wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 05:40 am GMT

PDB ID	:	6T9R
Title	:	Aplysia californica AChBP in complex with a cytisine derivative
Authors	:	Davis, S.; Hunter, W.N.
Deposited on	:	2019-10-28
Resolution	:	1.72 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 (i) 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 (i)) were used in the production of this report:

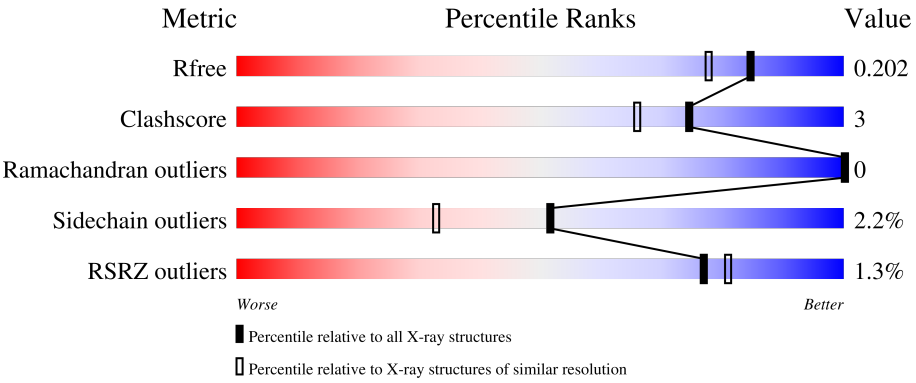
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.72 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.



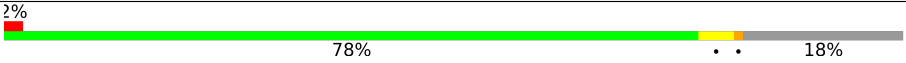
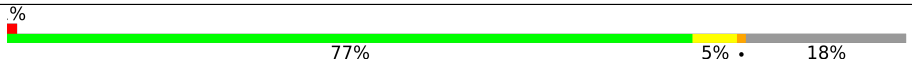
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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

Mol	Chain	Length	Quality of chain
1	AAA	249	78% · 18%
1	BBB	249	2% 78% 6% 15%
1	CCC	249	77% · · 17%
1	DDD	249	78% · 18%
1	EEE	249	78% · 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	249	
1	GGG	249	
1	HHH	249	
1	III	249	
1	JJJ	249	

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
4	GOL	CCC	303	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 38198 atoms, of which 17501 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 Acetylcholine binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	205	Total	C	H	N	O	S	96	18	0
			3431	1109	1701	273	337	11			
1	BBB	212	Total	C	H	N	O	S	98	18	0
			3557	1149	1767	289	341	11			
1	CCC	206	Total	C	H	N	O	S	96	14	0
			3384	1092	1674	274	335	9			
1	DDD	205	Total	C	H	N	O	S	91	13	0
			3376	1095	1671	270	330	10			
1	EEE	205	Total	C	H	N	O	S	98	15	0
			3391	1096	1679	272	334	10			
1	FFF	205	Total	C	H	N	O	S	96	19	0
			3428	1109	1700	272	335	12			
1	GGG	205	Total	C	H	N	O	S	92	11	0
			3353	1080	1661	274	328	10			
1	HHH	205	Total	C	H	N	O	S	93	13	0
			3369	1090	1665	271	333	10			
1	III	205	Total	C	H	N	O	S	93	11	0
			3350	1083	1657	271	329	10			
1	JJJ	205	Total	C	H	N	O	S	94	12	0
			3356	1083	1658	272	333	10			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	60	VAL	ALA	conflict	UNP Q8WSF8
AAA	155	VAL	ALA	conflict	UNP Q8WSF8
AAA	237	GLU	-	expression tag	UNP Q8WSF8
AAA	238	ASN	-	expression tag	UNP Q8WSF8
AAA	239	LEU	-	expression tag	UNP Q8WSF8
AAA	240	TYR	-	expression tag	UNP Q8WSF8
AAA	241	PHE	-	expression tag	UNP Q8WSF8
AAA	242	GLN	-	expression tag	UNP Q8WSF8
AAA	243	GLY	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	244	HIS	-	expression tag	UNP Q8WSF8
AAA	245	HIS	-	expression tag	UNP Q8WSF8
AAA	246	HIS	-	expression tag	UNP Q8WSF8
AAA	247	HIS	-	expression tag	UNP Q8WSF8
AAA	248	HIS	-	expression tag	UNP Q8WSF8
AAA	249	HIS	-	expression tag	UNP Q8WSF8
BBB	60	VAL	ALA	conflict	UNP Q8WSF8
BBB	155	VAL	ALA	conflict	UNP Q8WSF8
BBB	237	GLU	-	expression tag	UNP Q8WSF8
BBB	238	ASN	-	expression tag	UNP Q8WSF8
BBB	239	LEU	-	expression tag	UNP Q8WSF8
BBB	240	TYR	-	expression tag	UNP Q8WSF8
BBB	241	PHE	-	expression tag	UNP Q8WSF8
BBB	242	GLN	-	expression tag	UNP Q8WSF8
BBB	243	GLY	-	expression tag	UNP Q8WSF8
BBB	244	HIS	-	expression tag	UNP Q8WSF8
BBB	245	HIS	-	expression tag	UNP Q8WSF8
BBB	246	HIS	-	expression tag	UNP Q8WSF8
BBB	247	HIS	-	expression tag	UNP Q8WSF8
BBB	248	HIS	-	expression tag	UNP Q8WSF8
BBB	249	HIS	-	expression tag	UNP Q8WSF8
CCC	60	VAL	ALA	conflict	UNP Q8WSF8
CCC	155	VAL	ALA	conflict	UNP Q8WSF8
CCC	237	GLU	-	expression tag	UNP Q8WSF8
CCC	238	ASN	-	expression tag	UNP Q8WSF8
CCC	239	LEU	-	expression tag	UNP Q8WSF8
CCC	240	TYR	-	expression tag	UNP Q8WSF8
CCC	241	PHE	-	expression tag	UNP Q8WSF8
CCC	242	GLN	-	expression tag	UNP Q8WSF8
CCC	243	GLY	-	expression tag	UNP Q8WSF8
CCC	244	HIS	-	expression tag	UNP Q8WSF8
CCC	245	HIS	-	expression tag	UNP Q8WSF8
CCC	246	HIS	-	expression tag	UNP Q8WSF8
CCC	247	HIS	-	expression tag	UNP Q8WSF8
CCC	248	HIS	-	expression tag	UNP Q8WSF8
CCC	249	HIS	-	expression tag	UNP Q8WSF8
DDD	60	VAL	ALA	conflict	UNP Q8WSF8
DDD	155	VAL	ALA	conflict	UNP Q8WSF8
DDD	237	GLU	-	expression tag	UNP Q8WSF8
DDD	238	ASN	-	expression tag	UNP Q8WSF8
DDD	239	LEU	-	expression tag	UNP Q8WSF8
DDD	240	TYR	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	241	PHE	-	expression tag	UNP Q8WSF8
DDD	242	GLN	-	expression tag	UNP Q8WSF8
DDD	243	GLY	-	expression tag	UNP Q8WSF8
DDD	244	HIS	-	expression tag	UNP Q8WSF8
DDD	245	HIS	-	expression tag	UNP Q8WSF8
DDD	246	HIS	-	expression tag	UNP Q8WSF8
DDD	247	HIS	-	expression tag	UNP Q8WSF8
DDD	248	HIS	-	expression tag	UNP Q8WSF8
DDD	249	HIS	-	expression tag	UNP Q8WSF8
EEE	60	VAL	ALA	conflict	UNP Q8WSF8
EEE	155	VAL	ALA	conflict	UNP Q8WSF8
EEE	237	GLU	-	expression tag	UNP Q8WSF8
EEE	238	ASN	-	expression tag	UNP Q8WSF8
EEE	239	LEU	-	expression tag	UNP Q8WSF8
EEE	240	TYR	-	expression tag	UNP Q8WSF8
EEE	241	PHE	-	expression tag	UNP Q8WSF8
EEE	242	GLN	-	expression tag	UNP Q8WSF8
EEE	243	GLY	-	expression tag	UNP Q8WSF8
EEE	244	HIS	-	expression tag	UNP Q8WSF8
EEE	245	HIS	-	expression tag	UNP Q8WSF8
EEE	246	HIS	-	expression tag	UNP Q8WSF8
EEE	247	HIS	-	expression tag	UNP Q8WSF8
EEE	248	HIS	-	expression tag	UNP Q8WSF8
EEE	249	HIS	-	expression tag	UNP Q8WSF8
FFF	60	VAL	ALA	conflict	UNP Q8WSF8
FFF	155	VAL	ALA	conflict	UNP Q8WSF8
FFF	237	GLU	-	expression tag	UNP Q8WSF8
FFF	238	ASN	-	expression tag	UNP Q8WSF8
FFF	239	LEU	-	expression tag	UNP Q8WSF8
FFF	240	TYR	-	expression tag	UNP Q8WSF8
FFF	241	PHE	-	expression tag	UNP Q8WSF8
FFF	242	GLN	-	expression tag	UNP Q8WSF8
FFF	243	GLY	-	expression tag	UNP Q8WSF8
FFF	244	HIS	-	expression tag	UNP Q8WSF8
FFF	245	HIS	-	expression tag	UNP Q8WSF8
FFF	246	HIS	-	expression tag	UNP Q8WSF8
FFF	247	HIS	-	expression tag	UNP Q8WSF8
FFF	248	HIS	-	expression tag	UNP Q8WSF8
FFF	249	HIS	-	expression tag	UNP Q8WSF8
GGG	60	VAL	ALA	conflict	UNP Q8WSF8
GGG	155	VAL	ALA	conflict	UNP Q8WSF8
GGG	237	GLU	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

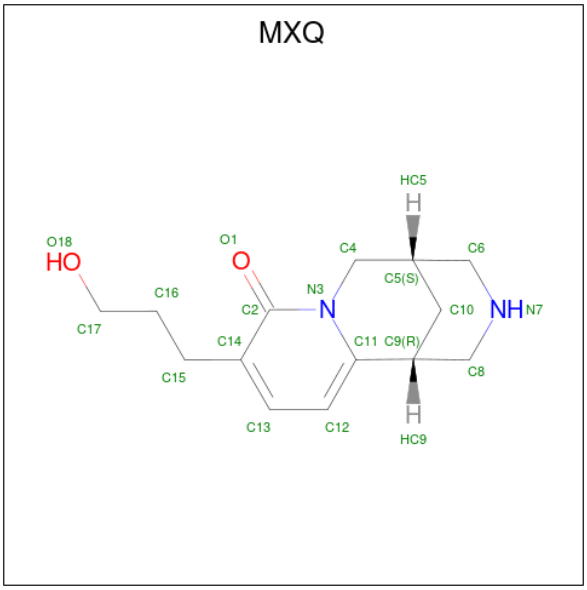
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	238	ASN	-	expression tag	UNP Q8WSF8
GGG	239	LEU	-	expression tag	UNP Q8WSF8
GGG	240	TYR	-	expression tag	UNP Q8WSF8
GGG	241	PHE	-	expression tag	UNP Q8WSF8
GGG	242	GLN	-	expression tag	UNP Q8WSF8
GGG	243	GLY	-	expression tag	UNP Q8WSF8
GGG	244	HIS	-	expression tag	UNP Q8WSF8
GGG	245	HIS	-	expression tag	UNP Q8WSF8
GGG	246	HIS	-	expression tag	UNP Q8WSF8
GGG	247	HIS	-	expression tag	UNP Q8WSF8
GGG	248	HIS	-	expression tag	UNP Q8WSF8
GGG	249	HIS	-	expression tag	UNP Q8WSF8
HHH	60	VAL	ALA	conflict	UNP Q8WSF8
HHH	155	VAL	ALA	conflict	UNP Q8WSF8
HHH	237	GLU	-	expression tag	UNP Q8WSF8
HHH	238	ASN	-	expression tag	UNP Q8WSF8
HHH	239	LEU	-	expression tag	UNP Q8WSF8
HHH	240	TYR	-	expression tag	UNP Q8WSF8
HHH	241	PHE	-	expression tag	UNP Q8WSF8
HHH	242	GLN	-	expression tag	UNP Q8WSF8
HHH	243	GLY	-	expression tag	UNP Q8WSF8
HHH	244	HIS	-	expression tag	UNP Q8WSF8
HHH	245	HIS	-	expression tag	UNP Q8WSF8
HHH	246	HIS	-	expression tag	UNP Q8WSF8
HHH	247	HIS	-	expression tag	UNP Q8WSF8
HHH	248	HIS	-	expression tag	UNP Q8WSF8
HHH	249	HIS	-	expression tag	UNP Q8WSF8
III	60	VAL	ALA	conflict	UNP Q8WSF8
III	155	VAL	ALA	conflict	UNP Q8WSF8
III	237	GLU	-	expression tag	UNP Q8WSF8
III	238	ASN	-	expression tag	UNP Q8WSF8
III	239	LEU	-	expression tag	UNP Q8WSF8
III	240	TYR	-	expression tag	UNP Q8WSF8
III	241	PHE	-	expression tag	UNP Q8WSF8
III	242	GLN	-	expression tag	UNP Q8WSF8
III	243	GLY	-	expression tag	UNP Q8WSF8
III	244	HIS	-	expression tag	UNP Q8WSF8
III	245	HIS	-	expression tag	UNP Q8WSF8
III	246	HIS	-	expression tag	UNP Q8WSF8
III	247	HIS	-	expression tag	UNP Q8WSF8
III	248	HIS	-	expression tag	UNP Q8WSF8
III	249	HIS	-	expression tag	UNP Q8WSF8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
JJJ	60	VAL	ALA	conflict	UNP Q8WSF8
JJJ	155	VAL	ALA	conflict	UNP Q8WSF8
JJJ	237	GLU	-	expression tag	UNP Q8WSF8
JJJ	238	ASN	-	expression tag	UNP Q8WSF8
JJJ	239	LEU	-	expression tag	UNP Q8WSF8
JJJ	240	TYR	-	expression tag	UNP Q8WSF8
JJJ	241	PHE	-	expression tag	UNP Q8WSF8
JJJ	242	GLN	-	expression tag	UNP Q8WSF8
JJJ	243	GLY	-	expression tag	UNP Q8WSF8
JJJ	244	HIS	-	expression tag	UNP Q8WSF8
JJJ	245	HIS	-	expression tag	UNP Q8WSF8
JJJ	246	HIS	-	expression tag	UNP Q8WSF8
JJJ	247	HIS	-	expression tag	UNP Q8WSF8
JJJ	248	HIS	-	expression tag	UNP Q8WSF8
JJJ	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is (1 {R},9 {S})-5-(3-oxidanylpropyl)-7,11-diazatricyclo[7.3.1.0^{2,7}]trideca-2,4-dien-6-one (three-letter code: MXQ) (formula: $C_{14}H_{20}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



