wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 08:48 am GMT

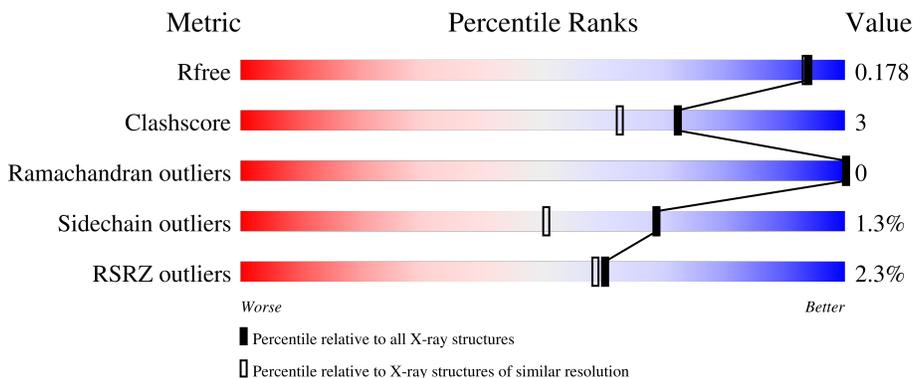|		
PDB ID	:	4AVV
Title	:	Structure of CPHPC bound to Serum Amyloid P Component
Authors	:	Kolstoe, S.E.; Jenvey, M.C.; Wood, S.P.
Deposited on	:	2012-05-29
Resolution	:	1.60 Å(reported)

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 1.60 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.
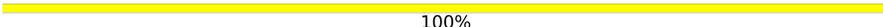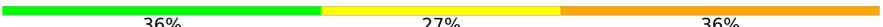
Metric	Percentile Ranks	Value
Rfree		0.178
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		2.3%

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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	204	93% 7%
1	B	204	.% 94% 6%
1	C	204	93% 6%
1	D	204	5% 94% 6%
1	E	204	4% 94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	100%
3	G	11	36% 27% 36%

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
3	MAN	G	4	-	-	-	X
3	NAG	G	9	-	-	-	X
4	ACT	A	1206	-	-	X	-
4	ACT	A	1208	-	-	X	-
4	ACT	B	1208	-	-	X	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 10255 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 SERUM AMYLOID P-COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	8	0
			1710	1107	283	315	5			
1	B	204	Total	C	N	O	S	0	4	0
			1675	1086	276	308	5			
1	C	204	Total	C	N	O	S	0	4	0
			1675	1086	276	308	5			
1	D	204	Total	C	N	O	S	0	6	0
			1691	1093	279	314	5			
1	E	204	Total	C	N	O	S	0	4	0
			1675	1084	277	309	5			

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

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

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1 -3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deox y-beta-D-glucopyranose-(1-2)-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-glucopyranos e.
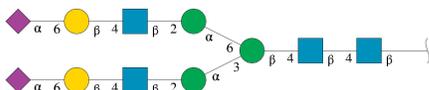
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	11	Total 151	C 84	N 6	O 61	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

- Molecule 5 is (2R)-1-[6-[(2R)-2-carboxypyrrolidin-1-yl]-6-oxidanylidene-hexanoyl]pyrrolidine-2-carboxylic acid (three-letter code: GHE) (formula: $C_{16}H_{24}N_2O_6$).

GHE
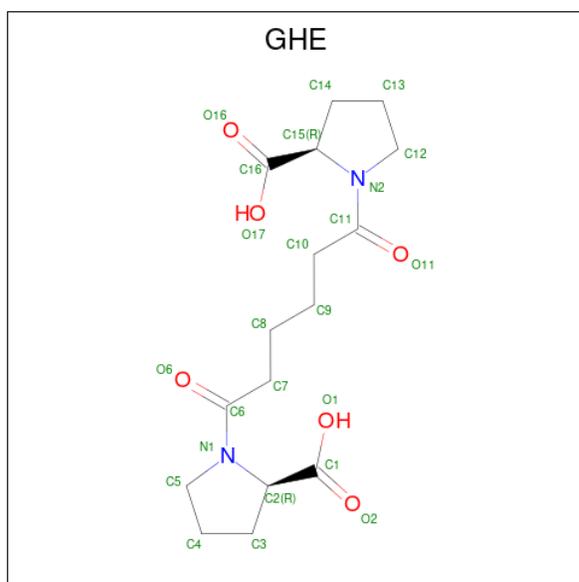
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 24	C 16	N 2	O 6	0	0
5	B	1	Total 24	C 16	N 2	O 6	0	0
5	C	1	Total 24	C 16	N 2	O 6	0	0
5	D	1	Total 24	C 16	N 2	O 6	0	0
5	E	1	Total 24	C 16	N 2	O 6	0	0

- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	Cd 8	0	0
6	B	7	Total 7	Cd 7	0	0
6	C	6	Total 6	Cd 6	0	0
6	D	5	Total 5	Cd 5	0	0
6	E	9	Total 9	Cd 9	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

O6
OH

O5
O1
HO O

C1(R) C5(R)
C6

C2(R) C4(S)
C3(R)
N2
HN
OH
O4

C7
OH
O3

C8 O
O7
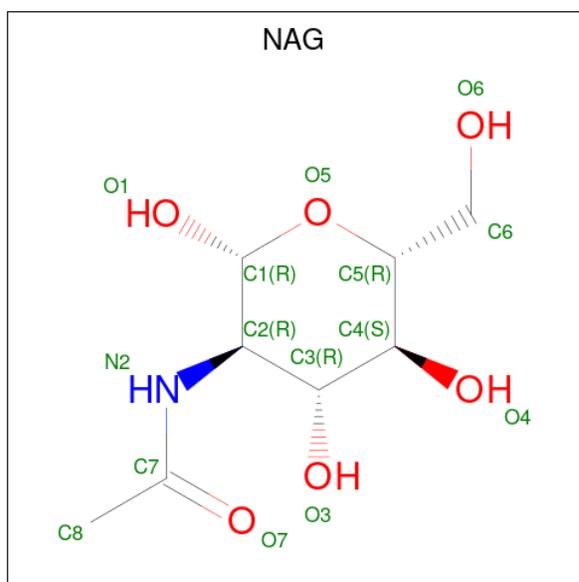
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).

SIA

O7
OH
O1B
HO
O6 C1
O1A
C9
C8(R) C7(R)
HO C6(R)
O9 C2(R)
OH O2

C5(R)
OH C4(S) C3
O8
N5
HN

C10
OH
O4
C11 O
O10
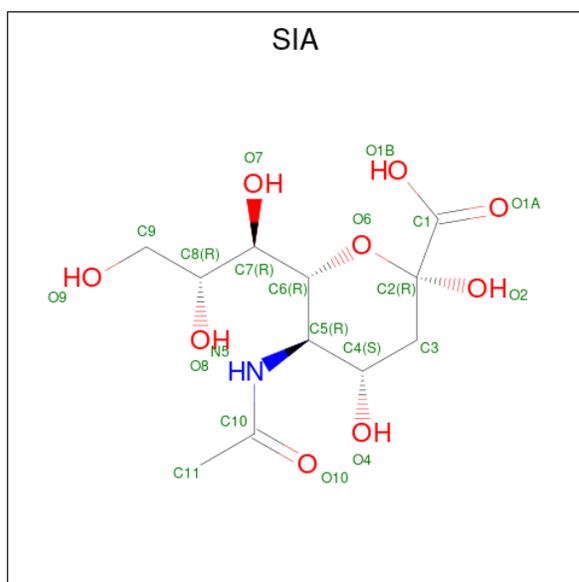
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			20	11	1	8		

WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 9 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	327	Total O 327 327		0	0
9	B	275	Total O 275 275		0	0
9	C	283	Total O 283 283		0	0
9	D	277	Total O 277 277		0	0
9	E	239	Total O 239 239		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: SERUM AMYLOID P-COMPONENT

Chain A:

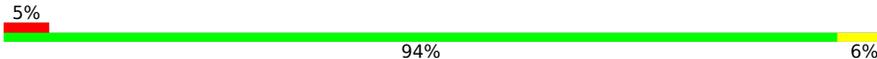- Molecule 1: SERUM AMYLOID P-COMPONENT

Chain B:
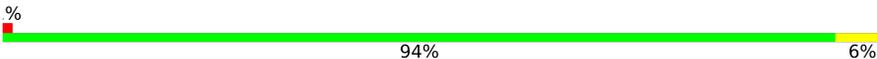
- Molecule 1: SERUM AMYLOID P-COMPONENT

Chain C:

- Molecule 1: SERUM AMYLOID P-COMPONENT

Chain D:

- Molecule 1: SERUM AMYLOID P-COMPONENT

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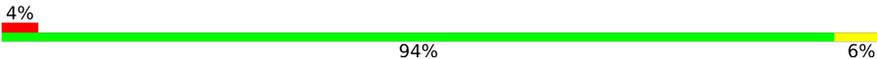
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1
NAG2

• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 G:
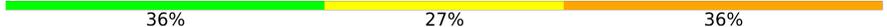
36%   27%   36%

NAG1
NAG2
BMA3
MAN4
NAG5
GAL6
SIA7
MAN8
NAG9
GAL10
SIA11

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.38Å 108.58Å 120.26Å 90.00° 138.53° 90.00°	Depositor
Resolution (Å)	37.87 – 1.60 80.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.87-1.60) 99.1 (80.56-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 1.60Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.150 , 0.175 0.157 , 0.178	Depositor DCC
R_{free} test set	2005 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h+2*l,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/1757	0.71	0/2389
1	B	0.50	0/1722	0.70	0/2341
1	C	0.50	0/1722	0.70	0/2341
1	D	0.48	0/1738	0.69	0/2362
1	E	0.49	0/1722	0.69	1/2341 (0.0%)
All	All	0.50	0/8661	0.70	1/11774 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ARG	NE-CZ-NH2	-5.17	117.72	120.30

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	1710	0	1679	12	0
1	B	1675	0	1645	11	0
1	C	1675	0	1644	7	0
1	D	1691	0	1651	10	0
1	E	1675	0	1639	7	0

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	0	0
3	G	151	0	127	3	0
4	A	16	0	12	4	0
4	B	4	0	3	3	0
4	E	12	0	9	1	0
5	A	24	0	22	0	0
5	B	24	0	22	0	0
5	C	24	0	22	1	0
5	D	24	0	22	0	0
5	E	24	0	22	0	0
6	A	8	0	0	0	0
6	B	7	0	0	0	0
6	C	6	0	0	0	0
6	D	5	0	0	0	0
6	E	9	0	0	0	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
7	E	14	0	13	1	0
8	B	20	0	18	1	0
9	A	327	0	0	6	0
9	B	275	0	0	4	1
9	C	283	0	0	2	0
9	D	277	0	0	1	1
9	E	239	0	0	1	0
All	All	10255	0	8601	58	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 3.

The worst 5 of 58 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)
4:A:1206:ACT:H3	9:A:7145:HOH:O	1.70	0.90
1:B:120:ARG:HH12	4:B:1208:ACT:H3	1.42	0.84
1:E:95[B]:CYS:SG	1:E:169:ILE:HD12	2.21	0.80
1:B:31:GLN:HG2	1:B:124:PHE:CE2	2.19	0.78
1:B:181:ASN:ND2	9:B:7228:HOH:O	2.20	0.74

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)
9:B:7052:HOH:O	9:D:7209:HOH:O[2_557]	2.12	0.08

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	210/204 (103%)	203 (97%)	7 (3%)	0	100	100
1	B	206/204 (101%)	199 (97%)	7 (3%)	0	100	100
1	C	206/204 (101%)	201 (98%)	5 (2%)	0	100	100
1	D	208/204 (102%)	203 (98%)	5 (2%)	0	100	100
1	E	206/204 (101%)	202 (98%)	4 (2%)	0	100	100
All	All	1036/1020 (102%)	1008 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	189/181 (104%)	187 (99%)	2 (1%)	73	57
1	B	185/181 (102%)	183 (99%)	2 (1%)	73	57
1	C	185/181 (102%)	183 (99%)	2 (1%)	73	57
1	D	187/181 (103%)	184 (98%)	3 (2%)	62	41
1	E	185/181 (102%)	182 (98%)	3 (2%)	62	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	931/905 (103%)	919 (99%)	12 (1%)	69	50

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	TYR
1	D	164	LEU
1	E	52	TYR
1	E	1	HIS
1	B	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

13 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	F	1	1,2	14,14,15	0.54	0	17,19,21	1.08	1 (5%)
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.64	0	17,19,21	0.79	0
3	GAL	G	10	3	11,11,12	0.59	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SIA	G	11	3	20,20,21	2.18	7 (35%)	24,28,31	1.20	2 (8%)
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	0.85	0
3	BMA	G	3	3	11,11,12	1.96	3 (27%)	15,15,17	1.30	1 (6%)
3	MAN	G	4	3	11,11,12	0.99	0	15,15,17	4.66	6 (40%)
3	NAG	G	5	3	14,14,15	0.39	0	17,19,21	1.28	2 (11%)
3	GAL	G	6	3	11,11,12	0.68	0	15,15,17	2.62	5 (33%)
3	SIA	G	7	3	20,20,21	1.93	5 (25%)	24,28,31	1.41	4 (16%)
3	MAN	G	8	3	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
3	NAG	G	9	3	14,14,15	0.30	0	17,19,21	0.62	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
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	GAL	G	10	3	-	0/2/19/22	0/1/1/1
3	SIA	G	11	3	-	4/18/34/38	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	1/1/1/1
3	NAG	G	5	3	-	4/6/23/26	0/1/1/1
3	GAL	G	6	3	-	1/2/19/22	0/1/1/1
3	SIA	G	7	3	-	0/18/34/38	0/1/1/1
3	MAN	G	8	3	-	1/2/19/22	0/1/1/1
3	NAG	G	9	3	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	11	SIA	O6-C6	-4.55	1.36	1.44
3	G	3	BMA	C2-C3	4.47	1.59	1.52
3	G	7	SIA	C4-C5	-3.71	1.49	1.53
3	G	7	SIA	O6-C6	-3.69	1.38	1.44
3	G	3	BMA	O3-C3	3.46	1.51	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	4	MAN	O2-C2-C1	13.86	137.51	109.15
3	G	4	MAN	C1-C2-C3	-9.99	97.39	109.67
3	G	6	GAL	O5-C5-C6	7.95	119.67	107.20
3	G	3	BMA	O3-C3-C2	4.49	118.60	109.99
3	G	6	GAL	C1-C2-C3	3.25	113.67	109.67

