



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:07 AM UTC

PDB ID : 8X27 / pdb_00008x27
Title : Crystal structure of H5 hemagglutinin from human-infecting H5N8 influenza virus in complex with LSTc
Authors : Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.
Deposited on : 2023-11-09
Resolution : 3.04 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:

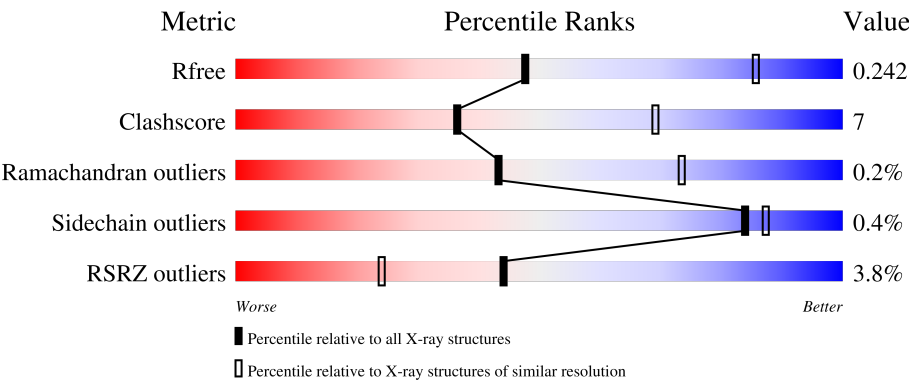
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	506	4% 81% 14% .
1	B	506	4% 78% 18% .
1	C	506	2% 81% 14% ..
1	D	506	2% 81% 15% .
1	E	506	3% 75% 21% .

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Mol	Chain	Length	Quality of chain
1	F	506	7% 75% 20%
2	G	3	67% 33%
2	J	3	33% 67%
3	H	4	50% 25% 25%
3	I	4	50% 25% 25%
4	K	4	50% 50%
5	L	2	100%

2 Entry composition [i](#)

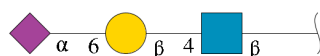
There are 6 unique types of molecules in this entry. The entry contains 23757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	484	Total	C	N	O	S	0	0	0
			3879	2439	675	743	22			
1	C	484	Total	C	N	O	S	0	0	0
			3878	2438	675	743	22			
1	D	485	Total	C	N	O	S	0	0	0
			3885	2443	676	744	22			
1	B	485	Total	C	N	O	S	0	0	0
			3883	2441	676	744	22			
1	E	485	Total	C	N	O	S	0	0	0
			3882	2440	676	744	22			
1	F	486	Total	C	N	O	S	0	0	0
			3891	2447	677	745	22			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	4	Total	C	N	O	0	0	0
			57	31	2	24			
3	I	4	Total	C	N	O	0	0	0
			57	31	2	24			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



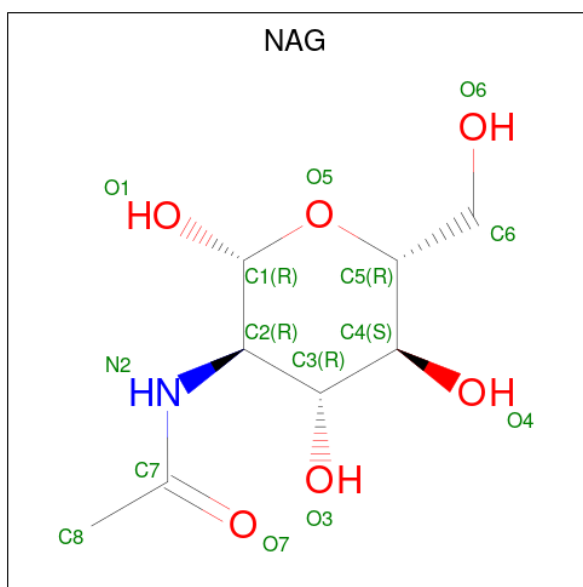
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	4	Total	C	N	O	0	0	0
			57	31	2	24			

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

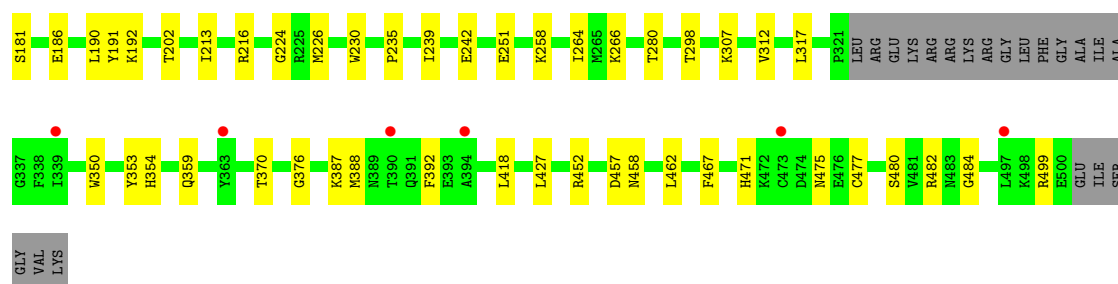


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

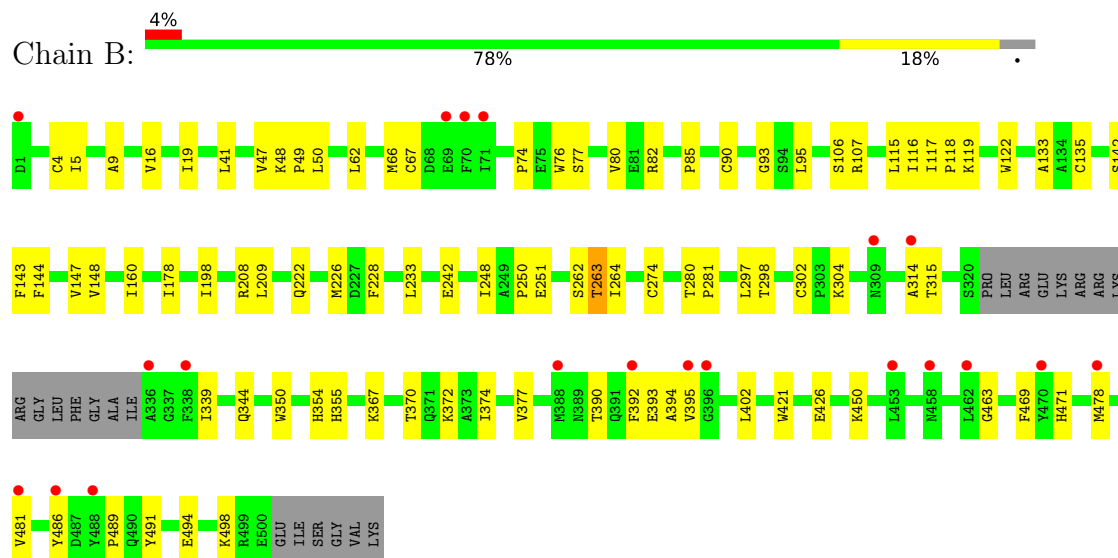
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



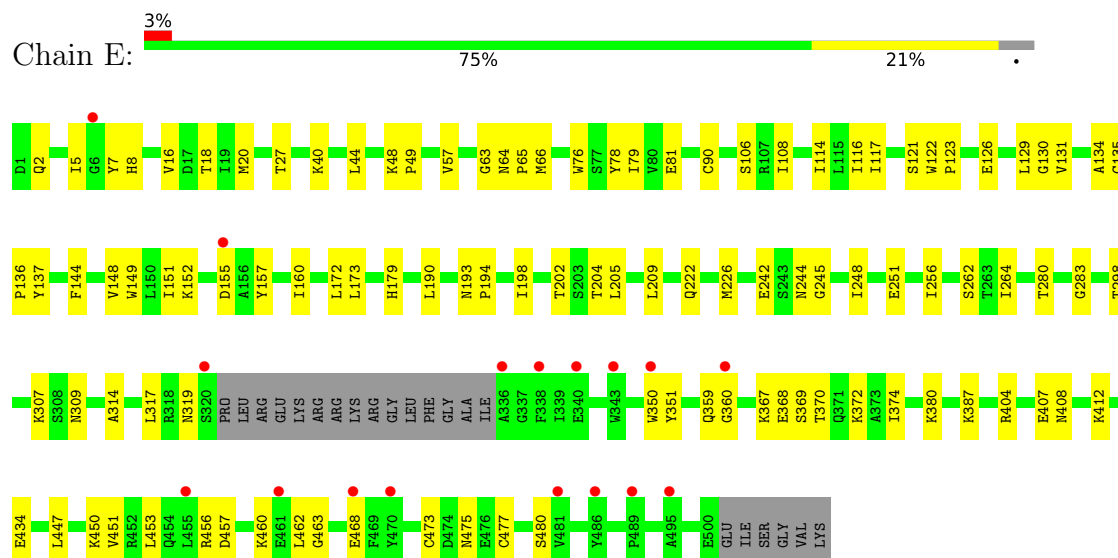
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1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



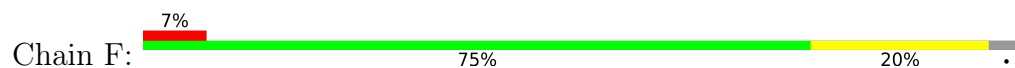
• Molecule 1: Hemagglutinin

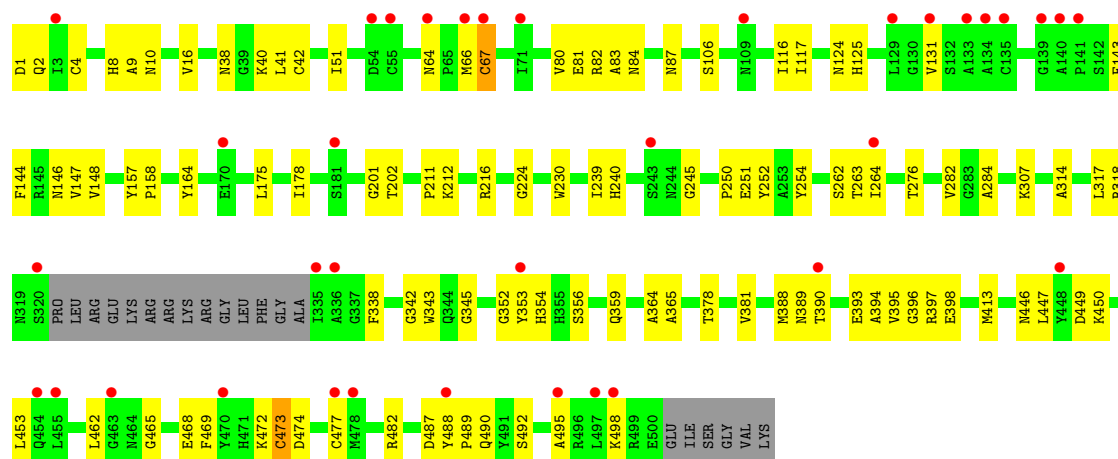


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 67% 33%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 33% 67%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain H: 50% 25% 25%



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain I: 50% 25% 25%



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain K: 50% 50%



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

Chain L:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.83Å 263.93Å 131.20Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	31.72 – 3.04 31.72 – 3.04	Depositor EDS
% Data completeness (in resolution range)	96.0 (31.72-3.04) 90.5 (31.72-3.04)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.242 0.211 , 0.242	Depositor DCC
R_{free} test set	1992 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23757	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA, 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	0.46	0/3968	0.68	0/5374
1	B	0.39	0/3972	0.55	0/5379
1	C	0.52	0/3967	0.74	3/5372 (0.1%)
1	D	0.47	0/3975	0.65	0/5384
1	E	0.43	0/3971	0.65	1/5377 (0.0%)
1	F	0.35	0/3980	0.52	0/5390
All	All	0.44	0/23833	0.64	4/32276 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	222	GLN	OE1-CD-NE2	8.17	130.77	122.60
1	C	88	ASP	N-CA-C	-5.67	100.69	109.14
1	C	62	LEU	CA-C-N	-5.61	110.41	121.41
1	C	62	LEU	C-N-CA	-5.61	110.41	121.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3879	0	3736	45	0
1	B	3883	0	3740	60	0
1	C	3878	0	3732	46	0
1	D	3885	0	3741	51	0
1	E	3882	0	3735	76	0
1	F	3891	0	3749	67	0
2	G	46	0	40	2	0
2	J	46	0	40	4	0
3	H	57	0	49	1	0
3	I	57	0	49	4	0
4	K	57	0	49	2	0
5	L	28	0	25	0	0
6	A	42	0	39	1	0
6	C	42	0	39	0	0
6	D	42	0	39	0	0
6	E	28	0	26	0	0
6	F	14	0	13	0	0
All	All	23757	0	22841	336	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 7.

