



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 02:48 PM BST

PDB ID : 4M7E
Title : Structural insight into BL-induced activation of the BRI1-BAK1 complex
Authors : Chai, J.; Han, Z.; Sun, Y.
Deposited on : 2013-08-12
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

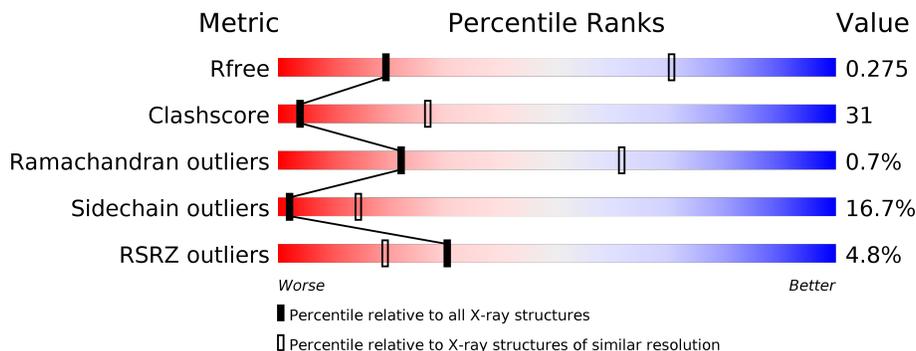
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



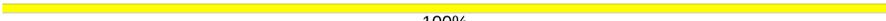
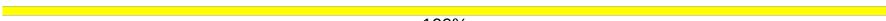
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	767	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 43% 44% 8% . . .</p>
1	B	767	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 44% 44% 8% .</p>
2	C	201	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 32% 37% 18% 13%</p>
2	D	201	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 42%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7% 28% 42% 16% 13%</p>
3	E	2	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="font-size: small; margin-top: 5px; text-align: center;">100%</p>
3	F	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: orange;"></div> </div> <p style="font-size: small; margin-top: 5px; text-align: center;">50% 50%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 100%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 13926 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	733	5542	3499	919	1093	31	0	0	0
1	B	734	5554	3506	921	1096	31	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	HIS	-	expression tag	UNP O22476
A	786	HIS	-	expression tag	UNP O22476
A	787	HIS	-	expression tag	UNP O22476
A	788	HIS	-	expression tag	UNP O22476
A	789	HIS	-	expression tag	UNP O22476
A	790	HIS	-	expression tag	UNP O22476
B	785	HIS	-	expression tag	UNP O22476
B	786	HIS	-	expression tag	UNP O22476
B	787	HIS	-	expression tag	UNP O22476
B	788	HIS	-	expression tag	UNP O22476
B	789	HIS	-	expression tag	UNP O22476
B	790	HIS	-	expression tag	UNP O22476

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	175	1299	821	221	254	3	0	0	0
2	C	175	1299	821	221	254	3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

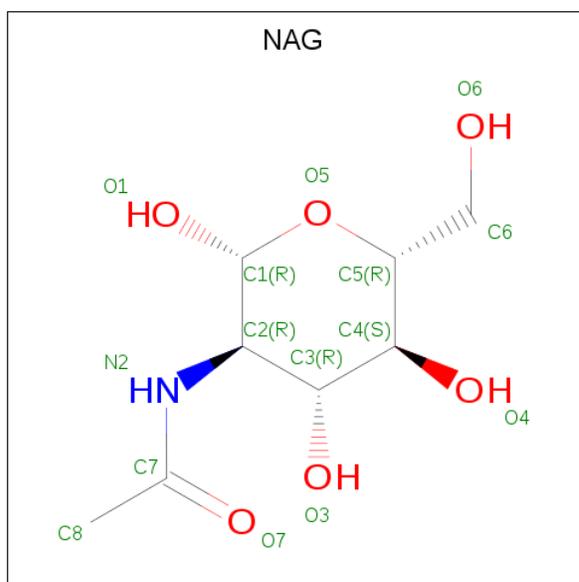
Chain	Residue	Modelled	Actual	Comment	Reference
D	221	HIS	-	expression tag	UNP Q94F62
D	222	HIS	-	expression tag	UNP Q94F62
D	223	HIS	-	expression tag	UNP Q94F62
D	224	HIS	-	expression tag	UNP Q94F62
D	225	HIS	-	expression tag	UNP Q94F62
D	226	HIS	-	expression tag	UNP Q94F62
C	221	HIS	-	expression tag	UNP Q94F62
C	222	HIS	-	expression tag	UNP Q94F62
C	223	HIS	-	expression tag	UNP Q94F62
C	224	HIS	-	expression tag	UNP Q94F62
C	225	HIS	-	expression tag	UNP Q94F62
C	226	HIS	-	expression tag	UNP Q94F62

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



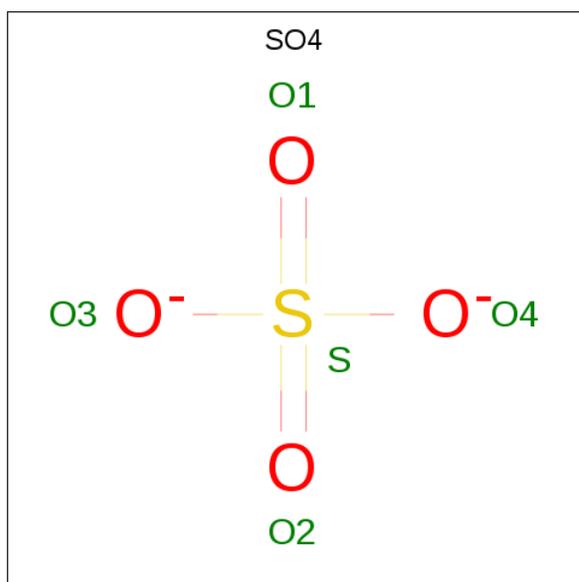
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0
3	F	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



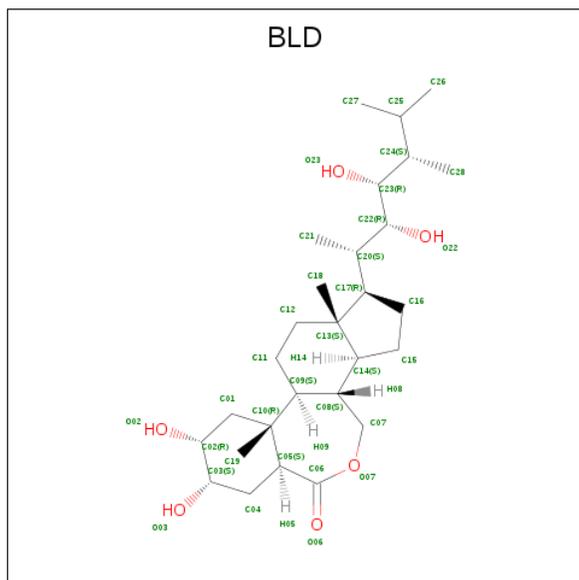
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0

