Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2024 – 02:38 pm GMT

PDB ID	:	8RQQ
Title	:	In meso structure of the adenosine A2a G protein-coupled receptor, A2aR, in 7.10 monoacylglycerol
Authors	:	Smithers, L.; Krawinski, P.; Caffrey, M.
Deposited on	:	2024-01-19
Resolution	:	2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

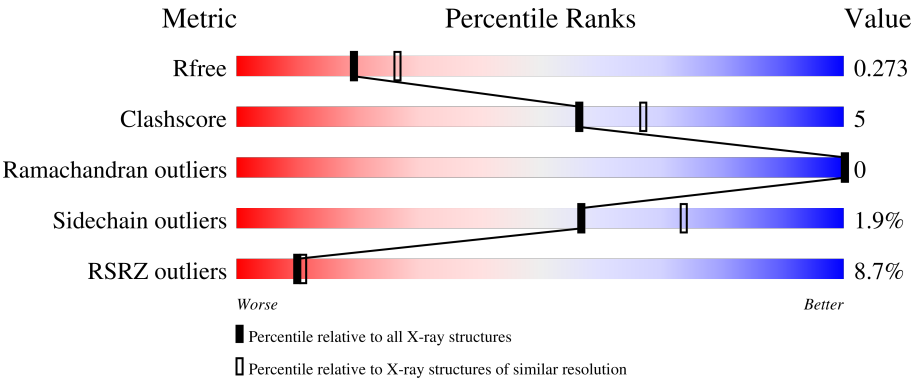
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	447	8% 77% 9% · 13%

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	A1H2K	A	1215	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6952 atoms, of which 3547 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 Adenosine receptor A2a,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	390	6083	1977	3047	515	522	22	0	23	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	1007	TRP	MET	variant	UNP P0ABE7

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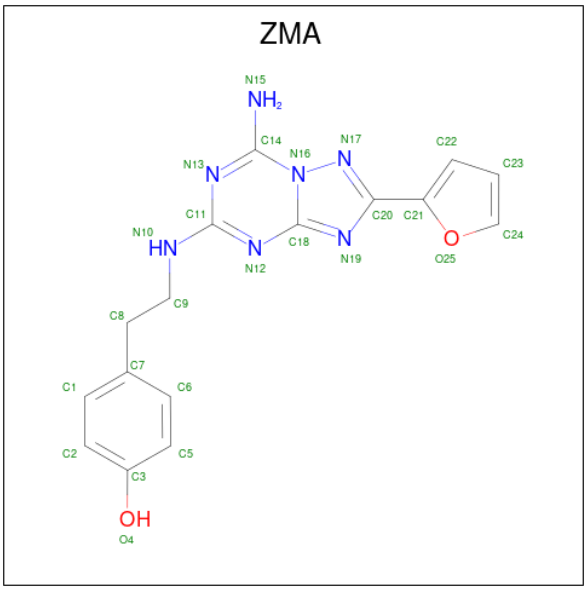
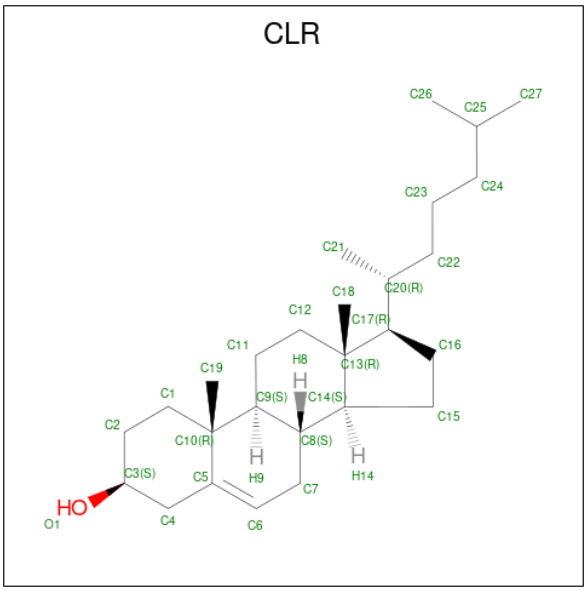
Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	ILE	HIS	variant	UNP P0ABE7
A	1106	LEU	ARG	variant	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: $C_{16}H_{15}N_7O_2$).



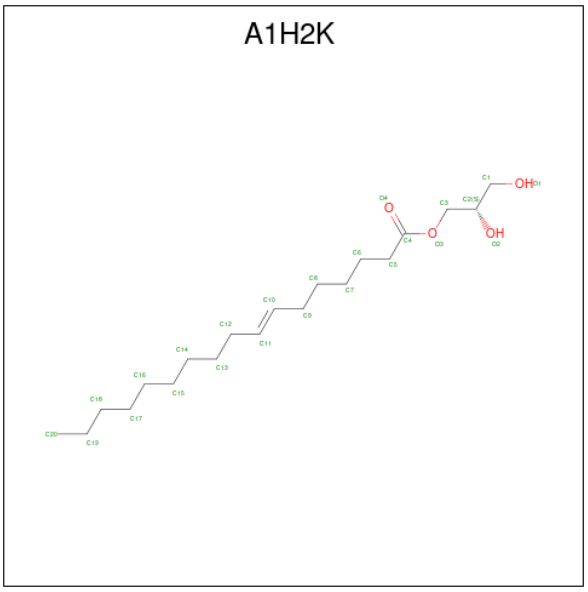
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			40	16	15	7	2		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



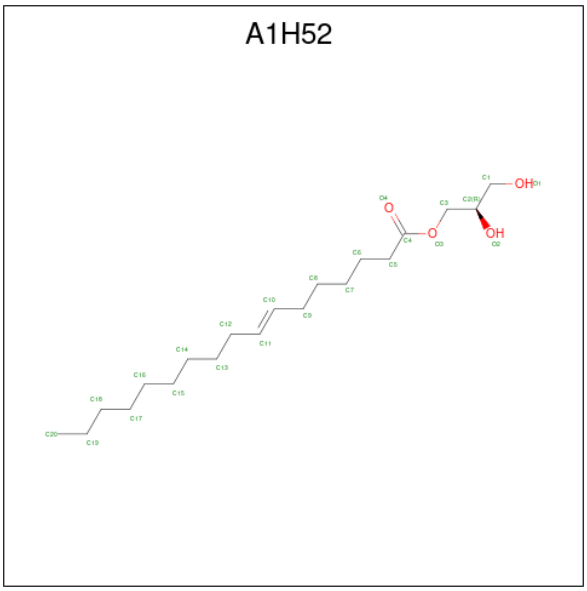
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			74	27	46	1		
3	A	1	Total	C	H	O	0	0
			74	27	46	1		
3	A	1	Total	C	H	O	0	0
			74	27	46	1		

- Molecule 4 is 7.10 monoacylglycerol (S-form) (three-letter code: A1H2K) (formula: $C_{20}H_{38}O_4$) (labeled as "Ligand of Interest" by depositor).



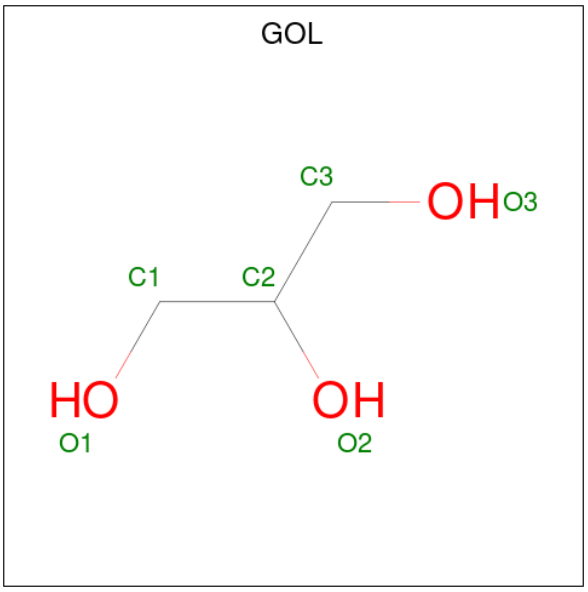
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			46	15	27	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		
4	A	1	Total	C	H	O	2	0
			62	20	38	4		

- Molecule 5 is 7.10 monoacylglycerol (R-form) (three-letter code: A1H52) (formula: $C_{20}H_{38}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	2	0
			62	20	38	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0
6	A	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

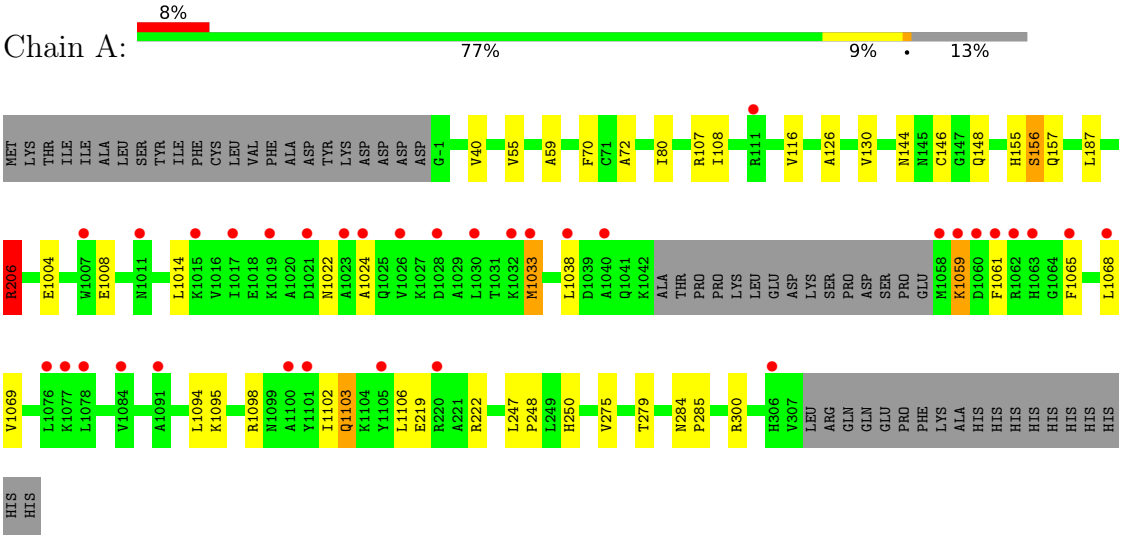
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	36	Total O 36 36	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: Adenosine receptor A2a,Soluble cytochrome b562



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.69Å 180.44Å 141.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.37 45.11 – 2.37	Depositor EDS
% Data completeness (in resolution range)	77.8 (47.17-2.37) 77.8 (45.11-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.274 0.221 , 0.273	Depositor DCC
R_{free} test set	843 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6952	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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: GOL, ZMA, NA, CLR, A1H52, A1H2K

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	0.27	0/3101	0.49	0/4215

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	206	ARG	Sidechain
1	A	300[A]	ARG	Sidechain

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	3036	3047	3024	32	0
2	A	25	15	15	1	0
3	A	84	138	138	2	0
4	A	187	293	0	2	0
5	A	24	38	0	0	0
6	A	12	16	16	0	0
7	A	1	0	0	0	0
8	A	36	0	0	0	0
All	All	3405	3547	3193	33	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 5.

