WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 09:06 am GMT

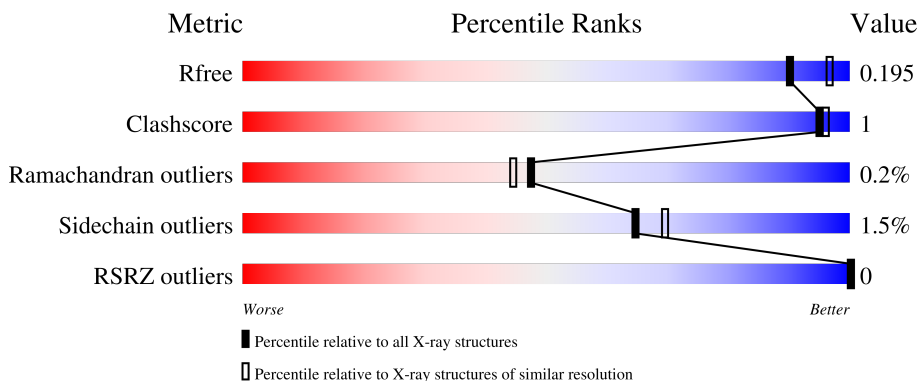|		
PDB ID	:	5FRA
Title	:	CBM40_CPF0721-6'SL
Authors	:	Ribeiro, J.P.; Pau, W.; Pifferi, C.; Renaudet, O.; Varrot, A.; Mahal, L.K.; Imberty, A.
Deposited on	:	2015-12-16
Resolution	:	2.00 Å(reported)

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 2.00 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.
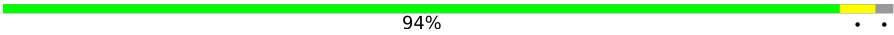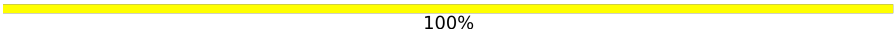
Metric	Percentile Ranks	Value
Rfree		0.195
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		1.5%
RSRZ outliers		0

Worse　　　　　　　　　　　　　　　　*Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	197	95%　　　　　5%
1	B	197	94%　　　　　· · ·
1	C	197	91%　　　　　8%　·
1	D	197	94%　　　　　· · ·
1	E	197	94%　　　　　· · ·

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Mol	Chain	Length	Quality of chain
1	F	197	94%
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10282 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	2	0
			1591	995	268	325	3			
1	B	194	Total	C	N	O	S	0	0	0
			1553	973	262	315	3			
1	C	194	Total	C	N	O	S	0	2	0
			1562	977	263	319	3			
1	D	194	Total	C	N	O	S	0	2	0
			1566	980	264	319	3			
1	E	193	Total	C	N	O	S	0	0	0
			1546	968	261	314	3			
1	F	193	Total	C	N	O	S	0	0	0
			1542	965	260	314	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP A0A0H2YQR1
A	-6	PRO	-	expression tag	UNP A0A0H2YQR1
A	-5	ASP	-	expression tag	UNP A0A0H2YQR1
A	-4	PRO	-	expression tag	UNP A0A0H2YQR1
A	-3	ASN	-	expression tag	UNP A0A0H2YQR1
A	-2	TRP	-	expression tag	UNP A0A0H2YQR1
A	-1	GLU	-	expression tag	UNP A0A0H2YQR1
A	0	LEU	-	expression tag	UNP A0A0H2YQR1
B	-7	SER	-	expression tag	UNP A0A0H2YQR1
B	-6	PRO	-	expression tag	UNP A0A0H2YQR1
B	-5	ASP	-	expression tag	UNP A0A0H2YQR1
B	-4	PRO	-	expression tag	UNP A0A0H2YQR1
B	-3	ASN	-	expression tag	UNP A0A0H2YQR1
B	-2	TRP	-	expression tag	UNP A0A0H2YQR1
B	-1	GLU	-	expression tag	UNP A0A0H2YQR1
B	0	LEU	-	expression tag	UNP A0A0H2YQR1
C	-7	SER	-	expression tag	UNP A0A0H2YQR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	PRO	-	expression tag	UNP A0A0H2YQR1
C	-5	ASP	-	expression tag	UNP A0A0H2YQR1
C	-4	PRO	-	expression tag	UNP A0A0H2YQR1
C	-3	ASN	-	expression tag	UNP A0A0H2YQR1
C	-2	TRP	-	expression tag	UNP A0A0H2YQR1
C	-1	GLU	-	expression tag	UNP A0A0H2YQR1
C	0	LEU	-	expression tag	UNP A0A0H2YQR1
D	-7	SER	-	expression tag	UNP A0A0H2YQR1
D	-6	PRO	-	expression tag	UNP A0A0H2YQR1
D	-5	ASP	-	expression tag	UNP A0A0H2YQR1
D	-4	PRO	-	expression tag	UNP A0A0H2YQR1
D	-3	ASN	-	expression tag	UNP A0A0H2YQR1
D	-2	TRP	-	expression tag	UNP A0A0H2YQR1
D	-1	GLU	-	expression tag	UNP A0A0H2YQR1
D	0	LEU	-	expression tag	UNP A0A0H2YQR1
E	-7	SER	-	expression tag	UNP A0A0H2YQR1
E	-6	PRO	-	expression tag	UNP A0A0H2YQR1
E	-5	ASP	-	expression tag	UNP A0A0H2YQR1
E	-4	PRO	-	expression tag	UNP A0A0H2YQR1
E	-3	ASN	-	expression tag	UNP A0A0H2YQR1
E	-2	TRP	-	expression tag	UNP A0A0H2YQR1
E	-1	GLU	-	expression tag	UNP A0A0H2YQR1
E	0	LEU	-	expression tag	UNP A0A0H2YQR1
F	-7	SER	-	expression tag	UNP A0A0H2YQR1
F	-6	PRO	-	expression tag	UNP A0A0H2YQR1
F	-5	ASP	-	expression tag	UNP A0A0H2YQR1
F	-4	PRO	-	expression tag	UNP A0A0H2YQR1
F	-3	ASN	-	expression tag	UNP A0A0H2YQR1
F	-2	TRP	-	expression tag	UNP A0A0H2YQR1
F	-1	GLU	-	expression tag	UNP A0A0H2YQR1
F	0	LEU	-	expression tag	UNP A0A0H2YQR1

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto
  pyranose.
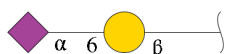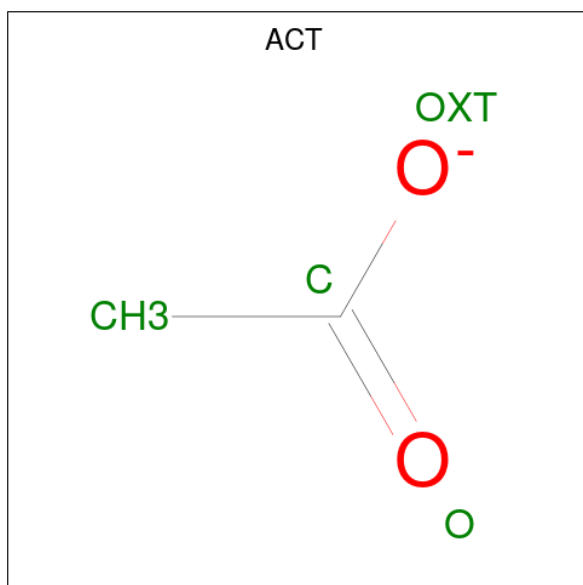

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	2	32	17	1	14	0	0	0

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).