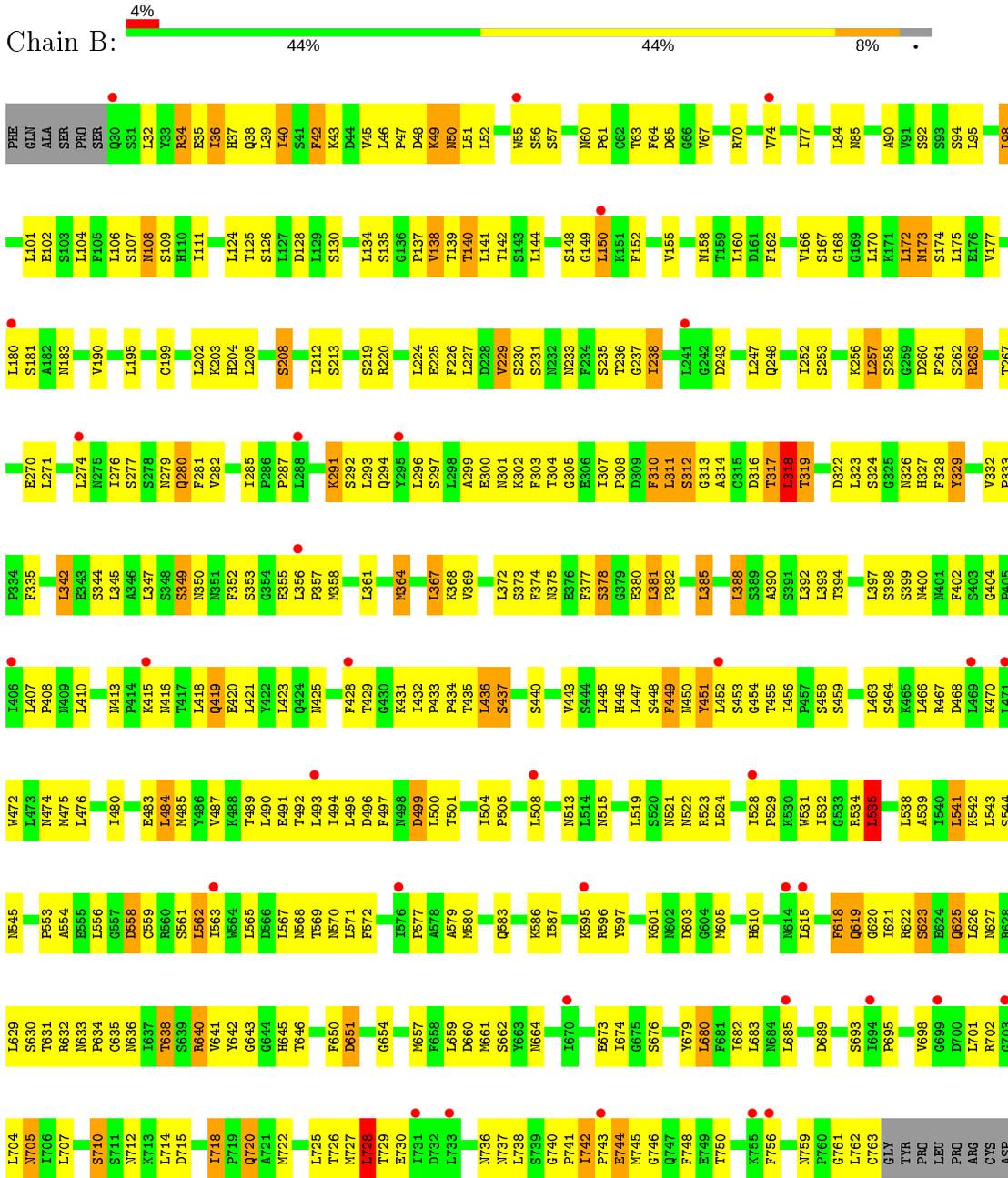
- Molecule 6 is Brassinolide (three-letter code: BLD) (formula: $C_{28}H_{48}O_6$).

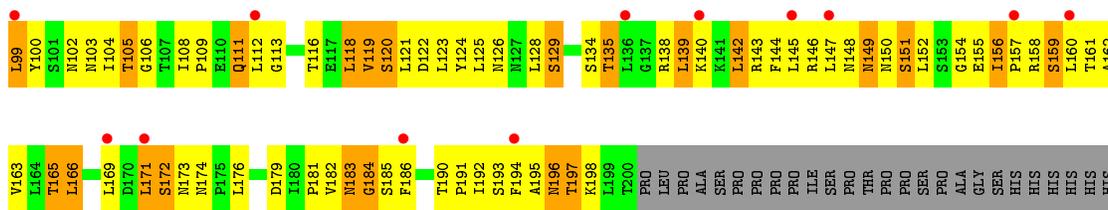


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 34 28 6	0	0
6	B	1	Total C O 34 28 6	0	0

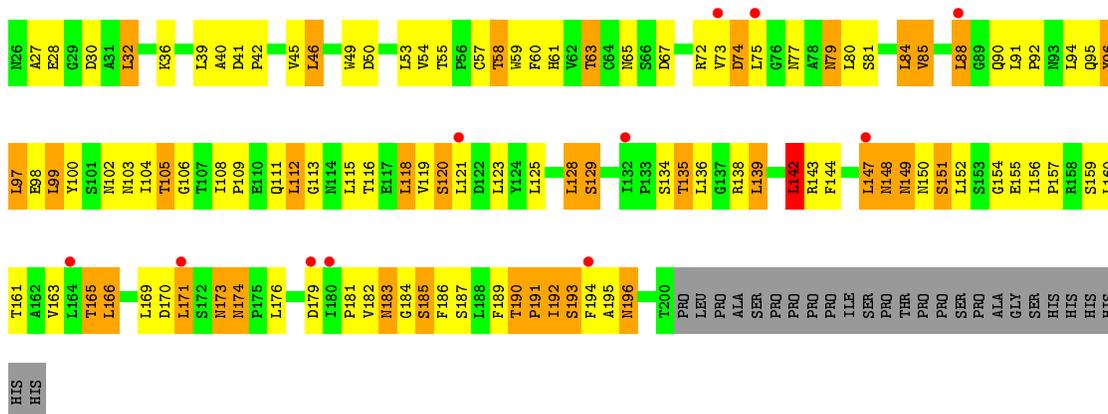
ALA
HIS
HIS
HIS
GLN
GLN
ARG
SER
SER
HIS
HIS
HIS
HIS
HIS

● Molecule 1: Protein BRASSINOSTEROID INSENSITIVE 1





- Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAP1
MAP2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	145.91Å 145.91Å 166.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.90 – 3.60 47.76 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.90-3.60) 98.3 (47.76-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.220 , 0.275 0.221 , 0.275	Depositor DCC
R_{free} test set	2269 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.873	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 0.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.310 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13926	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BLD, NAG, SO4