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
3	G	9	NAG	C4-C5-C6-O6
3	G	9	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	G	8	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5	NAG	1	0
3	G	3	BMA	1	0
3	G	4	MAN	2	0
3	G	11	SIA	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 F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
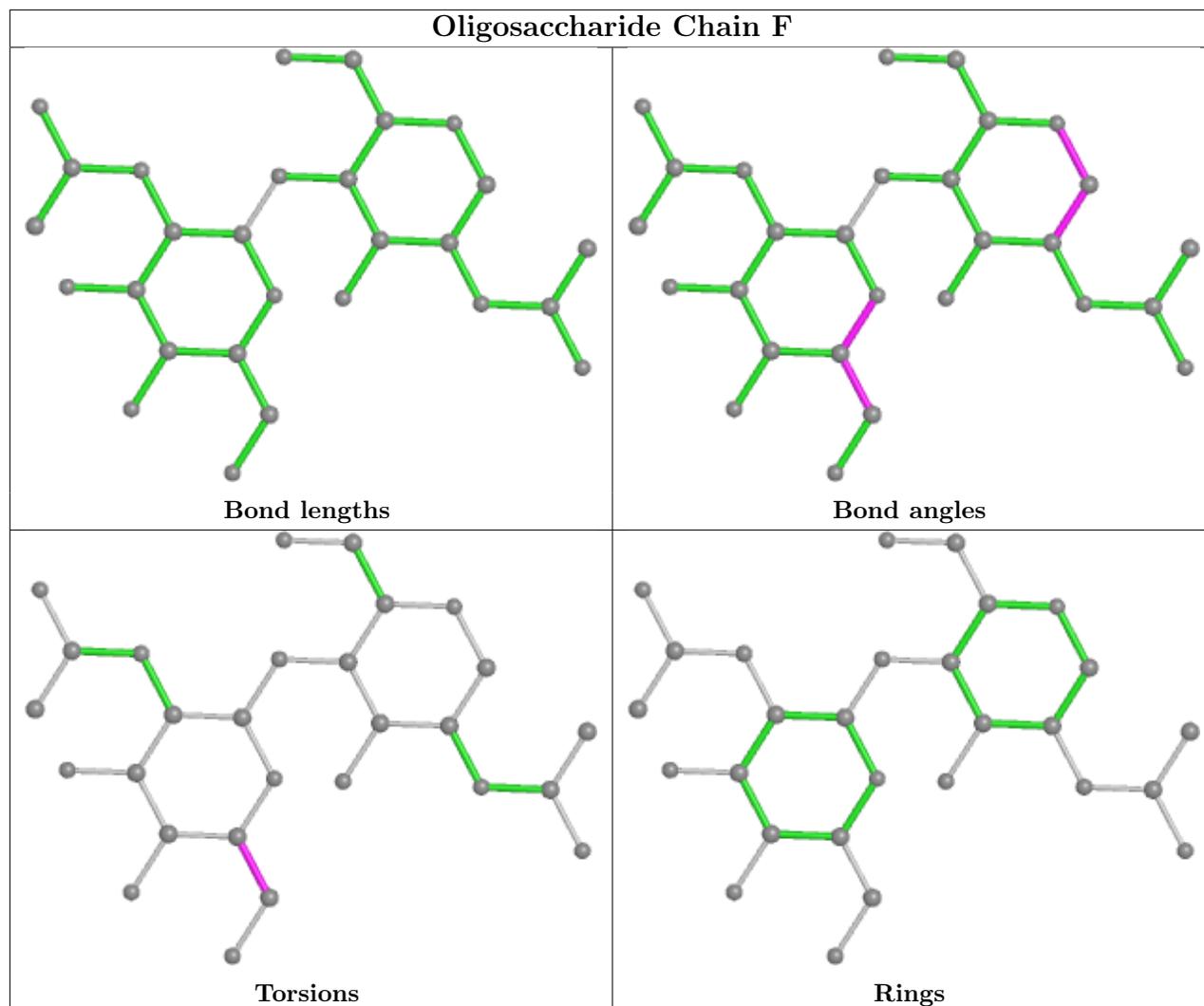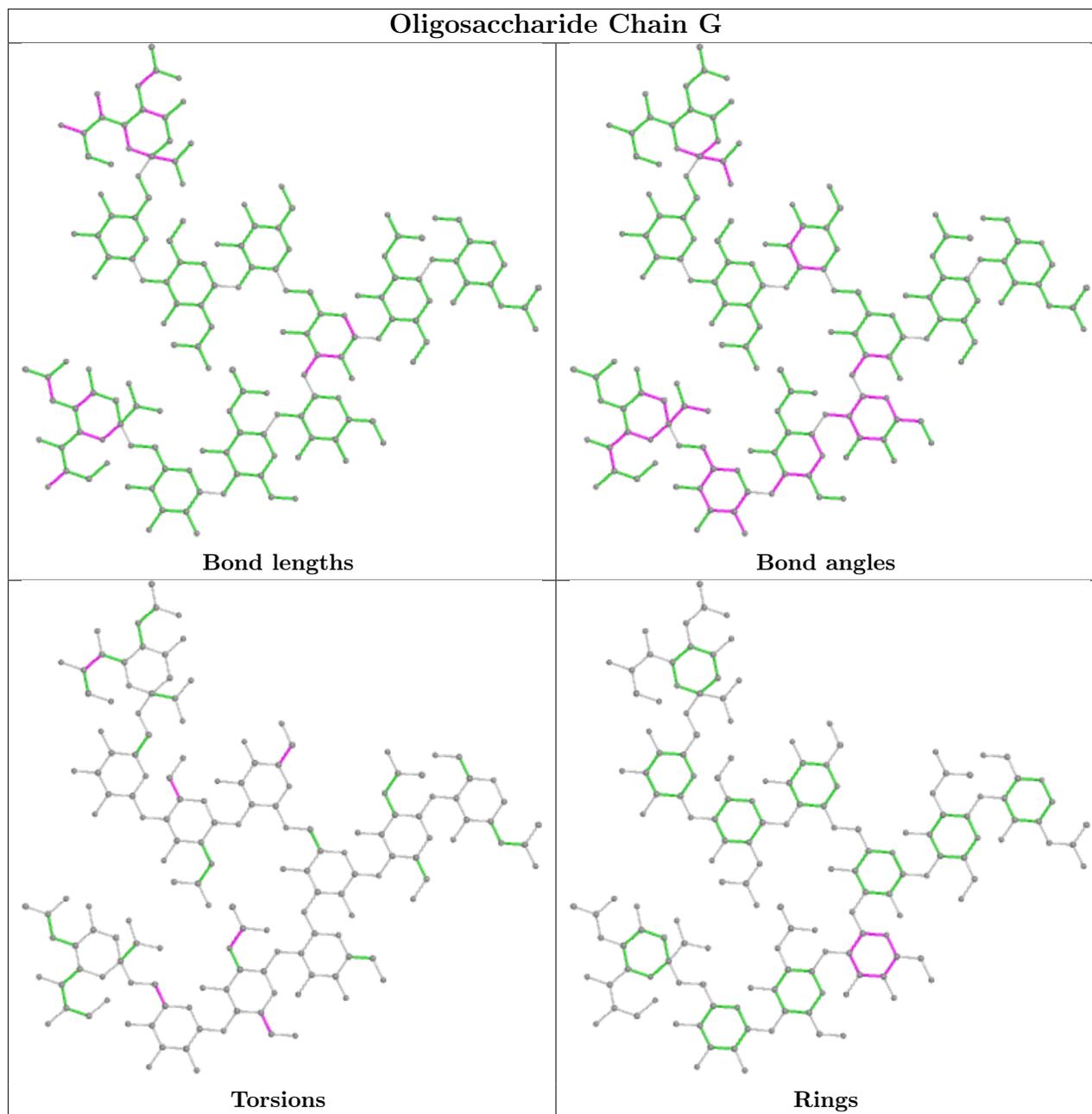
5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 35 are monoatomic - leaving 17 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
8	SIA	B	1213	-	20,20,21	1.01	1 (5%)	22,29,31	0.97	1 (4%)
4	ACT	A	1206	6	3,3,3	0.61	0	3,3,3	1.45	0
4	ACT	A	1205	6	3,3,3	0.64	0	3,3,3	0.98	0
5	GHE	A	1207	6	25,25,25	1.79	8 (32%)	34,34,34	1.02	3 (8%)
7	NAG	A	1214	1	14,14,15	0.53	0	17,19,21	1.17	3 (17%)
5	GHE	D	1207	6	25,25,25	1.63	6 (24%)	34,34,34	1.26	5 (14%)
5	GHE	E	1207	6	25,25,25	1.79	7 (28%)	34,34,34	0.90	0
4	ACT	A	1215	6	3,3,3	0.58	0	3,3,3	1.20	0
5	GHE	C	1207	6	25,25,25	1.74	7 (28%)	34,34,34	1.04	2 (5%)
7	NAG	C	1209	1	14,14,15	0.74	0	17,19,21	1.62	3 (17%)
5	GHE	B	1207	6	25,25,25	1.64	6 (24%)	34,34,34	1.32	4 (11%)
4	ACT	A	1208	6	3,3,3	0.98	0	3,3,3	1.61	1 (33%)
4	ACT	E	1214	6	3,3,3	1.08	0	3,3,3	0.26	0
7	NAG	E	1213	1	14,14,15	0.55	0	17,19,21	1.21	3 (17%)
4	ACT	B	1208	6	3,3,3	0.47	0	3,3,3	1.86	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SIA	B	1213	-	-	6/19/37/38	0/1/1/1
5	GHE	A	1207	6	-	0/23/43/43	0/2/2/2
7	NAG	A	1214	1	-	0/6/23/26	0/1/1/1
5	GHE	D	1207	6	-	1/23/43/43	0/2/2/2
5	GHE	E	1207	6	-	0/23/43/43	0/2/2/2
7	NAG	C	1209	1	-	2/6/23/26	0/1/1/1
5	GHE	C	1207	6	-	0/23/43/43	0/2/2/2
5	GHE	B	1207	6	-	1/23/43/43	0/2/2/2
7	NAG	E	1213	1	-	0/6/23/26	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1207	GHE	C3-C2	-3.76	1.44	1.53
5	A	1207	GHE	C3-C2	-3.74	1.44	1.53
5	C	1207	GHE	C3-C2	-3.72	1.44	1.53
5	D	1207	GHE	C3-C2	-3.65	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1207	GHE	C3-C2	-3.39	1.45	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1209	NAG	C3-C4-C5	3.68	116.81	110.24
8	B	1213	SIA	O1A-C1-C2	-3.36	118.50	123.59
5	B	1207	GHE	C3-C2-C1	-3.18	106.14	111.36
7	C	1209	NAG	O5-C1-C2	-3.04	106.49	111.29
5	B	1207	GHE	C1-C2-N1	2.79	117.92	112.26

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1213	SIA	O1B-C1-C2-O6
8	B	1213	SIA	C4-C5-N5-C10
7	C	1209	NAG	C4-C5-C6-O6
7	C	1209	NAG	O5-C5-C6-O6
5	D	1207	GHE	C6-C7-C8-C9

