



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:28 PM UTC

PDB ID : 5MDR / pdb_00005mdr
Title : Crystal structure of in vitro folded Chitoporin VhChip from *Vibrio harveyi* in complex with chitohexaose
Authors : Zahn, M.; van den Berg, B.
Deposited on : 2016-11-13
Resolution : 1.90 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

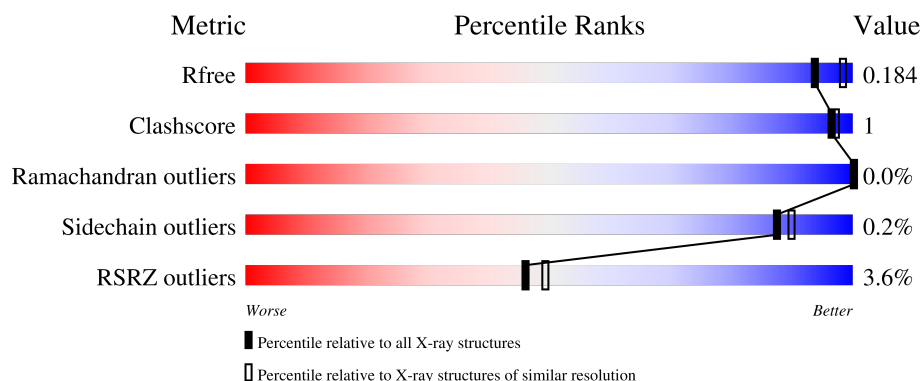
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	352	4% 95% ..
1	B	352	3% 96% ..
1	C	352	3% 95% ..
1	D	352	3% 95% ..
1	E	352	4% 95% ..

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Mol	Chain	Length	Quality of chain
1	F	352	4% 96%
2	G	6	67% 33%
2	H	6	17% 50% 33%
2	I	6	33% 67%
2	J	6	33% 67%
2	K	6	17% 50% 33%
2	L	6	67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18479 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 Chitoporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	Se	0	1	0
			2677	1689	439	540	9			
1	B	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	C	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	D	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	E	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	F	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			

There are 12 discrepancies between the modelled and reference sequences:

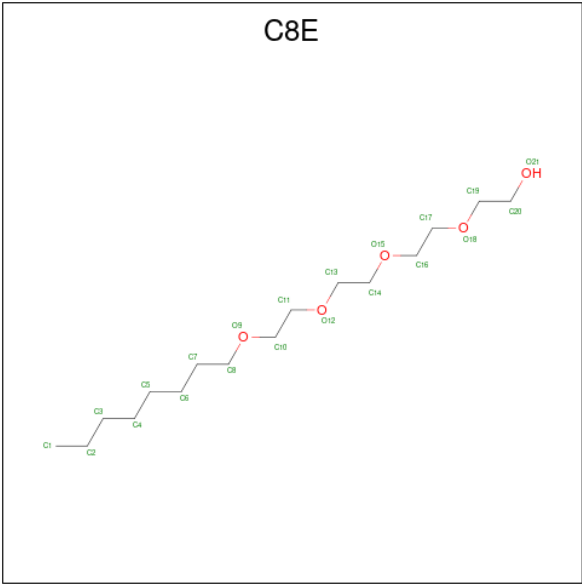
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	initiating methionine	UNP L0RVU0
A	0	GLY	-	expression tag	UNP L0RVU0
B	-1	MSE	-	initiating methionine	UNP L0RVU0
B	0	GLY	-	expression tag	UNP L0RVU0
C	-1	MSE	-	initiating methionine	UNP L0RVU0
C	0	GLY	-	expression tag	UNP L0RVU0
D	-1	MSE	-	initiating methionine	UNP L0RVU0
D	0	GLY	-	expression tag	UNP L0RVU0
E	-1	MSE	-	initiating methionine	UNP L0RVU0
E	0	GLY	-	expression tag	UNP L0RVU0
F	-1	MSE	-	initiating methionine	UNP L0RVU0
F	0	GLY	-	expression tag	UNP L0RVU0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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
2	G	6	Total	C	N	O	0	0	0
			85	48	6	31			
2	H	6	Total	C	N	O	0	0	0
			85	48	6	31			
2	I	6	Total	C	N	O	0	0	0
			85	48	6	31			
2	J	6	Total	C	N	O	0	0	0
			85	48	6	31			
2	K	6	Total	C	N	O	0	0	0
			85	48	6	31			
2	L	6	Total	C	N	O	0	0	0
			85	48	6	31			

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	8	4		
3	A	1	Total	C	O	0	0
			9	6	3		
3	A	1	Total	C	O	0	0
			14	9	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 8 1	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 21 16 5	0	0
3	B	1	Total C O 13 11 2	0	0
3	B	1	Total C O 12 10 2	0	0
3	C	1	Total C O 21 16 5	0	0
3	D	1	Total C O 14 12 2	0	0
3	D	1	Total C O 13 11 2	0	0
3	D	1	Total C O 11 10 1	0	0
3	E	1	Total C O 12 10 2	0	0
3	E	1	Total C O 15 12 3	0	0
3	F	1	Total C O 17 14 3	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Na 4 4	0	0
4	B	3	Total Na 3 3	0	0
4	C	2	Total Na 2 2	0	0
4	D	4	Total Na 4 4	0	0
4	E	3	Total Na 3 3	0	0
4	F	2	Total Na 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total 314	O 314	0	0
5	B	275	Total 275	O 275	0	0
5	C	288	Total 288	O 288	0	0
5	D	280	Total 280	O 280	0	0
5	E	279	Total 279	O 279	0	0
5	F	312	Total 312	O 312	0	0

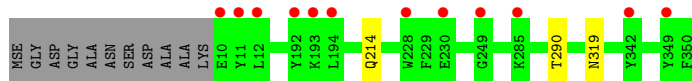
3 Residue-property plots [i](#)

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

- Molecule 1: Chitoporin



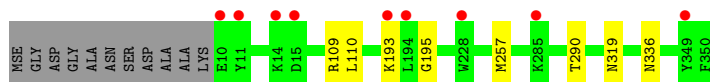
- Molecule 1: Chitoporin



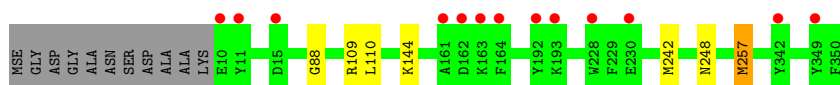
- Molecule 1: Chitoporin



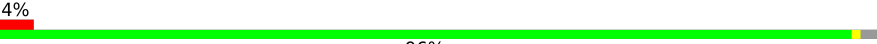
- Molecule 1: Chitoporin

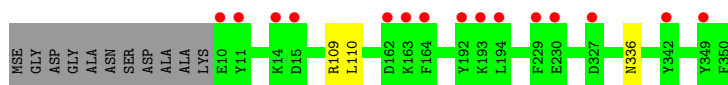


- Molecule 1: Chitoporin



- Molecule 1: Chitoporin

Chain F:  4% 96%

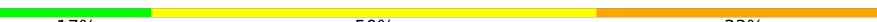


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%



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

Chain H:  17% 50% 33%



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

Chain I:  33% 67%



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

Chain J:  33% 67%



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

Chain K:  17% 50% 33%

MAG1	MAG2	MAG3	MAG4	MAG5	MAG6
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%

MAG1	MAG2	MAG3	MAG4	MAG5	MAG6
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.55Å 121.94Å 147.16Å 90.00° 117.92° 90.00°	Depositor
Resolution (Å)	130.02 – 1.90 130.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (130.02-1.90) 99.6 (130.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.172 , 0.183 (Not available) , 0.184	Depositor DCC
R_{free} test set	3476 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h-l,k,h 0.010 for l,k,-h-l 0.015 for h,-k,-h-l 0.017 for -h-l,-k,l 0.125 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18479	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, C8E, NA

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	0.76	0/2738	0.80	2/3695 (0.1%)
1	B	0.76	0/2725	0.79	0/3677
1	C	0.74	1/2725 (0.0%)	0.81	4/3677 (0.1%)
1	D	0.79	1/2725 (0.0%)	0.83	4/3677 (0.1%)
1	E	0.71	0/2725	0.79	1/3677 (0.0%)
1	F	0.77	0/2725	0.79	0/3677
All	All	0.76	2/16363 (0.0%)	0.80	11/22080 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	LYS	CA-C	-7.07	1.44	1.52
1	D	193	LYS	CA-C	-6.91	1.44	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MSE	CG-SE-CE	-8.73	79.71	98.92
1	D	195	GLY	CA-C-N	-8.33	112.33	120.83
1	D	195	GLY	C-N-CA	-8.33	112.33	120.83
1	C	195	GLY	CA-C-N	-8.31	112.36	120.83
1	C	195	GLY	C-N-CA	-8.31	112.36	120.83
1	D	193	LYS	CB-CA-C	-6.82	99.14	110.19
1	E	257	MSE	CG-SE-CE	6.57	113.37	98.92
1	C	257	MSE	CG-SE-CE	-6.35	84.95	98.92
1	A	257	MSE	CG-SE-CE	6.11	112.36	98.92
1	C	193	LYS	CB-CA-C	-5.88	100.66	110.19
1	A	193	LYS	CB-CA-C	5.62	119.01	109.80

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	2677	0	2428	3	0
1	B	2665	0	2420	2	0
1	C	2665	0	2420	3	0
1	D	2665	0	2420	3	0
1	E	2665	0	2420	4	0
1	F	2665	0	2420	2	0
2	G	85	0	75	3	0
2	H	85	0	75	4	0
2	I	85	0	75	5	0
2	J	85	0	75	3	0
2	K	85	0	75	1	0
2	L	85	0	75	2	0
3	A	73	0	109	1	0
3	B	25	0	42	0	0
3	C	21	0	34	0	0
3	D	38	0	63	0	0
3	E	27	0	46	0	0
3	F	17	0	27	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	314	0	0	1	0
5	B	275	0	0	3	0
5	C	288	0	0	0	0
5	D	280	0	0	1	0
5	E	279	0	0	1	0
5	F	312	0	0	1	0
All	All	18479	0	15299	33	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 1.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4:NAG:O3	2:G:5:NAG:O5	1.96	0.83
2:I:4:NAG:O3	2:I:5:NAG:O5	2.06	0.72
2:K:4:NAG:O3	2:K:5:NAG:O5	2.07	0.71
1:A:291:SER:OG	3:A:403:C8E:H171	1.90	0.69
2:H:4:NAG:O3	2:H:5:NAG:O5	2.11	0.66
1:F:336:ASN:OD1	5:F:501:HOH:O	2.14	0.66
2:L:4:NAG:O3	2:L:5:NAG:O5	2.12	0.62
2:J:4:NAG:O3	2:J:5:NAG:O5	2.15	0.59
1:D:336:ASN:OD1	5:D:501:HOH:O	2.17	0.58
5:B:557:HOH:O	2:H:4:NAG:H61	2.04	0.58
1:C:136:TRP:CH2	2:I:4:NAG:H83	2.39	0.57
2:G:4:NAG:HO3	2:G:5:NAG:C1	2.21	0.52
2:J:4:NAG:HO3	2:J:5:NAG:C5	2.21	0.52
2:H:5:NAG:O3	2:H:5:NAG:H82	2.11	0.51
2:I:4:NAG:O3	2:I:4:NAG:H82	2.14	0.46
2:I:4:NAG:HO3	2:I:5:NAG:C1	2.21	0.46
5:B:584:HOH:O	2:H:4:NAG:H81	2.16	0.45
2:L:4:NAG:HO3	2:L:5:NAG:C1	2.24	0.45
2:J:1:NAG:O3	2:J:2:NAG:O5	2.34	0.45
1:D:109:ARG:C	1:D:110:LEU:HD12	2.43	0.44
1:B:214:GLN:NE2	5:B:509:HOH:O	2.49	0.43
1:E:88:GLY:O	5:E:501:HOH:O	2.21	0.43
1:A:175:LYS:NZ	5:A:513:HOH:O	2.51	0.42
1:D:290:THR:HA	1:D:319:ASN:HB2	2.01	0.42
2:I:1:NAG:O3	2:I:2:NAG:O5	2.38	0.42
1:A:144:LYS:HD3	1:A:242:MSE:SE	2.70	0.41
1:E:144:LYS:HD3	1:E:242:MSE:SE	2.69	0.41
1:B:290:THR:HA	1:B:319:ASN:HB2	2.03	0.41
1:E:109:ARG:C	1:E:110:LEU:HD12	2.45	0.41
2:G:4:NAG:O3	2:G:5:NAG:C1	2.69	0.41
1:C:290:THR:HA	1:C:319:ASN:HB2	2.03	0.41
1:C:248:ASN:HA	1:E:248:ASN:HA	2.03	0.40
1:F:109:ARG:C	1:F:110:LEU:HD12	2.46	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	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
1	B	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
1	C	339/352 (96%)	331 (98%)	7 (2%)	1 (0%)	36	29
1	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
1	E	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
1	F	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
All	All	2035/2112 (96%)	1990 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	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	263/258 (102%)	262 (100%)	1 (0%)	84	87
1	B	262/258 (102%)	262 (100%)	0	100	100
1	C	262/258 (102%)	261 (100%)	1 (0%)	84	87
1	D	262/258 (102%)	262 (100%)	0	100	100
1	E	262/258 (102%)	261 (100%)	1 (0%)	84	87
1	F	262/258 (102%)	262 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1573/1548 (102%)	1570 (100%)	3 (0%)	87 90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	MSE
1	C	257	MSE
1	E	257	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	336	ASN
1	B	336	ASN
1	C	336	ASN
1	D	336	ASN
1	E	336	ASN
1	F	336	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 ⓘ

