



## Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:38 AM BST

PDB ID : 6S0Q  
Title : Structure of the A2A adenosine receptor determined at SwissFEL using native-SAD at 4.57 keV from 50,000 diffraction patterns  
Authors : Nass, K.; Cheng, R.; Vera, L.; Mozzanica, A.; Redford, S.; Ozerov, D.; Basu, S.; James, D.; Knopp, G.; Cirelli, C.; Martiel, I.; Casadei, C.; Weinert, T.; Nogly, P.; Skopintsev, P.; Usov, I.; Leonarski, F.; Geng, T.; Rappas, M.; Dore, A.S.; Cooke, R.; Nasrollahi Shirazi, S.; Dworkowski, F.; Sharpe, M.; Olieric, N.; Steinmetz, M.O.; Schertler, G.; Abela, R.; Patthey, L.; Schmitt, B.; Hennig, M.; Standfuss, J.; Wang, M.; Milne, J.C.  
Deposited on : 2019-06-18  
Resolution : 2.65 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](mailto: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.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

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

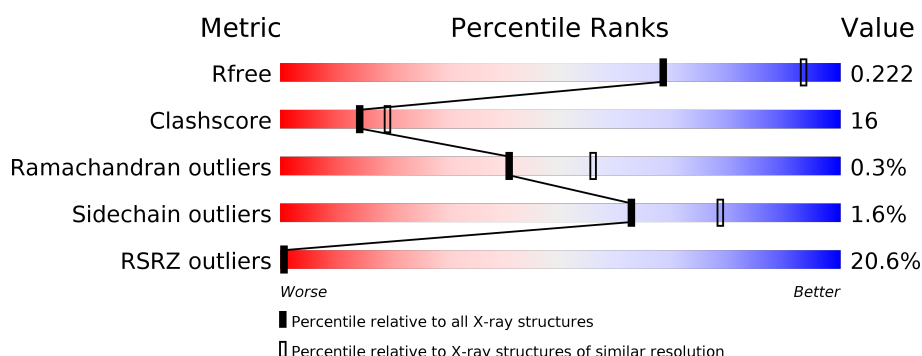
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	433	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLA	A	1205	-	-	-	X
4	OLB	A	1210	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLR	A	1213	X	-	-	-
6	CLR	A	1214	X	-	-	-
6	CLR	A	1215	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3286 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2998	1953	506	517	22			

There are 33 discrepancies between the modelled and reference sequences:

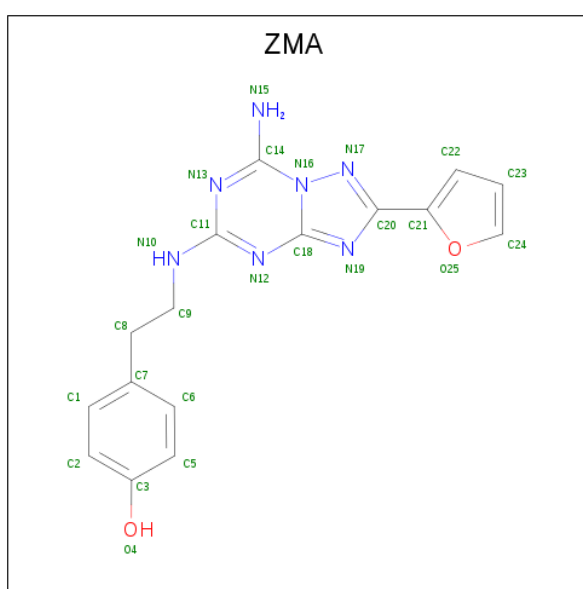
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	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

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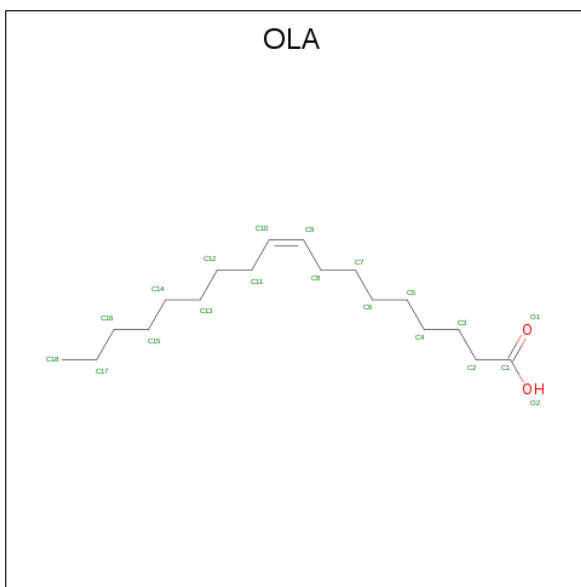
Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	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<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).



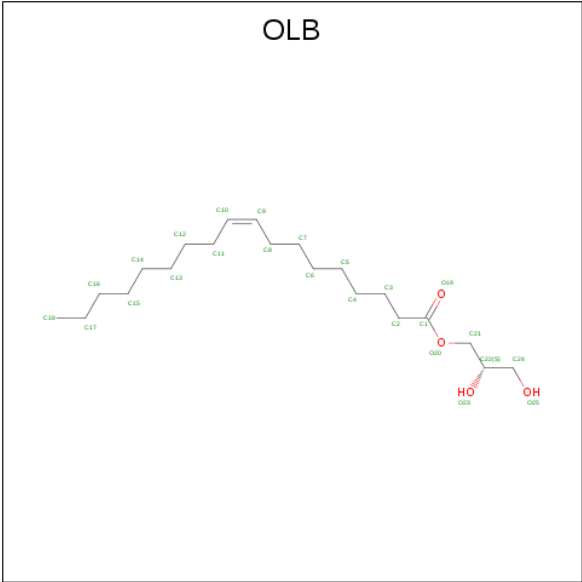
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



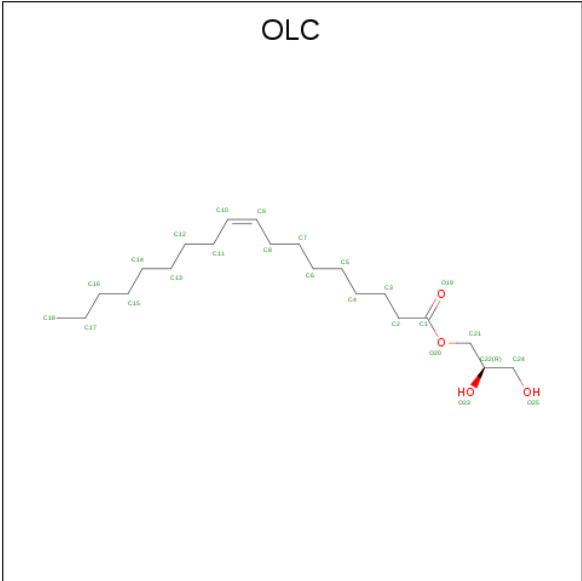
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			15	13	2		
3	A	1	Total	C	O	0	0
			9	7	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C		0	0
			10	10			
3	A	1	Total	C		0	0
			7	7			
3	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	15	4		
4	A	1	Total	C	O	0	0
			20	16	4		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		

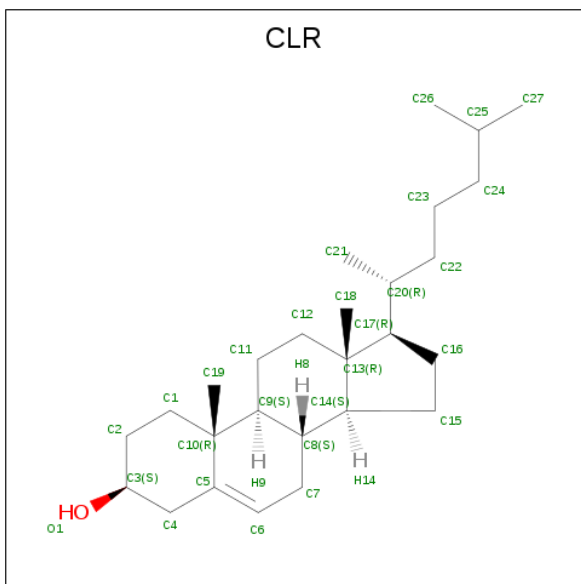
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	15	4		

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).

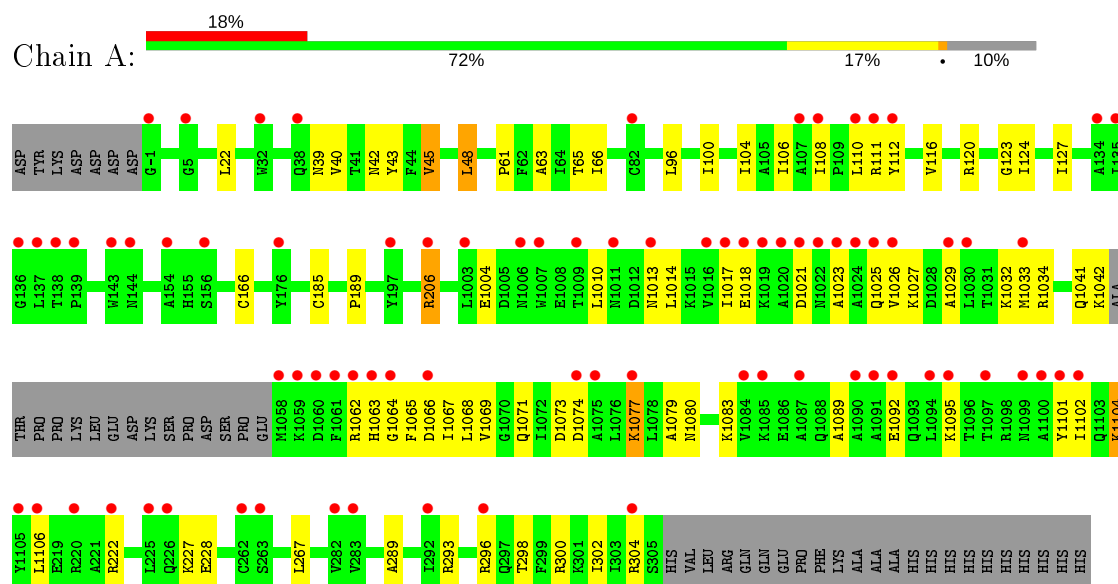


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	27	1		
6	A	1	Total	C	O	0	0
			28	27	1		
6	A	1	Total	C	O	0	0
			28	27	1		

### 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,Adenosine receptor A2a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.34Å 180.66Å 143.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.49 – 2.65 35.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.49-2.65) 93.8 (35.76-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.87 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.194 , 0.221 0.195 , 0.222	Depositor DCC
$R_{free}$ test set	786 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLB, ZMA, OLC, CLR

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	0.50	1/3062 (0.0%)	0.58	1/4164 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CB-CG1	-6.90	1.38	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LEU	CA-CB-CG	5.33	127.55	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2998	0	3068	65	0
2	A	25	0	15	0	0
3	A	96	0	141	3	0
4	A	39	0	52	1	0
5	A	44	0	65	2	0
6	A	84	0	117	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3286	0	3458	105	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 16.