There are no ring outliers.
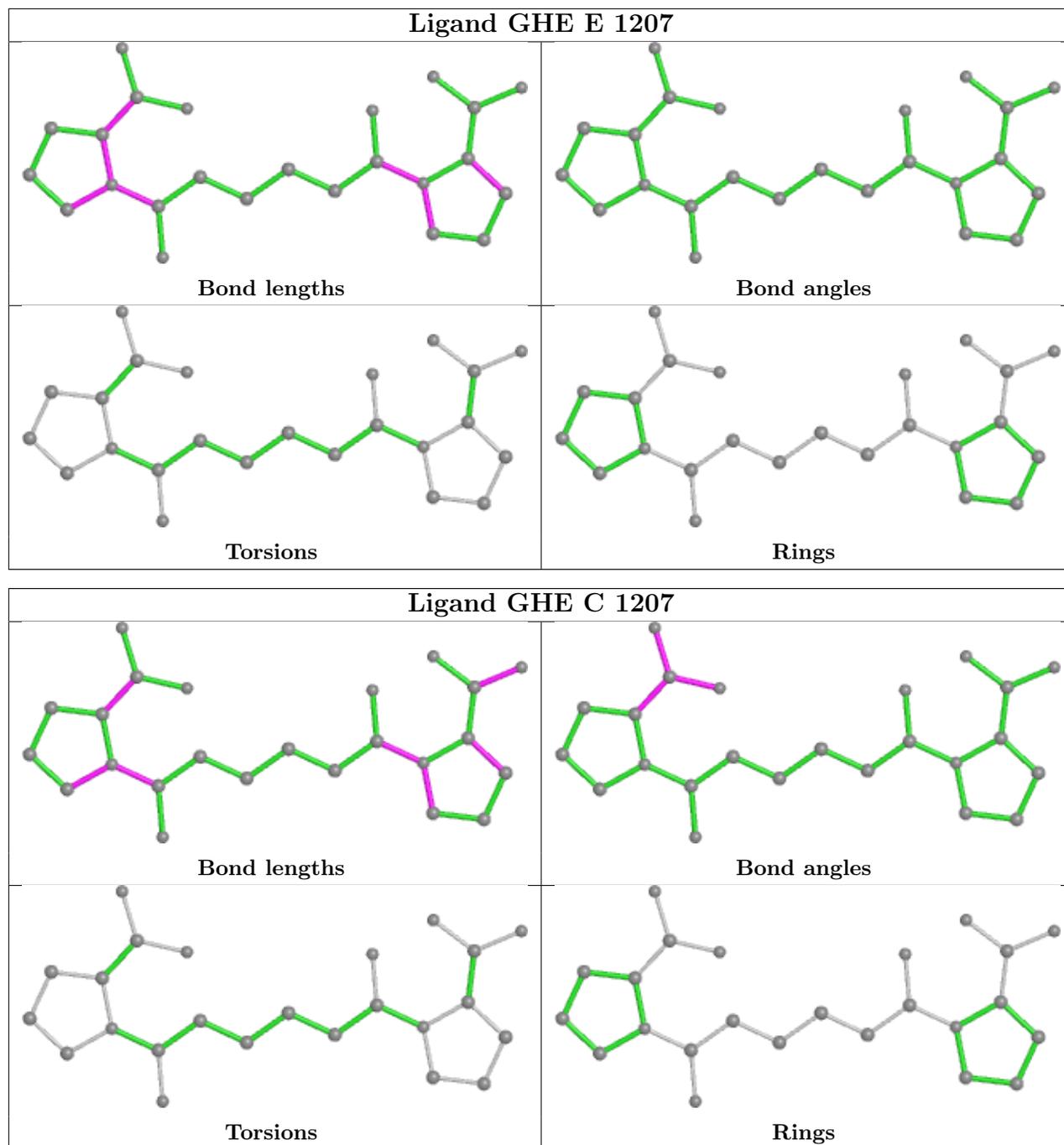
9 monomers are involved in 11 short contacts:

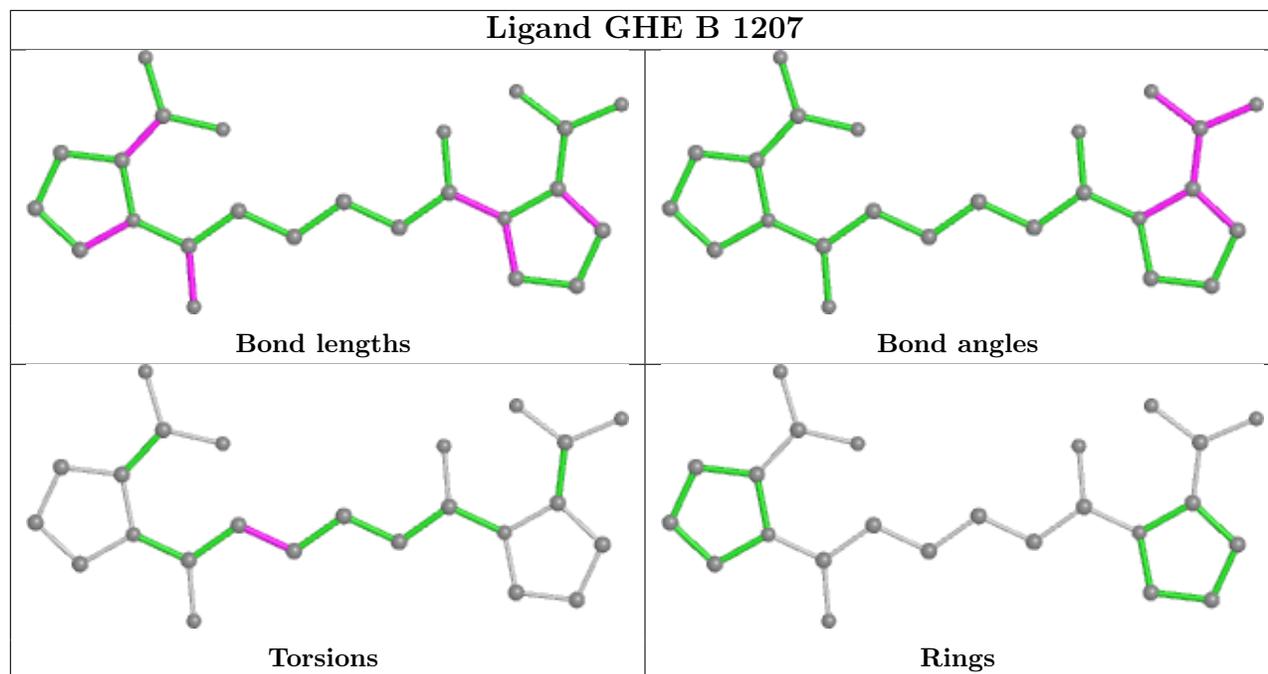| Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1213	SIA	1	0
4	A	1206	ACT	2	0
4	A	1205	ACT	1	0
4	A	1215	ACT	1	0
5	C	1207	GHE	1	0
4	A	1208	ACT	2	0
4	E	1214	ACT	1	0
7	E	1213	NAG	1	0
4	B	1208	ACT	3	0