All (336) 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:487:ASP:HB2	1:C:490:GLN:HG2	1.57	0.86
1:C:173:LEU:HB2	1:C:256:ILE:HD11	1.58	0.85
1:E:179:HIS:HB2	1:E:226:MET:HE2	1.62	0.80
1:F:81:GLU:HB2	1:F:264:ILE:HD11	1.65	0.79
1:F:124:ASN:HB2	1:F:158:PRO:HG3	1.64	0.79
1:C:7:TYR:HB2	1:C:317:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:HIS:CD2	1:A:495:ALA:H	2.01	0.77
1:D:280:THR:HG22	1:D:298:THR:HG22	1.67	0.77
1:B:208:ARG:HD3	1:F:212:LYS:HD2	1.65	0.77
1:B:4:CYS:HB2	1:B:354:HIS:HB3	1.67	0.77
1:E:18:THR:HG22	1:E:20:MET:H	1.51	0.74
1:E:202:THR:HG22	1:E:205:LEU:HB3	1.67	0.74
1:E:408:ASN:HD21	1:F:395:VAL:HG21	1.52	0.74
1:E:157:TYR:CE2	1:E:245:GLY:HA2	2.23	0.73
1:A:280:THR:HG22	1:A:298:THR:HG22	1.71	0.73
1:C:460:LYS:HB3	1:C:468:GLU:HB3	1.71	0.72
1:F:1:ASP:HB2	1:F:469:PHE:HB3	1.70	0.72
1:D:457:ASP:HB2	1:D:499:ARG:HH22	1.56	0.70
1:B:262:SER:HA	1:B:393:GLU:HG2	1.74	0.69
1:F:353:TYR:HB2	1:F:364:ALA:HB3	1.73	0.69
1:A:41:LEU:HG	1:A:269:VAL:HG23	1.75	0.69
1:E:173:LEU:HB2	1:E:256:ILE:HD11	1.74	0.69
1:B:297:LEU:HB3	1:B:395:VAL:HG22	1.75	0.68
1:E:280:THR:HG22	1:E:298:THR:HG22	1.75	0.67
1:B:463:GLY:HA3	1:E:453:LEU:HD11	1.76	0.67
1:E:2:GLN:HG2	1:E:468:GLU:HG2	1.75	0.67
1:D:216:ARG:HH21	1:D:224:GLY:HA2	1.60	0.66
1:B:106:SER:HB2	1:B:262:SER:O	1.94	0.66
1:C:130:GLY:HA2	3:H:4:SIA:H113	1.79	0.65
1:D:350:TRP:HB2	1:D:370:THR:HG23	1.79	0.65
1:B:226:MET:HE3	1:B:248:ILE:HG13	1.77	0.65
1:B:16:VAL:HG21	1:B:314:ALA:HB2	1.78	0.65
1:E:462:LEU:HD11	1:E:468:GLU:HG3	1.77	0.65
1:C:181:SER:HB2	1:C:213:ILE:HG12	1.80	0.64
1:F:338:PHE:HD2	1:F:465:GLY:HA2	1.63	0.64
1:E:477:CYS:HA	1:E:480:SER:HB2	1.80	0.63
1:A:18:THR:HB	1:A:434:GLU:HB2	1.79	0.63
1:D:7:TYR:HB2	1:D:317:LEU:HD13	1.80	0.63
1:C:3:ILE:HG22	1:C:467:PHE:HB2	1.80	0.62
1:F:216:ARG:HH21	1:F:224:GLY:HA2	1.63	0.62
1:A:317:LEU:HD21	1:A:440:HIS:HB3	1.81	0.62
1:E:126:GLU:HB3	1:E:151:ILE:HG22	1.81	0.62
1:E:151:ILE:HD11	1:E:190:LEU:HB3	1.81	0.62
1:C:102:LYS:HB3	1:C:264:ILE:HD11	1.83	0.61
1:E:90:CYS:HG	1:E:135:CYS:HG	1.48	0.61
1:A:308:SER:HB2	1:A:311:LEU:HD11	1.82	0.61
1:B:263:THR:HG22	1:B:393:GLU:HB3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:495:ALA:HB1	1:F:498:LYS:HB2	1.83	0.61
1:D:75:GLU:HG3	1:D:109:ASN:HA	1.82	0.61
1:E:351:TYR:H	1:E:370:THR:HG22	1.65	0.61
1:F:106:SER:HB2	1:F:262:SER:O	2.01	0.61
1:F:488:TYR:CG	1:F:489:PRO:HD3	2.36	0.61
1:E:63:GLY:O	1:E:144:PHE:HD1	1.84	0.60
1:B:178:ILE:HD12	1:B:209:LEU:HB3	1.83	0.60
1:A:16:VAL:HG21	1:A:314:ALA:HB2	1.82	0.60
1:D:181:SER:HB2	1:D:213:ILE:HG12	1.82	0.60
1:F:164:TYR:H	1:F:239:ILE:HG22	1.66	0.60
1:B:222:GLN:NE2	2:J:2:GAL:H61	2.17	0.59
1:D:130:GLY:HA2	3:I:4:SIA:H113	1.84	0.59
1:A:160:ILE:O	1:A:242:GLU:HA	2.02	0.59
1:E:16:VAL:HG21	1:E:314:ALA:HB2	1.85	0.59
1:B:9:ALA:HB3	1:B:344:GLN:HA	1.85	0.59
1:B:280:THR:HG22	1:B:298:THR:HG22	1.85	0.58
1:E:27:THR:HG23	1:E:317:LEU:O	2.04	0.58
1:C:16:VAL:HG21	1:C:314:ALA:HB2	1.86	0.57
1:B:148:VAL:HG23	1:B:251:GLU:HB2	1.87	0.57
1:F:157:TYR:CE2	1:F:245:GLY:HA2	2.40	0.57
1:D:458:ASN:HB3	1:D:471:HIS:CE1	2.40	0.57
1:F:2:GLN:HB2	1:F:356:SER:HB3	1.87	0.57
1:F:201:GLY:O	1:F:240:HIS:HB2	2.04	0.57
1:C:114:ILE:HD11	1:C:172:LEU:HD21	1.86	0.56
1:B:281:PRO:HD3	1:B:297:LEU:O	2.06	0.56
1:E:202:THR:HG23	1:E:204:THR:H	1.71	0.56
1:F:131:VAL:HG22	1:F:143:PHE:HB2	1.88	0.56
1:D:72:ARG:HH22	1:D:113:LYS:H	1.54	0.56
1:A:345:GLY:O	1:A:347:VAL:HG13	2.06	0.56
1:B:355:HIS:HB3	1:B:478:MET:HE3	1.88	0.56
1:B:469:PHE:CE2	1:B:471:HIS:HB3	2.40	0.56
1:D:307:LYS:HB2	1:D:418:LEU:HD11	1.88	0.56
1:E:7:TYR:HB2	1:E:317:LEU:HD13	1.87	0.56
1:E:412:LYS:HE2	1:F:413:MET:HE1	1.88	0.56
1:F:64:ASN:HB3	1:F:67:CYS:HB2	1.88	0.55
1:C:181:SER:OG	1:C:187:GLN:OE1	2.23	0.55
1:D:452:ARG:HG2	1:D:467:PHE:HZ	1.71	0.55
1:F:462:LEU:HG	1:F:468:GLU:HB2	1.89	0.54
1:A:92:PRO:HB2	1:A:225:ARG:HE	1.73	0.54
1:C:102:LYS:HB3	1:C:264:ILE:CD1	2.38	0.54
1:B:62:LEU:HB3	1:B:144:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ARG:HH21	1:F:84:ASN:H	1.55	0.54
1:B:50:LEU:HD12	1:B:76:TRP:CD2	2.43	0.54
1:D:477:CYS:O	1:D:480:SER:HB2	2.08	0.53
1:F:488:TYR:CD2	1:F:489:PRO:HD3	2.43	0.53
1:B:116:ILE:HG22	1:B:117:ILE:HG13	1.89	0.53
1:E:160:ILE:O	1:E:242:GLU:HA	2.09	0.53
1:A:307:LYS:HB2	1:A:418:LEU:HD21	1.91	0.53
1:A:43:ASP:OD1	1:A:48:LYS:HA	2.09	0.52
1:F:263:THR:HG21	1:F:396:GLY:H	1.74	0.52
1:E:367:LYS:HG3	1:E:368:GLU:H	1.74	0.52
1:F:144:PHE:HB2	1:F:147:VAL:HG12	1.91	0.52
1:F:4:CYS:HB2	1:F:354:HIS:HB3	1.91	0.52
1:B:133:ALA:N	2:J:3:SIA:O1A	2.23	0.52
1:E:126:GLU:HG2	1:E:129:LEU:HD13	1.90	0.52
2:G:3:SIA:O1B	2:G:3:SIA:H6	2.09	0.52
1:B:494:GLU:O	1:B:498:LYS:HG2	2.10	0.52
1:F:487:ASP:HB3	1:F:490:GLN:HB3	1.91	0.52
1:D:359:GLN:HB3	1:D:475:ASN:OD1	2.09	0.51
1:C:3:ILE:HB	1:C:469:PHE:HE2	1.74	0.51
1:D:48:LYS:HG2	1:D:49:PRO:HD2	1.92	0.51
4:K:2:NAG:H83	4:K:4:SIA:H5	1.93	0.51
1:B:19:ILE:HG22	1:E:380:LYS:HG2	1.92	0.51
1:A:57:VAL:O	1:A:61:LEU:HB2	2.10	0.51
1:D:452:ARG:HG2	1:D:467:PHE:CZ	2.45	0.51
1:E:64:ASN:HD22	1:E:66:MET:H	1.59	0.51
1:A:310:LYS:C	1:A:311:LEU:HD12	2.36	0.51
1:D:186:GLU:OE2	3:I:4:SIA:O9	2.18	0.50
1:E:48:LYS:HG2	1:E:49:PRO:HD2	1.92	0.50
1:C:93:GLY:HA3	1:C:226:MET:O	2.11	0.50
1:F:178:ILE:HD11	1:F:211:PRO:HG3	1.92	0.50
1:F:317:LEU:HD12	1:F:318:ARG:H	1.76	0.50
1:F:365:ALA:H	1:F:482:ARG:HH21	1.59	0.50
1:E:65:PRO:HB3	1:E:137:TYR:HB2	1.94	0.50
1:A:448:TYR:HE1	1:A:452:ARG:HD2	1.76	0.49
1:C:469:PHE:HB3	1:C:471:HIS:O	2.12	0.49
1:E:193:ASN:ND2	1:E:244:ASN:O	2.45	0.49
1:A:49:PRO:HB3	1:A:78:TYR:CZ	2.47	0.49
1:B:62:LEU:HB3	1:B:144:PHE:HD2	1.78	0.49
1:F:82:ARG:NH2	1:F:83:ALA:HB3	2.27	0.49
1:F:359:GLN:HG2	1:F:474:ASP:HA	1.94	0.49
1:E:57:VAL:HG23	1:E:81:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLU:O	1:D:266:LYS:HA	2.12	0.49
1:B:5:ILE:O	1:B:339:ILE:HG12	2.13	0.49
1:A:33:LEU:HB2	1:A:311:LEU:HD13	1.95	0.49
1:C:106:SER:HB2	1:C:262:SER:O	2.13	0.49
1:B:263:THR:OG1	1:B:264:ILE:N	2.45	0.49
1:C:350:TRP:CZ3	1:C:374:ILE:HG22	2.48	0.49
1:B:390:THR:HG23	1:B:392:PHE:HD2	1.77	0.49
1:A:474:ASP:O	1:A:478:MET:HG2	2.13	0.48
1:C:20:MET:HG2	1:D:376:GLY:O	2.13	0.48
1:A:102:LYS:HD2	1:A:264:ILE:HD12	1.95	0.48
1:A:35:LYS:HE3	1:A:293:ASN:HD21	1.78	0.48
1:E:18:THR:HG23	1:E:434:GLU:HB2	1.95	0.48
1:B:198:ILE:HB	1:B:209:LEU:HB2	1.94	0.48
1:E:8:HIS:HB2	1:E:350:TRP:HA	1.94	0.48
1:F:307:LYS:HA	1:F:307:LYS:HD3	1.66	0.48
1:B:350:TRP:CZ3	1:B:374:ILE:HG12	2.48	0.48
1:B:426:GLU:HB3	1:E:387:LYS:HD2	1.96	0.48
1:C:27:THR:HG22	1:C:319:ASN:OD1	2.14	0.48
1:F:148:VAL:HG23	1:F:251:GLU:HG2	1.96	0.48
1:A:460:LYS:HB2	1:A:470:TYR:CZ	2.49	0.47
1:D:4:CYS:HB2	1:D:354:HIS:HB3	1.96	0.47
1:F:175:LEU:HD23	1:F:230:TRP:HB3	1.96	0.47
1:C:175:LEU:O	1:C:250:PRO:HB3	2.13	0.47
1:E:79:ILE:HB	1:E:264:ILE:HD13	1.95	0.47
1:A:101:LEU:HD22	1:A:230:TRP:CD1	2.49	0.47
1:C:88:ASP:O	1:C:89:LEU:C	2.57	0.47
1:D:55:CYS:HB3	1:D:67:CYS:SG	2.53	0.47
1:C:280:THR:HG22	1:C:298:THR:HG22	1.95	0.47
1:A:427:LEU:O	1:A:431:MET:HG3	2.15	0.47
1:B:48:LYS:HG2	1:B:49:PRO:HD2	1.96	0.47
1:E:198:ILE:HB	1:E:209:LEU:HB2	1.97	0.47
2:J:3:SIA:O1B	2:J:3:SIA:H6	2.14	0.47
1:C:353:TYR:CD2	1:C:482:ARG:HG2	2.50	0.47
1:B:298:THR:H	1:B:394:ALA:HB3	1.80	0.47
1:F:393:GLU:HG3	1:F:394:ALA:N	2.30	0.47
1:E:130:GLY:HA3	1:E:149:TRP:HB3	1.97	0.47
1:C:263:THR:HG21	1:C:396:GLY:HA3	1.96	0.46
1:D:152:LYS:HD3	1:D:155:ASP:HA	1.97	0.46
1:A:172:LEU:HD12	1:A:254:TYR:O	2.15	0.46
1:C:171:ASP:OD1	1:C:235:PRO:HD3	2.14	0.46
1:B:302:CYS:HB2	1:B:392:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:TRP:CZ2	1:E:108:ILE:HG12	2.49	0.46
1:A:2:GLN:HA	1:A:467:PHE:O	2.15	0.46
1:C:426:GLU:HB3	1:D:387:LYS:HG3	1.97	0.46