All (105) 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)
6:A:1215:CLR:C14	6:A:1215:CLR:C8	1.78	1.61
6:A:1213:CLR:C7	6:A:1213:CLR:C8	1.75	1.59
6:A:1213:CLR:C8	6:A:1213:CLR:C14	1.78	1.58
6:A:1214:CLR:C8	6:A:1214:CLR:C7	1.76	1.57
6:A:1214:CLR:C8	6:A:1214:CLR:C14	1.79	1.57
6:A:1215:CLR:C7	6:A:1215:CLR:C8	1.76	1.57
6:A:1214:CLR:C13	6:A:1214:CLR:C17	1.81	1.42
6:A:1213:CLR:C13	6:A:1213:CLR:C17	1.81	1.41
6:A:1215:CLR:C13	6:A:1215:CLR:C17	1.82	1.36
1:A:108:ILE:O	1:A:108:ILE:HD12	1.45	1.16
1:A:123:GLY:O	1:A:127:ILE:HD12	1.54	1.04
1:A:1013:ASN:HD21	1:A:1032:LYS:HB2	1.13	1.03
1:A:1074:ASP:HA	1:A:1077:LYS:HE2	1.48	0.95
1:A:123:GLY:O	1:A:127:ILE:CD1	2.15	0.94
6:A:1214:CLR:C17	6:A:1214:CLR:C18	2.46	0.93
6:A:1213:CLR:H14	6:A:1213:CLR:C8	1.99	0.92
6:A:1215:CLR:C8	6:A:1215:CLR:H14	2.00	0.91
6:A:1213:CLR:C17	6:A:1213:CLR:C18	2.49	0.90
6:A:1214:CLR:C8	6:A:1214:CLR:H14	1.98	0.90
1:A:1017:ILE:HD12	1:A:1026:VAL:HG23	1.58	0.85
1:A:45:VAL:HA	1:A:48:LEU:CD2	2.05	0.85
6:A:1215:CLR:C17	6:A:1215:CLR:C18	2.54	0.85
1:A:108:ILE:HD13	1:A:111:ARG:HB3	1.60	0.82
1:A:1021:ASP:HB2	1:A:1025:GLN:HE22	1.43	0.82
1:A:1013:ASN:ND2	1:A:1032:LYS:HB2	1.96	0.80
1:A:108:ILE:CD1	1:A:108:ILE:O	2.29	0.79
1:A:42:ASN:HA	1:A:45:VAL:HG12	1.65	0.78
6:A:1213:CLR:C6	6:A:1213:CLR:C8	2.36	0.78
1:A:1041:GLN:HB3	1:A:1042:LYS:HE2	1.67	0.77
6:A:1215:CLR:C6	6:A:1215:CLR:C8	2.40	0.77
6:A:1213:CLR:C9	6:A:1213:CLR:C7	2.46	0.75
4:A:1210:OLB:H26	5:A:1212:OLC:H10	1.69	0.73
6:A:1215:CLR:C7	6:A:1215:CLR:C9	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD22	1:A:110:LEU:H	1.59	0.67
1:A:298:THR:O	1:A:302:ILE:HG13	1.95	0.66
1:A:106:ILE:HD11	1:A:228:GLU:HB3	1.76	0.66
1:A:1065:PHE:O	1:A:1069:VAL:HG12	1.98	0.63
1:A:300:ARG:HD2	1:A:304:ARG:HH11	1.65	0.62
1:A:42:ASN:HA	1:A:45:VAL:CG1	2.29	0.62
1:A:65:THR:HG22	3:A:1202:OLA:H71	1.80	0.61
1:A:1101:TYR:O	1:A:1104:LYS:HG3	2.01	0.61
6:A:1214:CLR:H181	6:A:1214:CLR:C16	2.27	0.61
1:A:61:PRO:O	1:A:65:THR:HG23	2.01	0.59
1:A:1068:LEU:HD22	1:A:1102:ILE:HG12	1.84	0.59
1:A:45:VAL:O	1:A:48:LEU:HD23	2.03	0.57
1:A:1062:ARG:NH1	1:A:1066:ASP:OD2	2.37	0.57
6:A:1213:CLR:C16	6:A:1213:CLR:H181	2.33	0.56
6:A:1214:CLR:C16	6:A:1214:CLR:C18	2.78	0.56
6:A:1214:CLR:C6	6:A:1214:CLR:C8	2.41	0.55
1:A:1017:ILE:HD12	1:A:1026:VAL:CG2	2.34	0.55
1:A:1017:ILE:CD1	1:A:1026:VAL:HA	2.38	0.54
1:A:45:VAL:HA	1:A:48:LEU:HD21	1.87	0.54
6:A:1213:CLR:C9	6:A:1213:CLR:C14	2.48	0.54
1:A:123:GLY:O	1:A:127:ILE:HD13	2.08	0.53
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.43	0.53
6:A:1214:CLR:C9	6:A:1214:CLR:C14	2.47	0.52
6:A:1213:CLR:C7	6:A:1213:CLR:C14	2.86	0.52
1:A:1010:LEU:HD12	1:A:1033:MET:HG2	1.92	0.52
6:A:1214:CLR:C9	6:A:1214:CLR:C7	2.48	0.51
1:A:1017:ILE:CD1	1:A:1029:ALA:HB3	2.41	0.51
6:A:1213:CLR:C16	6:A:1213:CLR:C18	2.83	0.51
6:A:1215:CLR:C16	6:A:1215:CLR:C18	2.82	0.50
1:A:1106:LEU:HD11	1:A:222:ARG:HH21	1.77	0.50
1:A:227:LYS:HD2	1:A:227:LYS:O	2.11	0.50
3:A:1202:OLA:H152	5:A:1211:OLC:H13	1.95	0.49
6:A:1214:CLR:C18	6:A:1214:CLR:C20	2.90	0.49
1:A:63:ALA:O	1:A:66:ILE:HG22	2.12	0.48
6:A:1215:CLR:C14	6:A:1215:CLR:C9	2.47	0.48
1:A:1017:ILE:HD11	1:A:1029:ALA:HB3	1.96	0.48
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.79	0.48
6:A:1213:CLR:C20	6:A:1213:CLR:C18	2.91	0.48
1:A:289:ALA:O	1:A:296:ARG:HB2	2.14	0.47
1:A:108:ILE:HD13	1:A:111:ARG:CB	2.39	0.47
1:A:120:ARG:O	1:A:124:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1215:CLR:H273	6:A:1215:CLR:H231	1.76	0.47
1:A:293:ARG:HE	1:A:296:ARG:HH22	1.63	0.47
1:A:1063:HIS:CE1	1:A:1067:ILE:HD11	2.50	0.47
6:A:1215:CLR:H181	6:A:1215:CLR:C16	2.33	0.47
1:A:1027:LYS:HD2	1:A:1080:ASN:OD1	2.16	0.46
1:A:1067:ILE:O	1:A:1071:GLN:HG3	2.16	0.46
1:A:1014:LEU:O	1:A:1018:GLU:HG2	2.16	0.46
6:A:1215:CLR:C14	6:A:1215:CLR:C7	2.90	0.46
1:A:1017:ILE:HD12	1:A:1026:VAL:HA	1.99	0.45
1:A:65:THR:HG22	3:A:1202:OLA:C7	2.47	0.45
1:A:1004:GLU:OE2	1:A:222:ARG:NH2	2.50	0.44
6:A:1214:CLR:H181	6:A:1214:CLR:H152	1.73	0.44
1:A:1034:ARG:HH21	1:A:1073:ASP:CG	2.20	0.44
1:A:1023:ALA:HB1	1:A:1079:ALA:O	2.19	0.43
1:A:127:ILE:H	1:A:127:ILE:HD12	1.83	0.43
1:A:1023:ALA:HA	1:A:1026:VAL:HG12	1.99	0.43
1:A:206:ARG:HA	1:A:206:ARG:HD3	1.62	0.43
1:A:96:LEU:O	1:A:100:ILE:HG13	2.19	0.43
1:A:40:VAL:HG21	1:A:116:VAL:CG1	2.49	0.42
1:A:66:ILE:HD12	1:A:166:CYS:SG	2.60	0.42
6:A:1215:CLR:H181	6:A:1215:CLR:H152	1.63	0.42
1:A:1092:GLU:O	1:A:1095:LYS:HB2	2.19	0.41
1:A:300:ARG:O	1:A:304:ARG:HG3	2.20	0.41
1:A:185:CYS:O	1:A:189:PRO:HG2	2.21	0.41
6:A:1214:CLR:C14	6:A:1214:CLR:C7	2.92	0.41
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.93	0.40
1:A:1089:ALA:HA	1:A:1092:GLU:OE1	2.21	0.40
1:A:40:VAL:HG21	1:A:116:VAL:HG12	2.02	0.40
1:A:1106:LEU:HD11	1:A:222:ARG:NH2	2.36	0.40
1:A:110:LEU:H	1:A:110:LEU:CD2	2.32	0.40
1:A:267:LEU:HA	1:A:267:LEU:HD12	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	384/433 (89%)	375 (98%)	8 (2%)	1 (0%)	41	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1064	GLY

