



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 10:29 PM EDT

PDB ID : 3SH1
Title : Ac-AChBP ligand binding domain mutated to human alpha-7 nAChR
Authors : Nemezc, A.; Taylor, P.W.
Deposited on : 2011-06-15
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

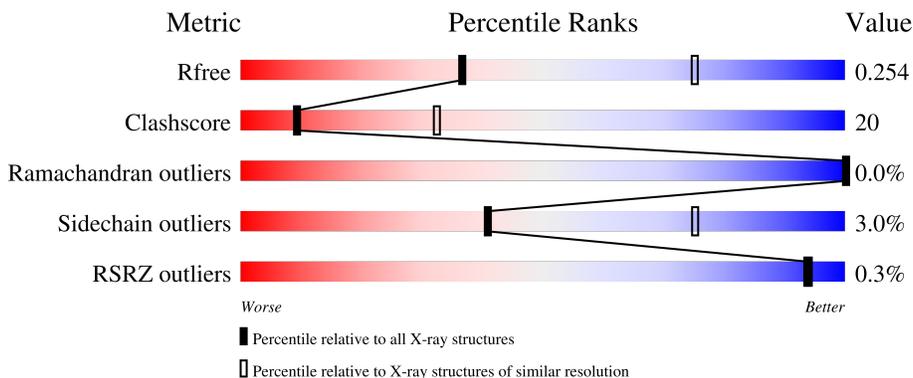
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	67% 25% 7%
1	B	230	67% 27% 7%
1	C	230	63% 30% 6%
1	D	230	67% 25% 7%
1	E	230	68% 24% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	230	 % 72% 21% 7%
1	G	230	 % 65% 27% 7%
1	H	230	 % 64% 29% 7%
1	I	230	 % 61% 30% 7%
1	J	230	 % 62% 30% 7%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 50% 50%
3	O	3	 33% 67%
3	P	3	 33% 67%

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	NAG	P	1	-	-	X	-
8	NAG	I	275[B]	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 18393 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	Total 1734	C 1092	N 286	O 348	S 8	22	2	0
1	B	215	Total 1743	C 1097	N 285	O 353	S 8	10	3	0
1	C	216	Total 1764	C 1111	N 292	O 353	S 8	8	5	0
1	D	214	Total 1733	C 1092	N 283	O 350	S 8	3	3	0
1	E	215	Total 1751	C 1101	N 292	O 350	S 8	12	3	0
1	F	214	Total 1733	C 1092	N 285	O 348	S 8	0	2	0
1	G	214	Total 1716	C 1081	N 280	O 347	S 8	4	0	0
1	H	215	Total 1741	C 1096	N 287	O 350	S 8	0	2	0
1	I	214	Total 1728	C 1087	N 283	O 350	S 8	0	2	0
1	J	215	Total 1754	C 1103	N 292	O 351	S 8	8	4	0

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	TYR	THR	engineered mutation	UNP Q8WSF8
A	34	SER	GLY	engineered mutation	UNP Q8WSF8
A	36	SER	THR	engineered mutation	UNP Q8WSF8
A	38	LEU	GLN	engineered mutation	UNP Q8WSF8
A	55	TRP	TYR	engineered mutation	UNP Q8WSF8
A	59	SER	ARG	engineered mutation	UNP Q8WSF8
A	106	ASN	ILE	engineered mutation	UNP Q8WSF8
A	108	LEU	VAL	engineered mutation	UNP Q8WSF8
A	110	ASN	THR	engineered mutation	UNP Q8WSF8
A	111	SER	HIS	engineered mutation	UNP Q8WSF8
A	112	SER	ASP	engineered mutation	UNP Q8WSF8
A	114	HIS	SER	engineered mutation	UNP Q8WSF8
A	116	GLN	MET	engineered mutation	UNP Q8WSF8
A	117	TYR	PHE	engineered mutation	UNP Q8WSF8
A	118	LEU	ILE	engineered mutation	UNP Q8WSF8
A	148	SER	VAL	engineered mutation	UNP Q8WSF8
A	150	GLY	SER	engineered mutation	UNP Q8WSF8
A	152	TRP	PHE	engineered mutation	UNP Q8WSF8
A	184	SER	GLN	engineered mutation	UNP Q8WSF8
A	185	GLU	VAL	engineered mutation	UNP Q8WSF8
A	186	ARG	GLN	engineered mutation	UNP Q8WSF8
A	187	PHE	HIS	engineered mutation	UNP Q8WSF8
A	189	GLU	SER	engineered mutation	UNP Q8WSF8
A	192	LYS	PRO	engineered mutation	UNP Q8WSF8
A	196	PRO	ILE	engineered mutation	UNP Q8WSF8
A	220	SER	-	expression tag	UNP Q8WSF8
A	221	ARG	-	expression tag	UNP Q8WSF8
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
B	32	TYR	THR	engineered mutation	UNP Q8WSF8
B	34	SER	GLY	engineered mutation	UNP Q8WSF8
B	36	SER	THR	engineered mutation	UNP Q8WSF8
B	38	LEU	GLN	engineered mutation	UNP Q8WSF8
B	55	TRP	TYR	engineered mutation	UNP Q8WSF8
B	59	SER	ARG	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ASN	ILE	engineered mutation	UNP Q8WSF8
B	108	LEU	VAL	engineered mutation	UNP Q8WSF8
B	110	ASN	THR	engineered mutation	UNP Q8WSF8
B	111	SER	HIS	engineered mutation	UNP Q8WSF8
B	112	SER	ASP	engineered mutation	UNP Q8WSF8
B	114	HIS	SER	engineered mutation	UNP Q8WSF8
B	116	GLN	MET	engineered mutation	UNP Q8WSF8
B	117	TYR	PHE	engineered mutation	UNP Q8WSF8
B	118	LEU	ILE	engineered mutation	UNP Q8WSF8
B	148	SER	VAL	engineered mutation	UNP Q8WSF8
B	150	GLY	SER	engineered mutation	UNP Q8WSF8
B	152	TRP	PHE	engineered mutation	UNP Q8WSF8
B	184	SER	GLN	engineered mutation	UNP Q8WSF8
B	185	GLU	VAL	engineered mutation	UNP Q8WSF8
B	186	ARG	GLN	engineered mutation	UNP Q8WSF8
B	187	PHE	HIS	engineered mutation	UNP Q8WSF8
B	189	GLU	SER	engineered mutation	UNP Q8WSF8
B	192	LYS	PRO	engineered mutation	UNP Q8WSF8
B	196	PRO	ILE	engineered mutation	UNP Q8WSF8
B	220	SER	-	expression tag	UNP Q8WSF8
B	221	ARG	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
C	32	TYR	THR	engineered mutation	UNP Q8WSF8
C	34	SER	GLY	engineered mutation	UNP Q8WSF8
C	36	SER	THR	engineered mutation	UNP Q8WSF8
C	38	LEU	GLN	engineered mutation	UNP Q8WSF8
C	55	TRP	TYR	engineered mutation	UNP Q8WSF8
C	59	SER	ARG	engineered mutation	UNP Q8WSF8
C	106	ASN	ILE	engineered mutation	UNP Q8WSF8
C	108	LEU	VAL	engineered mutation	UNP Q8WSF8
C	110	ASN	THR	engineered mutation	UNP Q8WSF8
C	111	SER	HIS	engineered mutation	UNP Q8WSF8
C	112	SER	ASP	engineered mutation	UNP Q8WSF8
C	114	HIS	SER	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	116	GLN	MET	engineered mutation	UNP Q8WSF8
C	117	TYR	PHE	engineered mutation	UNP Q8WSF8
C	118	LEU	ILE	engineered mutation	UNP Q8WSF8
C	148	SER	VAL	engineered mutation	UNP Q8WSF8
C	150	GLY	SER	engineered mutation	UNP Q8WSF8
C	152	TRP	PHE	engineered mutation	UNP Q8WSF8
C	184	SER	GLN	engineered mutation	UNP Q8WSF8
C	185	GLU	VAL	engineered mutation	UNP Q8WSF8
C	186	ARG	GLN	engineered mutation	UNP Q8WSF8
C	187	PHE	HIS	engineered mutation	UNP Q8WSF8
C	189	GLU	SER	engineered mutation	UNP Q8WSF8
C	192	LYS	PRO	engineered mutation	UNP Q8WSF8
C	196	PRO	ILE	engineered mutation	UNP Q8WSF8
C	220	SER	-	expression tag	UNP Q8WSF8
C	221	ARG	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
D	32	TYR	THR	engineered mutation	UNP Q8WSF8
D	34	SER	GLY	engineered mutation	UNP Q8WSF8
D	36	SER	THR	engineered mutation	UNP Q8WSF8
D	38	LEU	GLN	engineered mutation	UNP Q8WSF8
D	55	TRP	TYR	engineered mutation	UNP Q8WSF8
D	59	SER	ARG	engineered mutation	UNP Q8WSF8
D	106	ASN	ILE	engineered mutation	UNP Q8WSF8
D	108	LEU	VAL	engineered mutation	UNP Q8WSF8
D	110	ASN	THR	engineered mutation	UNP Q8WSF8
D	111	SER	HIS	engineered mutation	UNP Q8WSF8
D	112	SER	ASP	engineered mutation	UNP Q8WSF8
D	114	HIS	SER	engineered mutation	UNP Q8WSF8
D	116	GLN	MET	engineered mutation	UNP Q8WSF8
D	117	TYR	PHE	engineered mutation	UNP Q8WSF8
D	118	LEU	ILE	engineered mutation	UNP Q8WSF8
D	148	SER	VAL	engineered mutation	UNP Q8WSF8
D	150	GLY	SER	engineered mutation	UNP Q8WSF8
D	152	TRP	PHE	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	184	SER	GLN	engineered mutation	UNP Q8WSF8
D	185	GLU	VAL	engineered mutation	UNP Q8WSF8
D	186	ARG	GLN	engineered mutation	UNP Q8WSF8
D	187	PHE	HIS	engineered mutation	UNP Q8WSF8
D	189	GLU	SER	engineered mutation	UNP Q8WSF8
D	192	LYS	PRO	engineered mutation	UNP Q8WSF8
D	196	PRO	ILE	engineered mutation	UNP Q8WSF8
D	220	SER	-	expression tag	UNP Q8WSF8
D	221	ARG	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
E	32	TYR	THR	engineered mutation	UNP Q8WSF8
E	34	SER	GLY	engineered mutation	UNP Q8WSF8
E	36	SER	THR	engineered mutation	UNP Q8WSF8
E	38	LEU	GLN	engineered mutation	UNP Q8WSF8
E	55	TRP	TYR	engineered mutation	UNP Q8WSF8
E	59	SER	ARG	engineered mutation	UNP Q8WSF8
E	106	ASN	ILE	engineered mutation	UNP Q8WSF8
E	108	LEU	VAL	engineered mutation	UNP Q8WSF8
E	110	ASN	THR	engineered mutation	UNP Q8WSF8
E	111	SER	HIS	engineered mutation	UNP Q8WSF8
E	112	SER	ASP	engineered mutation	UNP Q8WSF8
E	114	HIS	SER	engineered mutation	UNP Q8WSF8
E	116	GLN	MET	engineered mutation	UNP Q8WSF8
E	117	TYR	PHE	engineered mutation	UNP Q8WSF8
E	118	LEU	ILE	engineered mutation	UNP Q8WSF8
E	148	SER	VAL	engineered mutation	UNP Q8WSF8
E	150	GLY	SER	engineered mutation	UNP Q8WSF8
E	152	TRP	PHE	engineered mutation	UNP Q8WSF8
E	184	SER	GLN	engineered mutation	UNP Q8WSF8
E	185	GLU	VAL	engineered mutation	UNP Q8WSF8
E	186	ARG	GLN	engineered mutation	UNP Q8WSF8
E	187	PHE	HIS	engineered mutation	UNP Q8WSF8
E	189	GLU	SER	engineered mutation	UNP Q8WSF8
E	192	LYS	PRO	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	196	PRO	ILE	engineered mutation	UNP Q8WSF8
E	220	SER	-	expression tag	UNP Q8WSF8
E	221	ARG	-	expression tag	UNP Q8WSF8
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
F	32	TYR	THR	engineered mutation	UNP Q8WSF8
F	34	SER	GLY	engineered mutation	UNP Q8WSF8
F	36	SER	THR	engineered mutation	UNP Q8WSF8
F	38	LEU	GLN	engineered mutation	UNP Q8WSF8
F	55	TRP	TYR	engineered mutation	UNP Q8WSF8
F	59	SER	ARG	engineered mutation	UNP Q8WSF8
F	106	ASN	ILE	engineered mutation	UNP Q8WSF8
F	108	LEU	VAL	engineered mutation	UNP Q8WSF8
F	110	ASN	THR	engineered mutation	UNP Q8WSF8
F	111	SER	HIS	engineered mutation	UNP Q8WSF8
F	112	SER	ASP	engineered mutation	UNP Q8WSF8
F	114	HIS	SER	engineered mutation	UNP Q8WSF8
F	116	GLN	MET	engineered mutation	UNP Q8WSF8
F	117	TYR	PHE	engineered mutation	UNP Q8WSF8
F	118	LEU	ILE	engineered mutation	UNP Q8WSF8
F	148	SER	VAL	engineered mutation	UNP Q8WSF8
F	150	GLY	SER	engineered mutation	UNP Q8WSF8
F	152	TRP	PHE	engineered mutation	UNP Q8WSF8
F	184	SER	GLN	engineered mutation	UNP Q8WSF8
F	185	GLU	VAL	engineered mutation	UNP Q8WSF8
F	186	ARG	GLN	engineered mutation	UNP Q8WSF8
F	187	PHE	HIS	engineered mutation	UNP Q8WSF8
F	189	GLU	SER	engineered mutation	UNP Q8WSF8
F	192	LYS	PRO	engineered mutation	UNP Q8WSF8
F	196	PRO	ILE	engineered mutation	UNP Q8WSF8
F	220	SER	-	expression tag	UNP Q8WSF8
F	221	ARG	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
G	32	TYR	THR	engineered mutation	UNP Q8WSF8
G	34	SER	GLY	engineered mutation	UNP Q8WSF8
G	36	SER	THR	engineered mutation	UNP Q8WSF8
G	38	LEU	GLN	engineered mutation	UNP Q8WSF8
G	55	TRP	TYR	engineered mutation	UNP Q8WSF8
G	59	SER	ARG	engineered mutation	UNP Q8WSF8
G	106	ASN	ILE	engineered mutation	UNP Q8WSF8
G	108	LEU	VAL	engineered mutation	UNP Q8WSF8
G	110	ASN	THR	engineered mutation	UNP Q8WSF8
G	111	SER	HIS	engineered mutation	UNP Q8WSF8
G	112	SER	ASP	engineered mutation	UNP Q8WSF8
G	114	HIS	SER	engineered mutation	UNP Q8WSF8
G	116	GLN	MET	engineered mutation	UNP Q8WSF8
G	117	TYR	PHE	engineered mutation	UNP Q8WSF8
G	118	LEU	ILE	engineered mutation	UNP Q8WSF8
G	148	SER	VAL	engineered mutation	UNP Q8WSF8
G	150	GLY	SER	engineered mutation	UNP Q8WSF8
G	152	TRP	PHE	engineered mutation	UNP Q8WSF8
G	184	SER	GLN	engineered mutation	UNP Q8WSF8
G	185	GLU	VAL	engineered mutation	UNP Q8WSF8
G	186	ARG	GLN	engineered mutation	UNP Q8WSF8
G	187	PHE	HIS	engineered mutation	UNP Q8WSF8
G	189	GLU	SER	engineered mutation	UNP Q8WSF8
G	192	LYS	PRO	engineered mutation	UNP Q8WSF8
G	196	PRO	ILE	engineered mutation	UNP Q8WSF8
G	220	SER	-	expression tag	UNP Q8WSF8
G	221	ARG	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	32	TYR	THR	engineered mutation	UNP Q8WSF8
H	34	SER	GLY	engineered mutation	UNP Q8WSF8
H	36	SER	THR	engineered mutation	UNP Q8WSF8
H	38	LEU	GLN	engineered mutation	UNP Q8WSF8
H	55	TRP	TYR	engineered mutation	UNP Q8WSF8
H	59	SER	ARG	engineered mutation	UNP Q8WSF8
H	106	ASN	ILE	engineered mutation	UNP Q8WSF8
H	108	LEU	VAL	engineered mutation	UNP Q8WSF8
H	110	ASN	THR	engineered mutation	UNP Q8WSF8
H	111	SER	HIS	engineered mutation	UNP Q8WSF8
H	112	SER	ASP	engineered mutation	UNP Q8WSF8
H	114	HIS	SER	engineered mutation	UNP Q8WSF8
H	116	GLN	MET	engineered mutation	UNP Q8WSF8
H	117	TYR	PHE	engineered mutation	UNP Q8WSF8
H	118	LEU	ILE	engineered mutation	UNP Q8WSF8
H	148	SER	VAL	engineered mutation	UNP Q8WSF8
H	150	GLY	SER	engineered mutation	UNP Q8WSF8
H	152	TRP	PHE	engineered mutation	UNP Q8WSF8
H	184	SER	GLN	engineered mutation	UNP Q8WSF8
H	185	GLU	VAL	engineered mutation	UNP Q8WSF8
H	186	ARG	GLN	engineered mutation	UNP Q8WSF8
H	187	PHE	HIS	engineered mutation	UNP Q8WSF8
H	189	GLU	SER	engineered mutation	UNP Q8WSF8
H	192	LYS	PRO	engineered mutation	UNP Q8WSF8
H	196	PRO	ILE	engineered mutation	UNP Q8WSF8
H	220	SER	-	expression tag	UNP Q8WSF8
H	221	ARG	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
I	32	TYR	THR	engineered mutation	UNP Q8WSF8
I	34	SER	GLY	engineered mutation	UNP Q8WSF8
I	36	SER	THR	engineered mutation	UNP Q8WSF8
I	38	LEU	GLN	engineered mutation	UNP Q8WSF8
I	55	TRP	TYR	engineered mutation	UNP Q8WSF8
I	59	SER	ARG	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	106	ASN	ILE	engineered mutation	UNP Q8WSF8
I	108	LEU	VAL	engineered mutation	UNP Q8WSF8
I	110	ASN	THR	engineered mutation	UNP Q8WSF8
I	111	SER	HIS	engineered mutation	UNP Q8WSF8
I	112	SER	ASP	engineered mutation	UNP Q8WSF8
I	114	HIS	SER	engineered mutation	UNP Q8WSF8
I	116	GLN	MET	engineered mutation	UNP Q8WSF8
I	117	TYR	PHE	engineered mutation	UNP Q8WSF8
I	118	LEU	ILE	engineered mutation	UNP Q8WSF8
I	148	SER	VAL	engineered mutation	UNP Q8WSF8
I	150	GLY	SER	engineered mutation	UNP Q8WSF8
I	152	TRP	PHE	engineered mutation	UNP Q8WSF8
I	184	SER	GLN	engineered mutation	UNP Q8WSF8
I	185	GLU	VAL	engineered mutation	UNP Q8WSF8
I	186	ARG	GLN	engineered mutation	UNP Q8WSF8
I	187	PHE	HIS	engineered mutation	UNP Q8WSF8
I	189	GLU	SER	engineered mutation	UNP Q8WSF8
I	192	LYS	PRO	engineered mutation	UNP Q8WSF8
I	196	PRO	ILE	engineered mutation	UNP Q8WSF8
I	220	SER	-	expression tag	UNP Q8WSF8
I	221	ARG	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8
J	32	TYR	THR	engineered mutation	UNP Q8WSF8
J	34	SER	GLY	engineered mutation	UNP Q8WSF8
J	36	SER	THR	engineered mutation	UNP Q8WSF8
J	38	LEU	GLN	engineered mutation	UNP Q8WSF8
J	55	TRP	TYR	engineered mutation	UNP Q8WSF8
J	59	SER	ARG	engineered mutation	UNP Q8WSF8
J	106	ASN	ILE	engineered mutation	UNP Q8WSF8
J	108	LEU	VAL	engineered mutation	UNP Q8WSF8
J	110	ASN	THR	engineered mutation	UNP Q8WSF8
J	111	SER	HIS	engineered mutation	UNP Q8WSF8
J	112	SER	ASP	engineered mutation	UNP Q8WSF8
J	114	HIS	SER	engineered mutation	UNP Q8WSF8