SIA
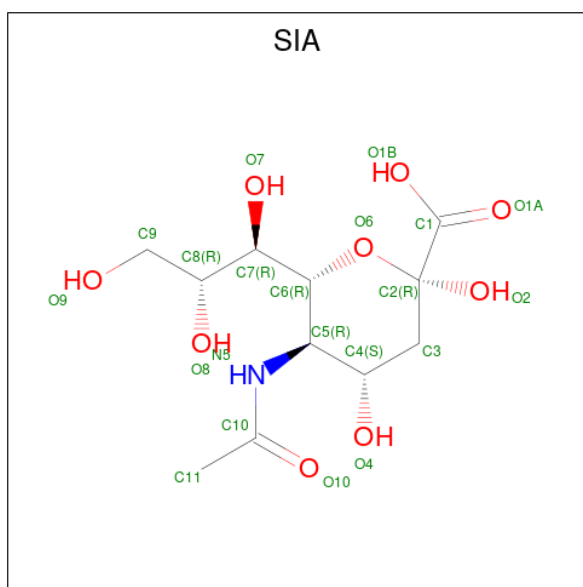
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 21	C 11	N 1	O 9	0	0
4	E	1	Total 21	C 11	N 1	O 9	0	0
4	F	1	Total 21	C 11	N 1	O 9	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total 131	O 131	0	0
5	B	127	Total 127	O 127	0	0
5	C	137	Total 137	O 137	0	0
5	D	137	Total 137	O 137	0	0
5	E	149	Total 149	O 149	0	0
5	F	74	Total 74	O 74	0	0

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.

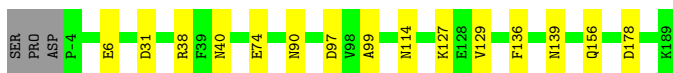- Molecule 1: SIALIDASE

Chain A:

95%   5%

S-7 R38 K45 K56 E74 K96 D97 K115 D178 T188 K189

- Molecule 1: SIALIDASE

Chain B:

94%

SER PRO ASP P-4 N-3 W-2 E-1 L0 N16 A17 K28 D97 K115 K189

- Molecule 1: SIALIDASE

Chain C:

91%   8%

SER PRO ASP P-4 E6 D31 R38 F39 N40 E74 N90 D97 V98 A99 N114 K127 E128 V129 F136 N139 Q156 D178 K189

- Molecule 1: SIALIDASE

Chain D:

94%

SER PRO ASP P-4 N-3 K28 D31 K58 N138 Q156 E159 K189

- Molecule 1: SIALIDASE

Chain E:

94%

SER PRO ASP PRO N-3 E13 D31 R38 D102 Y154 N165 D178 S183 K189

- Molecule 1: SIALIDASE

Chain F:

94%

SER PRO ASP PRO N-3 E25 K28 R38 K42 K58 Y154 K184 K189

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain G: 100%

GAL1 SIA2

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain H: 50% 50%

GAL1 SIA2

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain I: 50% 50%

GAL1 SIA2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.50Å 84.27Å 90.00Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	39.69 – 2.00 39.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.69-2.00) 99.3 (39.69-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.179 , 0.210 0.188 , 0.195	Depositor DCC
R_{free} test set	4080 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10282	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, ACT, GAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.89	0/1619	0.91	3/2177 (0.1%)
1	B	0.88	0/1577	0.92	2/2119 (0.1%)
1	C	0.89	0/1586	0.94	4/2133 (0.2%)
1	D	0.89	1/1593 (0.1%)	0.89	0/2141
1	E	0.94	1/1569 (0.1%)	0.92	5/2108 (0.2%)
1	F	0.90	0/1565	0.88	0/2104
All	All	0.90	2/9509 (0.0%)	0.91	14/12782 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	GLU	CD-OE2	5.59	1.31	1.25
1	E	183	SER	CB-OG	-5.37	1.35	1.42

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	97	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	31[A]	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	C	31[B]	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	97	ASP	CB-CG-OD1	7.14	124.73	118.30
1	E	31	ASP	CB-CG-OD1	6.66	124.29	118.30

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	1591	0	1548	3	0
1	B	1553	0	1512	4	0
1	C	1562	0	1505	10	0
1	D	1566	0	1521	2	0
1	E	1546	0	1505	2	0
1	F	1542	0	1494	2	0
2	G	32	0	28	0	0
2	H	32	0	28	1	0
2	I	32	0	28	1	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
4	D	21	0	18	0	0
4	E	21	0	18	0	0
4	F	21	0	18	0	0
5	A	131	0	0	1	0
5	B	127	0	0	2	0
5	C	137	0	0	5	0
5	D	137	0	0	0	0
5	E	149	0	0	0	0
5	F	74	0	0	1	0
All	All	10282	0	9229	22	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.

The worst 5 of 22 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ALA:HB1	1:E:154:TYR:CE1	2.30	0.66
1:C:136:PHE:H	1:C:139:ASN:HD22	1.44	0.65
5:C:2137:HOH:O	2:I:1:GAL:H4	1.97	0.64
5:B:2126:HOH:O	2:H:1:GAL:O3	2.17	0.57
1:D:31[A]:ASP:OD1	1:D:138[A]:ASN:ND2	2.38	0.57

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	197/197 (100%)	190 (96%)	7 (4%)	0	100	100
1	B	192/197 (98%)	184 (96%)	7 (4%)	1 (0%)	29	23
1	C	194/197 (98%)	188 (97%)	6 (3%)	0	100	100
1	D	194/197 (98%)	187 (96%)	6 (3%)	1 (0%)	29	23
1	E	191/197 (97%)	184 (96%)	7 (4%)	0	100	100
1	F	191/197 (97%)	182 (95%)	9 (5%)	0	100	100
All	All	1159/1182 (98%)	1115 (96%)	42 (4%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	ALA
1	D	-3	ASN

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	179/177 (101%)	176 (98%)	3 (2%)	60	65
1	B	173/177 (98%)	172 (99%)	1 (1%)	86	90
1	C	173/177 (98%)	171 (99%)	2 (1%)	71	76
1	D	175/177 (99%)	170 (97%)	5 (3%)	42	43
1	E	172/177 (97%)	171 (99%)	1 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	171/177 (97%)	167 (98%)	4 (2%)	50	53
All	All	1043/1062 (98%)	1027 (98%)	16 (2%)	65	69

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	42	LYS
1	F	28	LYS
1	D	58	LYS
1	F	25	GLU
1	D	28	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	16	ASN
1	F	156	GLN
1	C	139	ASN
1	C	161	ASN
1	D	161	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 ⓘ

6 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	GAL	G	1	2	12,12,12	0.87	0	17,17,17	1.04	1 (5%)
2	SIA	G	2	2	20,20,21	0.96	0	24,28,31	1.36	4 (16%)
2	GAL	H	1	2	12,12,12	0.81	0	17,17,17	1.38	2 (11%)
2	SIA	H	2	2	20,20,21	1.10	1 (5%)	24,28,31	1.69	9 (37%)
2	GAL	I	1	2	12,12,12	0.83	0	17,17,17	1.45	2 (11%)
2	SIA	I	2	2	20,20,21	1.26	4 (20%)	24,28,31	1.66	6 (25%)

