



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 5E66 / pdb_00005e66
Title : The complex structure of Hemagglutinin-esterase-fusion mutant protein from the influenza D virus with receptor analog 9-N-Ac-Sia
Authors : Song, H.; Qi, J.; Shi, Y.; Gao, G.F.
Deposited on : 2015-10-09
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

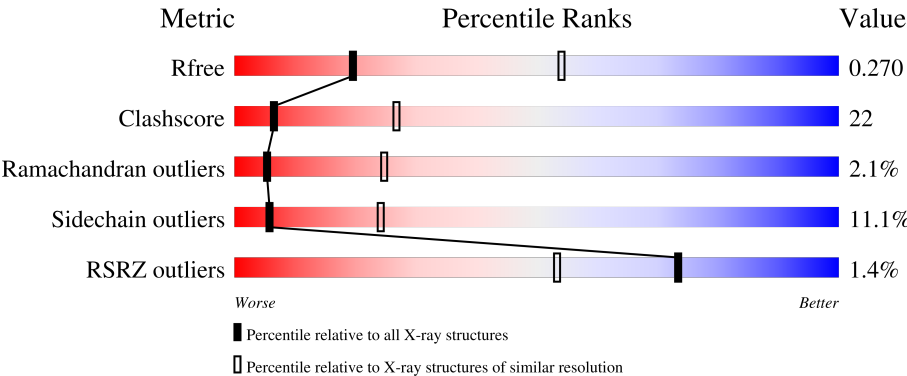
1 Overall quality at a glance ⓘ

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	427	56% 39% ...
2	B	166	2% 45% 33% 12% 10%
3	C	6	100%
4	D	2	50% 50%
4	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CAC	A	501	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4575 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.

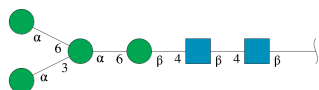
- Molecule 1 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3249	2043	542	642	22			

- Molecule 2 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1104	689	194	217	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



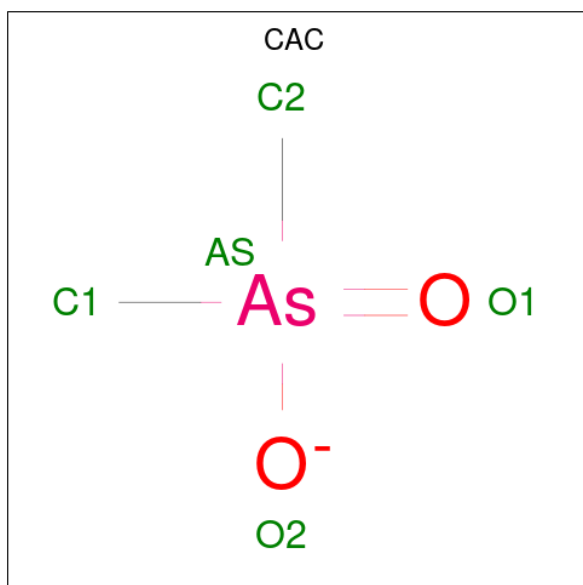
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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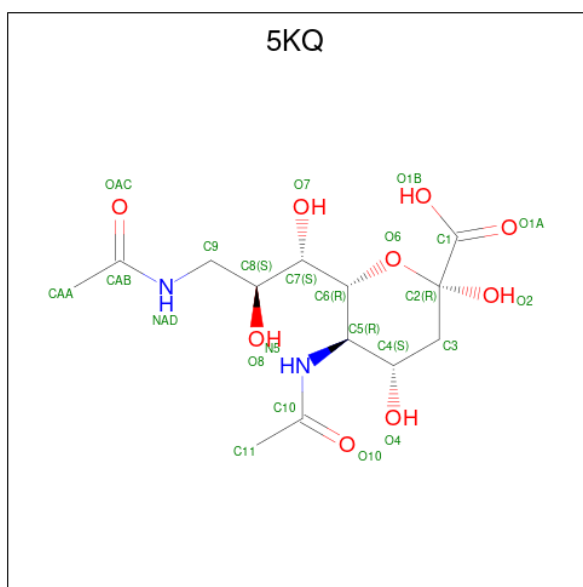
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



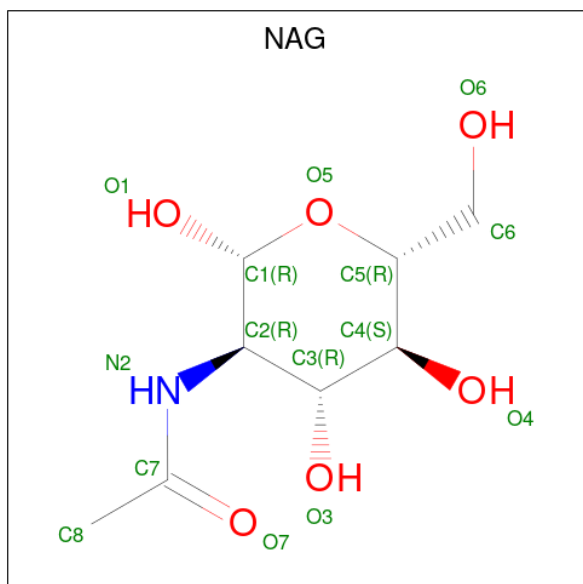
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	As	C	O	0	0
			4	1	2	1		

- Molecule 6 is (6R)-5-acetamido-6-[(1S,2S)-3-acetamido-1,2-dihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranosonic acid (CCD ID: 5KQ) (formula: $\text{C}_{13}\text{H}_{22}\text{N}_2\text{O}_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 24	C 13	N 2	O 9	0	0
6	A	1	Total 24	C 13	N 2	O 9	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).