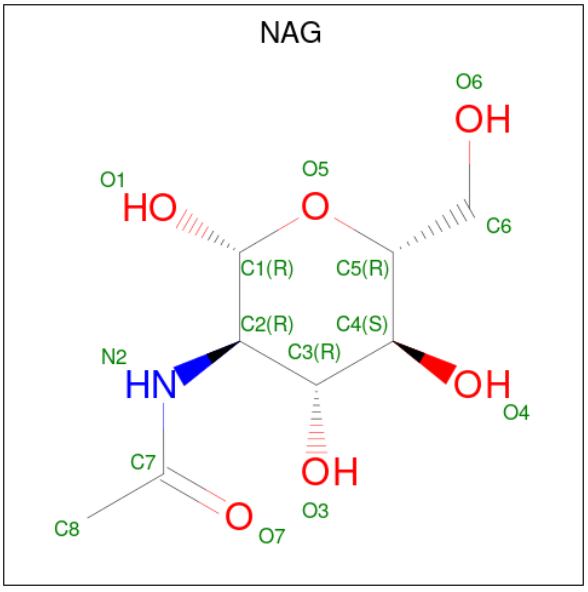
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	BBB	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	CCC	1	Total	C	H	N	O	1	0
			38	14	20	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	DDD	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	EEE	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	FFF	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	GGG	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	HHH	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	III	1	Total	C	H	N	O	1	0
			38	14	20	2	2		
2	JJJ	1	Total	C	H	N	O	1	0
			38	14	20	2	2		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



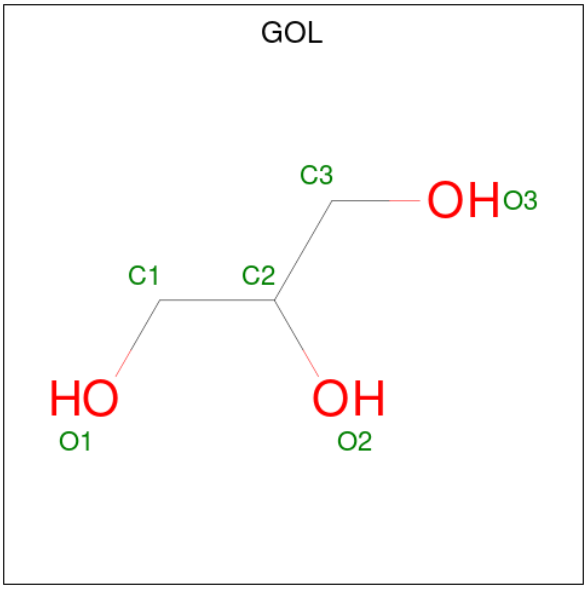
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	CCC	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	DDD	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	EEE	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	FFF	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	GGG	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	HHH	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	III	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	JJJ	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
4	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

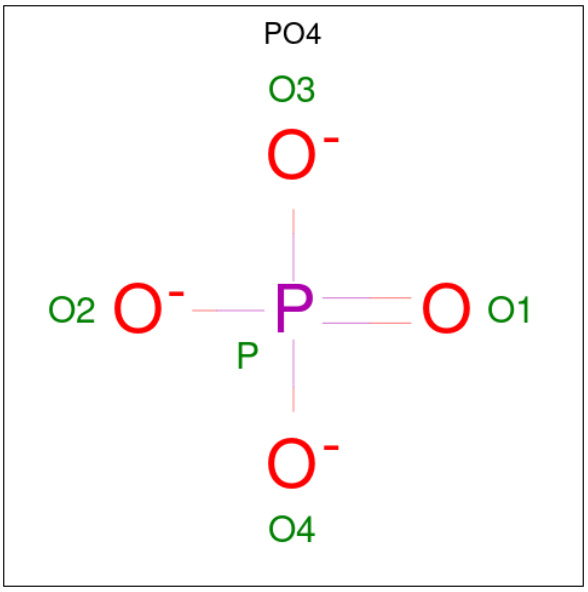
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
4	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	CCC	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
4	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
4	EEE	1	Total	C	H	O	2	0
			14	3	8	3		
4	EEE	1	Total	C	H	O	2	0
			14	3	8	3		
4	EEE	1	Total	C	H	O	2	0
			14	3	8	3		
4	EEE	1	Total	C	H	O	2	0
			14	3	8	3		
4	EEE	1	Total	C	H	O	2	0
			14	3	8	3		
4	FFF	1	Total	C	H	O	2	0
			14	3	8	3		
4	FFF	1	Total	C	H	O	2	0
			14	3	8	3		
4	FFF	1	Total	C	H	O	2	0
			14	3	8	3		
4	GGG	1	Total	C	H	O	2	0
			14	3	8	3		
4	GGG	1	Total	C	H	O	2	0
			14	3	8	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	GGG	1	Total C H O 14 3 8 3	2	0
4	GGG	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	HHH	1	Total C H O 14 3 8 3	2	0
4	III	1	Total C H O 14 3 8 3	2	0
4	III	1	Total C H O 14 3 8 3	2	0
4	III	1	Total C H O 14 3 8 3	2	0
4	III	1	Total C H O 14 3 8 3	2	0
4	JJJ	1	Total C H O 14 3 8 3	2	0
4	JJJ	1	Total C H O 14 3 8 3	2	0
4	JJJ	1	Total C H O 14 3 8 3	2	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O P 5 4 1	0	0
5	BBB	1	Total O P 5 4 1	0	0
5	CCC	1	Total O P 5 4 1	0	0
5	DDD	1	Total O P 5 4 1	0	0
5	EEE	1	Total O P 5 4 1	0	0
5	FFF	1	Total O P 5 4 1	0	0
5	GGG	1	Total O P 5 4 1	0	0
5	HHH	1	Total O P 5 4 1	0	0
5	III	1	Total O P 5 4 1	0	0
5	JJJ	1	Total O P 5 4 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Cl 1 1	0	0
6	BBB	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total Cl 1 1	0	0
6	DDD	1	Total Cl 1 1	0	0
6	EEE	1	Total Cl 1 1	0	0
6	FFF	1	Total Cl 1 1	0	0
6	GGG	1	Total Cl 1 1	0	0
6	HHH	1	Total Cl 1 1	0	0
6	III	1	Total Cl 1 1	0	0
6	JJJ	1	Total Cl 1 1	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total K 1 1	0	0
7	BBB	1	Total K 1 1	0	0
7	CCC	1	Total K 1 1	0	0
7	DDD	1	Total K 1 1	0	0
7	EEE	1	Total K 1 1	0	0
7	FFF	1	Total K 1 1	0	0
7	GGG	1	Total K 1 1	0	0
7	HHH	1	Total K 1 1	0	0
7	III	1	Total K 1 1	0	0
7	JJJ	1	Total K 1 1	0	0

- Molecule 8 is water.

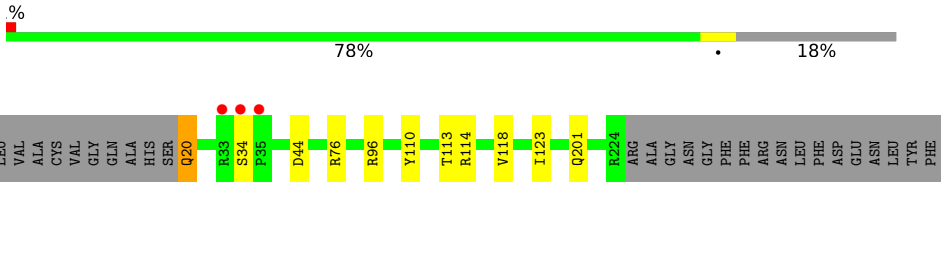
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	310	Total O 310 310	0	0
8	BBB	315	Total O 315 315	0	0
8	CCC	291	Total O 291 291	0	0
8	DDD	312	Total O 312 312	0	0
8	EEE	284	Total O 284 284	0	0
8	FFF	278	Total O 278 278	0	0
8	GGG	282	Total O 282 282	0	0
8	HHH	288	Total O 288 288	0	0
8	III	273	Total O 273 273	0	0
8	JJJ	266	Total O 266 266	0	0

3 Residue-property plots (i)

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

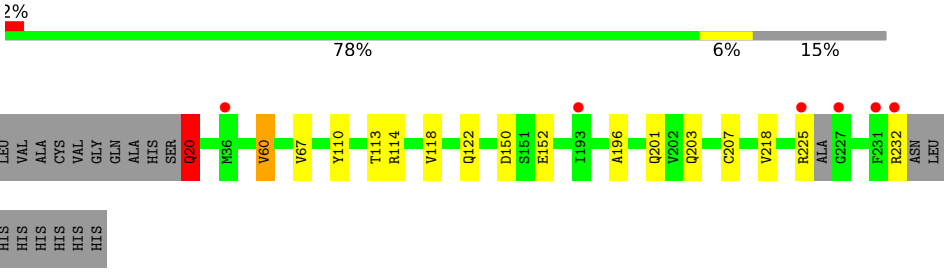
• Molecule 1: Acetylcholine binding protein

Chain AAA:



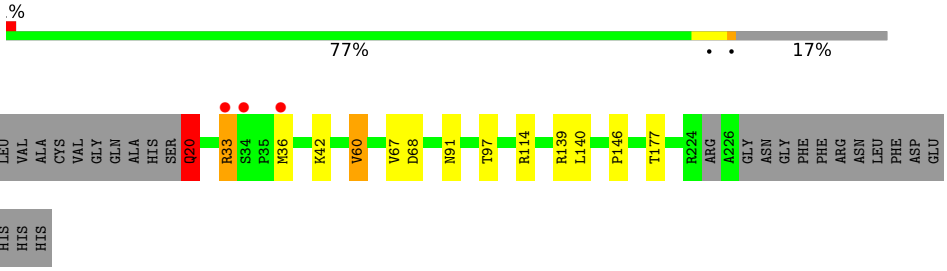
• Molecule 1: Acetylcholine binding protein

Chain BBB:



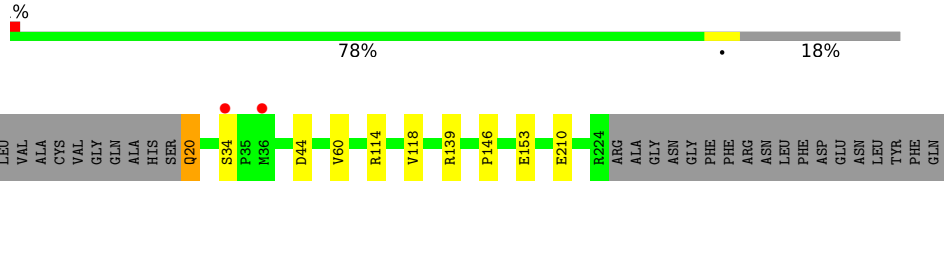
• Molecule 1: Acetylcholine binding protein

Chain CCC:



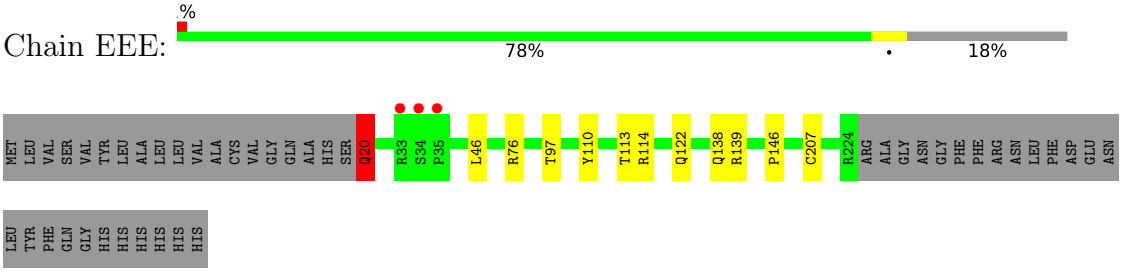
• Molecule 1: Acetylcholine binding protein

Chain DDD:



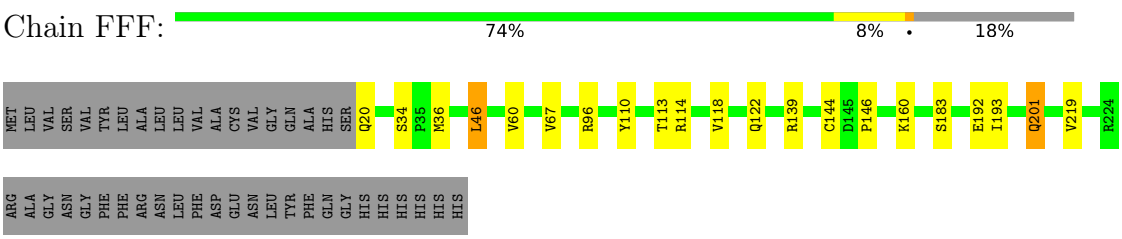
• Molecule 1: Acetylcholine binding protein

Chain EEE:



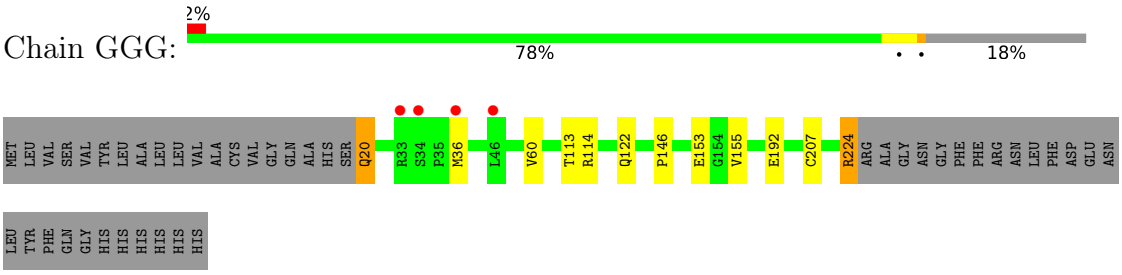
• Molecule 1: Acetylcholine binding protein

Chain FFF:



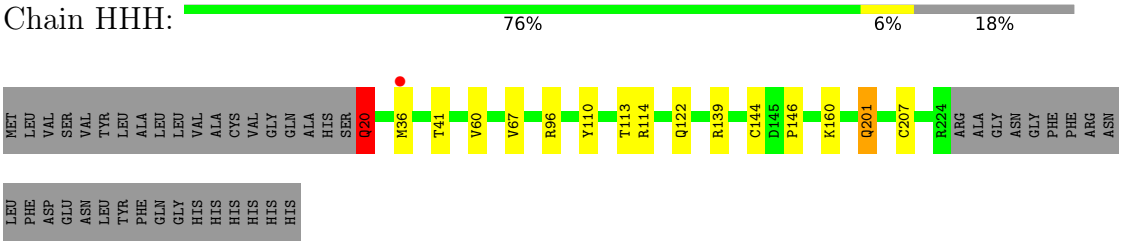
• Molecule 1: Acetylcholine binding protein

Chain GGG:



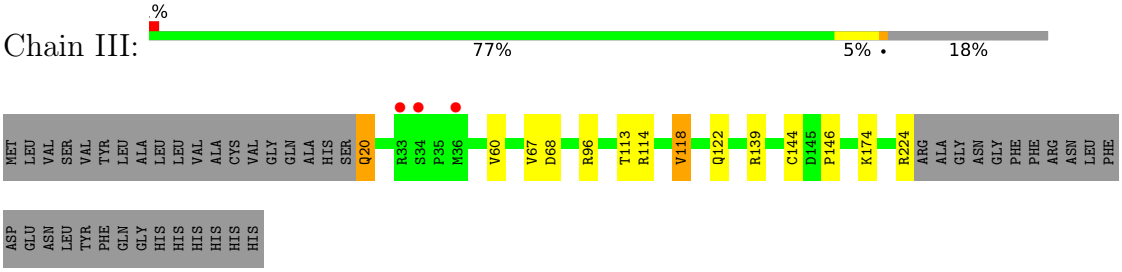
• Molecule 1: Acetylcholine binding protein

Chain HHH:



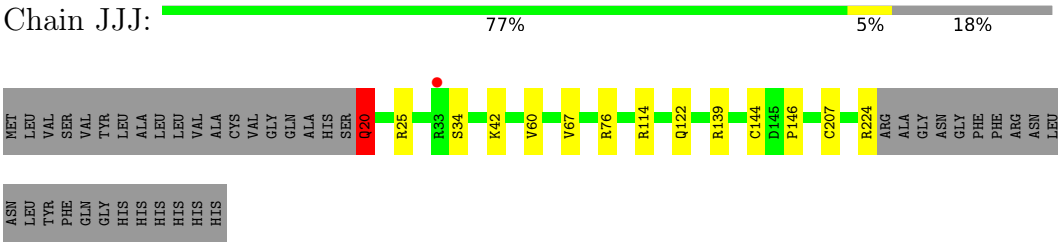
• Molecule 1: Acetylcholine binding protein

Chain III:



• Molecule 1: Acetylcholine binding protein

Chain JJJ:


77%
5%
18%
MET LEU VAL SER VAL TYR LEU ALA LEU LEU VAL ALA CYS VAL GLY GLN ALA HIS SER Q20 R25 R33 S34 K42 V60 V67 R76 R114 Q122 R139 C144 D145 P146 C207 R224 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP GLU
ASN LEU TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.47Å 132.87Å 131.09Å 90.00° 102.52° 90.00°	Depositor
Resolution (Å)	111.67 – 1.72 111.42 – 1.72	Depositor EDS
% Data completeness (in resolution range)	95.5 (111.67-1.72) 95.5 (111.42-1.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.162 , 0.192 0.173 , 0.202	Depositor DCC
R_{free} test set	17388 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	38198	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NAG, MXQ, PO4, GOL, K

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	AAA	0.80	0/1825	0.97	1/2489 (0.0%)
1	BBB	0.83	0/1886	0.99	1/2567 (0.0%)
1	CCC	0.79	0/1791	0.99	0/2445
1	DDD	0.86	2/1786 (0.1%)	0.98	0/2439
1	EEE	0.79	0/1799	0.97	0/2457
1	FFF	0.80	0/1826	0.98	0/2492
1	GGG	0.79	0/1764	1.00	0/2405
1	HHH	0.81	0/1784	0.98	3/2436 (0.1%)
1	III	0.79	0/1767	0.99	3/2412 (0.1%)
1	JJJ	0.79	0/1774	0.99	3/2420 (0.1%)
All	All	0.80	2/18002 (0.0%)	0.98	11/24562 (0.0%)

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	BBB	0	2
1	CCC	0	1
1	EEE	0	2
1	GGG	0	2
1	HHH	0	2
1	JJJ	0	2
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	153	GLU	CD-OE1	6.65	1.32	1.25
1	DDD	153	GLU	CD-OE2	5.56	1.31	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	HHH	122[A]	GLN	CB-CA-C	5.73	121.86	110.40
1	HHH	122[B]	GLN	CB-CA-C	5.73	121.86	110.40
1	JJJ	122[A]	GLN	CB-CA-C	5.26	120.92	110.40
1	JJJ	122[B]	GLN	CB-CA-C	5.26	120.92	110.40
1	HHH	201	GLN	CB-CA-C	-5.24	99.91	110.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	20	GLN	Peptide
1	BBB	207	CYS	Peptide
1	CCC	20	GLN	Peptide
1	EEE	20	GLN	Peptide
1	EEE	207	CYS	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	AAA	1730	1701	1716	10	0
1	BBB	1790	1767	1781	16	0
1	CCC	1710	1674	1684	11	0
1	DDD	1705	1671	1681	10	0
1	EEE	1712	1679	1685	10	0
1	FFF	1728	1700	1716	17	0
1	GGG	1692	1661	1668	6	0
1	HHH	1704	1665	1675	14	0
1	III	1693	1657	1665	11	0
1	JJJ	1698	1658	1667	7	0
2	AAA	18	20	0	0	0
2	BBB	18	20	0	0	0
2	CCC	18	20	0	0	0
2	DDD	18	20	0	0	0
2	EEE	18	20	0	0	0
2	FFF	18	20	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	GGG	18	20	0	0	0
2	HHH	18	20	0	0	0
2	III	18	20	0	0	0
2	JJJ	18	20	0	0	0
3	AAA	14	14	13	0	0
3	BBB	14	14	13	0	0
3	CCC	14	14	13	1	0
3	DDD	14	14	13	0	0
3	EEE	14	14	13	0	0
3	FFF	14	14	13	0	0
3	GGG	14	14	13	0	0
3	HHH	14	14	13	0	0
3	III	14	14	13	0	0
3	JJJ	14	14	13	0	0
4	AAA	12	16	16	0	0
4	BBB	36	48	48	0	0
4	CCC	24	32	32	6	0
4	DDD	24	32	32	2	0
4	EEE	30	40	40	2	0
4	FFF	18	24	24	0	0
4	GGG	24	32	32	1	0
4	HHH	36	48	48	3	0
4	III	24	32	32	0	0
4	JJJ	18	24	24	0	0
5	AAA	5	0	0	0	0
5	BBB	5	0	0	0	0
5	CCC	5	0	0	0	0
5	DDD	5	0	0	0	0
5	EEE	5	0	0	0	0
5	FFF	5	0	0	0	0
5	GGG	5	0	0	0	0
5	HHH	5	0	0	0	0
5	III	5	0	0	0	0
5	JJJ	5	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
6	EEE	1	0	0	0	0
6	FFF	1	0	0	0	0
6	GGG	1	0	0	0	0
6	HHH	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	III	1	0	0	0	0
6	JJJ	1	0	0	0	0
7	AAA	1	0	0	0	0
7	BBB	1	0	0	0	0
7	CCC	1	0	0	0	0
7	DDD	1	0	0	0	0
7	EEE	1	0	0	0	0
7	FFF	1	0	0	0	0
7	GGG	1	0	0	0	0
7	HHH	1	0	0	0	0
7	III	1	0	0	0	0
7	JJJ	1	0	0	0	0
8	AAA	310	0	0	4	0
8	BBB	315	0	0	5	0
8	CCC	291	0	0	7	0
8	DDD	312	0	0	7	0
8	EEE	284	0	0	5	0
8	FFF	278	0	0	7	0
8	GGG	282	0	0	3	1
8	HHH	288	0	0	6	0
8	III	273	0	0	2	0
8	JJJ	266	0	0	2	0
All	All	20697	17501	17396	111	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 111 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:BBB:110[B]:TYR:OH	8:BBB:401:HOH:O	1.81	0.98
1:EEE:110[B]:TYR:OH	8:EEE:4301:HOH:O	1.79	0.95
1:FFF:193[B]:ILE:HD11	1:FFF:219[B]:VAL:HG13	1.49	0.94
1:HHH:110[B]:TYR:OH	8:HHH:501:HOH:O	1.80	0.94
1:AAA:110[B]:TYR:OH	8:AAA:401:HOH:O	1.79	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:GGG:2731:HOH:O	8:GGG:2731:HOH:O[2_556]	1.42	0.78

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	AAA	221/249 (89%)	219 (99%)	2 (1%)	0	100	100
1	BBB	226/249 (91%)	224 (99%)	2 (1%)	0	100	100
1	CCC	217/249 (87%)	214 (99%)	3 (1%)	0	100	100
1	DDD	216/249 (87%)	214 (99%)	2 (1%)	0	100	100
1	EEE	218/249 (88%)	214 (98%)	4 (2%)	0	100	100
1	FFF	222/249 (89%)	219 (99%)	3 (1%)	0	100	100
1	GGG	213/249 (86%)	213 (100%)	0	0	100	100
1	HHH	216/249 (87%)	210 (97%)	6 (3%)	0	100	100
1	III	214/249 (86%)	213 (100%)	1 (0%)	0	100	100
1	JJJ	215/249 (86%)	213 (99%)	2 (1%)	0	100	100
All	All	2178/2490 (88%)	2153 (99%)	25 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	206/224 (92%)	200 (97%)	6 (3%)	42 22
1	BBB	211/224 (94%)	206 (98%)	5 (2%)	49 29
1	CCC	202/224 (90%)	196 (97%)	6 (3%)	41 21
1	DDD	201/224 (90%)	199 (99%)	2 (1%)	76 65
1	EEE	203/224 (91%)	197 (97%)	6 (3%)	41 21
1	FFF	207/224 (92%)	198 (96%)	9 (4%)	29 10
1	GGG	199/224 (89%)	190 (96%)	9 (4%)	27 9
1	HHH	201/224 (90%)	200 (100%)	1 (0%)	88 83
1	III	199/224 (89%)	195 (98%)	4 (2%)	55 37
1	JJJ	200/224 (89%)	195 (98%)	5 (2%)	47 27
All	All	2029/2240 (91%)	1976 (97%)	53 (3%)	52 26

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FFF	46[A]	LEU
1	GGG	36[A]	MET
1	JJJ	34	SER
1	FFF	46[B]	LEU
1	FFF	201[A]	GLN