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	GAL	G	1	2	-	0/2/22/22	0/1/1/1
2	SIA	G	2	2	-	0/18/34/38	0/1/1/1
2	GAL	H	1	2	-	0/2/22/22	0/1/1/1
2	SIA	H	2	2	-	1/18/34/38	0/1/1/1
2	GAL	I	1	2	-	0/2/22/22	0/1/1/1
2	SIA	I	2	2	-	1/18/34/38	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	SIA	C4-C5	3.35	1.56	1.53
2	I	2	SIA	O6-C2	2.14	1.46	1.43
2	I	2	SIA	C4-C5	2.14	1.55	1.53
2	I	2	SIA	C7-C6	-2.07	1.50	1.53
2	I	2	SIA	C2-C1	2.07	1.54	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	SIA	O1B-C1-C2	3.61	123.34	113.03
2	I	2	SIA	O1B-C1-O1A	-3.27	116.66	124.09
2	H	2	SIA	O1A-C1-C2	-3.11	115.22	122.57
2	I	2	SIA	C9-C8-C7	-3.07	105.75	112.41
2	G	2	SIA	O6-C2-C1	3.01	113.61	107.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	SIA	O1B-C1-C2-O6
2	I	2	SIA	O1B-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	GAL	1	0
2	H	1	GAL	1	0

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

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
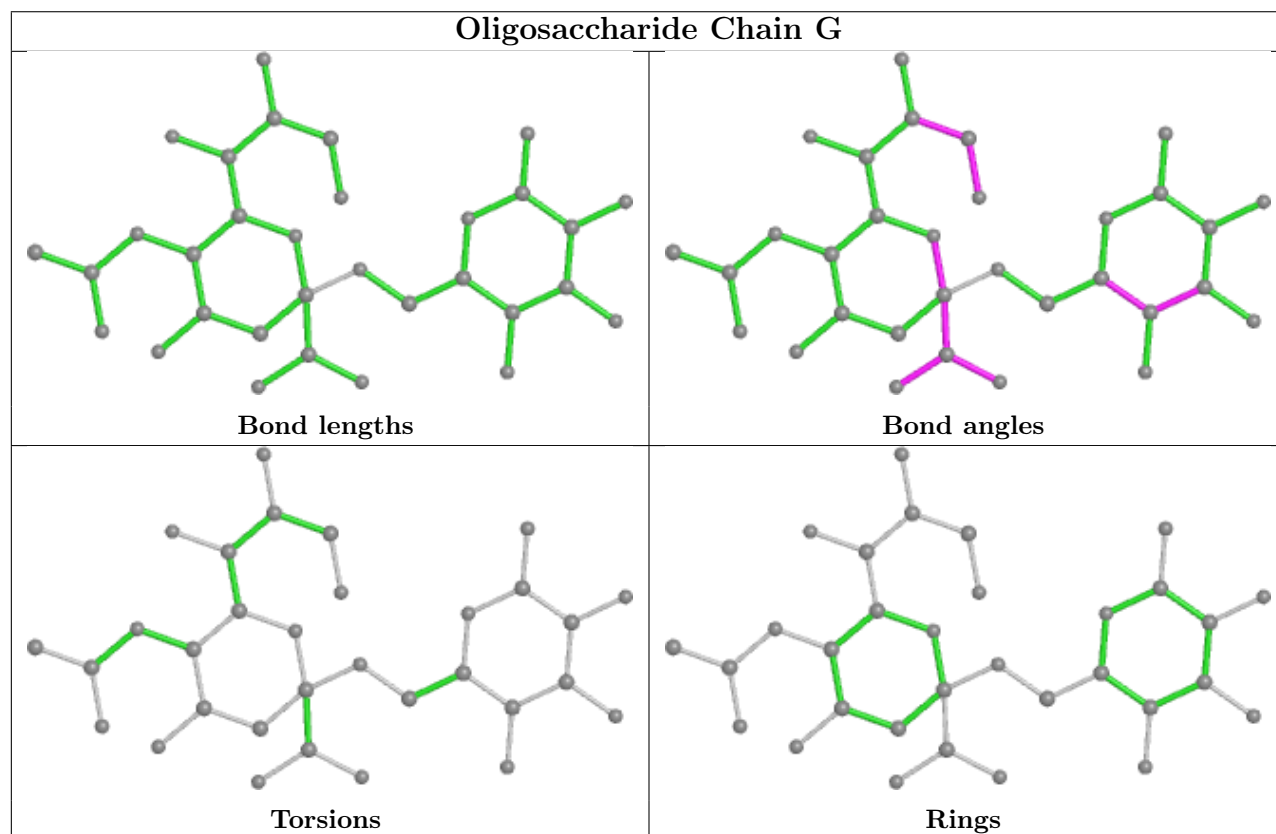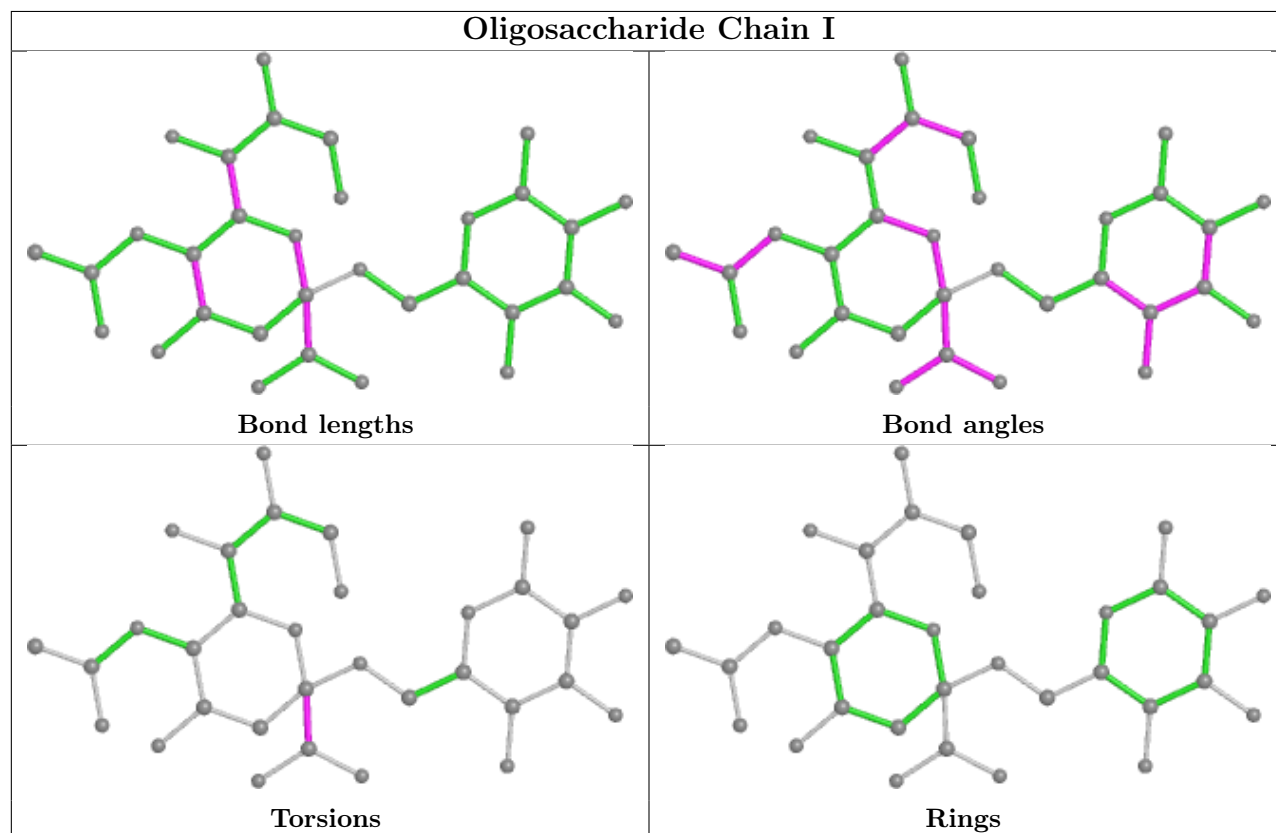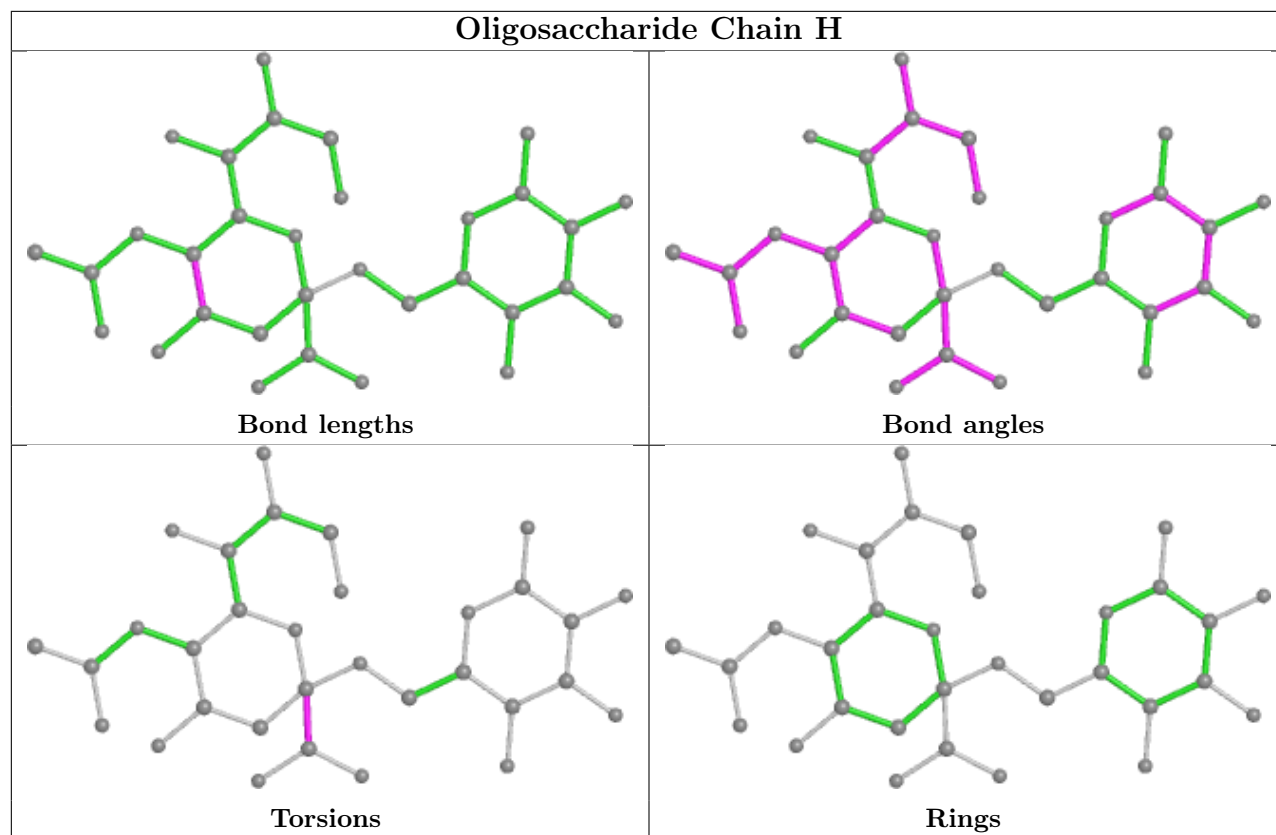
5.6 Ligand geometry (i)