### 5.3.2 Protein sidechains ⓘ

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	312/353 (88%)	307 (98%)	5 (2%)	62	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	206	ARG
1	A	1077	LYS
1	A	1083	LYS
1	A	1104	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	ASN
1	A	1093	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	CLR	A	1213	-	31,31,31	9.08	20 (64%)	48,48,48	3.66	21 (43%)
3	OLA	A	1205	-	14,17,19	0.74	1 (7%)	13,17,19	0.61	0
2	ZMA	A	1201	-	21,28,28	2.05	4 (19%)	22,39,39	2.81	9 (40%)
3	OLA	A	1202	-	16,19,19	0.73	1 (6%)	15,19,19	0.58	0
6	CLR	A	1215	-	31,31,31	9.16	22 (70%)	48,48,48	3.62	21 (43%)
5	OLC	A	1212	-	18,18,24	0.95	1 (5%)	18,19,25	1.13	2 (11%)
3	OLA	A	1206	-	9,9,19	1.04	1 (11%)	8,8,19	0.71	0
3	OLA	A	1208	-	13,16,19	0.86	1 (7%)	12,16,19	0.55	0
6	CLR	A	1214	-	31,31,31	9.07	19 (61%)	48,48,48	3.63	22 (45%)
5	OLC	A	1211	-	24,24,24	0.81	2 (8%)	25,25,25	1.17	2 (8%)
3	OLA	A	1203	-	11,14,19	0.86	1 (9%)	10,14,19	0.66	0
3	OLA	A	1207	-	6,6,19	0.32	0	5,5,19	0.42	0
4	OLB	A	1210	-	19,19,24	0.93	1 (5%)	20,20,25	1.21	1 (5%)
3	OLA	A	1204	-	5,8,19	0.32	0	4,8,19	0.80	0
4	OLB	A	1209	-	18,18,24	0.89	1 (5%)	18,19,25	1.21	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	A	1213	-	2/2/10/11	3/10/68/68	0/4/4/4
3	OLA	A	1205	-	-	11/13/15/17	-
2	ZMA	A	1201	-	-	0/6/10/10	0/4/4/4
6	CLR	A	1214	-	2/2/10/11	3/10/68/68	0/4/4/4
5	OLC	A	1212	-	-	7/18/18/24	-
3	OLA	A	1206	-	-	4/7/7/17	-
3	OLA	A	1203	-	-	5/10/12/17	-
3	OLA	A	1208	-	-	8/12/14/17	-
3	OLA	A	1202	-	-	10/15/17/17	-
5	OLC	A	1211	-	-	12/24/24/24	-
6	CLR	A	1215	-	2/2/10/11	1/10/68/68	0/4/4/4
3	OLA	A	1207	-	-	2/4/4/17	-
4	OLB	A	1210	-	-	8/19/19/24	-
3	OLA	A	1204	-	-	2/4/6/17	-
4	OLB	A	1209	-	-	5/18/18/24	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1213	CLR	C8-C9	-21.43	1.12	1.53
6	A	1215	CLR	C8-C9	-21.42	1.12	1.53
6	A	1214	CLR	C8-C9	-21.35	1.12	1.53
6	A	1213	CLR	C13-C14	-18.89	1.19	1.55
6	A	1215	CLR	C13-C14	-18.60	1.19	1.55
6	A	1214	CLR	C13-C14	-18.30	1.20	1.55
6	A	1213	CLR	C7-C6	-16.94	1.13	1.50
6	A	1214	CLR	C7-C6	-16.74	1.14	1.50
6	A	1215	CLR	C7-C6	-16.63	1.14	1.50
6	A	1213	CLR	C12-C13	-16.30	1.24	1.54
6	A	1215	CLR	C12-C13	-16.22	1.25	1.54
6	A	1214	CLR	C12-C13	-15.99	1.25	1.54
6	A	1215	CLR	C11-C9	-14.64	1.29	1.53
6	A	1214	CLR	C11-C9	-14.58	1.29	1.53
6	A	1215	CLR	C13-C17	14.35	1.82	1.55
6	A	1213	CLR	C11-C9	-14.30	1.29	1.53
6	A	1213	CLR	C13-C17	14.10	1.81	1.55
6	A	1214	CLR	C13-C17	13.98	1.81	1.55
6	A	1215	CLR	C10-C9	-13.84	1.32	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1214	CLR	C7-C8	13.74	1.76	1.53
6	A	1214	CLR	C8-C14	13.70	1.79	1.53
6	A	1215	CLR	C7-C8	13.63	1.76	1.53
6	A	1213	CLR	C7-C8	13.24	1.75	1.53
6	A	1215	CLR	C8-C14	13.23	1.78	1.53
6	A	1214	CLR	C10-C9	-12.94	1.34	1.56
6	A	1213	CLR	C8-C14	12.77	1.78	1.53
6	A	1213	CLR	C10-C9	-12.71	1.34	1.56
6	A	1215	CLR	C15-C14	8.54	1.72	1.54
6	A	1214	CLR	C15-C14	8.39	1.71	1.54
6	A	1213	CLR	C15-C14	8.31	1.71	1.54
6	A	1214	CLR	C12-C11	7.15	1.68	1.53
6	A	1213	CLR	C12-C11	7.04	1.68	1.53
6	A	1215	CLR	C12-C11	6.74	1.67	1.53
6	A	1213	CLR	C20-C17	-6.30	1.43	1.54
2	A	1201	ZMA	C11-N10	6.23	1.43	1.34
6	A	1214	CLR	C20-C17	-6.13	1.43	1.54
6	A	1215	CLR	C20-C17	-5.96	1.44	1.54
6	A	1215	CLR	C4-C3	5.88	1.62	1.52
6	A	1213	CLR	C4-C3	5.38	1.61	1.52
6	A	1214	CLR	C4-C3	5.09	1.61	1.52
6	A	1213	CLR	C1-C10	4.89	1.63	1.54
2	A	1201	ZMA	C14-N15	4.89	1.44	1.34
6	A	1214	CLR	C1-C10	4.36	1.62	1.54
6	A	1215	CLR	C1-C10	4.32	1.62	1.54
6	A	1214	CLR	C16-C17	-4.18	1.45	1.54
6	A	1215	CLR	C16-C17	-4.13	1.45	1.54
6	A	1215	CLR	C19-C10	4.07	1.61	1.54
6	A	1213	CLR	C16-C17	-3.72	1.46	1.54
6	A	1213	CLR	C22-C20	3.65	1.63	1.54
2	A	1201	ZMA	C21-C20	-3.51	1.38	1.48
6	A	1213	CLR	C19-C10	3.31	1.60	1.54
6	A	1215	CLR	C22-C20	3.16	1.62	1.54
6	A	1214	CLR	C19-C10	3.12	1.59	1.54
5	A	1212	OLC	O20-C1	3.01	1.42	1.33
3	A	1206	OLA	C9-C10	2.97	1.48	1.28
6	A	1214	CLR	C22-C20	2.96	1.62	1.54
3	A	1208	OLA	C10-C9	2.83	1.48	1.31
4	A	1210	OLB	O20-C1	2.83	1.41	1.33
6	A	1213	CLR	C10-C5	2.80	1.58	1.52
3	A	1203	OLA	C10-C9	2.71	1.47	1.31
3	A	1202	OLA	C10-C9	2.62	1.47	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	OLA	C10-C9	2.58	1.46	1.31
6	A	1215	CLR	O1-C3	-2.58	1.35	1.43
6	A	1214	CLR	O1-C3	-2.55	1.35	1.43
6	A	1213	CLR	C2-C3	2.51	1.57	1.51
4	A	1209	OLB	O20-C1	2.49	1.40	1.33
6	A	1214	CLR	C10-C5	2.37	1.57	1.52
5	A	1211	OLC	O20-C1	2.32	1.40	1.33
6	A	1213	CLR	O1-C3	-2.29	1.36	1.43
5	A	1211	OLC	O20-C21	-2.25	1.40	1.45
6	A	1215	CLR	C18-C13	2.24	1.58	1.54
6	A	1215	CLR	C6-C5	2.22	1.37	1.33
6	A	1215	CLR	C10-C5	2.12	1.57	1.52
6	A	1215	CLR	C4-C5	2.09	1.56	1.51
2	A	1201	ZMA	C14-N13	-2.04	1.32	1.34

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1215	CLR	C18-C13-C12	-13.11	89.88	110.59
6	A	1215	CLR	C12-C13-C14	11.72	125.46	107.27
6	A	1213	CLR	C18-C13-C12	-11.59	92.29	110.59
6	A	1214	CLR	C18-C13-C12	-11.34	92.68	110.59
6	A	1213	CLR	C12-C13-C14	10.95	124.26	107.27
6	A	1214	CLR	C12-C13-C14	10.68	123.84	107.27
6	A	1214	CLR	C18-C13-C17	-9.97	93.12	111.71
6	A	1213	CLR	C18-C13-C17	-9.10	94.75	111.71
6	A	1215	CLR	C18-C13-C17	-8.09	96.62	111.71
2	A	1201	ZMA	N17-C20-N19	-8.06	109.22	114.56
6	A	1214	CLR	C12-C13-C17	8.02	128.57	116.57
6	A	1213	CLR	C12-C13-C17	7.80	128.25	116.57
6	A	1215	CLR	C12-C13-C17	7.39	127.63	116.57
6	A	1214	CLR	C7-C8-C9	5.87	116.83	109.71
2	A	1201	ZMA	C9-C8-C7	-5.76	99.51	112.87
6	A	1213	CLR	C7-C8-C9	5.55	116.43	109.71
6	A	1213	CLR	C14-C8-C9	5.19	116.04	109.09
6	A	1214	CLR	C7-C6-C5	-5.03	115.78	125.06
2	A	1201	ZMA	C9-N10-C11	-4.86	115.35	123.75
6	A	1215	CLR	C7-C8-C9	4.85	115.58	109.71
6	A	1213	CLR	C7-C6-C5	-4.82	116.17	125.06
6	A	1214	CLR	C15-C14-C8	4.50	126.48	119.08
6	A	1215	CLR	C15-C14-C8	4.41	126.34	119.08
6	A	1213	CLR	C1-C10-C9	4.19	114.58	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1215	CLR	C7-C6-C5	-4.18	117.34	125.06
6	A	1215	CLR	C14-C8-C9	4.14	114.64	109.09
6	A	1213	CLR	C19-C10-C9	-3.98	106.93	111.68
6	A	1213	CLR	C11-C9-C10	3.86	118.17	113.08
6	A	1213	CLR	C15-C14-C8	3.78	125.31	119.08
6	A	1213	CLR	C18-C13-C14	-3.67	104.88	111.71
6	A	1214	CLR	C14-C8-C9	3.62	113.94	109.09
6	A	1215	CLR	C18-C13-C14	-3.56	105.07	111.71
6	A	1213	CLR	C8-C7-C6	-3.43	107.81	112.73
6	A	1215	CLR	C9-C10-C5	3.35	114.91	109.65
2	A	1201	ZMA	N12-C11-N13	-3.34	120.94	126.23
6	A	1214	CLR	C19-C10-C1	-3.19	104.38	109.43
6	A	1215	CLR	C4-C5-C6	3.17	125.18	120.61
6	A	1214	CLR	C10-C9-C8	3.14	117.44	112.73
6	A	1214	CLR	C9-C10-C5	3.08	114.48	109.65
5	A	1211	OLC	O20-C1-C2	3.07	121.53	111.91
4	A	1210	OLB	O20-C1-C2	3.06	121.50	111.91
6	A	1213	CLR	C16-C17-C13	-3.04	100.18	103.84
6	A	1214	CLR	C22-C20-C17	-3.02	104.05	110.28
6	A	1213	CLR	C9-C10-C5	3.00	114.36	109.65
4	A	1209	OLB	O20-C1-C2	3.00	121.33	111.91
6	A	1215	CLR	C16-C17-C13	-2.92	100.33	103.84
6	A	1214	CLR	C1-C10-C9	2.91	112.79	108.73
6	A	1214	CLR	C21-C20-C22	-2.89	105.83	110.36
6	A	1215	CLR	C10-C9-C8	2.75	116.86	112.73
6	A	1213	CLR	C19-C10-C1	-2.70	105.16	109.43
6	A	1213	CLR	C15-C16-C17	2.67	110.42	105.13
6	A	1215	CLR	C19-C10-C9	-2.66	108.51	111.68
6	A	1214	CLR	C19-C10-C5	-2.63	104.09	108.34
6	A	1215	CLR	C19-C10-C5	-2.61	104.11	108.34
6	A	1214	CLR	C11-C9-C10	2.59	116.48	113.08
6	A	1213	CLR	C17-C13-C14	2.54	103.09	100.07
6	A	1215	CLR	C22-C20-C17	-2.52	105.08	110.28
2	A	1201	ZMA	N15-C14-N13	2.52	120.34	117.03
6	A	1213	CLR	C22-C20-C17	-2.49	105.15	110.28
6	A	1214	CLR	C18-C13-C14	-2.44	107.17	111.71
5	A	1212	OLC	O20-C1-C2	2.43	119.53	111.91
2	A	1201	ZMA	C1-C2-C3	-2.39	117.25	119.88
6	A	1214	CLR	C16-C17-C13	-2.38	100.97	103.84
2	A	1201	ZMA	N15-C14-N16	2.38	119.57	117.97
6	A	1215	CLR	C11-C9-C10	2.35	116.18	113.08
6	A	1213	CLR	C16-C15-C14	-2.35	100.47	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1214	CLR	C23-C24-C25	-2.35	104.93	115.98
6	A	1215	CLR	C17-C13-C14	2.30	102.80	100.07
2	A	1201	ZMA	C5-C6-C7	-2.29	117.88	121.03
6	A	1214	CLR	C17-C13-C14	2.28	102.78	100.07
6	A	1214	CLR	C19-C10-C9	-2.26	108.99	111.68
5	A	1211	OLC	O20-C1-O19	-2.15	118.16	123.59
2	A	1201	ZMA	C21-C20-N17	2.14	127.19	123.44
6	A	1215	CLR	C15-C16-C17	2.14	109.38	105.13
6	A	1213	CLR	C15-C14-C13	2.12	106.40	103.84
6	A	1215	CLR	C4-C5-C10	-2.07	113.67	116.42
6	A	1214	CLR	C15-C16-C17	2.06	109.22	105.13
6	A	1215	CLR	C21-C20-C22	-2.04	107.17	110.36
5	A	1212	OLC	C5-C6-C7	-2.04	104.09	114.42

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1213	CLR	C8
6	A	1213	CLR	C9
6	A	1215	CLR	C8
6	A	1215	CLR	C9
6	A	1214	CLR	C8
6	A	1214	CLR	C9