All (33) 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:A:187:LEU:HD23	4:A:1212:A1H2K:C16	2.21	0.69
1:A:148:GLN:O	1:A:148:GLN:OE1	2.12	0.67
1:A:1014:LEU:HD23	1:A:1033:MET:CE	2.25	0.66
1:A:1059:LYS:O	1:A:1059:LYS:HD3	1.96	0.66
1:A:1106:LEU:HD11	1:A:222:ARG:HH12	1.61	0.65
3:A:1202:CLR:H183	3:A:1202:CLR:H212	1.82	0.60
1:A:1038:LEU:HD21	1:A:1069:VAL:HG21	1.83	0.59
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.84	0.58
1:A:70:PHE:CE2	1:A:72:ALA:HB2	2.43	0.54
1:A:275:VAL:O	1:A:279[A]:THR:HG23	2.10	0.51
1:A:1014:LEU:CD1	1:A:1095:LYS:HD2	2.40	0.51
1:A:1022:ASN:ND2	1:A:1024:ALA:HB3	2.27	0.49
1:A:1106:LEU:HD11	1:A:222:ARG:NH1	2.25	0.49
1:A:108:ILE:HG13	1:A:108:ILE:O	2.13	0.48
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.45	0.46
1:A:1068:LEU:HD12	1:A:1094:LEU:HD22	1.97	0.46
1:A:1103:GLN:O	1:A:219:GLU:HG3	2.16	0.46
1:A:1004:GLU:O	1:A:1008:GLU:HG3	2.17	0.45
1:A:1102:ILE:HD13	1:A:1102:ILE:N	2.31	0.45
1:A:1098:ARG:HA	1:A:1102:ILE:HG12	1.97	0.45
1:A:1004:GLU:HB2	1:A:222:ARG:HH22	1.81	0.45
1:A:80[A]:ILE:HD11	3:A:1203:CLR:H182	2.00	0.44
1:A:156:SER:OG	1:A:157:GLN:N	2.51	0.44
1:A:250:HIS:CE1	2:A:1201:ZMA:H24	2.54	0.43
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.00	0.43
1:A:247:LEU:N	1:A:248:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD23	4:A:1212:A1H2K:C15	2.48	0.43
1:A:284:ASN:HB2	1:A:285:PRO:HD3	2.00	0.42
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.84	0.42
1:A:126:ALA:O	1:A:130:VAL:HG23	2.19	0.41
1:A:144:ASN:OD1	1:A:146:CYS:HB2	2.19	0.41
1:A:1061:PHE:CE1	1:A:1065:PHE:HE2	2.38	0.41
1:A:1014:LEU:HD23	1:A:1033:MET:HE2	2.00	0.41

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	386/447 (86%)	379 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/374 (86%)	315 (98%)	6 (2%)	57 73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	156	SER
1	A	206	ARG
1	A	1033	MET
1	A	1059	LYS
1	A	1103	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	1025	GLN
1	A	306	HIS

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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
3	CLR	A	1202	-	31,31,31	0.39	0	48,48,48	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	A1H2K	A	1205	-	23,23,23	0.24	0	24,24,24	0.34	0
4	A1H2K	A	1209	-	23,23,23	0.32	0	24,24,24	0.56	0
4	A1H2K	A	1208	-	18,18,23	0.33	0	19,19,24	0.56	0
4	A1H2K	A	1215	-	23,23,23	0.27	0	24,24,24	0.45	0
6	GOL	A	1214	-	5,5,5	0.94	0	5,5,5	0.94	0
2	ZMA	A	1201	-	21,28,28	2.09	2 (9%)	20,39,39	1.53	5 (25%)
4	A1H2K	A	1206	-	23,23,23	0.32	0	24,24,24	0.61	0
6	GOL	A	1213	-	5,5,5	1.01	0	5,5,5	0.84	0
4	A1H2K	A	1211	-	23,23,23	0.21	0	24,24,24	0.56	0
4	A1H2K	A	1207	-	23,23,23	0.25	0	24,24,24	0.57	0
4	A1H2K	A	1212	-	23,23,23	0.25	0	24,24,24	0.72	0
5	A1H52	A	1210	-	23,23,23	0.39	0	24,24,24	0.86	2 (8%)
3	CLR	A	1203	-	31,31,31	0.39	0	48,48,48	0.71	0
3	CLR	A	1204	-	31,31,31	0.35	0	48,48,48	0.75	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
3	CLR	A	1202	-	-	6/10/68/68	0/4/4/4
4	A1H2K	A	1205	-	-	5/23/23/23	-
4	A1H2K	A	1209	-	-	7/23/23/23	-
4	A1H2K	A	1208	-	-	10/18/18/23	-
4	A1H2K	A	1215	-	-	8/23/23/23	-
6	GOL	A	1214	-	-	2/4/4/4	-
2	ZMA	A	1201	-	-	0/6/10/10	0/4/4/4
4	A1H2K	A	1206	-	-	12/23/23/23	-
6	GOL	A	1213	-	-	2/4/4/4	-
4	A1H2K	A	1211	-	-	8/23/23/23	-
4	A1H2K	A	1207	-	-	8/23/23/23	-
4	A1H2K	A	1212	-	-	9/23/23/23	-
5	A1H52	A	1210	-	-	9/23/23/23	-
3	CLR	A	1203	-	-	5/10/68/68	0/4/4/4
3	CLR	A	1204	-	-	4/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ZMA	C11-N10	7.01	1.45	1.34
2	A	1201	ZMA	C14-N15	5.48	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	ZMA	N12-C11-N13	-3.23	121.13	126.23
2	A	1201	ZMA	N15-C14-N16	2.83	119.87	117.97
5	A	1210	A1H52	O2-C2-C3	2.82	119.44	109.56
2	A	1201	ZMA	N15-C14-N13	2.54	120.37	117.03
2	A	1201	ZMA	C9-C8-C7	-2.37	107.39	112.87
2	A	1201	ZMA	C9-N10-C11	-2.03	120.24	123.75
5	A	1210	A1H52	O2-C2-C1	2.01	118.00	109.12

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1206	A1H2K	O2-C2-C3-O3
4	A	1206	A1H2K	O4-C4-O3-C3
4	A	1206	A1H2K	C5-C4-O3-C3
4	A	1208	A1H2K	C1-C2-C3-O3
4	A	1208	A1H2K	O2-C2-C3-O3
4	A	1209	A1H2K	O4-C4-O3-C3
4	A	1209	A1H2K	C5-C4-O3-C3
4	A	1211	A1H2K	O1-C1-C2-C3
4	A	1211	A1H2K	C1-C2-C3-O3
5	A	1210	A1H52	O4-C4-O3-C3
5	A	1210	A1H52	C5-C4-O3-C3
6	A	1214	GOL	O1-C1-C2-C3
4	A	1208	A1H2K	O4-C4-O3-C3
4	A	1208	A1H2K	C5-C4-O3-C3
4	A	1211	A1H2K	O2-C2-C3-O3
4	A	1212	A1H2K	C5-C4-O3-C3
3	A	1203	CLR	C20-C22-C23-C24
4	A	1215	A1H2K	O2-C2-C3-O3
5	A	1210	A1H52	C12-C13-C14-C15
4	A	1215	A1H2K	C1-C2-C3-O3
5	A	1210	A1H52	C5-C6-C7-C8
4	A	1206	A1H2K	C13-C14-C15-C16
4	A	1207	A1H2K	O1-C1-C2-C3
4	A	1208	A1H2K	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	1213	GOL	O1-C1-C2-C3
5	A	1210	A1H52	C11-C12-C13-C14
4	A	1205	A1H2K	C6-C7-C8-C9
4	A	1212	A1H2K	C13-C14-C15-C16
4	A	1211	A1H2K	O1-C1-C2-O2
6	A	1213	GOL	O1-C1-C2-O2
4	A	1207	A1H2K	C14-C15-C16-C17
4	A	1212	A1H2K	O4-C4-O3-C3
3	A	1202	CLR	C23-C24-C25-C26
4	A	1206	A1H2K	C15-C16-C17-C18
4	A	1215	A1H2K	C13-C14-C15-C16
4	A	1207	A1H2K	C7-C8-C9-C10
3	A	1202	CLR	C23-C24-C25-C27
4	A	1209	A1H2K	C10-C11-C12-C13
3	A	1204	CLR	C13-C17-C20-C22
4	A	1206	A1H2K	C17-C18-C19-C20
6	A	1214	GOL	O1-C1-C2-O2
4	A	1205	A1H2K	C17-C18-C19-C20
4	A	1208	A1H2K	C4-C5-C6-C7
4	A	1209	A1H2K	C17-C18-C19-C20
4	A	1208	A1H2K	C6-C7-C8-C9
4	A	1207	A1H2K	C11-C12-C13-C14
3	A	1203	CLR	C17-C20-C22-C23
4	A	1207	A1H2K	C5-C4-O3-C3
4	A	1215	A1H2K	C11-C10-C9-C8
4	A	1206	A1H2K	C16-C17-C18-C19
4	A	1207	A1H2K	C13-C14-C15-C16
3	A	1204	CLR	C16-C17-C20-C22
4	A	1215	A1H2K	C16-C17-C18-C19
3	A	1202	CLR	C13-C17-C20-C21
3	A	1204	CLR	C13-C17-C20-C21
4	A	1205	A1H2K	O1-C1-C2-O2
3	A	1202	CLR	C16-C17-C20-C22
5	A	1210	A1H52	C16-C17-C18-C19
4	A	1211	A1H2K	C10-C11-C12-C13
3	A	1204	CLR	C16-C17-C20-C21
4	A	1206	A1H2K	C12-C13-C14-C15
4	A	1207	A1H2K	C10-C11-C12-C13
4	A	1212	A1H2K	C16-C17-C18-C19
4	A	1211	A1H2K	C12-C13-C14-C15
5	A	1210	A1H52	C15-C16-C17-C18
4	A	1205	A1H2K	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	1212	A1H2K	C7-C8-C9-C10
4	A	1206	A1H2K	C1-C2-C3-O3
3	A	1203	CLR	C21-C20-C22-C23
4	A	1206	A1H2K	C6-C7-C8-C9
4	A	1208	A1H2K	C11-C10-C9-C8
3	A	1203	CLR	C23-C24-C25-C26
4	A	1209	A1H2K	C5-C6-C7-C8
4	A	1212	A1H2K	C17-C18-C19-C20
4	A	1215	A1H2K	C15-C16-C17-C18
5	A	1210	A1H52	C10-C11-C12-C13
4	A	1212	A1H2K	C11-C12-C13-C14
4	A	1206	A1H2K	C11-C10-C9-C8
4	A	1215	A1H2K	C17-C18-C19-C20
3	A	1202	CLR	C16-C17-C20-C21
4	A	1208	A1H2K	C10-C11-C12-C13
4	A	1209	A1H2K	C13-C14-C15-C16
4	A	1211	A1H2K	C7-C8-C9-C10
5	A	1210	A1H52	C14-C15-C16-C17
4	A	1215	A1H2K	C10-C11-C12-C13
4	A	1206	A1H2K	C11-C12-C13-C14
4	A	1205	A1H2K	O1-C1-C2-C3
3	A	1203	CLR	C23-C24-C25-C27
3	A	1202	CLR	C21-C20-C22-C23
4	A	1211	A1H2K	C14-C15-C16-C17
4	A	1208	A1H2K	O1-C1-C2-O2
4	A	1209	A1H2K	C4-C5-C6-C7
4	A	1212	A1H2K	C14-C15-C16-C17
4	A	1212	A1H2K	C10-C11-C12-C13
4	A	1207	A1H2K	C11-C10-C9-C8