5 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	#$|Z| > 2$
4	SIA	D	201	-	21,21,21	1.15	1 (4%)	25,31,31	1.69	7 (28%)
3	ACT	B	1190	-	3,3,3	0.87	0	3,3,3	0.55	0
3	ACT	A	1190	-	3,3,3	1.00	0	3,3,3	0.99	0
4	SIA	F	201	-	21,21,21	1.51	1 (4%)	25,31,31	1.54	4 (16%)
4	SIA	E	201	-	21,21,21	1.05	1 (4%)	25,31,31	1.73	3 (12%)

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
4	SIA	F	201	-	-	0/20/38/38	0/1/1/1
4	SIA	D	201	-	-	3/20/38/38	0/1/1/1
4	SIA	E	201	-	-	3/20/38/38	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	201	SIA	O2-C2	5.83	1.47	1.39
4	D	201	SIA	O6-C2	3.17	1.46	1.43
4	E	201	SIA	O2-C2	2.64	1.43	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	201	SIA	O9-C9-C8	-4.72	100.78	111.07
4	E	201	SIA	O1A-C1-C2	-4.69	116.48	123.59
4	E	201	SIA	O2-C2-C1	-4.00	102.62	110.76
4	D	201	SIA	O1A-C1-C2	-3.93	117.64	123.59

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	201	SIA	O9-C9-C8	-3.93	102.51	111.07

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	201	SIA	O1A-C1-C2-O6
4	D	201	SIA	O1A-C1-C2-O6
4	D	201	SIA	O1A-C1-C2-O2
4	E	201	SIA	O1A-C1-C2-O2
4	D	201	SIA	O1B-C1-C2-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1190	ACT	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 then 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.