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1205	OLA	C1-C2-C3-C4
3	A	1202	OLA	C1-C2-C3-C4
3	A	1208	OLA	C1-C2-C3-C4
5	A	1211	OLC	C21-C22-C24-O25
5	A	1211	OLC	O23-C22-C24-O25
3	A	1203	OLA	C1-C2-C3-C4
3	A	1204	OLA	C1-C2-C3-C4
4	A	1209	OLB	C21-C22-C24-O25
4	A	1210	OLB	O19-C1-O20-C21
4	A	1210	OLB	C2-C1-O20-C21
3	A	1205	OLA	C11-C10-C9-C8
3	A	1208	OLA	C11-C10-C9-C8
5	A	1212	OLC	C2-C1-O20-C21
4	A	1209	OLB	O23-C22-C24-O25
5	A	1212	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
6	A	1215	CLR	C22-C23-C24-C25
3	A	1206	OLA	C12-C13-C14-C15
4	A	1210	OLB	C3-C4-C5-C6
6	A	1214	CLR	C23-C24-C25-C26
3	A	1202	OLA	C3-C4-C5-C6
3	A	1203	OLA	C5-C6-C7-C8
4	A	1210	OLB	C2-C3-C4-C5
4	A	1210	OLB	C5-C6-C7-C8
5	A	1211	OLC	C4-C5-C6-C7
3	A	1208	OLA	C3-C4-C5-C6
6	A	1214	CLR	C23-C24-C25-C27
3	A	1203	OLA	C3-C4-C5-C6
3	A	1205	OLA	C2-C3-C4-C5
5	A	1211	OLC	C3-C4-C5-C6
3	A	1202	OLA	C4-C5-C6-C7
3	A	1202	OLA	C11-C12-C13-C14
3	A	1208	OLA	C4-C5-C6-C7
5	A	1211	OLC	C14-C15-C16-C17
5	A	1211	OLC	C11-C12-C13-C14
5	A	1211	OLC	C6-C7-C8-C9
4	A	1210	OLB	C6-C7-C8-C9
6	A	1214	CLR	C21-C20-C22-C23
3	A	1206	OLA	C11-C12-C13-C14
3	A	1205	OLA	C4-C5-C6-C7
4	A	1209	OLB	C4-C5-C6-C7
4	A	1210	OLB	C7-C8-C9-C10
3	A	1205	OLA	C3-C4-C5-C6
5	A	1211	OLC	C10-C11-C12-C13
5	A	1211	OLC	C12-C13-C14-C15
3	A	1208	OLA	C2-C3-C4-C5
5	A	1212	OLC	C2-C3-C4-C5
4	A	1209	OLB	C3-C4-C5-C6
5	A	1212	OLC	O20-C21-C22-C24
6	A	1213	CLR	C21-C20-C22-C23
3	A	1205	OLA	C12-C13-C14-C15
6	A	1213	CLR	C23-C24-C25-C26
5	A	1212	OLC	C9-C10-C11-C12
3	A	1204	OLA	C3-C4-C5-C6
6	A	1213	CLR	C23-C24-C25-C27
5	A	1211	OLC	C5-C6-C7-C8
3	A	1207	OLA	C3-C4-C5-C6
3	A	1205	OLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	1202	OLA	C14-C15-C16-C17
3	A	1202	OLA	C13-C14-C15-C16
5	A	1212	OLC	C5-C6-C7-C8
3	A	1205	OLA	C9-C10-C11-C12
3	A	1206	OLA	C9-C10-C11-C12
5	A	1211	OLC	C15-C16-C17-C18
3	A	1202	OLA	C11-C10-C9-C8
3	A	1203	OLA	C4-C5-C6-C7
5	A	1212	OLC	O20-C21-C22-O23
3	A	1207	OLA	C6-C7-C8-C9
3	A	1205	OLA	C13-C14-C15-C16
3	A	1206	OLA	C10-C11-C12-C13
3	A	1202	OLA	C10-C11-C12-C13
4	A	1209	OLB	C9-C10-C11-C12
3	A	1208	OLA	C5-C6-C7-C8
3	A	1208	OLA	C9-C10-C11-C12
5	A	1211	OLC	C7-C8-C9-C10
3	A	1202	OLA	C7-C8-C9-C10
3	A	1208	OLA	C7-C8-C9-C10
3	A	1205	OLA	C10-C11-C12-C13
3	A	1202	OLA	C9-C10-C11-C12
3	A	1203	OLA	C9-C10-C11-C12
4	A	1210	OLB	C9-C10-C11-C12
3	A	1205	OLA	C7-C8-C9-C10

There are no ring outliers.

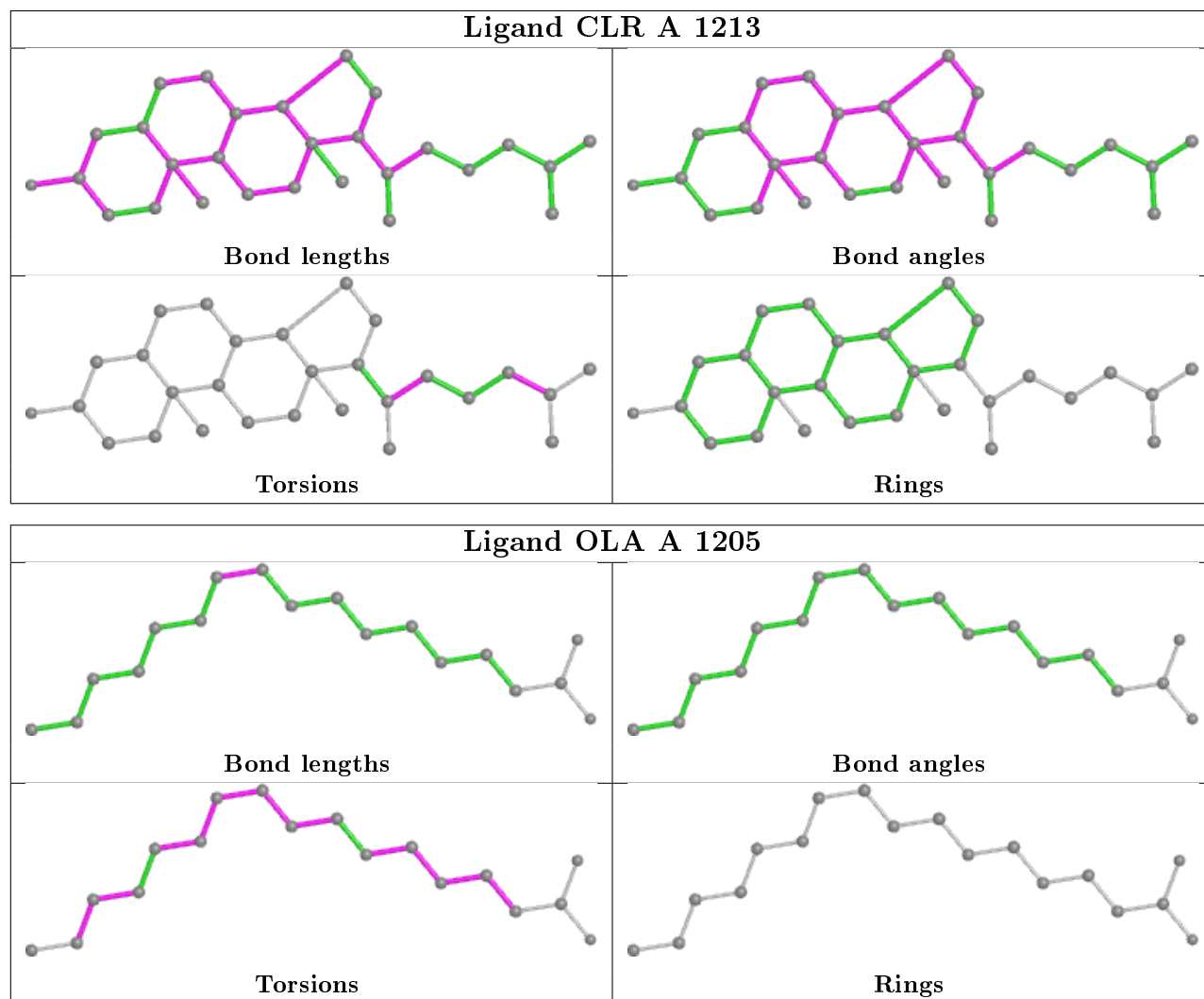
7 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1213	CLR	12	0
3	A	1202	OLA	3	0
6	A	1215	CLR	13	0
5	A	1212	OLC	1	0
6	A	1214	CLR	13	0
5	A	1211	OLC	1	0
4	A	1210	OLB	1	0

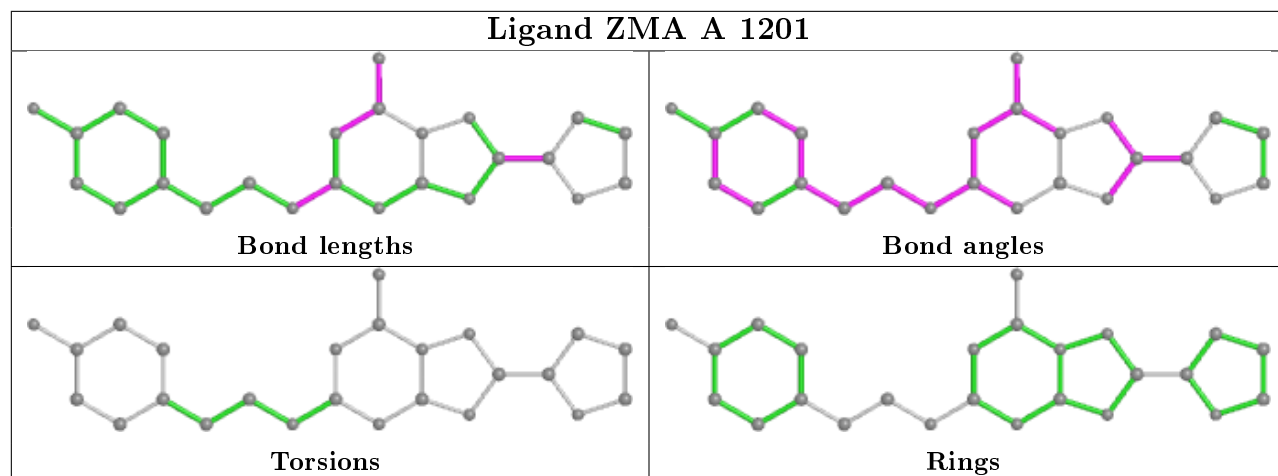
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



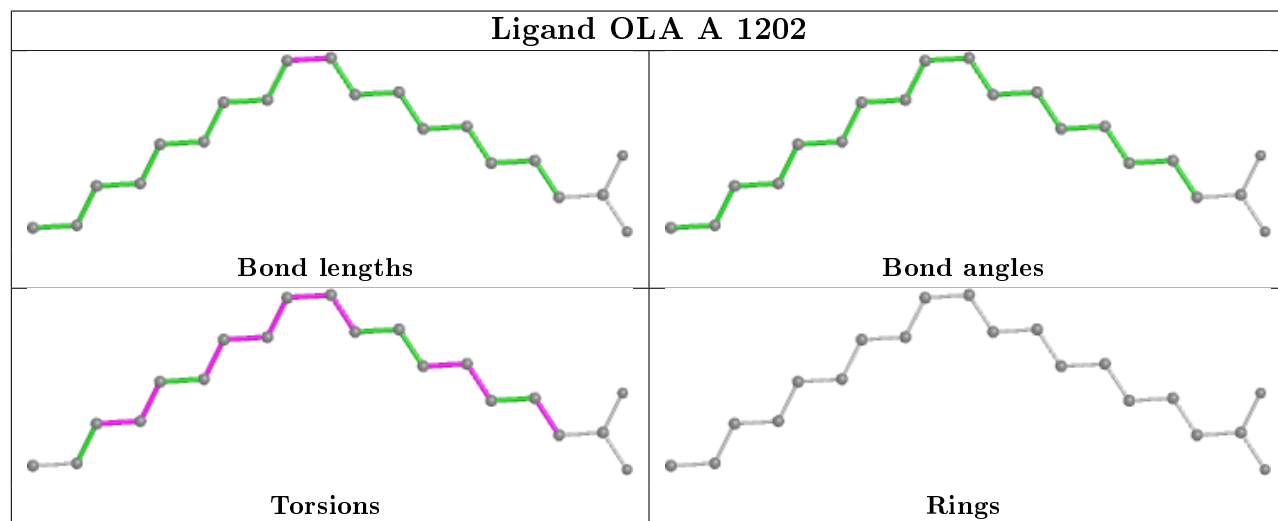
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



