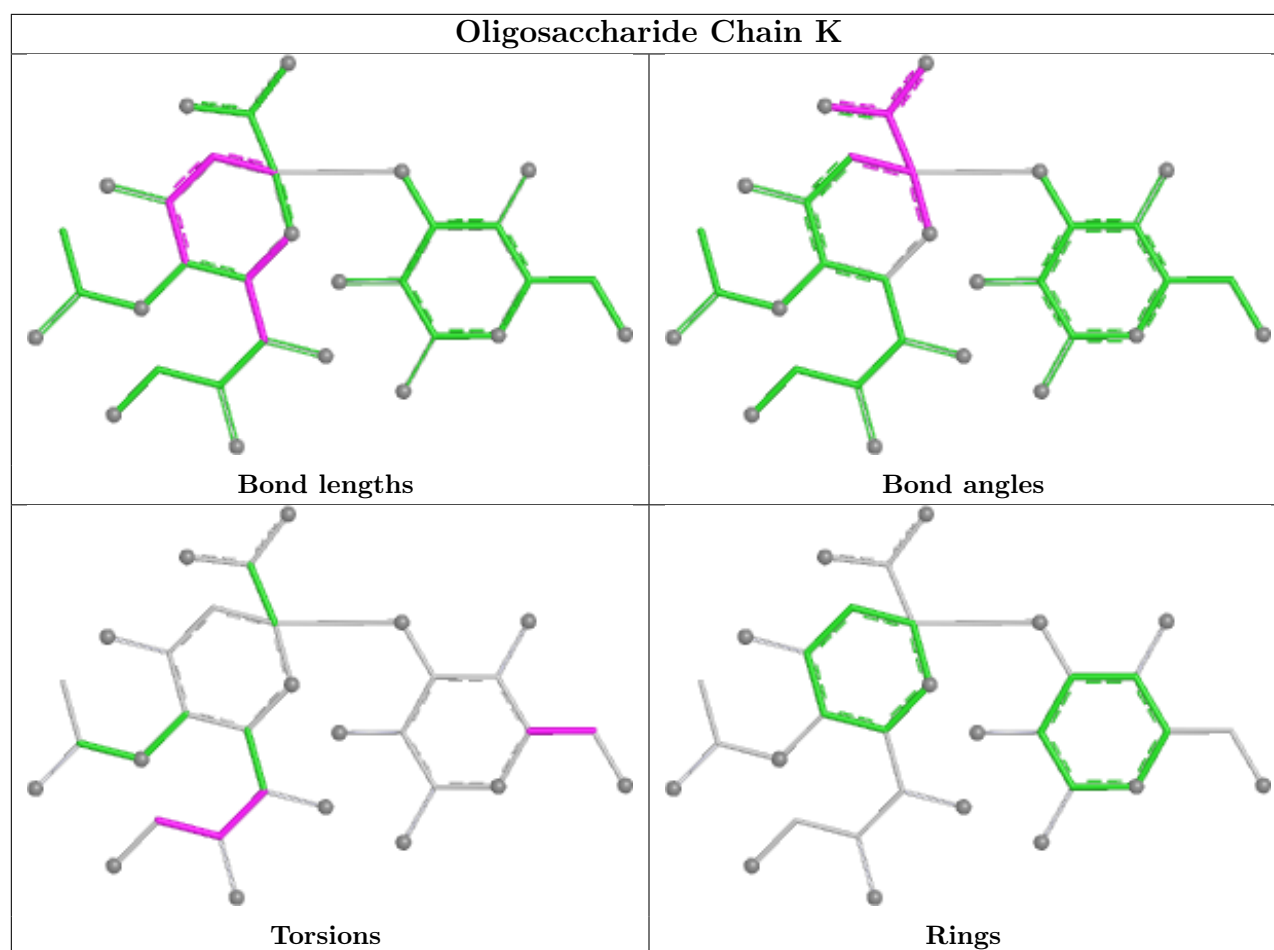
7 monomers are involved in 5 short contacts:

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







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	0.48	0	17,19,21	0.96	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	2.74	115.86	112.19
5	E	601	NAG	C1-O5-C5	2.24	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 [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	321/321 (100%)	-0.98	0 100 100	3, 37, 92, 128	0
1	C	321/321 (100%)	-0.90	0 100 100	8, 41, 106, 167	0