36 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	0.89	0	21,21,21	1.59	4 (19%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	1.24	2 (11%)
2	NAG	G	3	2	14,14,15	0.42	0	17,19,21	0.98	1 (5%)
2	NAG	G	4	2	14,14,15	0.71	0	17,19,21	2.20	6 (35%)
2	NAG	G	5	2	14,14,15	0.80	0	17,19,21	3.10	11 (64%)
2	NAG	G	6	2	14,14,15	0.88	1 (7%)	17,19,21	2.99	6 (35%)
2	NAG	H	1	2	15,15,15	0.84	0	21,21,21	1.80	5 (23%)
2	NAG	H	2	2	14,14,15	0.56	0	17,19,21	1.14	2 (11%)
2	NAG	H	3	2	14,14,15	0.42	0	17,19,21	1.01	0
2	NAG	H	4	2	14,14,15	0.59	0	17,19,21	2.16	7 (41%)
2	NAG	H	5	2	14,14,15	0.81	0	17,19,21	2.34	7 (41%)
2	NAG	H	6	2	14,14,15	0.87	0	17,19,21	2.54	4 (23%)
2	NAG	I	1	2	15,15,15	0.96	1 (6%)	21,21,21	1.86	5 (23%)
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
2	NAG	I	3	2	14,14,15	0.35	0	17,19,21	1.24	1 (5%)
2	NAG	I	4	2	14,14,15	0.56	0	17,19,21	2.11	4 (23%)
2	NAG	I	5	2	14,14,15	0.77	0	17,19,21	1.91	4 (23%)
2	NAG	I	6	2	14,14,15	0.89	1 (7%)	17,19,21	2.98	5 (29%)
2	NAG	J	1	2	15,15,15	0.90	1 (6%)	21,21,21	1.83	5 (23%)
2	NAG	J	2	2	14,14,15	0.58	0	17,19,21	1.36	2 (11%)
2	NAG	J	3	2	14,14,15	0.45	0	17,19,21	1.11	1 (5%)
2	NAG	J	4	2	14,14,15	0.60	0	17,19,21	1.76	5 (29%)
2	NAG	J	5	2	14,14,15	0.66	0	17,19,21	1.77	4 (23%)
2	NAG	J	6	2	14,14,15	0.83	0	17,19,21	2.78	5 (29%)
2	NAG	K	1	2	15,15,15	0.93	0	21,21,21	1.66	5 (23%)
2	NAG	K	2	2	14,14,15	0.39	0	17,19,21	1.12	1 (5%)
2	NAG	K	3	2	14,14,15	0.31	0	17,19,21	1.26	0
2	NAG	K	4	2	14,14,15	0.60	0	17,19,21	1.78	6 (35%)
2	NAG	K	5	2	14,14,15	0.60	0	17,19,21	1.51	3 (17%)
2	NAG	K	6	2	14,14,15	0.75	0	17,19,21	2.44	3 (17%)
2	NAG	L	1	2	15,15,15	0.86	0	21,21,21	1.85	4 (19%)
2	NAG	L	2	2	14,14,15	0.43	0	17,19,21	1.10	1 (5%)
2	NAG	L	3	2	14,14,15	0.29	0	17,19,21	0.85	1 (5%)
2	NAG	L	4	2	14,14,15	0.62	0	17,19,21	1.39	2 (11%)
2	NAG	L	5	2	14,14,15	0.80	0	17,19,21	3.06	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	6	2	14,14,15	0.68	0	17,19,21	2.88	6 (35%)

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	-	2/6/26/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	3	2	-	2/6/23/26	0/1/1/1
2	NAG	G	4	2	-	2/6/23/26	0/1/1/1
2	NAG	G	5	2	-	5/6/23/26	0/1/1/1
2	NAG	G	6	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	4/6/26/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	3	2	-	1/6/23/26	0/1/1/1
2	NAG	H	4	2	-	2/6/23/26	0/1/1/1
2	NAG	H	5	2	-	4/6/23/26	0/1/1/1
2	NAG	H	6	2	-	6/6/23/26	0/1/1/1
2	NAG	I	1	2	-	3/6/26/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	3	2	-	1/6/23/26	0/1/1/1
2	NAG	I	4	2	-	2/6/23/26	0/1/1/1
2	NAG	I	5	2	-	3/6/23/26	0/1/1/1
2	NAG	I	6	2	-	6/6/23/26	0/1/1/1
2	NAG	J	1	2	-	4/6/26/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	3	2	-	1/6/23/26	0/1/1/1
2	NAG	J	4	2	-	0/6/23/26	0/1/1/1
2	NAG	J	5	2	-	2/6/23/26	0/1/1/1
2	NAG	J	6	2	-	5/6/23/26	0/1/1/1
2	NAG	K	1	2	-	2/6/26/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	0/1/1/1
2	NAG	K	4	2	-	0/6/23/26	0/1/1/1
2	NAG	K	5	2	-	2/6/23/26	0/1/1/1
2	NAG	K	6	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	2	-	4/6/26/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	3	2	-	2/6/23/26	0/1/1/1
2	NAG	L	4	2	-	2/6/23/26	0/1/1/1
2	NAG	L	5	2	-	4/6/23/26	0/1/1/1
2	NAG	L	6	2	-	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	NAG	C1-C2	2.31	1.55	1.52
2	I	1	NAG	C2-N2	2.11	1.49	1.45
2	G	6	NAG	C1-C2	2.03	1.55	1.52
2	J	1	NAG	C2-N2	2.03	1.49	1.45