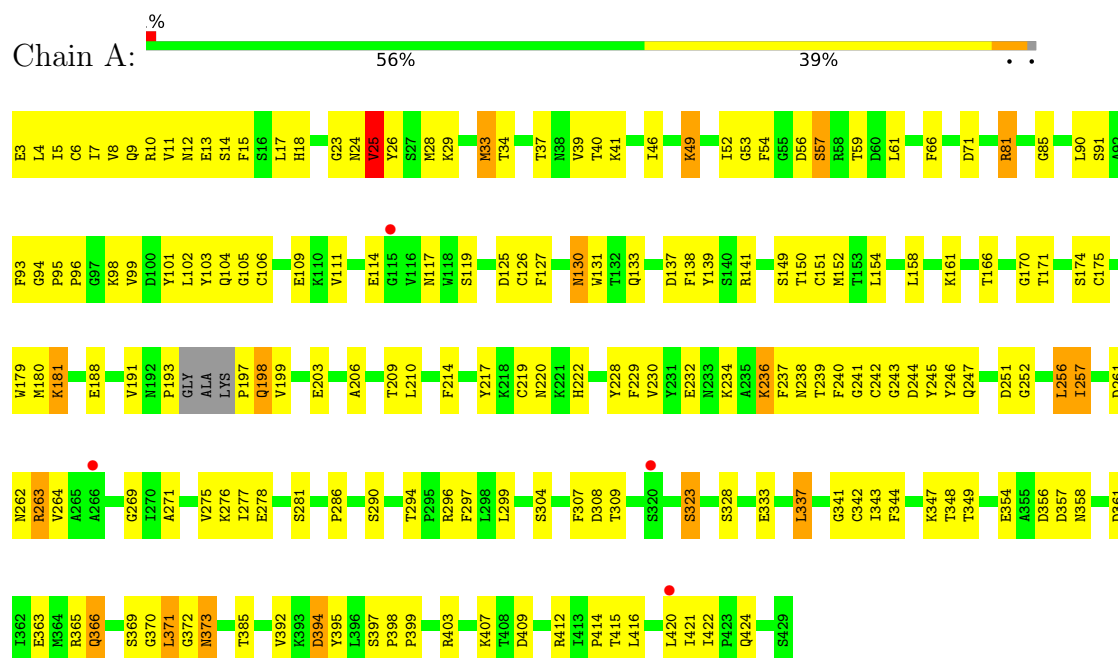


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

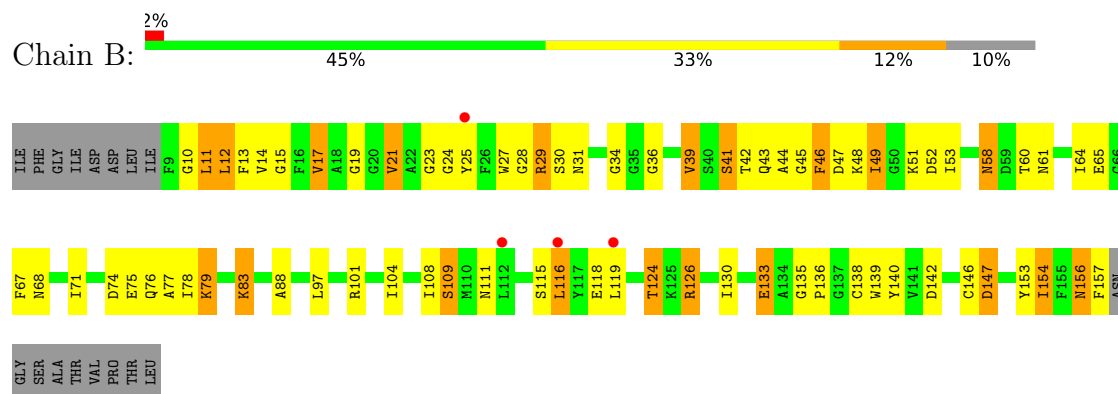
3 Residue-property plots

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

• Molecule 1: Hemagglutinin-esterase



• Molecule 2: Hemagglutinin-esterase



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

Chain C:  100%

MAG1
MAG2
BGA3
MAN4
MAN5
MAN6

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	165.30Å 165.30Å 165.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.96 – 3.10 38.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.96-3.10) 94.7 (38.96-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.265 0.238 , 0.270	Depositor DCC
R_{free} test set	666 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 96.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4575	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: CAC, BMA, MAN, 5KQ, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/3325	1.04	12/4507 (0.3%)
2	B	0.73	1/1120 (0.1%)	1.10	8/1506 (0.5%)
All	All	0.69	1/4445 (0.0%)	1.06	20/6013 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	147	ASP	CA-C	7.69	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	LEU	N-CA-C	8.22	123.31	113.28
2	B	135	GLY	CA-C-N	7.51	129.22	119.84
2	B	135	GLY	C-N-CA	7.51	129.22	119.84
2	B	147	ASP	N-CA-C	7.38	119.82	108.30
1	A	294	THR	CA-C-N	6.94	128.52	119.84
1	A	294	THR	C-N-CA	6.94	128.52	119.84
1	A	25	VAL	N-CA-C	6.27	116.53	107.88
1	A	119	SER	CA-C-N	-6.14	112.53	119.28
1	A	119	SER	C-N-CA	-6.14	112.53	119.28
1	A	170	GLY	N-CA-C	5.92	121.57	112.51
1	A	349	THR	CA-C-N	-5.89	112.48	119.84
1	A	349	THR	C-N-CA	-5.89	112.48	119.84
2	B	88	ALA	N-CA-C	-5.76	104.92	111.14
2	B	104	ILE	N-CA-C	-5.73	104.92	110.42
1	A	357	ASP	N-CA-C	-5.58	105.19	112.23
1	A	181	LYS	N-CA-C	-5.57	105.29	111.36
2	B	24	GLY	N-CA-C	5.55	117.53	110.20
2	B	116	LEU	N-CA-C	-5.46	105.88	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	166	THR	N-CA-C	-5.19	106.80	113.23
2	B	83	LYS	N-CA-C	5.05	116.86	111.36

There are no chirality outliers.

There are no planarity outliers.

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	3249	0	3114	142	1
2	B	1104	0	1060	67	0
3	C	72	0	61	0	0
4	D	28	0	25	1	0
4	E	28	0	25	3	0
4	F	28	0	25	1	0
5	A	4	0	0	9	0
6	A	48	0	0	8	1
7	B	14	0	13	0	0
All	All	4575	0	4323	194	1

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 22.