Continued on next page...

Continued from previous page...

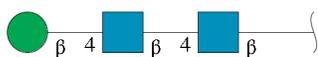
Chain	Residue	Modelled	Actual	Comment	Reference
J	116	GLN	MET	engineered mutation	UNP Q8WSF8
J	117	TYR	PHE	engineered mutation	UNP Q8WSF8
J	118	LEU	ILE	engineered mutation	UNP Q8WSF8
J	148	SER	VAL	engineered mutation	UNP Q8WSF8
J	150	GLY	SER	engineered mutation	UNP Q8WSF8
J	152	TRP	PHE	engineered mutation	UNP Q8WSF8
J	184	SER	GLN	engineered mutation	UNP Q8WSF8
J	185	GLU	VAL	engineered mutation	UNP Q8WSF8
J	186	ARG	GLN	engineered mutation	UNP Q8WSF8
J	187	PHE	HIS	engineered mutation	UNP Q8WSF8
J	189	GLU	SER	engineered mutation	UNP Q8WSF8
J	192	LYS	PRO	engineered mutation	UNP Q8WSF8
J	196	PRO	ILE	engineered mutation	UNP Q8WSF8
J	220	SER	-	expression tag	UNP Q8WSF8
J	221	ARG	-	expression tag	UNP Q8WSF8

- Molecule 2 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
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

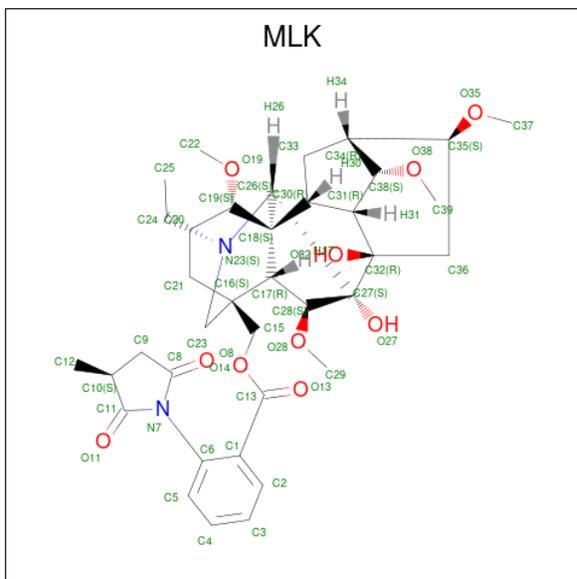


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		

- Molecule 5 is METHYLLYCACONITINE (three-letter code: MLK) (formula: C₃₇H₅₀N₂O₁₀).



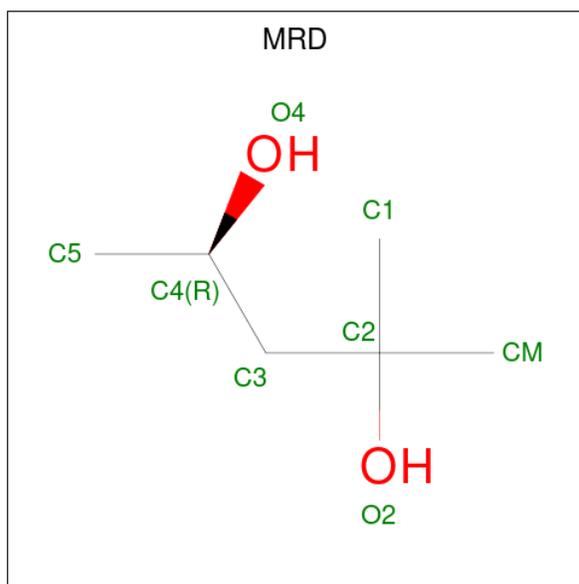
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			49	37	2	10		
5	B	1	Total	C	N	O	0	0
			49	37	2	10		
5	C	1	Total	C	N	O	0	0
			49	37	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			49	37	2	10		
5	E	1	Total	C	N	O	0	0
			49	37	2	10		
5	F	1	Total	C	N	O	0	0
			49	37	2	10		
5	G	1	Total	C	N	O	0	0
			49	37	2	10		
5	H	1	Total	C	N	O	0	0
			49	37	2	10		
5	I	1	Total	C	N	O	0	0
			49	37	2	10		
5	J	1	Total	C	N	O	0	0
			49	37	2	10		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



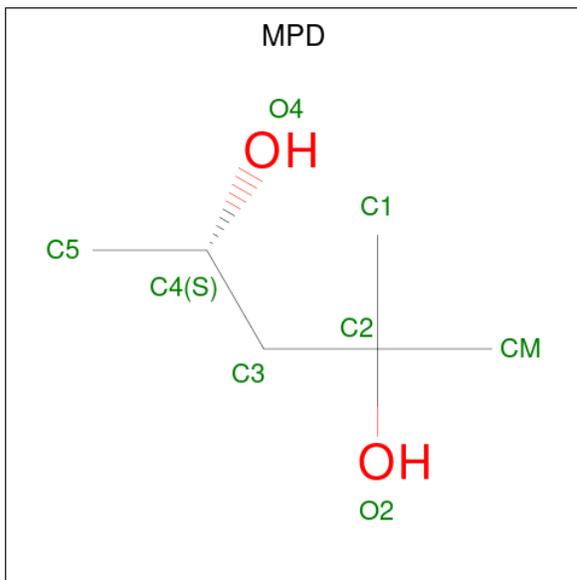
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			8	6 2		
6	B	1	Total	C O	0	0
			8	6 2		
6	D	1	Total	C O	0	0
			8	6 2		
6	E	1	Total	C O	0	0
			8	6 2		

Continued on next page...

Continued from previous page...

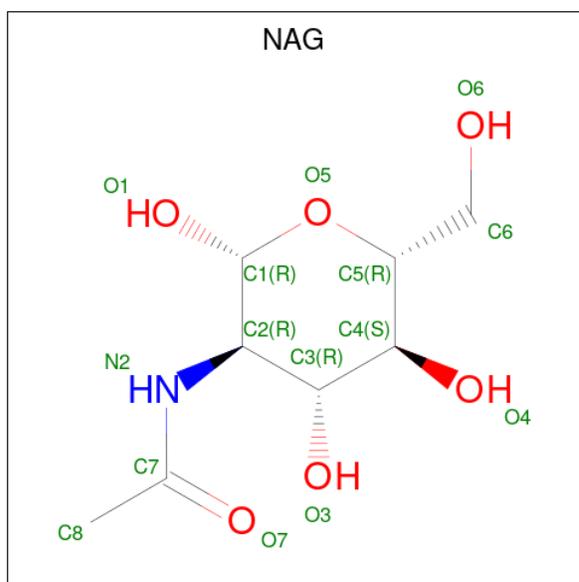
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



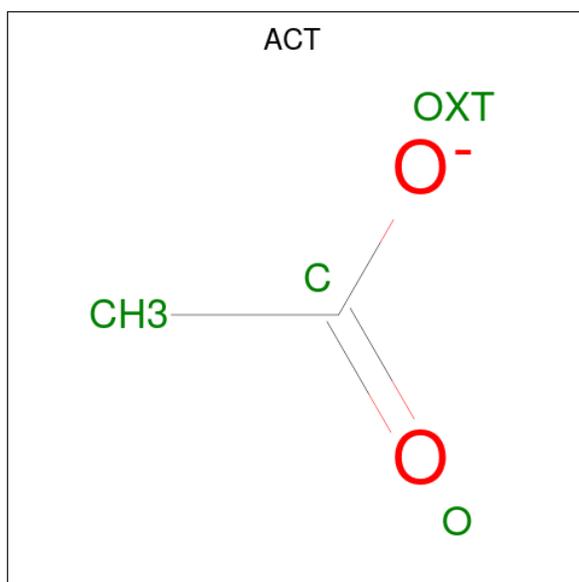
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	C	1	Total	C	O	0	0
			8	6	2		
7	G	1	Total	C	O	0	0
			8	6	2		
7	G	1	Total	C	O	0	0
			8	6	2		
7	I	1	Total	C	O	0	0
			8	6	2		
7	J	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	1
			28	16	2	10		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	1
			28	16	2	10		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	0
			14	8	1	5		
8	I	1	Total	C	N	O	0	1
			28	16	2	10		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	C O	0	0
			4	2 2		

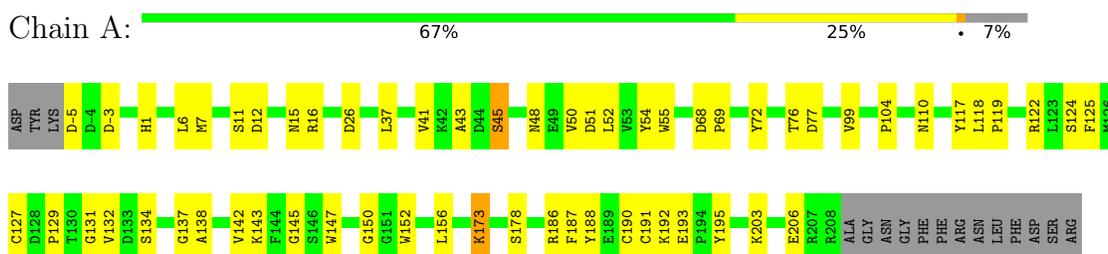
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	12	Total	O	0	0
			12	12		
10	B	12	Total	O	0	0
			12	12		
10	C	7	Total	O	0	0
			7	7		
10	D	3	Total	O	0	0
			3	3		
10	E	9	Total	O	0	0
			9	9		
10	F	5	Total	O	0	0
			5	5		
10	G	5	Total	O	0	0
			5	5		
10	H	5	Total	O	0	0
			5	5		
10	I	8	Total	O	0	0
			8	8		
10	J	5	Total	O	0	0
			5	5		

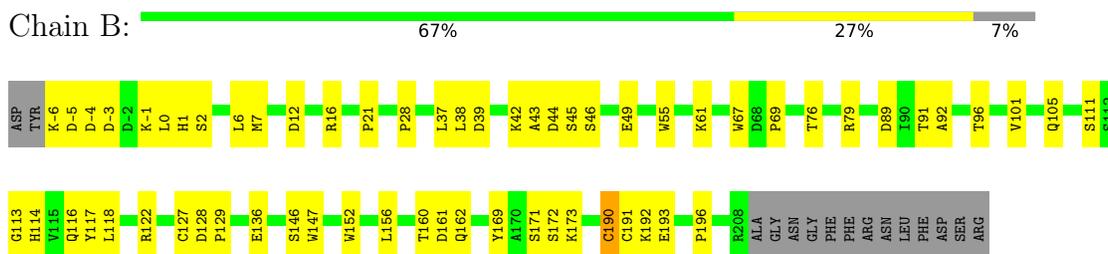
3 Residue-property plots [i](#)

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

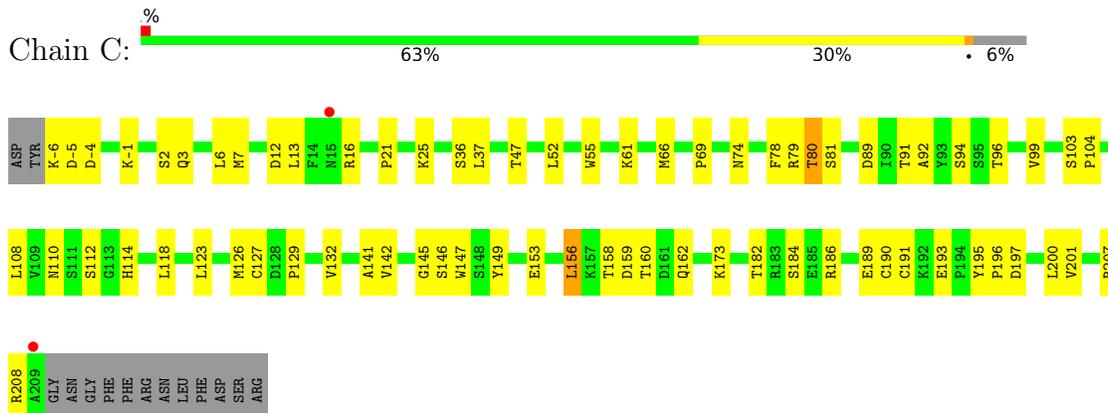
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor

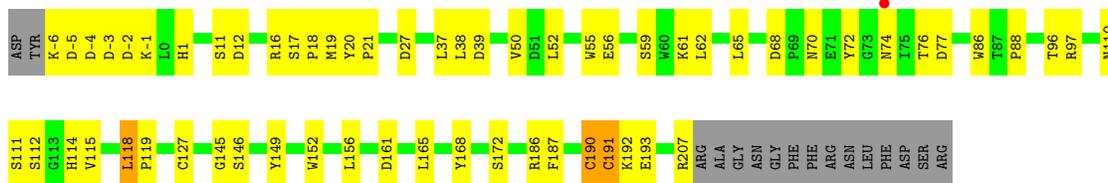


- Molecule 1: Soluble acetylcholine receptor

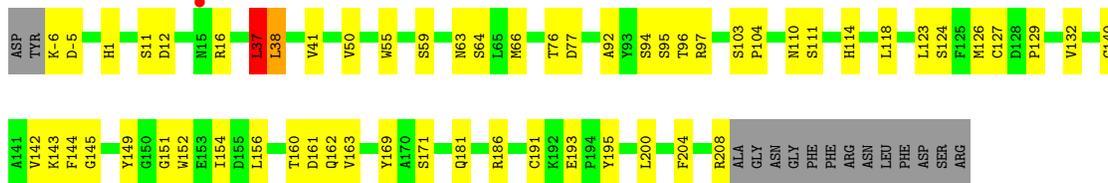


- Molecule 1: Soluble acetylcholine receptor

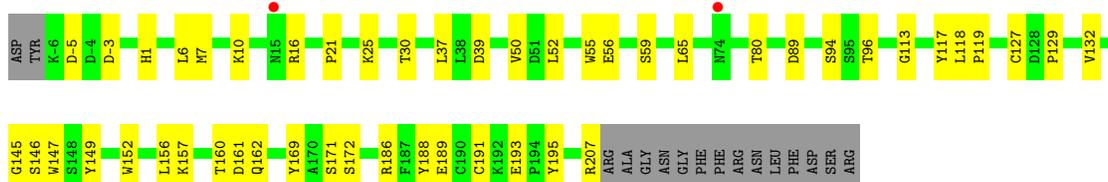




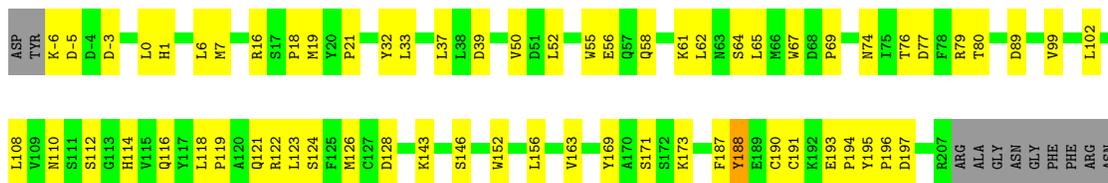
● Molecule 1: Soluble acetylcholine receptor



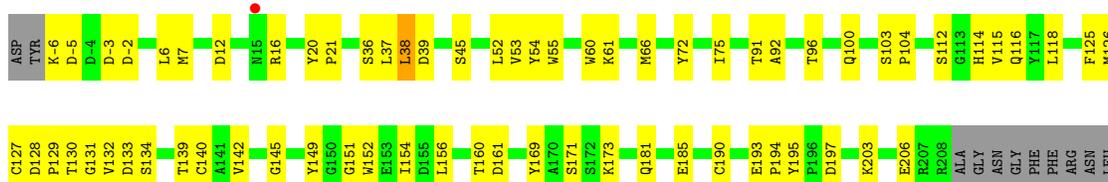
● Molecule 1: Soluble acetylcholine receptor



● Molecule 1: Soluble acetylcholine receptor



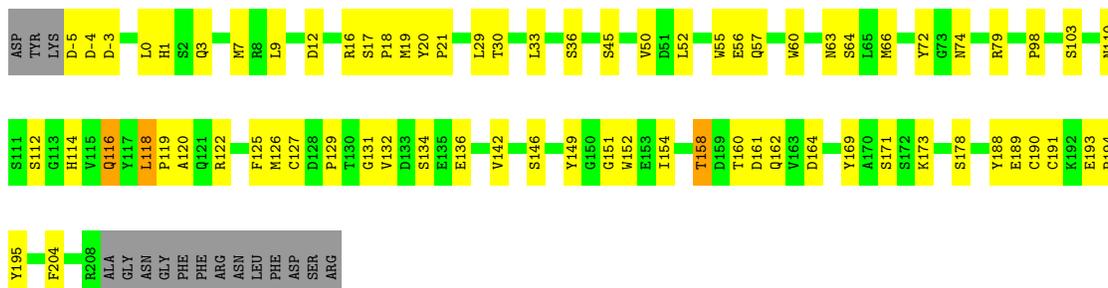
● Molecule 1: Soluble acetylcholine receptor



PHE
ASP
SER
ARG

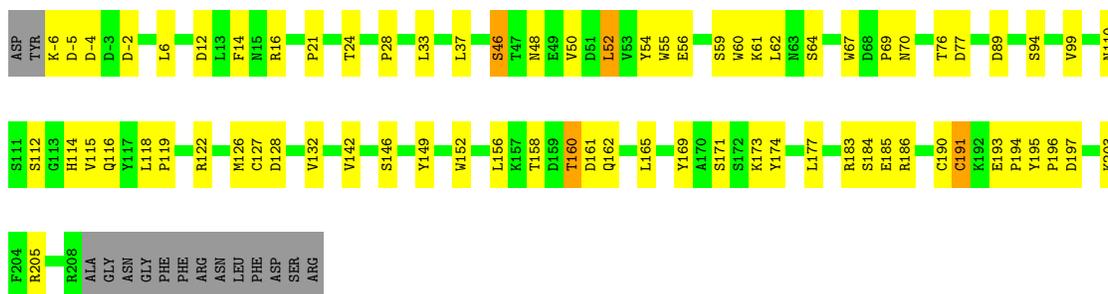
- Molecule 1: Soluble acetylcholine receptor

Chain I:  61% 30% 7%



- Molecule 1: Soluble acetylcholine receptor

Chain J:  62% 30% 7%



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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  50% 50%MAG1
MAG2

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

Chain O:  33% 67%MAG1
MAG2
BMA3

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

Chain P:  33% 67%MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.79Å 140.18Å 136.81Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	48.05 – 2.90 48.05 – 2.33	Depositor EDS
% Data completeness (in resolution range)	93.5 (48.05-2.90) 64.0 (48.05-2.33)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.213 , 0.258 0.210 , 0.254	Depositor DCC
R_{free} test set	2004 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtrriage
Anisotropy	0.694	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18393	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.86% 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: MRD, BMA, NAG, ACT, MG, MLK, MPD

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	0.45	0/1781	0.69	0/2428
1	B	0.47	0/1796	0.68	0/2446
1	C	0.57	0/1823	0.69	0/2481
1	D	0.47	0/1786	0.62	0/2433
1	E	0.45	0/1800	0.68	1/2449 (0.0%)
1	F	0.43	0/1780	0.67	0/2424
1	G	0.55	0/1760	0.62	0/2398
1	H	0.58	1/1791 (0.1%)	0.69	1/2439 (0.0%)
1	I	0.51	0/1778	0.64	0/2423
1	J	0.53	0/1807	0.67	1/2460 (0.0%)
All	All	0.51	1/17902 (0.0%)	0.66	3/24381 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	127	CYS	CB-SG	-5.22	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	38	LEU	CB-CA-C	-5.86	99.06	110.20
1	J	14	PHE	N-CA-C	5.56	126.02	111.00
1	E	37	LEU	CA-CB-CG	-5.49	102.67	115.30

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	1734	0	1647	56	0
1	B	1743	0	1648	68	0
1	C	1764	0	1689	80	0
1	D	1733	0	1645	76	0
1	E	1751	0	1664	77	0
1	F	1733	0	1649	56	0
1	G	1716	0	1621	74	0
1	H	1741	0	1653	67	0
1	I	1728	0	1628	84	0
1	J	1754	0	1672	93	0
2	K	28	0	25	3	0
2	L	28	0	25	6	0
2	M	28	0	25	5	0
2	N	28	0	25	4	0
3	O	39	0	34	3	0
3	P	39	0	34	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	49	0	50	9	0
5	B	49	0	50	11	0
5	C	49	0	50	18	0
5	D	49	0	50	4	0
5	E	49	0	50	15	0
5	F	49	0	50	20	0
5	G	49	0	50	10	0
5	H	49	0	50	15	0
5	I	49	0	50	15	0
5	J	49	0	50	10	0
6	A	8	0	14	1	0
6	B	8	0	14	2	0
6	D	8	0	14	4	0
6	E	8	0	14	0	0
6	F	8	0	14	3	0
7	A	16	0	28	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	8	0	14	3	0
7	G	16	0	28	1	0
7	I	8	0	14	1	0
7	J	8	0	14	0	0
8	B	42	0	39	2	0
8	C	14	0	13	3	0
8	E	28	0	26	2	0
8	F	14	0	13	0	0
8	I	42	0	39	7	0
9	G	4	0	3	0	0
10	A	12	0	0	0	0
10	B	12	0	0	0	0
10	C	7	0	0	1	0
10	D	3	0	0	0	0
10	E	9	0	0	1	0
10	F	5	0	0	0	0
10	G	5	0	0	0	0
10	H	5	0	0	1	0
10	I	8	0	0	0	0
10	J	5	0	0	0	0
All	All	18393	0	17485	699	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 20.

The worst 5 of 699 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:110:ASN:HD21	8:C:250:NAG:C1	1.05	1.65
1:J:110:ASN:HD21	3:P:1:NAG:C1	1.07	1.58
1:D:16:ARG:HG3	1:J:16:ARG:CD	1.44	1.46
1:D:16:ARG:CG	1:J:16:ARG:HD3	1.44	1.43
1:E:160:THR:HG22	1:E:162:GLN:H	0.99	1.12

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	214/230 (93%)	208 (97%)	5 (2%)	1 (0%)	29	61
1	B	216/230 (94%)	215 (100%)	1 (0%)	0	100	100
1	C	219/230 (95%)	216 (99%)	3 (1%)	0	100	100
1	D	215/230 (94%)	212 (99%)	3 (1%)	0	100	100
1	E	215/230 (94%)	208 (97%)	7 (3%)	0	100	100
1	F	214/230 (93%)	212 (99%)	2 (1%)	0	100	100
1	G	212/230 (92%)	208 (98%)	4 (2%)	0	100	100
1	H	215/230 (94%)	213 (99%)	2 (1%)	0	100	100
1	I	214/230 (93%)	211 (99%)	3 (1%)	0	100	100
1	J	217/230 (94%)	215 (99%)	2 (1%)	0	100	100
All	All	2151/2300 (94%)	2118 (98%)	32 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PRO

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	197/208 (95%)	190 (96%)	7 (4%)	35	69
1	B	199/208 (96%)	195 (98%)	4 (2%)	55	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	201/208 (97%)	192 (96%)	9 (4%)	27	61
1	D	198/208 (95%)	193 (98%)	5 (2%)	47	78
1	E	199/208 (96%)	192 (96%)	7 (4%)	36	70
1	F	197/208 (95%)	194 (98%)	3 (2%)	65	87
1	G	195/208 (94%)	192 (98%)	3 (2%)	65	87
1	H	198/208 (95%)	192 (97%)	6 (3%)	41	75
1	I	197/208 (95%)	188 (95%)	9 (5%)	27	60
1	J	200/208 (96%)	194 (97%)	6 (3%)	41	75
All	All	1981/2080 (95%)	1922 (97%)	59 (3%)	41	75

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	59	SER
1	J	52	LEU
1	G	64	SER
1	J	46	SER
1	I	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	116	GLN
1	I	116	GLN
1	J	116	GLN
1	J	70	ASN
1	D	162	GLN

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

14 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	K	1	1,2	14,14,15	1.33	1 (7%)	17,19,21	0.80	0
2	NAG	K	2	2	14,14,15	1.33	1 (7%)	17,19,21	0.79	0
2	NAG	L	1	1,2	14,14,15	0.56	0	17,19,21	1.83	2 (11%)
2	NAG	L	2	2	14,14,15	1.00	0	17,19,21	1.45	3 (17%)
2	NAG	M	1	1,2	14,14,15	0.60	0	17,19,21	1.51	2 (11%)
2	NAG	M	2	2	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
2	NAG	N	1	1,2	14,14,15	0.75	0	17,19,21	0.92	1 (5%)
2	NAG	N	2	2	14,14,15	0.56	0	17,19,21	1.01	0
3	NAG	O	1	1,3	14,14,15	0.68	0	17,19,21	1.53	5 (29%)
3	NAG	O	2	3	14,14,15	0.63	0	17,19,21	1.15	1 (5%)
3	BMA	O	3	3	11,11,12	0.45	0	15,15,17	1.08	1 (6%)
3	NAG	P	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.16	0
3	NAG	P	2	3	14,14,15	0.46	0	17,19,21	1.19	2 (11%)
3	BMA	P	3	3	11,11,12	0.52	0	15,15,17	0.92	1 (6%)

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	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	5/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	BMA	P	3	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	O7-C7	4.55	1.33	1.23
2	K	2	NAG	O7-C7	4.53	1.33	1.23
3	P	1	NAG	O5-C1	-2.30	1.40	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C1-O5-C5	4.85	118.77	112.19
2	M	1	NAG	C1-O5-C5	4.26	117.96	112.19
2	L	1	NAG	O5-C1-C2	3.87	117.39	111.29
2	M	2	NAG	C2-N2-C7	3.08	127.29	122.90
3	P	2	NAG	O5-C5-C6	2.95	111.82	107.20

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 30 short contacts:

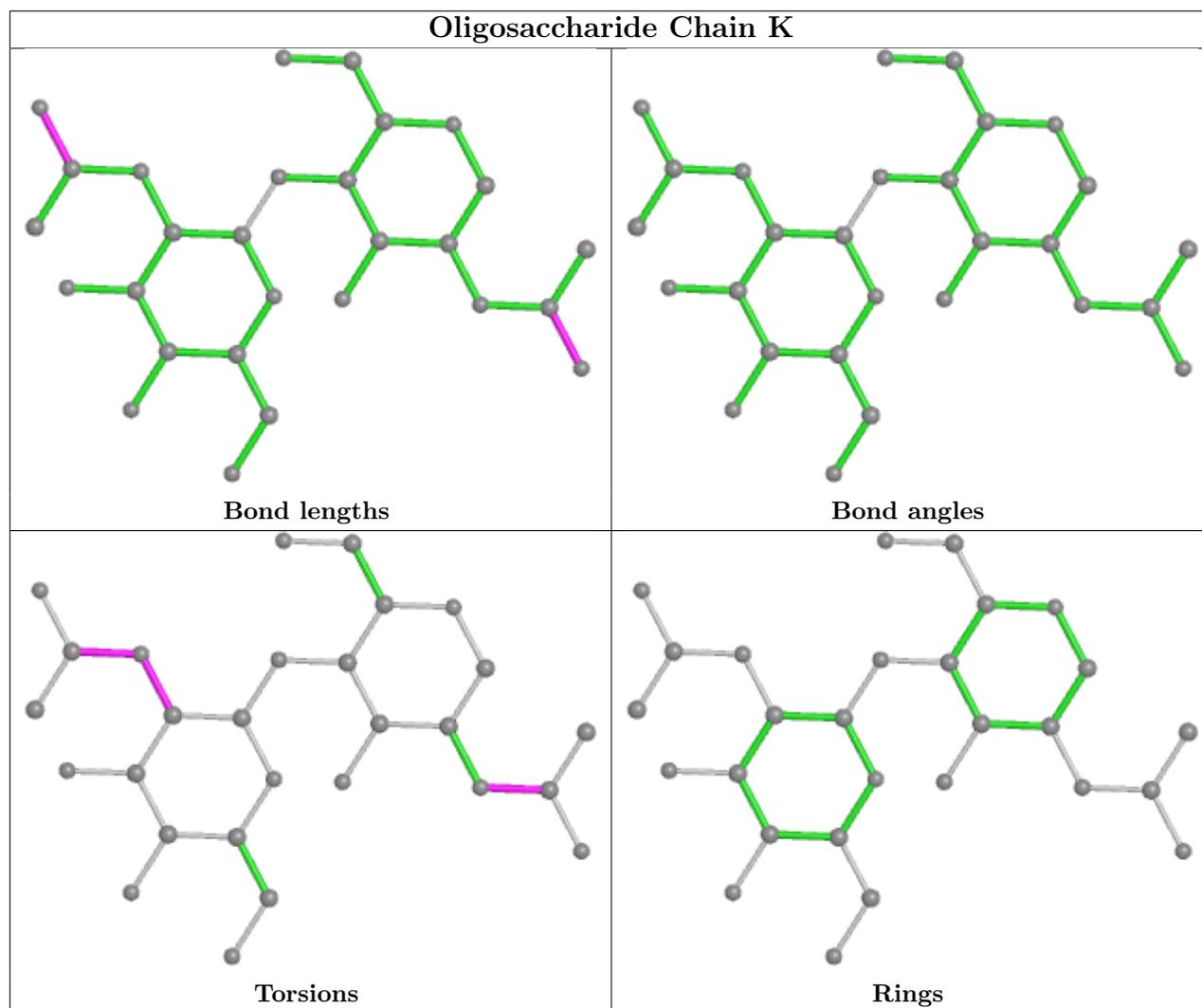
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	2	0