1:D:121:SER:O	1:D:123:PRO:HD3	2.16	0.46
1:E:456:ARG:HG3	1:E:457:ASP:H	1.79	0.46
1:A:370:THR:O	1:A:374:ILE:HG13	2.16	0.46
1:E:172:LEU:HD12	1:E:172:LEU:HA	1.76	0.46
1:D:101:LEU:HD22	1:D:230:TRP:CD1	2.51	0.46
1:D:202:THR:HG22	1:D:239:ILE:HA	1.98	0.46
1:C:173:LEU:HB2	1:C:256:ILE:CD1	2.38	0.46
1:E:134:ALA:C	1:E:136:PRO:HD3	2.40	0.46
1:E:450:LYS:HD3	1:E:450:LYS:C	2.41	0.46
1:F:41:LEU:HD13	1:F:80:VAL:HG21	1.98	0.46
1:E:106:SER:HB2	1:E:262:SER:HB3	1.98	0.45
1:C:265:MET:HB2	1:C:265:MET:HE3	1.82	0.45
1:B:41:LEU:HD21	1:B:80:VAL:HG11	1.98	0.45
1:F:16:VAL:HG21	1:F:314:ALA:HB2	1.97	0.45
1:F:276:THR:HG21	1:F:284:ALA:HB1	1.98	0.45
1:F:446:ASN:O	1:F:450:LYS:HG3	2.16	0.45
1:E:463:GLY:HA2	1:F:453:LEU:HD13	1.98	0.45
1:A:238:ALA:HB3	6:A:602:NAG:H82	1.99	0.45
1:C:343:TRP:HE3	1:C:346:MET:HG3	1.82	0.45
1:A:157:TYR:CE1	1:A:245:GLY:HA2	2.52	0.45
1:A:166:ASN:ND2	1:A:235:PRO:HA	2.31	0.45
1:D:90:CYS:HB2	1:D:134:ALA:O	2.16	0.45
1:A:2:GLN:O	1:A:356:SER:HB3	2.16	0.45
1:F:116:ILE:HG13	1:F:117:ILE:HG13	1.99	0.45
1:A:19:ILE:HG23	1:A:20:MET:HG3	1.98	0.45
1:B:481:VAL:HA	1:B:486:TYR:CE2	2.52	0.45
1:A:20:MET:HE1	1:C:439:PHE:CE2	2.51	0.45
1:B:107:ARG:HB2	1:B:262:SER:OG	2.17	0.45
1:F:1:ASP:OD2	1:F:472:LYS:HA	2.16	0.45
1:F:202:THR:HG22	1:F:239:ILE:HA	1.99	0.45
1:E:456:ARG:HE	1:E:456:ARG:HB2	1.62	0.44
1:D:191:TYR:O	1:D:192:LYS:C	2.60	0.44
1:B:147:VAL:HG12	1:B:250:PRO:HA	2.00	0.44
1:F:352:GLY:HA2	1:F:365:ALA:HA	1.98	0.44
1:A:448:TYR:CE1	1:A:452:ARG:HD2	2.53	0.44
1:D:91:TYR:HB3	1:D:226:MET:HE2	2.00	0.44
1:F:116:ILE:HG13	1:F:117:ILE:N	2.33	0.44
1:F:263:THR:OG1	1:F:398:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:MET:HE2	1:E:248:ILE:HD11	1.98	0.44
1:F:388:MET:HG3	1:F:390:THR:HG23	1.99	0.44
1:A:166:ASN:HD22	1:A:235:PRO:HA	1.82	0.44
1:C:160:ILE:O	1:C:242:GLU:HA	2.18	0.44
1:D:457:ASP:HB2	1:D:499:ARG:NH2	2.27	0.44
1:E:114:ILE:HD11	1:E:172:LEU:HD11	1.99	0.44
1:B:115:LEU:HD11	1:B:118:PRO:HG3	2.00	0.44
1:A:397:ARG:HH22	1:A:414:GLU:CD	2.23	0.44
1:D:121:SER:C	1:D:123:PRO:HD3	2.43	0.44
1:B:367:LYS:HD3	1:B:367:LYS:HA	1.81	0.44
1:C:418:LEU:HD23	1:D:392:PHE:HE2	1.82	0.44
1:D:49:PRO:HB3	1:D:78:TYR:CE1	2.53	0.44
1:D:66:MET:HE3	1:D:66:MET:HB3	1.92	0.44
1:B:304:LYS:HG2	1:B:421:TRP:CE2	2.53	0.44
1:A:197:TYR:CE1	1:A:244:ASN:HB2	2.53	0.43
1:D:79:ILE:HB	1:D:264:ILE:HD13	1.99	0.43
1:B:481:VAL:HA	1:B:486:TYR:HE2	1.83	0.43
1:E:40:LYS:O	1:E:283:GLY:HA2	2.18	0.43
1:E:121:SER:C	1:E:123:PRO:HD3	2.44	0.43
1:B:471:HIS:HB2	1:B:491:TYR:HB3	2.00	0.43
1:E:307:LYS:HD3	1:F:389:ASN:OD1	2.17	0.43
1:F:343:TRP:C	1:F:345:GLY:H	2.26	0.43
1:B:370:THR:O	1:B:374:ILE:HG13	2.17	0.43
1:F:397:ARG:C	1:F:398:GLU:HG3	2.44	0.43
1:C:404:ARG:NH1	1:C:407:GLU:OE1	2.51	0.43
1:B:143:PHE:CZ	1:B:226:MET:HE1	2.54	0.43
1:E:5:ILE:HD11	1:E:451:VAL:HG21	2.00	0.43
1:D:29:ALA:HB1	1:D:312:VAL:HG12	2.01	0.43
1:D:482:ARG:C	1:D:484:GLY:H	2.26	0.43
1:E:131:VAL:O	4:K:4:SIA:H4	2.19	0.43
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.85	0.43
1:C:400:ASN:OD1	1:C:400:ASN:N	2.41	0.43
1:C:454:GLN:NE2	1:C:484:GLY:HA2	2.34	0.43
1:D:151:ILE:HG21	3:I:4:SIA:H111	2.01	0.43
1:E:152:LYS:HD3	1:E:155:ASP:HA	2.01	0.43
1:C:431:MET:HE2	1:C:431:MET:HB2	1.83	0.43
1:D:353:TYR:CD2	1:D:482:ARG:HG2	2.54	0.43
1:E:116:ILE:HG13	1:E:117:ILE:HG13	2.00	0.43
1:F:251:GLU:HG3	1:F:252:TYR:H	1.84	0.43
1:B:143:PHE:HZ	1:B:226:MET:HE1	1.84	0.42
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:CYS:HB2	1:B:142:SER:O	2.19	0.42
1:E:350:TRP:CZ3	1:E:374:ILE:HG22	2.55	0.42
1:E:456:ARG:HG3	1:E:457:ASP:N	2.34	0.42
1:F:394:ALA:O	1:F:395:VAL:HG23	2.18	0.42
1:A:48:LYS:HG2	1:A:49:PRO:HD2	2.02	0.42
1:D:53:LYS:HE2	1:D:53:LYS:HB2	1.85	0.42
1:B:450:LYS:HA	1:B:450:LYS:HD3	1.87	0.42
1:F:42:CYS:HB2	1:F:276:THR:HG22	2.01	0.42
1:F:125:HIS:CE1	1:F:158:PRO:HG2	2.54	0.42
1:A:130:GLY:HA3	1:A:149:TRP:HB3	2.00	0.42
1:E:148:VAL:HG23	1:E:251:GLU:HB2	2.02	0.42
1:E:359:GLN:NE2	1:E:475:ASN:OD1	2.52	0.42
1:F:38:ASN:ND2	1:F:40:LYS:HB2	2.35	0.42
1:C:413:MET:HE2	1:C:413:MET:HB3	1.96	0.42
1:E:367:LYS:HG3	1:E:368:GLU:N	2.34	0.42
1:B:82:ARG:O	1:B:85:PRO:HD3	2.20	0.42
1:A:151:ILE:HD12	2:G:3:SIA:H111	2.01	0.42
1:C:406:ILE:HG21	1:C:406:ILE:HD13	1.76	0.42
1:B:93:GLY:HA3	1:B:226:MET:O	2.20	0.42
1:B:95:LEU:HD13	1:B:228:PHE:HB2	2.02	0.42
1:E:351:TYR:H	1:E:370:THR:CG2	2.31	0.42
1:F:146:ASN:OD1	1:F:254:TYR:OH	2.36	0.42
1:F:378:THR:HA	1:F:381:VAL:HG12	2.02	0.42
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.85	0.41
1:B:402:LEU:HA	1:B:402:LEU:HD23	1.81	0.41
1:E:49:PRO:HB3	1:E:78:TYR:CE1	2.55	0.41
1:F:64:ASN:HD22	1:F:87:ASN:HB3	1.84	0.41
1:F:449:ASP:O	1:F:453:LEU:HG	2.19	0.41
1:A:171:ASP:OD2	1:A:234:LYS:HD3	2.20	0.41
1:A:281:PRO:HD3	1:A:297:LEU:O	2.20	0.41
1:C:176:TRP:HZ3	1:C:231:THR:HG22	1.85	0.41
1:C:218:GLN:HG3	1:C:223:ARG:HG3	2.02	0.41
1:D:55:CYS:CB	1:D:67:CYS:SG	3.09	0.41
1:F:66:MET:HE2	1:F:66:MET:HB3	1.99	0.41
1:F:473:CYS:HB3	1:F:477:CYS:HB3	1.93	0.41
1:E:90:CYS:SG	1:E:135:CYS:SG	3.06	0.41
1:E:350:TRP:CH2	1:E:374:ILE:HG22	2.55	0.41
1:F:8:HIS:NE2	1:F:10:ASN:HB3	2.34	0.41
1:B:66:MET:HE1	1:B:90:CYS:HB3	2.02	0.41
1:E:44:LEU:HD12	1:E:44:LEU:HA	1.77	0.41
1:E:122:TRP:HZ3	1:E:160:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:PRO:HA	1:F:492:SER:HB3	2.00	0.41
1:A:192:LYS:HA	1:A:192:LYS:HD2	1.81	0.41
1:D:462:LEU:HA	1:D:462:LEU:HD23	1.84	0.41
1:B:119:LYS:HA	1:B:122:TRP:CE3	2.55	0.41
1:B:226:MET:CE	1:B:248:ILE:HG13	2.46	0.41
1:A:196:THR:HA	1:A:244:ASN:HB3	2.02	0.41
1:C:121:SER:C	1:C:123:PRO:HD3	2.45	0.41
1:D:171:ASP:OD1	1:D:235:PRO:HD3	2.21	0.41
1:E:66:MET:HE2	1:E:66:MET:HB3	1.69	0.41
1:E:307:LYS:HE2	1:E:307:LYS:HB3	1.87	0.41
1:F:9:ALA:HB2	1:F:342:GLY:HA3	2.03	0.41
1:A:176:TRP:NE1	1:A:200:VAL:HG21	2.36	0.41
1:C:162:ILE:HG22	1:C:241:PHE:HB2	2.03	0.41
1:D:387:LYS:HD2	1:D:387:LYS:HA	1.79	0.41
1:D:427:LEU:HA	1:D:427:LEU:HD23	1.76	0.41
1:B:160:ILE:O	1:B:242:GLU:HA	2.21	0.41
1:B:222:GLN:HE21	2:J:2:GAL:H61	1.84	0.41
1:B:372:LYS:HA	1:B:372:LYS:HD3	1.59	0.41
1:E:256:ILE:HG21	1:E:256:ILE:HD13	1.89	0.41
1:E:309:ASN:OD1	1:E:309:ASN:N	2.51	0.41
1:E:359:GLN:HG2	1:E:360:GLY:N	2.36	0.41
1:F:488:TYR:O	1:F:492:SER:HB3	2.21	0.41
1:C:92:PRO:O	1:C:225:ARG:HA	2.21	0.41
1:D:152:LYS:HG2	1:D:190:LEU:O	2.21	0.41
1:D:160:ILE:O	1:D:242:GLU:HA	2.21	0.41
1:A:397:ARG:NH2	1:A:414:GLU:OE1	2.44	0.40
1:C:81:GLU:O	1:C:266:LYS:HA	2.21	0.40
1:D:190:LEU:HD11	3:I:4:SIA:H92	2.04	0.40
1:E:453:LEU:HD13	1:E:453:LEU:C	2.46	0.40
1:F:51:ILE:HA	1:F:80:VAL:HB	2.03	0.40
1:F:175:LEU:O	1:F:250:PRO:HB3	2.21	0.40
1:D:388:MET:O	1:D:388:MET:HG3	2.21	0.40
1:E:368:GLU:O	1:E:372:LYS:HG3	2.20	0.40
1:E:404:ARG:NH1	1:E:407:GLU:OE1	2.54	0.40
1:E:460:LYS:HE3	1:E:460:LYS:HB3	1.88	0.40
1:D:104:LEU:HD12	1:D:258:LYS:HZ2	1.85	0.40
1:D:148:VAL:HG23	1:D:251:GLU:HB2	2.02	0.40
1:B:47:VAL:HB	1:B:77:SER:HB3	2.02	0.40
1:E:27:THR:HG22	1:E:319:ASN:HB2	2.03	0.40
1:E:367:LYS:C	1:E:369:SER:H	2.30	0.40
1:E:447:LEU:O	1:E:451:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:THR:O	1:B:377:VAL:HG11	2.21	0.40
1:F:447:LEU:HD12	1:F:450:LYS:HD2	2.04	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	480/506 (95%)	454 (95%)	26 (5%)	0	100	100
1	B	481/506 (95%)	450 (94%)	28 (6%)	3 (1%)	21	53
1	C	480/506 (95%)	465 (97%)	13 (3%)	2 (0%)	30	61
1	D	481/506 (95%)	460 (96%)	20 (4%)	1 (0%)	43	73
1	E	481/506 (95%)	456 (95%)	24 (5%)	1 (0%)	43	73
1	F	482/506 (95%)	453 (94%)	29 (6%)	0	100	100
All	All	2885/3036 (95%)	2738 (95%)	140 (5%)	7 (0%)	43	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	LEU
1	C	262	SER
1	B	263	THR
1	B	489	PRO
1	D	136	PRO
1	E	194	PRO
1	B	74	PRO