Ligand SIA D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA E 201

Bond lengths

Bond angles

Torsions

Rings
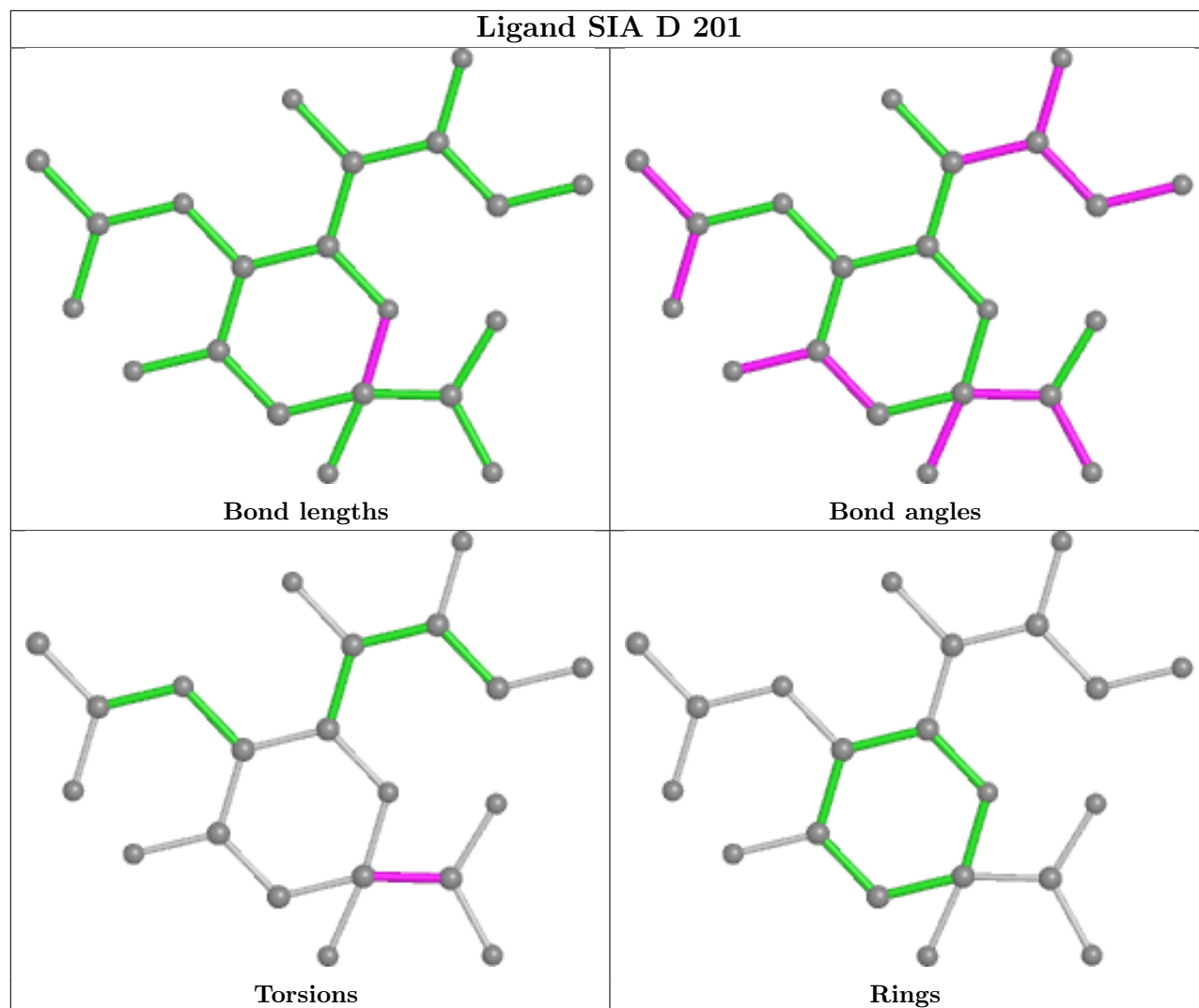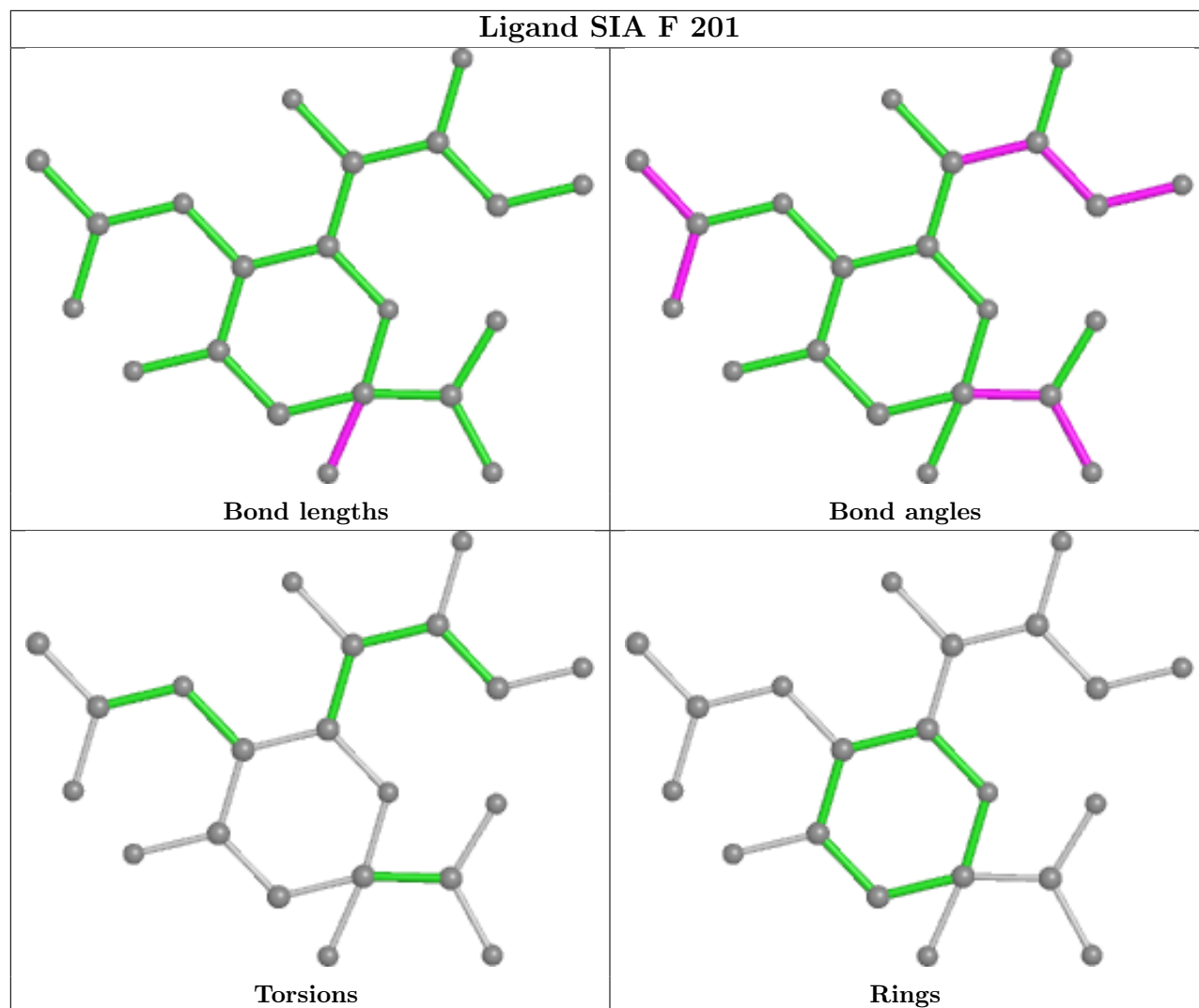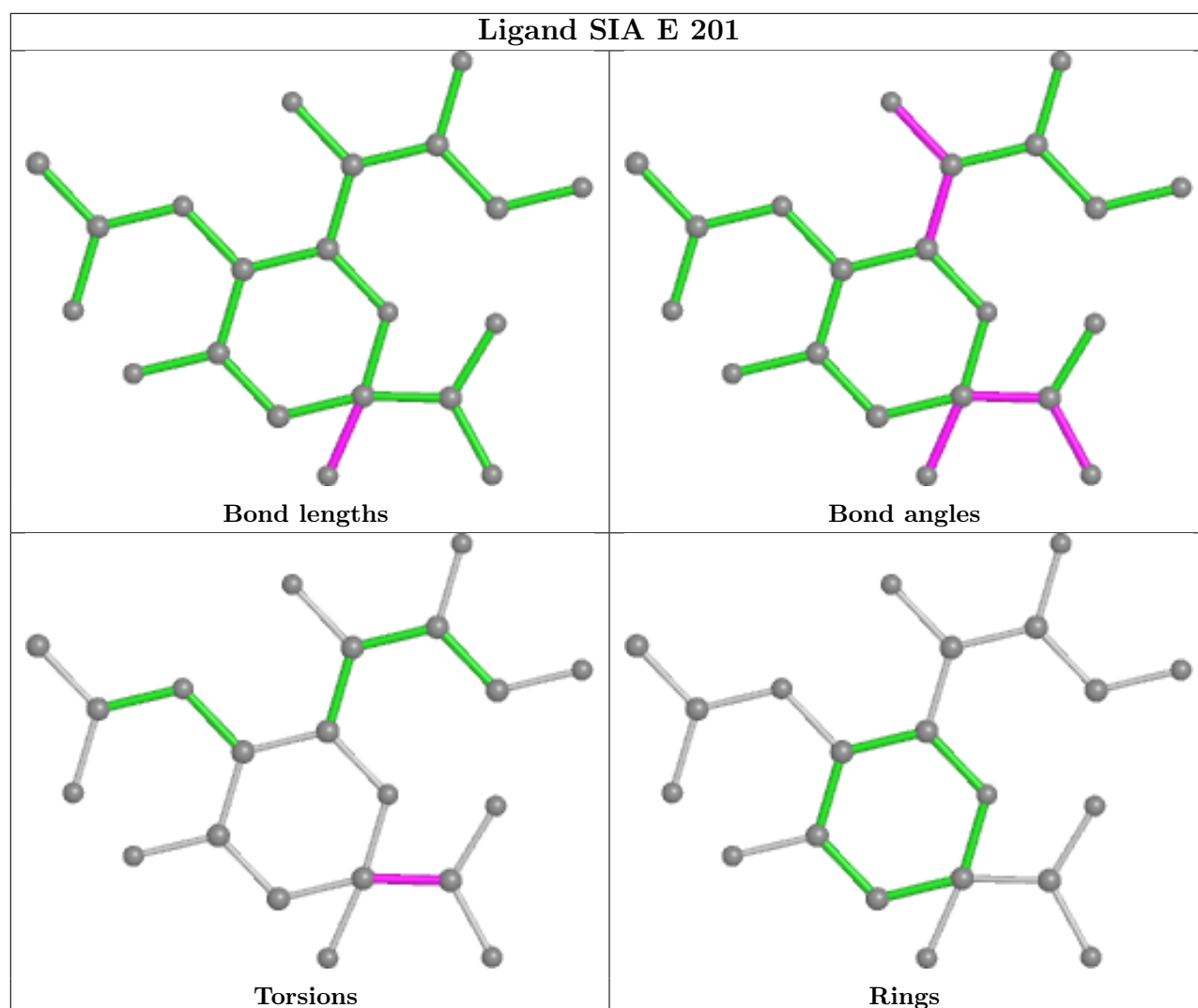
5.7 Other polymers (i)