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	0.65	1/5648 (0.0%)	0.96	14/7664 (0.2%)
1	B	0.61	0/5659	0.93	5/7678 (0.1%)
2	C	0.75	0/1321	1.05	4/1810 (0.2%)
2	D	0.74	0/1321	1.05	4/1810 (0.2%)
All	All	0.65	1/13949 (0.0%)	0.97	27/18962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	C	0	1
2	D	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	ARG	CG-CD	5.02	1.64	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	ARG	NE-CZ-NH2	8.67	124.63	120.30
1	A	288	LEU	CA-CB-CG	8.40	134.62	115.30
2	D	142	LEU	CA-CB-CG	7.16	131.76	115.30
2	C	142	LEU	CA-CB-CG	7.03	131.46	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	LEU	CA-CB-CG	6.52	130.30	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	PHE	Peptide
1	A	415	LYS	Peptide
1	B	172	LEU	Peptide
1	B	312	SER	Peptide
2	D	155	GLU	Peptide

5.2 Too-close contacts [i](#)

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	5542	0	5503	326	0
1	B	5554	0	5517	297	0
2	C	1299	0	1272	122	0
2	D	1299	0	1270	116	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	A	28	0	26	3	0
4	B	14	0	13	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	34	0	48	8	0
6	B	34	0	48	4	0
All	All	13926	0	13797	846	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 31.

The worst 5 of 846 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:D:190:THR:HG22	2:D:191:PRO:CD	1.46	1.42
2:D:196:ASN:O	2:D:198:LYS:N	1.58	1.35
2:D:190:THR:CG2	2:D:191:PRO:HD2	1.70	1.21
2:D:190:THR:CG2	2:D:191:PRO:CD	2.30	1.06
2:C:163:VAL:HG23	2:C:166:LEU:HD11	1.41	1.02

There are no symmetry-related clashes.

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	731/767 (95%)	695 (95%)	35 (5%)	1 (0%)	51	83
1	B	732/767 (95%)	699 (96%)	30 (4%)	3 (0%)	34	71
2	C	173/201 (86%)	146 (84%)	24 (14%)	3 (2%)	9	45
2	D	173/201 (86%)	147 (85%)	21 (12%)	5 (3%)	4	33
All	All	1809/1936 (93%)	1687 (93%)	110 (6%)	12 (1%)	22	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	197	THR
1	B	313	GLY
2	D	183	ASN
2	C	173	ASN
2	C	196	ASN

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	645/676 (95%)	552 (86%)	93 (14%)	3	20
1	B	647/676 (96%)	552 (85%)	95 (15%)	3	20
2	C	144/179 (80%)	103 (72%)	41 (28%)	0	3
2	D	144/179 (80%)	109 (76%)	35 (24%)	0	4
All	All	1580/1710 (92%)	1316 (83%)	264 (17%)	2	14

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	243	ASP
1	B	436	LEU
2	C	118	LEU
1	B	263	ARG
1	B	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	ASN
1	B	712	ASN
1	B	37	HIS
1	A	619	GLN
1	B	279	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
3	NAG	E	2	3	14,14,15	0.63	0	17,19,21	2.07	7 (41%)
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	1.41	2 (11%)
3	NAG	F	2	3	14,14,15	0.65	0	17,19,21	1.56	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.76	0	17,19,21	1.73	3 (17%)
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	1.87	3 (17%)
3	NAG	H	1	1,3	14,14,15	0.56	0	17,19,21	1.15	2 (11%)
3	NAG	H	2	3	14,14,15	0.52	0	17,19,21	1.80	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	5.96	120.27	112.19
3	H	2	NAG	C1-O5-C5	5.87	120.14	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O5-C1-C2	-5.20	103.07	111.29
3	E	1	NAG	O5-C1-C2	-5.16	103.14	111.29
3	F	2	NAG	C1-O5-C5	4.60	118.42	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

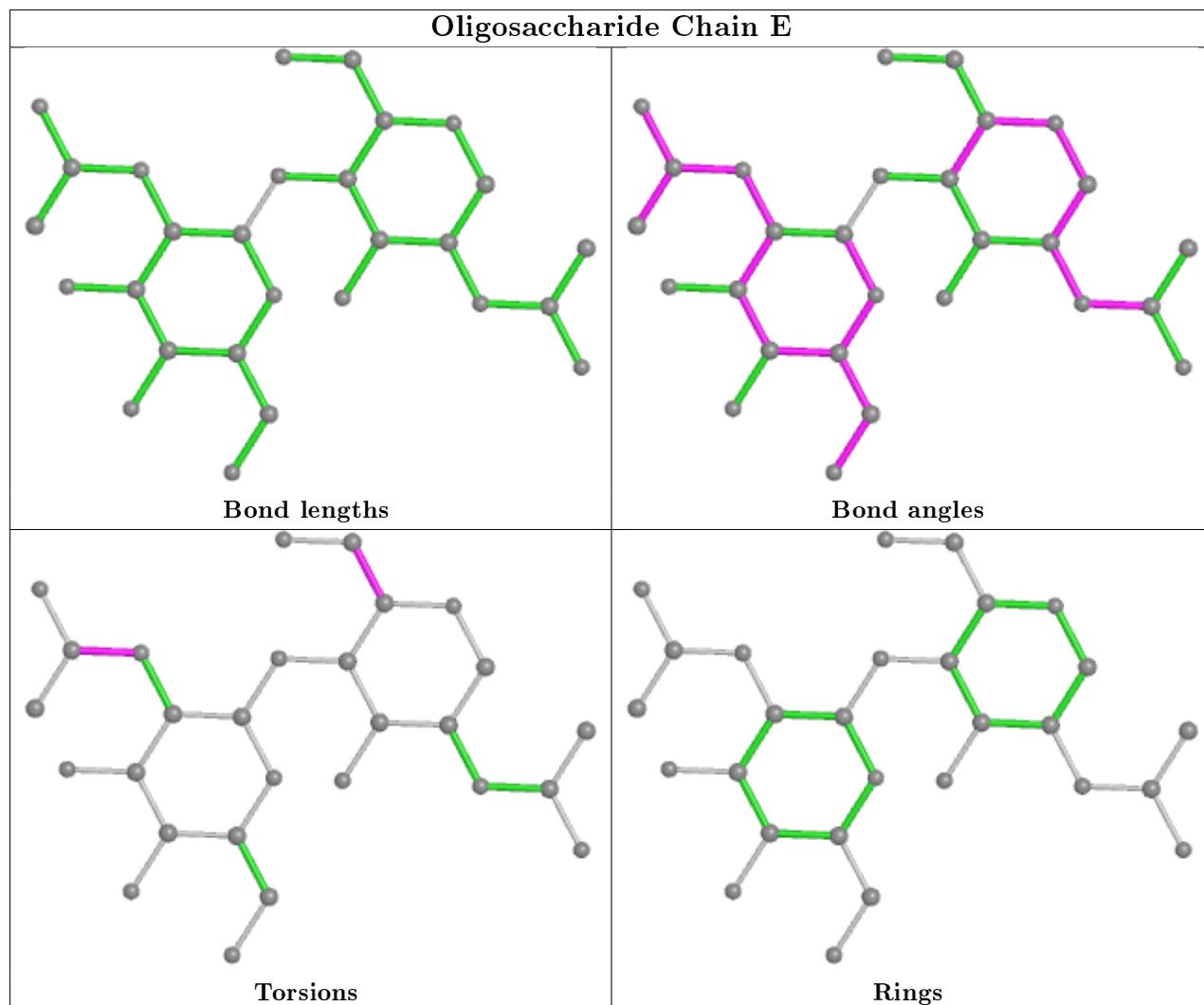
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2