All (194) 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:A:415:THR:O	2:B:101:ARG:NH1	2.03	0.91
2:B:23:GLY:N	4:E:1:NAG:O6	2.05	0.89
1:A:297:PHE:HE2	6:A:513:5KQ:OAC	1.55	0.88
1:A:33:MET:HE1	2:B:101:ARG:HB2	1.54	0.88
1:A:354:GLU:OE2	1:A:365:ARG:NH2	2.11	0.84
5:A:501:CAC:C1	6:A:502:5KQ:O8	2.28	0.81
2:B:64:ILE:O	2:B:68:ASN:ND2	2.14	0.80
1:A:275:VAL:HG21	6:A:513:5KQ:CAA	2.13	0.79
1:A:193:PRO:C	1:A:197:PRO:HA	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:HA2	5:A:501:CAC:O2	1.86	0.76
1:A:297:PHE:CE2	6:A:513:5KQ:OAC	2.39	0.75
1:A:373:ASN:N	1:A:373:ASN:OD1	2.21	0.73
1:A:85:GLY:N	5:A:501:CAC:O2	2.22	0.73
2:B:115:SER:HA	2:B:118:GLU:HB2	1.71	0.73
1:A:244:ASP:HB3	1:A:262:ASN:HB2	1.72	0.72
2:B:74:ASP:OD1	2:B:75:GLU:N	2.23	0.71
1:A:102:LEU:HA	1:A:154:LEU:HD23	1.71	0.71
1:A:137:ASP:OD1	1:A:281:SER:N	2.22	0.71
1:A:26:TYR:HB2	1:A:422:ILE:HB	1.73	0.70
1:A:49:LYS:HZ2	1:A:49:LYS:HB2	1.57	0.69
1:A:90:LEU:O	1:A:94:GLY:N	2.16	0.69
2:B:156:ASN:O	2:B:156:ASN:ND2	2.22	0.68
1:A:150:THR:N	1:A:308:ASP:OD1	2.15	0.68
1:A:85:GLY:CA	5:A:501:CAC:O2	2.42	0.67
2:B:17:VAL:HG11	2:B:21:VAL:HG11	1.76	0.67
1:A:7:ILE:O	2:B:10:GLY:HA2	1.95	0.66
1:A:130:ASN:O	1:A:133:GLN:N	2.28	0.66
1:A:236:LYS:O	1:A:239:THR:OG1	2.11	0.66
2:B:11:LEU:HD11	2:B:116:LEU:HD22	1.76	0.66
1:A:188:GLU:HB2	1:A:296:ARG:HA	1.77	0.66
1:A:261:ASP:CG	1:A:263:ARG:HH21	2.05	0.64
1:A:11:VAL:HG12	1:A:422:ILE:HD13	1.80	0.64
5:A:501:CAC:C1	6:A:502:5KQ:O7	2.47	0.62
1:A:409:ASP:HB3	1:A:412:ARG:NH1	2.14	0.62
2:B:108:ILE:O	2:B:111:ASN:N	2.32	0.61
1:A:10:ARG:HA	2:B:15:GLY:O	2.01	0.61
1:A:244:ASP:HB2	1:A:263:ARG:HG3	1.81	0.61
1:A:394:ASP:HA	1:A:407:LYS:HD2	1.82	0.61
2:B:31:ASN:OD1	2:B:36:GLY:N	2.34	0.61
1:A:5:ILE:HG23	2:B:28:GLY:O	2.00	0.60
2:B:133:GLU:HA	2:B:139:TRP:HD1	1.67	0.60
1:A:91:SER:HB3	1:A:154:LEU:HD22	1.84	0.59
1:A:395:TYR:CD1	1:A:407:LYS:HB3	2.38	0.59
1:A:232:GLU:CD	1:A:271:ALA:HA	2.27	0.59
1:A:371:LEU:N	1:A:372:GLY:HA3	2.17	0.59
1:A:12:ASN:OD1	2:B:17:VAL:HG23	2.02	0.58
2:B:10:GLY:HA3	2:B:138:CYS:SG	2.44	0.58
5:A:501:CAC:C1	6:A:502:5KQ:C8	2.82	0.58
2:B:23:GLY:O	4:E:1:NAG:O6	2.20	0.58
1:A:125:ASP:HB3	1:A:174:SER:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:HB3	1:A:358:ASN:H	1.69	0.57
2:B:67:PHE:CZ	2:B:97:LEU:HD22	2.39	0.56
1:A:395:TYR:CE2	1:A:407:LYS:HD3	2.40	0.56
1:A:71:ASP:HA	1:A:365:ARG:HG2	1.88	0.56
1:A:398:PRO:HB2	2:B:78:ILE:O	2.05	0.56
1:A:230:VAL:HG21	1:A:278:GLU:HG3	1.88	0.56
1:A:117:ASN:OD1	5:A:501:CAC:C2	2.54	0.56
1:A:179:TRP:CG	1:A:180:MET:H	2.24	0.55
1:A:333:GLU:HA	1:A:344:PHE:CE1	2.41	0.55
1:A:26:TYR:N	1:A:422:ILE:O	2.33	0.55
1:A:125:ASP:OD1	1:A:174:SER:HB2	2.06	0.55
2:B:147:ASP:OD1	2:B:147:ASP:N	2.40	0.55
1:A:214:PHE:N	1:A:217:TYR:O	2.25	0.55
2:B:61:ASN:O	2:B:65:GLU:N	2.29	0.54
1:A:210:LEU:HB2	1:A:286:PRO:HA	1.89	0.54
1:A:40:THR:HG22	1:A:41:LYS:O	2.08	0.54
1:A:234:LYS:HG2	1:A:238:ASN:OD1	2.08	0.53
2:B:27:TRP:CD1	2:B:44:ALA:HB2	2.44	0.53
2:B:133:GLU:HA	2:B:139:TRP:CD1	2.42	0.53
1:A:247:GLN:NE2	1:A:299:LEU:HB2	2.24	0.53
2:B:23:GLY:N	4:E:1:NAG:O5	2.42	0.53
2:B:45:GLY:O	2:B:47:ASP:N	2.41	0.53
1:A:191:VAL:HB	1:A:296:ARG:HD2	1.91	0.53
1:A:220:ASN:O	1:A:286:PRO:HD3	2.09	0.52
2:B:27:TRP:O	2:B:41:SER:N	2.37	0.52
4:F:1:NAG:H61	4:F:2:NAG:C7	2.40	0.52
1:A:191:VAL:HG11	1:A:296:ARG:HB2	1.92	0.52
1:A:403:ARG:HB3	2:B:71:ILE:HB	1.92	0.52
1:A:52:ILE:HG12	1:A:105:GLY:HA3	1.92	0.52
1:A:23:GLY:C	1:A:24:ASN:OD1	2.53	0.51
1:A:261:ASP:OD2	1:A:263:ARG:NH2	2.34	0.51
1:A:188:GLU:N	1:A:296:ARG:O	2.42	0.51
1:A:238:ASN:HD21	1:A:243:GLY:H	1.57	0.51
1:A:237:PHE:CZ	1:A:241:GLY:HA3	2.46	0.51
2:B:29:ARG:HB2	2:B:39:VAL:HG13	1.92	0.50
2:B:136:PRO:C	2:B:138:CYS:H	2.18	0.50
1:A:210:LEU:HD13	1:A:222:HIS:HB2	1.94	0.50
1:A:26:TYR:O	1:A:421:ILE:HA	2.12	0.50
1:A:403:ARG:HG2	2:B:71:ILE:O	2.12	0.50
1:A:141:ARG:HG3	1:A:281:SER:O	2.12	0.50
2:B:126:ARG:NH2	2:B:154:ILE:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:LEU:CD1	2:B:13:PHE:N	2.74	0.50
1:A:125:ASP:OD1	1:A:126:CYS:N	2.45	0.49
1:A:179:TRP:CG	1:A:180:MET:N	2.81	0.49
2:B:12:LEU:CD1	2:B:12:LEU:C	2.85	0.49
1:A:4:LEU:HD13	2:B:140:TYR:CZ	2.48	0.49
1:A:232:GLU:HA	1:A:269:GLY:O	2.13	0.49
1:A:361:ASP:O	1:A:365:ARG:HG3	2.13	0.49
1:A:18:HIS:N	1:A:25:VAL:O	2.45	0.48
1:A:323:SER:OG	1:A:358:ASN:OD1	2.30	0.48
1:A:39:VAL:HG22	1:A:385:THR:HG22	1.95	0.48
1:A:193:PRO:C	1:A:197:PRO:CA	2.84	0.48
1:A:244:ASP:CB	1:A:263:ARG:HG3	2.44	0.48
2:B:12:LEU:HD12	2:B:12:LEU:H	1.79	0.48
1:A:256:LEU:HG	1:A:257:ILE:N	2.26	0.48
2:B:126:ARG:NH2	2:B:153:TYR:O	2.47	0.48
1:A:203:GLU:OE1	1:A:246:TYR:OH	2.24	0.47
1:A:15:PHE:HZ	1:A:420:LEU:HD23	1.77	0.47
1:A:24:ASN:O	2:B:109:SER:OG	2.19	0.47
1:A:46:ILE:HG12	1:A:109:GLU:OE1	2.14	0.47
1:A:341:GLY:N	2:B:77:ALA:O	2.42	0.47
1:A:104:GLN:HA	1:A:152:MET:O	2.14	0.47
1:A:33:MET:HG3	1:A:416:LEU:HG	1.96	0.47
2:B:49:ILE:O	2:B:52:ASP:N	2.47	0.47
1:A:219:CYS:HB3	1:A:222:HIS:NE2	2.28	0.47
1:A:3:GLU:HG2	2:B:30:SER:H	1.79	0.47
2:B:12:LEU:C	2:B:12:LEU:HD13	2.39	0.47
1:A:240:PHE:HA	1:A:296:ARG:HH12	1.80	0.47
1:A:395:TYR:CE1	1:A:407:LYS:HB3	2.50	0.47
2:B:124:THR:OG1	2:B:139:TRP:NE1	2.48	0.47
1:A:52:ILE:HD11	1:A:81:ARG:HG2	1.97	0.46
1:A:61:LEU:HA	1:A:66:PHE:CD2	2.50	0.46
1:A:261:ASP:OD1	1:A:263:ARG:NE	2.42	0.46
1:A:409:ASP:HB3	1:A:412:ARG:HH11	1.79	0.46
2:B:64:ILE:HG22	2:B:68:ASN:HD21	1.81	0.46
1:A:161:LYS:O	1:A:206:ALA:HA	2.16	0.46
1:A:9:GLN:CD	2:B:11:LEU:HA	2.40	0.46
4:D:1:NAG:O3	4:D:2:NAG:O5	2.30	0.46
1:A:81:ARG:HB3	1:A:101:TYR:OH	2.16	0.46
2:B:29:ARG:HE	2:B:29:ARG:HB3	1.51	0.46
1:A:106:CYS:SG	1:A:217:TYR:HE1	2.39	0.46
1:A:11:VAL:HB	1:A:15:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:CYS:O	1:A:399:PRO:HG2	2.16	0.45
2:B:58:ASN:O	2:B:58:ASN:ND2	2.38	0.45
1:A:138:PHE:HD2	1:A:139:TYR:CD2	2.33	0.45
1:A:4:LEU:HD13	2:B:140:TYR:CE1	2.51	0.45
1:A:56:ASP:O	1:A:57:SER:C	2.59	0.45
2:B:48:LYS:NZ	2:B:52:ASP:OD2	2.49	0.45
1:A:347:LYS:HB3	1:A:363:GLU:OE1	2.16	0.45
1:A:395:TYR:CZ	1:A:407:LYS:HD3	2.52	0.45
1:A:17:LEU:HA	1:A:25:VAL:O	2.18	0.44
1:A:6:CYS:HA	2:B:138:CYS:HA	1.99	0.44
1:A:395:TYR:OH	2:B:83:LYS:NZ	2.42	0.44
1:A:241:GLY:C	1:A:242:CYS:SG	3.00	0.44
1:A:39:VAL:HG22	1:A:385:THR:CG2	2.47	0.43
1:A:342:CYS:SG	1:A:343:ILE:N	2.91	0.43
1:A:398:PRO:HA	1:A:399:PRO:C	2.43	0.43
1:A:18:HIS:HB2	1:A:25:VAL:HG12	1.98	0.43
1:A:366:GLN:O	1:A:366:GLN:HG3	2.17	0.43
2:B:25:TYR:CE1	2:B:116:LEU:HD11	2.53	0.43
1:A:101:TYR:CE2	1:A:103:TYR:HA	2.53	0.43
1:A:117:ASN:ND2	5:A:501:CAC:O2	2.52	0.43
1:A:228:TYR:CE1	1:A:278:GLU:HB2	2.53	0.43
2:B:12:LEU:HD13	2:B:13:PHE:N	2.34	0.43
1:A:229:PHE:HB2	1:A:245:TYR:CZ	2.53	0.43
1:A:232:GLU:OE1	1:A:236:LYS:HE2	2.18	0.43
1:A:337:LEU:O	2:B:79:LYS:HD3	2.19	0.43
2:B:47:ASP:O	2:B:51:LYS:HG3	2.19	0.43
1:A:414:PRO:HG2	2:B:97:LEU:HG	2.02	0.42
1:A:251:ASP:HB2	1:A:252:GLY:H	1.72	0.42
1:A:33:MET:CE	2:B:101:ARG:HB2	2.37	0.42
1:A:365:ARG:O	1:A:369:SER:HB3	2.19	0.42
1:A:276:LYS:HA	1:A:276:LYS:HD3	1.82	0.42
1:A:297:PHE:CE2	6:A:513:5KQ:CAB	3.02	0.42
1:A:53:GLY:HA2	1:A:111:VAL:O	2.19	0.42
1:A:370:GLY:C	1:A:372:GLY:HA3	2.45	0.42
1:A:95:PRO:O	1:A:98:LYS:HG2	2.20	0.42
2:B:12:LEU:HD12	2:B:13:PHE:N	2.35	0.41
2:B:61:ASN:O	2:B:65:GLU:HG3	2.20	0.41
1:A:28:MET:HE3	1:A:28:MET:HB2	1.82	0.41
1:A:117:ASN:OD1	5:A:501:CAC:AS	2.98	0.41
1:A:238:ASN:C	1:A:240:PHE:H	2.28	0.41
2:B:46:PHE:HB3	2:B:49:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ARG:CZ	2:B:153:TYR:O	2.68	0.41
1:A:106:CYS:SG	1:A:217:TYR:CE1	3.14	0.41
1:A:131:TRP:HA	1:A:131:TRP:CE3	2.55	0.41
1:A:95:PRO:HA	1:A:96:PRO:HD3	1.90	0.41
1:A:348:THR:N	1:A:363:GLU:OE2	2.32	0.41
6:A:513:5KQ:O7	6:A:513:5KQ:C10	2.69	0.41
1:A:149:SER:OG	1:A:308:ASP:N	2.49	0.41
1:A:333:GLU:HG3	1:A:344:PHE:CE2	2.56	0.41
2:B:60:THR:O	2:B:64:ILE:HG13	2.21	0.41
1:A:9:GLN:OE1	2:B:13:PHE:O	2.38	0.40
1:A:90:LEU:HD23	1:A:95:PRO:HD2	2.03	0.40
1:A:127:PHE:O	1:A:277:ILE:HG22	2.21	0.40
1:A:152:MET:HG3	1:A:307:PHE:CE2	2.56	0.40
2:B:48:LYS:HD3	2:B:119:LEU:HD13	2.03	0.40
2:B:58:ASN:HD22	2:B:58:ASN:C	2.25	0.40
2:B:130:ILE:HD13	2:B:146:CYS:SG	2.61	0.40
1:A:54:PHE:HB3	1:A:103:TYR:CD2	2.56	0.40
1:A:93:PHE:O	1:A:181:LYS:N	2.47	0.40
1:A:94:GLY:N	1:A:95:PRO:HD3	2.37	0.40
1:A:106:CYS:HA	1:A:151:CYS:HA	2.04	0.40
2:B:44:ALA:C	2:B:46:PHE:H	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:OG	6:A:502:5KQ:O4[14_545]	1.89	0.31