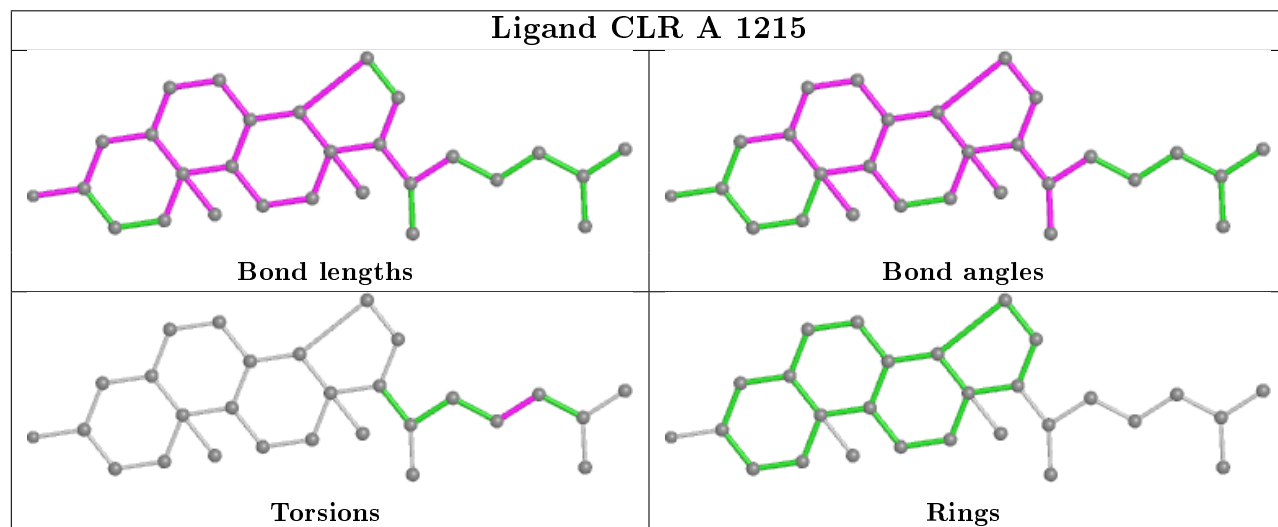
## Ligand ZMA A 1201

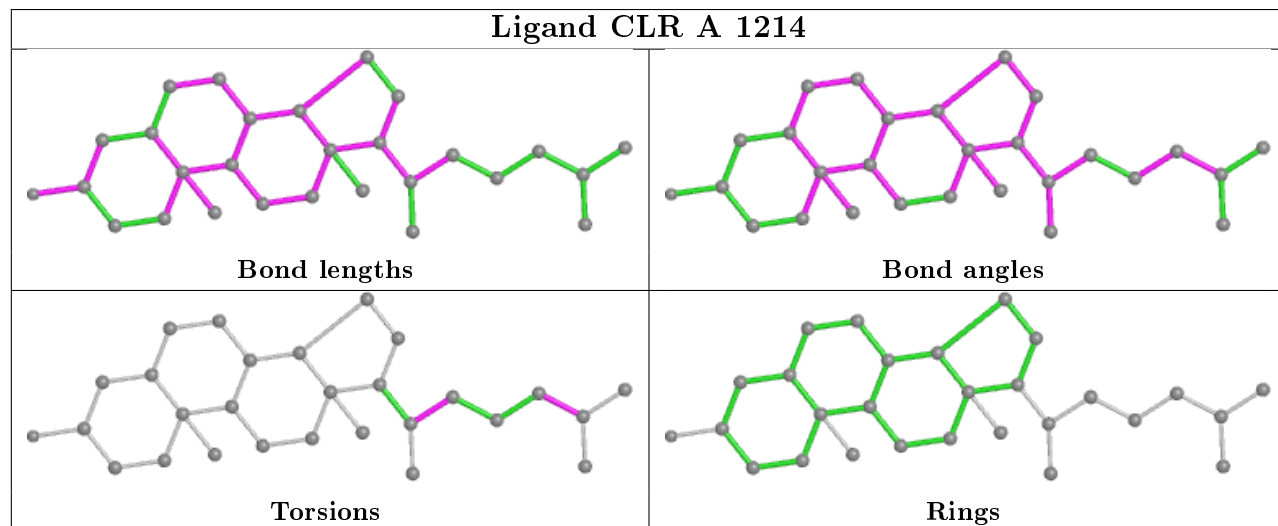
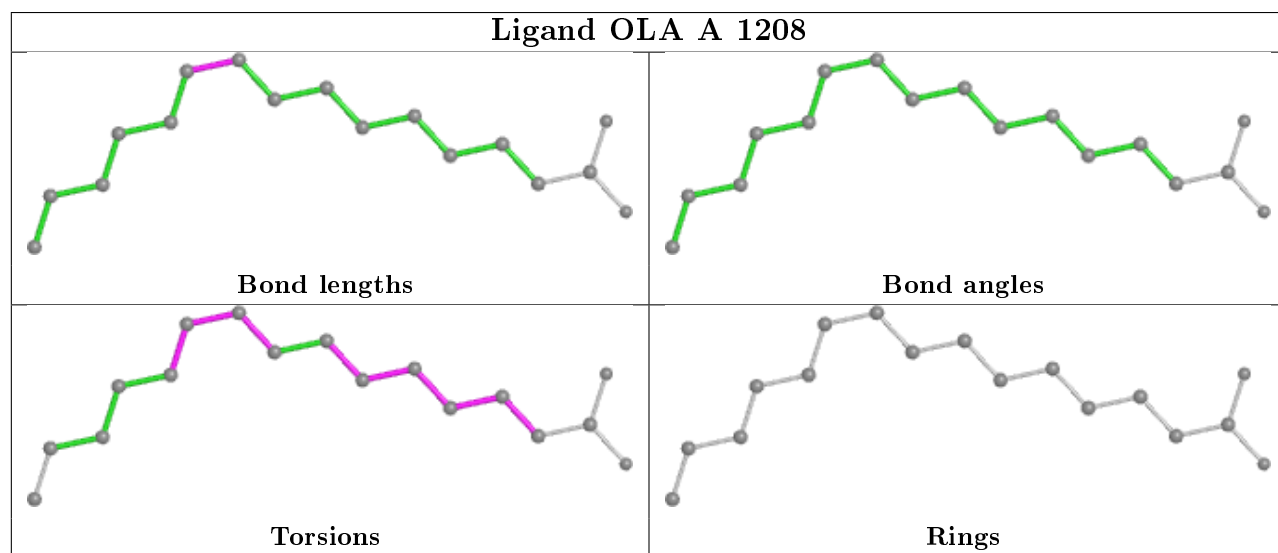
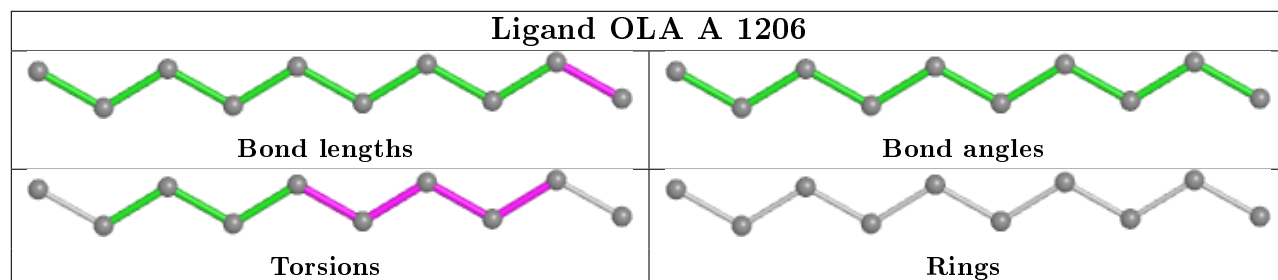
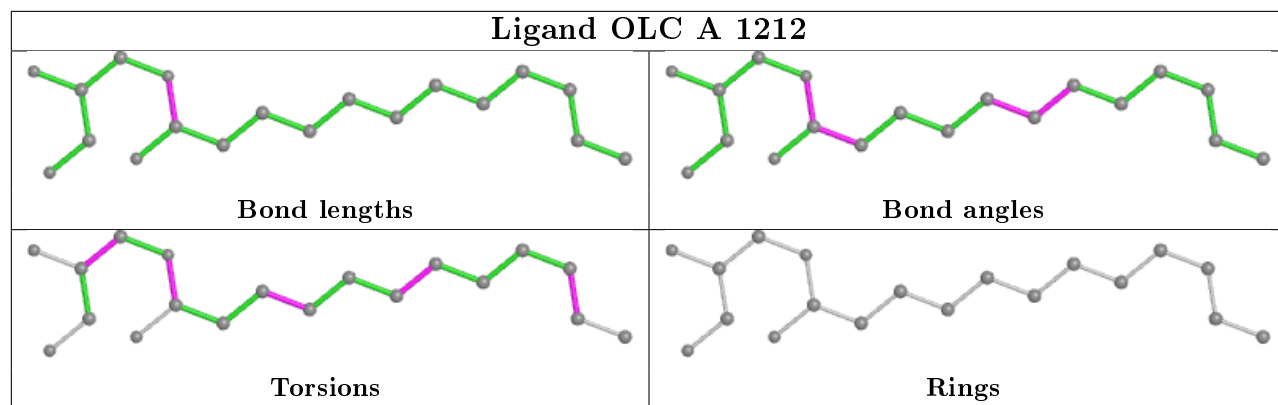