There are no ring outliers.

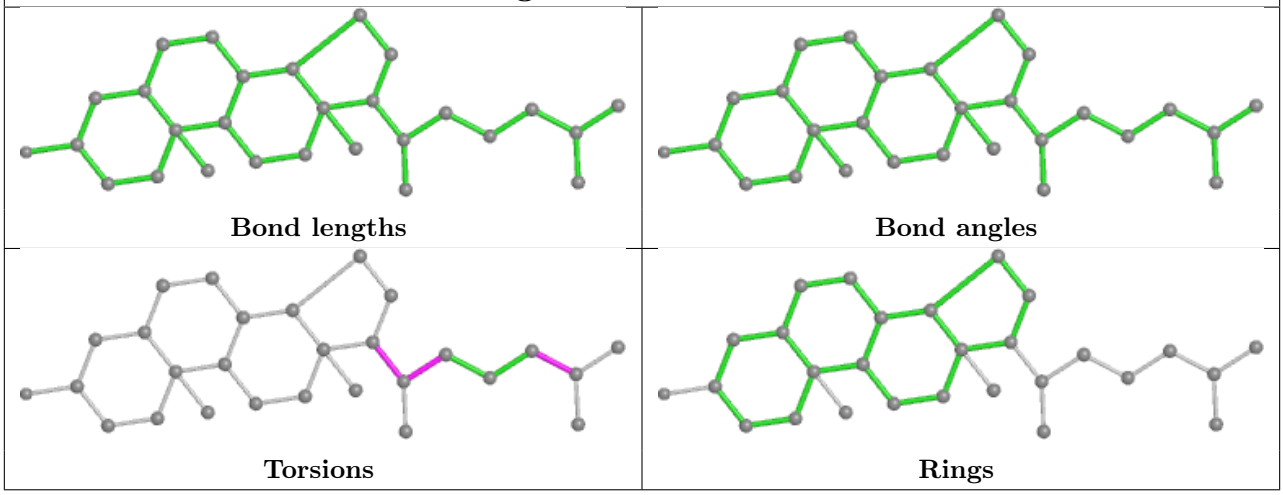
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	CLR	1	0
2	A	1201	ZMA	1	0
4	A	1212	A1H2K	2	0
3	A	1203	CLR	1	0

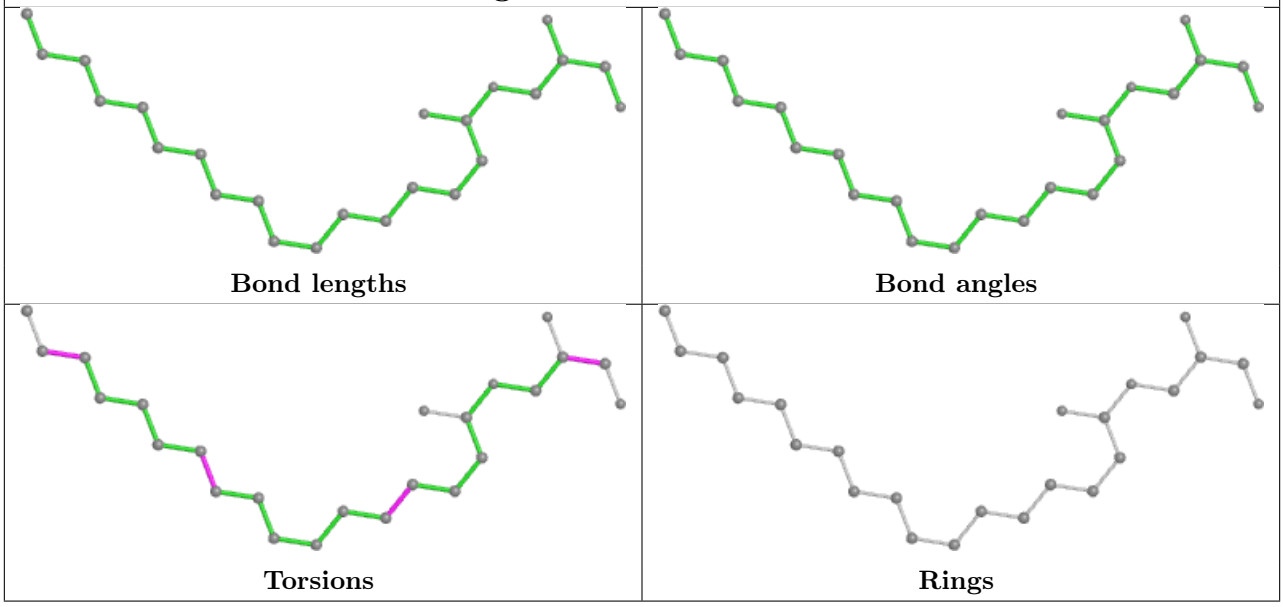
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