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

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 91 ligands modelled in this entry, 20 are monoatomic - leaving 71 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	$\#\|Z\| > 2$
4	GOL	CCC	304	-	5,5,5	0.44	0	5,5,5	0.92	0
2	MXQ	FFF	301	-	19,20,20	0.74	0	23,28,28	0.73	0
2	MXQ	EEE	4202	-	19,20,20	0.84	1 (5%)	23,28,28	0.86	0
3	NAG	CCC	302	1	14,14,15	0.78	0	17,19,21	1.95	4 (23%)
4	GOL	FFF	303	-	5,5,5	0.40	0	5,5,5	0.77	0
3	NAG	BBB	302	1	14,14,15	1.28	2 (14%)	17,19,21	2.69	5 (29%)
4	GOL	CCC	305	-	5,5,5	0.16	0	5,5,5	0.68	0
4	GOL	BBB	303	-	5,5,5	0.19	0	5,5,5	0.84	0
4	GOL	BBB	305	-	5,5,5	0.24	0	5,5,5	0.55	0
4	GOL	BBB	307	-	5,5,5	0.13	0	5,5,5	0.49	0
5	PO4	AAA	304	-	4,4,4	1.19	1 (25%)	6,6,6	0.77	0
3	NAG	DDD	504	1	14,14,15	1.02	2 (14%)	17,19,21	2.69	5 (29%)
4	GOL	EEE	4204	-	5,5,5	0.19	0	5,5,5	0.73	0
4	GOL	DDD	501	-	5,5,5	0.21	0	5,5,5	0.36	0
4	GOL	DDD	502	-	5,5,5	0.15	0	5,5,5	0.40	0
4	GOL	GGG	2601	-	5,5,5	0.20	0	5,5,5	0.53	0
4	GOL	HHH	409	-	5,5,5	0.25	0	5,5,5	0.46	0
2	MXQ	AAA	301	-	19,20,20	0.97	1 (5%)	23,28,28	0.85	2 (8%)
3	NAG	JJJ	302	1	14,14,15	0.90	0	17,19,21	1.80	5 (29%)
2	MXQ	GGG	2602	-	19,20,20	0.65	0	23,28,28	0.75	1 (4%)
4	GOL	III	307	-	5,5,5	0.14	0	5,5,5	0.38	0
4	GOL	JJJ	303	-	5,5,5	0.22	0	5,5,5	0.54	0
2	MXQ	HHH	402	-	19,20,20	0.77	1 (5%)	23,28,28	0.90	2 (8%)
3	NAG	GGG	2603	1	14,14,15	1.13	0	17,19,21	2.38	7 (41%)
4	GOL	AAA	303	-	5,5,5	0.45	0	5,5,5	0.89	0
4	GOL	AAA	305	-	5,5,5	0.16	0	5,5,5	0.66	0
4	GOL	HHH	401	-	5,5,5	0.18	0	5,5,5	0.37	0
4	GOL	BBB	304	-	5,5,5	0.17	0	5,5,5	0.39	0
4	GOL	EEE	4207	-	5,5,5	0.20	0	5,5,5	0.41	0
4	GOL	DDD	506	-	5,5,5	0.17	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	III	306	-	5,5,5	0.33	0	5,5,5	0.91	0
4	GOL	GGG	2604	-	5,5,5	0.32	0	5,5,5	1.17	0
4	GOL	GGG	2605	-	5,5,5	0.36	0	5,5,5	0.78	0
2	MXQ	JJJ	301	-	19,20,20	0.55	0	23,28,28	0.62	0
4	GOL	JJJ	304	-	5,5,5	0.28	0	5,5,5	0.75	0
5	PO4	III	304	-	4,4,4	1.15	1 (25%)	6,6,6	0.79	0
4	GOL	EEE	4208	-	5,5,5	0.22	0	5,5,5	0.40	0
2	MXQ	BBB	301	-	19,20,20	0.66	0	23,28,28	0.77	0
4	GOL	HHH	405	-	5,5,5	0.48	0	5,5,5	0.82	0
5	PO4	DDD	505	-	4,4,4	0.70	0	6,6,6	0.54	0
5	PO4	FFF	305	-	4,4,4	1.14	1 (25%)	6,6,6	0.47	0
4	GOL	FFF	306	-	5,5,5	0.14	0	5,5,5	0.30	0
4	GOL	CCC	307	-	5,5,5	0.17	0	5,5,5	1.00	0
4	GOL	CCC	303	-	5,5,5	0.23	0	5,5,5	0.66	0
5	PO4	CCC	306	-	4,4,4	1.01	0	6,6,6	0.85	0
4	GOL	HHH	407	-	5,5,5	0.15	0	5,5,5	0.33	0
5	PO4	HHH	406	-	4,4,4	0.92	0	6,6,6	0.55	0
4	GOL	EEE	4205	-	5,5,5	0.18	0	5,5,5	0.66	0
3	NAG	III	302	1	14,14,15	0.84	1 (7%)	17,19,21	1.95	5 (29%)
3	NAG	FFF	302	1	14,14,15	0.70	0	17,19,21	1.69	4 (23%)
2	MXQ	DDD	503	-	19,20,20	0.78	0	23,28,28	0.72	0
4	GOL	BBB	308	-	5,5,5	0.24	0	5,5,5	0.57	0
4	GOL	III	303	-	5,5,5	0.25	0	5,5,5	0.44	0
4	GOL	EEE	4201	-	5,5,5	0.18	0	5,5,5	0.44	0
4	GOL	HHH	404	-	5,5,5	0.35	0	5,5,5	0.56	0
4	GOL	III	305	-	5,5,5	0.14	0	5,5,5	0.40	0
4	GOL	JJJ	306	-	5,5,5	0.13	0	5,5,5	0.31	0
5	PO4	BBB	306	-	4,4,4	1.04	0	6,6,6	0.56	0
2	MXQ	III	301	-	19,20,20	0.96	2 (10%)	23,28,28	1.03	2 (8%)
4	GOL	GGG	2606	-	5,5,5	0.20	0	5,5,5	0.52	0
3	NAG	HHH	403	1	14,14,15	0.96	0	17,19,21	2.20	7 (41%)
4	GOL	BBB	309	-	5,5,5	0.17	0	5,5,5	0.48	0
4	GOL	FFF	304	-	5,5,5	0.21	0	5,5,5	0.41	0
3	NAG	AAA	302	1	14,14,15	0.88	0	17,19,21	2.18	4 (23%)
4	GOL	HHH	408	-	5,5,5	0.12	0	5,5,5	0.34	0
5	PO4	GGG	2607	-	4,4,4	1.13	0	6,6,6	0.65	0
4	GOL	DDD	507	-	5,5,5	0.29	0	5,5,5	0.37	0
3	NAG	EEE	4203	1	14,14,15	0.63	0	17,19,21	2.09	6 (35%)
5	PO4	JJJ	305	-	4,4,4	1.40	1 (25%)	6,6,6	0.50	0
2	MXQ	CCC	301	-	19,20,20	0.91	1 (5%)	23,28,28	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	EEE	4206	-	4,4,4	1.34	1 (25%)	6,6,6	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	CCC	304	-	-	2/4/4/4	-
2	MXQ	FFF	301	-	-	0/4/22/22	0/4/3/3
2	MXQ	EEE	4202	-	-	0/4/22/22	0/4/3/3
3	NAG	CCC	302	1	-	2/6/23/26	0/1/1/1
4	GOL	FFF	303	-	-	2/4/4/4	-
3	NAG	BBB	302	1	-	1/6/23/26	0/1/1/1
4	GOL	CCC	305	-	-	2/4/4/4	-
4	GOL	BBB	303	-	-	4/4/4/4	-
4	GOL	BBB	305	-	-	2/4/4/4	-
4	GOL	BBB	307	-	-	2/4/4/4	-
3	NAG	DDD	504	1	-	1/6/23/26	0/1/1/1
4	GOL	EEE	4204	-	-	3/4/4/4	-
4	GOL	DDD	501	-	-	0/4/4/4	-
4	GOL	DDD	502	-	-	2/4/4/4	-
4	GOL	GGG	2601	-	-	3/4/4/4	-
4	GOL	HHH	409	-	-	3/4/4/4	-
2	MXQ	AAA	301	-	-	0/4/22/22	0/4/3/3
3	NAG	JJJ	302	1	-	1/6/23/26	0/1/1/1
2	MXQ	GGG	2602	-	-	0/4/22/22	0/4/3/3
4	GOL	III	307	-	-	2/4/4/4	-
4	GOL	JJJ	303	-	-	0/4/4/4	-
2	MXQ	HHH	402	-	-	0/4/22/22	0/4/3/3
3	NAG	GGG	2603	1	-	4/6/23/26	0/1/1/1
4	GOL	AAA	303	-	-	2/4/4/4	-
4	GOL	AAA	305	-	-	2/4/4/4	-
4	GOL	HHH	401	-	-	0/4/4/4	-
4	GOL	BBB	304	-	-	2/4/4/4	-
4	GOL	EEE	4207	-	-	2/4/4/4	-
4	GOL	DDD	506	-	-	2/4/4/4	-
4	GOL	III	306	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	GGG	2604	-	-	2/4/4/4	-
4	GOL	GGG	2605	-	-	2/4/4/4	-
2	MXQ	JJJ	301	-	-	0/4/22/22	0/4/3/3
4	GOL	JJJ	304	-	-	2/4/4/4	-
4	GOL	EEE	4208	-	-	3/4/4/4	-
2	MXQ	BBB	301	-	-	0/4/22/22	0/4/3/3
4	GOL	HHH	405	-	-	2/4/4/4	-
4	GOL	FFF	306	-	-	2/4/4/4	-
4	GOL	CCC	307	-	-	4/4/4/4	-
4	GOL	CCC	303	-	-	4/4/4/4	-
4	GOL	HHH	407	-	-	0/4/4/4	-
4	GOL	EEE	4205	-	-	2/4/4/4	-
3	NAG	III	302	1	-	3/6/23/26	0/1/1/1
3	NAG	FFF	302	1	-	2/6/23/26	0/1/1/1
2	MXQ	DDD	503	-	-	0/4/22/22	0/4/3/3
4	GOL	BBB	308	-	-	2/4/4/4	-
4	GOL	III	303	-	-	2/4/4/4	-
4	GOL	EEE	4201	-	-	1/4/4/4	-
4	GOL	HHH	404	-	-	0/4/4/4	-
4	GOL	III	305	-	-	2/4/4/4	-
4	GOL	JJJ	306	-	-	0/4/4/4	-
2	MXQ	III	301	-	-	0/4/22/22	0/4/3/3
4	GOL	GGG	2606	-	-	2/4/4/4	-
3	NAG	HHH	403	1	-	4/6/23/26	0/1/1/1
4	GOL	BBB	309	-	-	2/4/4/4	-
4	GOL	FFF	304	-	-	4/4/4/4	-
3	NAG	AAA	302	1	-	2/6/23/26	0/1/1/1
4	GOL	HHH	408	-	-	0/4/4/4	-
4	GOL	DDD	507	-	-	2/4/4/4	-
3	NAG	EEE	4203	1	-	3/6/23/26	0/1/1/1
2	MXQ	CCC	301	-	-	0/4/22/22	0/4/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	301	MXQ	C2-N3	2.98	1.45	1.40
5	JJJ	305	PO4	P-O1	2.72	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	III	301	MXQ	C2-N3	2.49	1.44	1.40
5	EEE	4206	PO4	P-O1	2.38	1.56	1.50
3	BBB	302	NAG	O5-C1	2.35	1.47	1.43

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	302	NAG	C1-O5-C5	8.84	124.17	112.19
3	DDD	504	NAG	C1-O5-C5	8.56	123.79	112.19
3	AAA	302	NAG	C1-O5-C5	5.72	119.94	112.19
3	GGG	2603	NAG	C1-O5-C5	5.61	119.79	112.19
3	III	302	NAG	C1-O5-C5	4.97	118.93	112.19

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	303	GOL	C1-C2-C3-O3
4	AAA	303	GOL	O2-C2-C3-O3
4	BBB	303	GOL	O1-C1-C2-C3
4	BBB	303	GOL	C1-C2-C3-O3
4	BBB	303	GOL	O2-C2-C3-O3

There are no ring outliers.

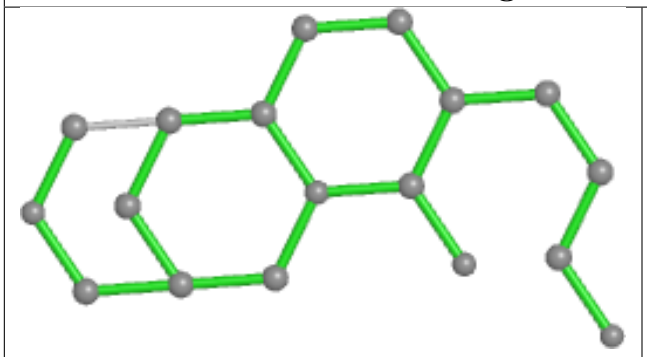
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	302	NAG	1	0
4	EEE	4204	GOL	1	0
4	DDD	501	GOL	1	0
4	HHH	401	GOL	1	0
4	EEE	4207	GOL	1	0
4	GGG	2604	GOL	1	0
4	CCC	307	GOL	1	0
4	CCC	303	GOL	5	0
4	HHH	404	GOL	2	0
4	DDD	507	GOL	1	0

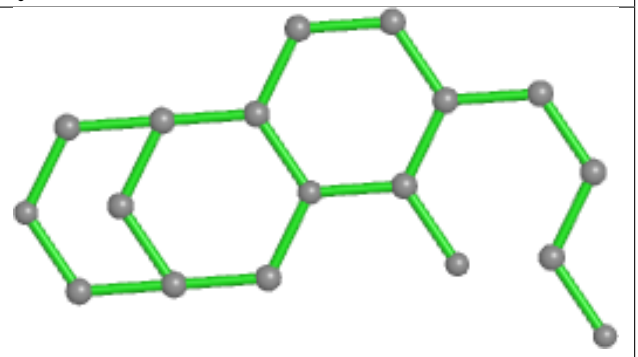
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