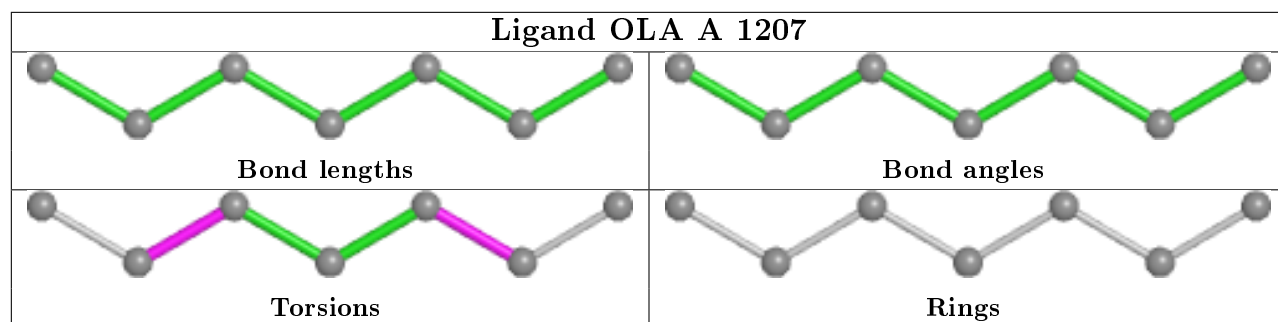
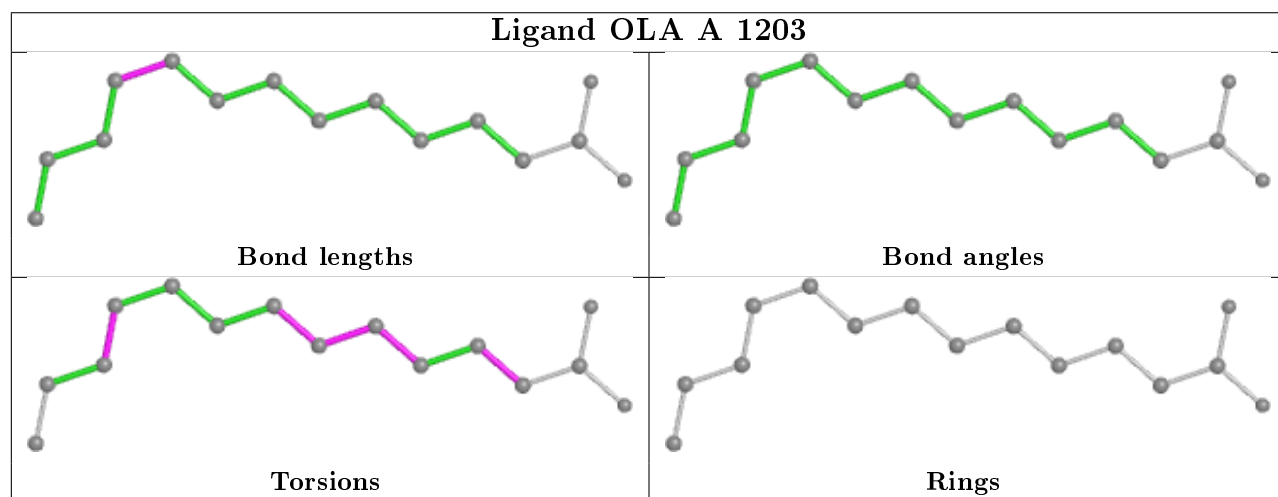
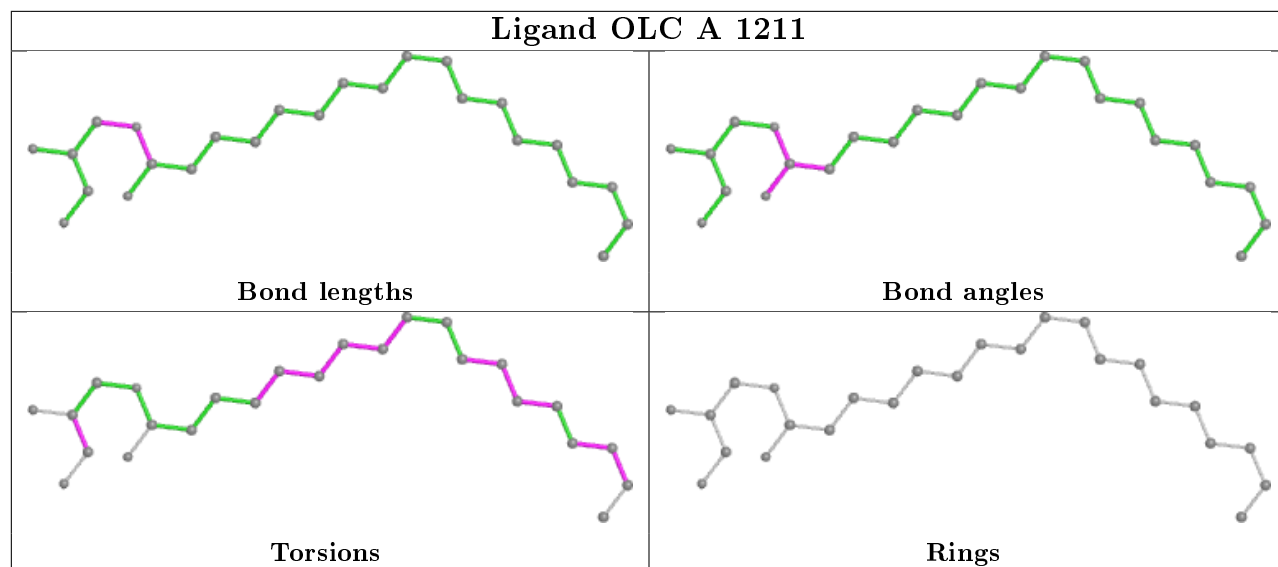
## Ligand OLA A 1202

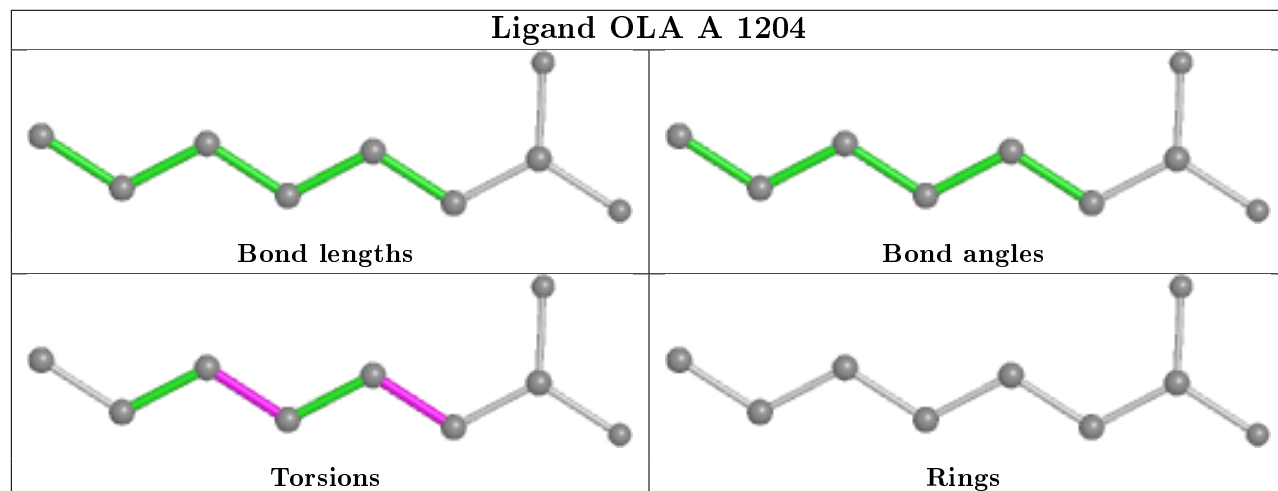
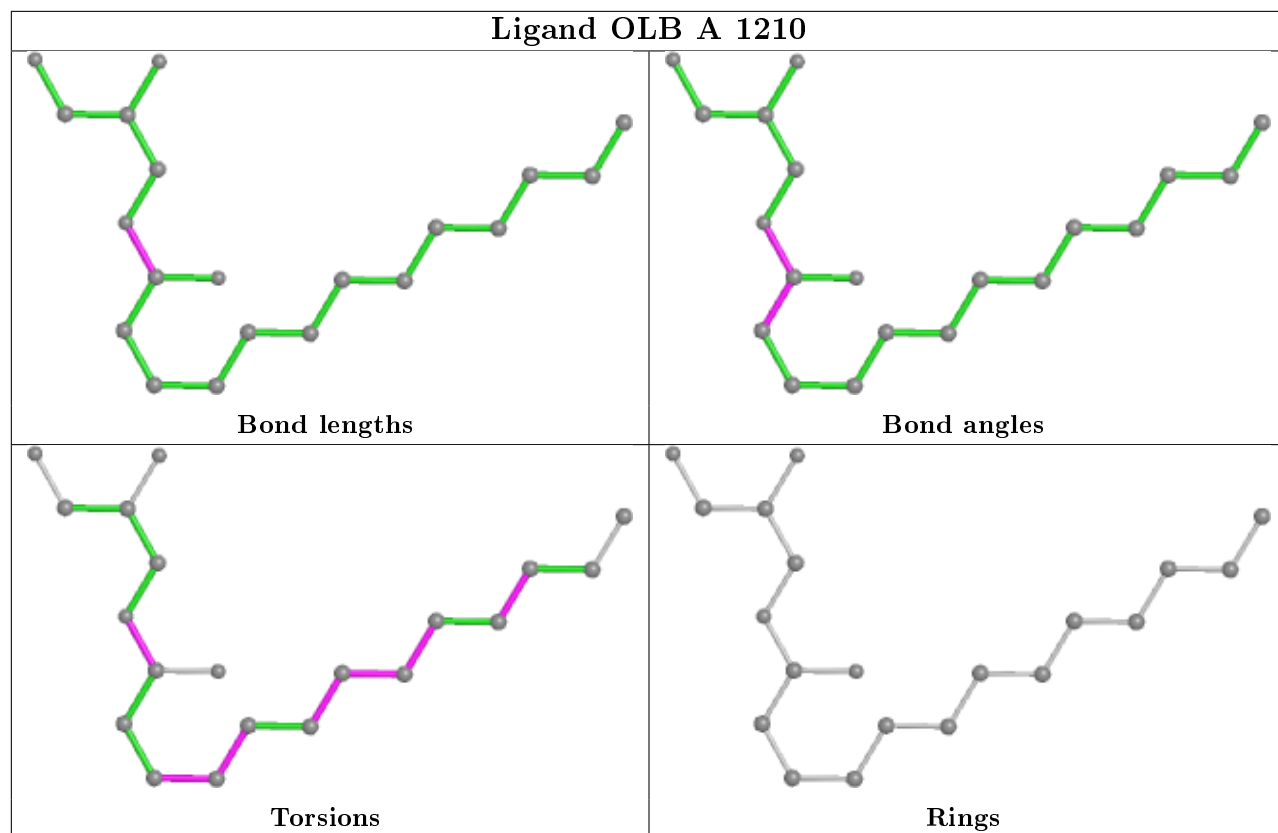