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 B 1213

Bond lengths

Bond angles

Torsions

Rings

Ligand GHE A 1207

Bond lengths

Bond angles

Torsions

Rings

Ligand GHE D 1207

Bond lengths

Bond angles

Torsions

Rings

Ligand GHE E 1207

Bond lengths

Bond angles

Torsions

Rings

Ligand GHE C 1207

Bond lengths

Bond angles

Torsions

Rings

Ligand GHE B 1207

Bond lengths

Bond angles

Torsions

Rings
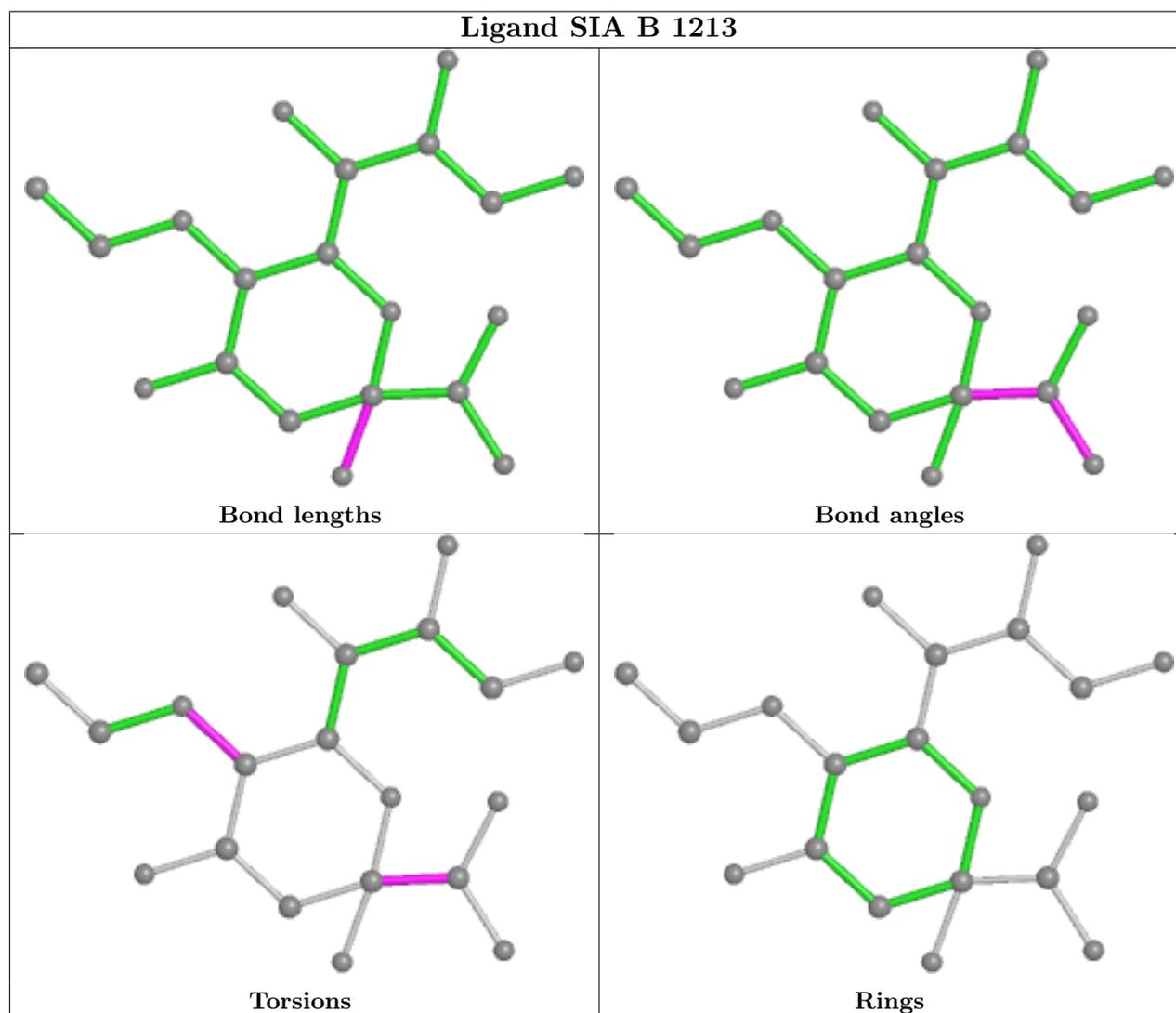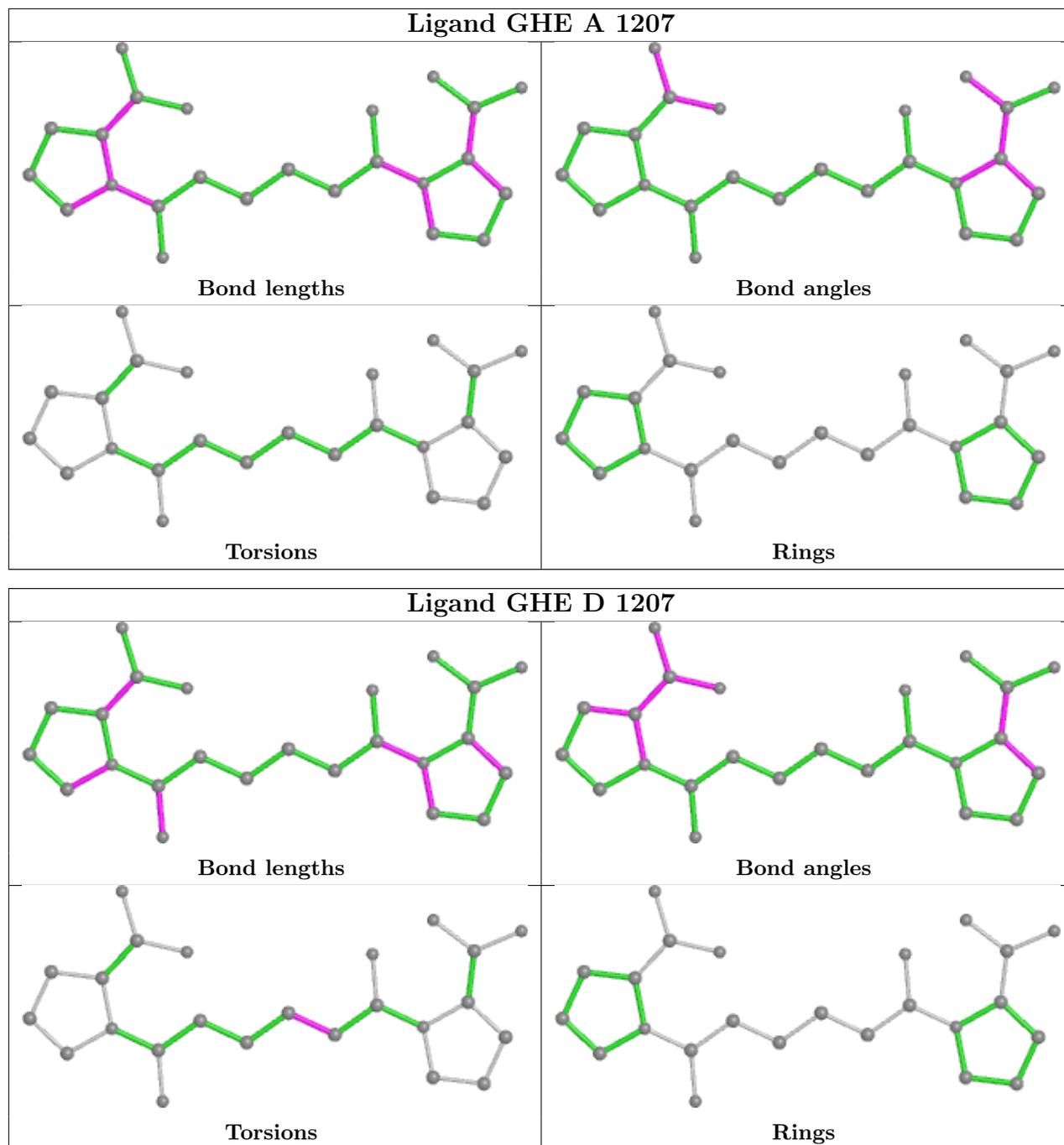
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	204/204 (100%)	-0.45	1 (0%)	91	90	10, 14, 24, 39	0
1	B	204/204 (100%)	-0.37	3 (1%)	73	73	10, 15, 30, 42	0
1	C	204/204 (100%)	-0.43	1 (0%)	91	90	10, 14, 26, 38	0
1	D	204/204 (100%)	-0.29	10 (4%)	29	27	10, 15, 34, 44	0
1	E	204/204 (100%)	-0.29	8 (3%)	39	36	10, 15, 32, 41	0
All	All	1020/1020 (100%)	-0.37	23 (2%)	60	59	10, 15, 31, 44	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	VAL	7.2
1	B	204	VAL	6.2
1	D	170	LEU	5.5
1	A	204	VAL	5.2
1	C	204	VAL	4.9