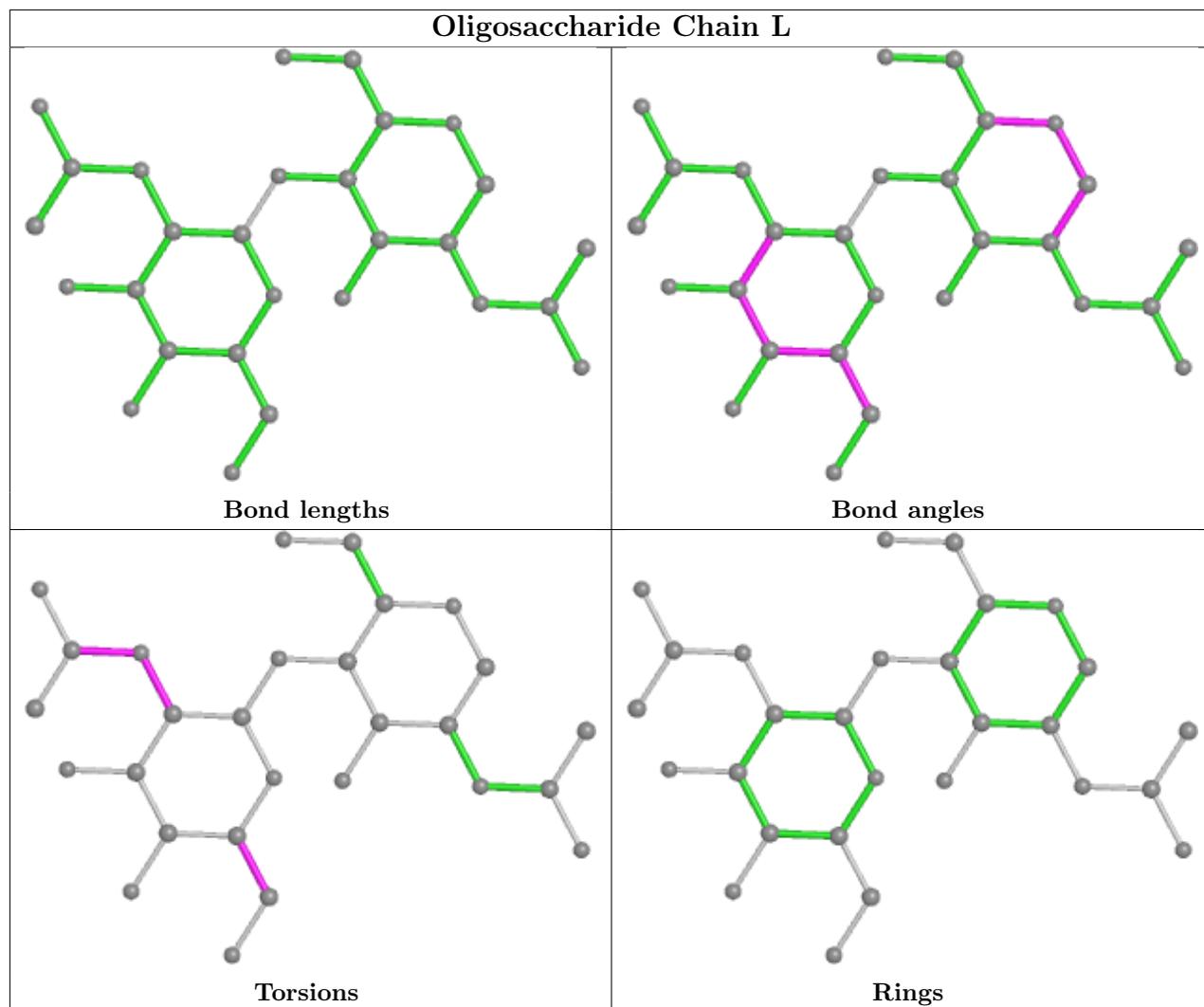
Continued on next page...

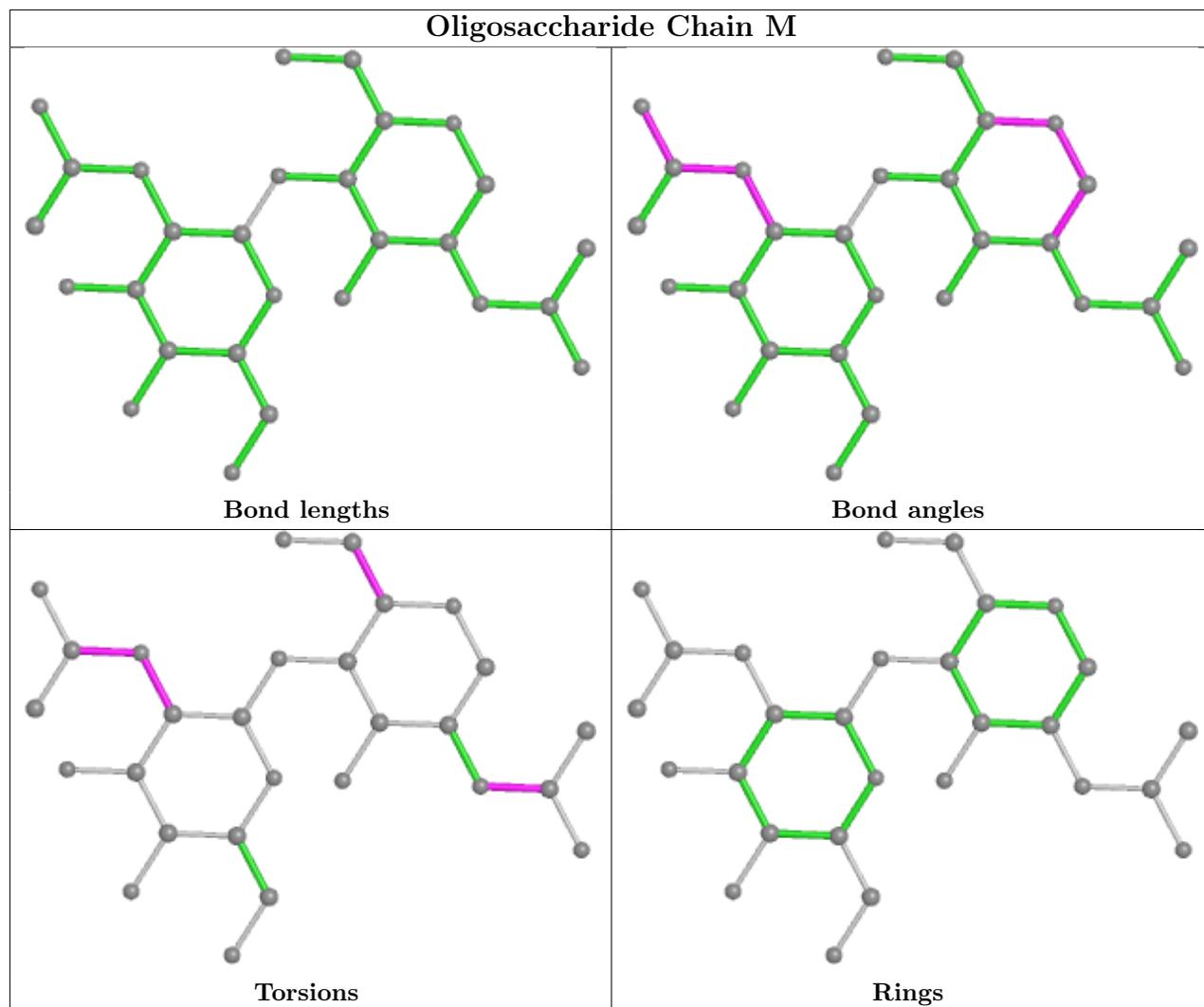
Continued from previous page...

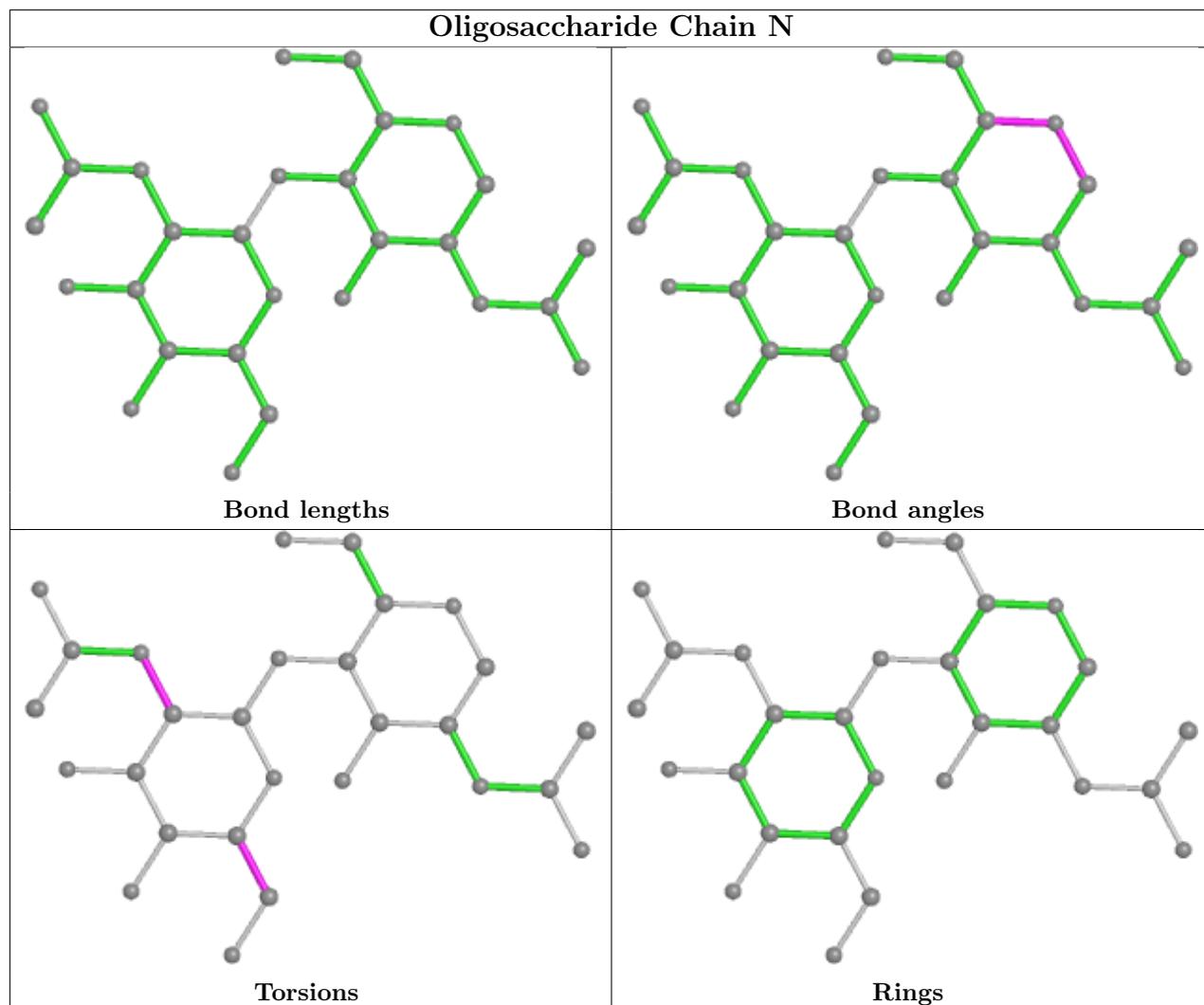
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	NAG	1	0
2	L	2	NAG	3	0
2	L	1	NAG	3	0
2	K	2	NAG	3	0
2	K	1	NAG	3	0
3	P	2	NAG	2	0
2	M	1	NAG	4	0
3	P	1	NAG	9	0
2	N	1	NAG	3	0
2	N	2	NAG	1	0
3	O	3	BMA	1	0