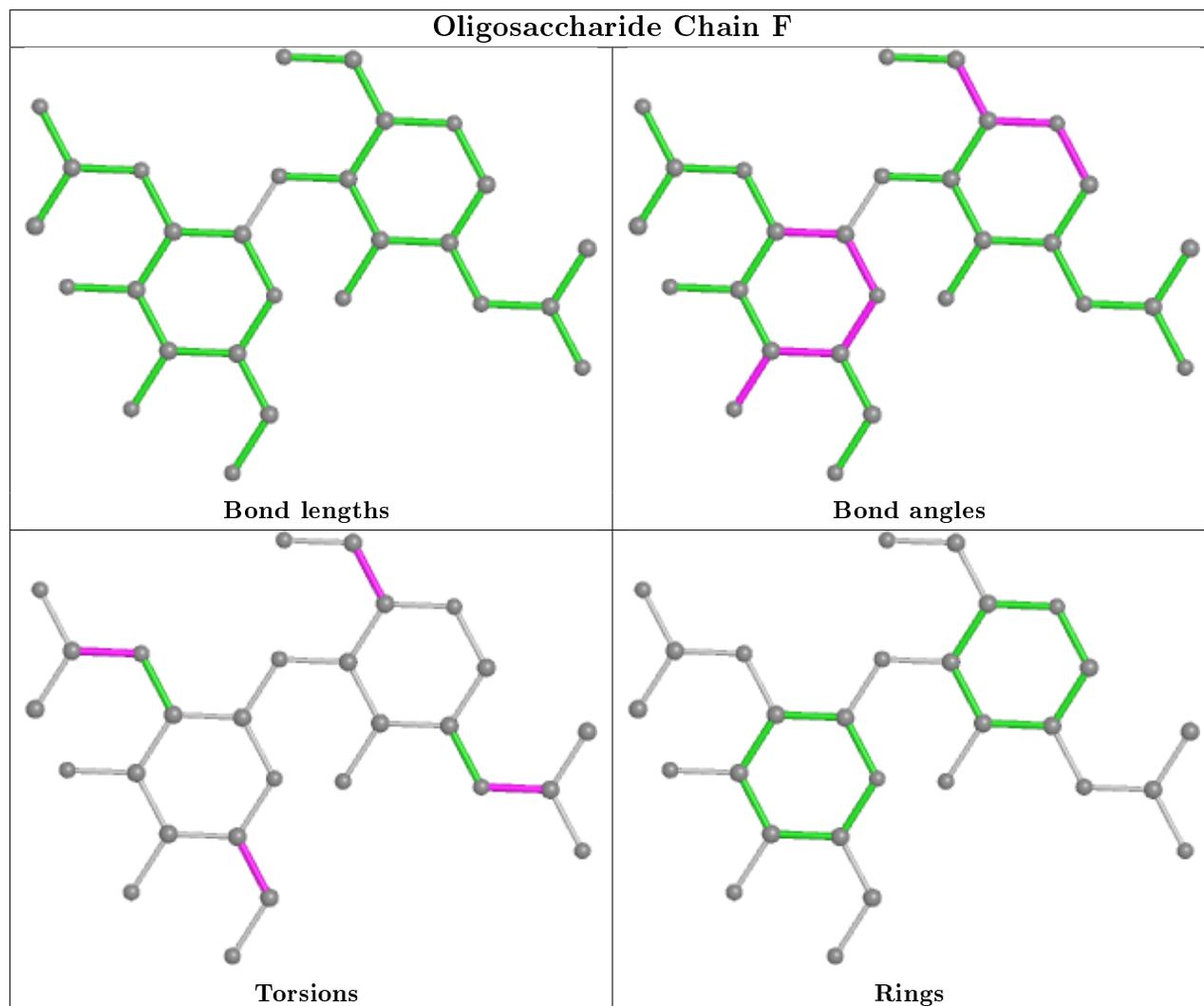
There are no ring outliers.

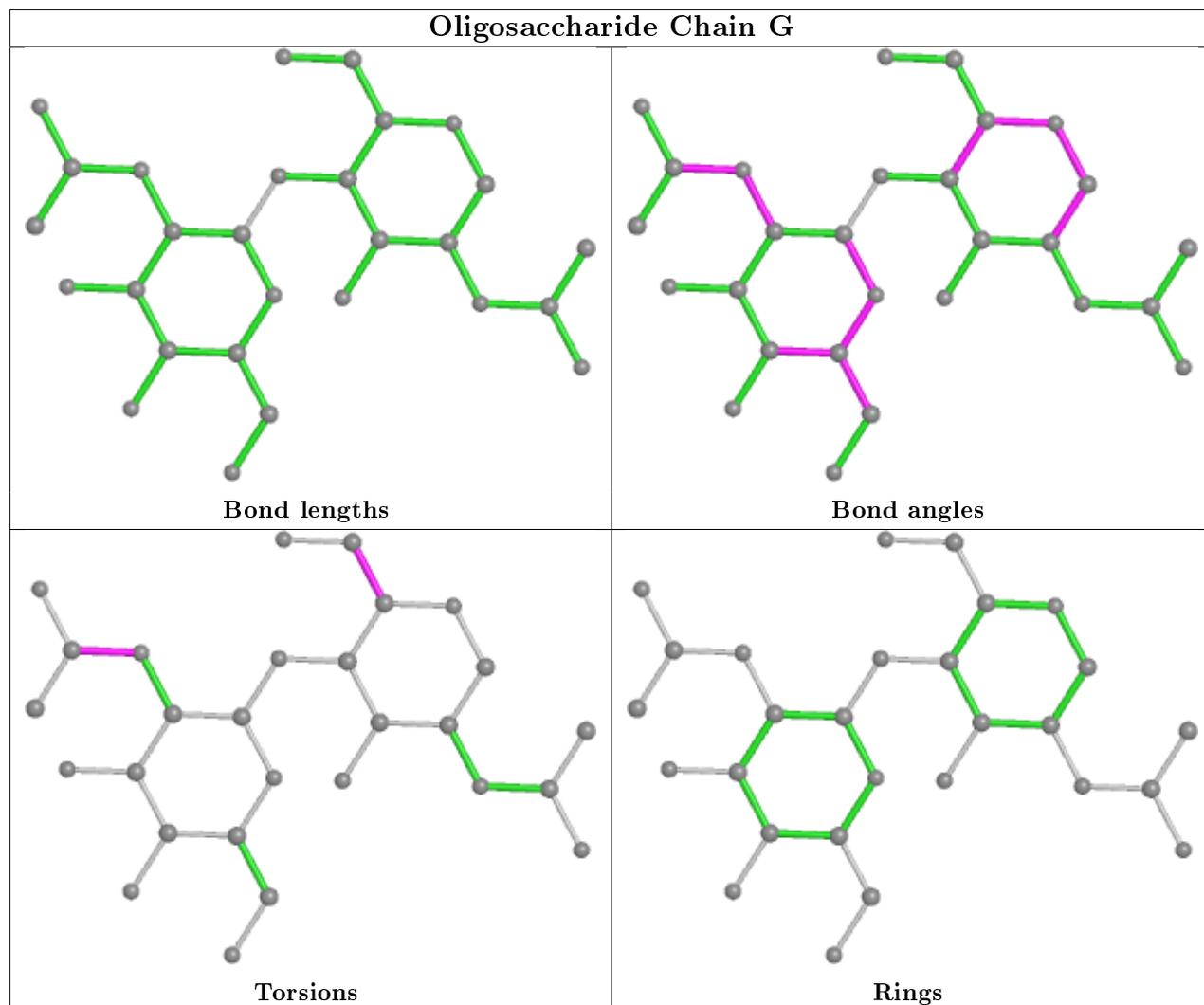
1 monomer is involved in 1 short contact:

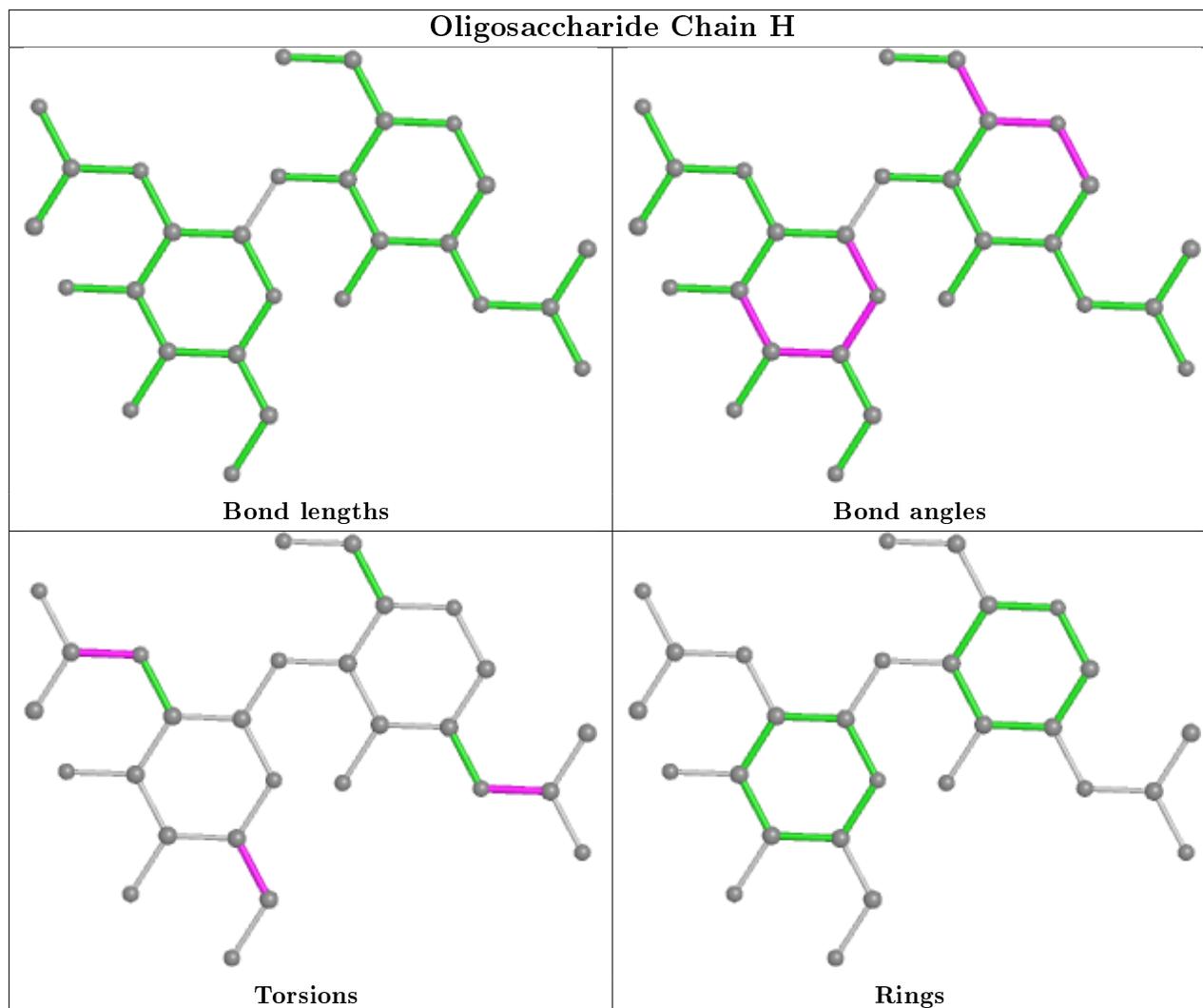
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0

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](#)

7 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	NAG	A	806	-	14,14,15	0.89	1 (7%)	17,19,21	1.54	3 (17%)
6	BLD	A	808	-	36,37,37	1.63	2 (5%)	46,59,59	1.99	11 (23%)
5	SO4	A	807	-	4,4,4	0.21	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	805	1	14,14,15	0.66	0	17,19,21	2.27	5 (29%)
5	SO4	B	806	-	4,4,4	0.15	0	6,6,6	0.41	0
6	BLD	B	807	-	36,37,37	1.64	2 (5%)	46,59,59	2.03	14 (30%)
4	NAG	B	805	1	14,14,15	0.45	0	17,19,21	2.49	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	805	1	-	2/6/23/26	0/1/1/1
4	NAG	A	806	-	-	5/6/23/26	0/1/1/1
6	BLD	A	808	-	-	7/20/85/85	0/4/4/4
6	BLD	B	807	-	-	5/20/85/85	0/4/4/4
4	NAG	B	805	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	807	BLD	O07-C06	8.65	1.45	1.34
6	A	808	BLD	O07-C06	8.32	1.44	1.34
4	A	806	NAG	O5-C1	-2.37	1.39	1.43
6	A	808	BLD	O07-C07	-2.13	1.42	1.45
6	B	807	BLD	O07-C07	-2.05	1.42	1.45

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	NAG	C1-O5-C5	6.70	121.27	112.19
4	B	805	NAG	C3-C4-C5	-5.91	99.70	110.24
6	A	808	BLD	C05-C04-C03	5.87	120.13	111.90
4	A	805	NAG	C2-N2-C7	-5.77	114.68	122.90
6	A	808	BLD	C14-C08-C09	-4.88	102.56	109.09

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	808	BLD	C23-C24-C25-C27

Continued on next page...

Continued from previous page...