1	E	321/321 (100%)	-0.88	0 100 100	21, 49, 99, 130	0
1	G	321/321 (100%)	-0.73	1 (0%) 90 80	23, 54, 117, 179	0
2	B	164/164 (100%)	-0.47	0 100 100	15, 88, 126, 140	0
2	D	164/164 (100%)	-0.28	0 100 100	18, 104, 151, 179	0
2	F	164/164 (100%)	-0.39	0 100 100	34, 98, 139, 153	0
2	H	164/164 (100%)	-0.16	0 100 100	31, 112, 156, 169	0
All	All	1940/1940 (100%)	-0.69	1 (0%) 92 86	3, 59, 133, 179	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	7	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](#)

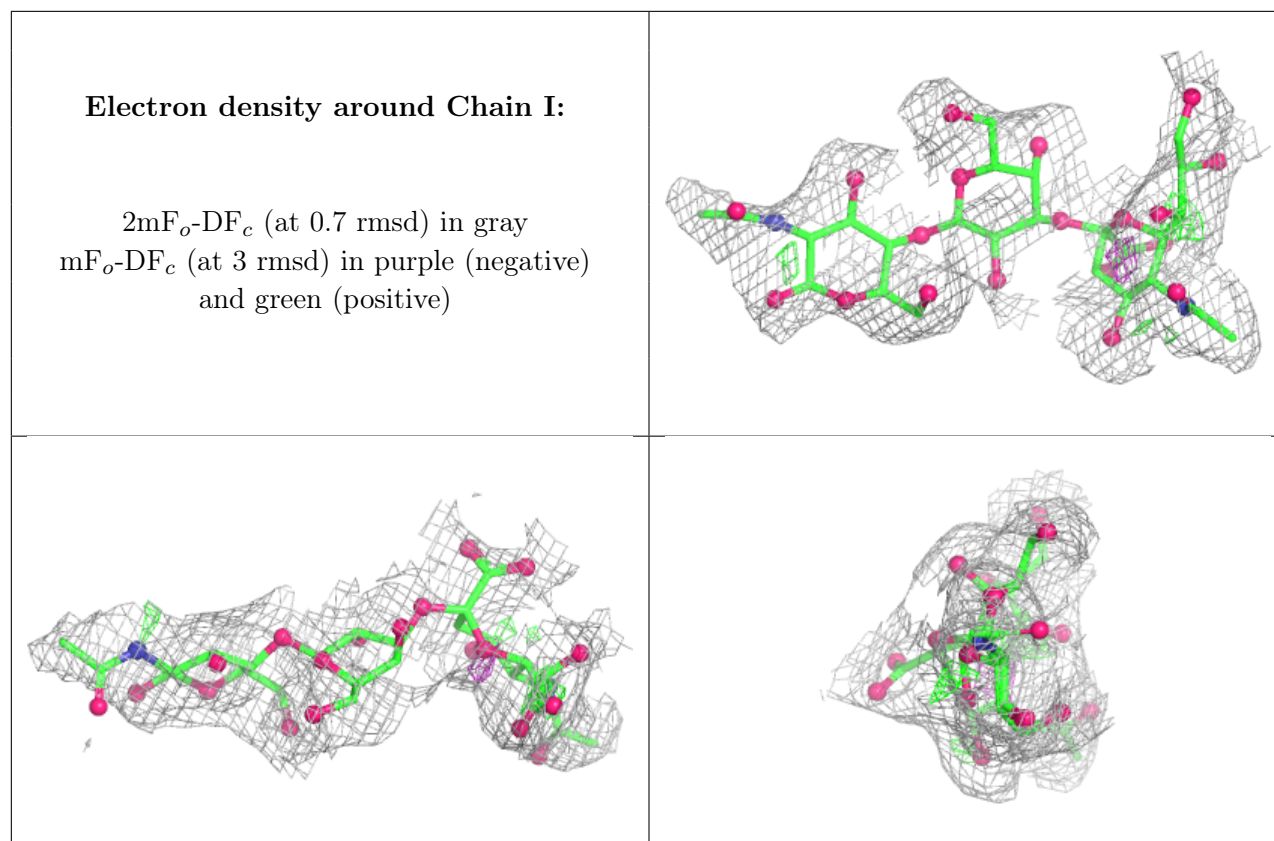
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