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6	NAG	C2-N2-C7	8.22	133.92	122.90
2	L	5	NAG	C2-N2-C7	8.01	133.63	122.90
2	G	5	NAG	C2-N2-C7	7.67	133.18	122.90
2	L	6	NAG	C2-N2-C7	7.52	132.98	122.90
2	I	6	NAG	C2-N2-C7	7.50	132.94	122.90
2	J	6	NAG	C2-N2-C7	7.10	132.42	122.90
2	H	6	NAG	C2-N2-C7	7.04	132.34	122.90
2	J	6	NAG	C1-O5-C5	6.99	121.55	112.19
2	K	6	NAG	C2-N2-C7	6.86	132.09	122.90
2	L	6	NAG	C1-O5-C5	6.76	121.25	112.19
2	G	6	NAG	C1-O5-C5	6.29	120.62	112.19
2	I	6	NAG	C1-O5-C5	6.25	120.57	112.19
2	L	5	NAG	C8-C7-N2	5.97	126.01	116.12
2	G	5	NAG	C8-C7-N2	5.46	125.17	116.12
2	H	6	NAG	C1-O5-C5	5.40	119.42	112.19
2	L	1	NAG	C3-C2-N2	5.09	120.00	110.62
2	K	6	NAG	C1-O5-C5	4.90	118.75	112.19
2	I	4	NAG	C2-N2-C7	4.87	129.43	122.90
2	I	6	NAG	C1-C2-N2	4.85	118.08	110.43
2	H	5	NAG	C8-C7-N2	4.68	123.88	116.12
2	H	1	NAG	C3-C2-N2	4.68	119.23	110.62
2	I	1	NAG	C3-C2-N2	4.66	119.20	110.62
2	G	6	NAG	C8-C7-N2	4.53	123.63	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	NAG	C2-N2-C7	4.43	128.84	122.90
2	J	1	NAG	C3-C2-N2	4.33	118.60	110.62
2	I	4	NAG	C8-C7-N2	4.33	123.30	116.12
2	I	5	NAG	C2-N2-C7	4.28	128.64	122.90
2	J	6	NAG	C8-C7-N2	4.27	123.19	116.12
2	I	6	NAG	C8-C7-N2	4.26	123.19	116.12
2	H	4	NAG	C2-N2-C7	4.24	128.58	122.90
2	H	5	NAG	C2-N2-C7	4.21	128.55	122.90
2	H	4	NAG	C3-C4-C5	-4.14	102.73	110.23
2	G	5	NAG	C1-O5-C5	4.13	117.73	112.19
2	K	6	NAG	C8-C7-N2	4.07	122.87	116.12
2	G	1	NAG	C3-C2-N2	4.03	118.05	110.62
2	L	6	NAG	C8-C7-N2	3.97	122.71	116.12
2	L	5	NAG	C1-O5-C5	3.87	117.37	112.19
2	G	4	NAG	O4-C4-C5	3.69	118.42	109.32
2	K	1	NAG	C3-C2-N2	3.65	117.35	110.62
2	I	5	NAG	C1-C2-N2	-3.63	104.71	110.43
2	H	5	NAG	C1-O5-C5	3.57	116.97	112.19
2	J	5	NAG	C1-O5-C5	3.54	116.93	112.19
2	G	4	NAG	C3-C4-C5	-3.38	104.10	110.23
2	I	3	NAG	C1-O5-C5	3.36	116.69	112.19
2	H	1	NAG	C1-C2-C3	-3.36	105.96	110.54
2	J	5	NAG	O5-C1-C2	-3.31	106.17	111.29
2	K	4	NAG	O3-C3-C2	-3.27	102.60	109.40
2	G	4	NAG	C8-C7-N2	3.27	121.54	116.12
2	K	5	NAG	C1-O5-C5	3.23	116.52	112.19
2	I	2	NAG	C1-O5-C5	3.21	116.49	112.19
2	J	1	NAG	C2-N2-C7	3.21	130.61	123.11
2	L	1	NAG	C1-C2-C3	-3.20	106.18	110.54
2	I	1	NAG	C2-N2-C7	3.19	130.57	123.11
2	G	5	NAG	C1-C2-N2	-3.18	105.42	110.43
2	H	6	NAG	C8-C7-N2	3.17	121.38	116.12
2	L	1	NAG	C2-N2-C7	3.17	130.53	123.11
2	K	4	NAG	C1-C2-N2	3.16	115.42	110.43
2	L	5	NAG	C1-C2-N2	-3.15	105.48	110.43
2	I	5	NAG	C1-O5-C5	3.13	116.38	112.19
2	J	5	NAG	C1-C2-N2	3.10	115.31	110.43
2	G	2	NAG	C1-O5-C5	3.07	116.30	112.19
2	G	5	NAG	O7-C7-C8	-3.06	116.61	122.05
2	H	5	NAG	O7-C7-C8	-2.96	116.78	122.05
2	G	4	NAG	C1-O5-C5	2.93	116.12	112.19
2	H	5	NAG	C4-C3-C2	2.92	115.29	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C2-N2-C7	2.92	129.93	123.11
2	J	4	NAG	O3-C3-C2	-2.89	103.39	109.40
2	H	4	NAG	C8-C7-N2	2.88	120.90	116.12
2	L	6	NAG	C1-C2-N2	2.87	114.96	110.43
2	G	5	NAG	O3-C3-C4	-2.87	103.62	110.38
2	L	5	NAG	O7-C7-C8	-2.84	117.00	122.05
2	L	5	NAG	O7-C7-N2	-2.83	116.98	121.98
2	G	1	NAG	C2-N2-C7	2.81	129.68	123.11
2	H	1	NAG	C2-N2-C7	2.80	129.66	123.11
2	G	5	NAG	C4-C3-C2	2.72	115.01	111.02
2	H	5	NAG	O5-C1-C2	-2.71	107.10	111.29
2	H	4	NAG	O4-C4-C5	2.66	115.89	109.32
2	I	2	NAG	O5-C1-C2	-2.66	107.17	111.29
2	I	1	NAG	O7-C7-N2	2.62	126.62	121.98
2	J	1	NAG	O7-C7-N2	2.60	126.58	121.98
2	K	4	NAG	O4-C4-C5	2.60	115.73	109.32
2	G	2	NAG	C2-N2-C7	2.58	126.35	122.90
2	J	4	NAG	C1-C2-N2	2.57	114.49	110.43
2	J	1	NAG	O4-C4-C3	2.52	116.33	110.38
2	J	3	NAG	C2-N2-C7	2.50	126.24	122.90
2	I	1	NAG	C1-C2-C3	-2.49	107.14	110.54
2	H	4	NAG	O7-C7-C8	-2.48	117.63	122.05
2	J	4	NAG	C2-N2-C7	2.47	126.22	122.90
2	K	1	NAG	C4-C3-C2	2.47	114.00	110.40
2	L	1	NAG	O7-C7-N2	2.47	126.34	121.98
2	G	5	NAG	O5-C1-C2	-2.45	107.50	111.29
2	I	1	NAG	C4-C3-C2	2.45	113.96	110.40
2	I	2	NAG	C2-N2-C7	2.44	126.17	122.90
2	H	4	NAG	C6-C5-C4	2.44	119.00	113.02
2	I	4	NAG	C1-O5-C5	2.42	115.43	112.19
2	K	1	NAG	O7-C7-N2	2.42	126.25	121.98
2	J	4	NAG	C1-O5-C5	2.40	115.41	112.19
2	J	5	NAG	O4-C4-C3	2.40	116.02	110.38
2	J	2	NAG	C2-N2-C7	2.39	126.10	122.90
2	L	4	NAG	C1-O5-C5	2.39	115.39	112.19
2	I	6	NAG	O7-C7-C8	-2.39	117.81	122.05
2	J	1	NAG	C4-C3-C2	2.36	113.84	110.40
2	L	4	NAG	C3-C4-C5	-2.36	105.95	110.23
2	J	2	NAG	C1-O5-C5	2.36	115.35	112.19
2	H	1	NAG	C4-C3-C2	2.36	113.83	110.40
2	I	4	NAG	O7-C7-C8	-2.35	117.87	122.05
2	H	6	NAG	O5-C5-C6	2.33	112.20	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	NAG	C1-O5-C5	2.31	115.28	112.19
2	H	5	NAG	O5-C5-C6	2.29	112.12	107.66
2	K	5	NAG	O5-C5-C6	2.28	112.11	107.66
2	G	6	NAG	O7-C7-C8	-2.25	118.06	122.05
2	L	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	L	6	NAG	O7-C7-N2	-2.19	118.12	121.98
2	K	5	NAG	O5-C1-C2	-2.19	107.91	111.29
2	G	6	NAG	O5-C5-C6	2.18	111.91	107.66
2	K	2	NAG	C2-N2-C7	2.17	125.81	122.90
2	K	4	NAG	C6-C5-C4	2.16	118.32	113.02
2	G	5	NAG	O7-C7-N2	-2.13	118.21	121.98
2	K	1	NAG	O4-C4-C3	2.12	115.38	110.38
2	H	2	NAG	C2-N2-C7	2.11	125.73	122.90
2	K	4	NAG	O3-C3-C4	2.11	115.34	110.38
2	H	4	NAG	O4-C4-C3	2.10	115.33	110.38
2	K	4	NAG	C3-C4-C5	-2.09	106.44	110.23
2	G	6	NAG	O7-C7-N2	-2.08	118.30	121.98
2	G	1	NAG	C4-C3-C2	2.08	113.43	110.40
2	G	5	NAG	O5-C5-C6	2.08	111.71	107.66
2	G	5	NAG	O4-C4-C3	2.06	115.22	110.38
2	G	4	NAG	O7-C7-C8	-2.06	118.39	122.05
2	L	5	NAG	O5-C1-C2	-2.06	108.11	111.29
2	G	1	NAG	O7-C7-N2	2.05	125.61	121.98
2	L	3	NAG	C1-O5-C5	2.05	114.94	112.19
2	H	1	NAG	O7-C7-N2	2.05	125.61	121.98
2	L	5	NAG	O4-C4-C3	2.05	115.20	110.38
2	J	6	NAG	O7-C7-C8	-2.04	118.42	122.05
2	J	6	NAG	O7-C7-N2	-2.03	118.39	121.98
2	J	4	NAG	O7-C7-C8	-2.03	118.44	122.05
2	L	6	NAG	O5-C5-C6	2.03	111.61	107.66
2	I	5	NAG	O4-C4-C3	2.00	115.09	110.38
2	H	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C1-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	G	5	NAG	C3-C2-N2-C7
2	G	6	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	H	6	NAG	C3-C2-N2-C7
2	I	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	I	5	NAG	C3-C2-N2-C7
2	I	6	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	J	6	NAG	C3-C2-N2-C7
2	K	1	NAG	C1-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	K	6	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	L	5	NAG	C3-C2-N2-C7
2	L	6	NAG	C3-C2-N2-C7
2	G	5	NAG	O5-C5-C6-O6
2	L	6	NAG	O5-C5-C6-O6
2	J	6	NAG	O5-C5-C6-O6
2	J	5	NAG	O5-C5-C6-O6
2	H	6	NAG	O5-C5-C6-O6
2	I	5	NAG	O5-C5-C6-O6
2	H	5	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	3	NAG	O5-C5-C6-O6
2	K	3	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	K	5	NAG	O5-C5-C6-O6
2	I	6	NAG	C4-C5-C6-O6
2	H	5	NAG	C4-C5-C6-O6
2	L	6	NAG	C4-C5-C6-O6
2	I	6	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	J	6	NAG	C4-C5-C6-O6
2	G	4	NAG	C8-C7-N2-C2
2	G	4	NAG	O7-C7-N2-C2
2	G	5	NAG	C8-C7-N2-C2
2	G	5	NAG	O7-C7-N2-C2
2	G	6	NAG	C8-C7-N2-C2
2	G	6	NAG	O7-C7-N2-C2
2	H	4	NAG	C8-C7-N2-C2
2	H	4	NAG	O7-C7-N2-C2
2	H	5	NAG	C8-C7-N2-C2
2	H	5	NAG	O7-C7-N2-C2
2	H	6	NAG	C8-C7-N2-C2

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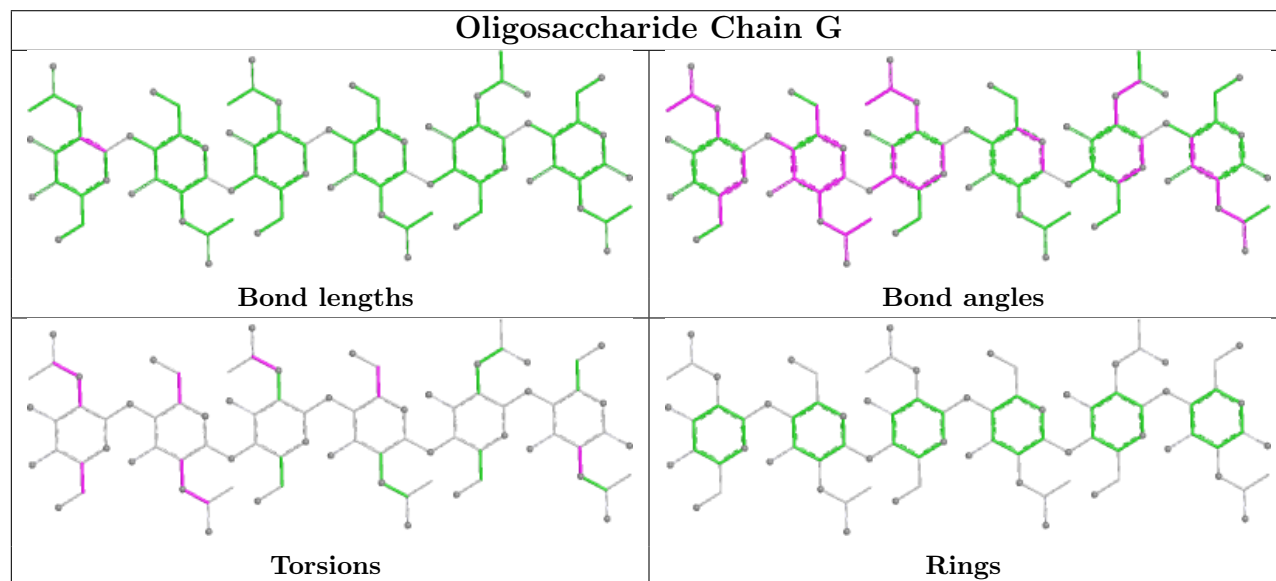
Mol	Chain	Res	Type	Atoms
2	H	6	NAG	O7-C7-N2-C2
2	I	4	NAG	C8-C7-N2-C2
2	I	4	NAG	O7-C7-N2-C2
2	I	6	NAG	C8-C7-N2-C2
2	I	6	NAG	O7-C7-N2-C2
2	J	6	NAG	C8-C7-N2-C2
2	J	6	NAG	O7-C7-N2-C2
2	K	6	NAG	C8-C7-N2-C2
2	K	6	NAG	O7-C7-N2-C2
2	L	5	NAG	C8-C7-N2-C2
2	L	5	NAG	O7-C7-N2-C2
2	L	6	NAG	C8-C7-N2-C2
2	L	6	NAG	O7-C7-N2-C2
2	L	1	NAG	O5-C5-C6-O6
2	G	5	NAG	C4-C5-C6-O6
2	J	5	NAG	C4-C5-C6-O6
2	H	6	NAG	C4-C5-C6-O6
2	L	3	NAG	O5-C5-C6-O6
2	G	3	NAG	C4-C5-C6-O6
2	K	3	NAG	C4-C5-C6-O6
2	G	6	NAG	O5-C5-C6-O6
2	J	3	NAG	O5-C5-C6-O6
2	L	4	NAG	C4-C5-C6-O6
2	K	5	NAG	C4-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
2	L	5	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	5	NAG	C4-C5-C6-O6
2	L	4	NAG	O5-C5-C6-O6
2	J	1	NAG	C1-C2-N2-C7
2	H	1	NAG	C4-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6
2	H	3	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	H	6	NAG	C1-C2-N2-C7
2	I	6	NAG	C1-C2-N2-C7
2	L	1	NAG	C1-C2-N2-C7
2	L	3	NAG	C4-C5-C6-O6