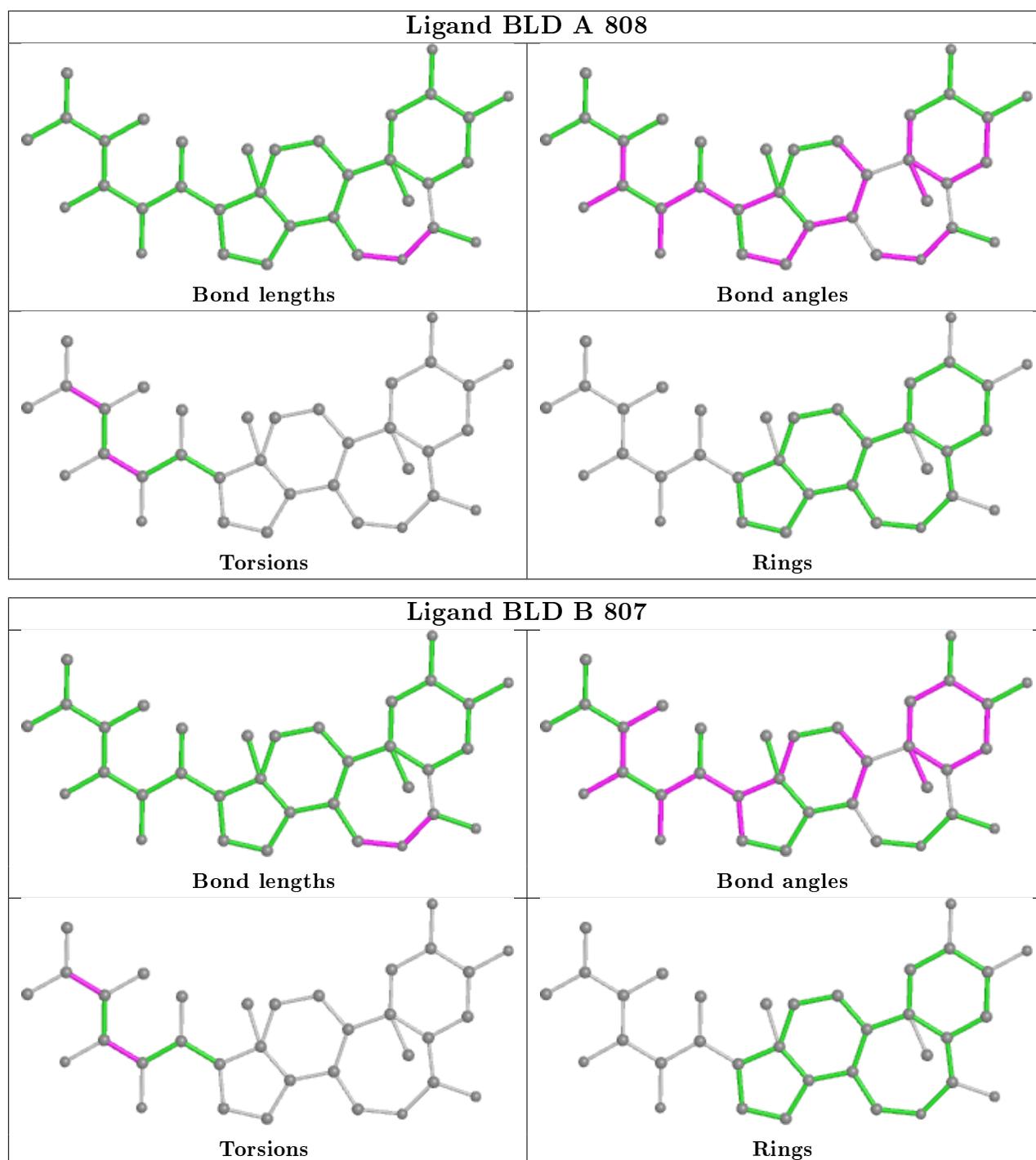
Mol	Chain	Res	Type	Atoms
6	B	807	BLD	C20-C22-C23-C24
6	B	807	BLD	C23-C24-C25-C27
4	A	805	NAG	C4-C5-C6-O6
4	A	806	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	806	NAG	1	0
6	A	808	BLD	8	0
4	A	805	NAG	3	0
6	B	807	BLD	4	0
4	B	805	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	733/767 (95%)	0.35	28 (3%) 40 26	0, 21, 83, 178	0
1	B	734/767 (95%)	0.35	34 (4%) 32 20	0, 28, 94, 199	0
2	C	175/201 (87%)	0.38	11 (6%) 20 11	0, 27, 76, 152	0
2	D	175/201 (87%)	0.37	15 (8%) 10 6	0, 27, 83, 133	0
All	All	1817/1936 (93%)	0.35	88 (4%) 30 19	0, 25, 89, 199	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	75	LEU	4.0
1	A	670	ILE	3.7
2	D	194	PHE	3.7
1	A	694	ILE	3.4
2	C	147	LEU	3.3

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

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

6.3 Carbohydrates [i](#)

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

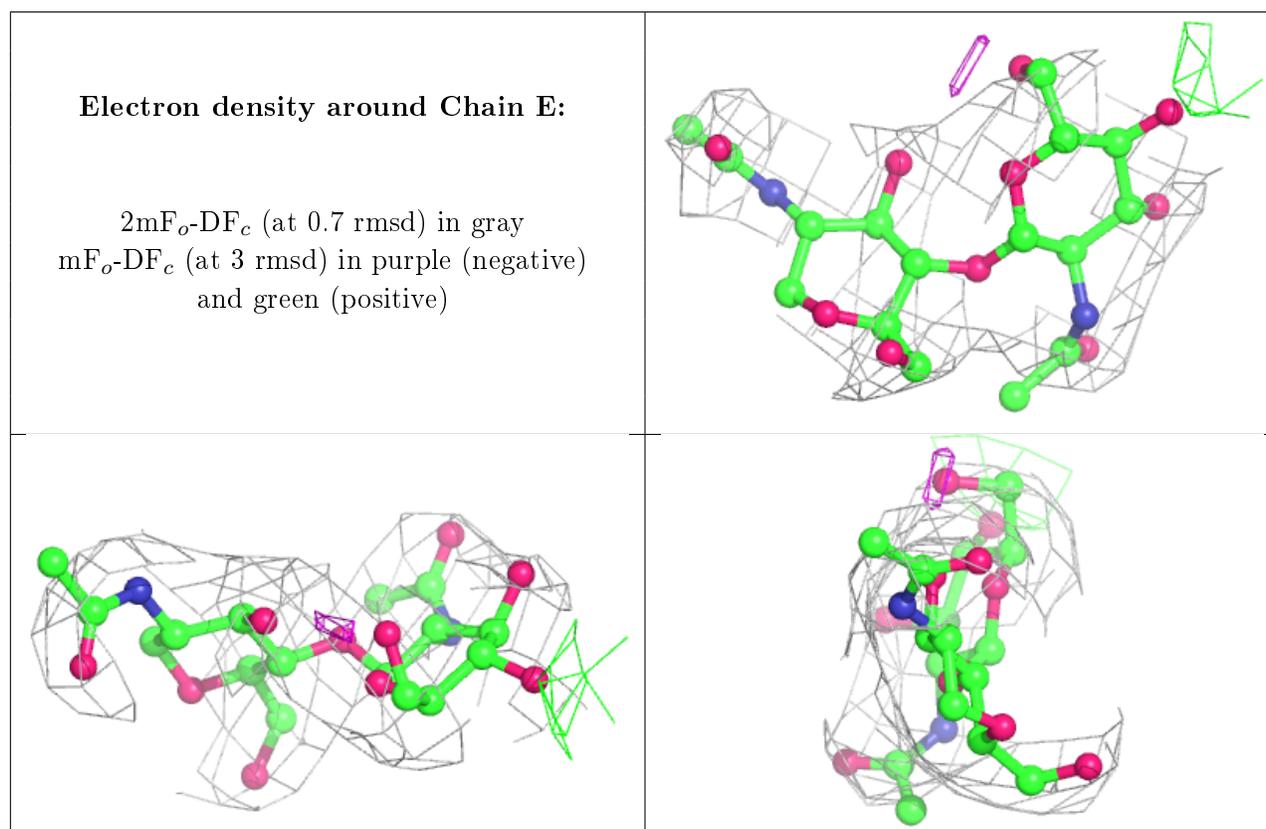
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.81	0.29	32,44,52,63	0
3	NAG	G	2	14/15	0.88	0.26	53,53,53,53	0