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	428/445 (96%)	427 (100%)	1 (0%)	87	90
1	B	428/445 (96%)	426 (100%)	2 (0%)	81	86
1	C	428/445 (96%)	426 (100%)	2 (0%)	81	86
1	D	429/445 (96%)	429 (100%)	0	100	100
1	E	426/445 (96%)	425 (100%)	1 (0%)	87	90
1	F	429/445 (96%)	426 (99%)	3 (1%)	76	84
All	All	2568/2670 (96%)	2559 (100%)	9 (0%)	84	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	CYS
1	C	274	CYS
1	C	473	CYS
1	B	67	CYS
1	B	274	CYS
1	E	473	CYS
1	F	67	CYS
1	F	282	VAL
1	F	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	168	ASN
1	A	240	HIS
1	A	246	ASN
1	A	293	ASN
1	A	401	ASN
1	C	168	ASN
1	C	179	HIS

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Mol	Chain	Res	Type
1	C	240	HIS
1	D	15	GLN
1	D	23	ASN
1	D	28	HIS
1	D	30	GLN
1	D	87	ASN
1	D	110	HIS
1	D	273	HIS
1	D	354	HIS
1	D	401	ASN
1	B	2	GLN
1	B	8	HIS
1	B	15	GLN
1	B	23	ASN
1	B	28	HIS
1	B	30	GLN
1	B	38	ASN
1	B	84	ASN
1	B	168	ASN
1	B	293	ASN
1	B	354	HIS
1	B	443	ASN
1	E	2	GLN
1	E	168	ASN
1	E	240	HIS
1	E	408	ASN
1	E	424	ASN
1	F	45	ASN
1	F	64	ASN
1	F	218	GLN
1	F	293	ASN
1	F	458	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 ⓘ

20 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$
2	NAG	G	1	2	15,15,15	2.05	6 (40%)	21,21,21	2.60	13 (61%)
2	GAL	G	2	2	11,11,12	1.39	2 (18%)	15,15,17	1.35	2 (13%)
2	SIA	G	3	2	20,20,21	1.73	8 (40%)	21,28,31	1.99	7 (33%)
3	GAL	H	1	3	12,12,12	0.14	0	17,17,17	0.19	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	0.42	0
3	GAL	H	3	3	11,11,12	0.75	0	15,15,17	1.09	1 (6%)
3	SIA	H	4	3	20,20,21	1.56	2 (10%)	21,28,31	1.93	5 (23%)
3	GAL	I	1	3	12,12,12	0.14	0	17,17,17	0.19	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	0.42	0
3	GAL	I	3	3	11,11,12	0.74	0	15,15,17	1.09	1 (6%)
3	SIA	I	4	3	20,20,21	1.56	2 (10%)	21,28,31	1.93	5 (23%)
2	NAG	J	1	2	15,15,15	2.30	7 (46%)	21,21,21	2.33	8 (38%)
2	GAL	J	2	2	11,11,12	1.90	3 (27%)	15,15,17	2.02	3 (20%)
2	SIA	J	3	2	20,20,21	2.12	6 (30%)	21,28,31	2.63	8 (38%)
4	GAL	K	1	4	12,12,12	1.95	4 (33%)	17,17,17	1.51	3 (17%)
4	NAG	K	2	4	14,14,15	2.40	5 (35%)	17,19,21	1.95	5 (29%)
4	GAL	K	3	4	11,11,12	2.33	3 (27%)	15,15,17	1.88	6 (40%)
4	SIA	K	4	4	20,20,21	1.54	3 (15%)	21,28,31	2.94	9 (42%)
5	NAG	L	1	5,1	14,14,15	1.96	3 (21%)	17,19,21	1.63	3 (17%)
5	NAG	L	2	5	14,14,15	2.30	5 (35%)	17,19,21	1.48	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	1/18/34/38	0/1/1/1
3	GAL	H	1	3	-	0/2/22/22	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	GAL	H	3	3	-	0/2/19/22	0/1/1/1
3	SIA	H	4	3	-	3/18/34/38	0/1/1/1
3	GAL	I	1	3	-	0/2/22/22	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	GAL	I	3	3	-	0/2/19/22	0/1/1/1
3	SIA	I	4	3	-	3/18/34/38	0/1/1/1
2	NAG	J	1	2	-	0/6/26/26	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	4/18/34/38	0/1/1/1
4	GAL	K	1	4	-	1/2/22/22	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	GAL	K	3	4	-	2/2/19/22	0/1/1/1
4	SIA	K	4	4	-	4/18/34/38	0/1/1/1
5	NAG	L	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	O5-C1	6.31	1.54	1.43
4	K	3	GAL	O5-C1	5.66	1.53	1.43
3	I	4	SIA	C2-C1	5.49	1.58	1.52
3	H	4	SIA	C2-C1	5.46	1.58	1.52
5	L	2	NAG	O5-C1	5.13	1.52	1.43
2	J	3	SIA	C2-C1	5.08	1.58	1.52
2	J	2	GAL	O5-C1	4.71	1.51	1.43
4	K	1	GAL	O5-C1	4.55	1.54	1.42
2	J	1	NAG	O5-C1	4.53	1.53	1.42
4	K	4	SIA	O6-C2	4.47	1.52	1.43
5	L	1	NAG	O5-C1	4.28	1.50	1.43
5	L	2	NAG	C7-N2	4.02	1.47	1.34
2	G	1	NAG	C2-N2	3.82	1.51	1.45
5	L	1	NAG	C7-N2	3.82	1.46	1.34
4	K	3	GAL	C1-C2	3.68	1.61	1.52
2	J	1	NAG	C2-N2	3.64	1.51	1.45
2	J	3	SIA	O6-C2	3.53	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	C7-N2	3.39	1.45	1.34
2	G	3	SIA	C10-N5	3.28	1.44	1.34
4	K	2	NAG	C1-C2	3.26	1.56	1.52
2	G	1	NAG	O5-C5	3.22	1.52	1.44
2	J	1	NAG	C1-C2	3.18	1.56	1.52
4	K	1	GAL	O5-C5	3.16	1.52	1.44
2	J	1	NAG	C7-N2	2.99	1.44	1.34
2	J	3	SIA	C10-N5	2.89	1.43	1.34
2	J	3	SIA	C11-C10	2.88	1.56	1.50
2	G	2	GAL	O5-C1	2.86	1.48	1.43
2	J	1	NAG	O5-C5	2.84	1.51	1.44
5	L	2	NAG	C2-N2	2.84	1.51	1.46
4	K	2	NAG	C7-N2	2.80	1.43	1.34
4	K	3	GAL	O5-C5	2.76	1.48	1.43
2	G	3	SIA	C4-C5	-2.73	1.50	1.53
5	L	2	NAG	O5-C5	2.70	1.48	1.43
2	J	2	GAL	O5-C5	2.70	1.48	1.43
4	K	2	NAG	C2-N2	2.69	1.50	1.46
2	G	3	SIA	O6-C2	2.68	1.48	1.43
2	G	3	SIA	C2-C1	2.66	1.55	1.52
2	G	1	NAG	O5-C1	2.65	1.49	1.42
2	G	2	GAL	O5-C5	2.63	1.48	1.43
2	G	3	SIA	O1A-C1	2.61	1.29	1.22
2	G	1	NAG	C1-C2	2.57	1.56	1.52
4	K	2	NAG	O5-C5	2.52	1.48	1.43
2	J	3	SIA	O1A-C1	2.47	1.29	1.22
2	J	1	NAG	C4-C5	2.46	1.58	1.53
4	K	4	SIA	C3-C4	-2.45	1.48	1.52
2	J	3	SIA	O4-C4	2.41	1.48	1.43
4	K	4	SIA	C10-N5	2.26	1.41	1.34
4	K	1	GAL	C4-C5	2.21	1.57	1.53
2	G	3	SIA	C11-C10	2.18	1.55	1.50
2	G	1	NAG	C8-C7	2.13	1.55	1.50
2	G	3	SIA	C3-C4	-2.11	1.48	1.52
5	L	2	NAG	C8-C7	2.11	1.54	1.50
4	K	1	GAL	C1-C2	2.10	1.57	1.52
2	J	2	GAL	C1-C2	2.10	1.57	1.52
2	G	3	SIA	O10-C10	2.06	1.27	1.23
2	J	1	NAG	C8-C7	2.04	1.54	1.50
3	H	4	SIA	O6-C2	2.03	1.47	1.43
3	I	4	SIA	O6-C2	2.02	1.47	1.43
5	L	1	NAG	C2-N2	2.01	1.49	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	SIA	C6-C5-N5	-6.50	100.53	110.91
4	K	4	SIA	O9-C9-C8	-6.32	97.89	111.16
4	K	4	SIA	O6-C2-C1	6.24	119.49	107.72
2	J	2	GAL	C1-O5-C5	-6.13	103.97	112.19
2	G	1	NAG	C8-C7-N2	5.48	125.21	116.12
4	K	4	SIA	C8-C7-C6	-5.35	103.00	113.05
3	H	4	SIA	O1A-C1-C2	-5.33	111.32	122.85
3	I	4	SIA	O1A-C1-C2	-5.33	111.34	122.85
2	G	3	SIA	C8-C7-C6	-4.94	103.78	113.05
2	J	3	SIA	C5-N5-C10	-4.84	111.78	123.11
2	J	1	NAG	O5-C1-C2	4.72	114.26	109.52
4	K	2	NAG	C8-C7-N2	4.58	123.71	116.12
2	J	1	NAG	C8-C7-N2	4.34	123.31	116.12
2	G	1	NAG	O5-C5-C4	4.22	117.30	109.70
4	K	4	SIA	O6-C2-C3	4.14	116.12	110.56
2	J	3	SIA	O6-C2-C3	4.03	115.97	110.56
4	K	4	SIA	O8-C8-C9	-3.98	99.98	109.03
2	G	3	SIA	C6-C5-N5	-3.85	104.77	110.91
3	I	4	SIA	C6-C5-N5	-3.78	104.87	110.91
3	H	4	SIA	C6-C5-N5	-3.75	104.92	110.91
2	J	3	SIA	O7-C7-C8	3.75	117.45	108.93
5	L	2	NAG	C8-C7-N2	3.75	122.33	116.12
2	J	3	SIA	C8-C7-C6	-3.59	106.31	113.05
2	G	1	NAG	O5-C1-C2	3.55	113.09	109.52
2	J	1	NAG	C1-O5-C5	-3.51	106.86	113.65
2	G	1	NAG	C1-C2-C3	3.42	115.21	110.54
5	L	1	NAG	C8-C7-N2	3.34	121.66	116.12
2	G	3	SIA	C11-C10-N5	-3.33	110.59	116.12
4	K	2	NAG	C1-C2-N2	-3.30	105.24	110.43
4	K	3	GAL	C2-C3-C4	-3.25	105.14	110.86
2	J	1	NAG	C1-C2-N2	-3.25	106.96	110.73
2	J	1	NAG	O3-C3-C2	3.25	116.05	109.58
2	G	2	GAL	C1-O5-C5	-3.23	107.86	112.19
2	G	2	GAL	O6-C6-C5	-3.22	100.35	111.33
4	K	3	GAL	C1-C2-C3	3.19	114.29	109.64
2	G	1	NAG	O7-C7-C8	-3.18	116.40	122.05
2	J	1	NAG	O5-C5-C4	3.16	115.39	109.70
2	J	2	GAL	O6-C6-C5	-3.12	100.70	111.33
2	J	3	SIA	O1B-C1-C2	3.05	120.64	112.71
2	J	1	NAG	O1-C1-C2	-3.01	102.97	109.22
2	G	1	NAG	O3-C3-C4	2.97	117.37	110.38
4	K	1	GAL	O5-C1-C2	2.96	115.50	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	GAL	O5-C5-C4	2.94	115.00	109.70
2	G	1	NAG	C4-C3-C2	2.89	114.61	110.40
2	J	1	NAG	O7-C7-C8	-2.88	116.92	122.05
4	K	4	SIA	O8-C8-C7	2.79	115.78	109.25
2	J	3	SIA	O1A-C1-C2	-2.69	117.05	122.85
4	K	2	NAG	C3-C4-C5	2.66	115.05	110.23
2	G	3	SIA	O9-C9-C8	-2.60	105.69	111.16
2	G	1	NAG	O5-C5-C6	2.60	112.88	106.44
4	K	3	GAL	O4-C4-C3	-2.50	104.48	110.38
3	I	4	SIA	O1B-C1-O1A	2.50	129.75	124.08
3	H	4	SIA	O1B-C1-O1A	2.48	129.71	124.08
4	K	4	SIA	C5-N5-C10	-2.46	117.36	123.11
4	K	1	GAL	O5-C5-C6	2.44	112.48	106.44
3	H	4	SIA	O1B-C1-C2	2.41	118.97	112.71
3	I	4	SIA	O1B-C1-C2	2.39	118.92	112.71
3	H	3	GAL	C1-O5-C5	2.38	115.38	112.19
3	I	3	GAL	C1-O5-C5	2.38	115.38	112.19
4	K	2	NAG	O7-C7-N2	-2.37	117.79	121.98
5	L	1	NAG	C1-C2-N2	-2.35	106.73	110.43
2	G	1	NAG	O4-C4-C3	2.35	115.92	110.38
4	K	2	NAG	O3-C3-C2	2.34	114.27	109.40
2	G	1	NAG	O3-C3-C2	-2.31	104.98	109.58
4	K	3	GAL	O5-C5-C6	-2.30	103.19	107.66
4	K	4	SIA	O1B-C1-C2	2.28	118.63	112.71
5	L	1	NAG	C1-O5-C5	2.28	115.24	112.19
2	G	3	SIA	O10-C10-N5	2.27	125.99	121.98
5	L	2	NAG	O4-C4-C5	2.26	114.89	109.32
4	K	3	GAL	O6-C6-C5	-2.19	103.89	111.33
2	J	2	GAL	C1-C2-C3	2.10	112.71	109.64
2	G	1	NAG	C6-C5-C4	-2.10	107.86	113.02
2	G	1	NAG	C1-C2-N2	2.10	113.16	110.73
4	K	4	SIA	O7-C7-C8	2.08	113.66	108.93
5	L	2	NAG	O7-C7-N2	-2.07	118.33	121.98
4	K	3	GAL	O5-C1-C2	2.07	115.72	110.79
2	G	3	SIA	C5-N5-C10	-2.06	118.29	123.11
2	G	3	SIA	O6-C2-C3	2.06	113.32	110.56
3	H	4	SIA	O6-C2-C3	-2.04	107.82	110.56
2	G	1	NAG	O7-C7-N2	-2.03	118.39	121.98
3	I	4	SIA	O6-C2-C3	-2.02	107.84	110.56
2	J	3	SIA	C9-C8-C7	2.02	116.28	112.17

There are no chirality outliers.