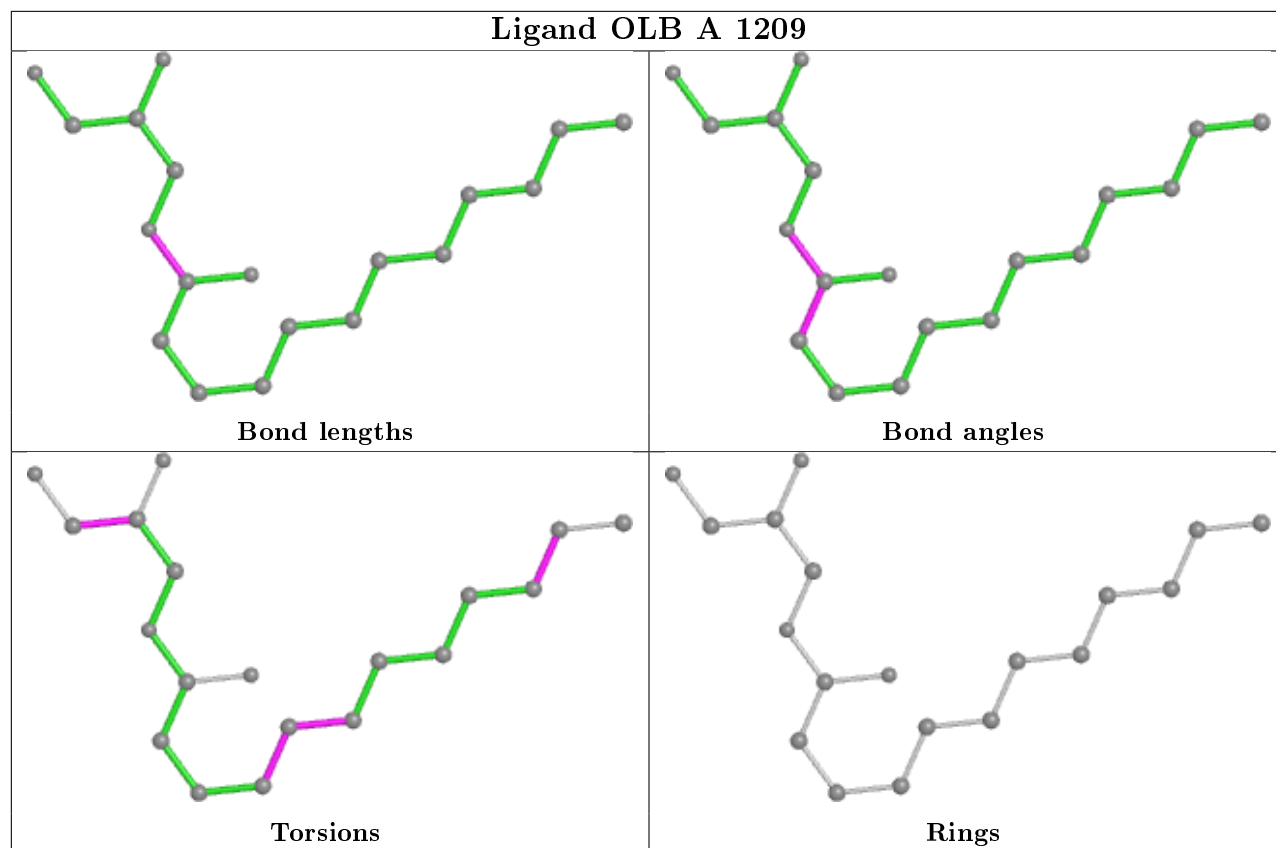
## Ligand CLR A 1215











## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/433 (89%)	1.19	80 (20%) <b>1</b> <b>1</b>	68, 93, 136, 175	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1091	ALA	8.5
1	A	1060	ASP	8.0
1	A	1061	PHE	7.2
1	A	111	ARG	6.8
1	A	1062	ARG	6.8
1	A	1101	TYR	6.3
1	A	1058	MET	6.0
1	A	-1	GLY	5.5
1	A	1059	LYS	5.4
1	A	1090	ALA	4.9
1	A	1087	ALA	4.8
1	A	1020	ALA	4.8
1	A	1026	VAL	4.7
1	A	1095	LYS	4.7
1	A	1016	VAL	4.6
1	A	1092	GLU	4.6
1	A	1063	HIS	4.5
1	A	225	LEU	4.4
1	A	304	ARG	4.2
1	A	1021	ASP	4.2
1	A	1030	LEU	4.2
1	A	1029	ALA	4.0
1	A	1064	GLY	3.9
1	A	1013	ASN	3.8
1	A	1077	LYS	3.8
1	A	1094	LEU	3.6
1	A	1019	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1007	TRP	3.4
1	A	134	ALA	3.3
1	A	112	TYR	3.3
1	A	282	VAL	3.2
1	A	138	THR	3.2
1	A	1006	ASN	3.1
1	A	1105	TYR	3.1
1	A	1100	ALA	3.0
1	A	1017	ILE	3.0
1	A	262	CYS	2.9
1	A	135	ILE	2.9
1	A	1003	LEU	2.9
1	A	1099	ASN	2.9
1	A	263	SER	2.8
1	A	1009	THR	2.8
1	A	1102	ILE	2.7
1	A	1085	LYS	2.7
1	A	139	PRO	2.6
1	A	226	GLN	2.6
1	A	1024	ALA	2.6
1	A	144	ASN	2.6
1	A	154	ALA	2.6
1	A	1033	MET	2.6
1	A	197	TYR	2.5
1	A	206	ARG	2.5
1	A	143	TRP	2.5
1	A	137	LEU	2.5
1	A	1022	ASN	2.4
1	A	38	GLN	2.4
1	A	222	ARG	2.4
1	A	292	ILE	2.4
1	A	1097	THR	2.3
1	A	108	ILE	2.3
1	A	1074	ASP	2.3
1	A	283	VAL	2.3
1	A	176	TYR	2.3
1	A	1066	ASP	2.3
1	A	1084	VAL	2.3
1	A	136	GLY	2.2
1	A	5	GLY	2.2
1	A	156	SER	2.2
1	A	1106	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	2.2
1	A	82	CYS	2.2
1	A	296	ARG	2.1
1	A	1011	ASN	2.1
1	A	1018	GLU	2.1
1	A	107	ALA	2.1
1	A	1023	ALA	2.1
1	A	32	TRP	2.1
1	A	220	ARG	2.1
1	A	1075	ALA	2.0
1	A	1025	GLN	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<sup>th</sup> 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.

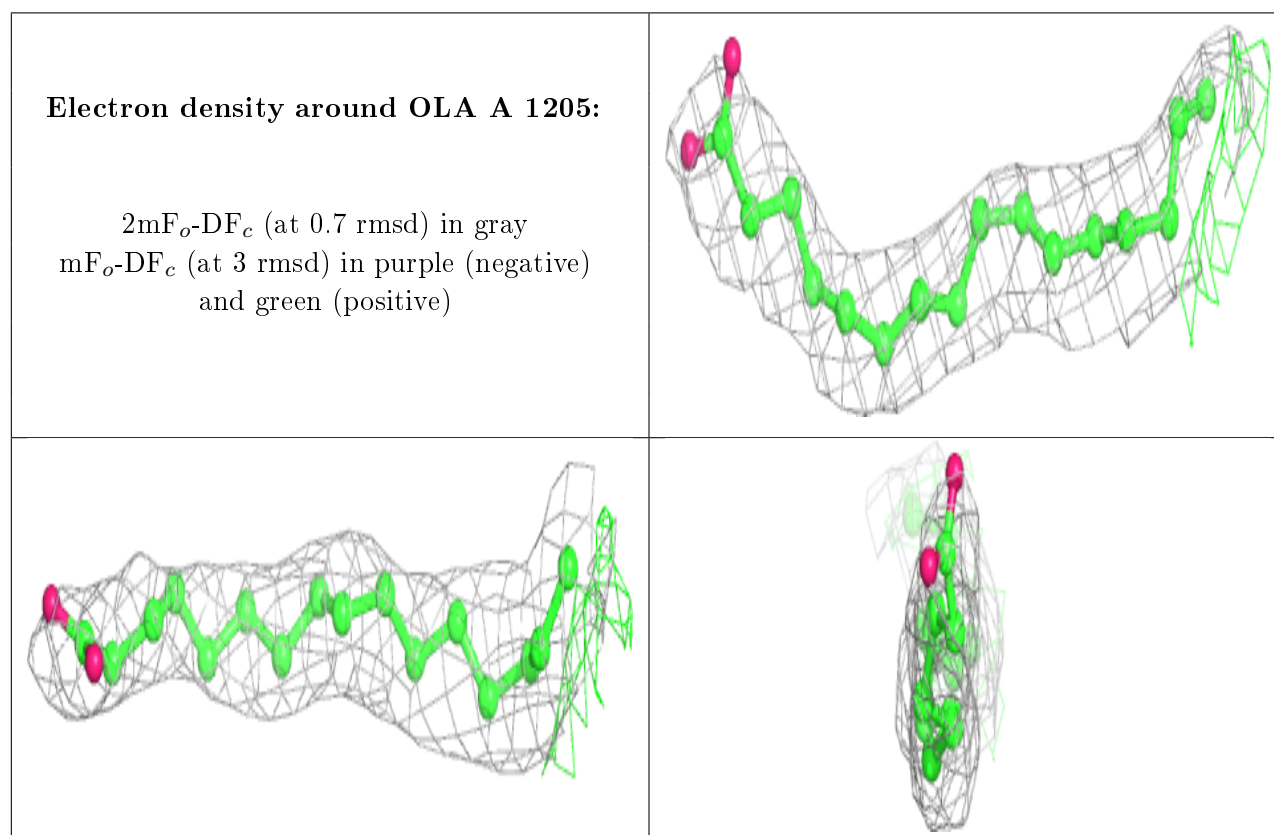
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OLA	A	1205	18/20	0.63	0.54	92,102,114,119	0
3	OLA	A	1203	15/20	0.66	0.18	103,107,120,125	0
5	OLC	A	1212	19/25	0.71	0.35	94,106,125,127	0
3	OLA	A	1204	9/20	0.71	0.34	93,97,105,116	0
3	OLA	A	1202	20/20	0.72	0.35	90,109,120,128	0
4	OLB	A	1210	20/25	0.75	0.41	104,116,121,125	0
3	OLA	A	1208	17/20	0.78	0.36	93,100,108,115	0
5	OLC	A	1211	25/25	0.81	0.56	92,104,120,124	0
4	OLB	A	1209	19/25	0.81	0.23	87,101,119,120	0
3	OLA	A	1207	7/20	0.83	0.37	89,96,100,104	0
6	CLR	A	1213	28/28	0.86	0.29	92,100,110,120	0
6	CLR	A	1215	28/28	0.86	0.28	88,97,108,110	0

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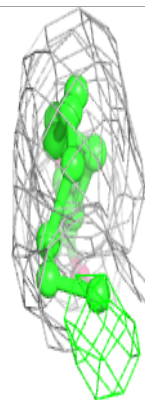
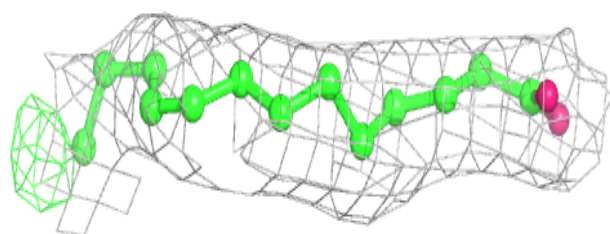
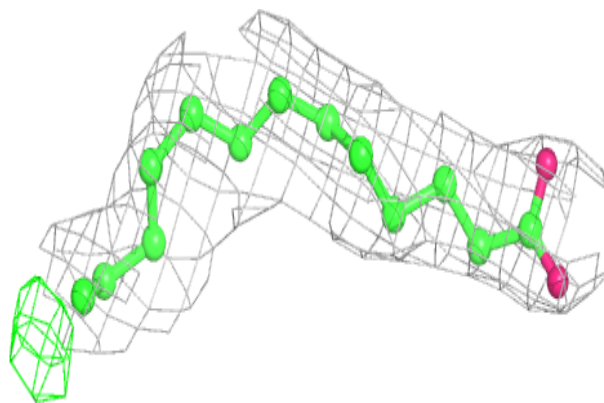
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OLA	A	1206	10/20	0.89	0.41	83,91,95,100	0
6	CLR	A	1214	28/28	0.92	0.23	90,97,101,114	0
2	ZMA	A	1201	25/25	0.93	0.28	69,77,91,105	0

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.