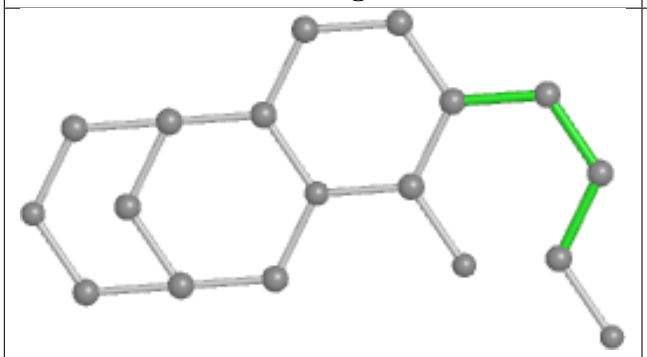
Ligand MXQ FFF 301



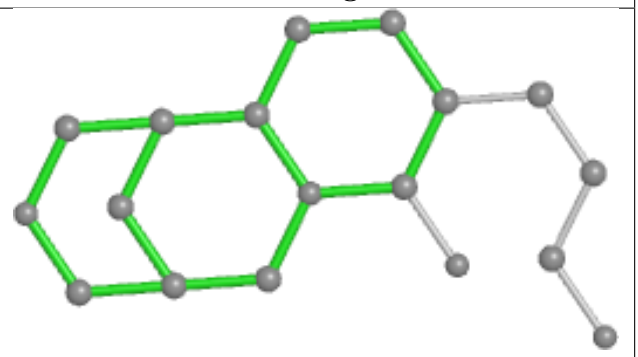
Bond lengths



Bond angles

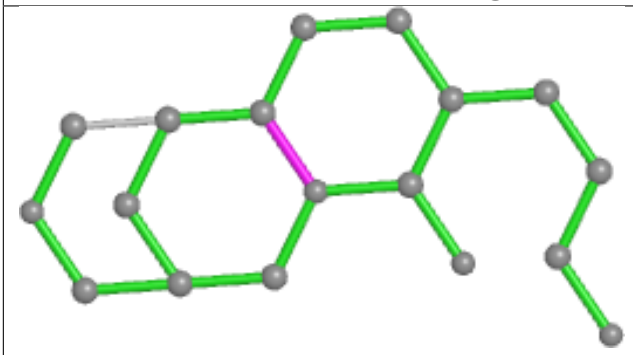


Torsions

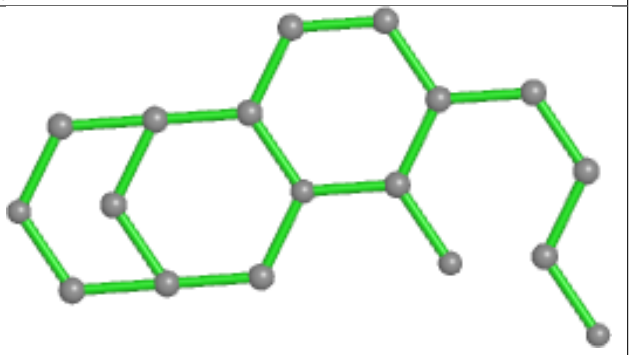


Rings

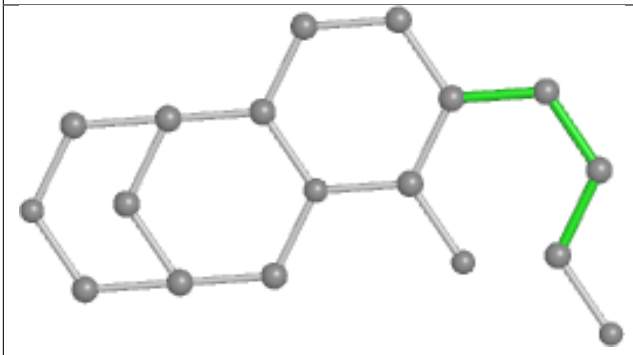
Ligand MXQ EEE 4202



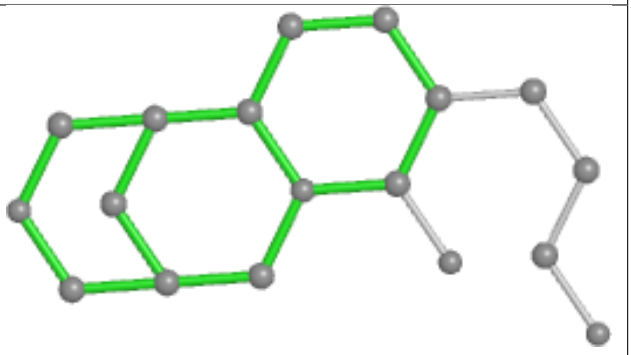
Bond lengths



Bond angles

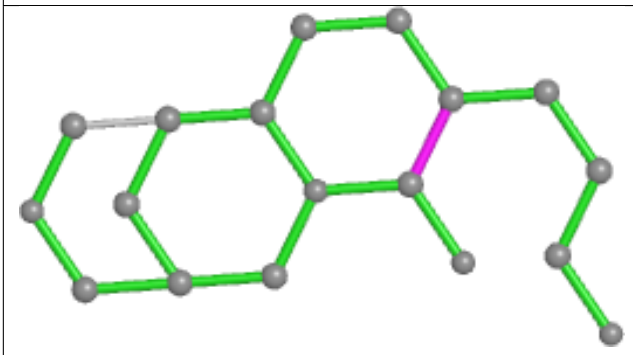


Torsions

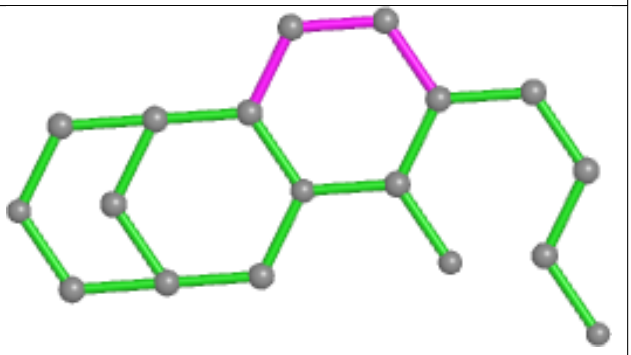


Rings

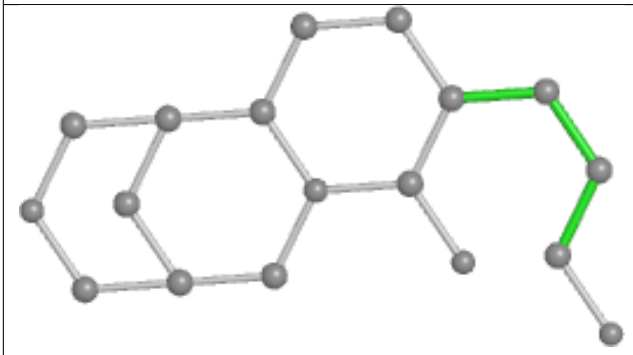
Ligand MXQ AAA 301



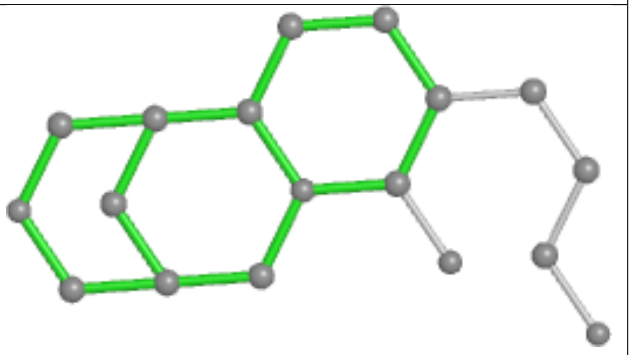
Bond lengths



Bond angles

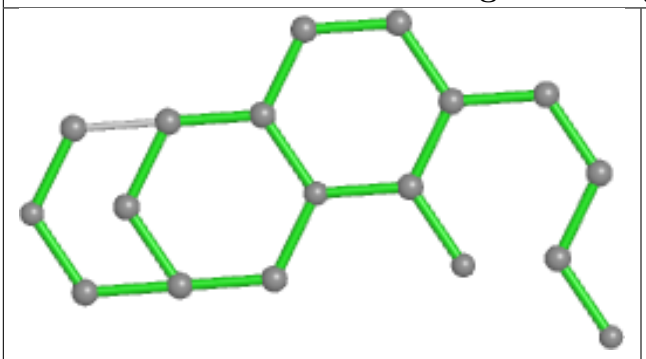


Torsions

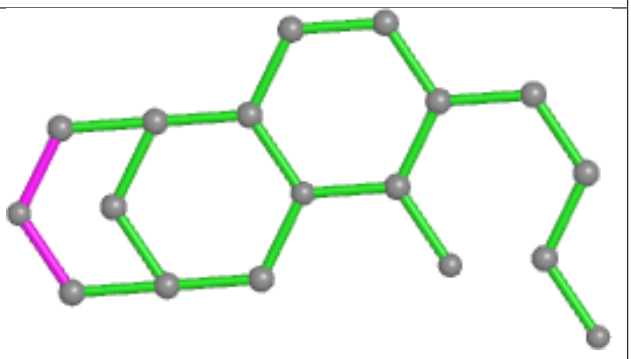


Rings

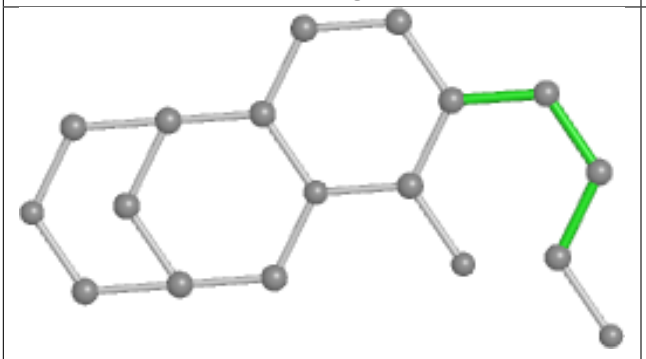
Ligand MXQ GGG 2602



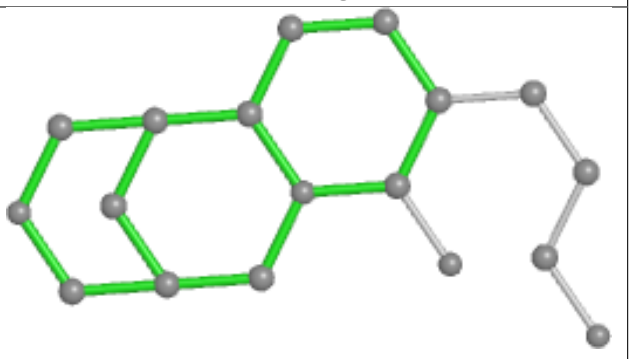
Bond lengths



Bond angles

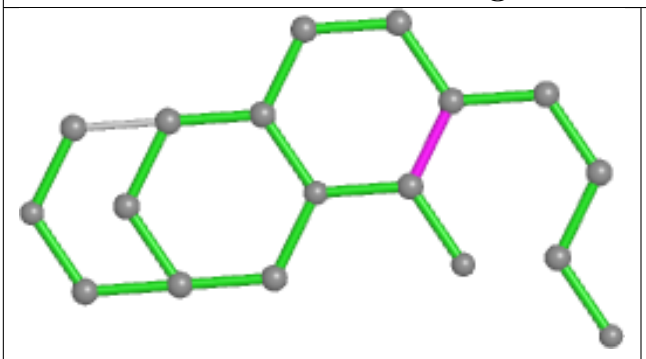


Torsions

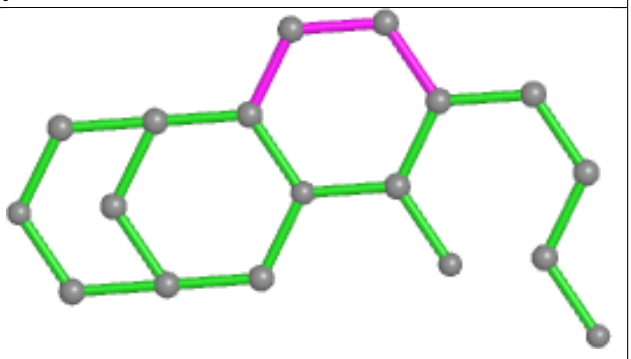


Rings

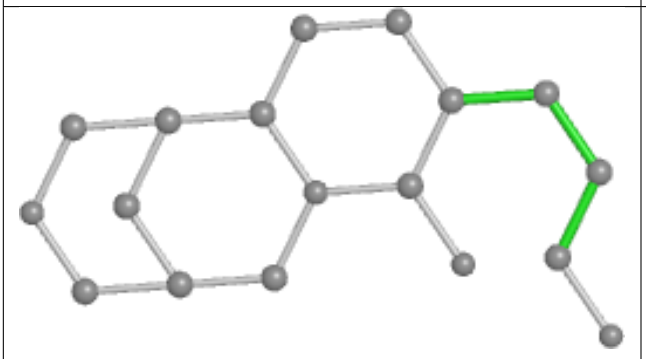
Ligand MXQ HHH 402



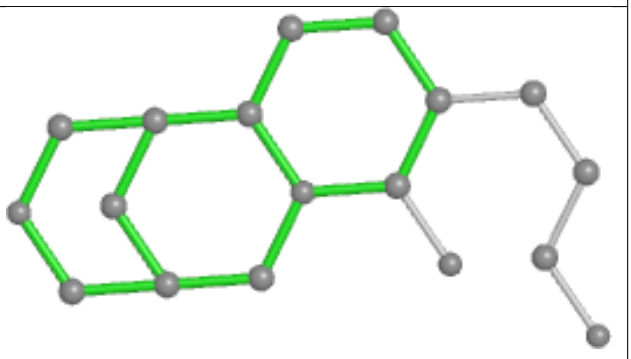
Bond lengths



Bond angles

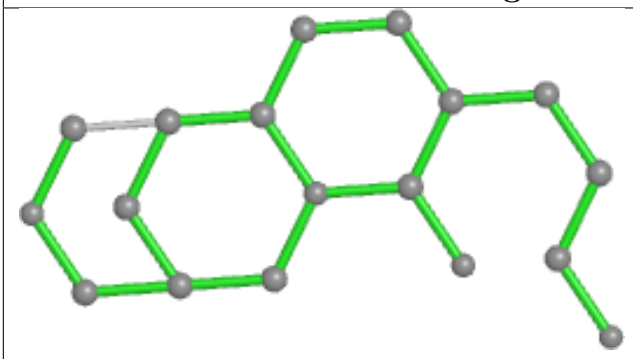


Torsions

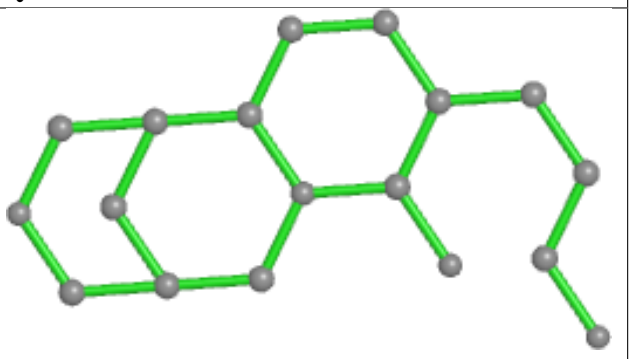


Rings

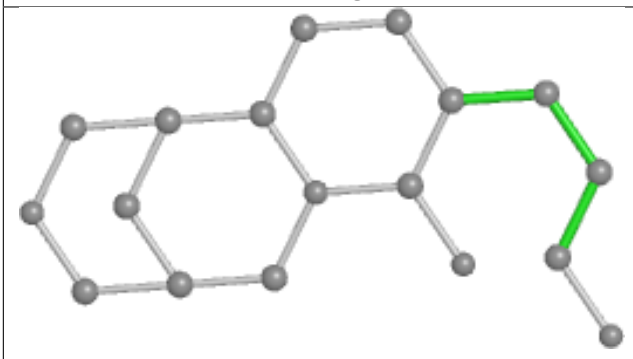
Ligand MXQ JJJ 301



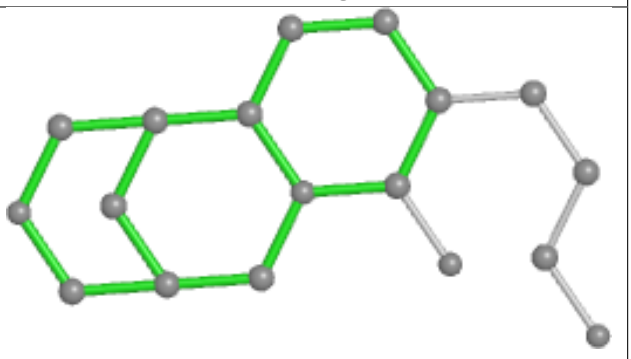
Bond lengths



Bond angles

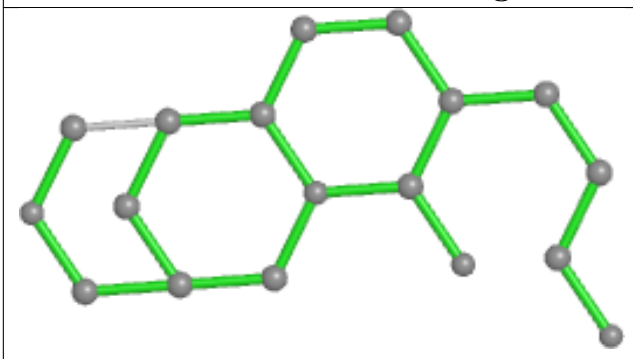


Torsions

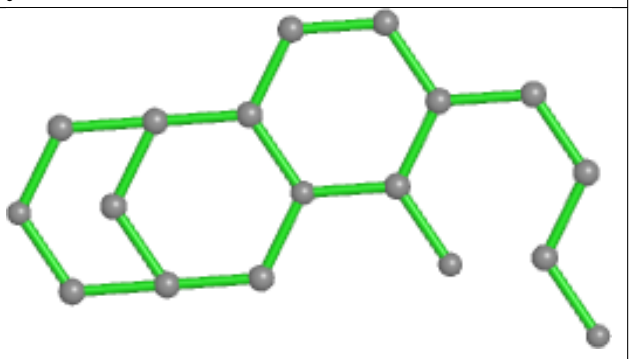


Rings

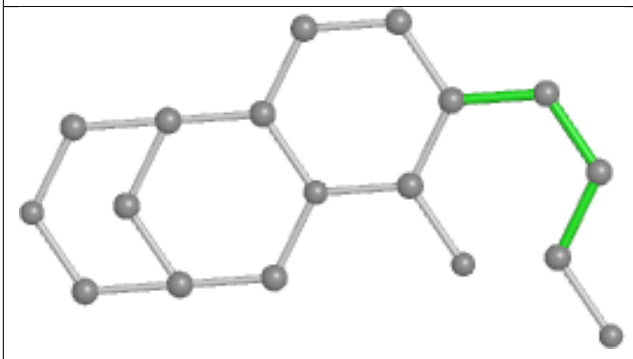
Ligand MXQ BBB 301



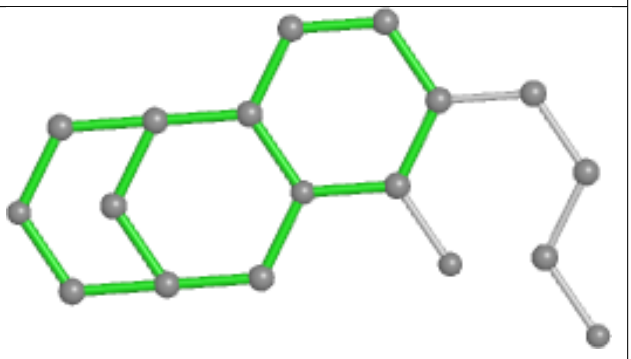
Bond lengths



Bond angles

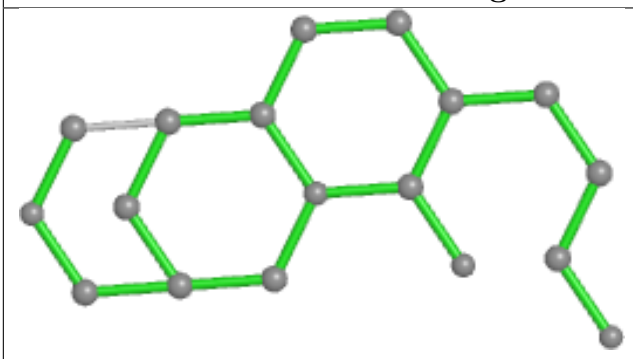


Torsions

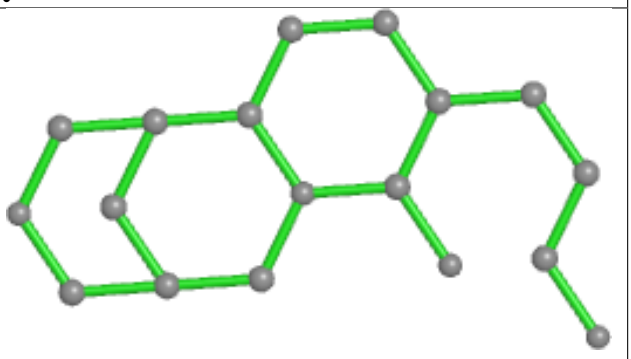


Rings

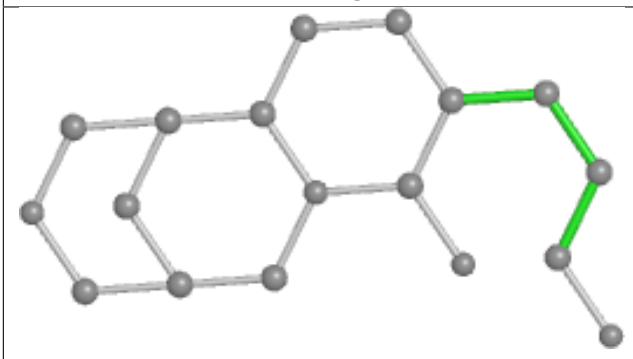
Ligand MXQ DDD 503



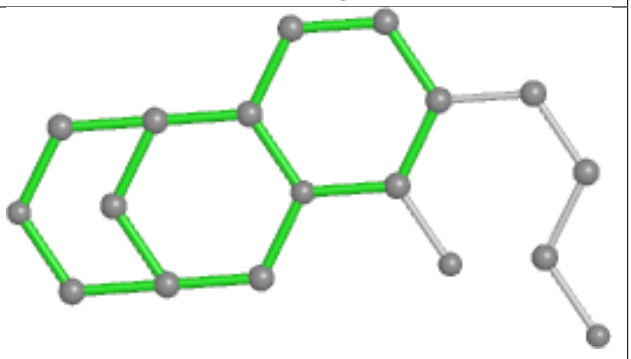
Bond lengths



Bond angles

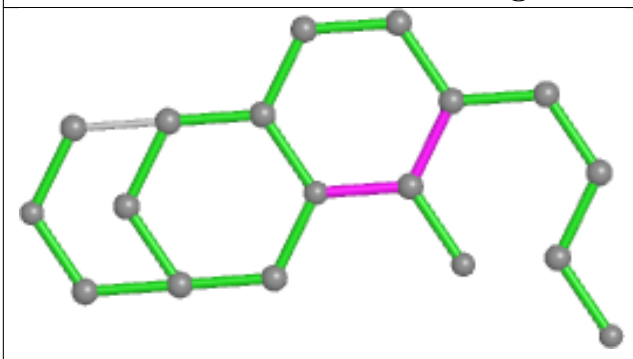


Torsions

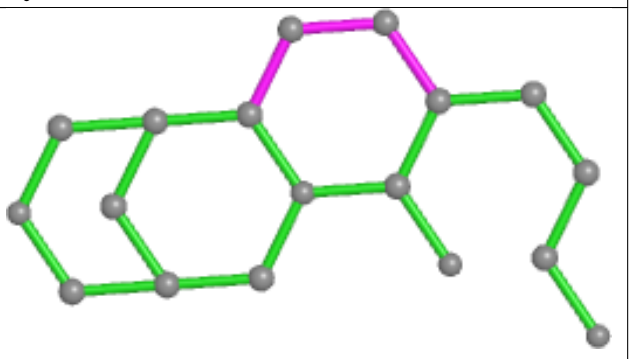


Rings

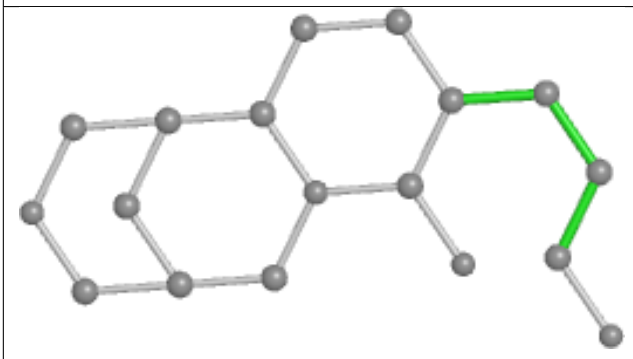
Ligand MXQ III 301



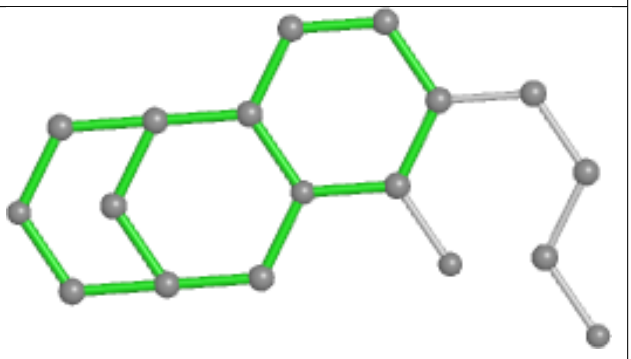
Bond lengths



Bond angles

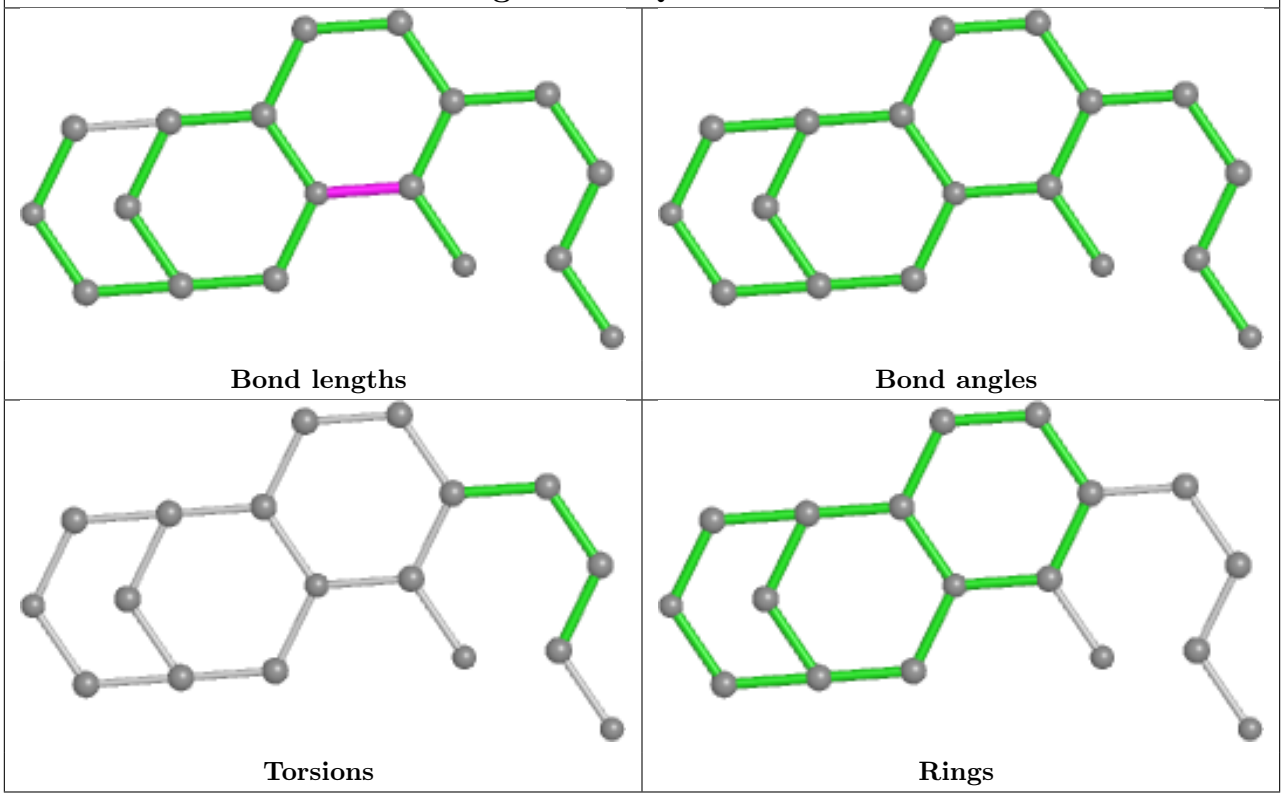


Torsions



Rings

Ligand MXQ CCC 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	AAA	205/249 (82%)	-0.04	3 (1%) 73 78	19, 27, 44, 70	0
1	BBB	212/249 (85%)	0.09	6 (2%) 53 57	18, 25, 51, 84	0
1	CCC	206/249 (82%)	-0.01	3 (1%) 73 78	19, 26, 50, 84	0
1	DDD	205/249 (82%)	-0.02	2 (0%) 82 85	19, 26, 46, 74	0
1	EEE	205/249 (82%)	0.00	3 (1%) 73 78	20, 27, 49, 84	0
1	FFF	205/249 (82%)	-0.07	0 100 100	20, 27, 48, 71	0
1	GGG	205/249 (82%)	-0.04	4 (1%) 65 69	20, 28, 45, 89	0
1	HHH	205/249 (82%)	-0.09	1 (0%) 91 92	22, 29, 48, 69	0
1	III	205/249 (82%)	-0.04	3 (1%) 73 78	23, 30, 52, 96	0
1	JJJ	205/249 (82%)	-0.07	1 (0%) 91 92	22, 31, 53, 81	0
All	All	2058/2490 (82%)	-0.03	26 (1%) 77 81	18, 28, 50, 96	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	232	ARG	5.9
1	BBB	231	PHE	4.1
1	III	34	SER	3.7
1	JJJ	33	ARG	3.6
1	GGG	33	ARG	3.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

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, 95^{th} 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	GGG	2603	14/15	0.43	0.25	90,104,113,114	3
3	NAG	BBB	302	14/15	0.57	0.33	69,90,106,110	3