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.
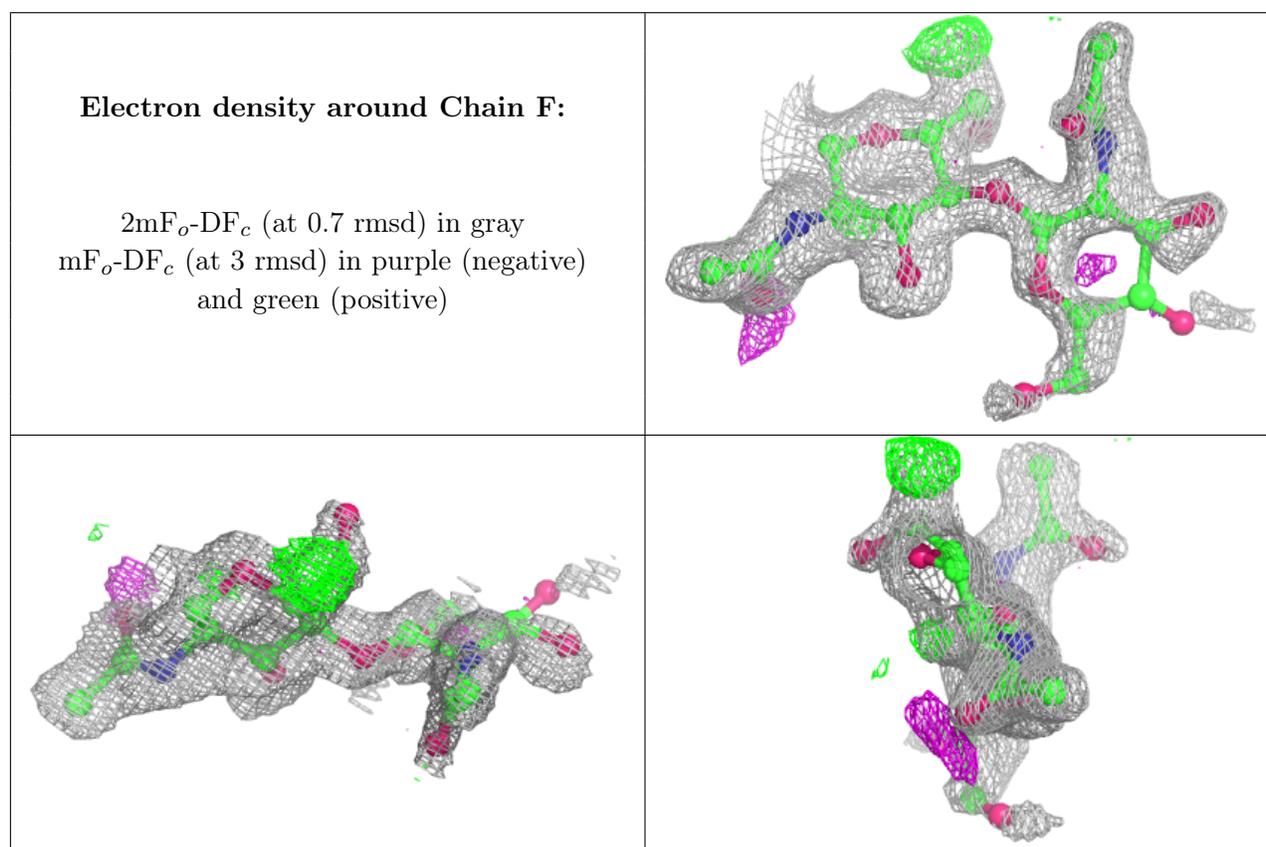
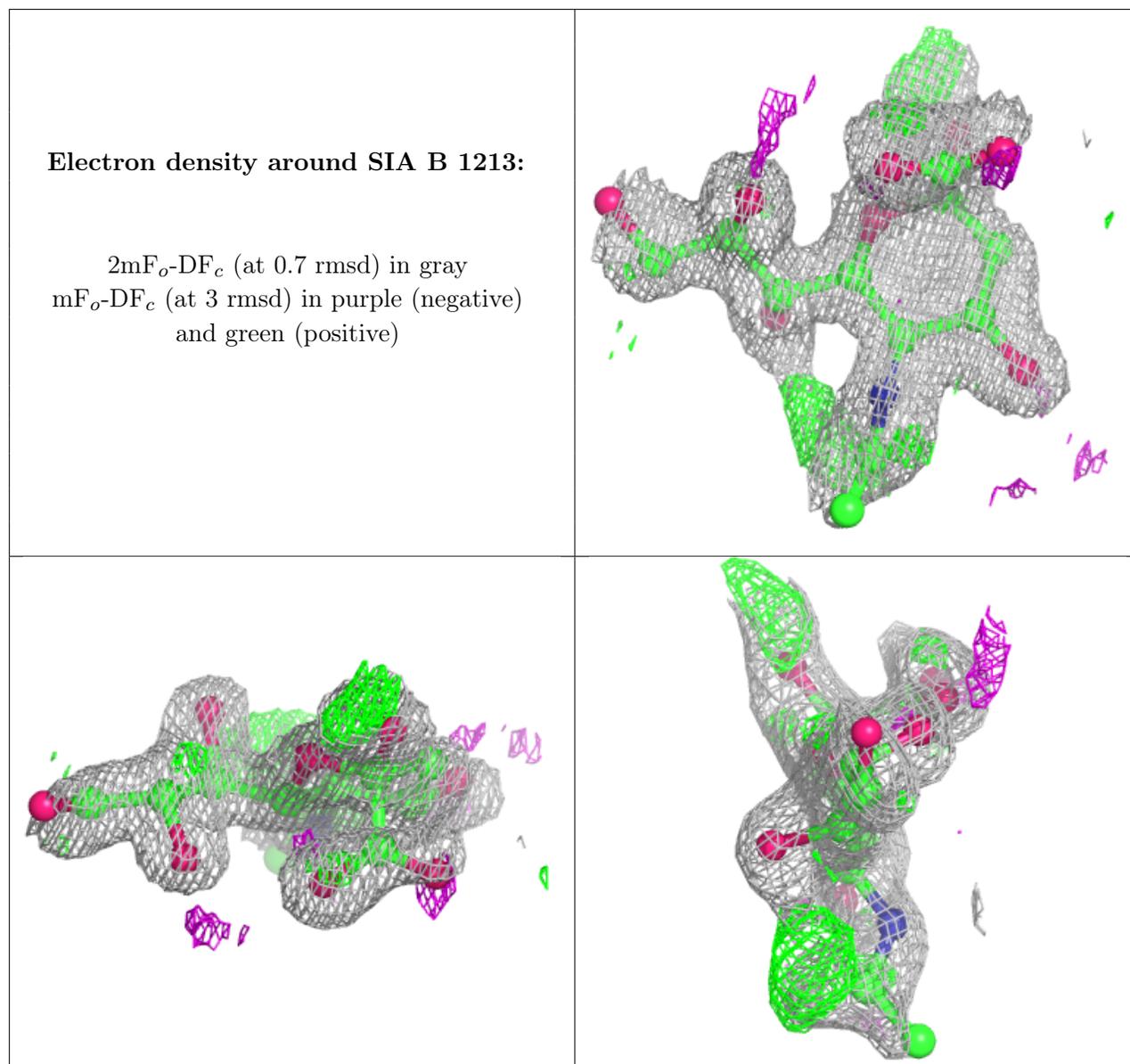| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	9	14/15	0.02	0.77	25,28,33,36	14

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	G	4	11/12	0.41	0.41	41,46,48,48	11
3	GAL	G	10	11/12	0.65	0.28	25,35,40,40	11
3	NAG	G	5	14/15	0.67	0.24	25,31,38,44	13
2	NAG	F	2	14/15	0.69	0.28	36,44,52,58	0
3	BMA	G	3	11/12	0.70	0.19	34,39,42,44	11
3	MAN	G	8	11/12	0.77	0.28	35,38,43,49	11
3	GAL	G	6	11/12	0.78	0.19	24,31,36,37	11
3	SIA	G	11	20/21	0.78	0.18	16,24,31,33	20
3	NAG	G	1	14/15	0.81	0.11	21,27,30,30	14
3	NAG	G	2	14/15	0.81	0.14	26,34,39,42	14
2	NAG	F	1	14/15	0.84	0.16	23,31,38,42	0
3	SIA	G	7	20/21	0.92	0.10	14,20,28,32	20

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 F:

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 G:

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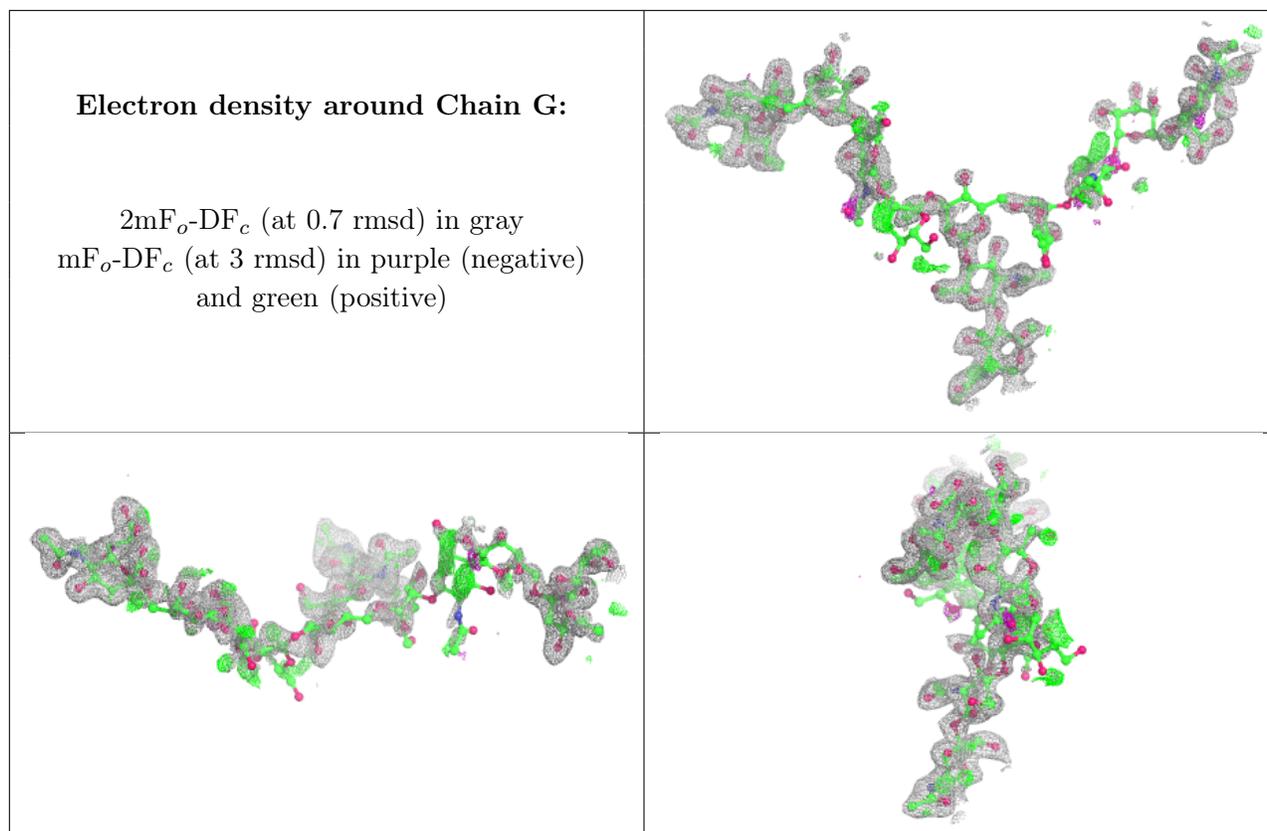
6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	E	1213	14/15	0.67	0.22	31,38,49,51	14
8	SIA	B	1213	20/21	0.76	0.18	15,21,30,31	20
7	NAG	A	1214	14/15	0.77	0.16	25,30,39,40	14
7	NAG	C	1209	14/15	0.77	0.20	26,34,42,47	14
4	ACT	A	1205	4/4	0.81	0.15	16,17,19,26	4
4	ACT	A	1215	4/4	0.84	0.15	12,14,16,31	4
4	ACT	B	1208	4/4	0.86	0.15	17,22,23,24	4
4	ACT	E	1215	4/4	0.86	0.11	14,16,22,24	4
4	ACT	A	1208	4/4	0.86	0.19	15,19,21,29	4
4	ACT	E	1214	4/4	0.88	0.15	8,18,22,33	0
4	ACT	A	1206	4/4	0.89	0.12	10,19,23,25	4
6	CD	A	1219	1/1	0.93	0.10	21,21,21,21	1
5	GHE	D	1207	24/24	0.94	0.12	11,14,21,22	24
5	GHE	B	1207	24/24	0.94	0.12	11,14,21,22	24