All (28) torsion outliers are listed below:

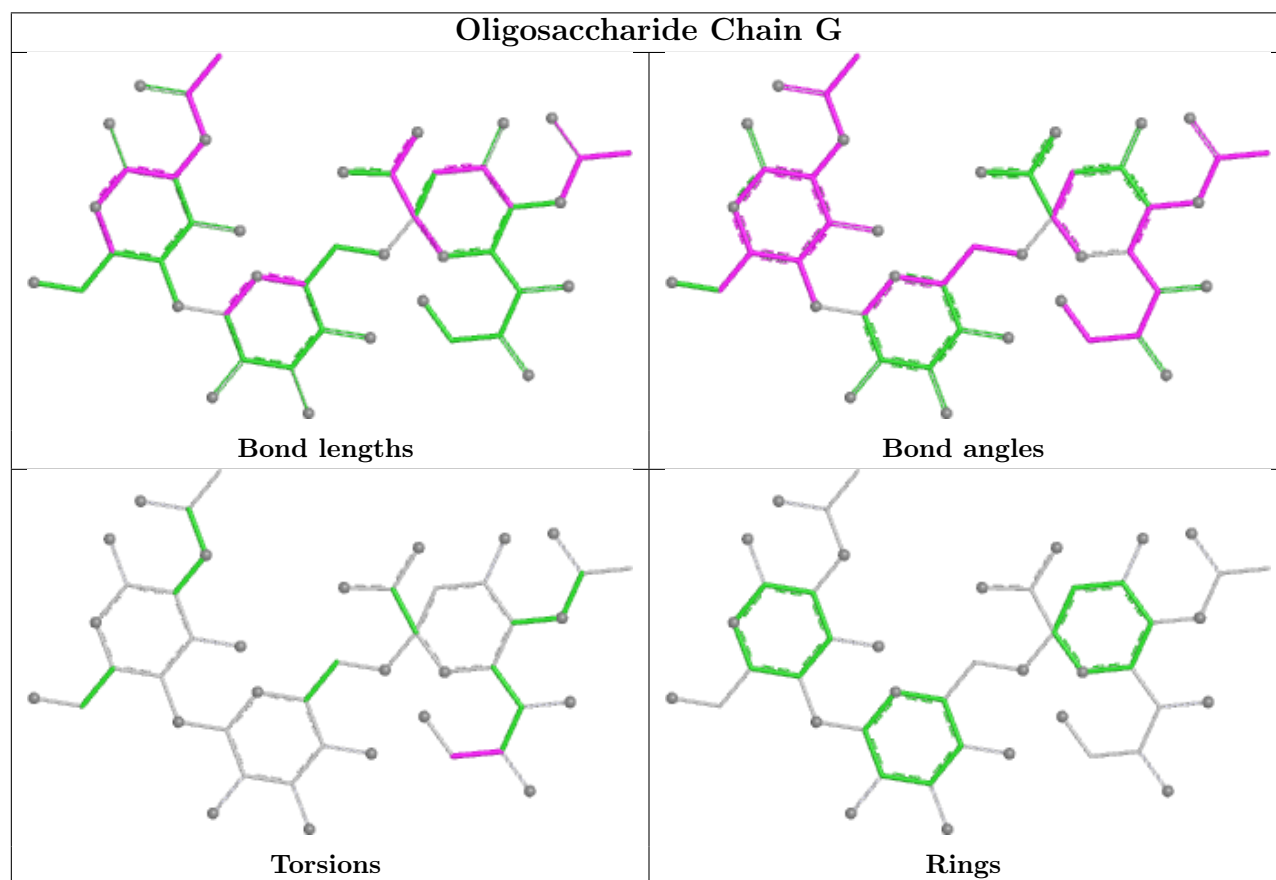
Mol	Chain	Res	Type	Atoms
4	K	4	SIA	C6-C7-C8-C9
4	K	4	SIA	O7-C7-C8-C9
4	K	4	SIA	O7-C7-C8-O8
4	K	3	GAL	O5-C5-C6-O6
4	K	4	SIA	C6-C7-C8-O8
4	K	3	GAL	C4-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
2	J	3	SIA	O8-C8-C9-O9
3	H	4	SIA	C6-C7-C8-O8
3	I	4	SIA	C6-C7-C8-O8
5	L	2	NAG	C4-C5-C6-O6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

There are no ring outliers.

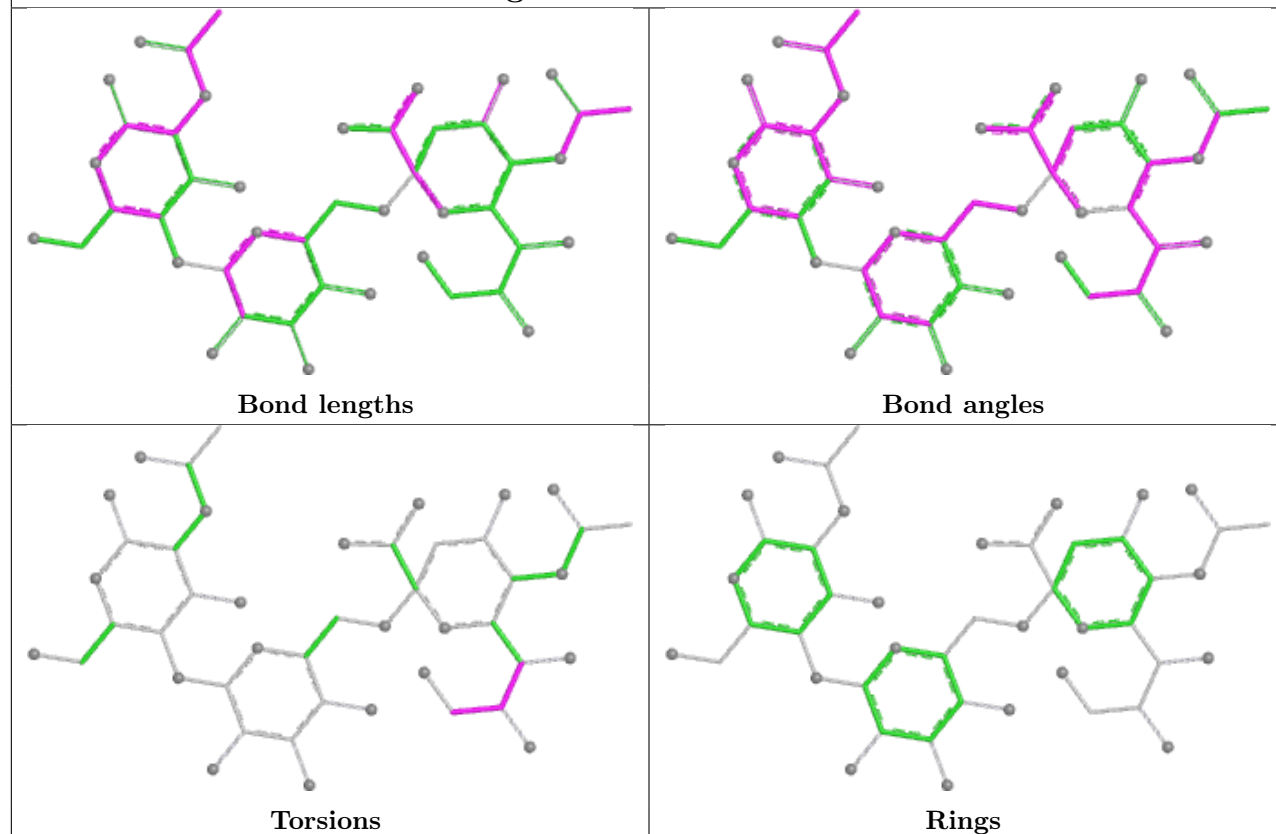
7 monomers are involved in 13 short contacts:

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

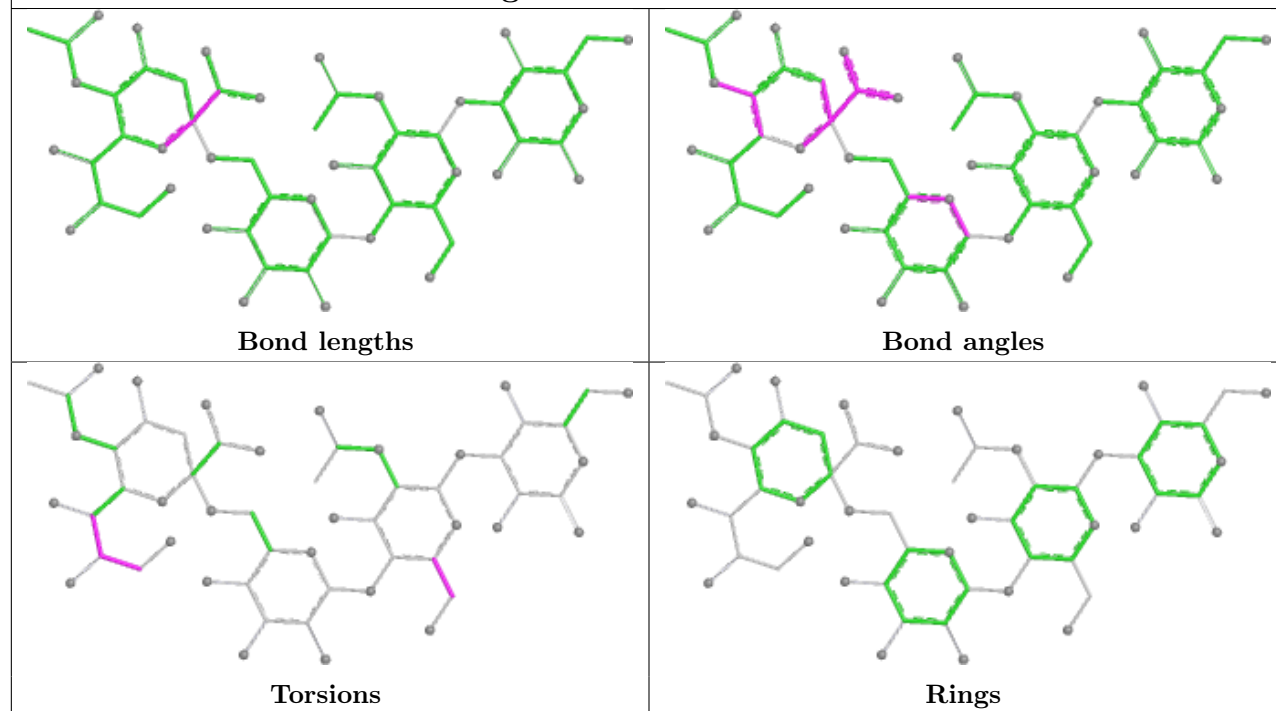
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