4	GOL	GGG	2606	6/6	0.60	0.28	60,71,90,90	2
3	NAG	AAA	302	14/15	0.62	0.22	65,94,103,106	3
3	NAG	CCC	302	14/15	0.62	0.28	73,108,127,129	3
3	NAG	JJJ	302	14/15	0.63	0.21	81,91,102,103	3
3	NAG	DDD	504	14/15	0.63	0.17	73,86,96,100	3
3	NAG	FFF	302	14/15	0.64	0.24	73,97,113,122	3
4	GOL	III	307	6/6	0.66	0.26	79,91,97,97	2
4	GOL	BBB	308	6/6	0.67	0.23	62,68,78,78	2
4	GOL	DDD	506	6/6	0.68	0.24	69,75,87,87	2
3	NAG	HHH	403	14/15	0.70	0.27	90,103,113,116	3
4	GOL	CCC	305	6/6	0.72	0.24	62,69,74,74	2
3	NAG	EEE	4203	14/15	0.72	0.22	82,99,107,125	3
3	NAG	III	302	14/15	0.74	0.24	88,99,108,112	3
4	GOL	FFF	304	6/6	0.76	0.24	54,64,69,69	2
4	GOL	BBB	305	6/6	0.77	0.21	63,70,76,76	2
4	GOL	HHH	409	6/6	0.78	0.30	56,63,66,66	2
4	GOL	BBB	303	6/6	0.79	0.13	45,48,62,62	2
4	GOL	CCC	307	6/6	0.80	0.22	57,65,69,69	2
4	GOL	CCC	303	6/6	0.81	0.16	47,54,68,68	2
4	GOL	EEE	4208	6/6	0.81	0.29	53,61,70,70	2
4	GOL	EEE	4207	6/6	0.82	0.22	53,56,63,63	2
4	GOL	BBB	307	6/6	0.82	0.29	69,75,90,90	2
4	GOL	JJJ	303	6/6	0.82	0.14	49,56,61,61	2
4	GOL	HHH	407	6/6	0.84	0.41	55,68,76,76	2
4	GOL	GGG	2604	6/6	0.85	0.18	42,49,70,70	2
4	GOL	EEE	4201	6/6	0.86	0.17	46,54,73,73	2
4	GOL	HHH	405	6/6	0.87	0.20	36,50,65,65	2
4	GOL	III	305	6/6	0.88	0.28	60,80,99,99	2
4	GOL	AAA	303	6/6	0.88	0.11	38,49,62,62	2
4	GOL	DDD	501	6/6	0.88	0.16	42,51,55,55	2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	CCC	304	6/6	0.89	0.16	37,46,55,55	2
4	GOL	HHH	408	6/6	0.89	0.20	54,65,83,83	2
4	GOL	GGG	2605	6/6	0.90	0.14	38,51,66,66	2
4	GOL	FFF	306	6/6	0.90	0.19	56,67,70,70	2
4	GOL	AAA	305	6/6	0.90	0.22	55,61,70,70	2
4	GOL	JJJ	306	6/6	0.90	0.12	53,61,66,66	2
4	GOL	HHH	401	6/6	0.91	0.13	39,50,63,63	2
4	GOL	HHH	404	6/6	0.91	0.15	42,46,51,51	2
4	GOL	BBB	309	6/6	0.91	0.28	40,70,82,82	2
4	GOL	DDD	502	6/6	0.91	0.18	40,55,70,70	2
4	GOL	JJJ	304	6/6	0.91	0.17	34,48,54,54	2
4	GOL	GGG	2601	6/6	0.91	0.24	47,64,74,74	2
4	GOL	EEE	4204	6/6	0.92	0.17	46,52,61,61	2
4	GOL	III	306	6/6	0.92	0.19	39,48,54,54	2
4	GOL	III	303	6/6	0.92	0.15	52,55,68,68	2
5	PO4	HHH	406	5/5	0.92	0.20	63,64,76,77	0
4	GOL	DDD	507	6/6	0.93	0.20	34,55,66,66	2
4	GOL	FFF	303	6/6	0.93	0.12	30,45,62,62	2
4	GOL	EEE	4205	6/6	0.94	0.22	34,47,71,71	2
4	GOL	BBB	304	6/6	0.94	0.17	38,45,62,62	2
5	PO4	JJJ	305	5/5	0.94	0.13	43,56,65,66	0
5	PO4	DDD	505	5/5	0.95	0.17	46,61,71,74	0
5	PO4	GGG	2607	5/5	0.95	0.11	46,54,61,64	0
2	MXQ	III	301	18/18	0.95	0.11	28,33,38,38	1
5	PO4	AAA	304	5/5	0.95	0.14	45,55,61,66	0
5	PO4	EEE	4206	5/5	0.96	0.15	38,50,50,56	0
2	MXQ	FFF	301	18/18	0.96	0.08	25,30,33,35	1
5	PO4	CCC	306	5/5	0.96	0.15	44,55,65,65	0
2	MXQ	HHH	402	18/18	0.96	0.10	28,32,39,39	1
2	MXQ	BBB	301	18/18	0.97	0.09	24,27,32,33	1
2	MXQ	EEE	4202	18/18	0.97	0.09	24,27,33,33	1
5	PO4	FFF	305	5/5	0.97	0.12	37,50,53,53	0
2	MXQ	JJJ	301	18/18	0.97	0.07	27,30,38,38	1
5	PO4	BBB	306	5/5	0.97	0.15	47,53,55,60	0
5	PO4	III	304	5/5	0.97	0.14	44,46,57,60	0
2	MXQ	AAA	301	18/18	0.97	0.08	23,27,31,32	1
7	K	III	309	1/1	0.97	0.06	43,43,43,43	0
2	MXQ	GGG	2602	18/18	0.98	0.09	21,23,28,30	1
2	MXQ	CCC	301	18/18	0.98	0.08	20,22,28,28	1
6	CL	BBB	310	1/1	0.98	0.08	34,34,34,34	0
6	CL	GGG	2608	1/1	0.98	0.08	37,37,37,37	0
6	CL	III	308	1/1	0.98	0.08	35,35,35,35	0

Continued on next page...