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	GHE	C	1207	24/24	0.94	0.11	10,13,23,24	24
6	CD	B	1216	1/1	0.95	0.08	49,49,49,49	1
5	GHE	A	1207	24/24	0.96	0.10	9,14,20,21	24
4	ACT	E	1206	4/4	0.96	0.09	16,17,18,22	4
5	GHE	E	1207	24/24	0.96	0.11	9,14,20,21	24
6	CD	C	1210	1/1	0.98	0.12	15,15,15,15	1
6	CD	D	6043	1/1	0.98	0.11	16,16,16,16	1
6	CD	E	1212	1/1	0.98	0.12	16,16,16,16	1
6	CD	E	1218	1/1	0.98	0.10	16,16,16,16	1
6	CD	A	1211	1/1	0.98	0.11	15,15,15,15	1
6	CD	B	1211	1/1	0.98	0.12	18,18,18,18	1
6	CD	B	1214	1/1	0.98	0.10	16,16,16,16	1
6	CD	A	1216	1/1	0.98	0.06	23,23,23,23	1
6	CD	B	1215	1/1	0.99	0.07	22,22,22,22	1
6	CD	D	6044	1/1	0.99	0.07	15,15,15,15	1
6	CD	E	1211	1/1	0.99	0.11	11,11,11,11	1
6	CD	A	1218	1/1	0.99	0.06	16,16,16,16	1
6	CD	E	1216	1/1	0.99	0.09	17,17,17,17	1
6	CD	E	1217	1/1	0.99	0.12	13,13,13,13	1
6	CD	C	1208	1/1	0.99	0.11	13,13,13,13	1
6	CD	E	1219	1/1	0.99	0.04	19,19,19,19	1
6	CD	A	1212	1/1	0.99	0.11	11,11,11,11	1
6	CD	C	1211	1/1	0.99	0.08	16,16,16,16	1
6	CD	C	1212	1/1	0.99	0.06	23,23,23,23	1
6	CD	D	6042	1/1	0.99	0.11	12,12,12,12	1
6	CD	E	1208	1/1	1.00	0.08	11,11,11,11	0
6	CD	E	1209	1/1	1.00	0.07	12,12,12,12	0
6	CD	E	1210	1/1	1.00	0.11	8,8,8,8	1
6	CD	C	1206	1/1	1.00	0.07	13,13,13,13	0
6	CD	B	1210	1/1	1.00	0.07	13,13,13,13	0
6	CD	A	1209	1/1	1.00	0.07	12,12,12,12	0
6	CD	B	1212	1/1	1.00	0.12	11,11,11,11	1
6	CD	A	1210	1/1	1.00	0.07	12,12,12,12	0
6	CD	D	6040	1/1	1.00	0.07	12,12,12,12	0
6	CD	D	6041	1/1	1.00	0.07	11,11,11,11	0
6	CD	A	1213	1/1	1.00	0.11	11,11,11,11	1
6	CD	B	1209	1/1	1.00	0.07	12,12,12,12	0
6	CD	C	1205	1/1	1.00	0.07	13,13,13,13	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.
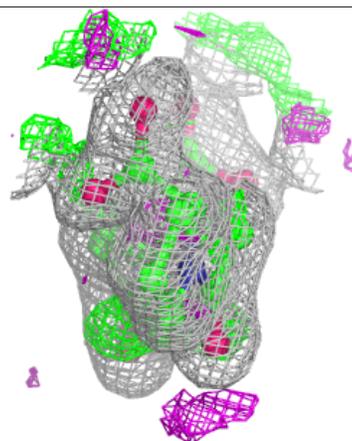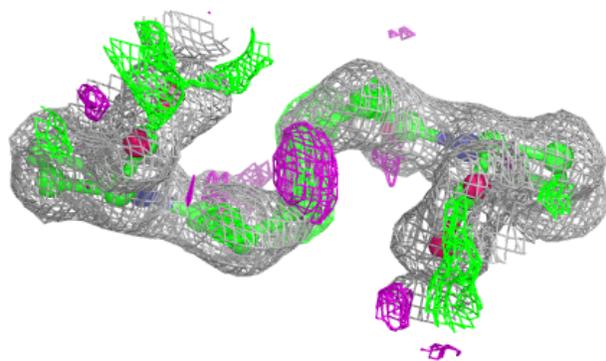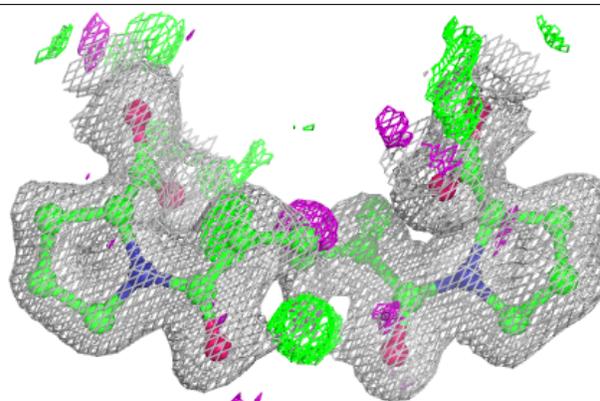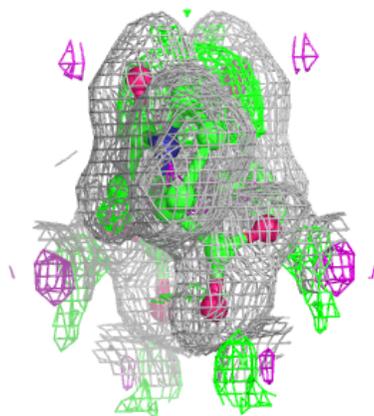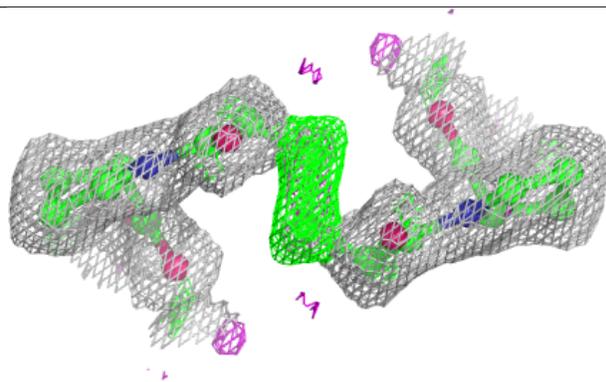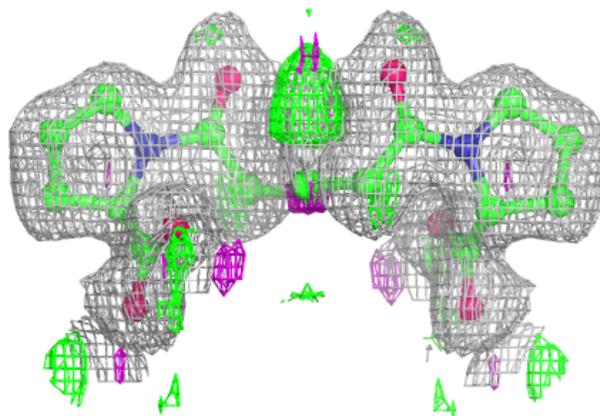
Electron density around SIA B 1213:

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

Electron density around GHE D 1207:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
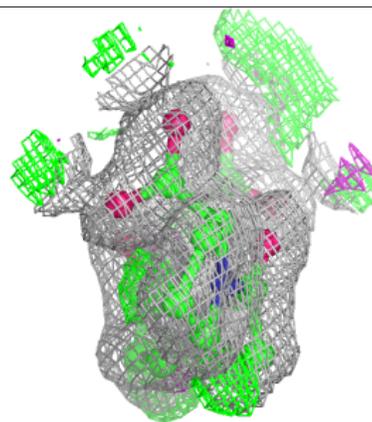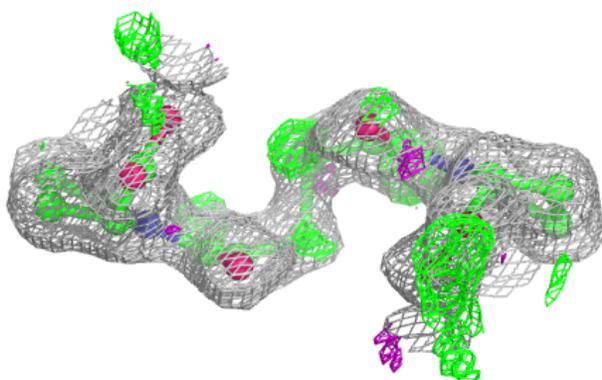$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
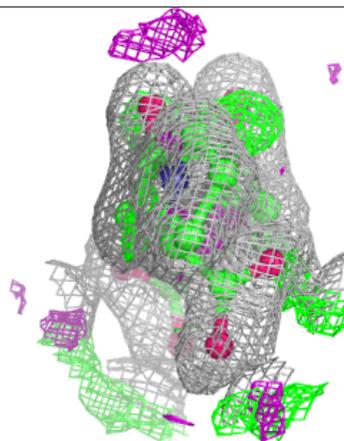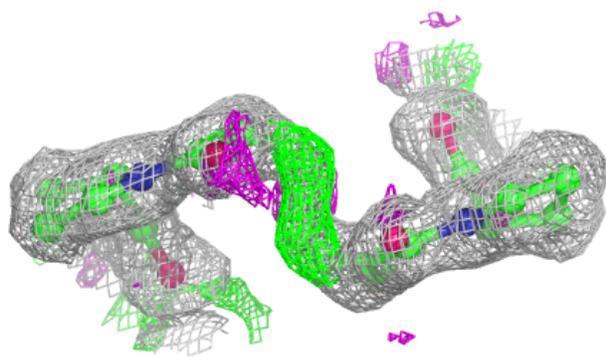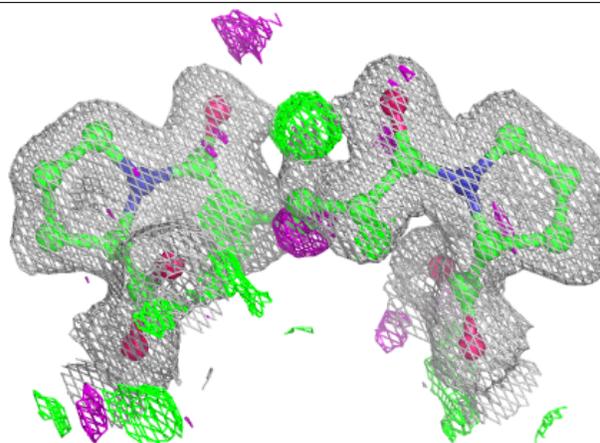
Electron density around GHE B 1207:

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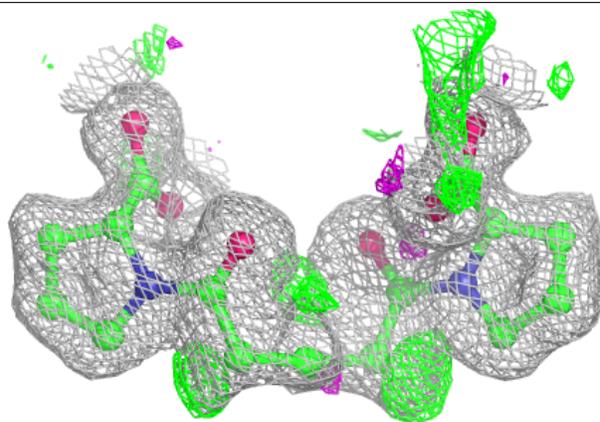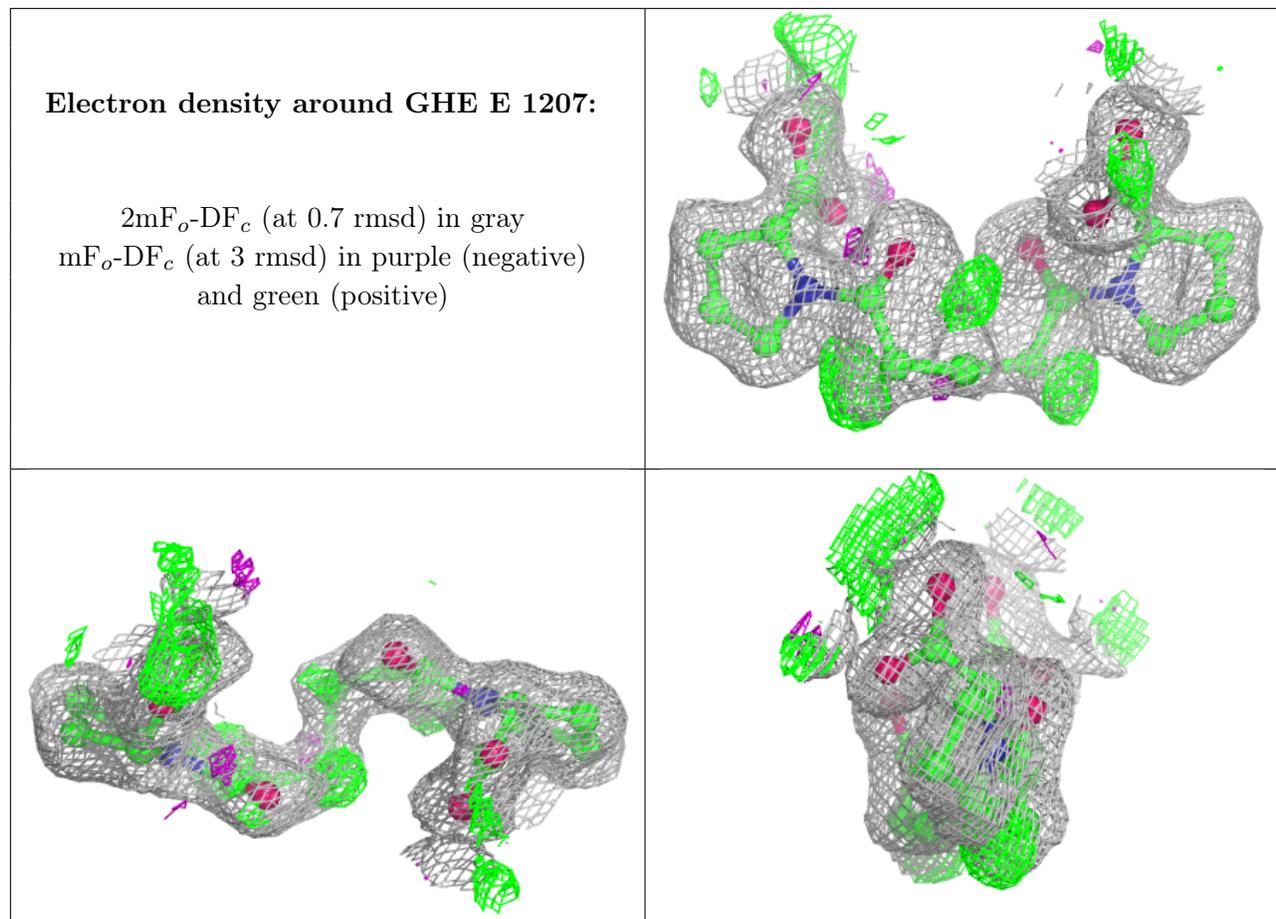and green (positive)

Electron density around GHE C 1207:

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

Electron density around GHE A 1207:

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

Electron density around GHE E 1207:

$2mF_o$-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.