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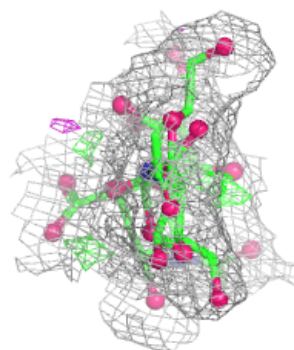
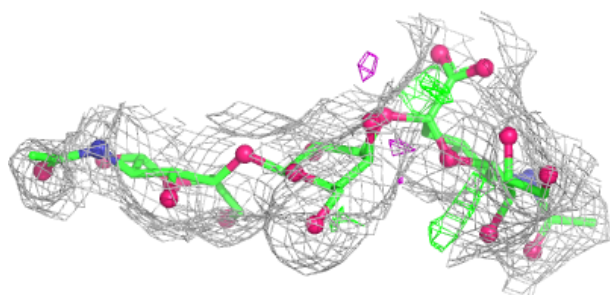
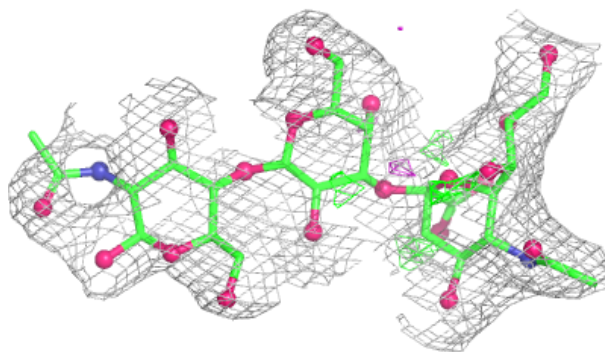
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	J	1	15/15	0.95	0.07	57,65,79,83	0
3	NAG	L	1	15/15	0.95	0.08	59,73,84,84	0
3	NAG	I	1	15/15	0.96	0.05	67,79,91,97	0
3	GAL	J	2	11/12	0.97	0.06	25,43,49,50	0
3	SIA	L	3	20/21	0.97	0.06	30,42,48,53	0
4	GAL	K	1	12/12	0.97	0.05	52,60,67,72	0
4	SIA	K	2	20/21	0.97	0.06	22,35,47,50	0
3	GAL	L	2	11/12	0.98	0.05	44,53,60,65	0