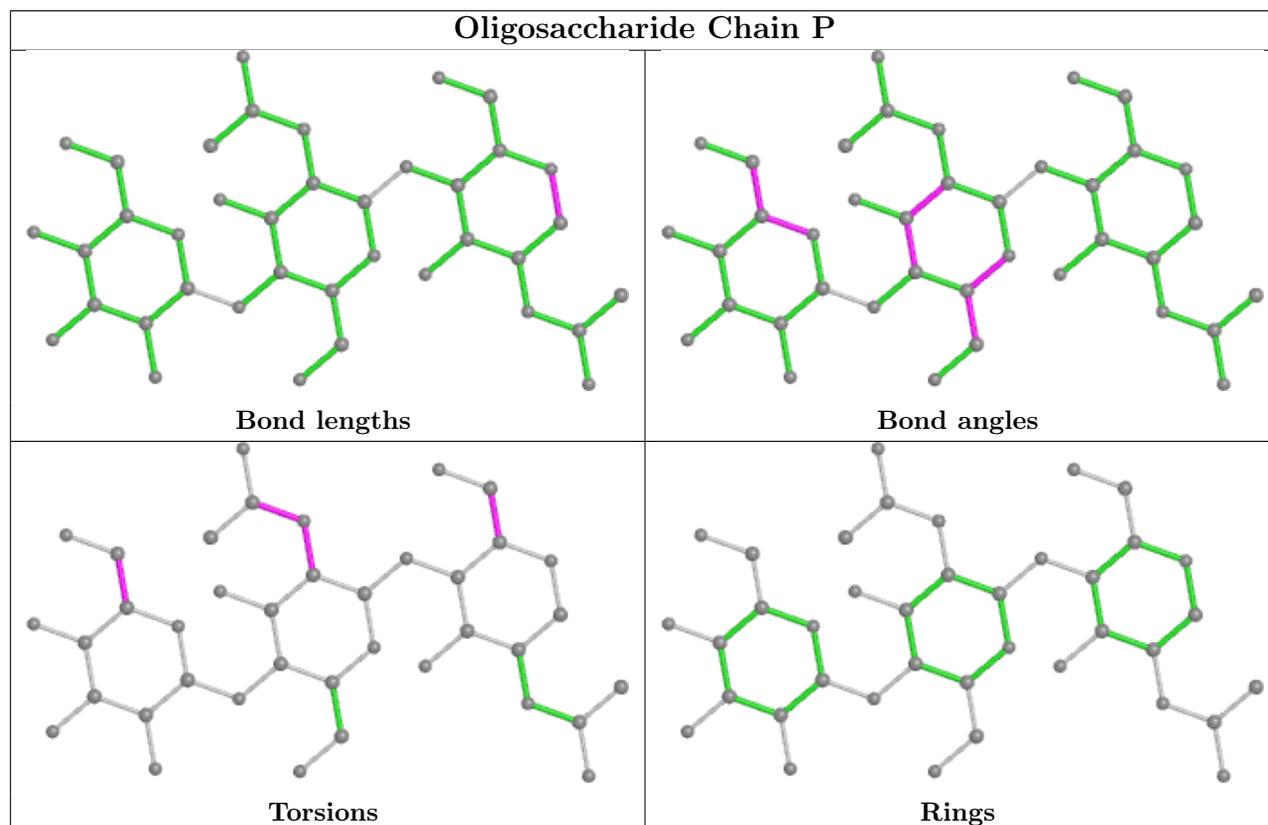
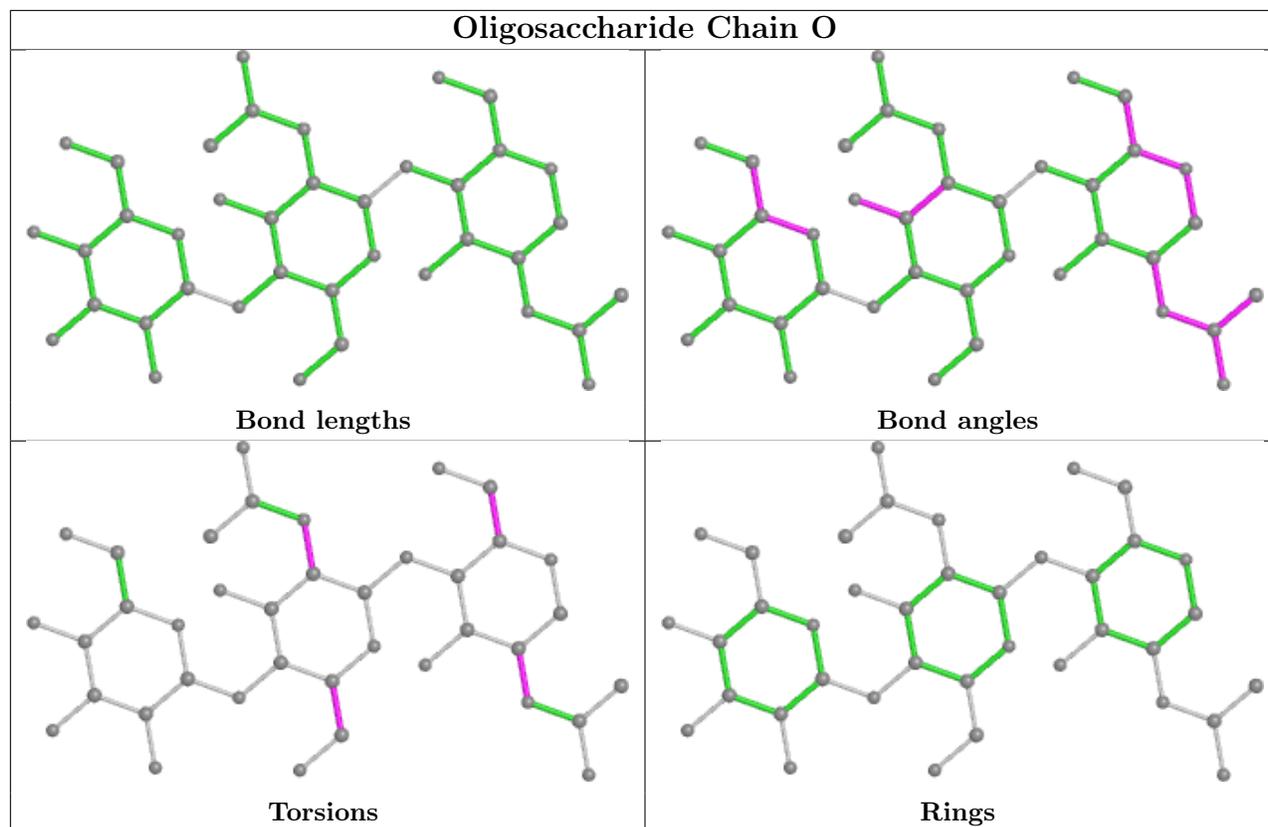
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 5 are monoatomic - leaving 33 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
6	MRD	E	305	-	7,7,7	0.38	0	9,10,10	0.28	0
8	NAG	I	275[A]	1	14,14,15	1.32	1 (7%)	17,19,21	1.02	1 (5%)
5	MLK	G	301	-	54,56,56	1.04	2 (3%)	78,92,92	1.85	21 (26%)
5	MLK	H	301	-	54,56,56	1.04	3 (5%)	78,92,92	2.19	24 (30%)
5	MLK	A	301	-	54,56,56	1.08	4 (7%)	78,92,92	2.00	18 (23%)
8	NAG	E	275[B]	1	14,14,15	0.49	0	17,19,21	1.56	4 (23%)
6	MRD	F	305	-	7,7,7	0.34	0	9,10,10	0.50	0
7	MPD	G	222	-	7,7,7	0.27	0	9,10,10	0.22	0
7	MPD	G	305	-	7,7,7	0.50	0	9,10,10	0.38	0
8	NAG	F	250	1	14,14,15	0.52	0	17,19,21	0.96	1 (5%)
5	MLK	E	301	-	54,56,56	1.01	3 (5%)	78,92,92	2.12	24 (30%)
5	MLK	I	301	-	54,56,56	1.13	4 (7%)	78,92,92	1.66	19 (24%)
8	NAG	B	275[A]	1	14,14,15	0.61	0	17,19,21	1.00	0
7	MPD	J	305	-	7,7,7	0.40	0	9,10,10	0.72	0
8	NAG	I	250	1	14,14,15	0.62	0	17,19,21	1.18	3 (17%)
8	NAG	C	250	1	14,14,15	1.11	1 (7%)	17,19,21	1.98	4 (23%)
5	MLK	B	301	-	54,56,56	1.07	4 (7%)	78,92,92	1.82	19 (24%)
8	NAG	E	275[A]	1	14,14,15	1.32	1 (7%)	17,19,21	1.05	1 (5%)
7	MPD	C	306	-	7,7,7	0.47	0	9,10,10	0.33	0
6	MRD	D	305	-	7,7,7	0.38	0	9,10,10	0.39	0
9	ACT	G	308	-	3,3,3	1.81	1 (33%)	3,3,3	0.95	0
5	MLK	J	301	-	54,56,56	1.09	4 (7%)	78,92,92	1.87	17 (21%)
6	MRD	A	305	-	7,7,7	0.28	0	9,10,10	0.70	0
5	MLK	F	301	-	54,56,56	1.14	4 (7%)	78,92,92	1.76	18 (23%)
8	NAG	I	275[B]	1	14,14,15	0.71	0	17,19,21	1.67	3 (17%)
5	MLK	C	301	-	54,56,56	1.15	3 (5%)	78,92,92	1.88	17 (21%)
6	MRD	B	305	-	7,7,7	0.54	0	9,10,10	0.53	0
7	MPD	A	306	-	7,7,7	0.42	0	9,10,10	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	250	1	14,14,15	0.67	0	17,19,21	1.11	0
7	MPD	I	305	-	7,7,7	0.42	0	9,10,10	0.92	0
7	MPD	A	223	-	7,7,7	0.39	0	9,10,10	0.54	0
5	MLK	D	301	-	54,56,56	1.15	4 (7%)	78,92,92	1.76	17 (21%)
8	NAG	B	275[B]	1	14,14,15	0.53	0	17,19,21	1.75	2 (11%)

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
6	MRD	E	305	-	-	3/5/5/5	-
8	NAG	I	275[A]	1	-	4/6/23/26	0/1/1/1
5	MLK	G	301	-	-	2/24/141/141	0/2/8/8
5	MLK	H	301	-	-	2/24/141/141	0/2/8/8
5	MLK	A	301	-	-	4/24/141/141	0/2/8/8
8	NAG	E	275[B]	1	-	5/6/23/26	0/1/1/1
6	MRD	F	305	-	-	2/5/5/5	-
7	MPD	G	222	-	-	5/5/5/5	-
7	MPD	G	305	-	-	1/5/5/5	-
8	NAG	F	250	1	-	4/6/23/26	0/1/1/1
5	MLK	E	301	-	-	6/24/141/141	0/2/8/8
5	MLK	I	301	-	-	6/24/141/141	0/2/8/8
8	NAG	B	275[A]	1	-	0/6/23/26	0/1/1/1
7	MPD	J	305	-	-	4/5/5/5	-
8	NAG	I	250	1	-	0/6/23/26	0/1/1/1
8	NAG	C	250	1	-	2/6/23/26	0/1/1/1
5	MLK	B	301	-	-	7/24/141/141	0/2/8/8
8	NAG	E	275[A]	1	-	0/6/23/26	0/1/1/1
7	MPD	C	306	-	-	5/5/5/5	-
6	MRD	D	305	-	-	2/5/5/5	-
5	MLK	J	301	-	-	7/24/141/141	0/2/8/8
6	MRD	A	305	-	-	3/5/5/5	-
5	MLK	F	301	-	-	3/24/141/141	0/2/8/8
8	NAG	I	275[B]	1	1/1/5/7	5/6/23/26	0/1/1/1
5	MLK	C	301	-	-	9/24/141/141	0/2/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MRD	B	305	-	-	2/5/5/5	-
7	MPD	A	306	-	-	3/5/5/5	-
8	NAG	B	250	1	-	0/6/23/26	0/1/1/1
7	MPD	I	305	-	-	3/5/5/5	-
7	MPD	A	223	-	-	0/5/5/5	-
5	MLK	D	301	-	-	1/24/141/141	0/2/8/8
8	NAG	B	275[B]	1	-	3/6/23/26	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	275[A]	NAG	O7-C7	4.55	1.33	1.23
8	E	275[A]	NAG	O7-C7	4.53	1.33	1.23
5	I	301	MLK	C8-N7	-4.50	1.34	1.40
5	C	301	MLK	C8-N7	-4.26	1.34	1.40
5	D	301	MLK	C8-N7	-4.14	1.34	1.40

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	301	MLK	C1-C6-N7	6.94	127.41	120.88
5	E	301	MLK	C1-C6-N7	6.72	127.21	120.88
5	A	301	MLK	C9-C10-C11	-6.62	98.16	103.95
5	H	301	MLK	C24-N23-C26	-6.51	106.50	114.64
5	C	301	MLK	C1-C6-N7	5.95	126.48	120.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	275[B]	NAG	C1

5 of 103 torsion outliers are listed below:

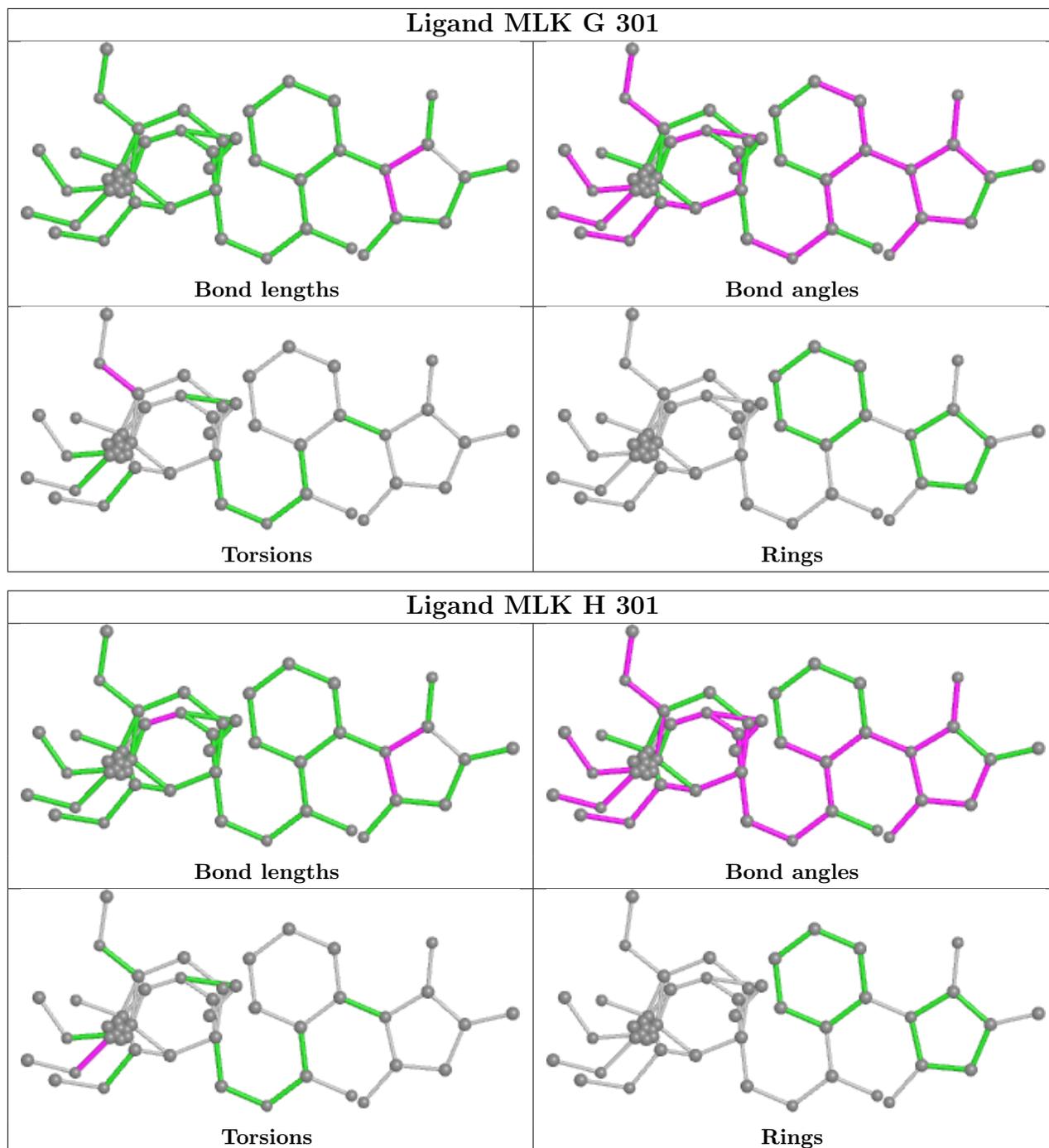
Mol	Chain	Res	Type	Atoms
5	A	301	MLK	C25-C24-N23-C26
5	A	301	MLK	C17-C28-O28-C29
5	B	301	MLK	O14-C15-C16-C21
5	B	301	MLK	O14-C15-C16-C17
5	B	301	MLK	O14-C15-C16-C23

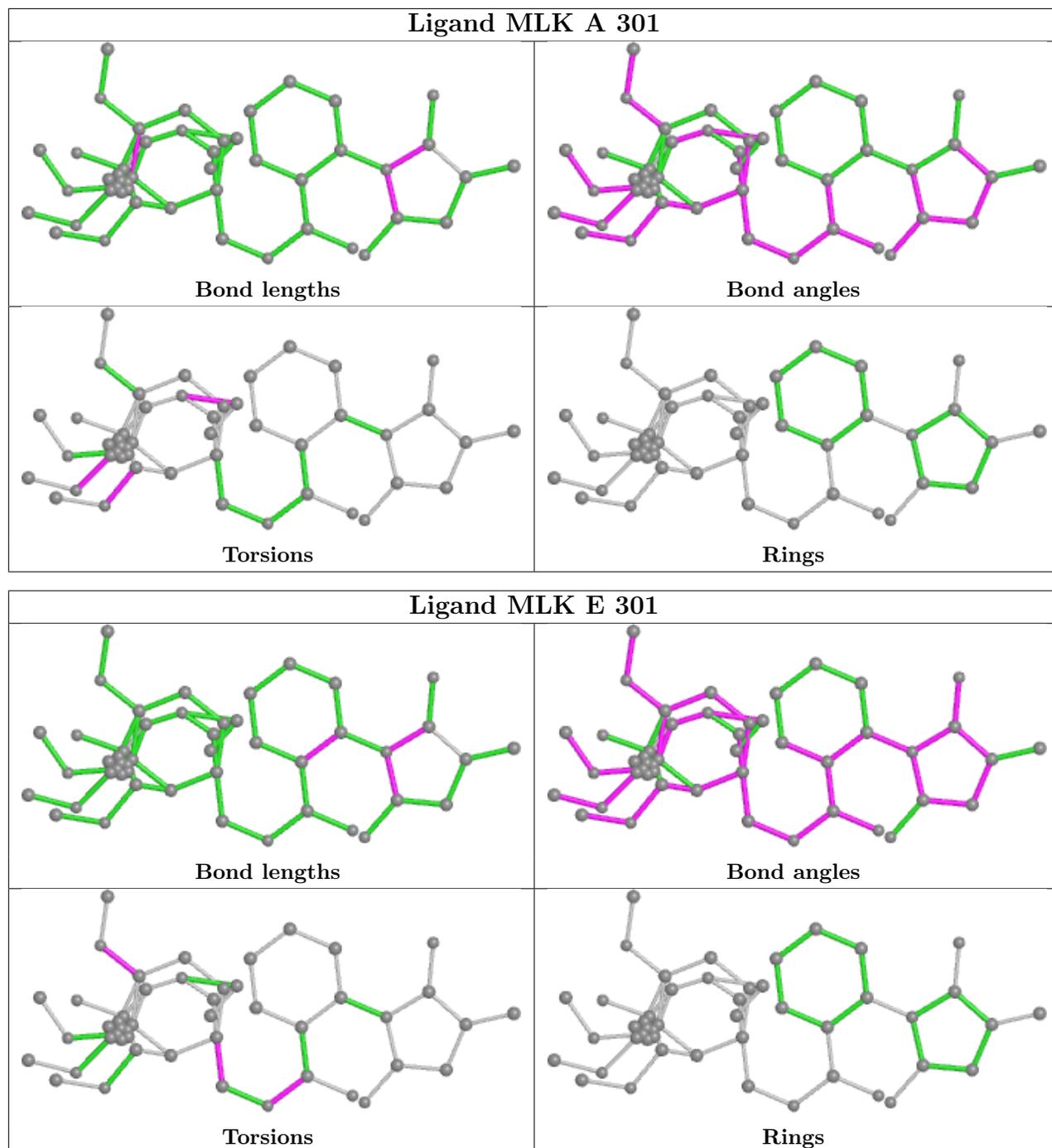
There are no ring outliers.