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	420/427 (98%)	371 (88%)	47 (11%)	2 (0%)	24	57
2	B	147/166 (89%)	112 (76%)	25 (17%)	10 (7%)	1	5
All	All	567/593 (96%)	483 (85%)	72 (13%)	12 (2%)	5	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	46	PHE
2	B	109	SER
2	B	49	ILE
2	B	133	GLU
2	B	154	ILE
1	A	198	GLN
2	B	21	VAL
1	A	130	ASN
2	B	11	LEU
2	B	19	GLY
2	B	43	GLN
2	B	34	GLY

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	360/361 (100%)	324 (90%)	36 (10%)	7	29
2	B	108/123 (88%)	92 (85%)	16 (15%)	3	13
All	All	468/484 (97%)	416 (89%)	52 (11%)	6	24

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	13	GLU
1	A	25	VAL
1	A	29	LYS

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Mol	Chain	Res	Type
1	A	33	MET
1	A	34	THR
1	A	37	THR
1	A	49	LYS
1	A	57	SER
1	A	59	THR
1	A	81	ARG
1	A	99	VAL
1	A	114	GLU
1	A	158	LEU
1	A	171	THR
1	A	175	CYS
1	A	198	GLN
1	A	199	VAL
1	A	209	THR
1	A	236	LYS
1	A	256	LEU
1	A	257	ILE
1	A	263	ARG
1	A	264	VAL
1	A	290	SER
1	A	304	SER
1	A	309	THR
1	A	323	SER
1	A	328	SER
1	A	337	LEU
1	A	366	GLN
1	A	373	ASN
1	A	392	VAL
1	A	394	ASP
1	A	397	SER
1	A	424	GLN
2	B	12	LEU
2	B	14	VAL
2	B	17	VAL
2	B	29	ARG
2	B	39	VAL
2	B	41	SER
2	B	42	THR
2	B	53	ILE
2	B	58	ASN
2	B	76	GLN

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Mol	Chain	Res	Type
2	B	79	LYS
2	B	124	THR
2	B	126	ARG
2	B	142	ASP
2	B	156	ASN
2	B	157	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	238	ASN
2	B	73	HIS

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 ⓘ

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.89	2 (14%)	17,19,21	0.46	0
3	NAG	C	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.72	0
3	BMA	C	3	3	11,11,12	2.03	6 (54%)	15,15,17	2.43	8 (53%)
3	MAN	C	4	3	11,11,12	1.02	0	15,15,17	1.54	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	C	5	3	11,11,12	2.26	4 (36%)	15,15,17	2.08	4 (26%)
3	MAN	C	6	3	11,11,12	1.38	3 (27%)	15,15,17	1.15	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.36	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.37	0	17,19,21	1.07	2 (11%)
4	NAG	E	1	1,4	14,14,15	0.45	0	17,19,21	0.85	1 (5%)
4	NAG	E	2	4	14,14,15	1.25	3 (21%)	17,19,21	0.67	0
4	NAG	F	1	2,4	14,14,15	1.03	2 (14%)	17,19,21	0.60	0
4	NAG	F	2	4	14,14,15	0.44	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	MAN	O2-C2	5.96	1.55	1.43
4	E	2	NAG	C1-C2	3.52	1.57	1.52
3	C	3	BMA	C2-C3	3.08	1.57	1.52
4	F	1	NAG	O5-C1	-2.86	1.38	1.43
3	C	6	MAN	O5-C1	-2.71	1.39	1.43
3	C	3	BMA	O3-C3	2.66	1.49	1.43
3	C	3	BMA	C1-C2	2.62	1.58	1.52
3	C	3	BMA	O4-C4	2.62	1.49	1.43
3	C	5	MAN	O5-C5	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	O5-C1	-2.46	1.39	1.43
3	C	2	NAG	O5-C1	-2.45	1.39	1.43
3	C	3	BMA	C4-C5	2.34	1.58	1.53
3	C	6	MAN	C4-C5	2.29	1.57	1.53
3	C	1	NAG	C1-C2	2.27	1.55	1.52
4	F	1	NAG	C1-C2	2.27	1.55	1.52
3	C	6	MAN	C4-C3	2.24	1.58	1.52
3	C	5	MAN	C2-C3	2.23	1.55	1.52
3	C	1	NAG	O5-C1	-2.21	1.40	1.43
3	C	5	MAN	C4-C5	2.20	1.57	1.53
4	E	2	NAG	O5-C1	-2.19	1.40	1.43
4	E	2	NAG	C3-C2	2.10	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	MAN	C1-C2-C3	-5.92	101.03	109.64
3	C	3	BMA	C1-O5-C5	5.24	119.22	112.19
3	C	4	MAN	C1-O5-C5	4.00	117.55	112.19
3	C	3	BMA	C3-C4-C5	-3.87	103.22	110.23
3	C	3	BMA	O3-C3-C2	3.12	116.43	110.05
3	C	5	MAN	C1-O5-C5	3.10	116.34	112.19
3	C	5	MAN	O3-C3-C2	2.93	116.04	110.05
4	D	2	NAG	O4-C4-C5	-2.80	102.44	109.32
3	C	3	BMA	C2-C3-C4	-2.77	105.99	110.86
3	C	6	MAN	C1-C2-C3	-2.70	105.71	109.64
3	C	3	BMA	O3-C3-C4	2.69	116.71	110.38
4	E	1	NAG	C1-O5-C5	2.62	115.70	112.19
3	C	5	MAN	O2-C2-C1	2.47	114.88	109.22
3	C	4	MAN	O2-C2-C3	-2.37	105.25	110.15
3	C	3	BMA	O2-C2-C3	-2.35	105.29	110.15
3	C	3	BMA	O4-C4-C3	2.29	115.77	110.38
3	C	3	BMA	O4-C4-C5	2.23	114.83	109.32
4	D	2	NAG	O3-C3-C2	-2.17	104.89	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6

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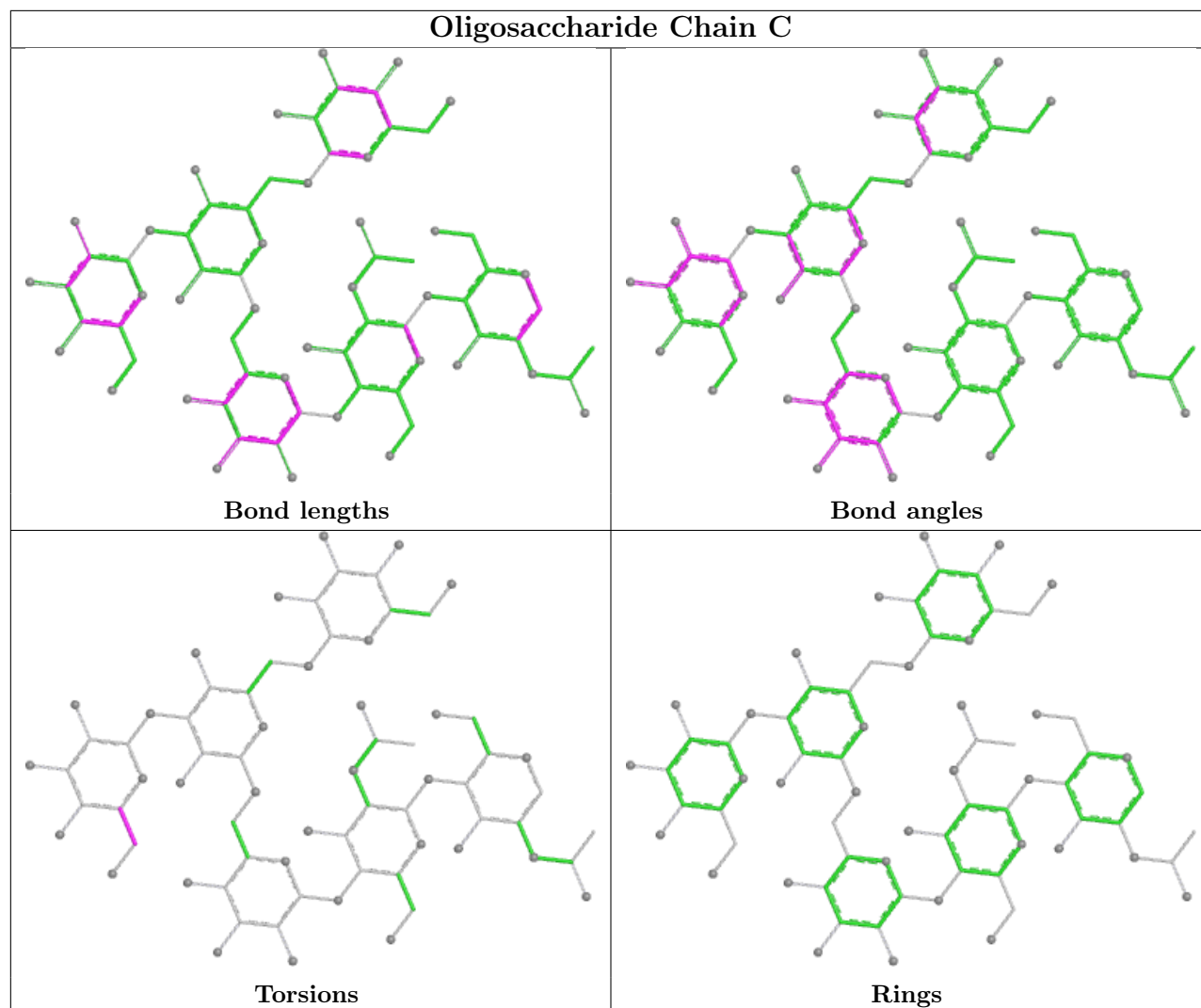
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6