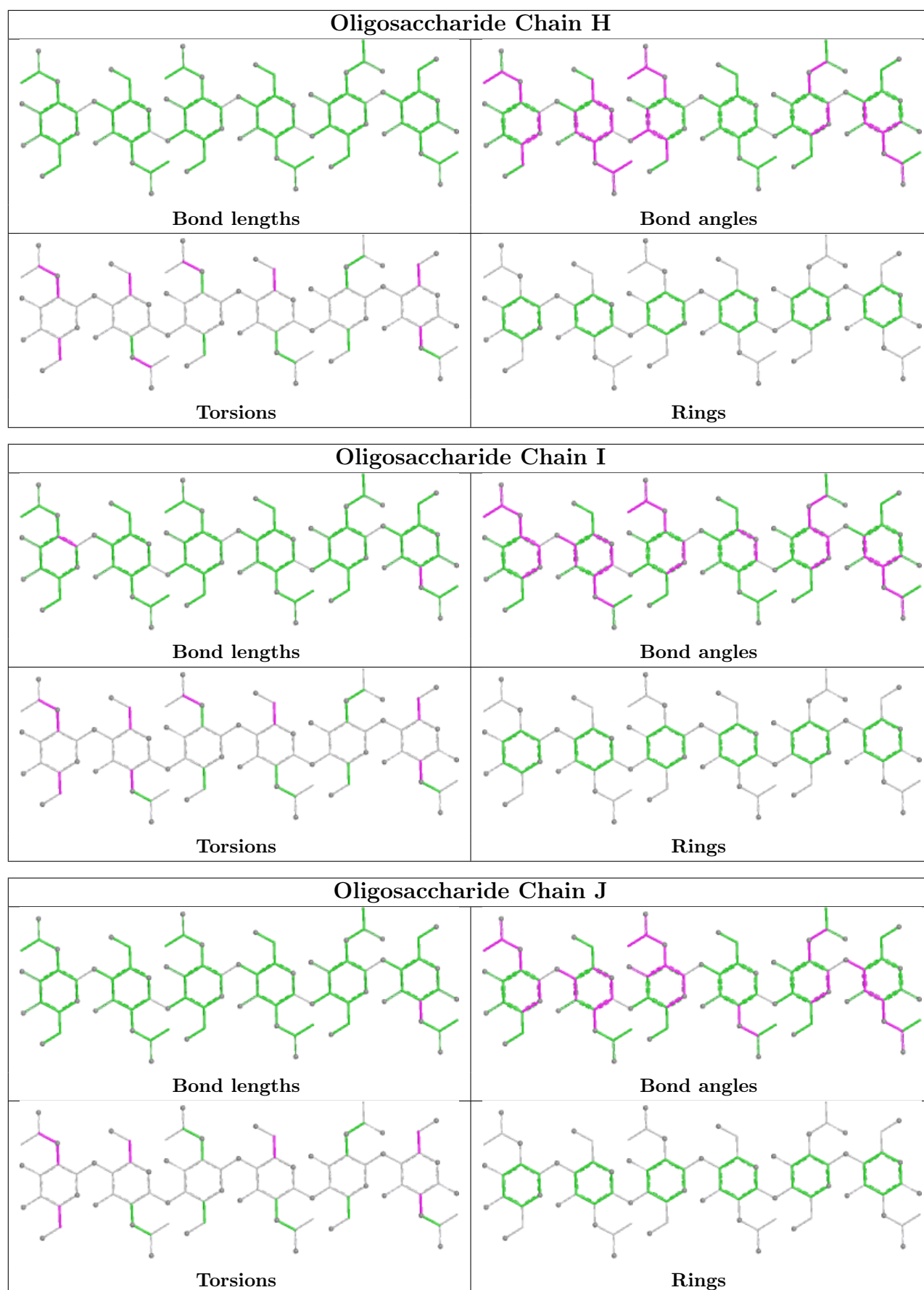
There are no ring outliers.

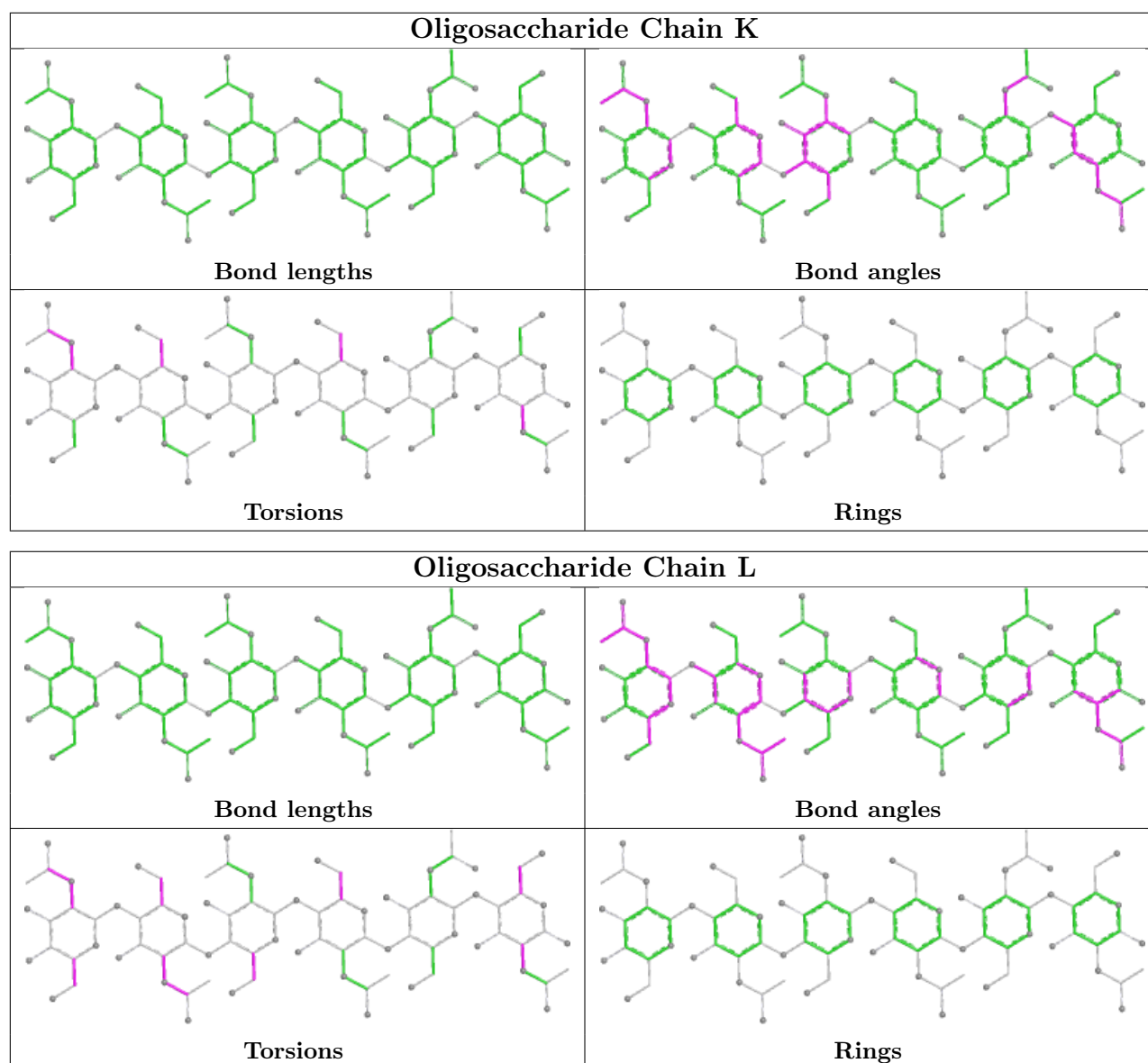
16 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	5	NAG	2	0
2	J	5	NAG	2	0
2	L	4	NAG	2	0
2	H	5	NAG	2	0
2	K	5	NAG	1	0
2	G	4	NAG	3	0
2	J	2	NAG	1	0
2	J	4	NAG	2	0
2	I	4	NAG	4	0
2	I	2	NAG	1	0
2	K	4	NAG	1	0
2	I	5	NAG	2	0
2	H	4	NAG	3	0
2	G	5	NAG	3	0
2	I	1	NAG	1	0
2	J	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](#)

Of 33 ligands modelled in this entry, 18 are monoatomic - leaving 15 for Mogul analysis.

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	C8E	A	401	-	11,11,20	0.42	0	10,10,19	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	E	402	-	14,14,20	0.37	0	13,13,19	0.70	0
3	C8E	D	402	-	12,12,20	0.47	0	11,11,19	0.47	0
3	C8E	E	401	-	11,11,20	0.24	0	10,10,19	0.48	0
3	C8E	A	403	-	13,13,20	0.45	0	12,12,19	0.55	0
3	C8E	A	406	-	20,20,20	0.49	0	19,19,19	0.67	0
3	C8E	D	403	-	10,10,20	0.45	0	9,9,19	0.38	0
3	C8E	A	404	-	8,8,20	0.26	0	7,7,19	0.38	0
3	C8E	A	402	-	8,8,20	0.56	0	7,7,19	0.26	0
3	C8E	C	401	-	20,20,20	0.43	0	19,19,19	0.46	0
3	C8E	F	401	-	16,16,20	0.37	0	15,15,19	0.33	0
3	C8E	B	401	-	12,12,20	0.43	0	11,11,19	0.45	0
3	C8E	D	401	-	13,13,20	0.52	0	12,12,19	0.65	0
3	C8E	A	405	-	7,7,20	0.28	0	6,6,19	0.39	0
3	C8E	B	402	-	11,11,20	0.30	0	10,10,19	0.47	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	C8E	A	401	-	-	3/9/9/18	-
3	C8E	E	402	-	-	6/12/12/18	-
3	C8E	D	402	-	-	5/10/10/18	-
3	C8E	E	401	-	-	2/9/9/18	-
3	C8E	A	403	-	-	4/11/11/18	-
3	C8E	A	406	-	-	8/18/18/18	-
3	C8E	D	403	-	-	2/8/8/18	-
3	C8E	A	404	-	-	3/6/6/18	-
3	C8E	A	402	-	-	0/6/6/18	-
3	C8E	C	401	-	-	7/18/18/18	-
3	C8E	F	401	-	-	3/14/14/18	-
3	C8E	B	401	-	-	3/10/10/18	-
3	C8E	D	401	-	-	2/11/11/18	-
3	C8E	A	405	-	-	1/5/5/18	-
3	C8E	B	402	-	-	4/9/9/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	C8E	O12-C13-C14-O15
3	A	406	C8E	O15-C16-C17-O18
3	A	406	C8E	O9-C10-C11-O12
3	C	401	C8E	O9-C10-C11-O12
3	E	402	C8E	O9-C10-C11-O12
3	C	401	C8E	C6-C7-C8-O9
3	B	402	C8E	C6-C7-C8-O9
3	D	402	C8E	C3-C4-C5-C6
3	A	406	C8E	O18-C19-C20-O21
3	F	401	C8E	O12-C13-C14-O15
3	D	401	C8E	C5-C6-C7-C8
3	A	406	C8E	C6-C7-C8-O9
3	B	401	C8E	C6-C7-C8-O9
3	A	403	C8E	O9-C10-C11-O12
3	D	402	C8E	C1-C2-C3-C4
3	C	401	C8E	C1-C2-C3-C4
3	D	402	C8E	C6-C7-C8-O9
3	B	402	C8E	C1-C2-C3-C4
3	B	401	C8E	O9-C10-C11-O12
3	D	403	C8E	C1-C2-C3-C4
3	F	401	C8E	C6-C7-C8-O9
3	A	403	C8E	O12-C13-C14-O15
3	C	401	C8E	O12-C13-C14-O15
3	B	401	C8E	C4-C5-C6-C7
3	A	403	C8E	C13-C14-O15-C16
3	B	402	C8E	C11-C10-O9-C8
3	E	402	C8E	C14-C13-O12-C11
3	A	404	C8E	C4-C5-C6-C7
3	A	405	C8E	C4-C5-C6-C7
3	D	402	C8E	C11-C10-O9-C8
3	E	401	C8E	C6-C7-C8-O9
3	D	401	C8E	O9-C10-C11-O12
3	C	401	C8E	C2-C3-C4-C5
3	A	404	C8E	C3-C4-C5-C6
3	A	406	C8E	C13-C14-O15-C16
3	E	401	C8E	C7-C8-O9-C10
3	A	406	C8E	C10-C11-O12-C13
3	A	403	C8E	O15-C16-C17-O18
3	A	404	C8E	C6-C7-C8-O9
3	E	402	C8E	C10-C11-O12-C13

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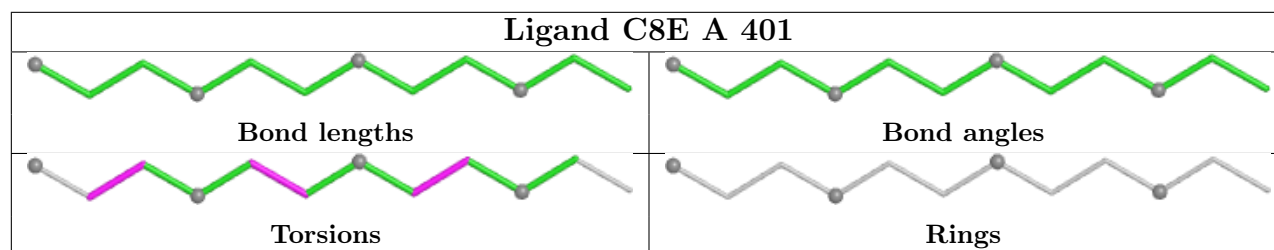
Mol	Chain	Res	Type	Atoms
3	C	401	C8E	C3-C4-C5-C6
3	F	401	C8E	C5-C6-C7-C8
3	A	406	C8E	C16-C17-O18-C19
3	A	401	C8E	O18-C19-C20-O21
3	D	403	C8E	C4-C5-C6-C7
3	A	401	C8E	O15-C16-C17-O18
3	D	402	C8E	C7-C8-O9-C10
3	E	402	C8E	C4-C5-C6-C7
3	E	402	C8E	O12-C13-C14-O15
3	C	401	C8E	O18-C19-C20-O21
3	B	402	C8E	O9-C10-C11-O12
3	A	406	C8E	O12-C13-C14-O15
3	E	402	C8E	C3-C4-C5-C6