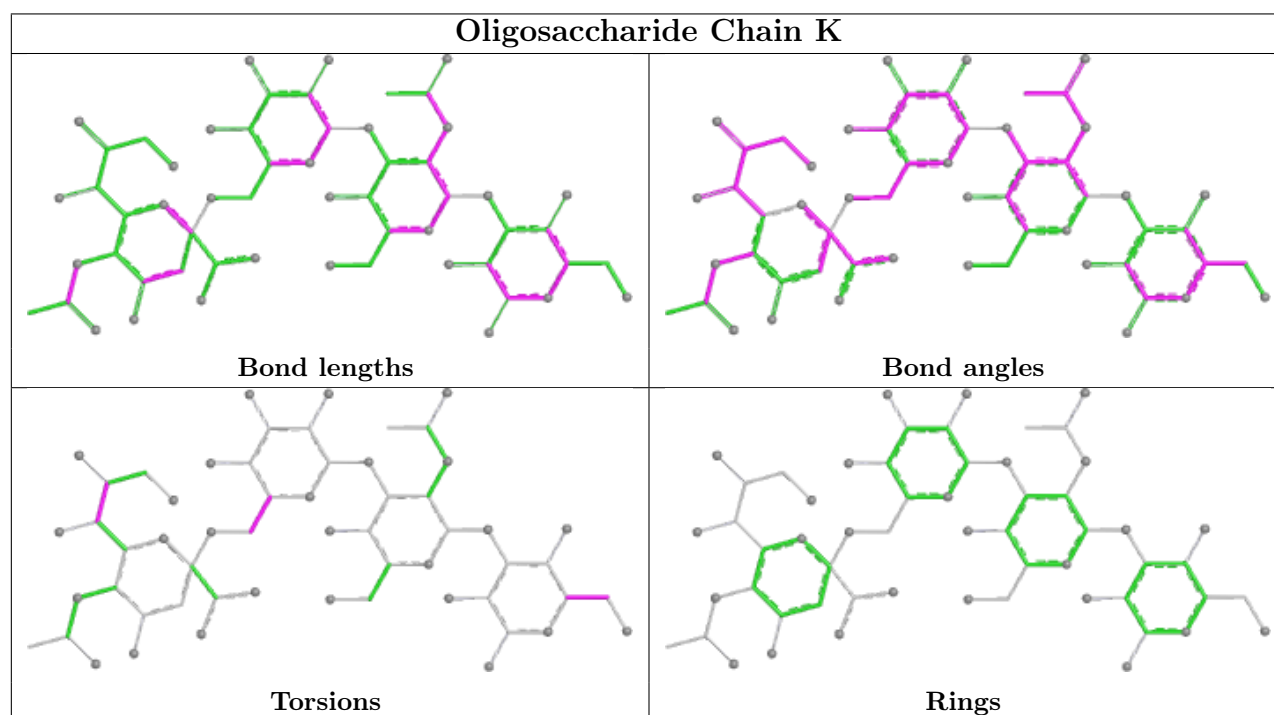
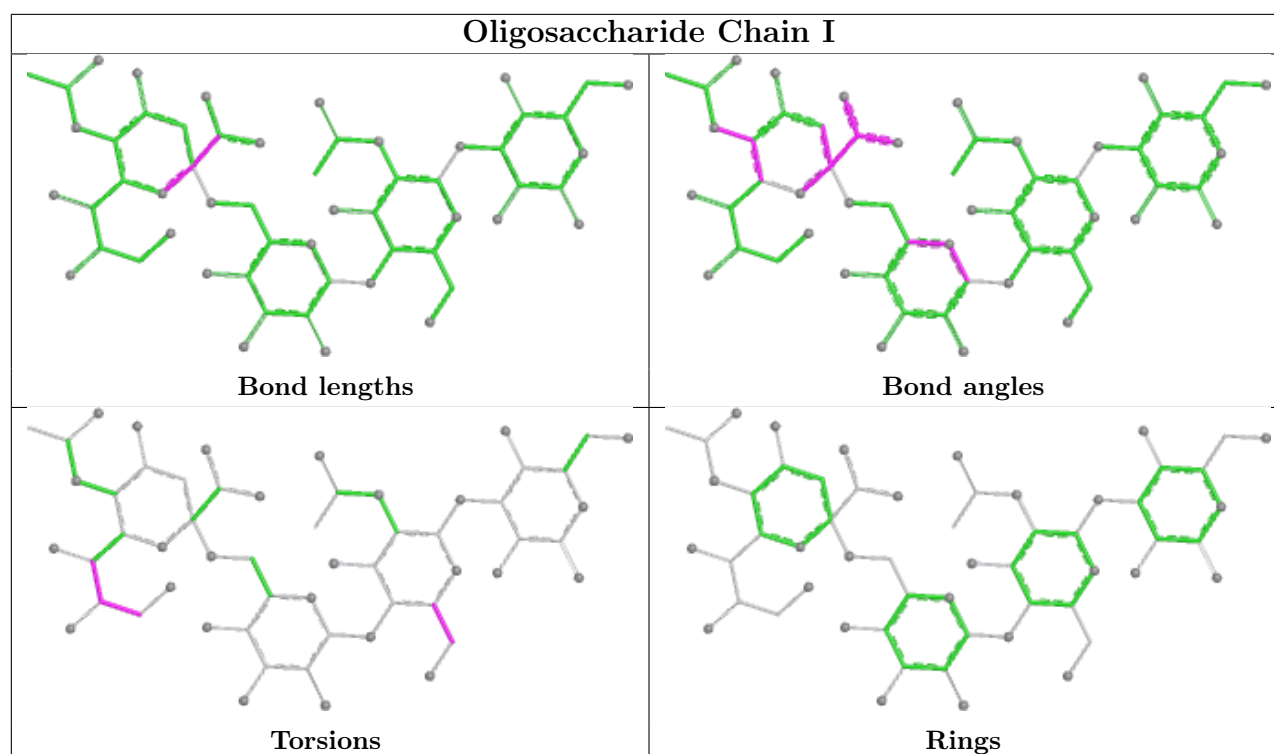