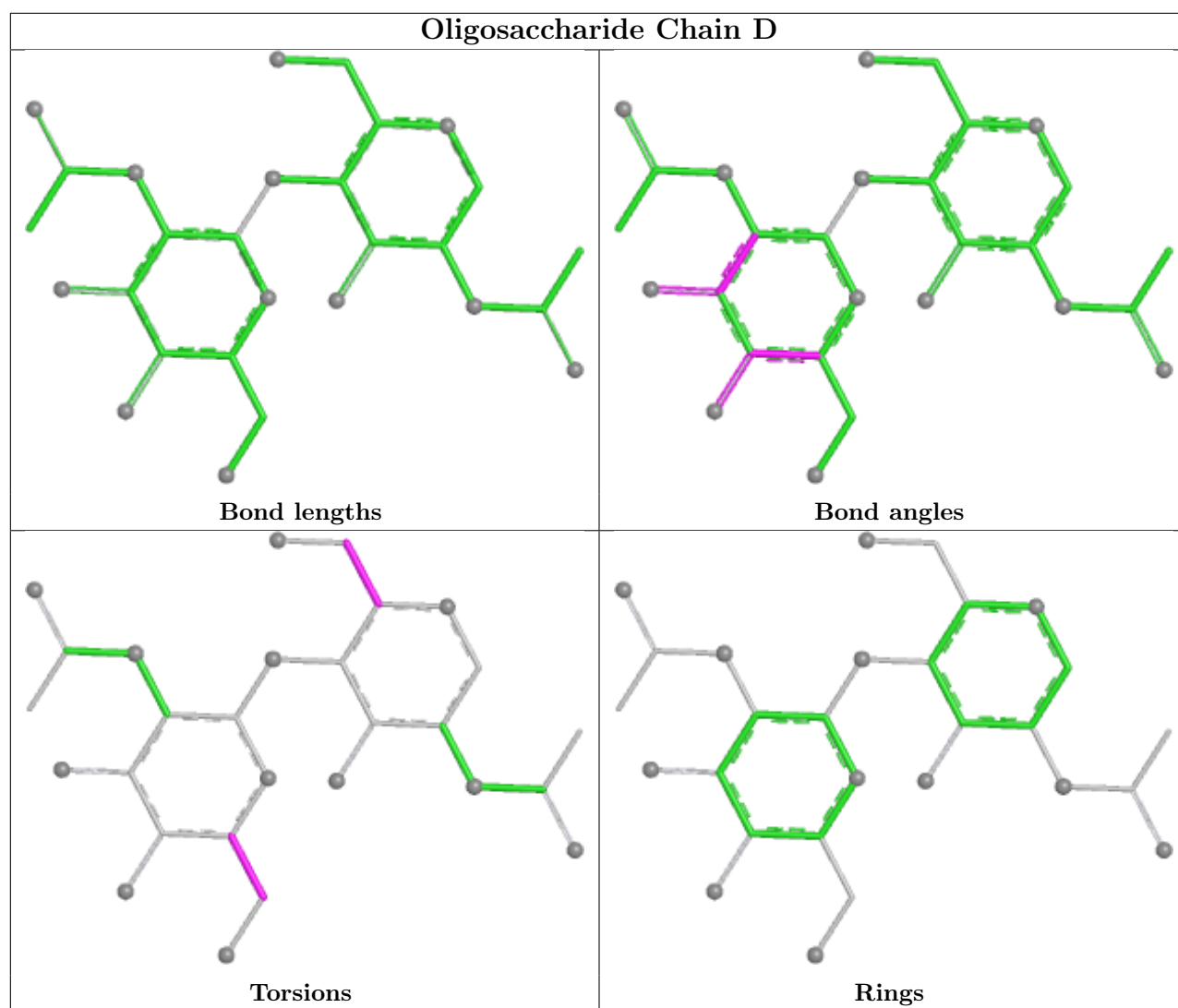
There are no ring outliers.

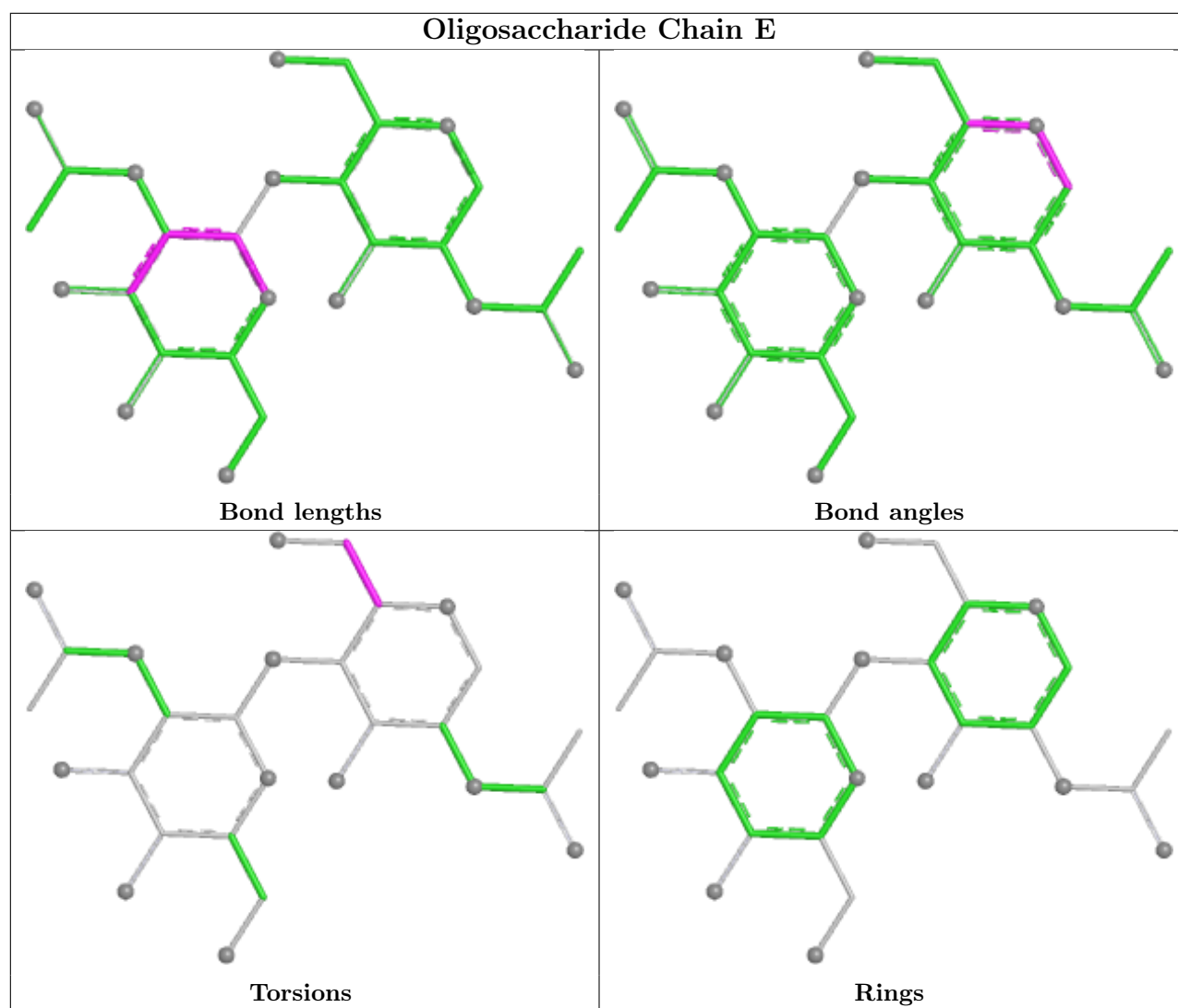
5 monomers are involved in 5 short contacts:

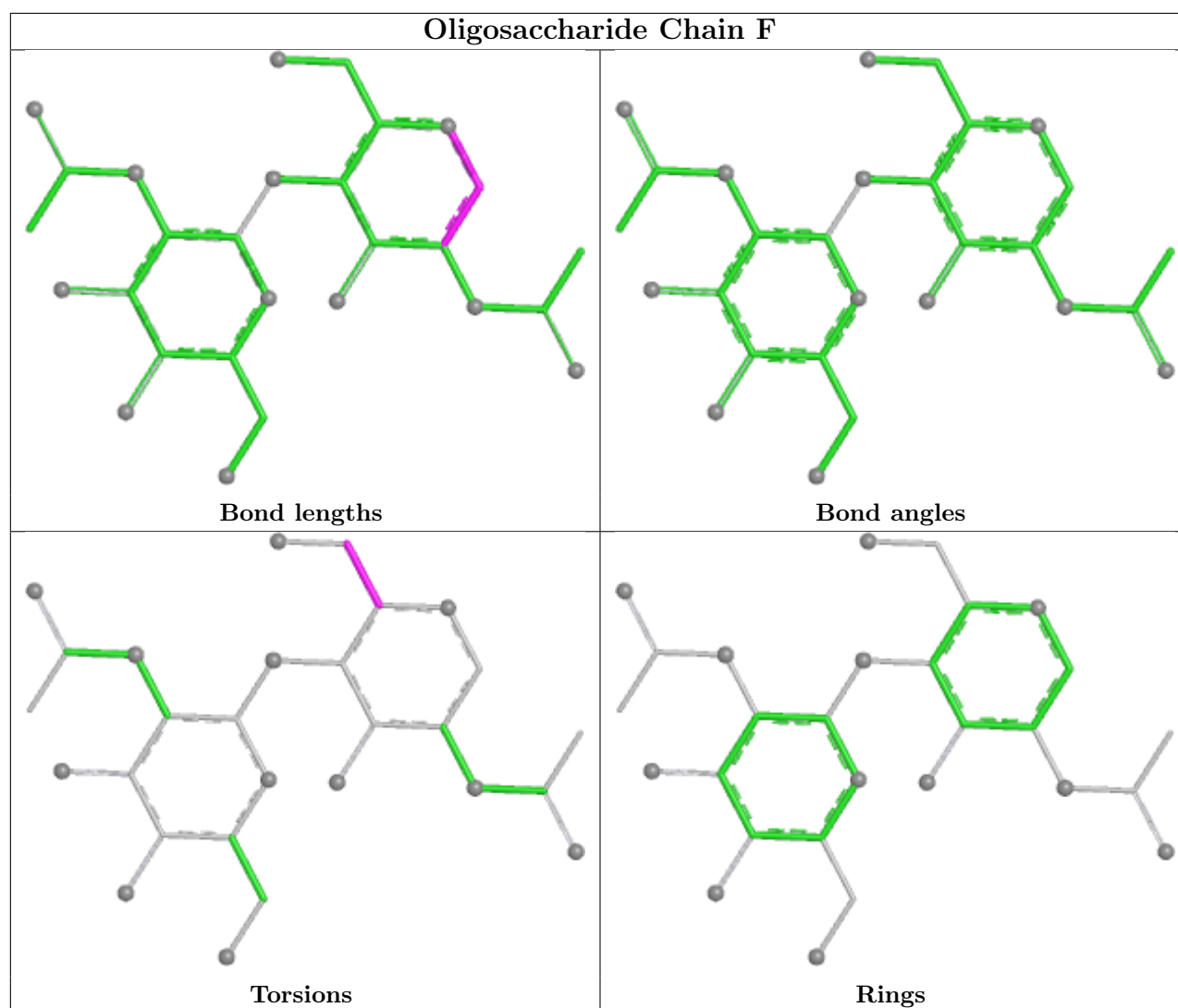
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	F	2	NAG	1	0
4	E	1	NAG	3	0
4	D	2	NAG	1	0
4	D	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
7	NAG	B	703	2	14,14,15	0.43	0	17,19,21	0.66	0
6	5KQ	A	502	-	24,24,24	0.94	1 (4%)	28,35,35	1.12	1 (3%)
6	5KQ	A	513	-	24,24,24	1.09	1 (4%)	28,35,35	1.59	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CAC	A	501	-	0,3,4	-	-	1,3,6	8.67	1 (100%)

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
7	NAG	B	703	2	-	3/6/23/26	0/1/1/1
6	5KQ	A	502	-	-	3/23/41/41	0/1/1/1
6	5KQ	A	513	-	-	6/23/41/41	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	502	5KQ	O2-C2	3.08	1.44	1.39
6	A	513	5KQ	O2-C2	2.93	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	CAC	C1-AS-C2	8.67	109.53	97.34
6	A	513	5KQ	O7-C7-C6	5.18	120.65	109.44
6	A	513	5KQ	O1A-C1-C2	-4.19	116.86	123.85
6	A	502	5KQ	O1A-C1-C2	-4.09	117.02	123.85
6	A	513	5KQ	C8-C7-C6	-3.18	107.08	113.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	5KQ	C7-C8-C9-NAD
6	A	502	5KQ	O8-C8-C9-NAD
6	A	513	5KQ	C5-C6-C7-O7
6	A	513	5KQ	C5-C6-C7-C8
6	A	513	5KQ	O6-C6-C7-O7
6	A	513	5KQ	O6-C6-C7-C8
7	B	703	NAG	O5-C5-C6-O6
6	A	513	5KQ	C8-C9-NAD-CAB
7	B	703	NAG	C4-C5-C6-O6

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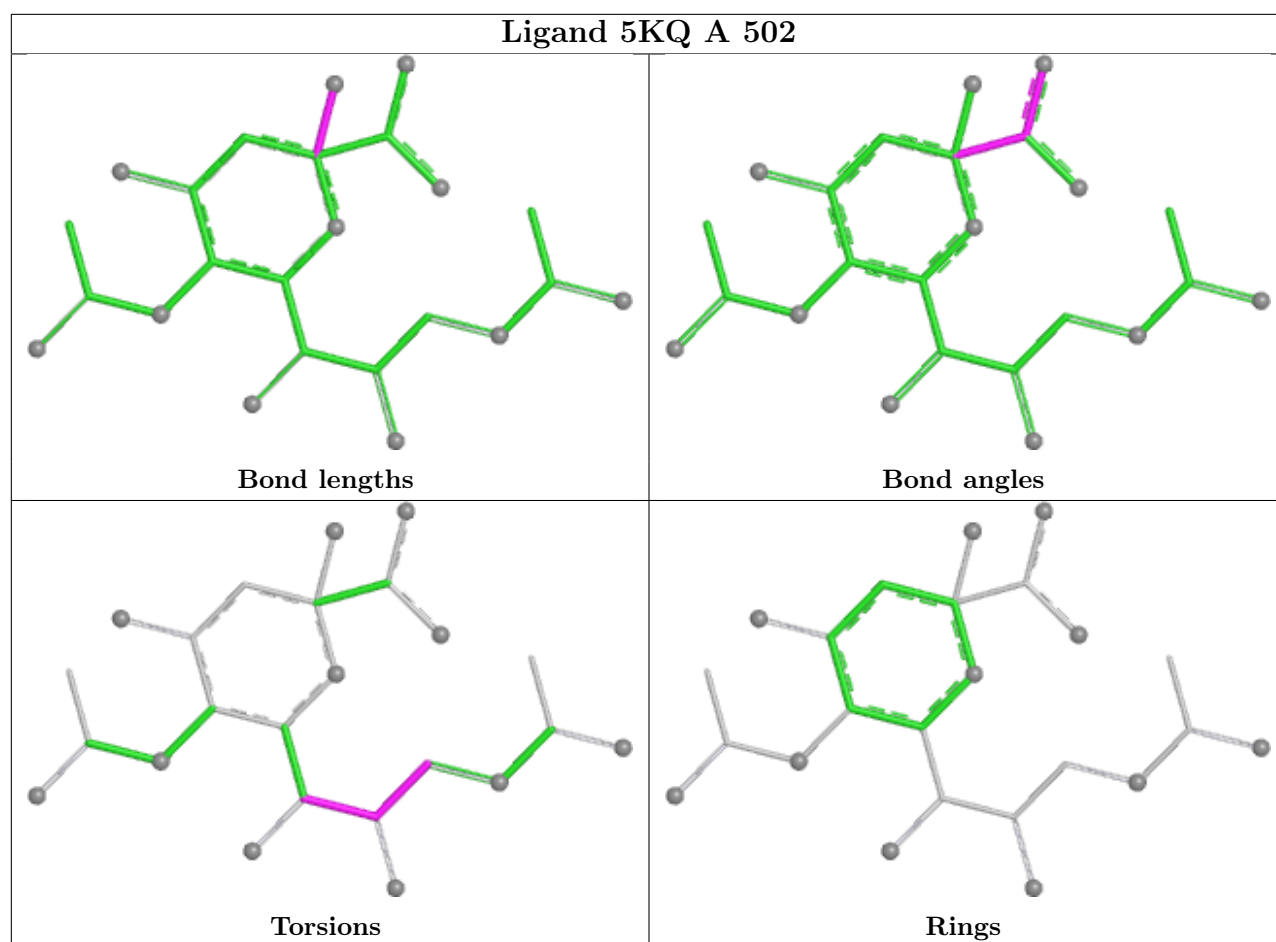
Mol	Chain	Res	Type	Atoms
6	A	513	5KQ	O7-C7-C8-O8
7	B	703	NAG	C1-C2-N2-C7
6	A	502	5KQ	O7-C7-C8-O8