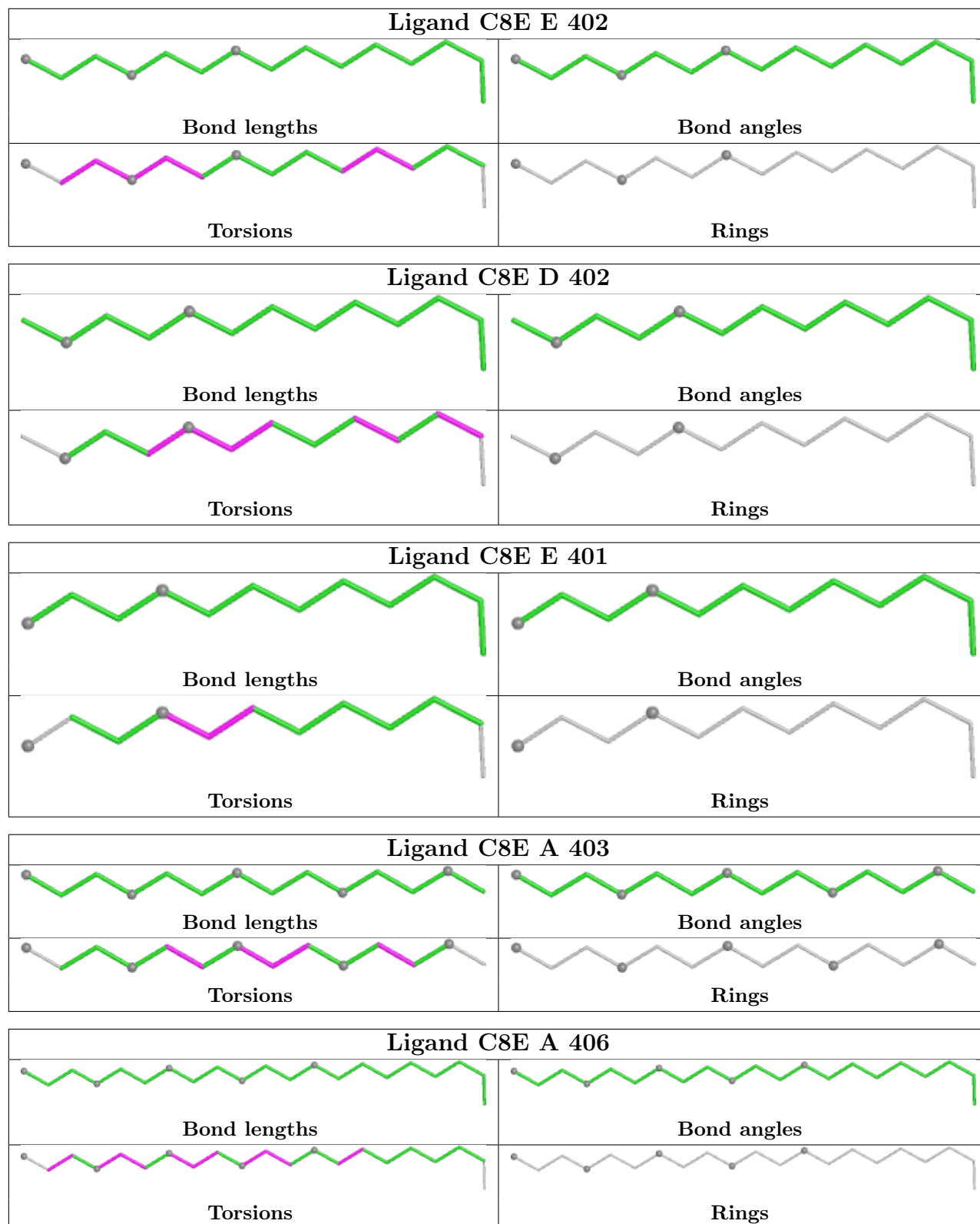
There are no ring outliers.

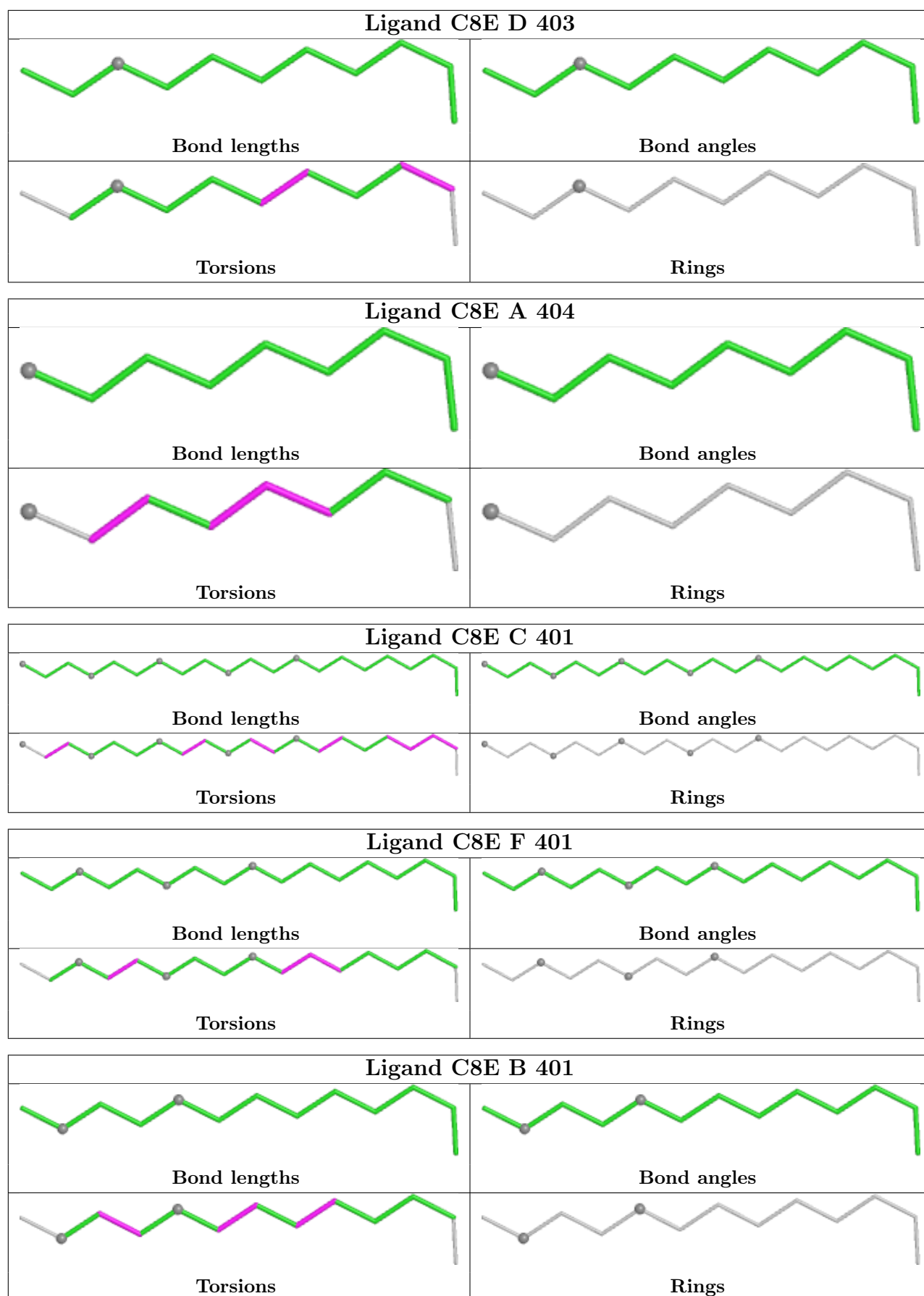
1 monomer is involved in 1 short contact:

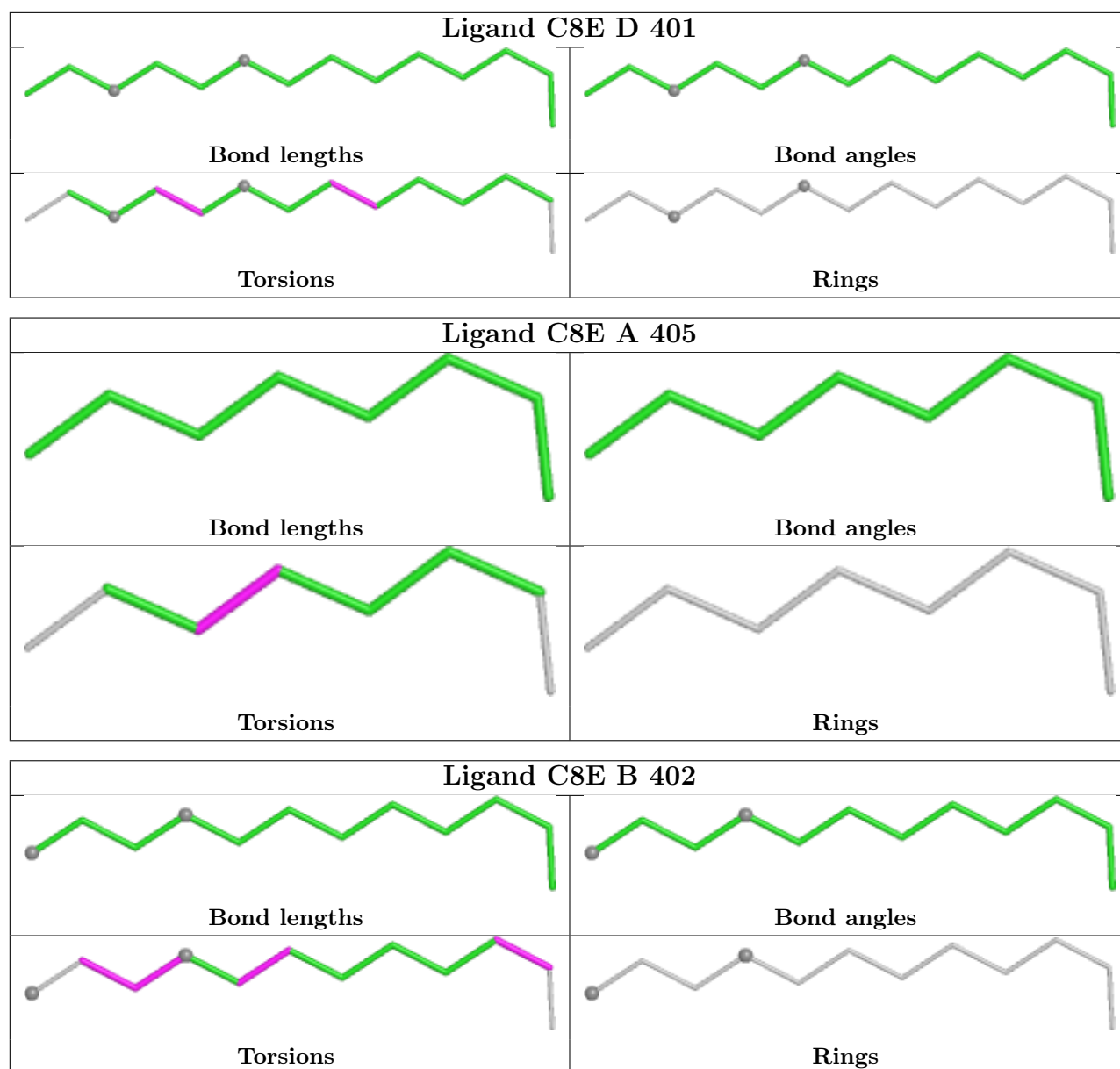
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	C8E	1	0