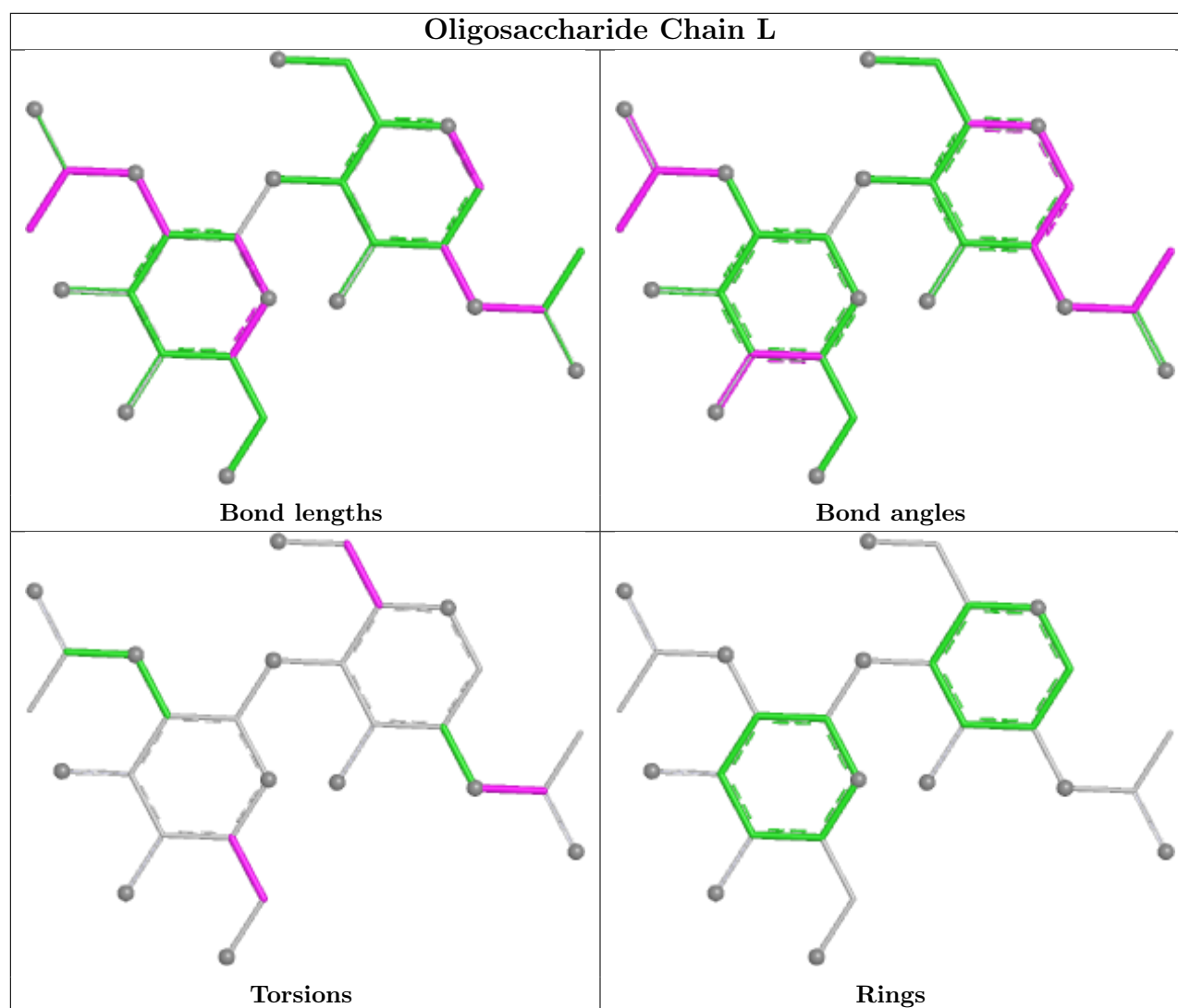
Oligosaccharide Chain J



Oligosaccharide Chain H







5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
6	NAG	E	602	1	14,14,15	2.26	4 (28%)	17,19,21	1.26	2 (11%)
6	NAG	D	701	1	14,14,15	2.11	5 (35%)	17,19,21	1.74	4 (23%)
6	NAG	E	601	1	14,14,15	2.02	4 (28%)	17,19,21	1.30	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	603	1	14,14,15	2.21	4 (28%)	17,19,21	1.32	2 (11%)
6	NAG	A	601	1	14,14,15	2.08	4 (28%)	17,19,21	1.17	2 (11%)
6	NAG	C	702	1	14,14,15	2.11	4 (28%)	17,19,21	1.48	4 (23%)
6	NAG	D	703	1	14,14,15	2.07	4 (28%)	17,19,21	1.17	1 (5%)
6	NAG	D	702	1	14,14,15	2.10	4 (28%)	17,19,21	1.08	1 (5%)
6	NAG	C	703	1	14,14,15	2.20	5 (35%)	17,19,21	1.99	4 (23%)
6	NAG	F	601	1	14,14,15	2.18	5 (35%)	17,19,21	1.36	3 (17%)
6	NAG	C	701	1	14,14,15	2.10	4 (28%)	17,19,21	1.55	2 (11%)
6	NAG	A	602	1	14,14,15	2.43	5 (35%)	17,19,21	1.87	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	602	1	-	2/6/23/26	0/1/1/1
6	NAG	D	701	1	-	0/6/23/26	0/1/1/1
6	NAG	E	601	1	-	3/6/23/26	0/1/1/1
6	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1	-	1/6/23/26	0/1/1/1
6	NAG	C	702	1	-	0/6/23/26	0/1/1/1
6	NAG	D	703	1	-	1/6/23/26	0/1/1/1
6	NAG	D	702	1	-	1/6/23/26	0/1/1/1
6	NAG	C	703	1	-	1/6/23/26	0/1/1/1
6	NAG	F	601	1	-	0/6/23/26	0/1/1/1
6	NAG	C	701	1	-	2/6/23/26	0/1/1/1
6	NAG	A	602	1	-	2/6/23/26	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	NAG	O5-C1	5.03	1.52	1.43
6	C	702	NAG	O5-C1	4.97	1.52	1.43
6	F	601	NAG	O5-C1	4.94	1.52	1.43
6	A	603	NAG	O5-C1	4.80	1.51	1.43
6	E	602	NAG	O5-C1	4.74	1.51	1.43
6	C	703	NAG	O5-C1	4.63	1.51	1.43
6	D	701	NAG	O5-C1	4.61	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	701	NAG	O5-C1	4.53	1.51	1.43
6	A	602	NAG	C7-N2	4.53	1.48	1.34
6	D	703	NAG	O5-C1	4.51	1.51	1.43
6	E	601	NAG	O5-C1	4.43	1.51	1.43
6	A	601	NAG	O5-C1	4.37	1.51	1.43
6	E	602	NAG	C7-N2	4.24	1.48	1.34
6	D	702	NAG	O5-C1	4.22	1.50	1.43
6	C	703	NAG	C7-N2	4.11	1.47	1.34
6	A	603	NAG	C7-N2	4.08	1.47	1.34
6	A	601	NAG	C7-N2	4.06	1.47	1.34
6	D	702	NAG	C7-N2	4.06	1.47	1.34
6	D	703	NAG	C7-N2	4.03	1.47	1.34
6	E	601	NAG	C7-N2	3.91	1.47	1.34
6	D	701	NAG	C7-N2	3.82	1.46	1.34
6	F	601	NAG	C7-N2	3.80	1.46	1.34
6	C	701	NAG	C7-N2	3.78	1.46	1.34
6	C	702	NAG	C7-N2	3.70	1.46	1.34
6	A	602	NAG	C2-N2	3.67	1.52	1.46
6	E	602	NAG	C2-N2	3.43	1.51	1.46
6	C	703	NAG	C2-N2	3.17	1.51	1.46
6	D	702	NAG	C2-N2	3.10	1.51	1.46
6	D	703	NAG	C2-N2	3.06	1.51	1.46
6	A	603	NAG	C2-N2	2.95	1.51	1.46
6	F	601	NAG	C2-N2	2.79	1.50	1.46
6	A	601	NAG	C2-N2	2.76	1.50	1.46
6	A	602	NAG	O5-C5	2.75	1.48	1.43
6	F	601	NAG	O5-C5	2.73	1.48	1.43
6	C	702	NAG	O5-C5	2.68	1.48	1.43
6	A	603	NAG	O5-C5	2.65	1.48	1.43
6	D	701	NAG	C2-N2	2.64	1.50	1.46
6	C	701	NAG	C2-N2	2.59	1.50	1.46
6	E	601	NAG	C2-N2	2.46	1.50	1.46
6	C	701	NAG	O5-C5	2.43	1.48	1.43
6	E	602	NAG	O5-C5	2.43	1.48	1.43
6	D	701	NAG	O5-C5	2.41	1.48	1.43
6	E	601	NAG	O5-C5	2.32	1.47	1.43
6	D	702	NAG	O5-C5	2.30	1.47	1.43
6	A	601	NAG	O5-C5	2.16	1.47	1.43
6	C	702	NAG	C2-N2	2.15	1.49	1.46
6	C	703	NAG	C1-C2	2.14	1.55	1.52
6	F	601	NAG	O7-C7	-2.07	1.18	1.23
6	A	602	NAG	C1-C2	2.06	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	703	NAG	O5-C5	2.02	1.47	1.43
6	C	703	NAG	O5-C5	2.01	1.47	1.43
6	D	701	NAG	C1-C2	2.01	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	703	NAG	C4-C3-C2	4.61	117.78	111.02
6	C	703	NAG	C2-N2-C7	4.60	129.07	122.90
6	D	701	NAG	C1-O5-C5	4.48	118.19	112.19
6	C	701	NAG	C1-O5-C5	4.02	117.57	112.19
6	A	602	NAG	C8-C7-N2	3.84	122.49	116.12
6	C	702	NAG	C2-N2-C7	-3.43	118.31	122.90
6	D	703	NAG	C1-C2-N2	-3.30	105.24	110.43
6	D	701	NAG	C2-N2-C7	-3.30	118.48	122.90
6	A	602	NAG	O7-C7-C8	-3.15	116.44	122.05
6	A	602	NAG	C1-O5-C5	3.13	116.38	112.19
6	E	602	NAG	C8-C7-N2	3.01	121.12	116.12
6	E	601	NAG	O5-C1-C2	-2.96	106.71	111.29
6	F	601	NAG	C8-C7-N2	2.91	120.94	116.12
6	A	602	NAG	C1-C2-N2	2.81	114.86	110.43
6	D	702	NAG	C8-C7-N2	2.78	120.73	116.12
6	A	601	NAG	C8-C7-N2	2.77	120.71	116.12
6	F	601	NAG	C1-O5-C5	2.73	115.85	112.19
6	C	702	NAG	C1-C2-N2	-2.69	106.19	110.43
6	F	601	NAG	C2-N2-C7	-2.61	119.40	122.90
6	C	701	NAG	O5-C5-C4	2.59	117.14	110.83
6	D	701	NAG	C1-C2-N2	2.54	114.44	110.43
6	A	603	NAG	C8-C7-N2	2.41	120.12	116.12
6	C	702	NAG	C8-C7-N2	2.39	120.08	116.12
6	C	703	NAG	C3-C4-C5	2.32	114.44	110.23
6	A	603	NAG	C1-O5-C5	2.30	115.27	112.19
6	E	601	NAG	O4-C4-C5	2.24	114.84	109.32
6	A	601	NAG	C6-C5-C4	-2.13	107.78	113.02
6	D	701	NAG	O3-C3-C2	2.09	113.75	109.40
6	C	702	NAG	O7-C7-N2	-2.07	118.33	121.98
6	E	601	NAG	O3-C3-C2	2.06	113.69	109.40
6	C	703	NAG	C1-C2-N2	2.02	113.61	110.43
6	E	602	NAG	O5-C1-C2	2.01	114.40	111.29
6	A	602	NAG	O3-C3-C2	2.01	113.57	109.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	703	NAG	C1-C2-N2-C7
6	E	601	NAG	O5-C5-C6-O6
6	E	601	NAG	C4-C5-C6-O6
6	C	701	NAG	C4-C5-C6-O6
6	D	702	NAG	O5-C5-C6-O6
6	C	701	NAG	O5-C5-C6-O6
6	A	602	NAG	C4-C5-C6-O6
6	E	601	NAG	C3-C2-N2-C7
6	E	602	NAG	O5-C5-C6-O6
6	D	703	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
6	E	602	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	484/506 (95%)	0.16	19 (3%)	43	23	41, 72, 173, 207	0
1	B	485/506 (95%)	0.48	20 (4%)	41	22	48, 101, 184, 201	0
1	C	484/506 (95%)	-0.00	10 (2%)	63	39	33, 58, 168, 180	0
1	D	485/506 (95%)	0.06	8 (1%)	70	47	39, 68, 153, 185	0
1	E	485/506 (95%)	0.25	17 (3%)	47	26	44, 81, 191, 207	0
1	F	486/506 (96%)	0.70	36 (7%)	20	10	66, 117, 197, 233	0
All	All	2909/3036 (95%)	0.27	110 (3%)	44	24	33, 89, 182, 233	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	ILE	6.4
1	F	170	GLU	6.3
1	F	478	MET	5.7
1	A	497	LEU	4.7
1	F	67	CYS	4.4
1	C	338	PHE	4.3
1	F	497	LEU	4.1
1	F	495	ALA	3.9
1	F	134	ALA	3.8
1	F	335	ILE	3.7
1	F	135	CYS	3.7
1	A	1	ASP	3.5
1	C	355	HIS	3.4
1	B	70	PHE	3.4
1	B	478	MET	3.4
1	E	338	PHE	3.2
1	B	458	ASN	3.1
1	E	455	LEU	3.1
1	D	473	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	71	ILE	3.1
1	C	486	TYR	3.1
1	E	336	ALA	3.0
1	B	486	TYR	3.0
1	A	467	PHE	3.0
1	C	320	SER	3.0
1	F	390	THR	3.0
1	B	71	ILE	2.9
1	A	320	SER	2.9
1	A	458	ASN	2.9
1	F	320	SER	2.9
1	E	495	ALA	2.9
1	A	68	ASP	2.9
1	E	340	GLU	2.8
1	D	1	ASP	2.8
1	F	470	TYR	2.8
1	A	244	ASN	2.7
1	F	64	ASN	2.7
1	A	354	HIS	2.7
1	F	488	TYR	2.7
1	B	462	LEU	2.7
1	F	243	SER	2.7
1	B	470	TYR	2.7
1	B	69	GLU	2.7
1	B	336	ALA	2.7
1	F	140	ALA	2.7
1	A	71	ILE	2.6
1	A	491	TYR	2.6
1	E	489	PRO	2.6
1	F	498	LYS	2.6
1	E	468	GLU	2.6
1	F	336	ALA	2.6
1	B	314	ALA	2.6
1	C	473	CYS	2.6
1	F	131	VAL	2.6
1	E	486	TYR	2.5
1	F	133	ALA	2.5
1	D	390	THR	2.5
1	B	338	PHE	2.5
1	F	448	TYR	2.5
1	C	478	MET	2.4
1	B	396	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	477	CYS	2.4
1	C	10	ASN	2.4
1	B	309	ASN	2.4
1	B	392	PHE	2.4
1	A	453	LEU	2.4
1	C	455	LEU	2.4
1	E	461	GLU	2.3
1	A	356	SER	2.3
1	B	1	ASP	2.3
1	B	388	MET	2.3
1	F	129	LEU	2.3
1	A	13	THR	2.3
1	F	353	TYR	2.3
1	A	3	ILE	2.3
1	D	339	ILE	2.3
1	F	264	ILE	2.3
1	C	317	LEU	2.3
1	F	139	GLY	2.2
1	E	470	TYR	2.2
1	F	454	GLN	2.2
1	F	455	LEU	2.2
1	A	469	PHE	2.2
1	B	481	VAL	2.2
1	B	453	LEU	2.2
1	F	181	SER	2.2
1	B	395	VAL	2.1
1	D	394	ALA	2.1
1	B	488	TYR	2.1
1	E	360	GLY	2.1
1	F	463	GLY	2.1
1	E	481	VAL	2.1
1	F	141	PRO	2.1
1	A	361	SER	2.1
1	A	472	LYS	2.1
1	E	350	TRP	2.1
1	D	71	ILE	2.1
1	D	363	TYR	2.1
1	F	66	MET	2.1
1	A	337	GLY	2.1
1	E	320	SER	2.1
1	E	155	ASP	2.1
1	F	54	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	TYR	2.1
1	F	55	CYS	2.1
1	C	450	LYS	2.0
1	E	6	GLY	2.0
1	F	109	ASN	2.0
1	E	343	TRP	2.0
1	D	497	LEU	2.0

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

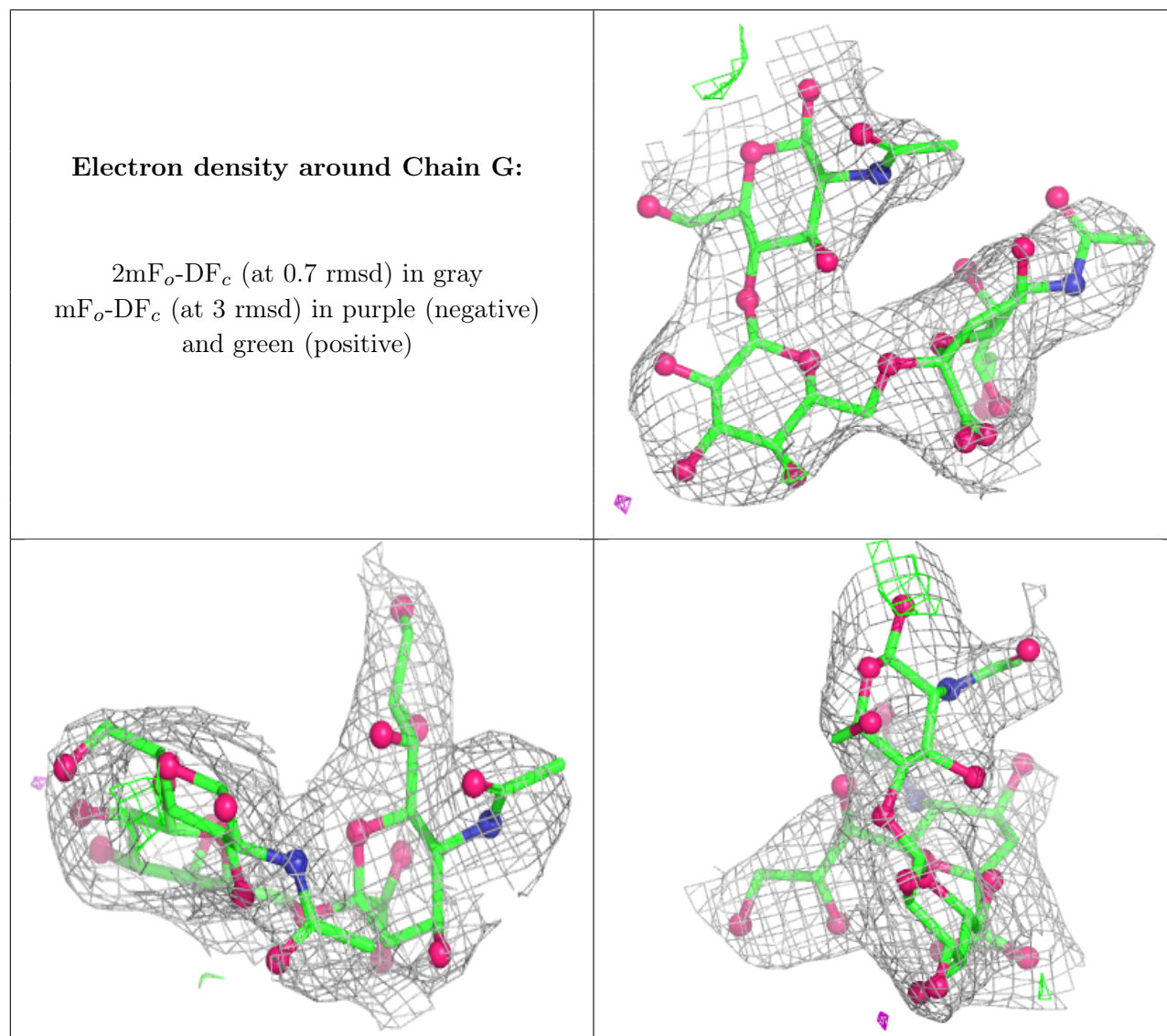
There are no non-standard protein/DNA/RNA residues in this entry.

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.

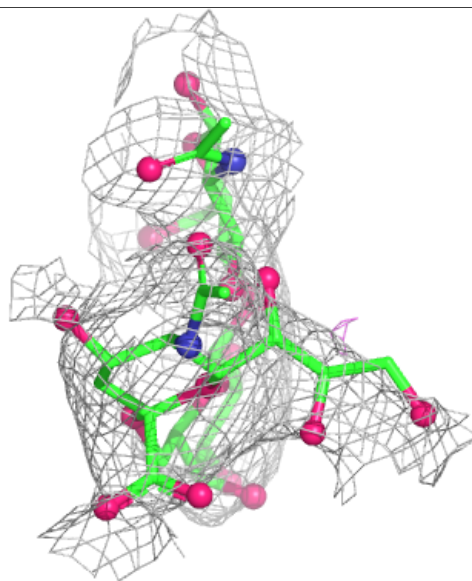
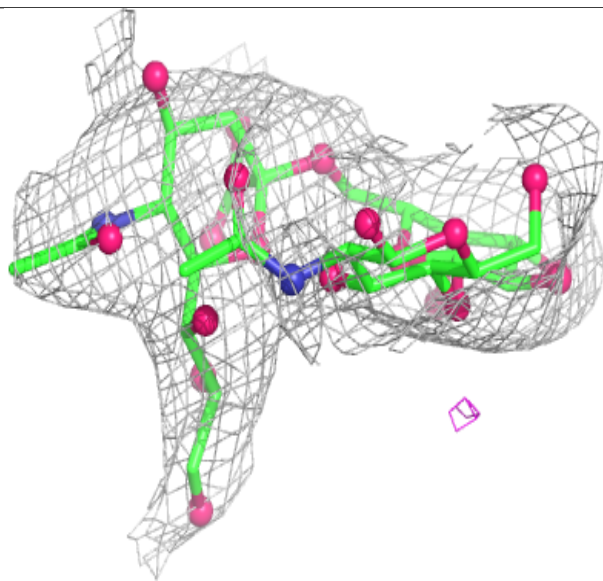
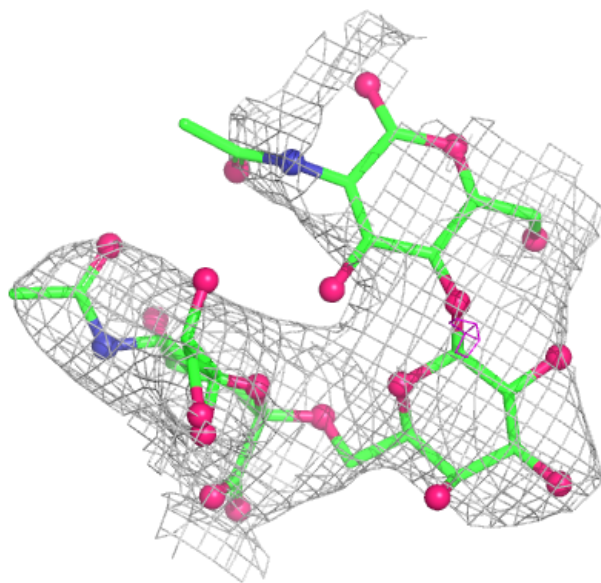
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GAL	K	1	12/12	0.33	0.16	136,143,158,159	0
3	GAL	H	1	12/12	0.43	0.17	63,78,83,87	0
4	NAG	K	2	14/15	0.44	0.17	128,146,165,168	0
3	NAG	I	2	14/15	0.47	0.18	67,72,76,78	0
3	GAL	I	1	12/12	0.56	0.17	63,78,83,87	0
3	NAG	H	2	14/15	0.60	0.19	67,72,76,78	0
2	NAG	J	1	15/15	0.62	0.17	111,121,136,139	0
3	GAL	H	3	11/12	0.62	0.14	57,63,69,69	0
3	GAL	I	3	11/12	0.70	0.13	57,63,69,69	0
2	NAG	G	1	15/15	0.71	0.13	86,115,128,129	0
5	NAG	L	2	14/15	0.75	0.13	82,119,141,144	0
2	GAL	J	2	11/12	0.77	0.12	93,111,126,132	0
2	GAL	G	2	11/12	0.82	0.10	89,102,107,109	0
4	GAL	K	3	11/12	0.83	0.10	97,120,128,133	0
3	SIA	I	4	20/21	0.84	0.14	44,57,65,67	0
5	NAG	L	1	14/15	0.85	0.13	85,99,114,117	0
3	SIA	H	4	20/21	0.88	0.13	44,57,65,67	0
2	SIA	J	3	20/21	0.92	0.12	75,100,121,134	0
4	SIA	K	4	20/21	0.93	0.12	70,87,115,122	0
2	SIA	G	3	20/21	0.96	0.09	54,67,92,101	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.