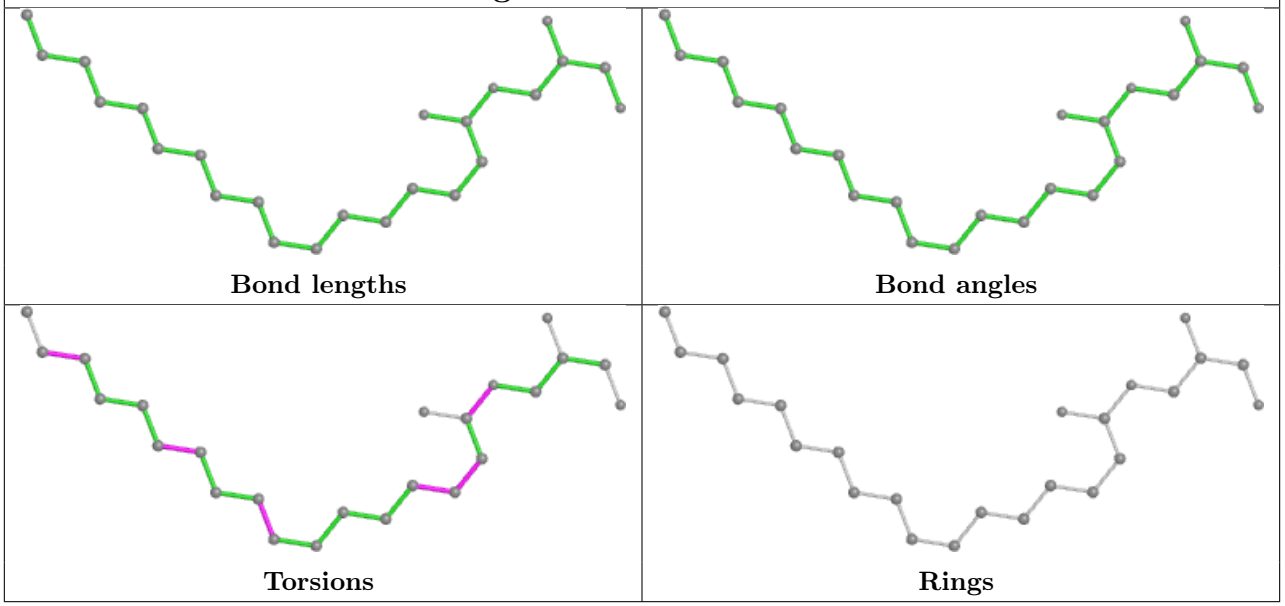
Ligand CLR A 1202



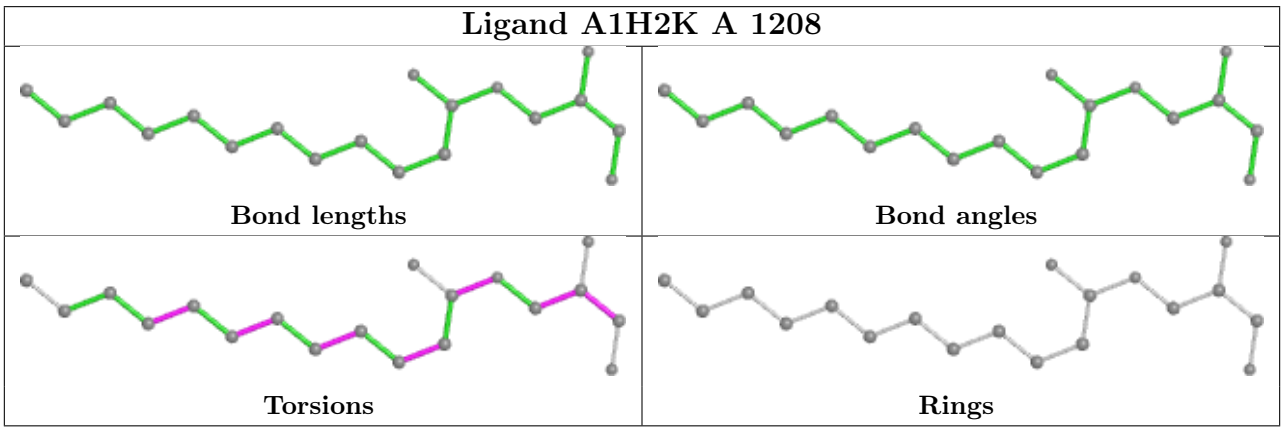
Ligand A1H2K A 1205



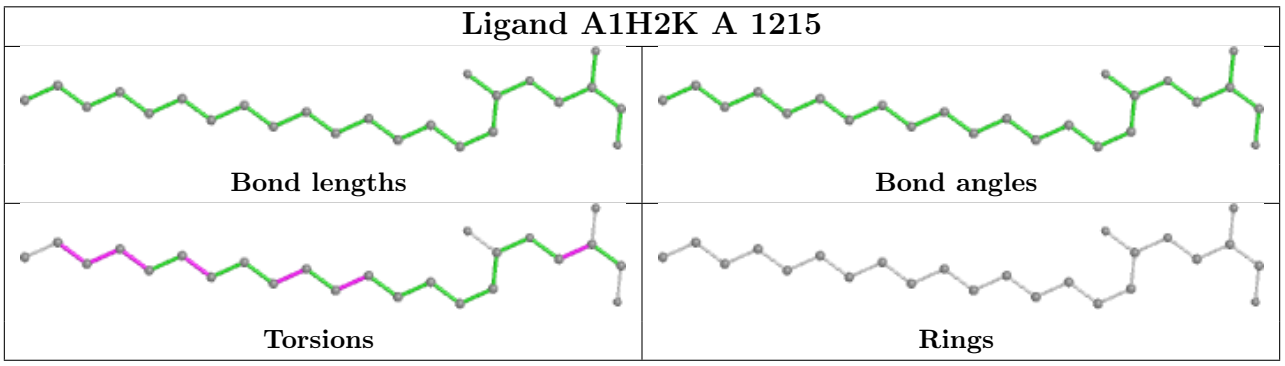
Ligand A1H2K A 1209



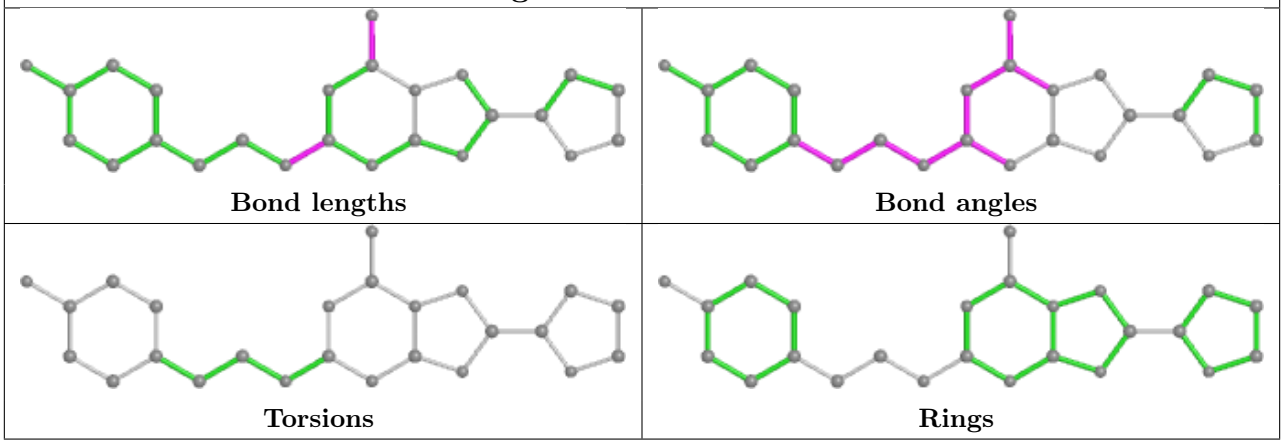
Ligand A1H2K A 1208



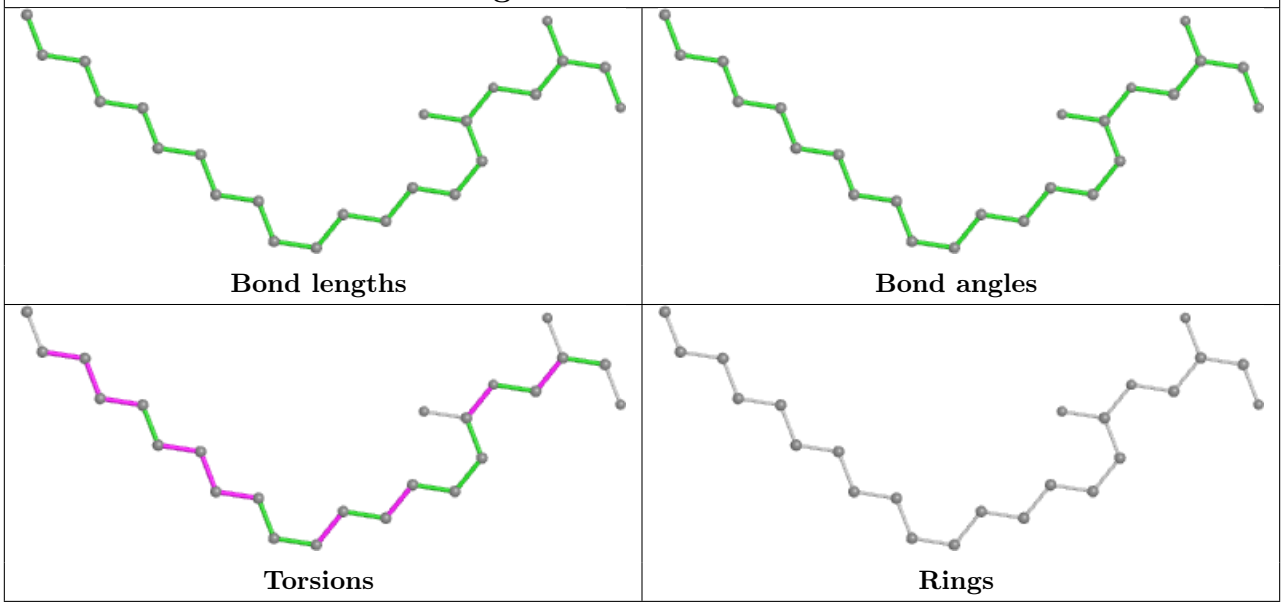
Ligand A1H2K A 1215



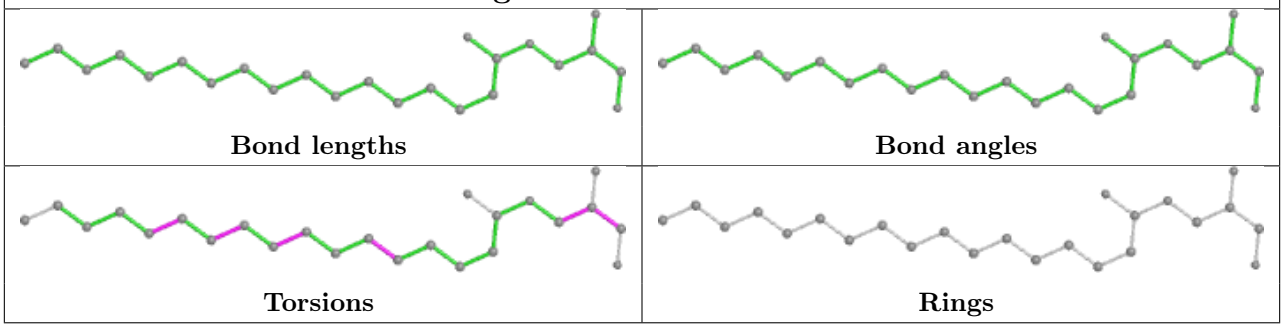
Ligand ZMA A 1201



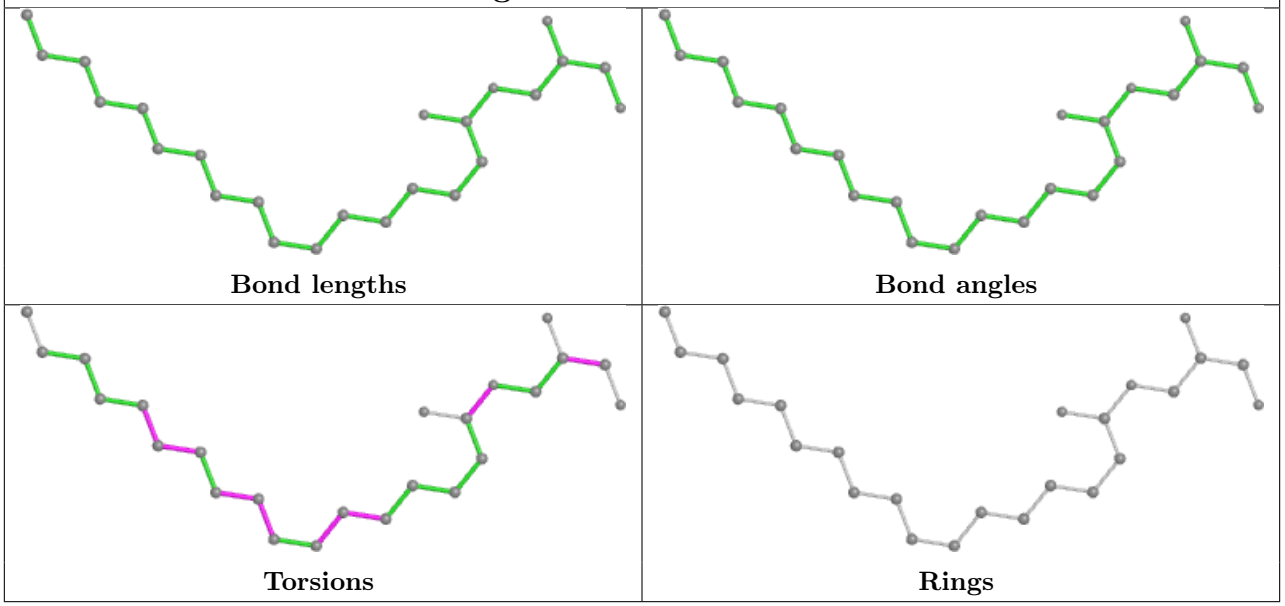
Ligand A1H2K A 1206



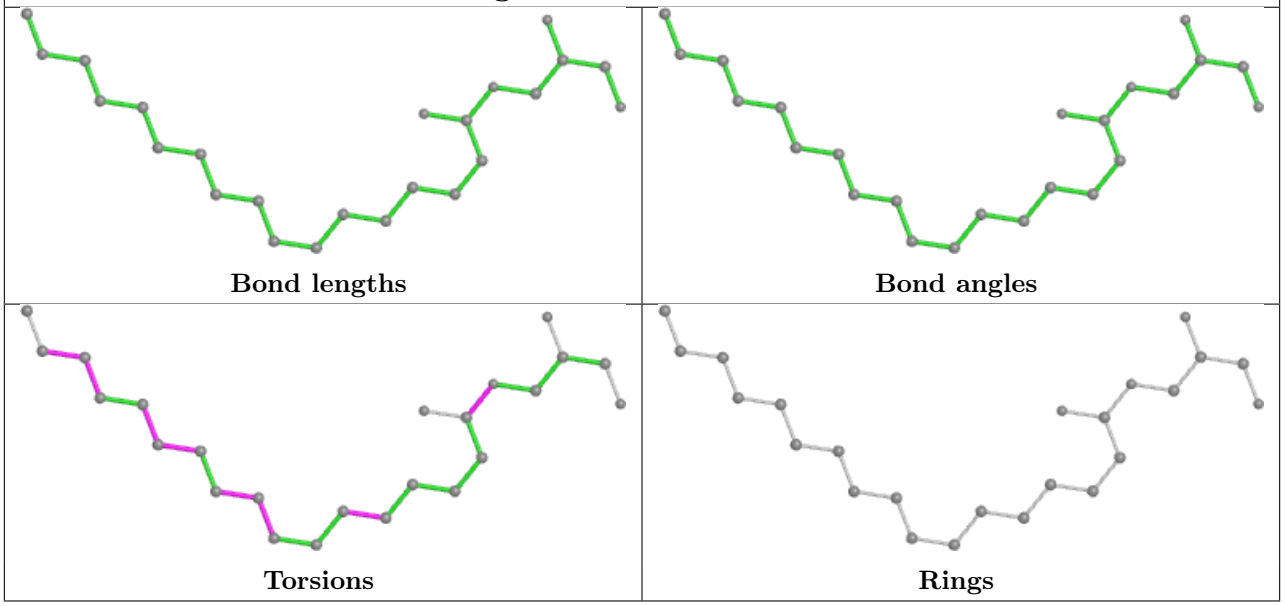
Ligand A1H2K A 1211



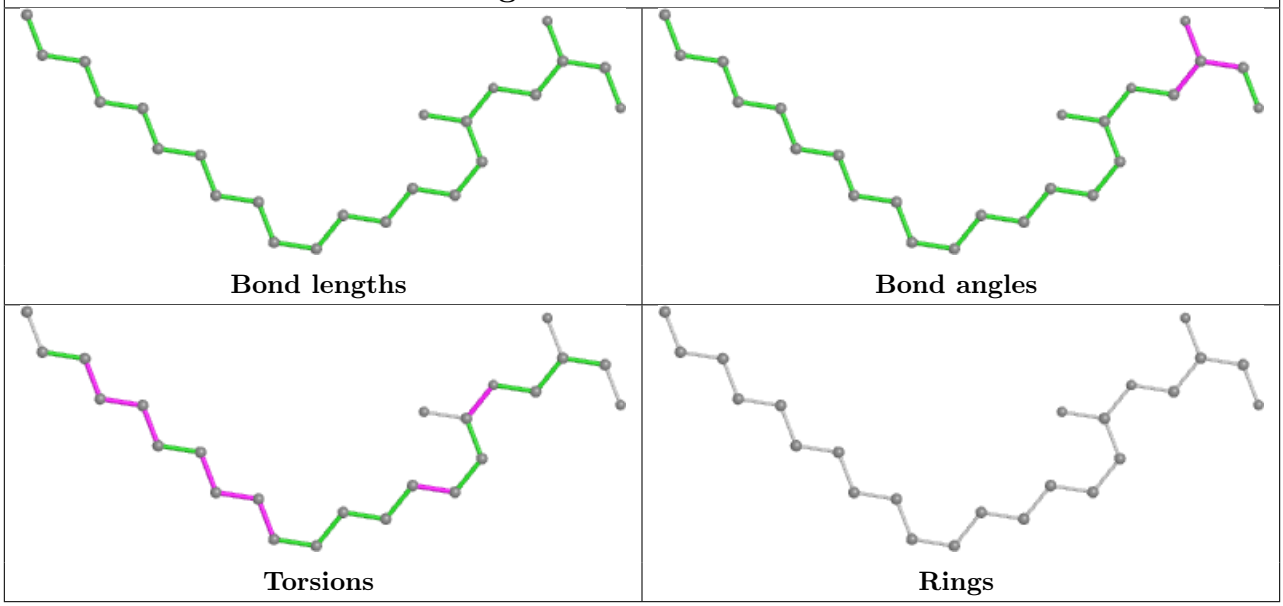
Ligand A1H2K A 1207



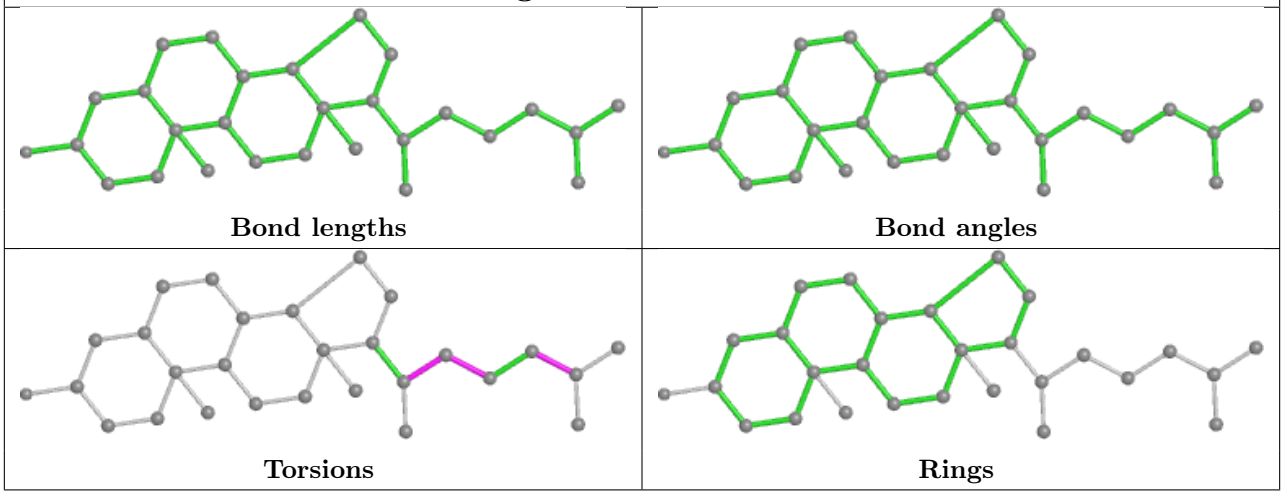
Ligand A1H2K A 1212



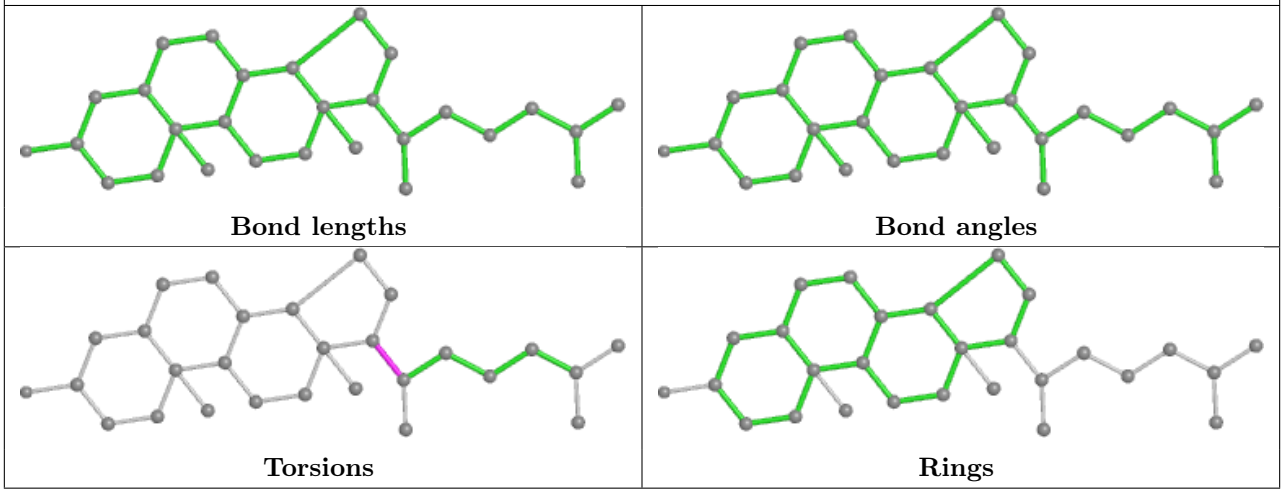
Ligand A1H52 A 1210



Ligand CLR A 1203



Ligand CLR A 1204