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

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	332/352 (94%)	-0.00	13 (3%)	43 46	18, 30, 46, 82	1 (0%)
1	B	332/352 (94%)	0.02	12 (3%)	46 49	21, 30, 48, 85	0
1	C	332/352 (94%)	0.00	10 (3%)	52 56	21, 32, 49, 75	0
1	D	332/352 (94%)	-0.05	9 (2%)	56 60	21, 30, 46, 81	0
1	E	332/352 (94%)	0.03	13 (3%)	43 46	21, 32, 49, 84	0
1	F	332/352 (94%)	-0.06	15 (4%)	38 40	20, 29, 46, 86	0
All	All	1992/2112 (94%)	-0.01	72 (3%)	46 49	18, 31, 48, 86	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	LEU	4.6
1	D	194	LEU	4.5
1	A	193	LYS	4.2
1	C	194	LEU	3.7
1	A	349	TYR	3.5
1	A	162	ASP	3.3
1	C	228	TRP	3.2
1	C	11	TYR	3.1
1	E	192	TYR	3.1
1	B	10	GLU	3.1
1	F	11	TYR	3.0
1	F	342	TYR	3.0
1	C	193	LYS	2.9
1	F	193	LYS	2.9
1	A	10	GLU	2.9
1	F	192	TYR	2.9
1	D	193	LYS	2.9
1	F	230	GLU	2.9
1	B	192	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	164	PHE	2.8
1	A	192	TYR	2.8
1	B	12	LEU	2.7
1	E	15	ASP	2.7
1	F	327	ASP	2.7
1	D	228	TRP	2.7
1	B	11	TYR	2.7
1	E	11	TYR	2.7
1	D	285	LYS	2.7
1	C	15	ASP	2.7
1	A	11	TYR	2.6
1	B	228	TRP	2.6
1	B	230	GLU	2.6
1	B	342	TYR	2.6
1	E	230	GLU	2.5
1	E	161	ALA	2.5
1	E	164	PHE	2.5
1	A	161	ALA	2.5
1	D	10	GLU	2.5
1	F	10	GLU	2.5
1	D	15	ASP	2.5
1	F	163	LYS	2.5
1	E	349	TYR	2.4
1	A	15	ASP	2.4
1	A	342[A]	TYR	2.4
1	B	249	GLY	2.4
1	E	162	ASP	2.3
1	F	162	ASP	2.3
1	E	10	GLU	2.3
1	F	14	LYS	2.3
1	D	14	LYS	2.3
1	E	163	LYS	2.3
1	C	10	GLU	2.2
1	D	11	TYR	2.2
1	D	349	TYR	2.2
1	E	342	TYR	2.2
1	B	285	LYS	2.2
1	F	194	LEU	2.2
1	B	349	TYR	2.2
1	F	164	PHE	2.2
1	E	193	LYS	2.2
1	C	342	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	349	TYR	2.1
1	C	162	ASP	2.1
1	F	15	ASP	2.1
1	C	14	LYS	2.1
1	E	228	TRP	2.1
1	A	229	PHE	2.1
1	A	194	LEU	2.1
1	A	14	LYS	2.0
1	B	193	LYS	2.0
1	F	229	PHE	2.0
1	C	349	TYR	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.

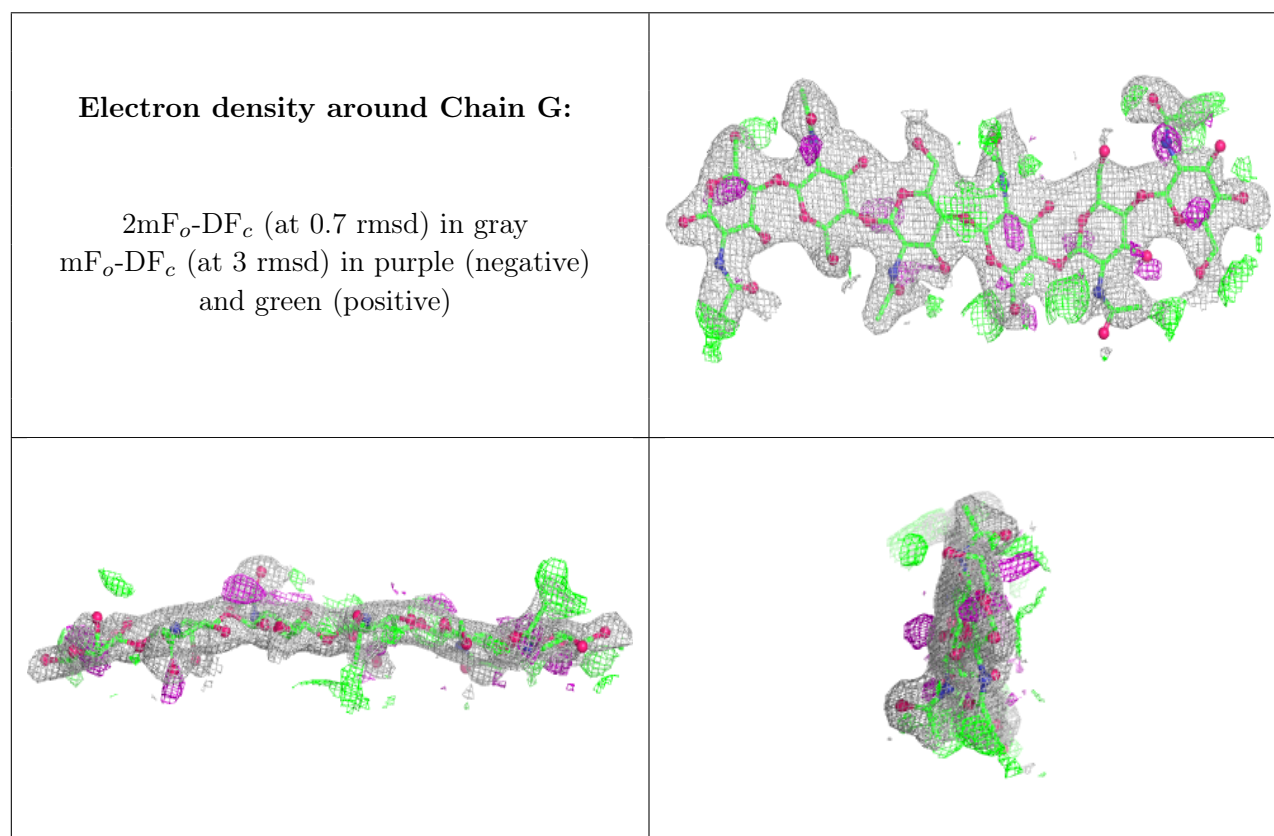
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	6	14/15	0.58	0.32	67,87,89,91	0
2	NAG	I	6	14/15	0.63	0.30	81,95,97,97	0
2	NAG	I	1	15/15	0.66	0.26	60,79,84,84	0
2	NAG	I	5	14/15	0.67	0.26	82,85,92,94	0
2	NAG	G	6	14/15	0.67	0.26	67,80,85,86	0
2	NAG	J	6	14/15	0.69	0.32	77,83,87,87	0
2	NAG	K	6	14/15	0.69	0.27	75,91,93,94	0
2	NAG	L	6	14/15	0.69	0.29	66,80,83,84	0
2	NAG	L	5	14/15	0.70	0.31	82,86,89,95	0
2	NAG	K	5	14/15	0.71	0.26	84,86,89,89	0
2	NAG	H	5	14/15	0.73	0.26	78,84,90,91	0
2	NAG	J	1	15/15	0.74	0.24	54,74,78,79	0
2	NAG	J	5	14/15	0.75	0.26	78,82,85,86	0
2	NAG	J	4	14/15	0.76	0.25	65,70,79,80	0
2	NAG	G	5	14/15	0.77	0.25	76,82,85,87	0
2	NAG	L	4	14/15	0.77	0.23	68,72,77,83	0
2	NAG	K	1	15/15	0.77	0.24	65,78,82,85	0

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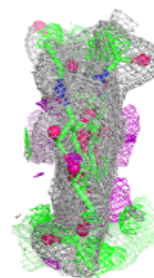
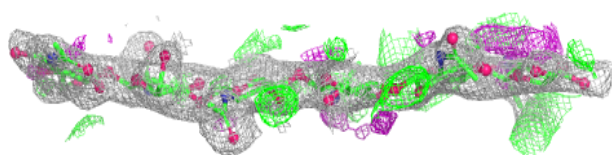
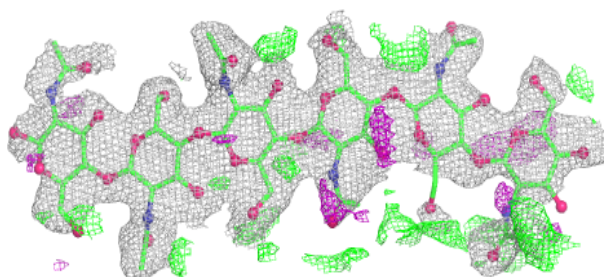
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	1	15/15	0.77	0.24	58,77,79,80	0
2	NAG	G	1	15/15	0.78	0.22	59,73,79,81	0
2	NAG	K	4	14/15	0.79	0.23	70,75,81,83	0
2	NAG	G	4	14/15	0.79	0.22	60,64,72,74	0
2	NAG	H	4	14/15	0.80	0.23	69,75,83,89	0
2	NAG	L	1	15/15	0.81	0.22	59,77,85,87	0
2	NAG	I	4	14/15	0.81	0.21	62,67,75,77	0
2	NAG	J	3	14/15	0.88	0.15	41,48,59,61	0
2	NAG	I	3	14/15	0.88	0.15	42,52,58,60	0
2	NAG	H	3	14/15	0.89	0.14	40,50,59,63	0
2	NAG	I	2	14/15	0.90	0.14	45,51,62,62	0
2	NAG	K	3	14/15	0.90	0.14	43,51,63,65	0
2	NAG	J	2	14/15	0.90	0.15	42,48,60,61	0
2	NAG	L	3	14/15	0.91	0.13	35,47,55,62	0
2	NAG	K	2	14/15	0.91	0.14	46,54,69,71	0
2	NAG	H	2	14/15	0.92	0.12	43,50,61,63	0
2	NAG	G	3	14/15	0.92	0.12	38,47,55,60	0
2	NAG	G	2	14/15	0.93	0.12	42,49,59,59	0
2	NAG	L	2	14/15	0.94	0.10	42,48,58,58	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.

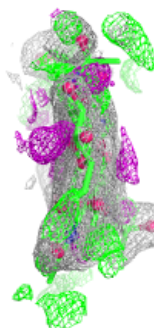
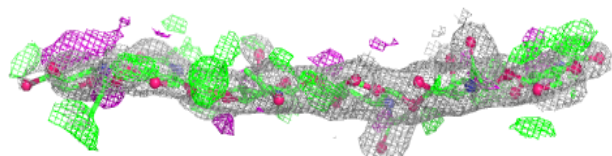
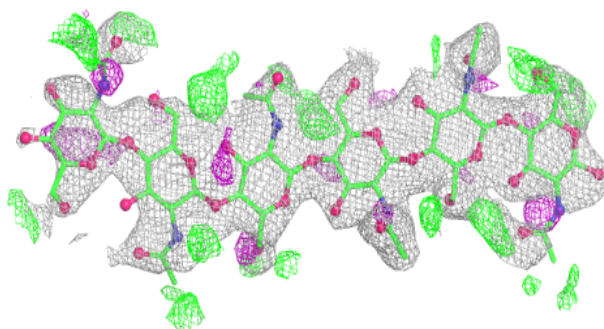


Electron density around Chain H:

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

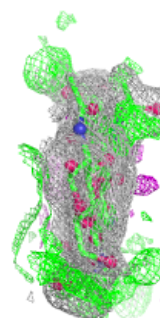
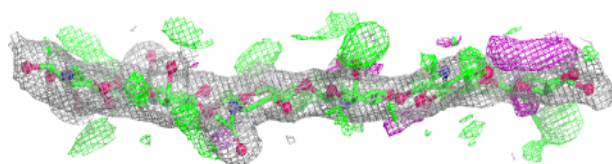
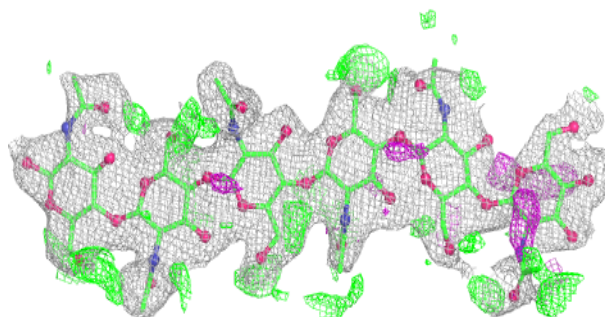
**Electron density around Chain I:**