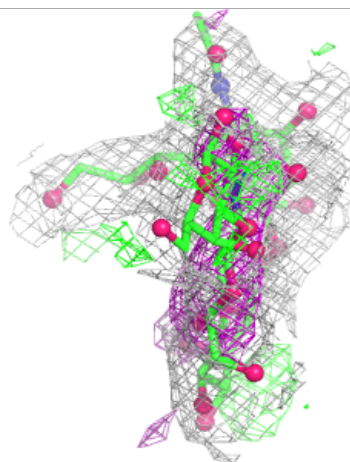
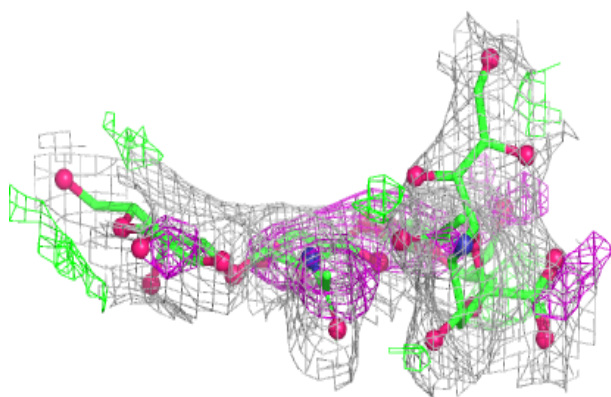
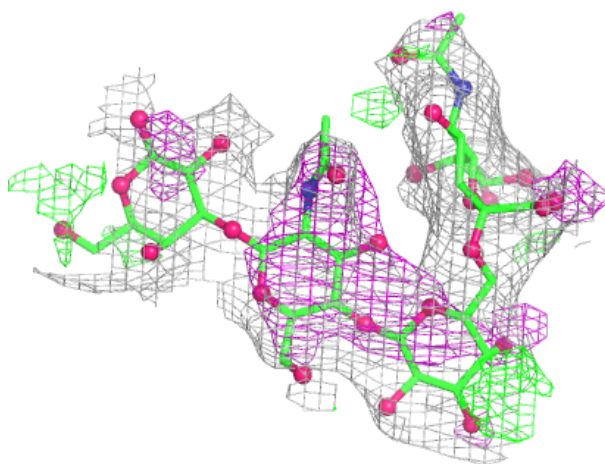
Electron density around Chain J:

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



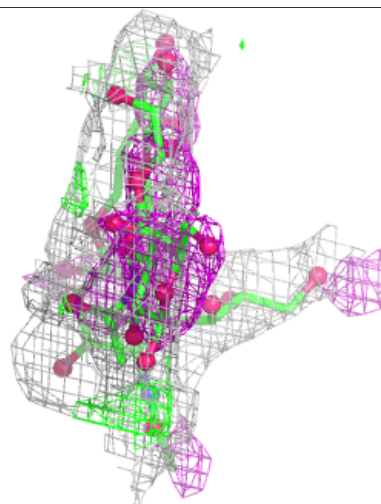
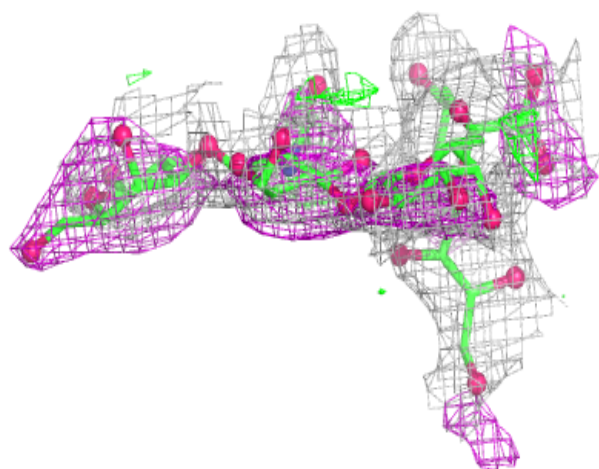
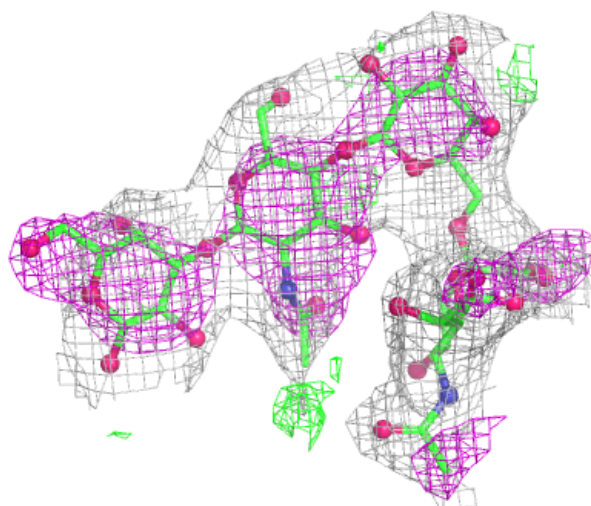
Electron density around Chain H:

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



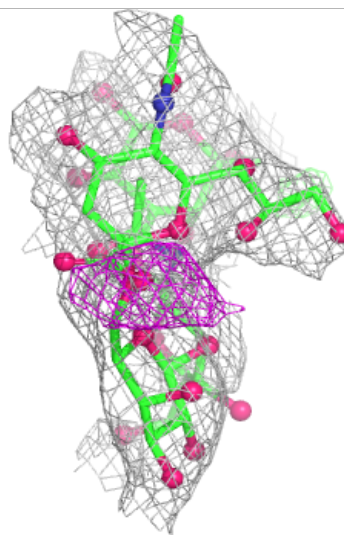
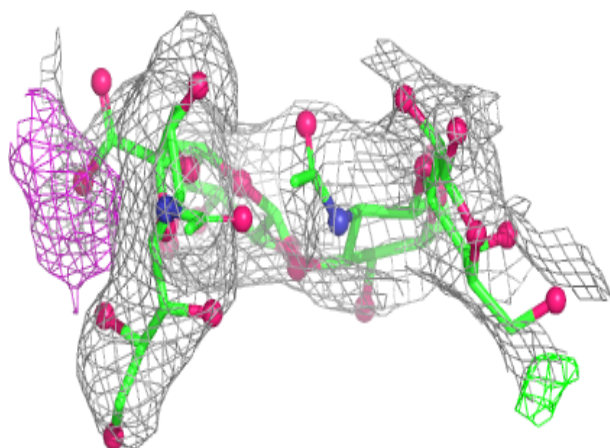
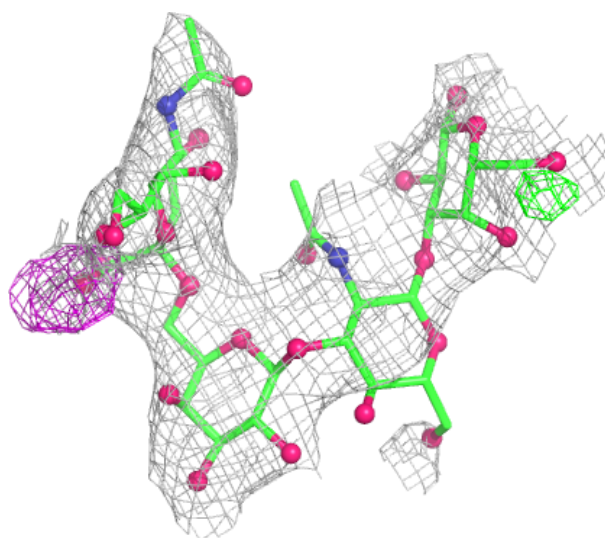
Electron density around Chain I:

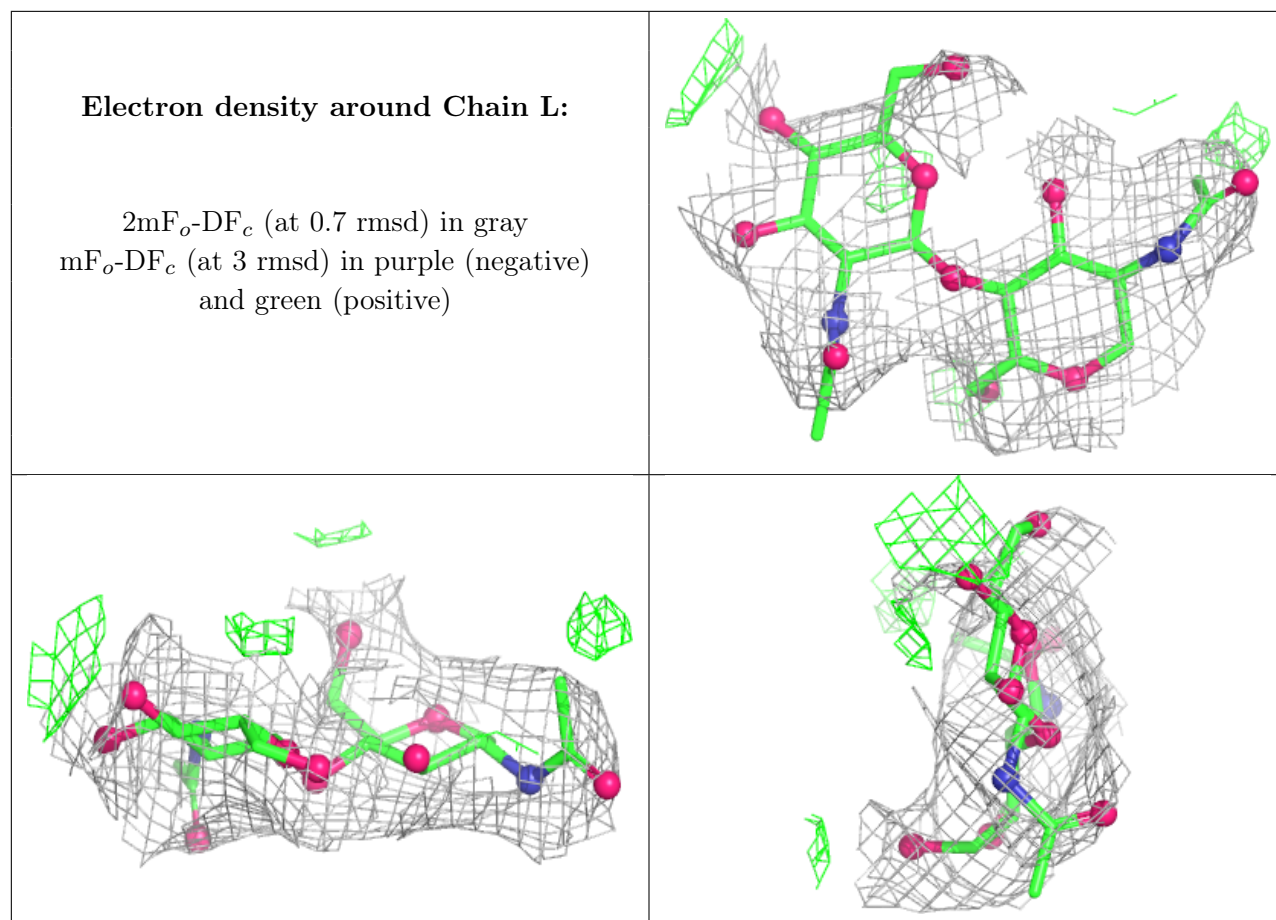
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





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
6	NAG	F	601	14/15	0.41	0.16	104,144,159,167	0
6	NAG	D	702	14/15	0.62	0.13	124,141,153,154	0
6	NAG	E	602	14/15	0.65	0.12	78,127,137,141	0
6	NAG	C	702	14/15	0.66	0.11	108,119,134,140	0
6	NAG	A	603	14/15	0.72	0.13	100,122,144,151	0
6	NAG	D	703	14/15	0.72	0.13	100,135,142,148	0
6	NAG	A	601	14/15	0.76	0.10	98,148,168,168	0
6	NAG	C	703	14/15	0.78	0.13	97,117,126,126	0
6	NAG	E	601	14/15	0.83	0.13	81,98,113,121	0
6	NAG	C	701	14/15	0.89	0.11	73,90,104,110	0
6	NAG	A	602	14/15	0.89	0.11	70,82,98,103	0
6	NAG	D	701	14/15	0.91	0.10	50,70,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.