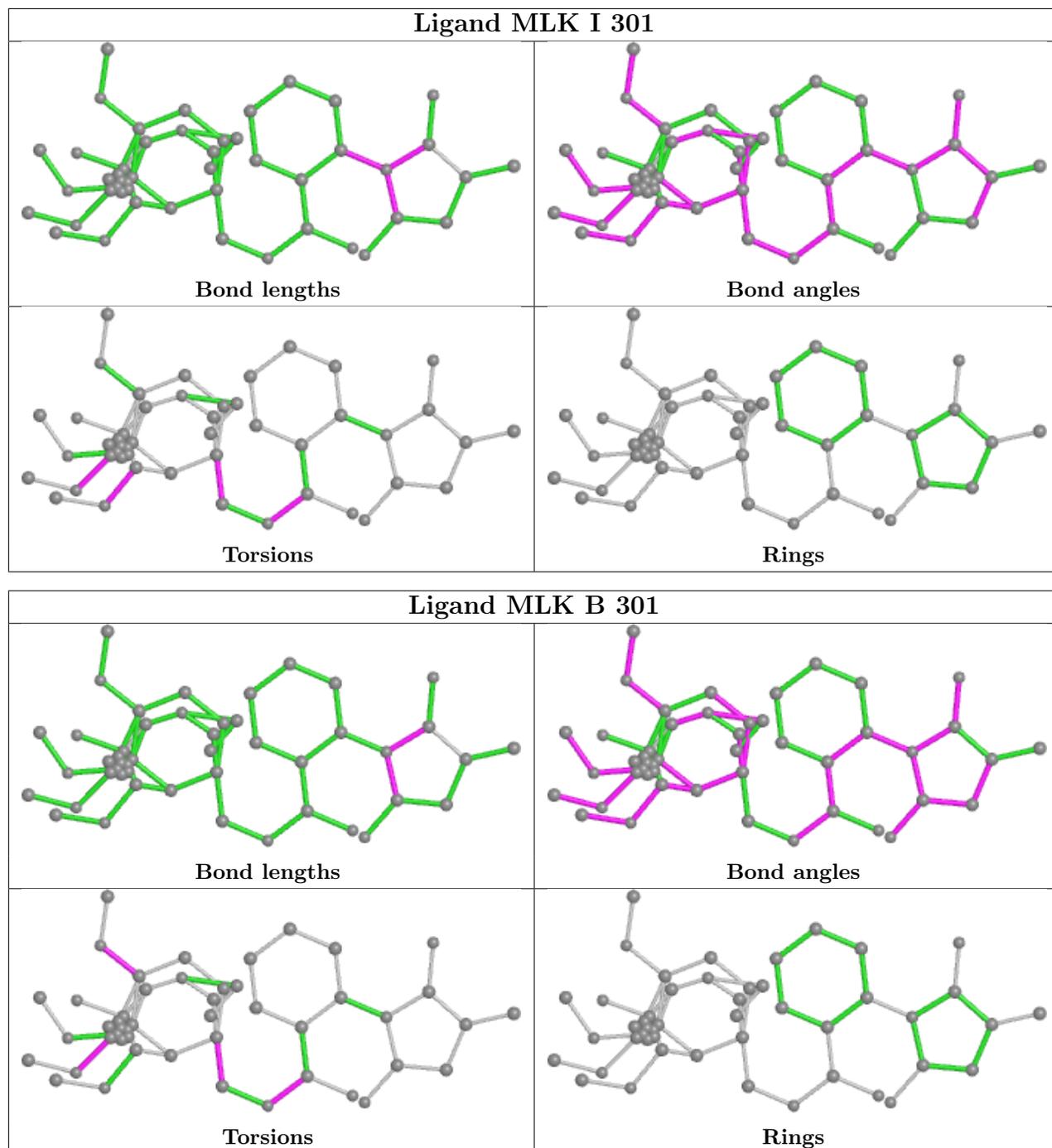
25 monomers are involved in 157 short contacts:

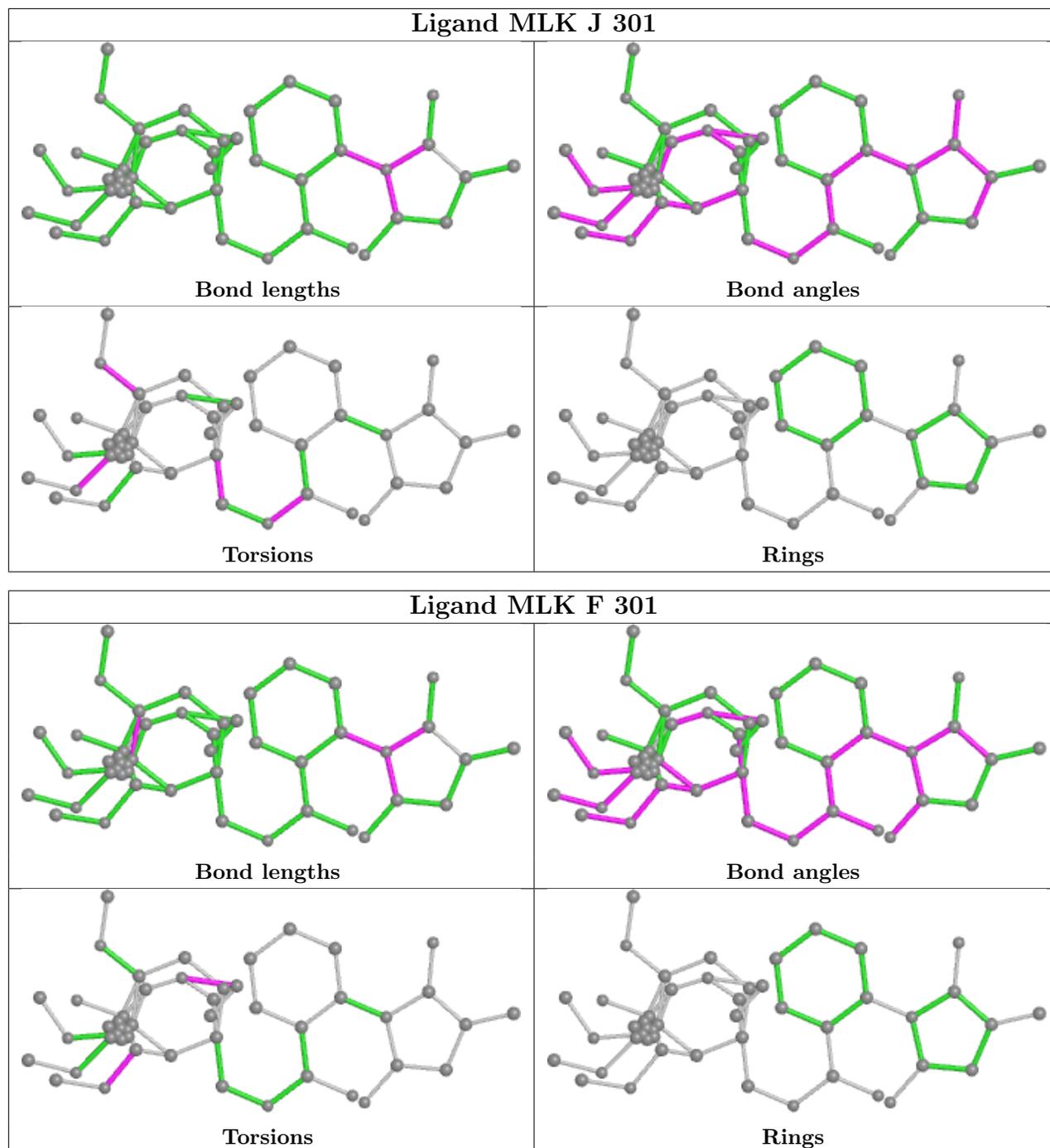
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	275[A]	NAG	2	0
5	G	301	MLK	10	0
5	H	301	MLK	15	0
5	A	301	MLK	9	0
8	E	275[B]	NAG	2	0
6	F	305	MRD	3	0
7	G	222	MPD	1	0
5	E	301	MLK	15	0
5	I	301	MLK	15	0
8	I	250	NAG	3	0
8	C	250	NAG	3	0
5	B	301	MLK	11	0
7	C	306	MPD	3	0
6	D	305	MRD	4	0
5	J	301	MLK	10	0
6	A	305	MRD	1	0
5	F	301	MLK	20	0
8	I	275[B]	NAG	2	0
5	C	301	MLK	18	0
6	B	305	MRD	2	0
8	B	250	NAG	1	0
7	I	305	MPD	1	0
7	A	223	MPD	1	0
5	D	301	MLK	4	0
8	B	275[B]	NAG	1	0

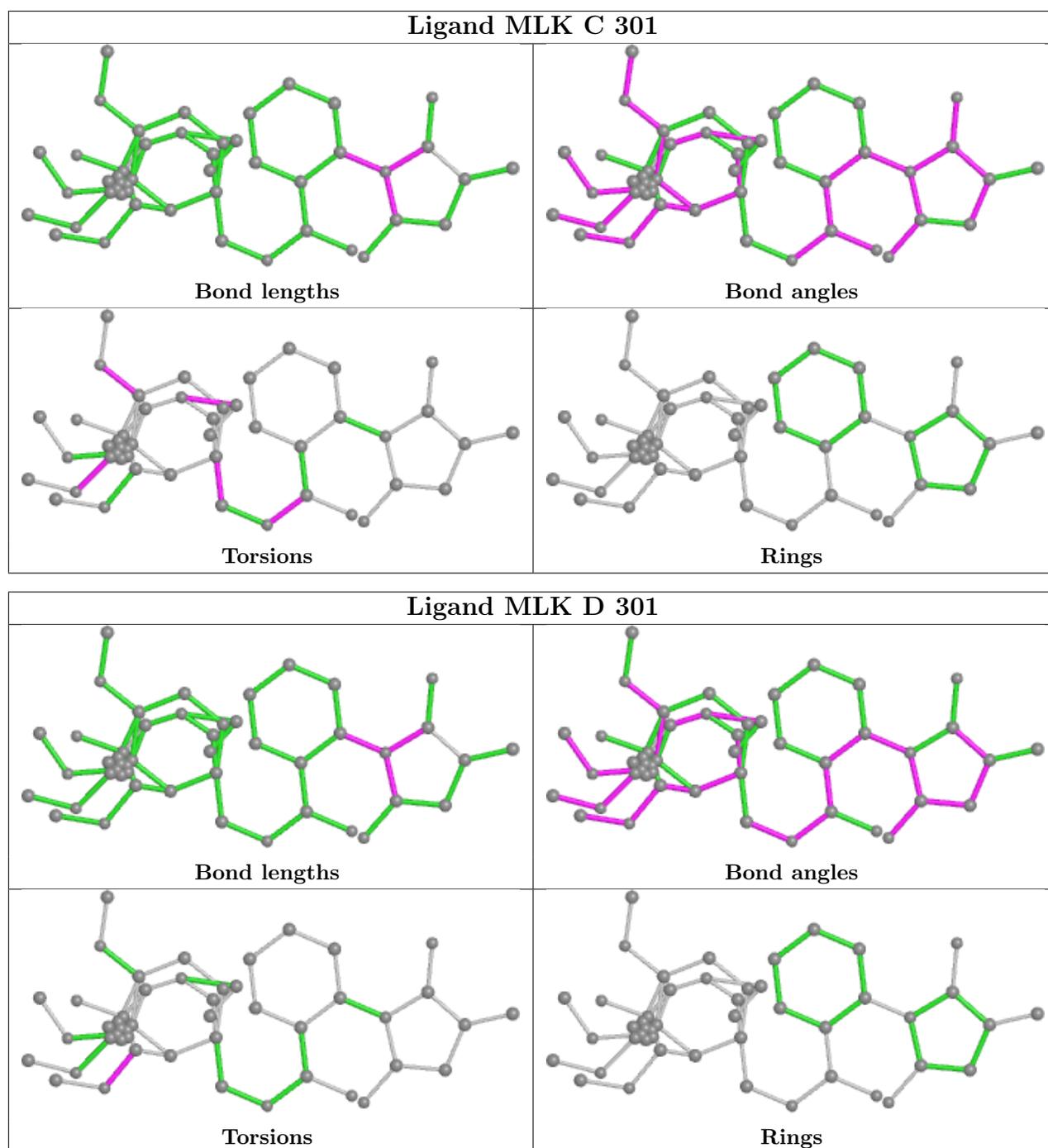
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	214/230 (93%)	-0.50	0 100 100	47, 66, 93, 117	5 (2%)
1	B	215/230 (93%)	-0.50	0 100 100	44, 61, 92, 122	2 (0%)
1	C	216/230 (93%)	-0.45	2 (0%) 84 84	40, 63, 96, 112	2 (0%)
1	D	214/230 (93%)	-0.53	1 (0%) 91 91	48, 67, 103, 114	1 (0%)
1	E	215/230 (93%)	-0.41	1 (0%) 91 91	44, 64, 96, 116	3 (1%)
1	F	214/230 (93%)	-0.40	2 (0%) 84 84	45, 65, 99, 118	0
1	G	214/230 (93%)	-0.54	0 100 100	47, 60, 93, 106	1 (0%)
1	H	215/230 (93%)	-0.49	1 (0%) 91 91	42, 61, 95, 109	0
1	I	214/230 (93%)	-0.43	0 100 100	48, 67, 105, 116	0
1	J	215/230 (93%)	-0.46	0 100 100	48, 63, 101, 119	2 (0%)
All	All	2146/2300 (93%)	-0.47	7 (0%) 94 94	40, 64, 97, 122	16 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	15	ASN	4.3
1	E	15	ASN	4.1
1	C	209	ALA	3.2
1	F	15	ASN	2.8
1	D	74	ASN	2.4

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

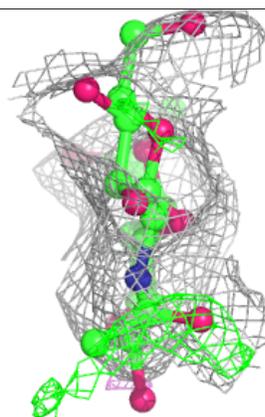
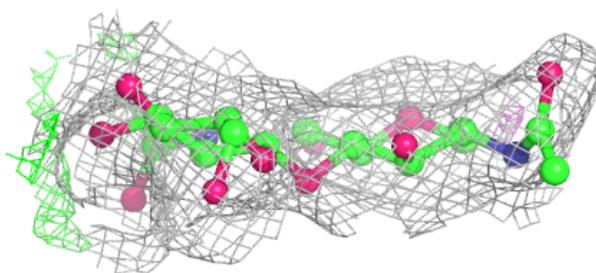
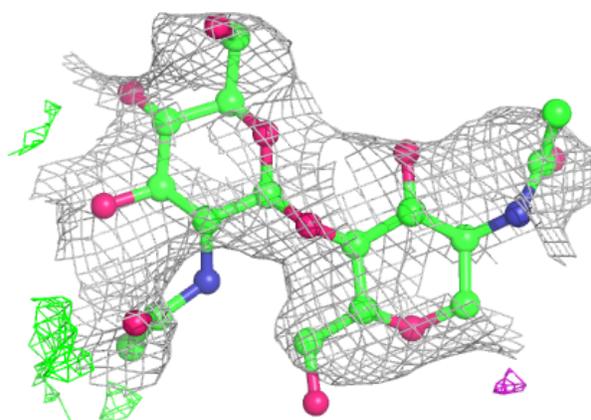
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	O	2	14/15	0.54	0.25	106,136,147,152	0
3	BMA	P	3	11/12	0.54	0.24	139,148,152,158	0
3	NAG	P	2	14/15	0.56	0.22	123,136,148,149	0
2	NAG	K	2	14/15	0.56	0.23	122,138,143,143	0
3	BMA	O	3	11/12	0.74	0.17	126,140,146,148	0
2	NAG	L	2	14/15	0.78	0.18	118,130,135,136	0
3	NAG	P	1	14/15	0.85	0.23	91,105,119,132	0
3	NAG	O	1	14/15	0.86	0.19	86,105,111,128	0
2	NAG	N	1	14/15	0.86	0.14	81,99,110,112	0
2	NAG	N	2	14/15	0.86	0.12	103,126,135,140	0
2	NAG	L	1	14/15	0.88	0.22	87,103,113,123	0
2	NAG	M	1	14/15	0.88	0.12	95,111,123,124	0
2	NAG	M	2	14/15	0.89	0.13	123,134,142,144	0
2	NAG	K	1	14/15	0.91	0.16	93,107,120,132	0