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

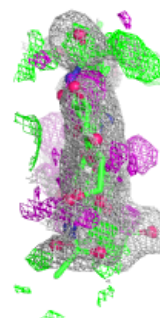
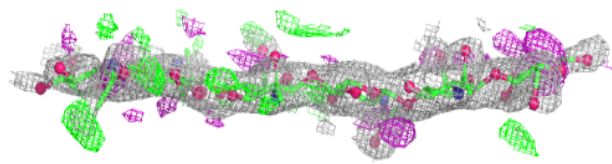
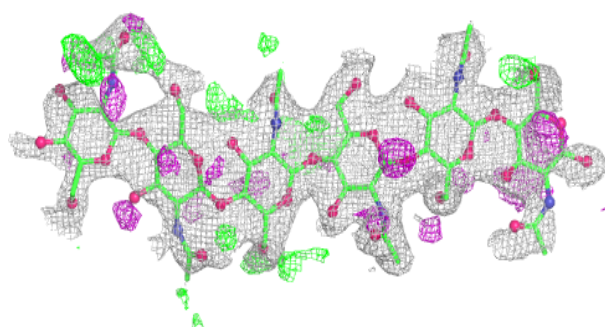


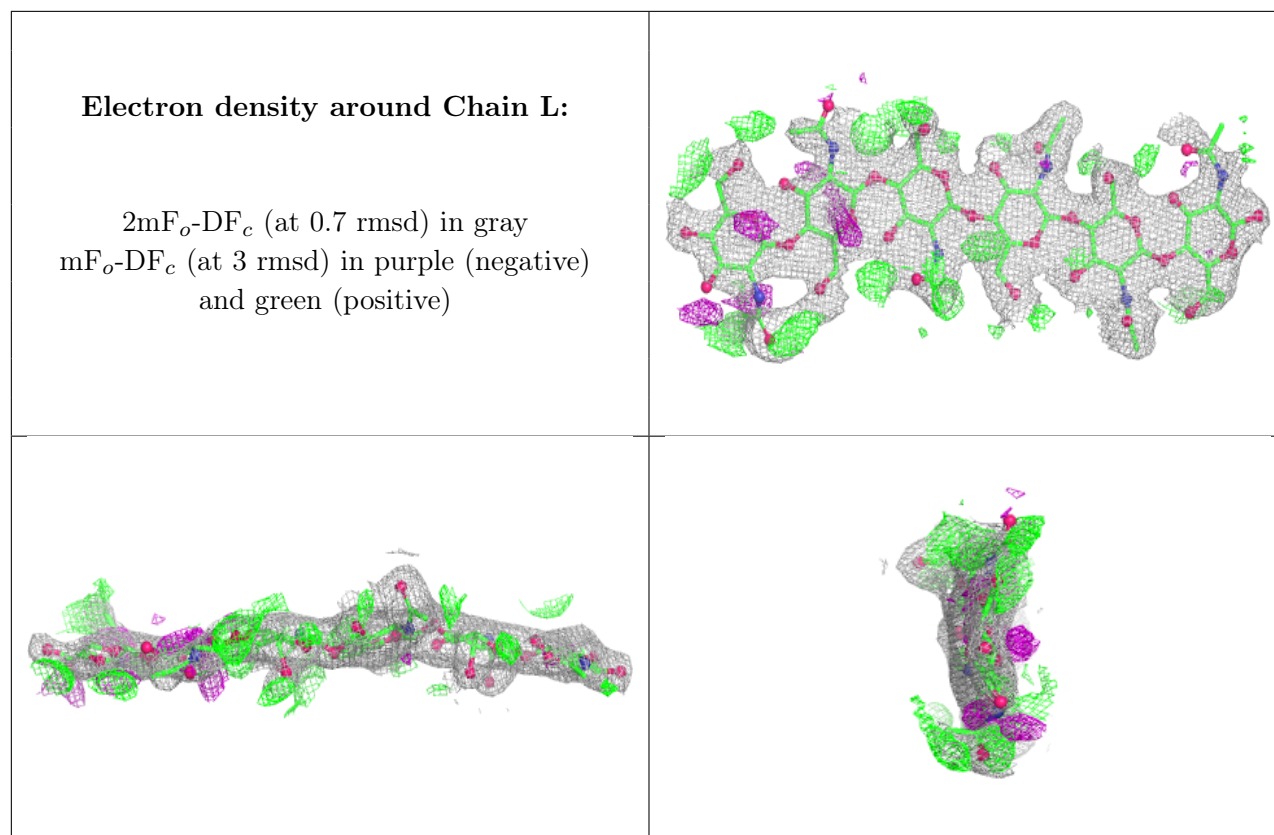
Electron density around Chain J:

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

**Electron density around Chain K:**

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





6.4 Ligands ⓘ

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
3	C8E	A	402	9/21	0.85	0.22	56,61,64,66	0
3	C8E	D	403	11/21	0.85	0.25	49,55,65,66	0
3	C8E	C	401	21/21	0.87	0.23	51,59,64,66	0
3	C8E	D	402	13/21	0.88	0.24	56,59,66,66	0
3	C8E	A	405	8/21	0.88	0.23	52,53,61,64	0
3	C8E	D	401	14/21	0.89	0.18	40,44,52,53	0
3	C8E	B	402	12/21	0.89	0.22	61,64,69,73	0
3	C8E	A	406	21/21	0.89	0.19	45,56,62,62	0
3	C8E	A	404	9/21	0.90	0.21	57,59,66,69	0
3	C8E	A	403	14/21	0.90	0.19	35,44,65,69	0
3	C8E	B	401	13/21	0.91	0.20	53,56,74,75	0
3	C8E	E	402	15/21	0.91	0.17	43,47,57,60	0
3	C8E	A	401	12/21	0.93	0.15	42,50,55,56	0
3	C8E	F	401	17/21	0.93	0.15	40,46,50,53	0

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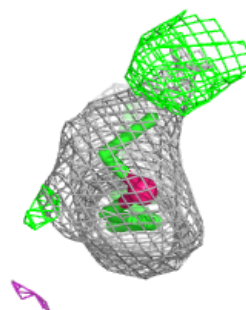
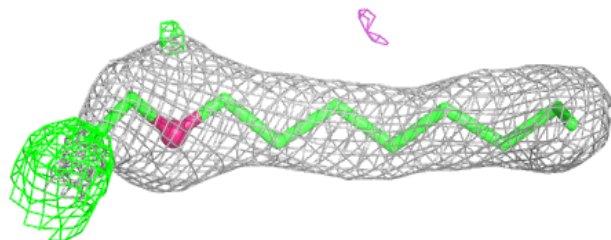
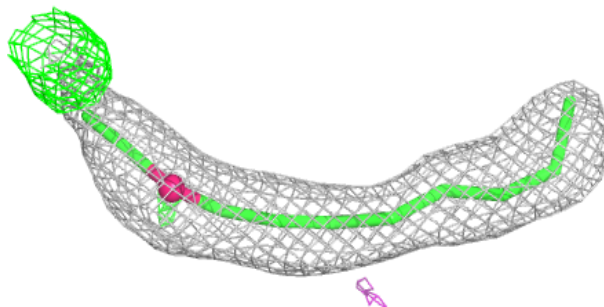
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	E	401	12/21	0.95	0.13	38,43,60,65	0
4	NA	E	409	1/1	0.96	0.05	31,31,31,31	0
4	NA	B	410	1/1	0.97	0.07	31,31,31,31	0
4	NA	A	413	1/1	0.98	0.04	26,26,26,26	0
4	NA	C	408	1/1	0.98	0.08	31,31,31,31	0
4	NA	D	410	1/1	0.98	0.04	25,25,25,25	0
4	NA	D	412	1/1	0.98	0.07	30,30,30,30	0
4	NA	A	414	1/1	0.98	0.04	28,28,28,28	0
4	NA	E	411	1/1	0.98	0.04	27,27,27,27	0
4	NA	C	409	1/1	0.99	0.09	31,31,31,31	0
4	NA	B	409	1/1	0.99	0.09	29,29,29,29	0
4	NA	D	411	1/1	0.99	0.07	29,29,29,29	0
4	NA	A	415	1/1	0.99	0.04	30,30,30,30	0
4	NA	D	413	1/1	0.99	0.05	29,29,29,29	0
4	NA	B	411	1/1	0.99	0.02	27,27,27,27	0
4	NA	E	410	1/1	0.99	0.13	32,32,32,32	0
4	NA	A	416	1/1	0.99	0.03	24,24,24,24	0
4	NA	F	408	1/1	0.99	0.07	26,26,26,26	0
4	NA	F	409	1/1	0.99	0.04	29,29,29,29	0

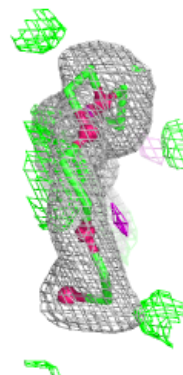
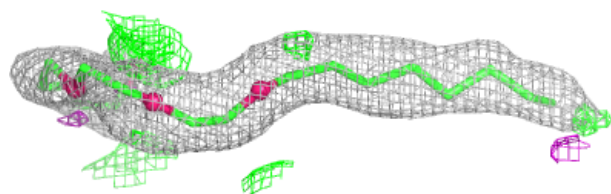
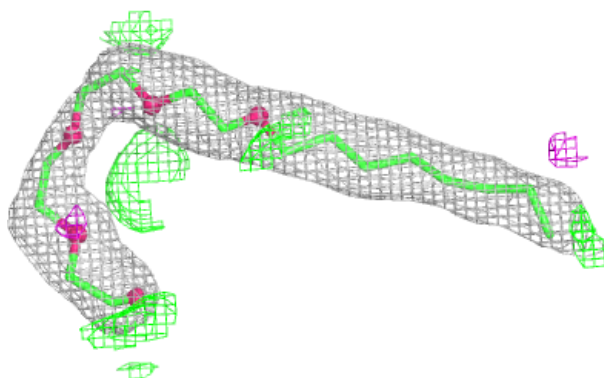
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E D 403:

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

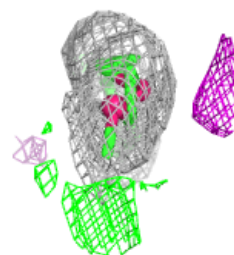
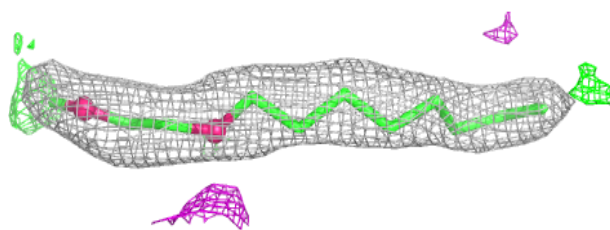
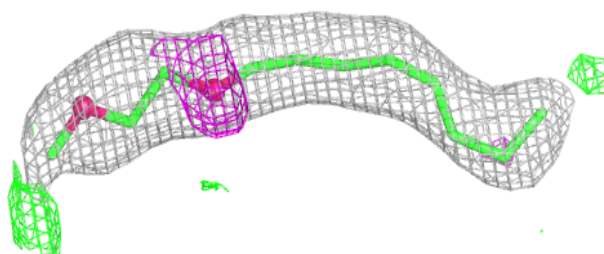
**Electron density around C8E C 401:**

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

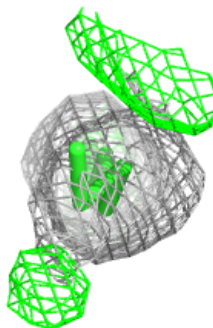
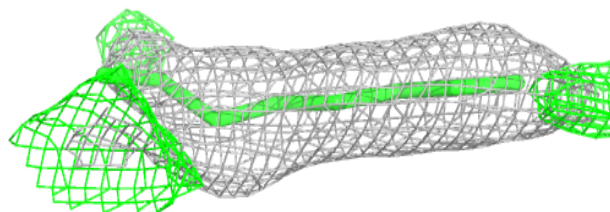
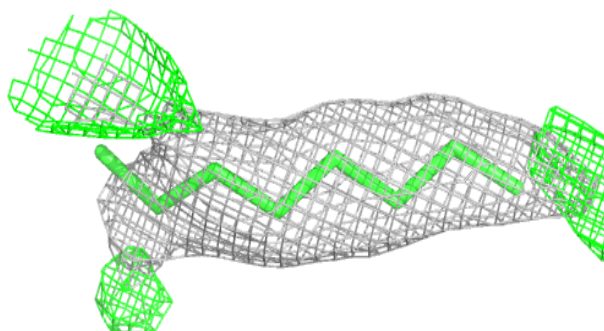


Electron density around C8E D 402:

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

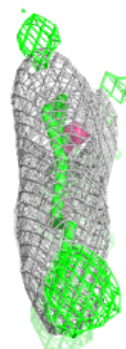
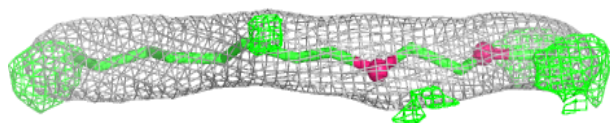
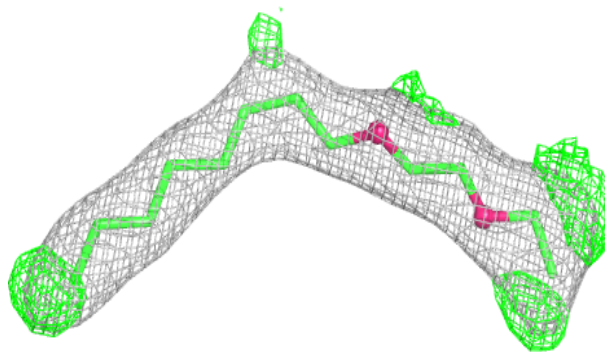
**Electron density around C8E A 405:**

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

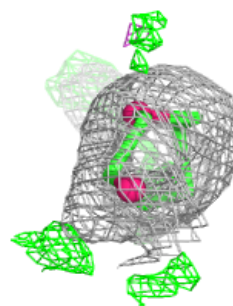
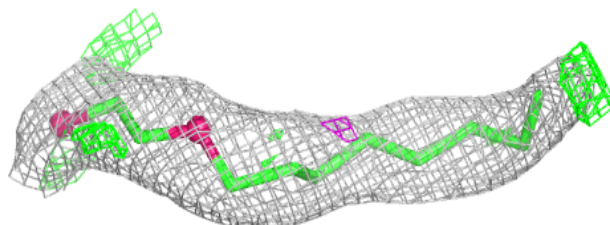
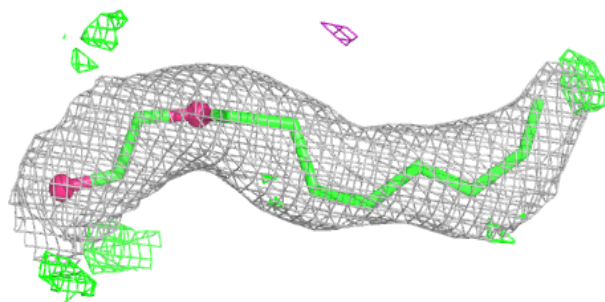


Electron density around C8E D 401:

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

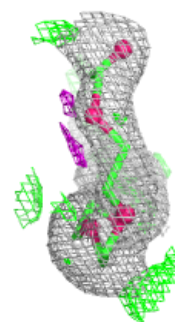
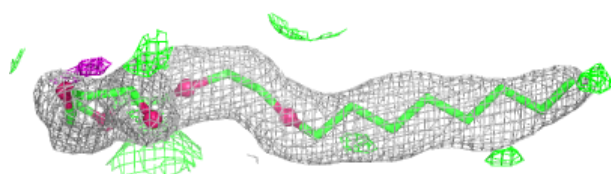
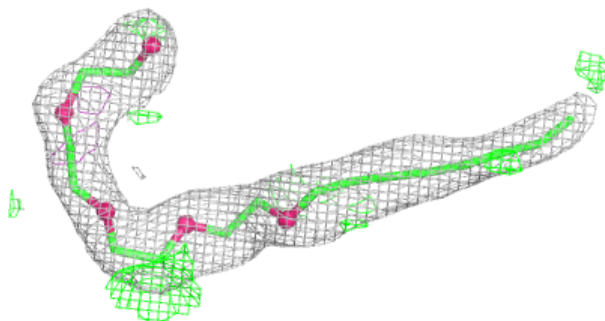
**Electron density around C8E B 402:**

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

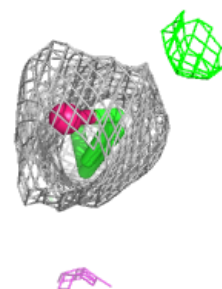
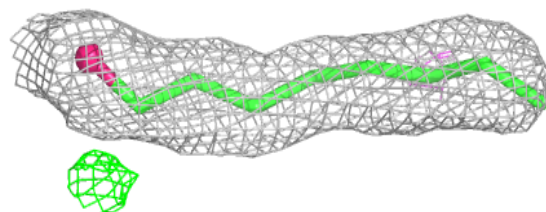
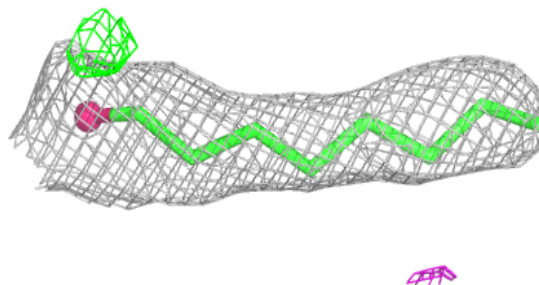


Electron density around C8E A 406:

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

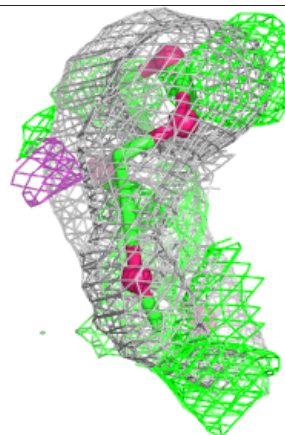
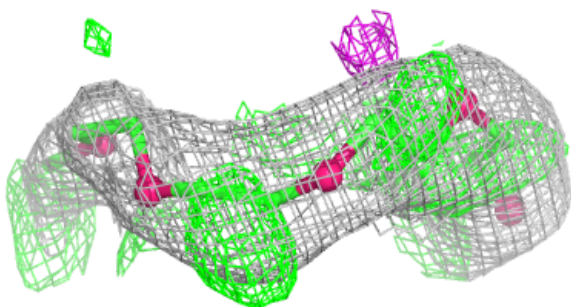
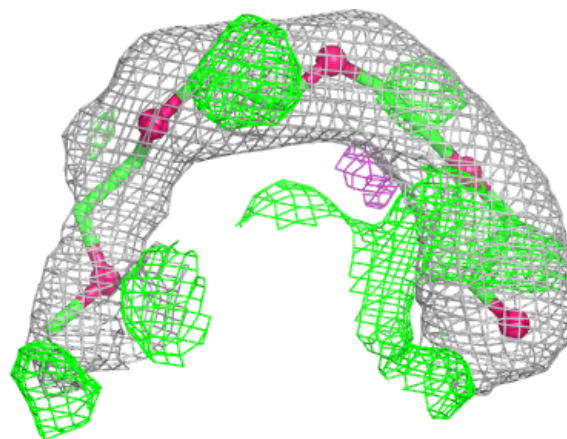
**Electron density around C8E A 404:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

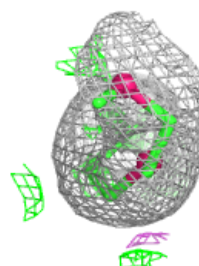
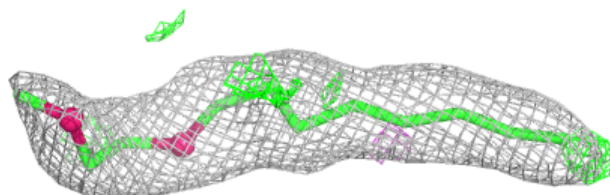
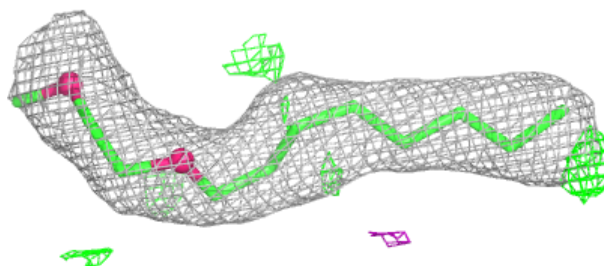


Electron density around C8E A 403:

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

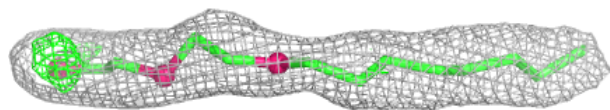
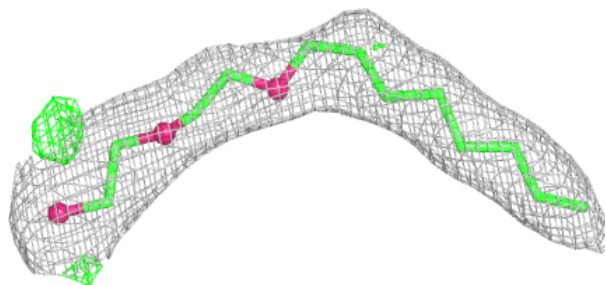
**Electron density around C8E B 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

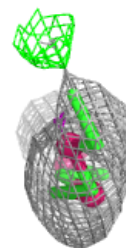
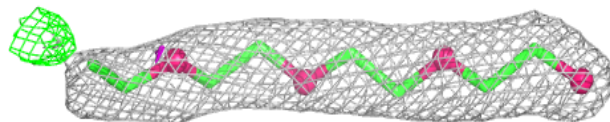
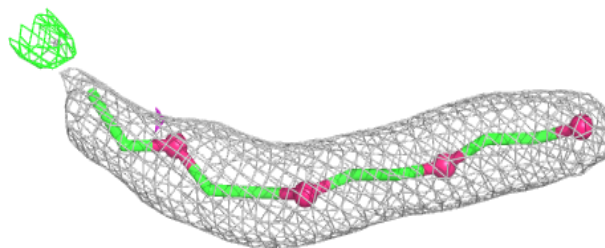


Electron density around C8E E 402:

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

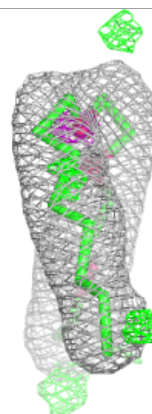
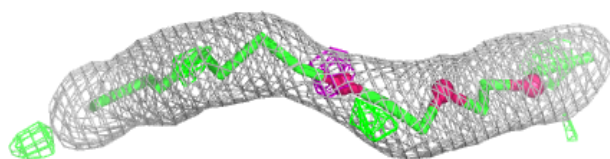
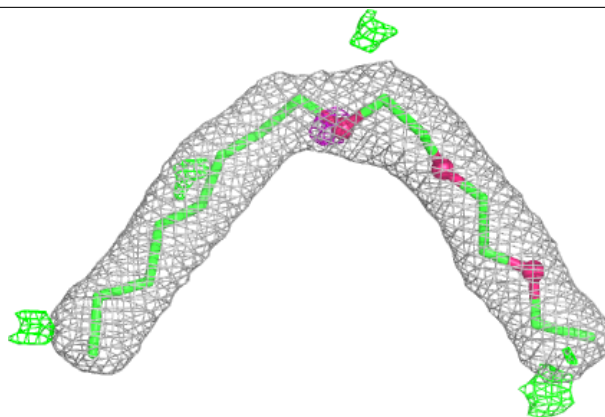
**Electron density around C8E A 401:**

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

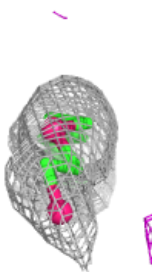
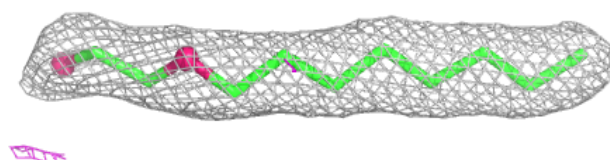
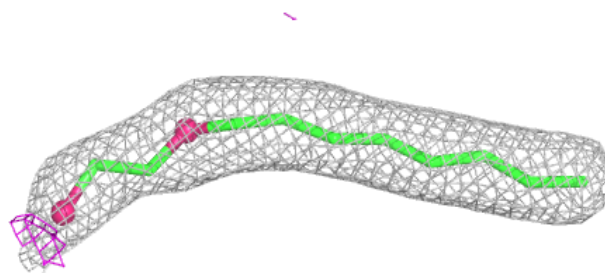


Electron density around C8E F 401:

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

**Electron density around C8E E 401:**

$2mF_o-DF_c$ (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.