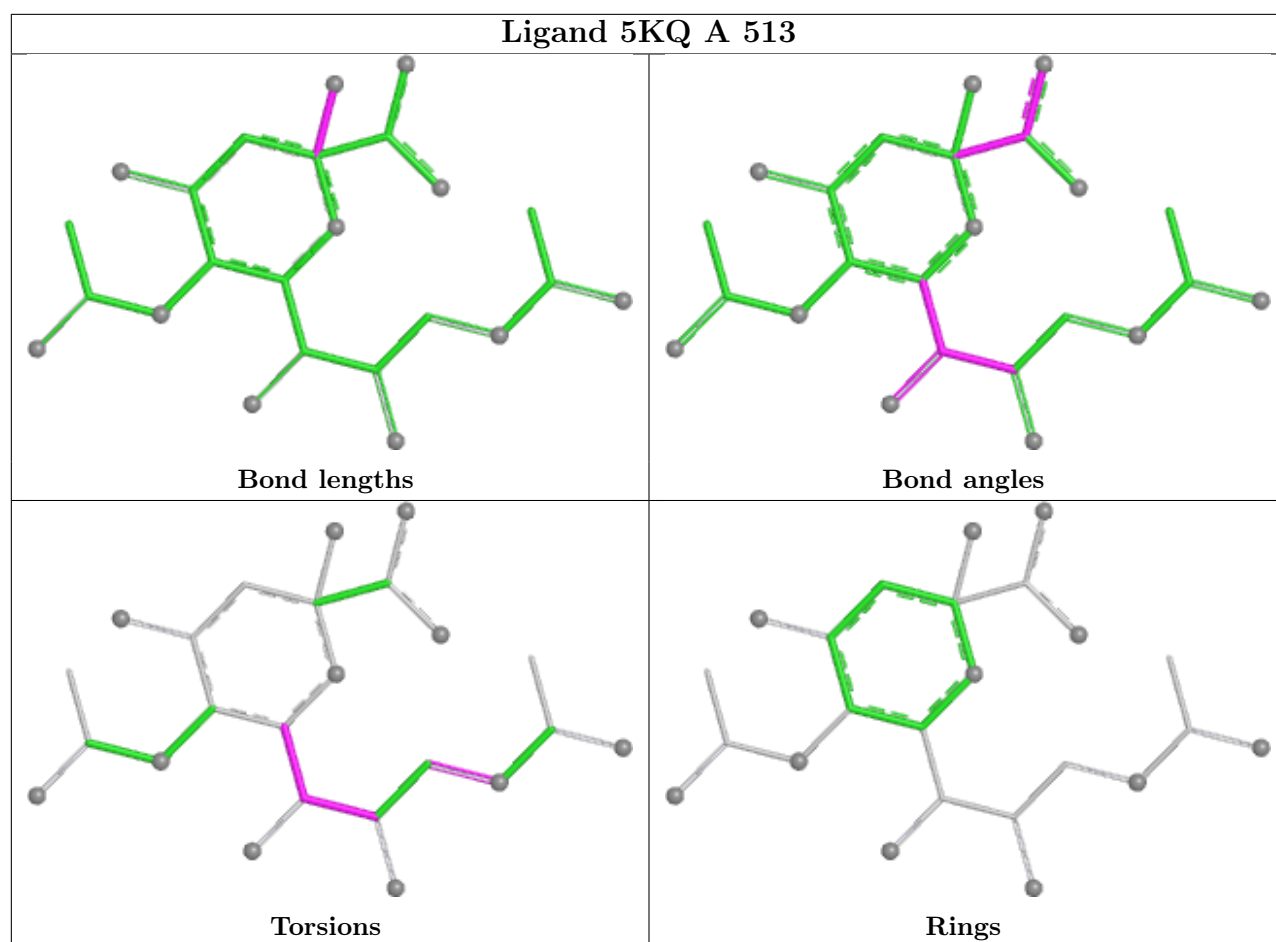
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	5KQ	3	1
6	A	513	5KQ	5	0
5	A	501	CAC	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	424/427 (99%)	-0.26	4 (0%) 81 63	61, 94, 168, 259	0
2	B	149/166 (89%)	0.15	4 (2%) 56 35	61, 154, 255, 358	0
All	All	573/593 (96%)	-0.15	8 (1%) 73 53	61, 101, 220, 358	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	TYR	4.0
2	B	112	LEU	3.1
1	A	320	SER	3.1
1	A	266	ALA	2.8
1	A	115	GLY	2.3
2	B	119	LEU	2.3
2	B	116	LEU	2.2
1	A	420	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.

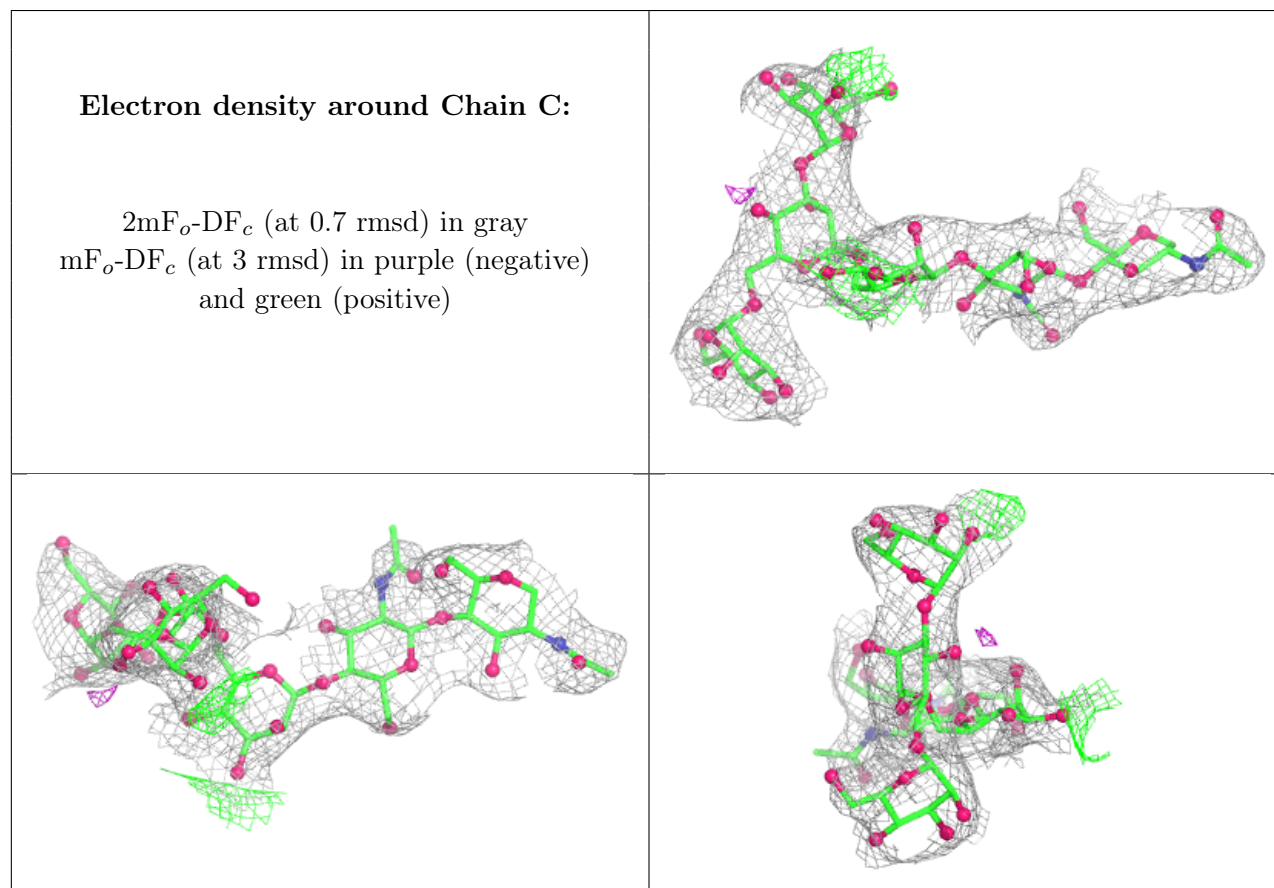
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	C	3	11/12	0.69	0.09	75,78,102,114	0

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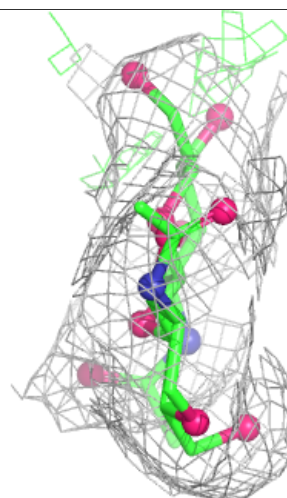
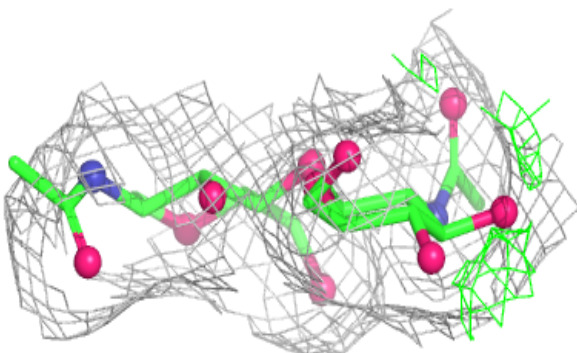
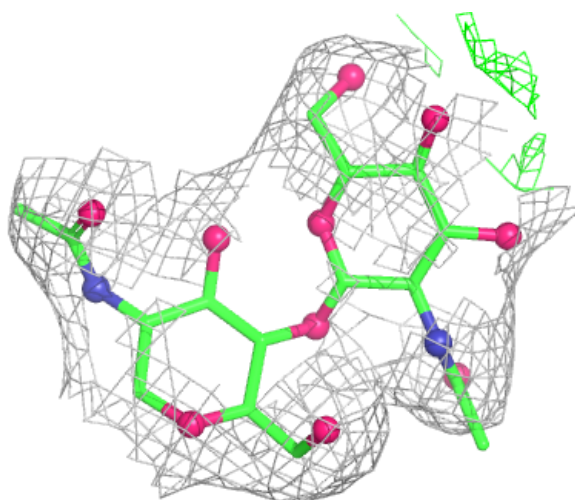
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	C	5	11/12	0.77	0.13	76,103,135,143	0
4	NAG	D	2	14/15	0.79	0.08	90,110,120,123	0
4	NAG	F	2	14/15	0.82	0.10	122,146,158,161	0
4	NAG	E	2	14/15	0.83	0.10	103,115,170,179	0
4	NAG	E	1	14/15	0.84	0.10	123,140,230,232	0
3	MAN	C	4	11/12	0.87	0.08	76,88,99,99	0
4	NAG	F	1	14/15	0.89	0.09	106,130,149,155	0
3	MAN	C	6	11/12	0.90	0.06	102,117,129,130	0
3	NAG	C	2	14/15	0.94	0.09	77,95,106,109	0
3	NAG	C	1	14/15	0.94	0.05	78,87,116,125	0
4	NAG	D	1	14/15	0.95	0.07	82,106,120,124	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.