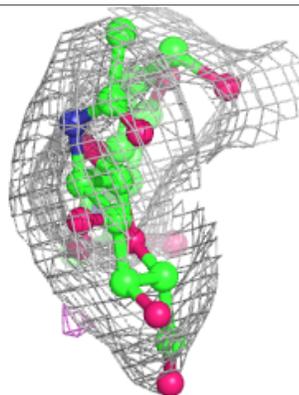
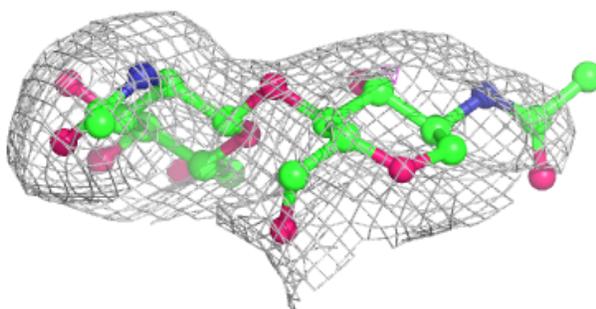
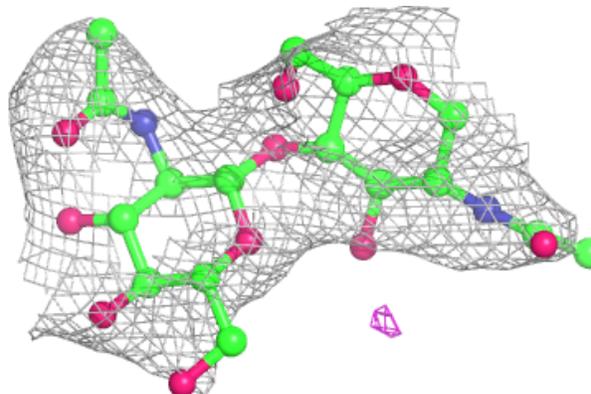
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

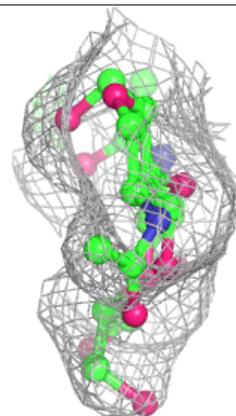
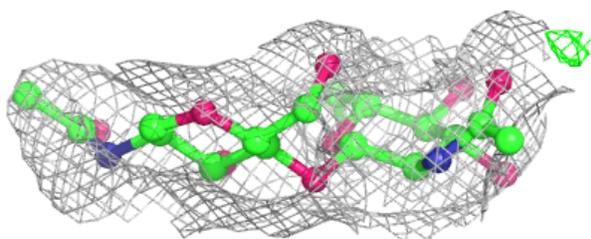
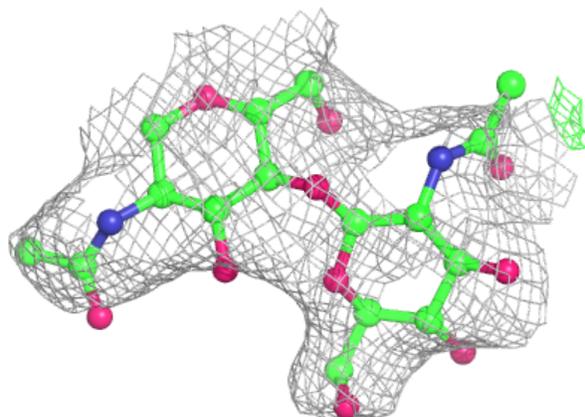
**Electron density around Chain L:**

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

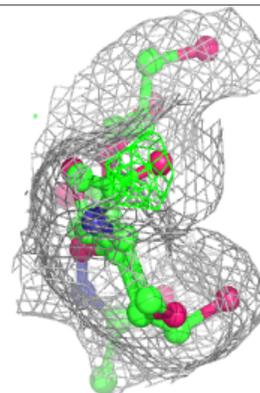
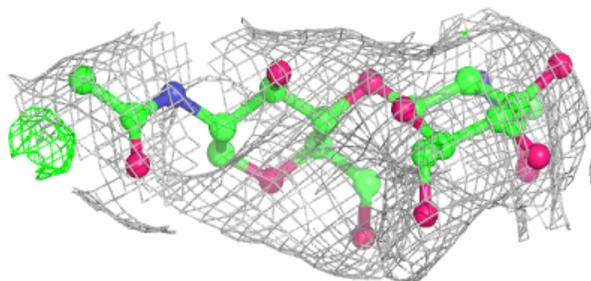
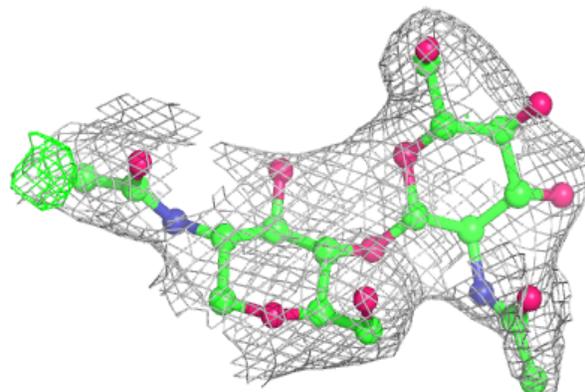


Electron density around Chain M:

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

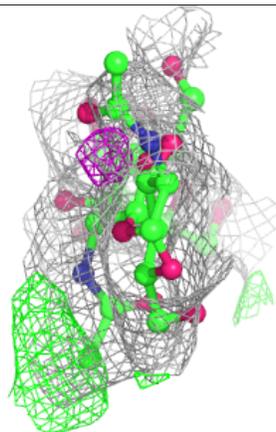
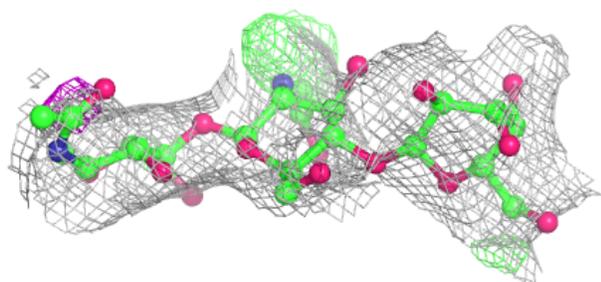
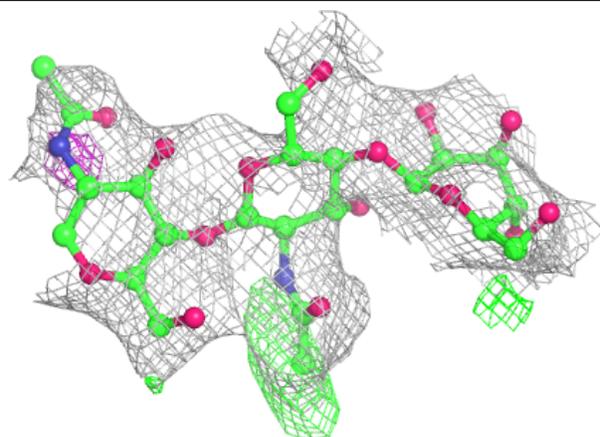
**Electron density around Chain N:**

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

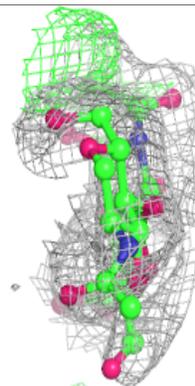
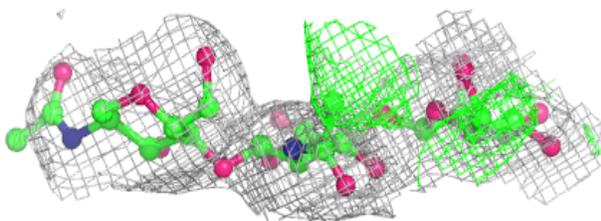
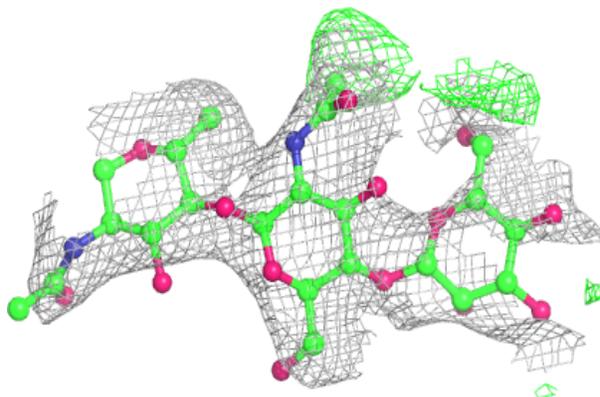


Electron density around Chain O:

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

**Electron density around Chain P:**

$2mF_o-DF_c$ (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.

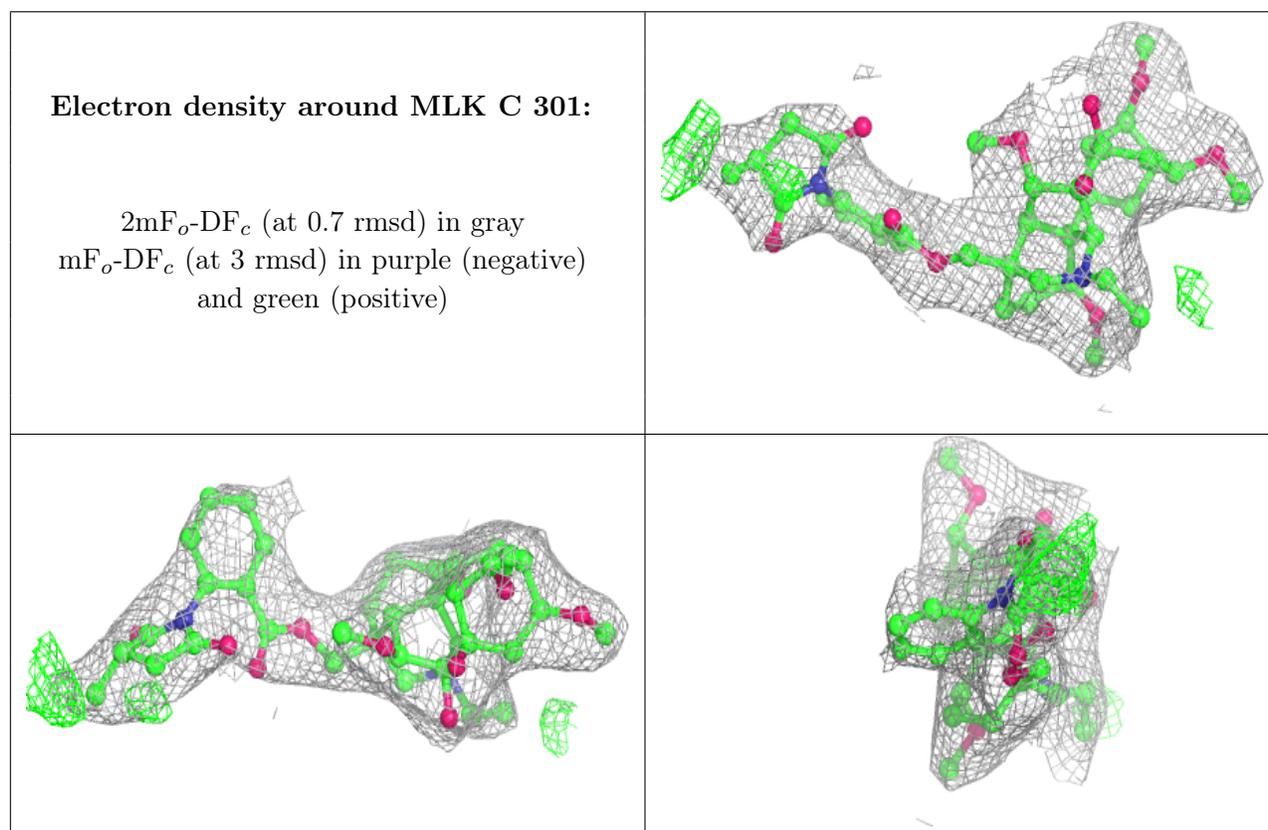
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	E	275[A]	14/15	0.59	0.39	105,111,115,117	14
8	NAG	E	275[B]	14/15	0.59	0.39	91,112,121,123	14
8	NAG	I	275[A]	14/15	0.66	0.26	96,99,103,105	14
8	NAG	I	275[B]	14/15	0.66	0.26	81,95,102,103	14
8	NAG	B	275[A]	14/15	0.67	0.35	78,98,105,106	14
8	NAG	B	275[B]	14/15	0.67	0.35	93,98,103,103	14
8	NAG	I	250	14/15	0.83	0.14	82,98,103,104	0
6	MRD	E	305	8/8	0.84	0.25	69,85,99,104	0
9	ACT	G	308	4/4	0.85	0.19	74,85,89,90	0
6	MRD	D	305	8/8	0.86	0.25	72,74,86,90	0
7	MPD	C	306	8/8	0.86	0.15	82,87,97,100	0
7	MPD	G	222	8/8	0.87	0.25	68,76,91,92	0
8	NAG	C	250	14/15	0.87	0.19	91,102,110,116	0
7	MPD	G	305	8/8	0.88	0.23	65,75,93,94	0
7	MPD	I	305	8/8	0.88	0.21	79,80,90,92	0
7	MPD	J	305	8/8	0.88	0.27	64,82,89,97	0
7	MPD	A	306	8/8	0.89	0.18	84,97,105,105	0
8	NAG	F	250	14/15	0.89	0.14	91,99,108,108	0
6	MRD	A	305	8/8	0.89	0.18	70,76,83,86	0
6	MRD	B	305	8/8	0.90	0.27	66,75,86,95	0
5	MLK	C	301	49/49	0.91	0.18	64,90,98,102	0
8	NAG	B	250	14/15	0.91	0.19	87,95,105,106	0
5	MLK	A	301	49/49	0.91	0.14	78,90,100,103	0
5	MLK	D	301	49/49	0.92	0.16	75,93,105,110	0
5	MLK	F	301	49/49	0.92	0.14	72,92,105,115	0
5	MLK	I	301	49/49	0.92	0.17	76,95,105,108	0
5	MLK	B	301	49/49	0.93	0.17	69,87,104,111	0
6	MRD	F	305	8/8	0.93	0.22	75,77,85,90	0
7	MPD	A	223	8/8	0.93	0.25	62,83,87,91	0
5	MLK	H	301	49/49	0.93	0.16	67,83,97,101	0
5	MLK	J	301	49/49	0.94	0.20	72,92,103,113	0
5	MLK	E	301	49/49	0.94	0.15	69,87,102,108	0
5	MLK	G	301	49/49	0.94	0.20	72,89,103,108	0
4	MG	E	222	1/1	0.96	0.29	57,57,57,57	0
4	MG	B	222	1/1	0.97	0.22	47,47,47,47	0
4	MG	C	222	1/1	0.97	0.29	57,57,57,57	0
4	MG	A	222	1/1	0.97	0.25	37,37,37,37	0

Continued on next page...

Continued from previous page...

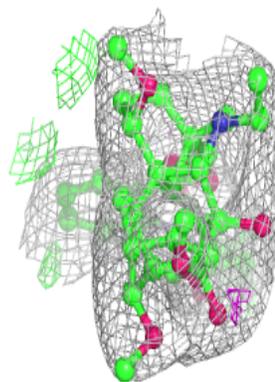
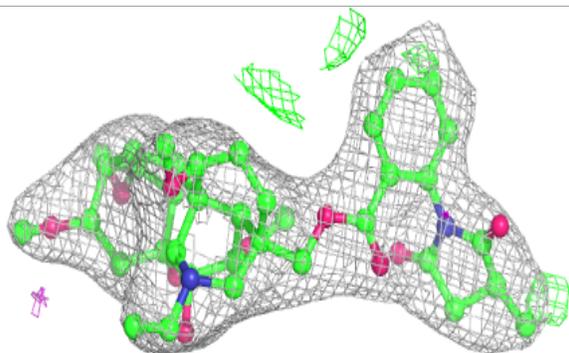
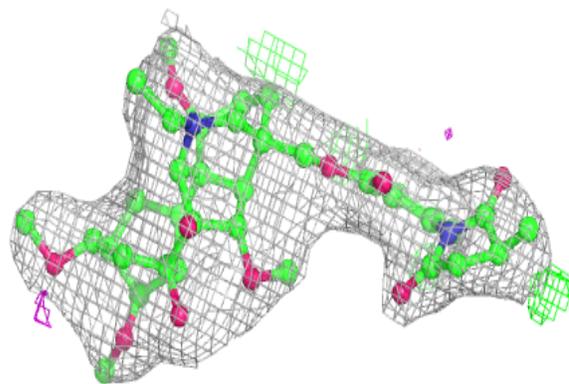
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	I	222	1/1	0.98	0.21	34,34,34,34	0

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.