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	197/197 (100%)	-0.40	0	100	100	17, 26, 41, 54	0
1	B	194/197 (98%)	-0.27	0	100	100	21, 30, 45, 57	0
1	C	194/197 (98%)	-0.46	0	100	100	16, 24, 39, 48	0
1	D	194/197 (98%)	-0.46	0	100	100	16, 25, 41, 58	0
1	E	193/197 (97%)	-0.50	0	100	100	16, 24, 37, 48	0
1	F	193/197 (97%)	-0.17	0	100	100	20, 32, 47, 57	1 (0%)
All	All	1165/1182 (98%)	-0.38	0	100	100	16, 27, 42, 58	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3   Carbohydrates ⓘ

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	GAL	H	1	12/12	0.82	0.18	42,54,59,59	0
2	GAL	I	1	12/12	0.91	0.17	31,51,70,70	0
2	SIA	H	2	20/21	0.95	0.11	27,31,34,35	0
2	GAL	G	1	12/12	0.96	0.10	26,30,33,34	0
2	SIA	G	2	20/21	0.97	0.10	19,22,27,32	0
2	SIA	I	2	20/21	0.97	0.09	21,24,28,32	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.
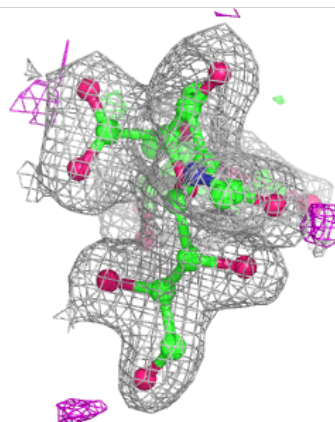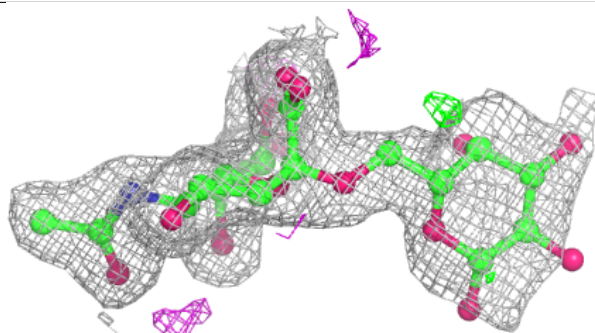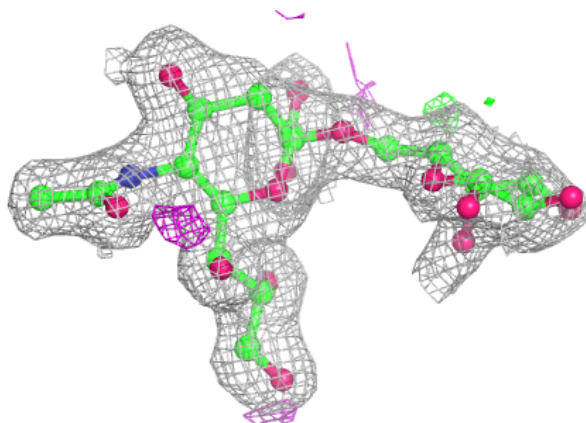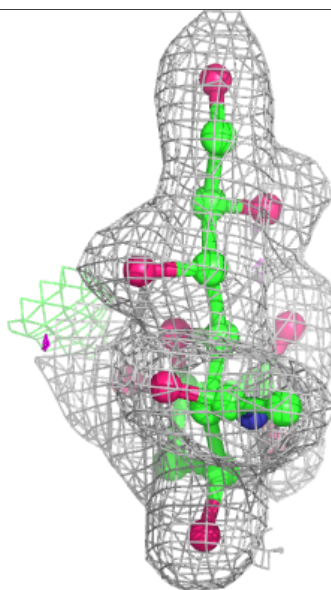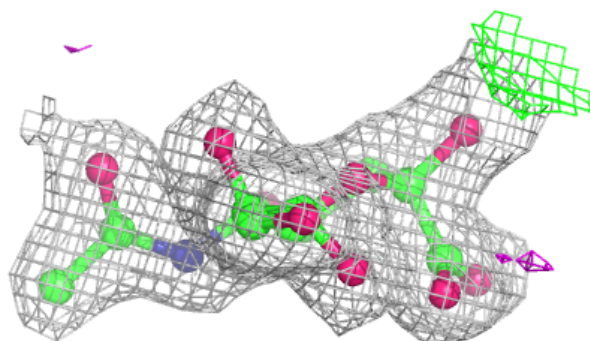
Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
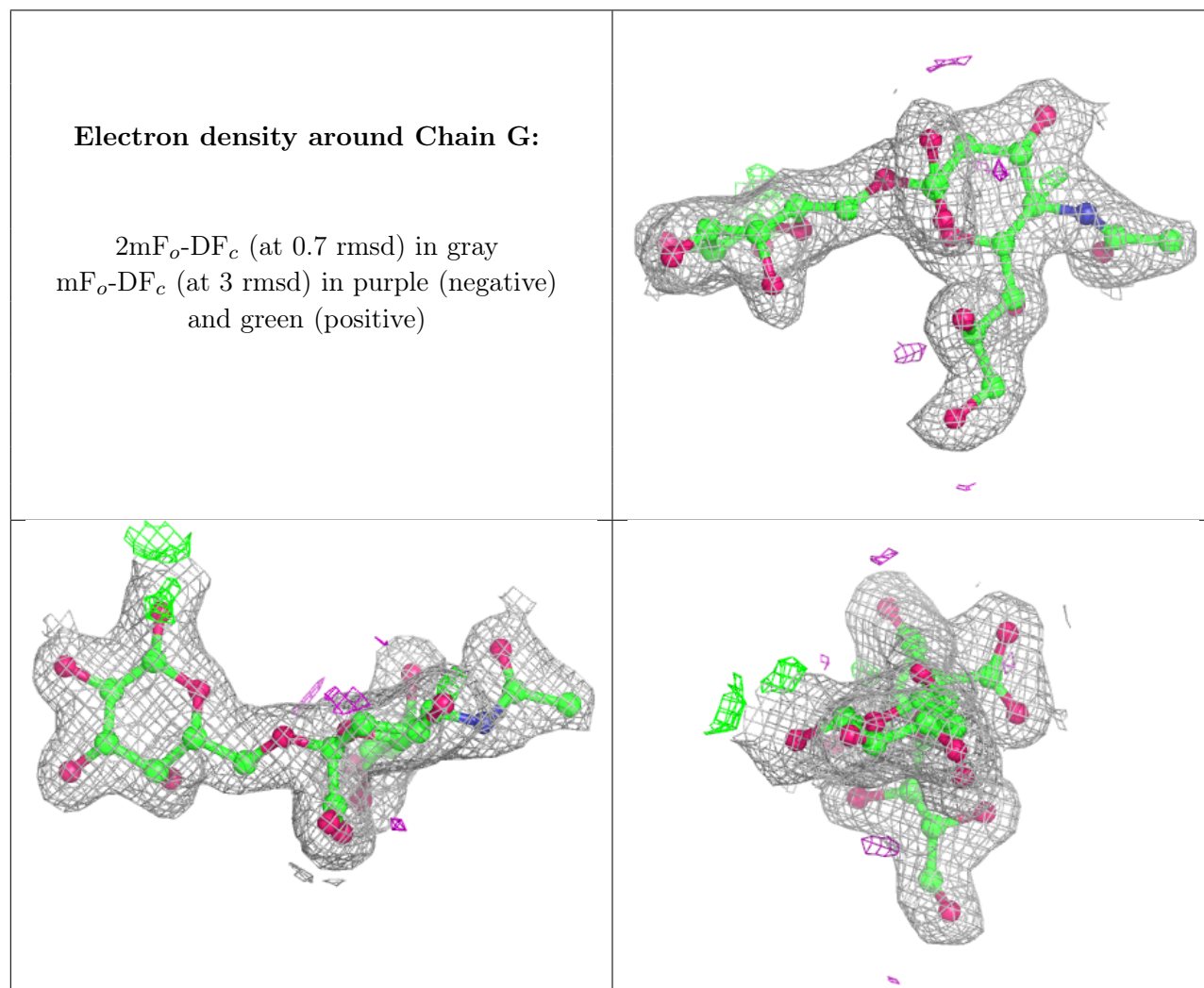
Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
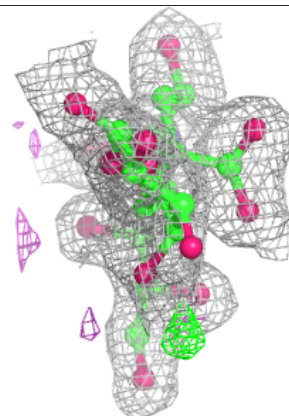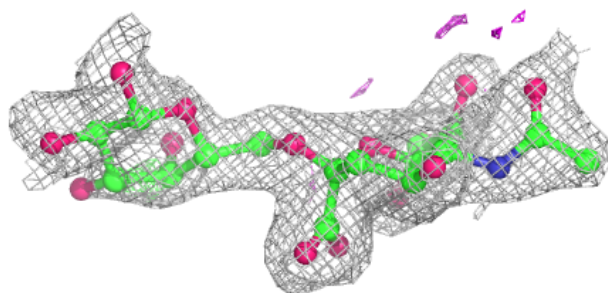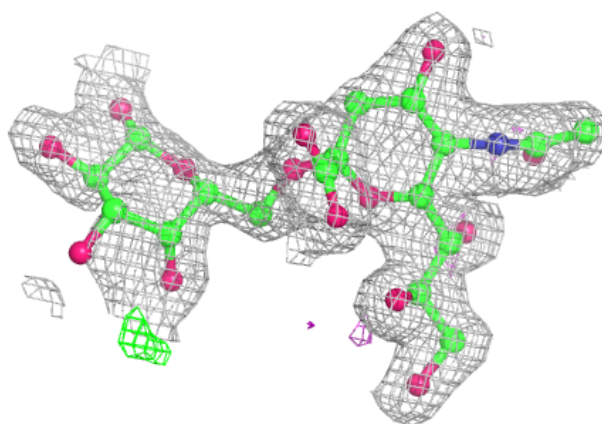
Electron density around Chain I:

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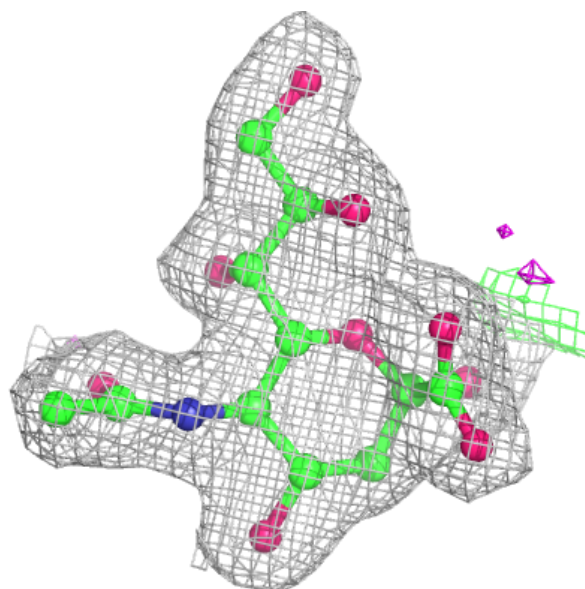and green (positive)