Continued on next page...

Continued from previous page...

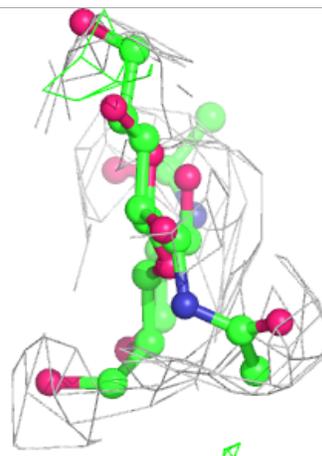
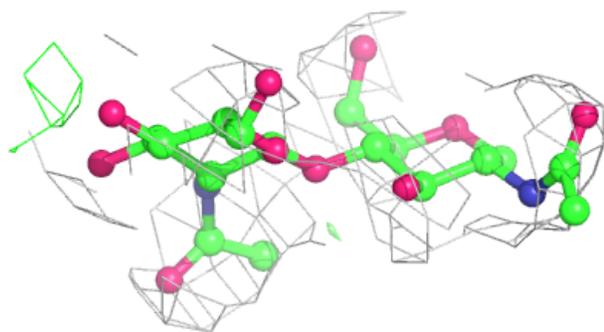
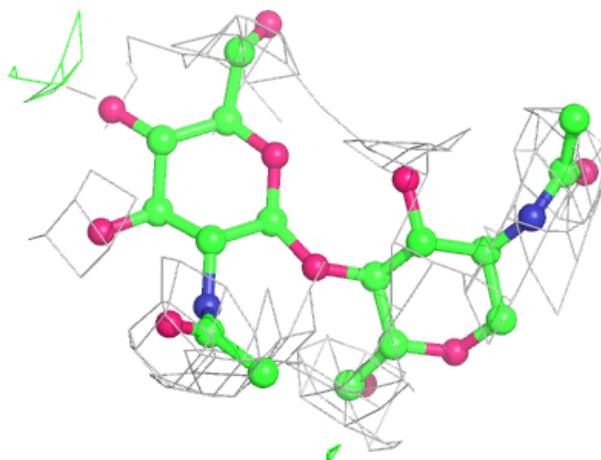
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	F	2	14/15	0.88	0.27	10,29,35,35	0
3	NAG	F	1	14/15	0.89	0.25	33,33,33,33	0
3	NAG	H	2	14/15	0.90	0.17	39,39,39,39	0
3	NAG	H	1	14/15	0.92	0.21	40,40,40,40	0
3	NAG	G	1	14/15	0.93	0.22	15,17,21,22	0
3	NAG	E	1	14/15	0.94	0.23	8,12,17,22	0

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.



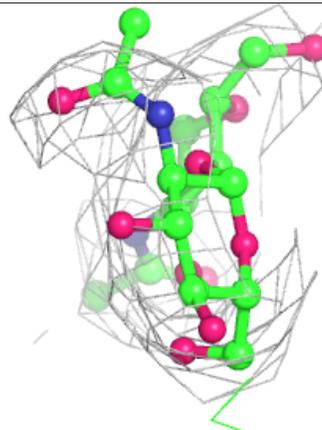
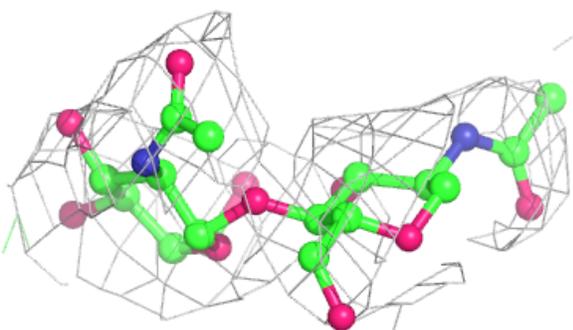
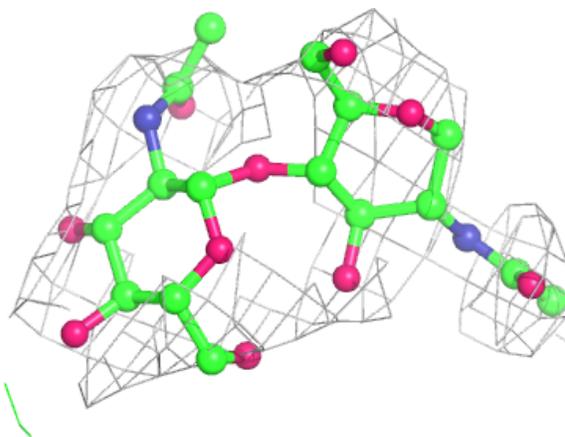
Electron density around Chain F:

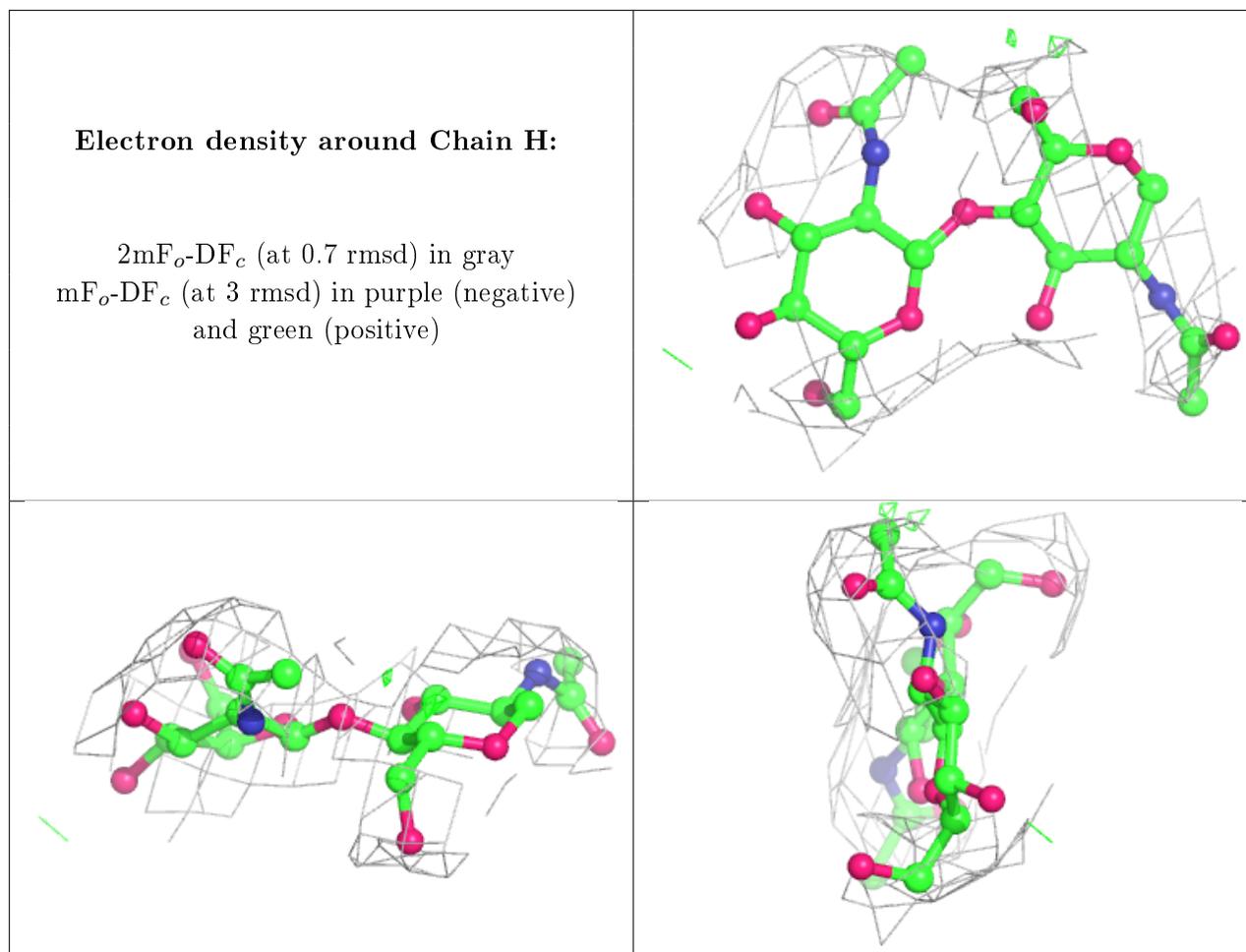
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.

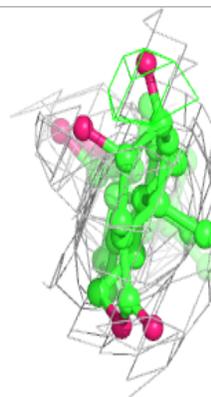
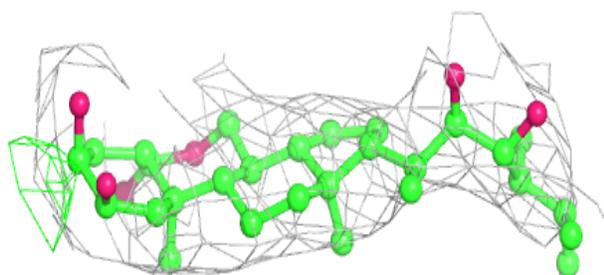
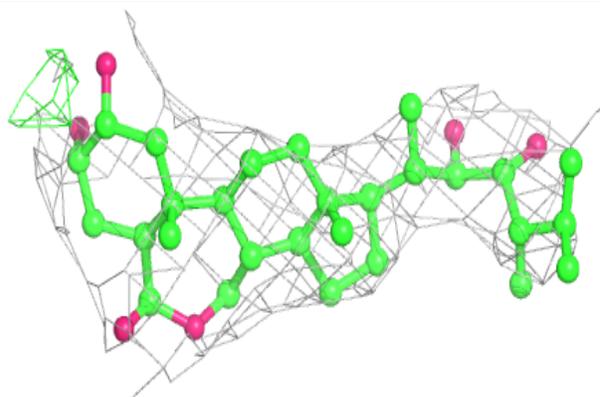
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	805	14/15	0.77	0.33	29,29,29,29	0
5	SO4	A	807	5/5	0.83	0.22	64,64,64,64	0
5	SO4	B	806	5/5	0.86	0.21	72,72,72,72	0
4	NAG	A	806	14/15	0.86	0.24	35,35,35,35	0
4	NAG	A	805	14/15	0.90	0.26	46,46,46,46	0
6	BLD	B	807	34/34	0.94	0.47	5,13,22,23	0
6	BLD	A	808	34/34	0.95	0.50	1,7,15,17	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.

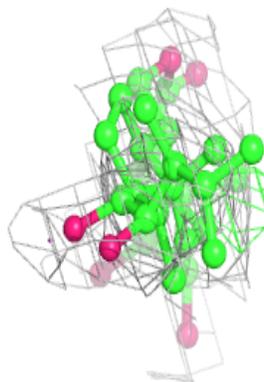
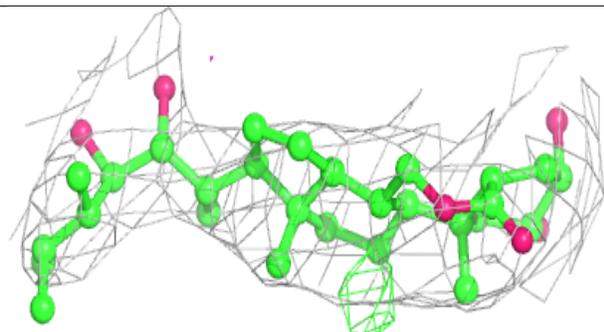
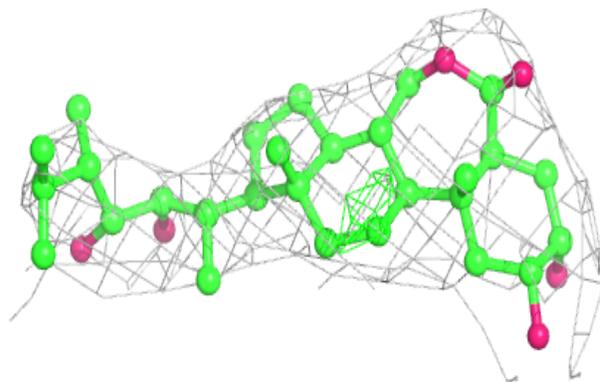
Electron density around BLD B 807:

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



Electron density around BLD A 808:

$2mF_o-DF_c$ (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.