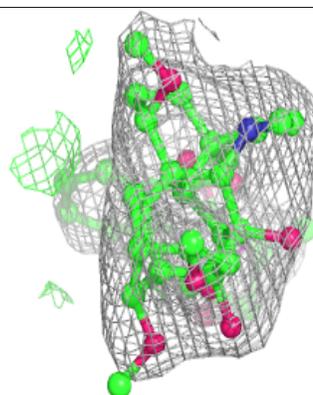
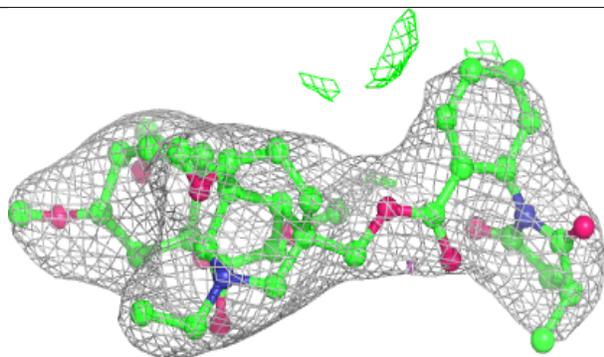
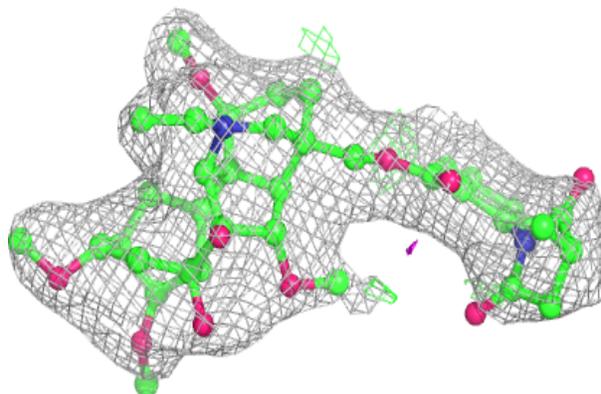


Electron density around MLK A 301:

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

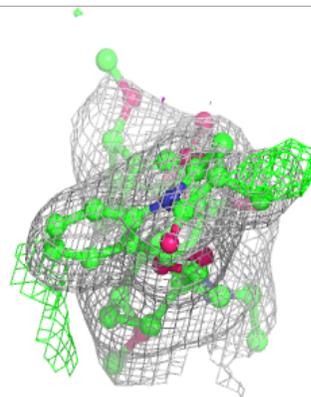
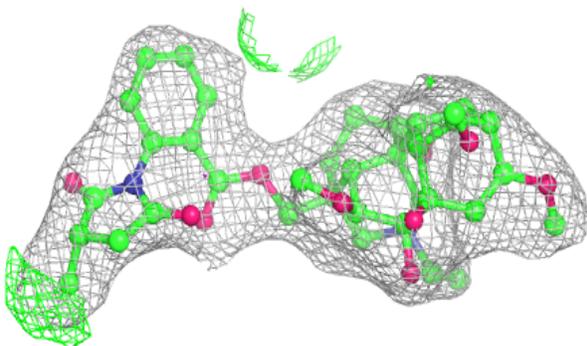
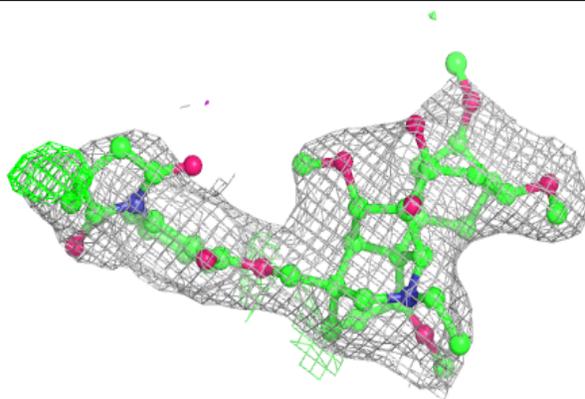
**Electron density around MLK D 301:**

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

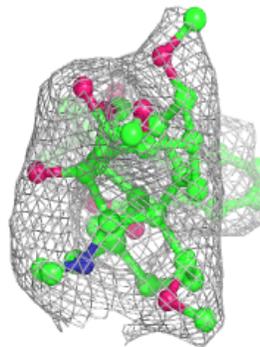
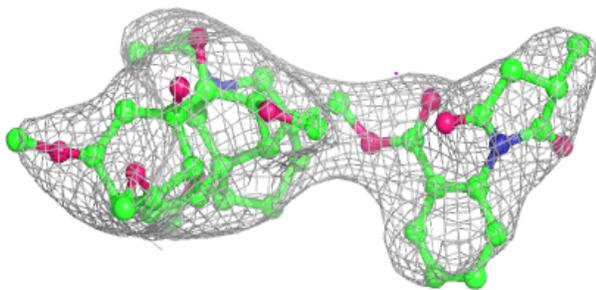
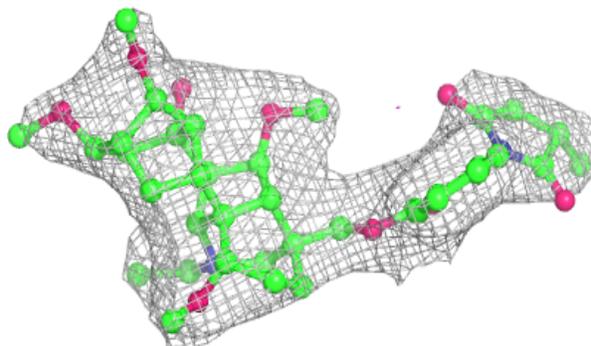


Electron density around MLK F 301:

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

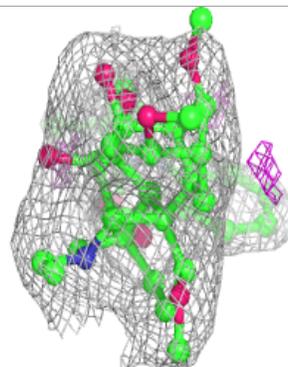
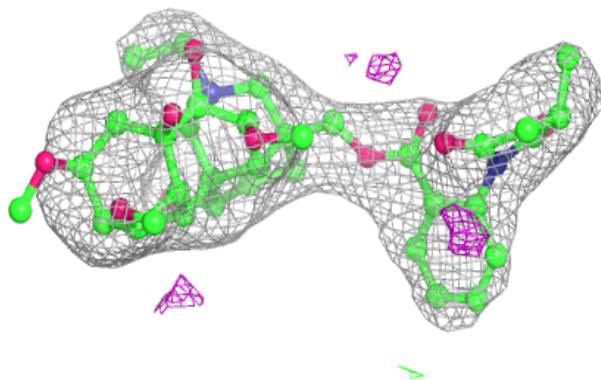
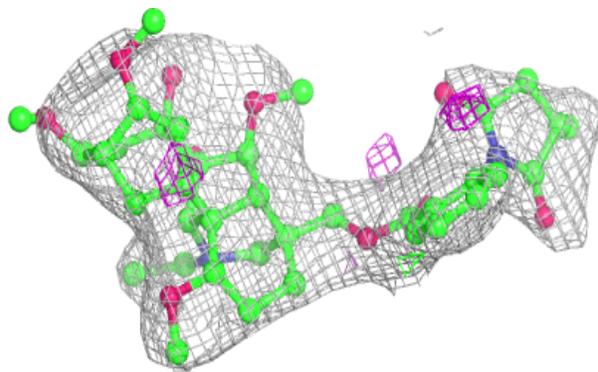
**Electron density around MLK I 301:**

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

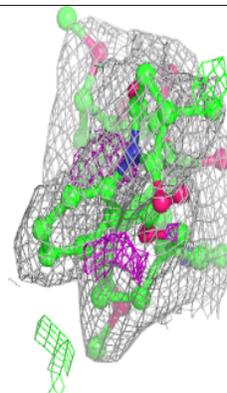
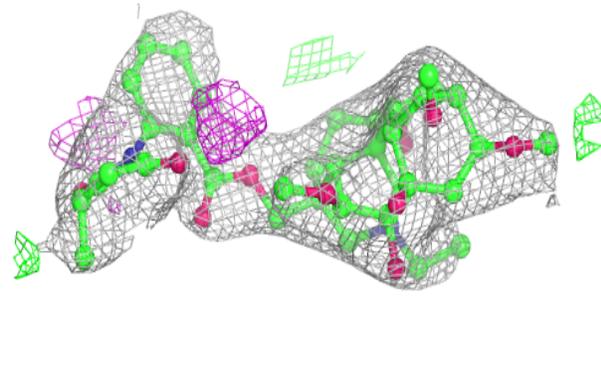
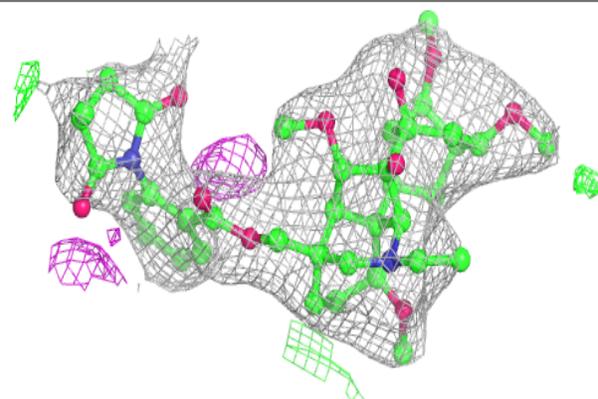


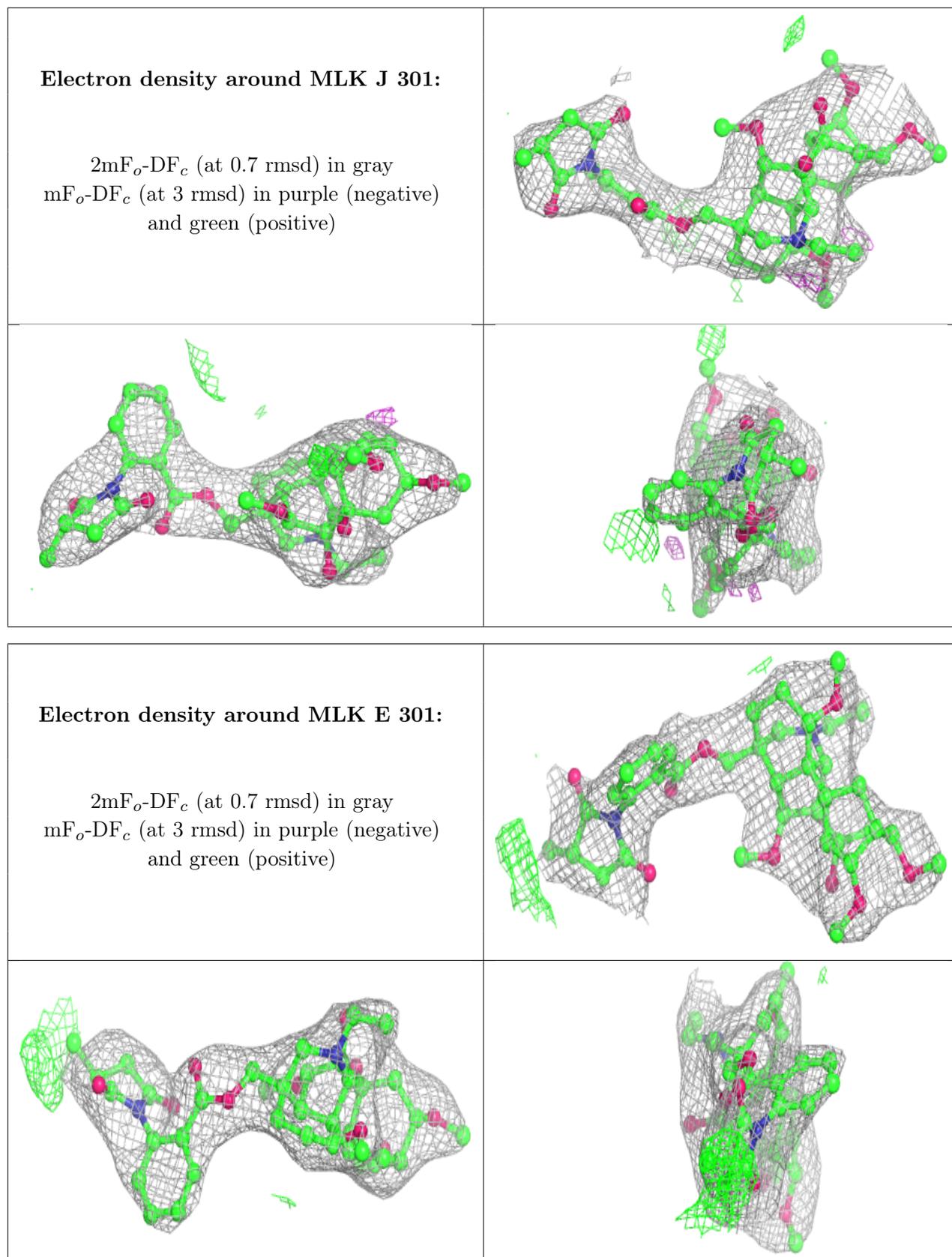
Electron density around MLK B 301:

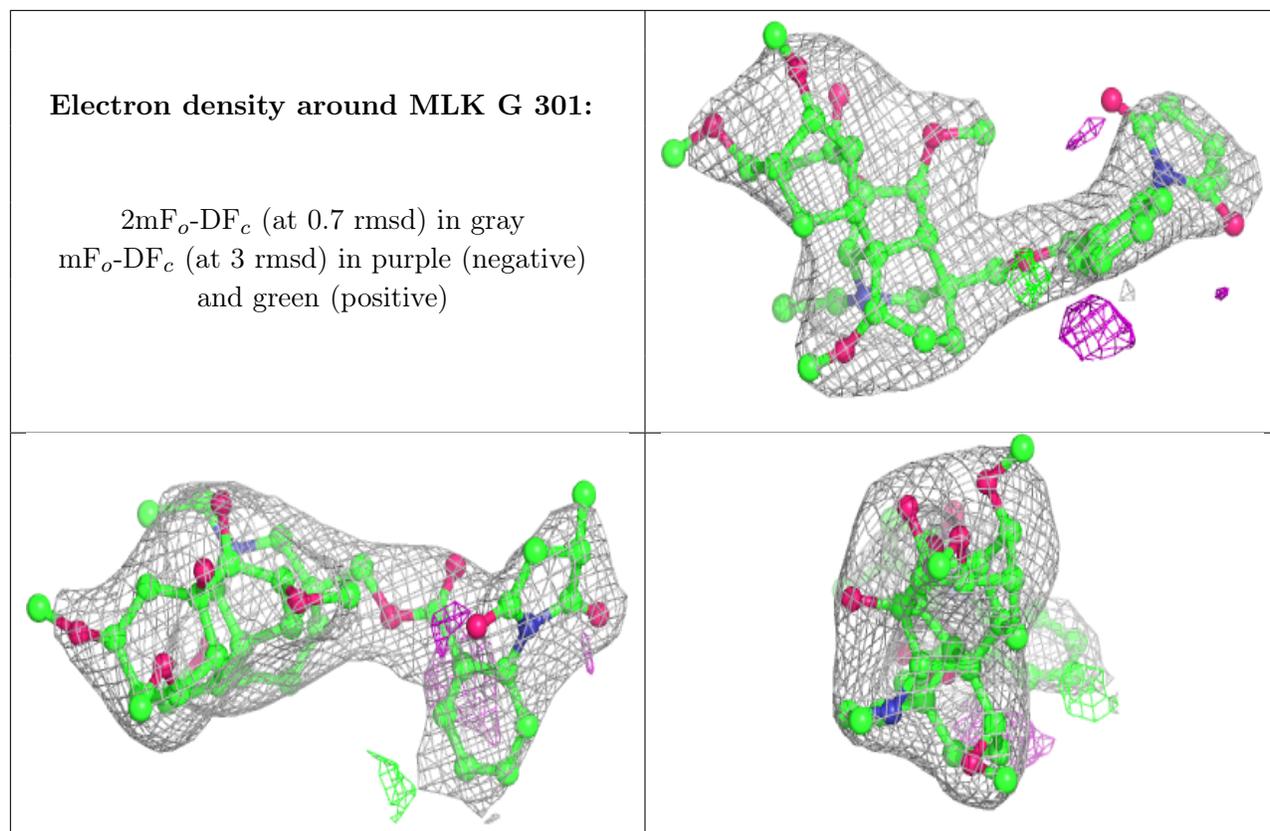
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MLK H 301:**

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







6.5 Other polymers [i](#)

There are no such residues in this entry.