3	SIA	I	3	20/21	0.98	0.06	19,37,43,44	0
3	SIA	J	3	20/21	0.98	0.05	22,26,40,42	0
3	GAL	I	2	11/12	0.98	0.05	47,54,61,65	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.

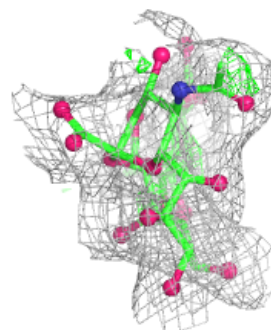
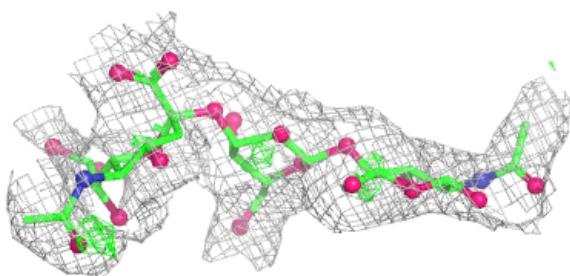
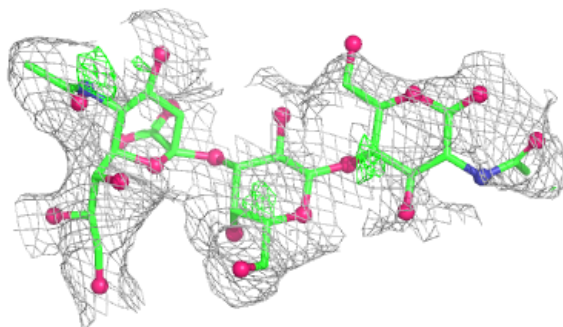


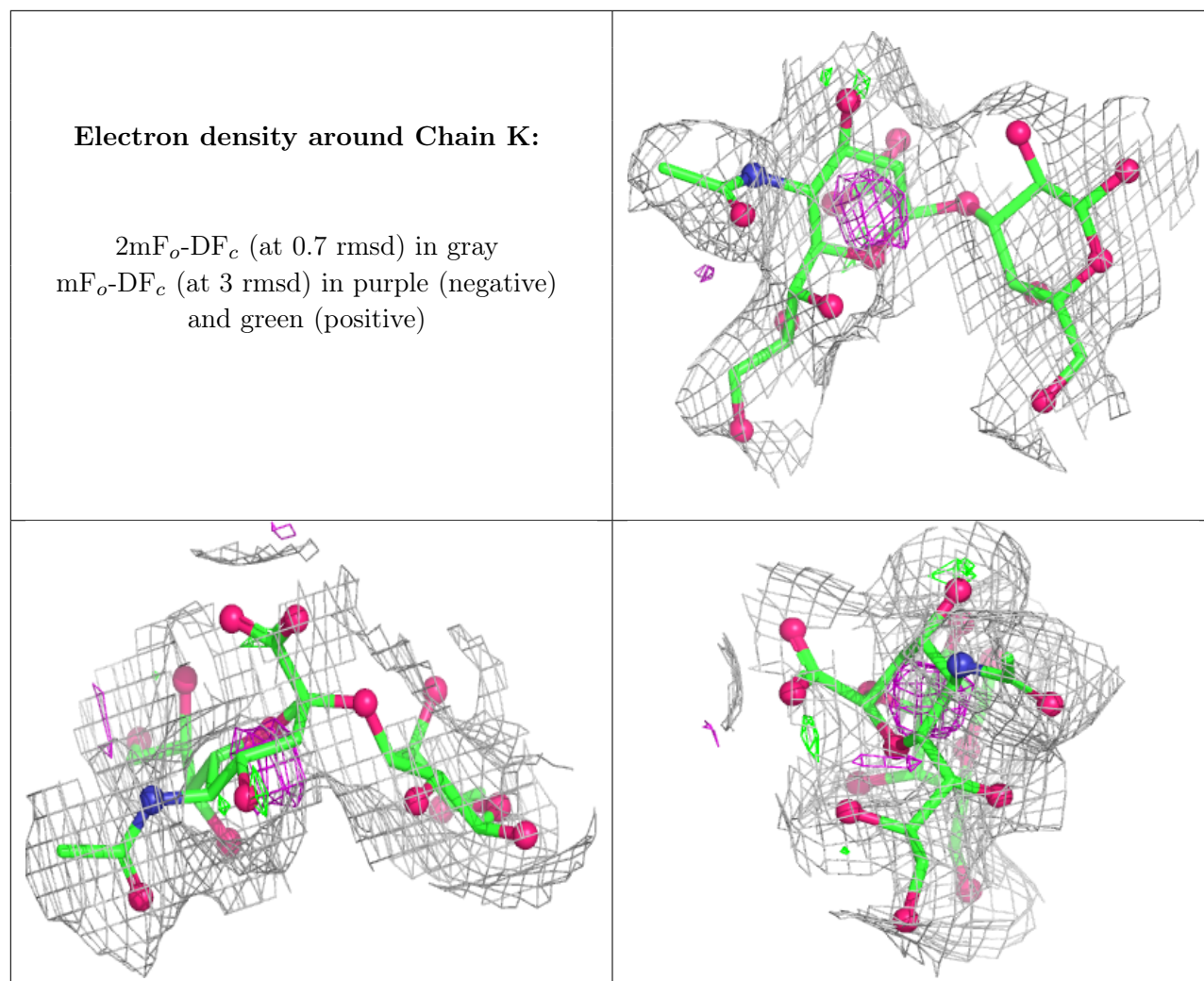
Electron density around Chain J:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
5	NAG	E	601	14/15	0.96	0.07	49,57,69,77	0
5	NAG	A	601	14/15	0.98	0.07	31,44,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.