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	A	390/447 (87%)	0.52	34 (8%)	10	11	26, 44, 105, 149	3 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	8.4
1	A	1063	HIS	6.3
1	A	1062	ARG	6.1
1	A	1058	MET	5.2
1	A	1105	TYR	3.9
1	A	1101	TYR	3.8
1	A	1023	ALA	3.8
1	A	1059	LYS	3.6
1	A	1030	LEU	3.6
1	A	1007	TRP	3.4
1	A	1015	LYS	3.4
1	A	1032	LYS	3.3
1	A	1084	VAL	3.3
1	A	111	ARG	3.2
1	A	220	ARG	3.2
1	A	1033	MET	2.9
1	A	306	HIS	2.9
1	A	1028	ASP	2.8
1	A	1065	PHE	2.7
1	A	1021	ASP	2.7
1	A	1076	LEU	2.4
1	A	1019	LYS	2.4
1	A	1078	LEU	2.4
1	A	1068	LEU	2.3
1	A	1026	VAL	2.3
1	A	1040	ALA	2.3
1	A	1100	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1038	LEU	2.2
1	A	1024	ALA	2.2
1	A	1077	LYS	2.1
1	A	1091	ALA	2.1
1	A	1060	ASP	2.0
1	A	1011	ASN	2.0
1	A	1017	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