6.4   Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	B	1190	4/4	0.94	0.14	24,29,29,35	0
4	SIA	F	201	21/21	0.95	0.09	23,27,30,31	0
4	SIA	D	201	21/21	0.96	0.08	20,24,27,28	0
4	SIA	E	201	21/21	0.96	0.08	18,22,25,29	0
3	ACT	A	1190	4/4	0.96	0.10	27,27,28,34	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.
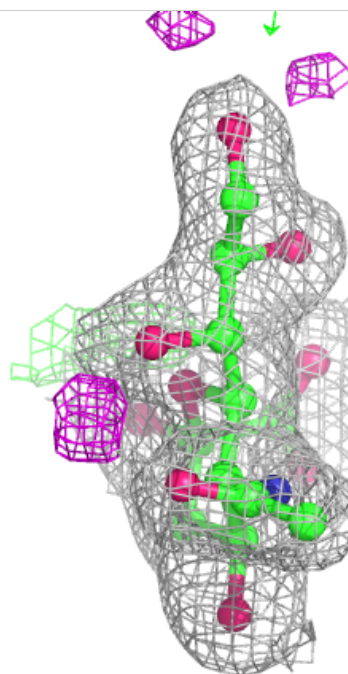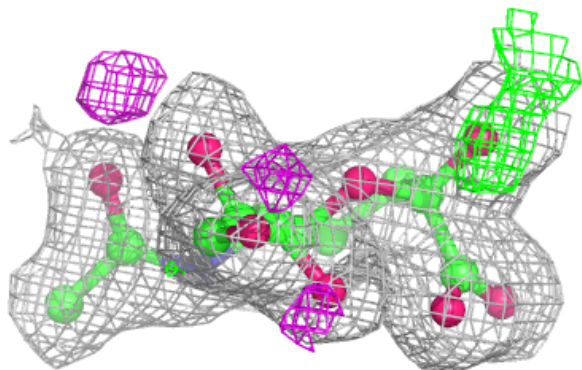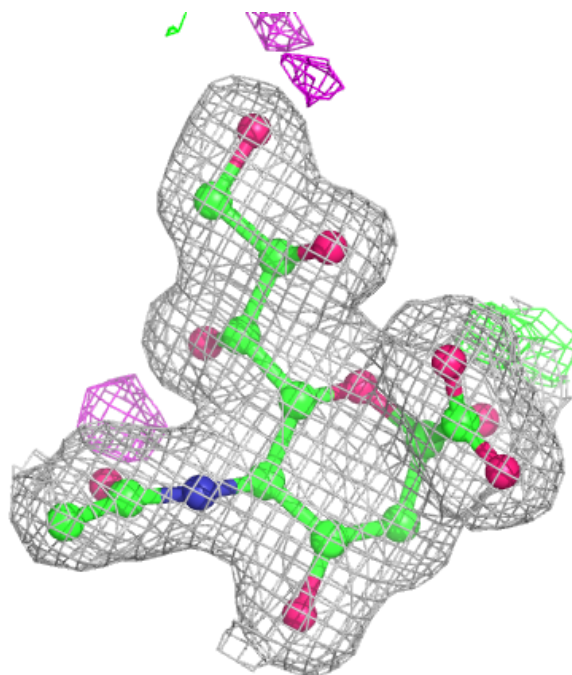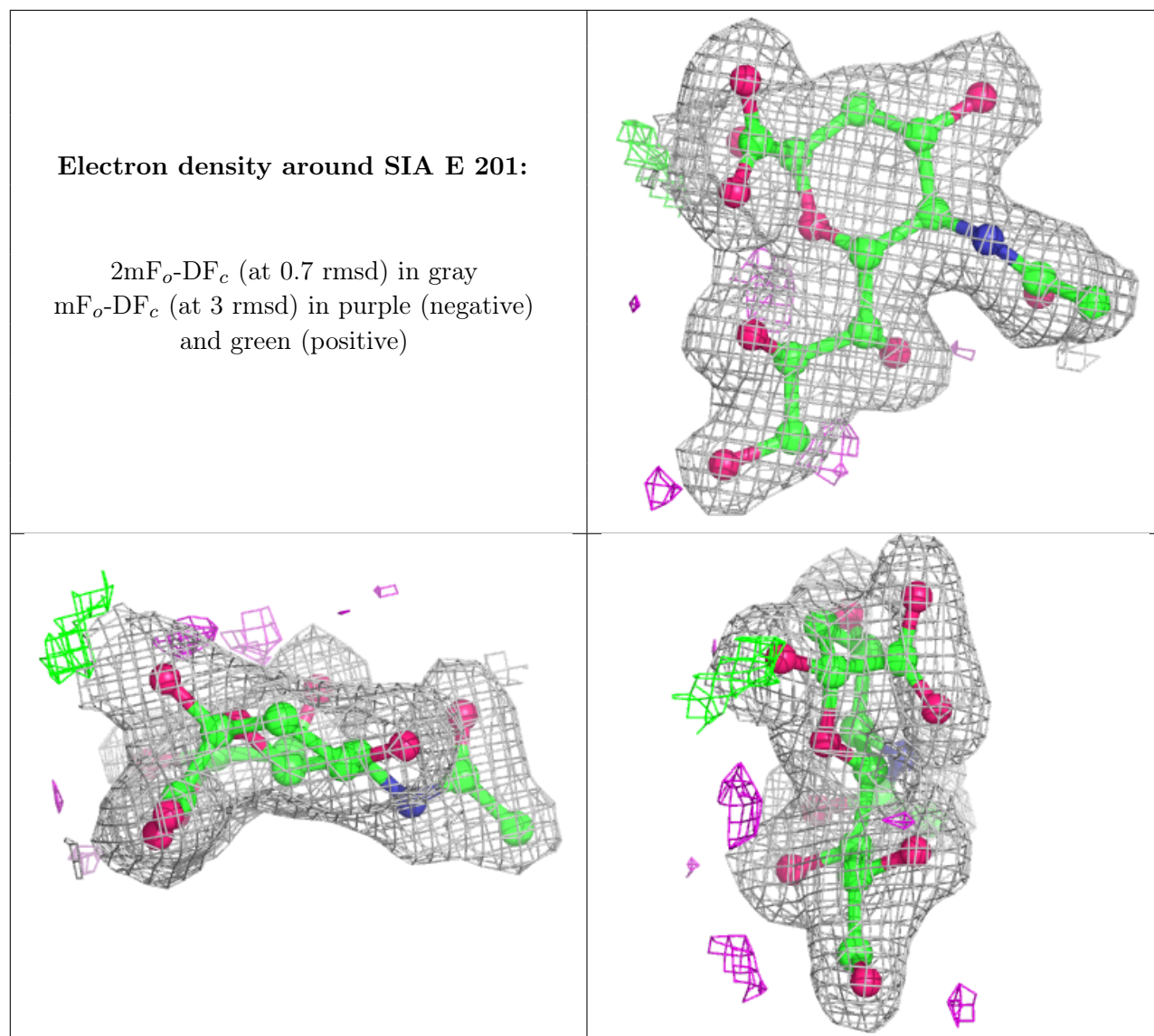
Electron density around SIA F 201:

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

Electron density around SIA D 201:

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

Electron density around SIA E 201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.