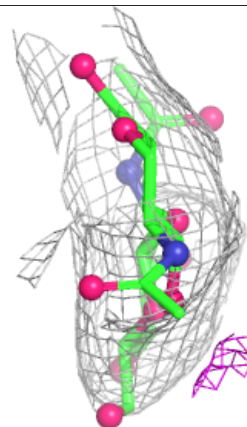
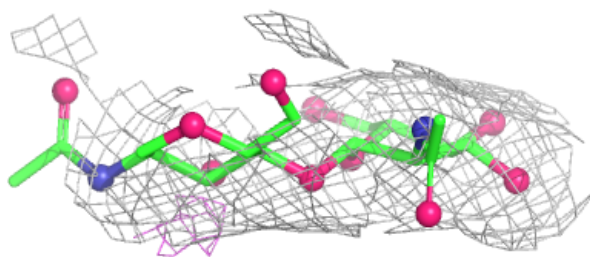
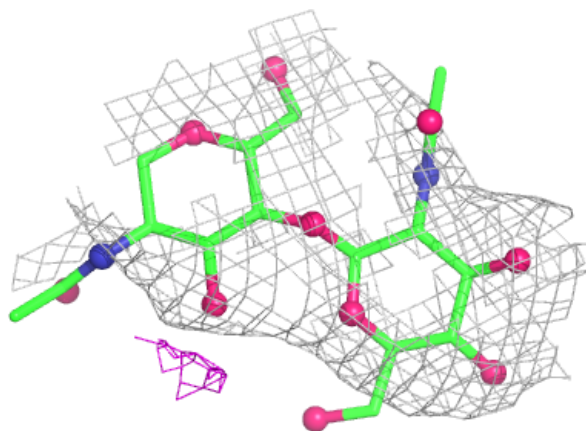
Electron density around Chain D:

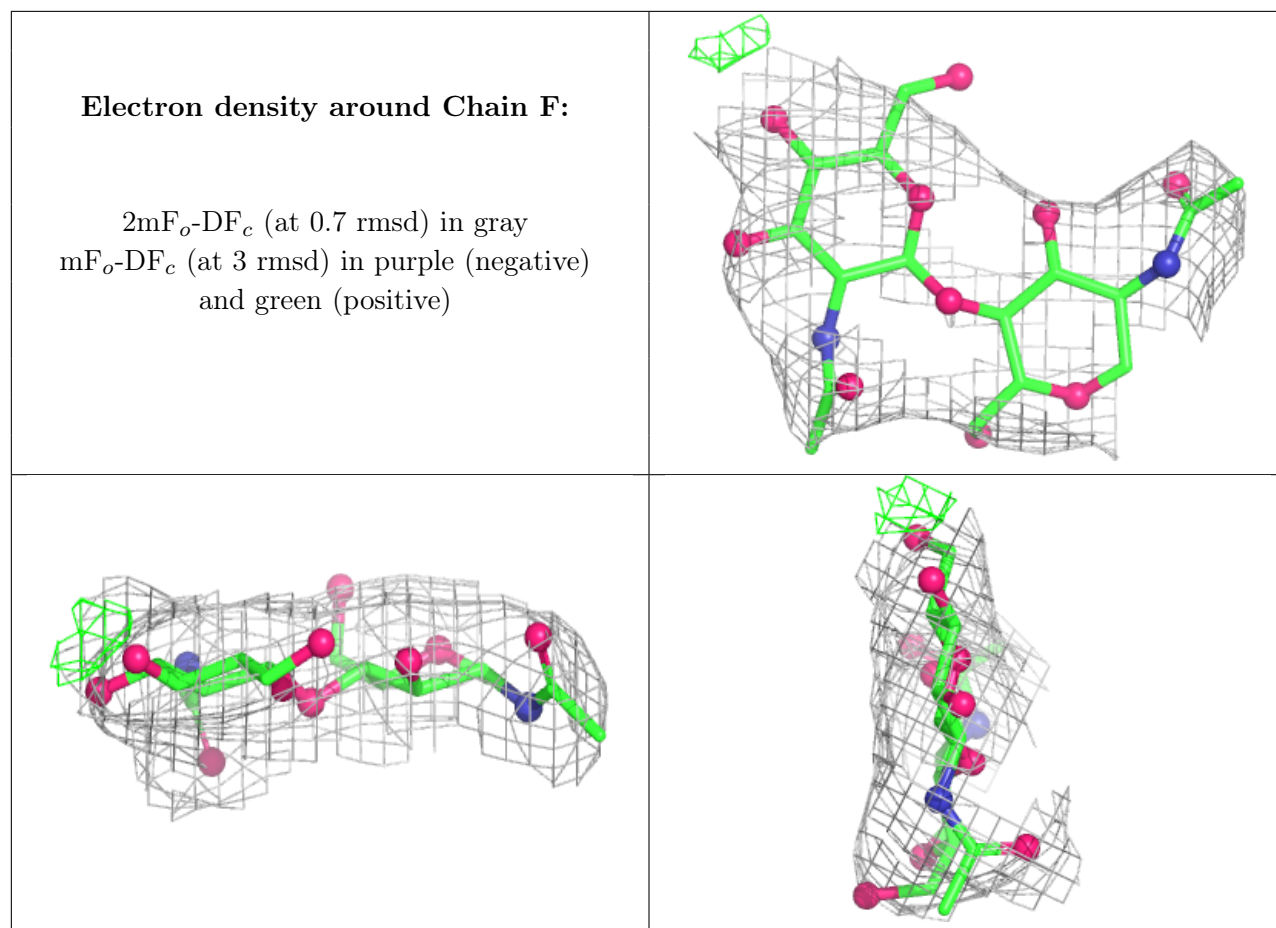
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands [i](#)

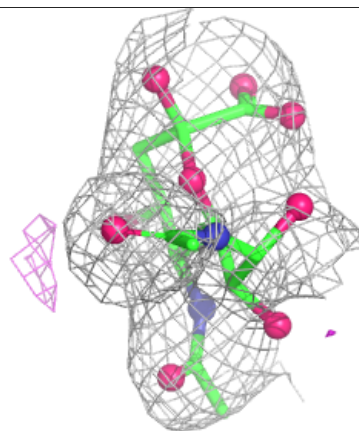
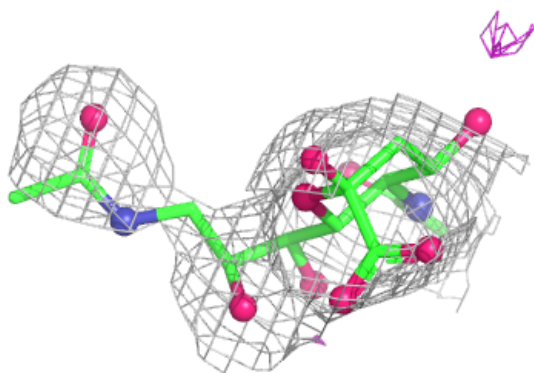
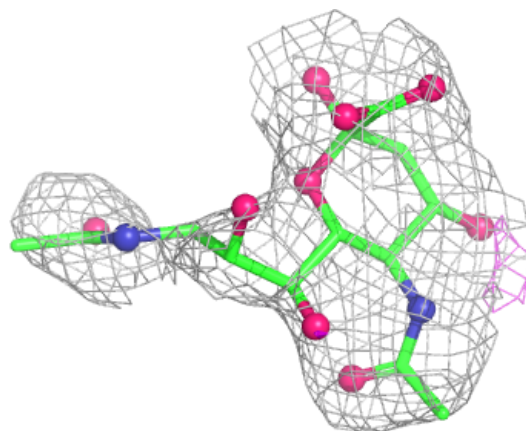
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	NAG	B	703	14/15	0.72	0.10	134,158,184,185	0
6	5KQ	A	502	24/24	0.73	0.10	72,153,168,181	0
6	5KQ	A	513	24/24	0.84	0.12	83,126,141,156	0
5	CAC	A	501	4/5	0.87	0.19	135,227,251,410	0

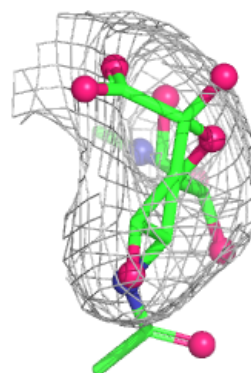
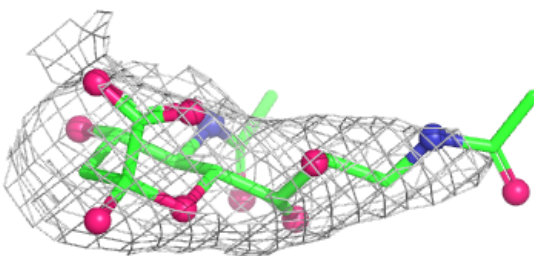
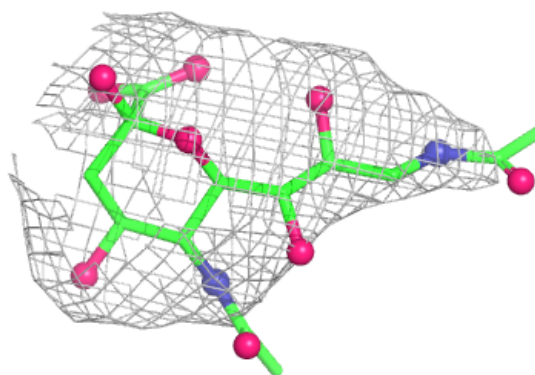
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5KQ A 502:

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

**Electron density around 5KQ A 513:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.