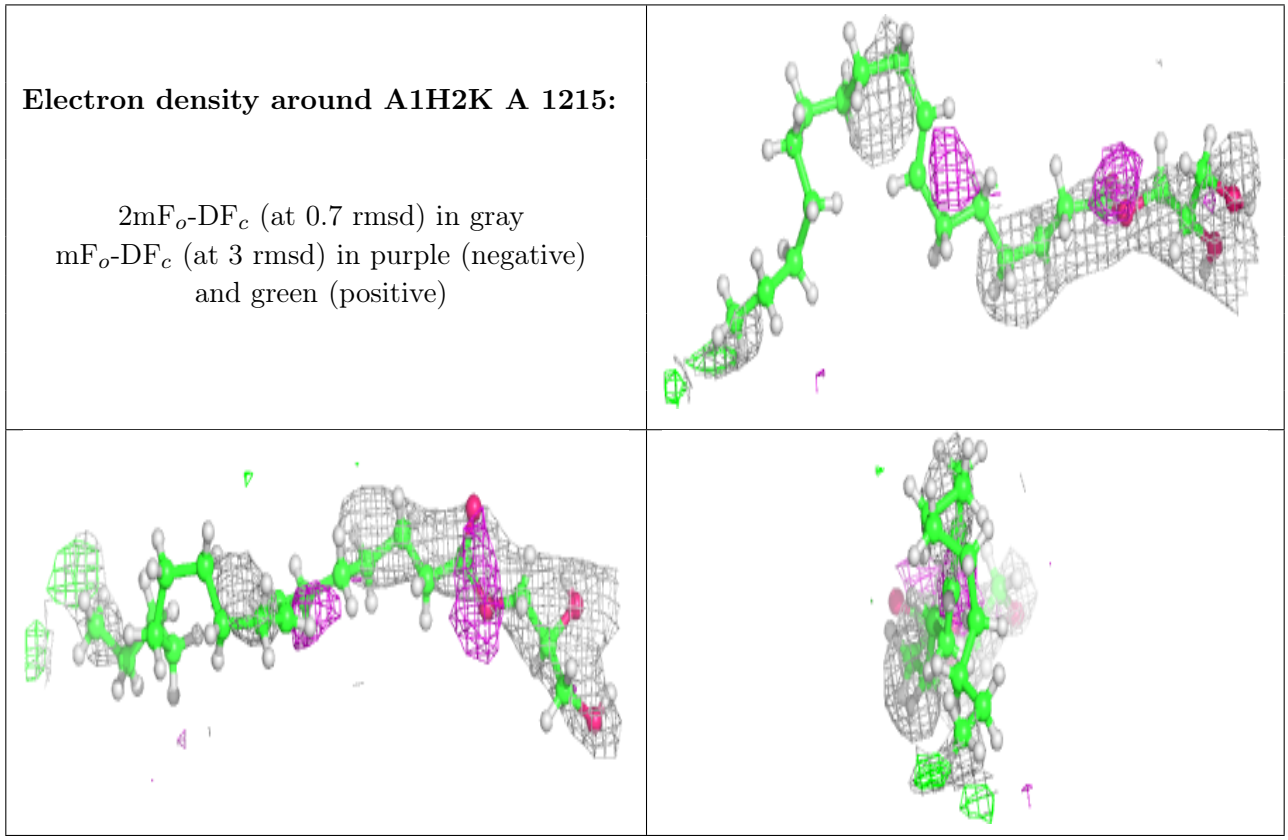
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	A	1214	6/6	0.62	0.27	65,79,95,95	0
4	A1H2K	A	1215	24/24	0.64	0.58	55,91,139,167	2
5	A1H52	A	1210	24/24	0.69	0.37	52,70,87,95	2
4	A1H2K	A	1209	24/24	0.75	0.33	47,70,98,105	2
6	GOL	A	1213	6/6	0.81	0.23	50,64,78,82	0
4	A1H2K	A	1206	24/24	0.82	0.26	48,72,88,96	2
4	A1H2K	A	1207	24/24	0.84	0.39	48,70,84,96	2
4	A1H2K	A	1205	24/24	0.84	0.29	46,69,97,110	2
4	A1H2K	A	1212	24/24	0.85	0.34	49,73,145,174	2
4	A1H2K	A	1211	24/24	0.86	0.31	39,75,124,139	2
7	NA	A	1216	1/1	0.87	0.11	50,50,50,50	0
4	A1H2K	A	1208	19/24	0.89	0.29	49,64,92,95	2
3	CLR	A	1202	28/28	0.92	0.18	37,54,78,79	0
3	CLR	A	1204	28/28	0.93	0.21	40,53,90,108	0
3	CLR	A	1203	28/28	0.94	0.16	47,60,81,93	0
2	ZMA	A	1201	25/25	0.95	0.17	24,37,68,85	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.

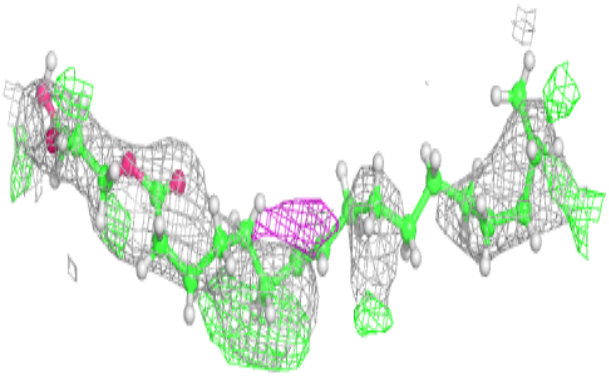
Electron density around A1H2K A 1215:

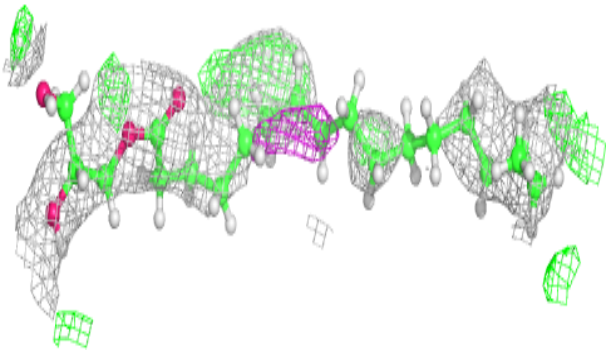
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

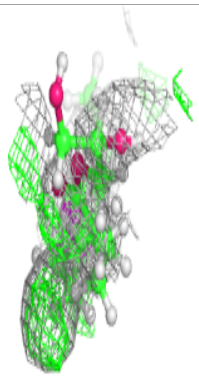


Electron density around A1H52 A 1210:

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

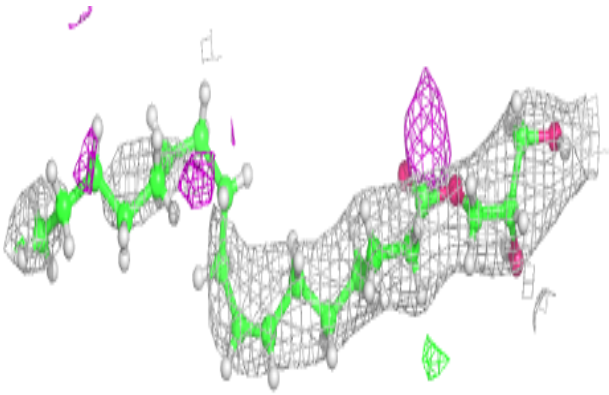


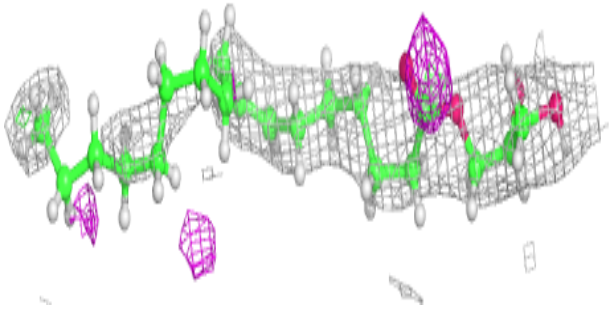


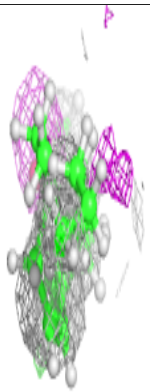


Electron density around A1H2K A 1209:

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

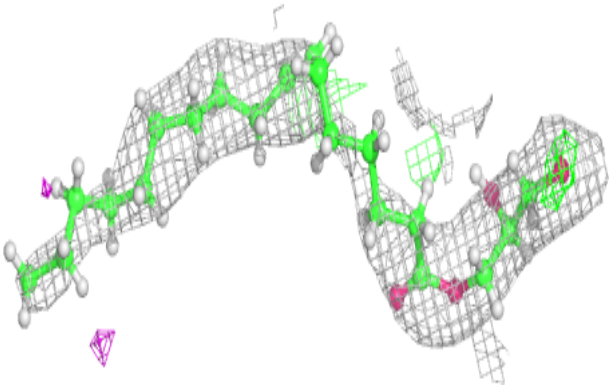


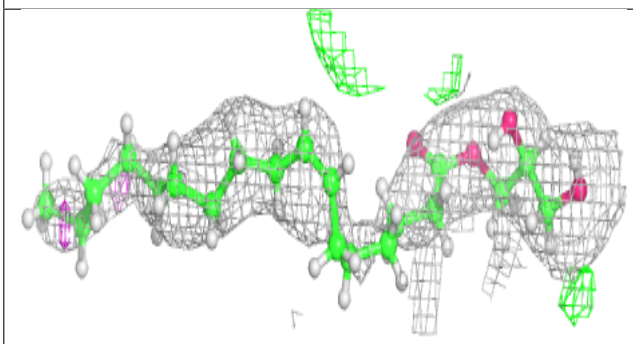


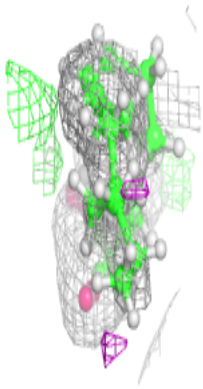


Electron density around A1H2K A 1206:

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

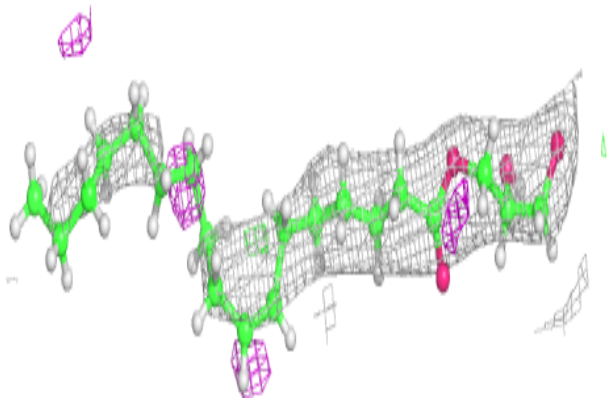


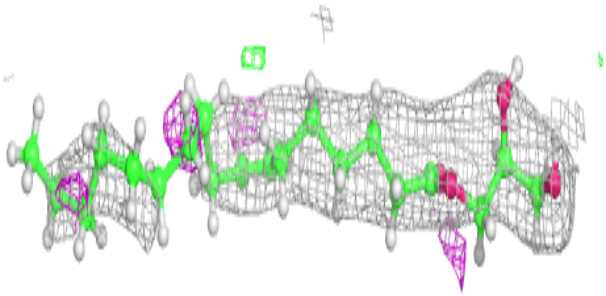


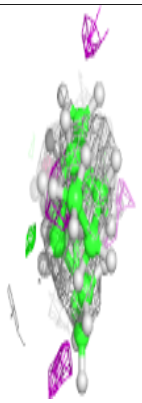


Electron density around A1H2K A 1207:

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

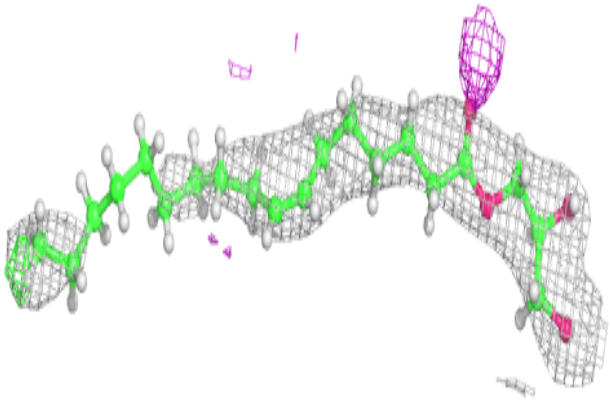


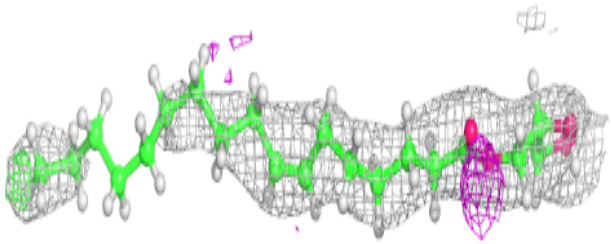


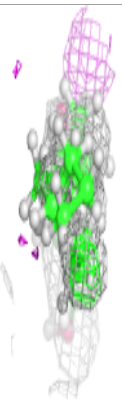


Electron density around A1H2K A 1205:

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

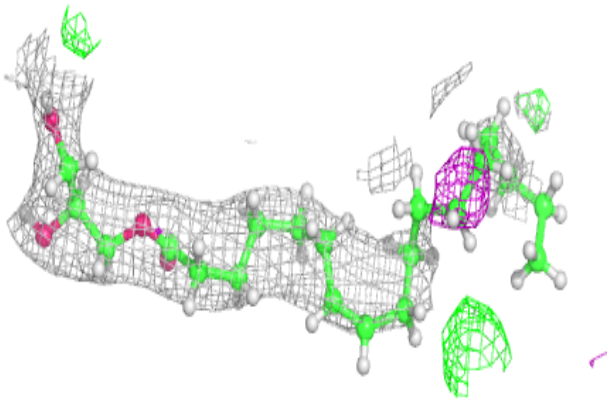


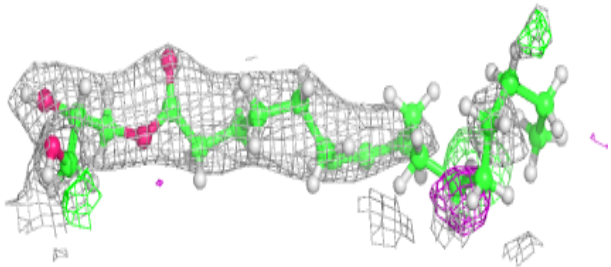


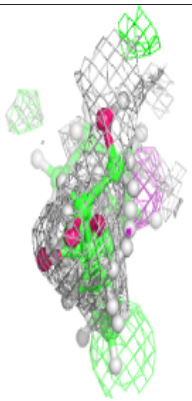


Electron density around A1H2K A 1212:

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

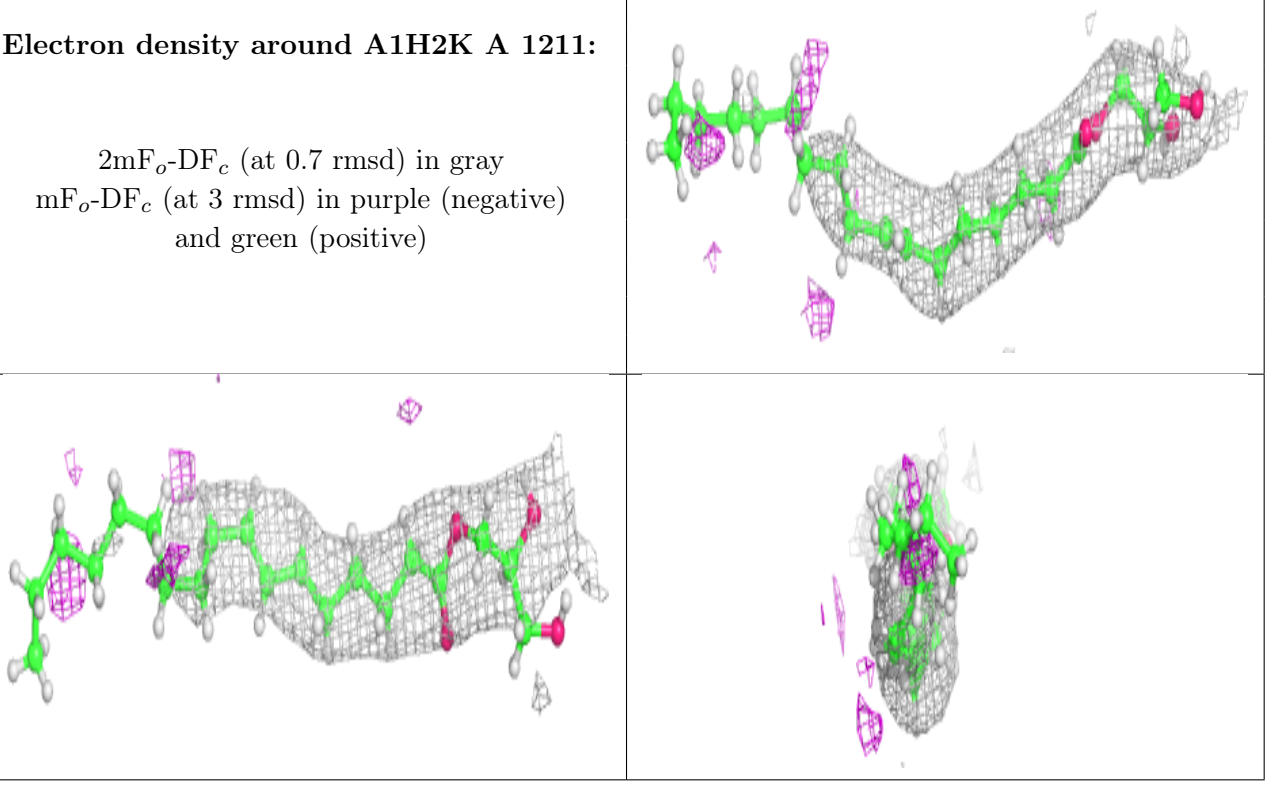






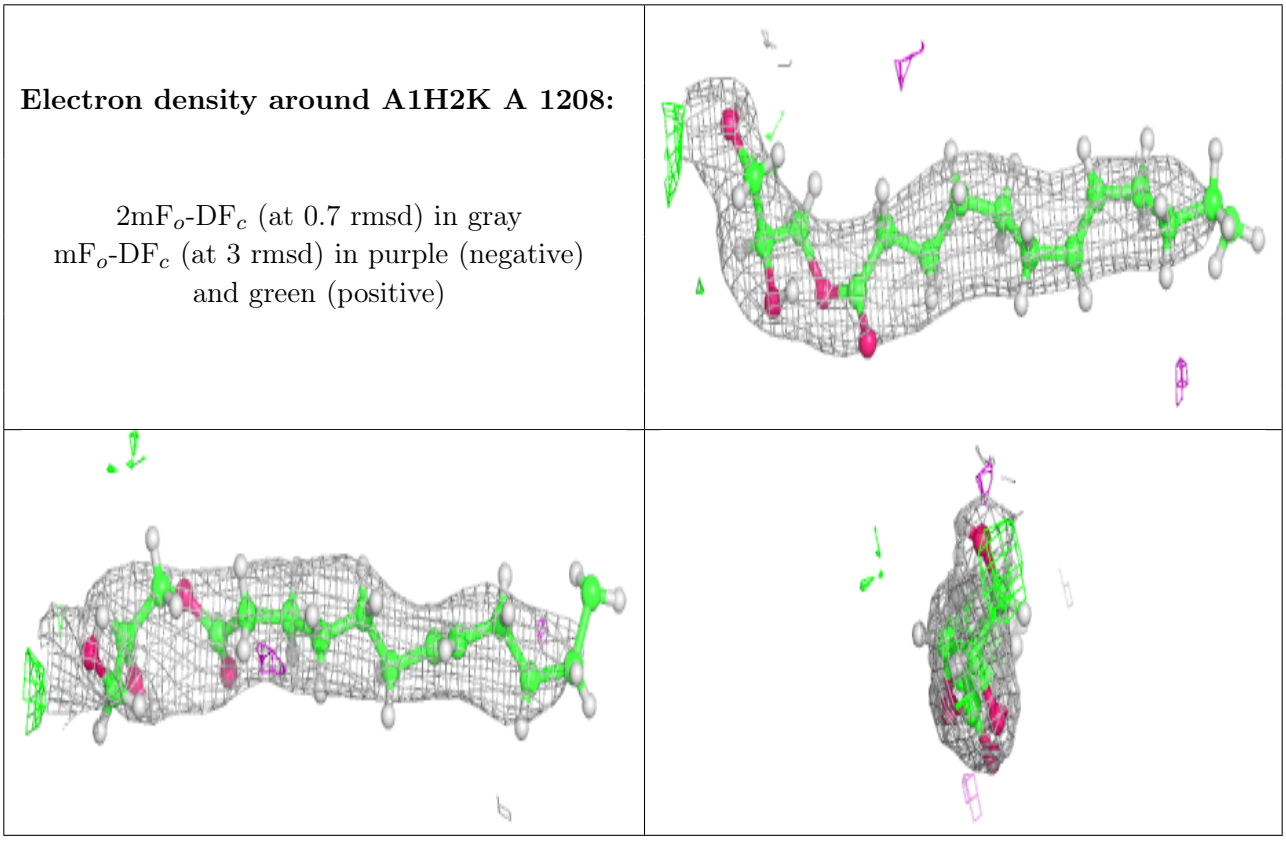
Electron density around A1H2K A 1211:

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



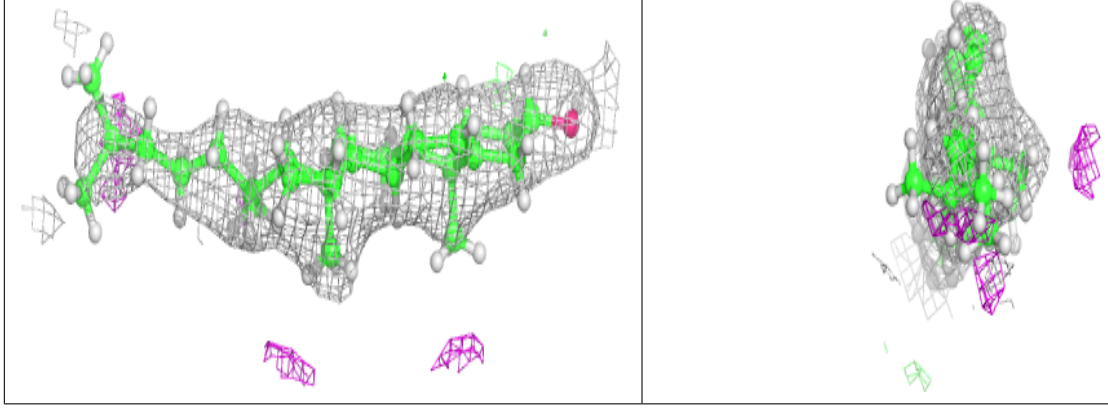
Electron density around A1H2K A 1208:

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



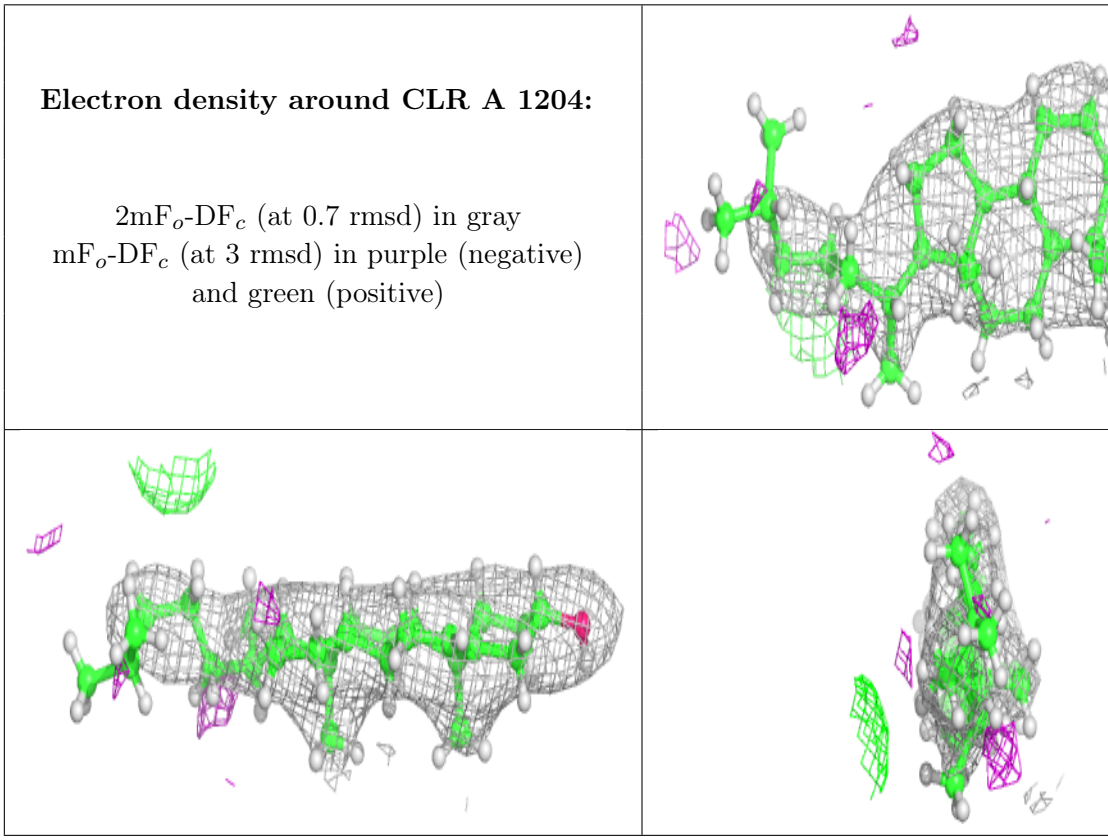
Electron density around CLR A 1202:

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



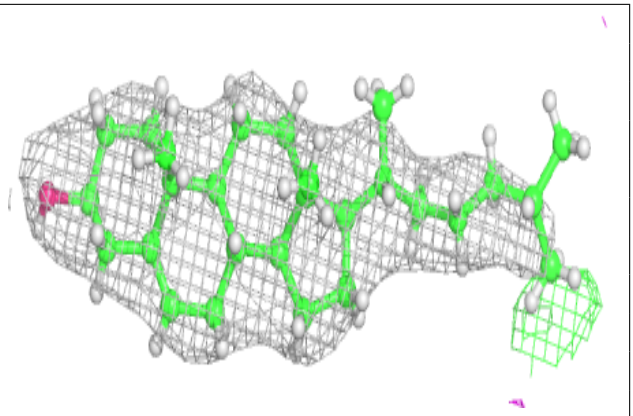
Electron density around CLR A 1204:

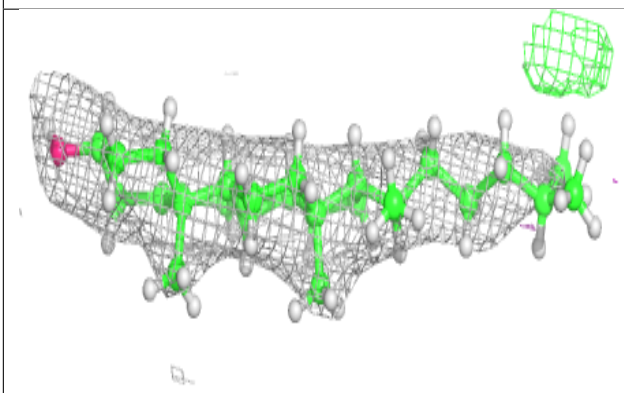
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

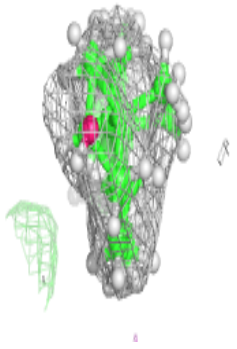


Electron density around CLR A 1203:

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

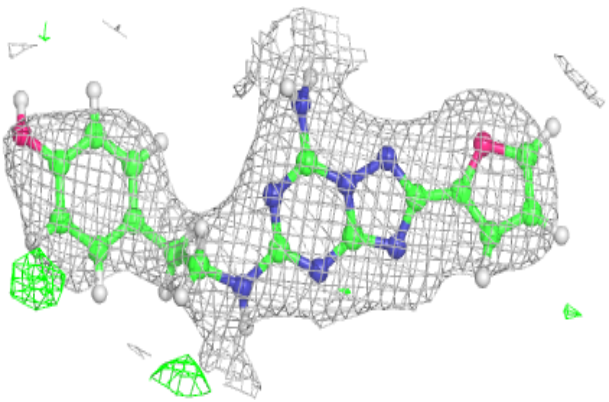


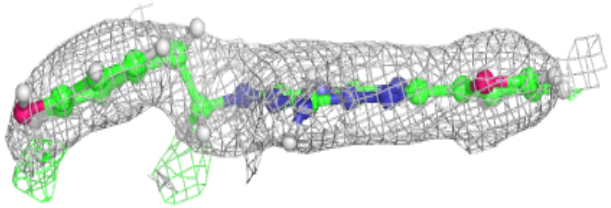


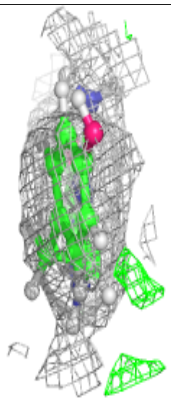


Electron density around ZMA A 1201:

$2mF_o$-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.