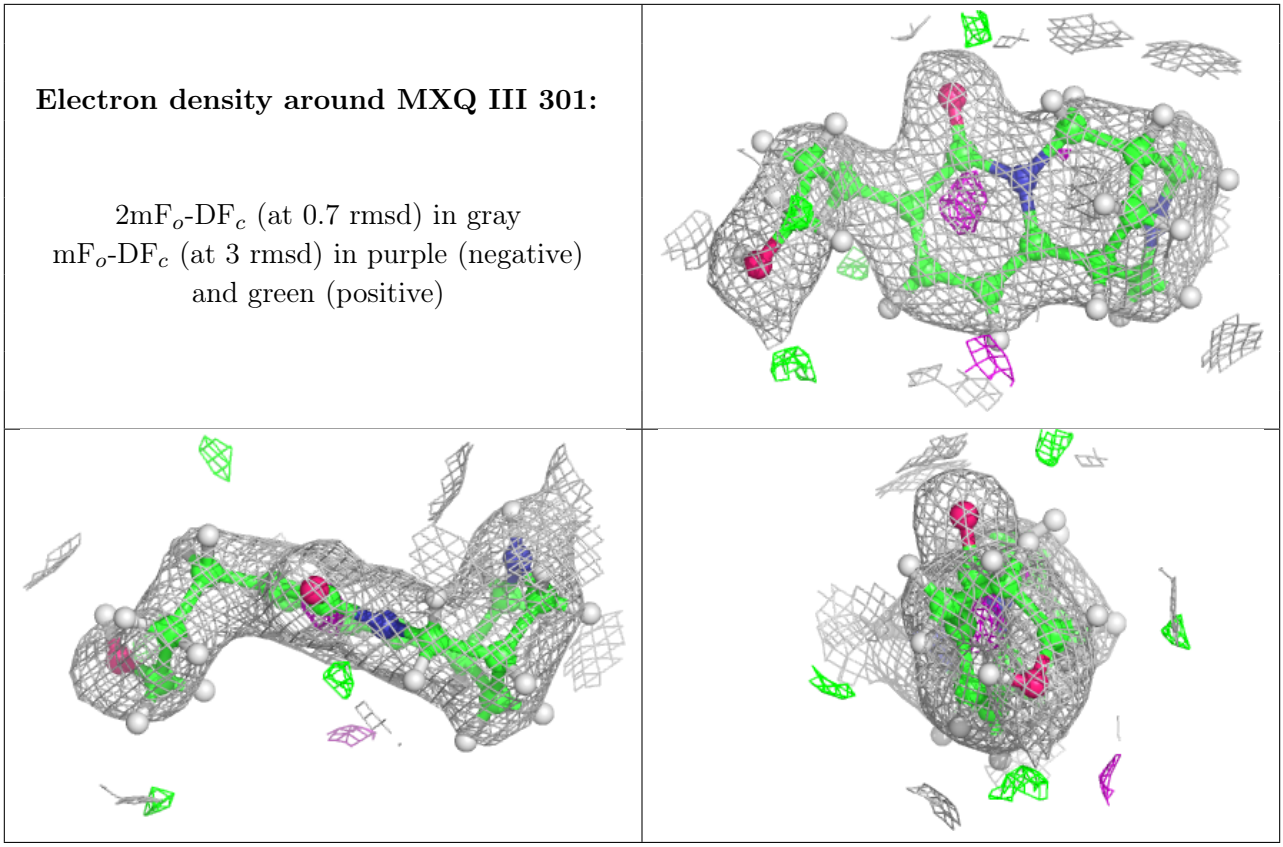
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CL	JJJ	307	1/1	0.98	0.09	37,37,37,37	0
7	K	GGG	2609	1/1	0.98	0.07	41,41,41,41	0
2	MXQ	DDD	503	18/18	0.98	0.08	17,21,27,30	1
6	CL	HHH	410	1/1	0.99	0.07	35,35,35,35	0
6	CL	CCC	308	1/1	0.99	0.09	31,31,31,31	0
6	CL	EEE	4209	1/1	0.99	0.09	33,33,33,33	0
7	K	AAA	307	1/1	0.99	0.06	37,37,37,37	0
7	K	BBB	311	1/1	0.99	0.07	37,37,37,37	0
7	K	CCC	309	1/1	0.99	0.08	38,38,38,38	0
7	K	DDD	509	1/1	0.99	0.06	40,40,40,40	0
7	K	FFF	308	1/1	0.99	0.07	40,40,40,40	0
6	CL	FFF	307	1/1	0.99	0.10	34,34,34,34	0
6	CL	AAA	306	1/1	0.99	0.06	33,33,33,33	0
7	K	JJJ	308	1/1	0.99	0.08	44,44,44,44	0
7	K	HHH	411	1/1	1.00	0.07	40,40,40,40	0
6	CL	DDD	508	1/1	1.00	0.09	32,32,32,32	0
7	K	EEE	4210	1/1	1.00	0.09	39,39,39,39	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.

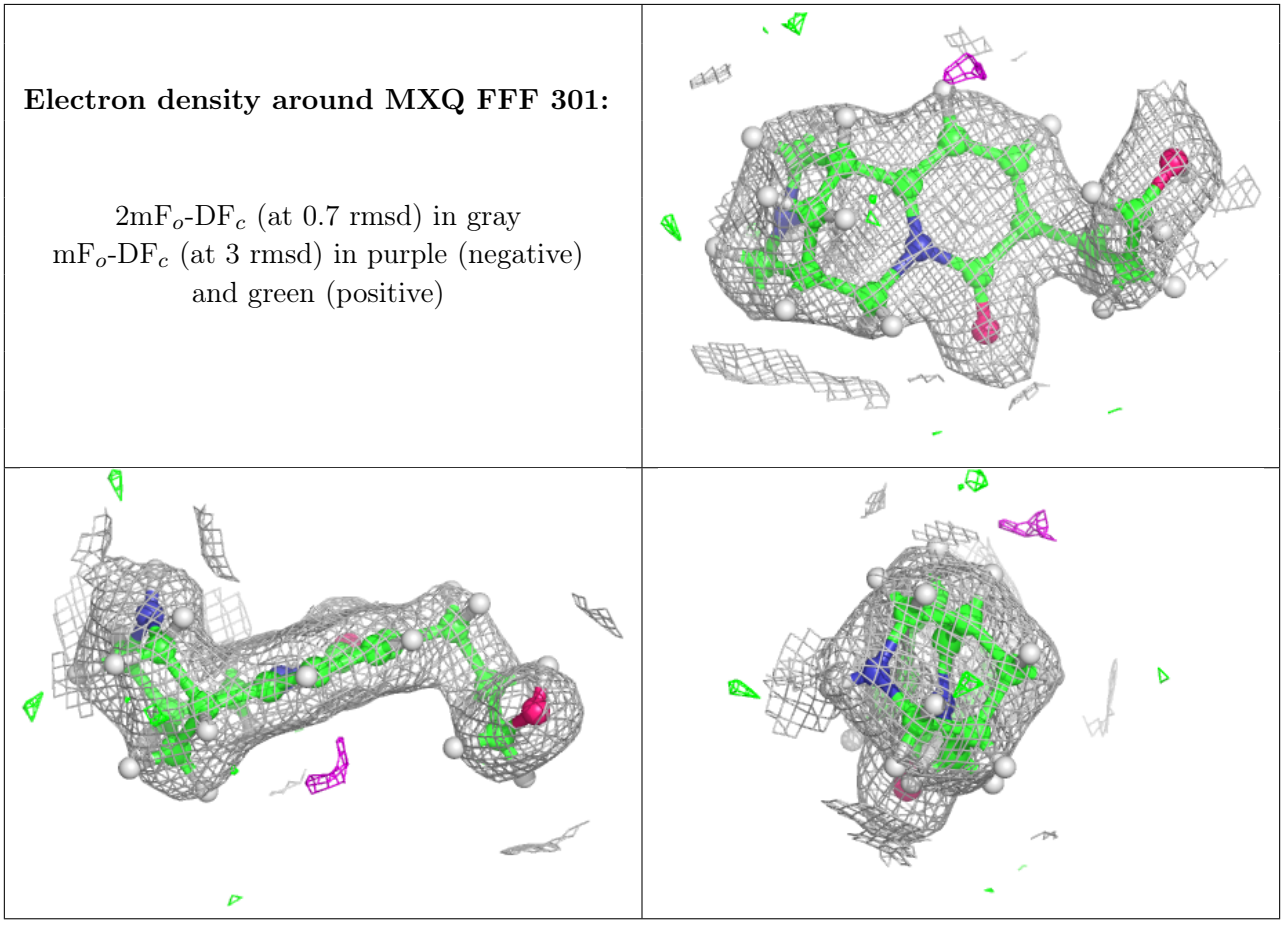
Electron density around MXQ III 301:

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



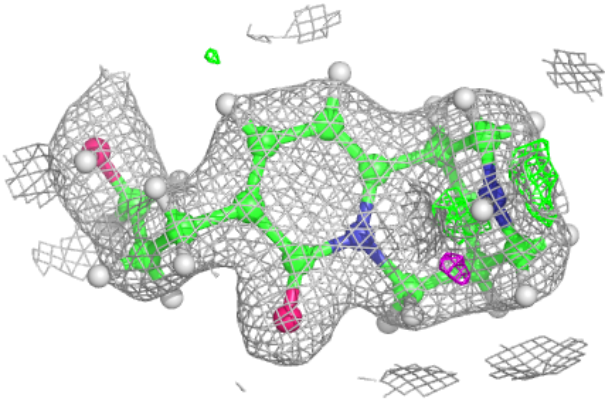
Electron density around MXQ FFF 301:

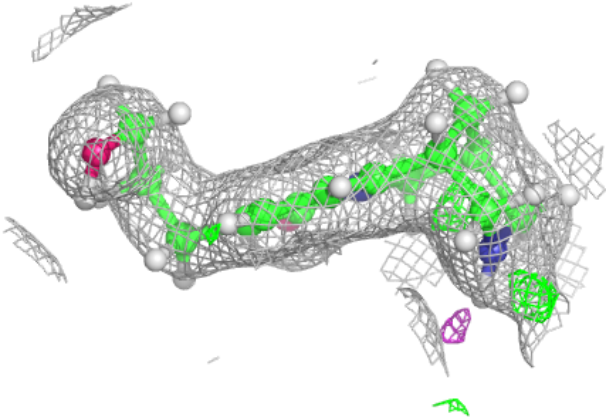
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

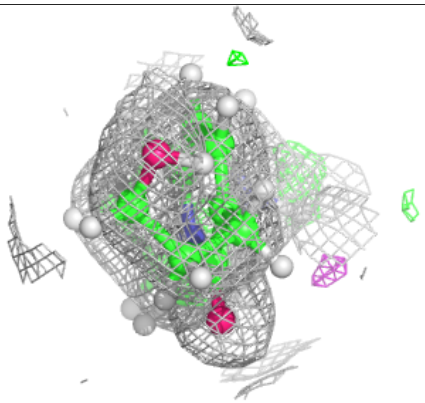


Electron density around MXQ HHH 402:

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

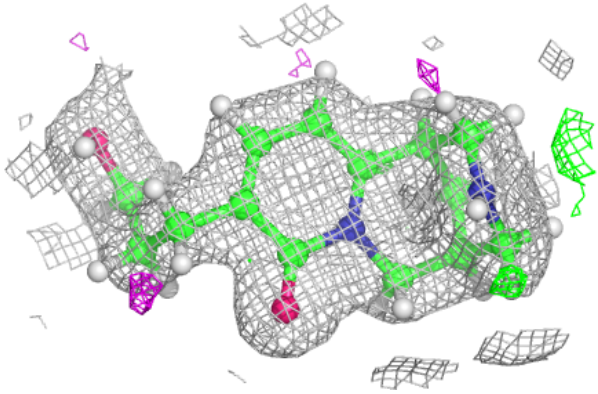


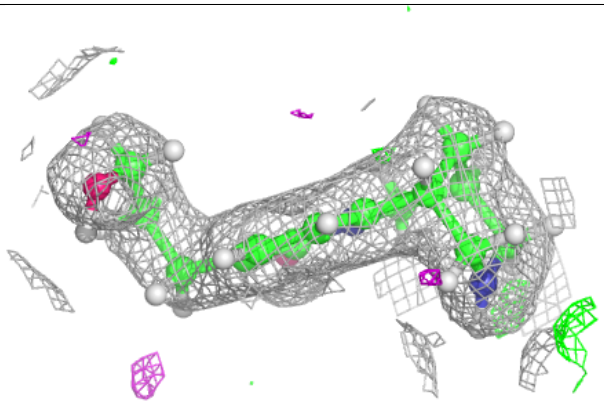


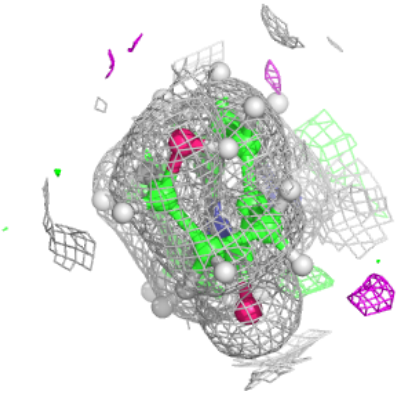


Electron density around MXQ BBB 301:

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

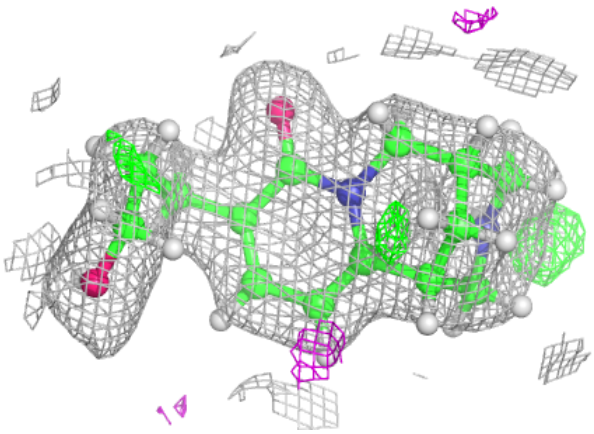


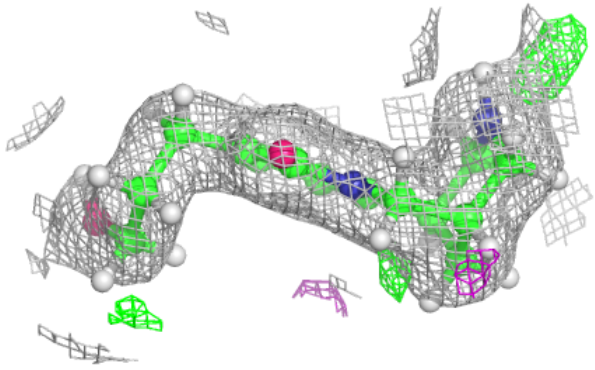


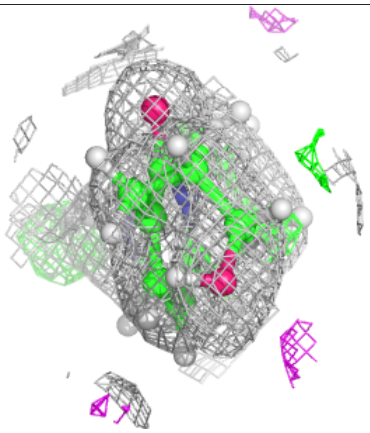


Electron density around MXQ EEE 4202:

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

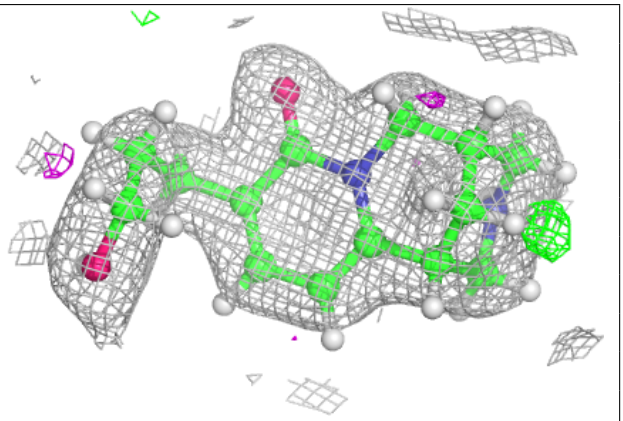


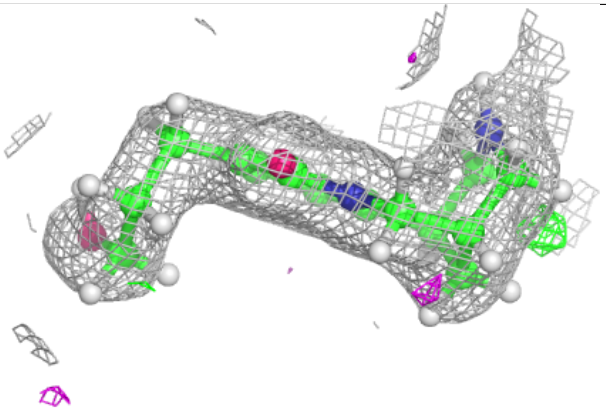


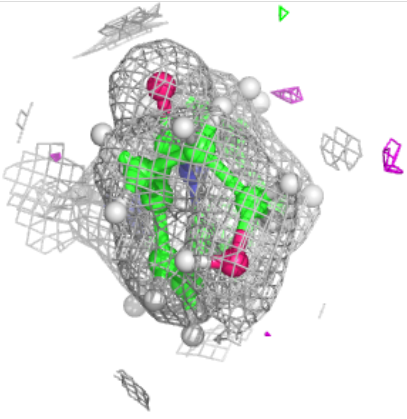


Electron density around MXQ JJJ 301:

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

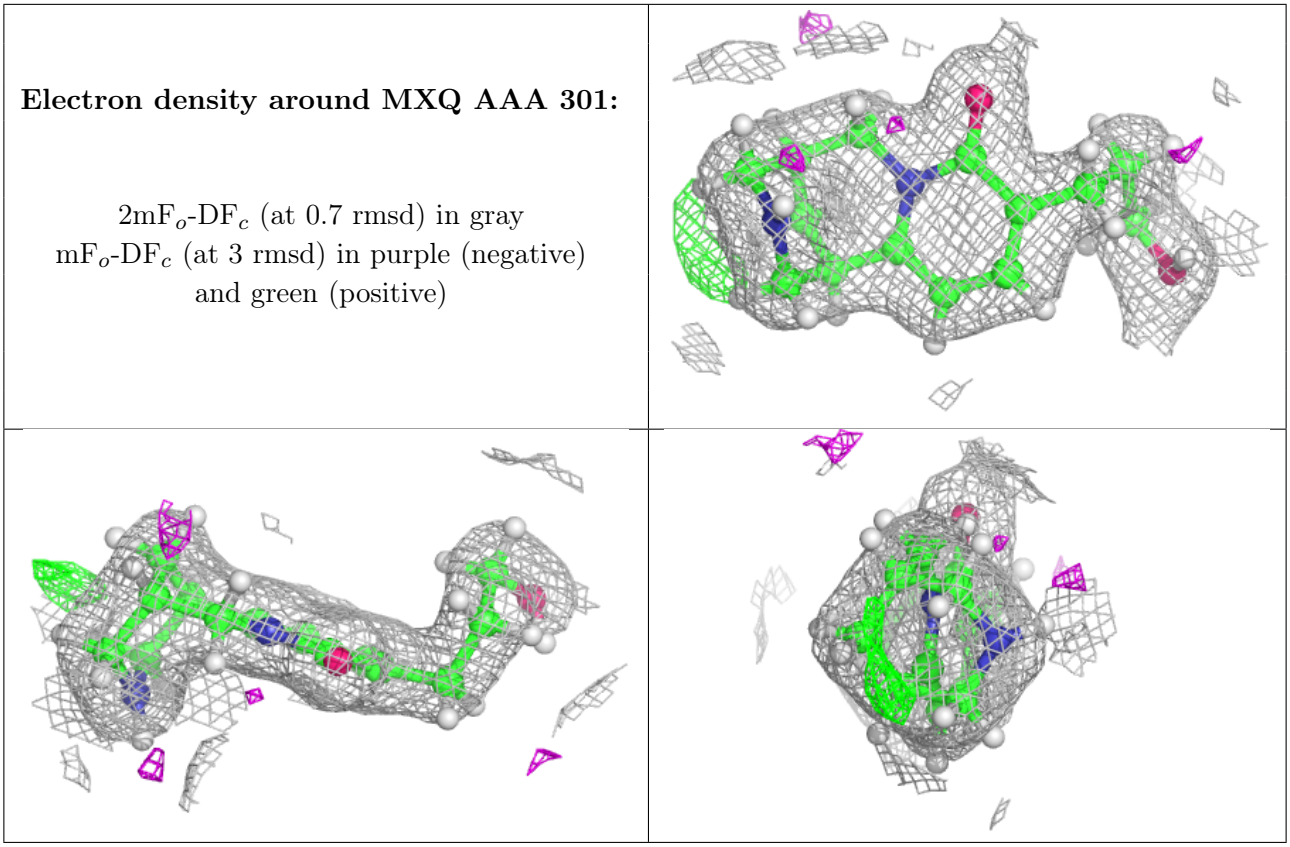






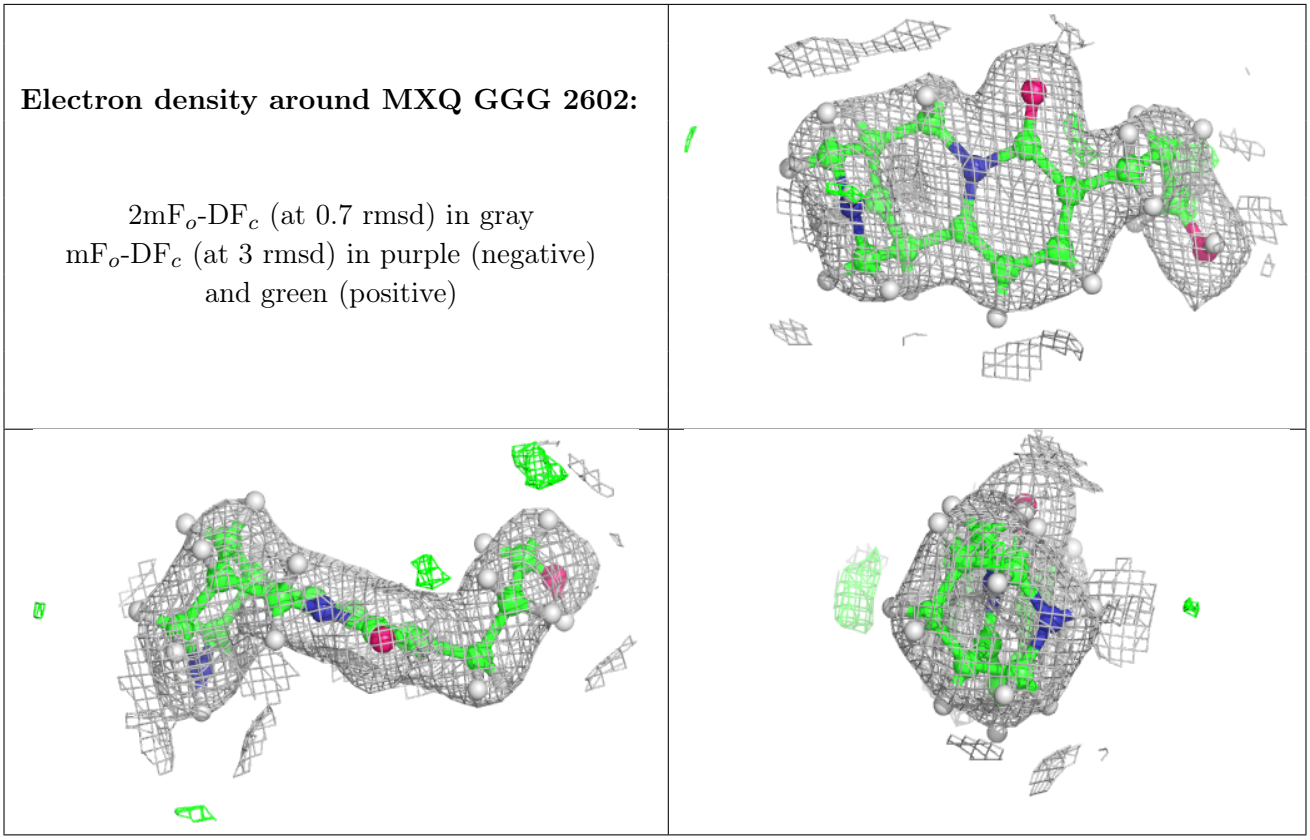
Electron density around MXQ AAA 301:

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



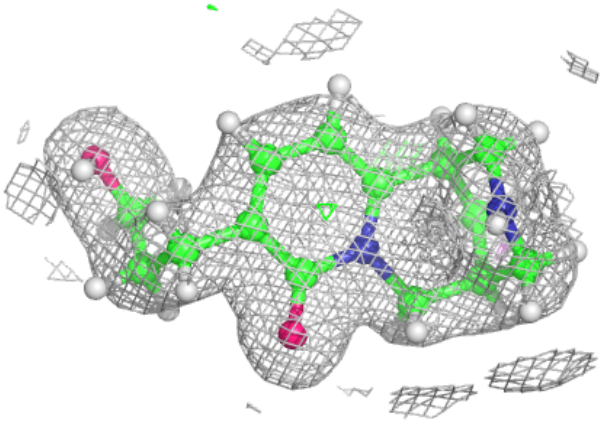
Electron density around MXQ GGG 2602:

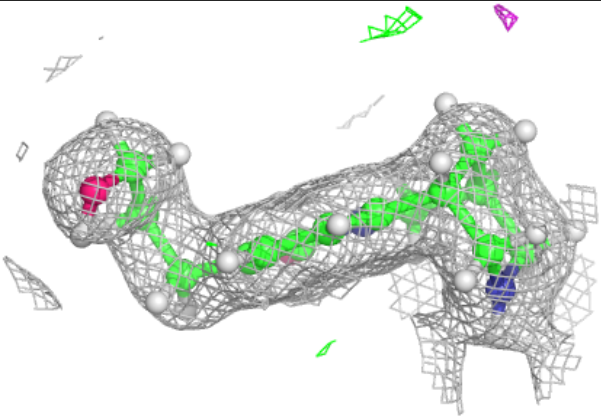
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

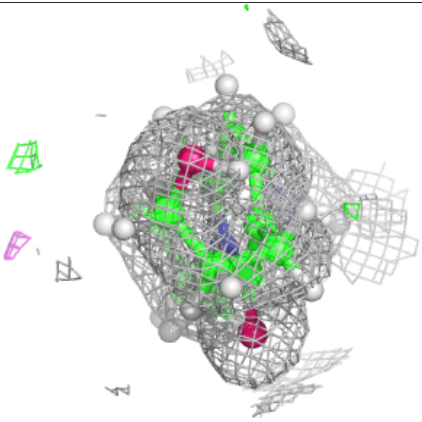


Electron density around MXQ CCC 301:

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

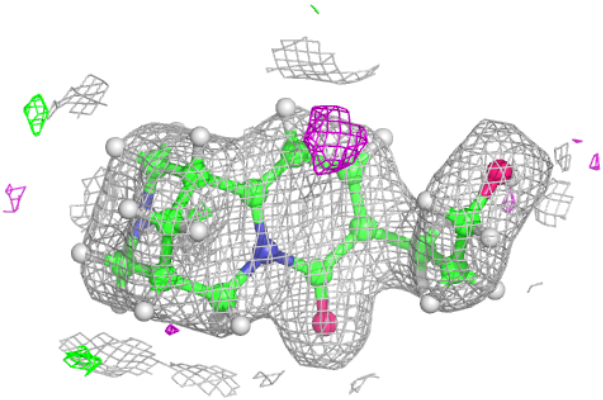


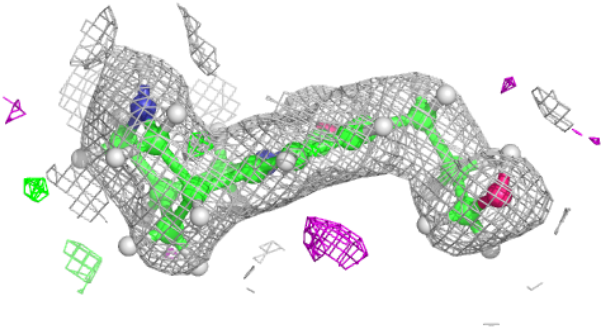


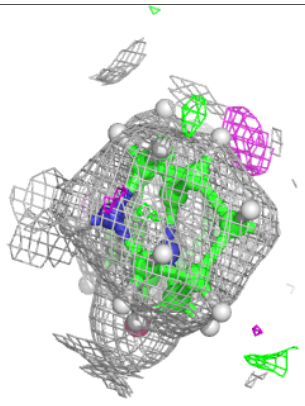


Electron density around MXQ DDD 503:

$2mF_o$-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.