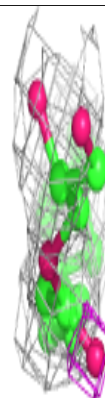
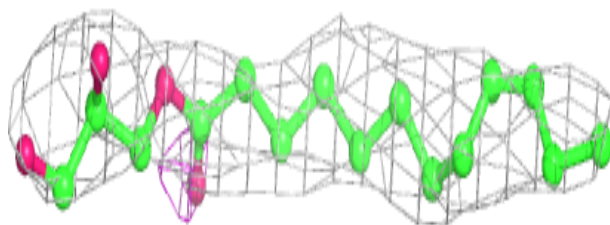
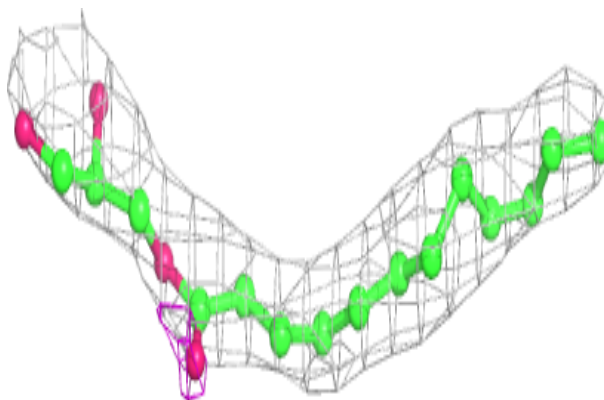


**Electron density around OLA A 1203:**

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

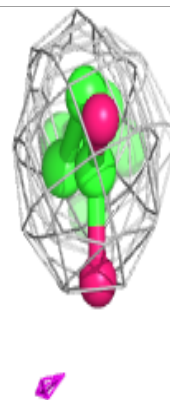
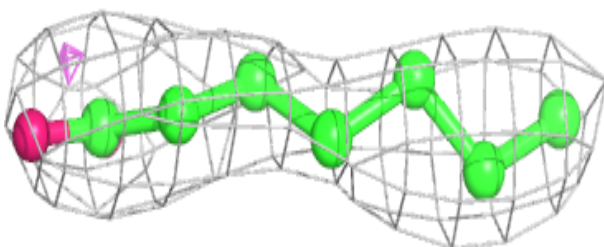
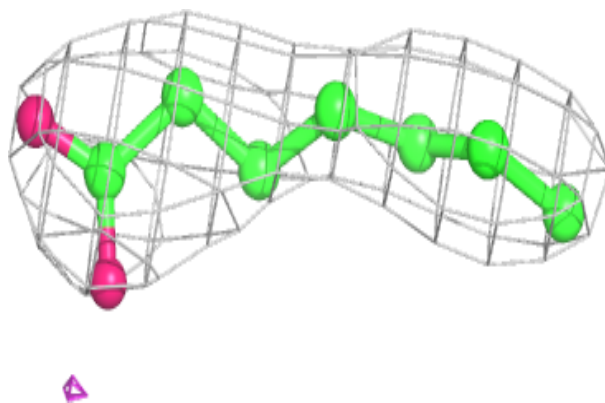
**Electron density around OLC A 1212:**

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

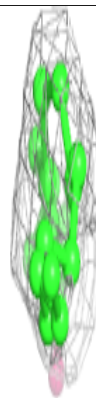
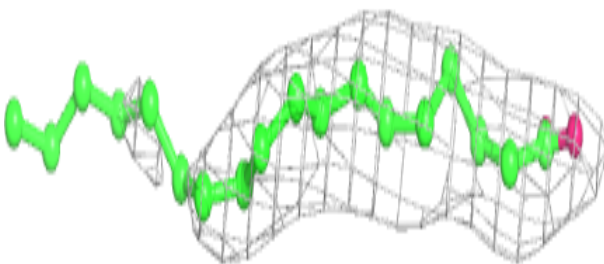
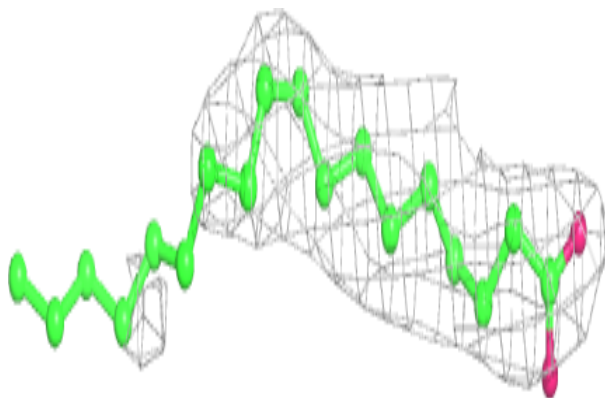


**Electron density around OLA A 1204:**

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

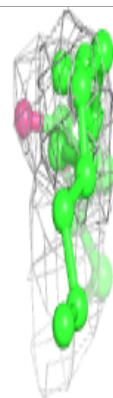
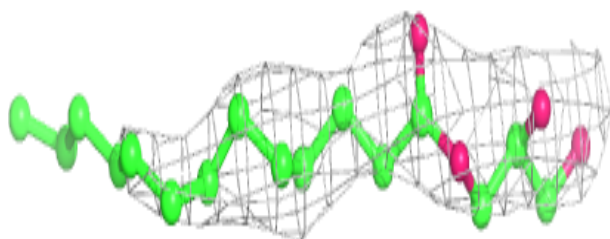
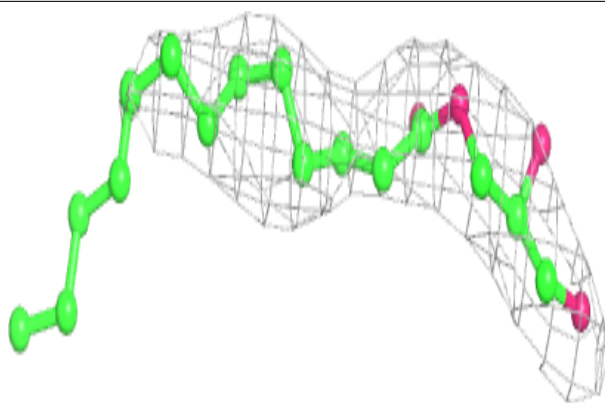
**Electron density around OLA A 1202:**

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

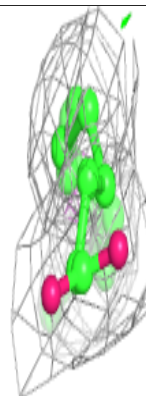
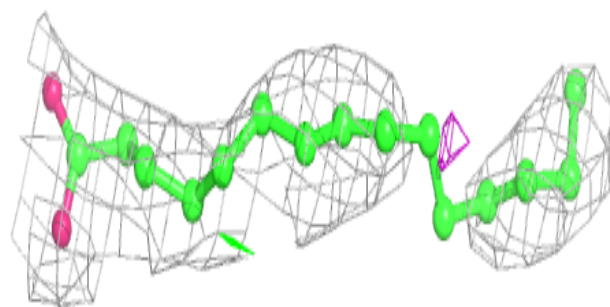
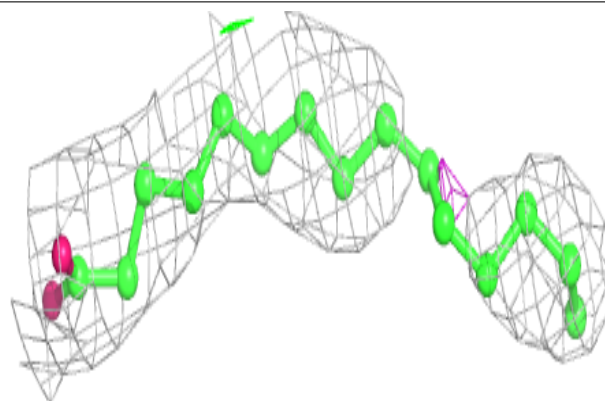


**Electron density around OLB A 1210:**

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

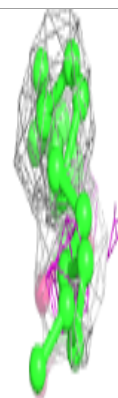
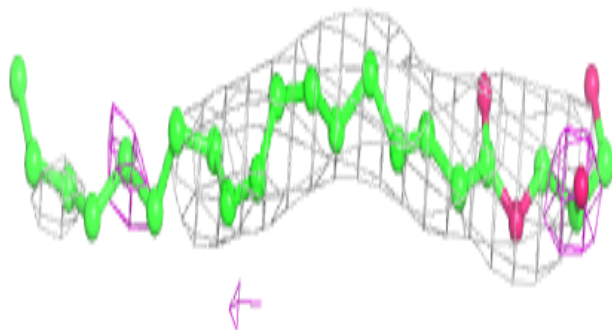
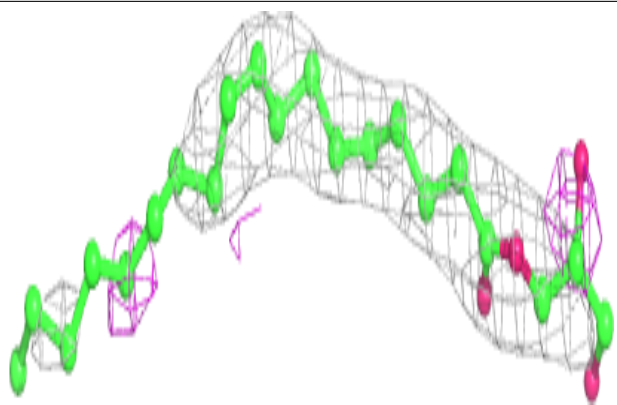
**Electron density around OLA A 1208:**

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

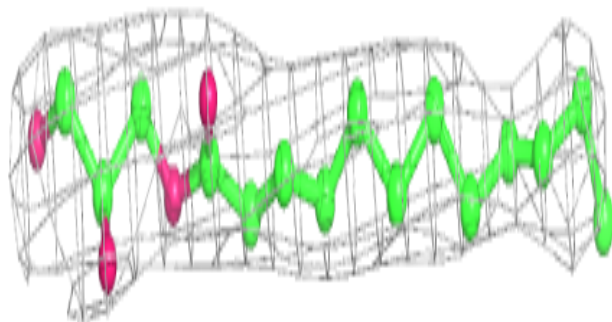
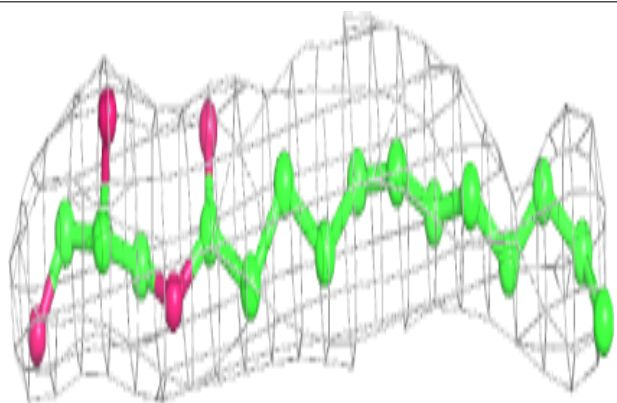


**Electron density around OLC A 1211:**

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

**Electron density around OLB A 1209:**

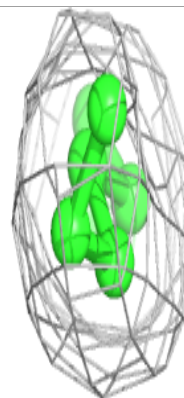
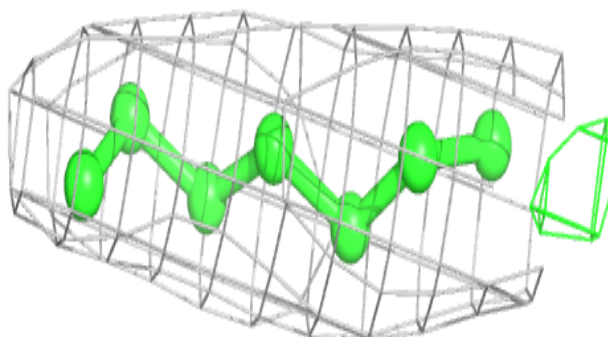
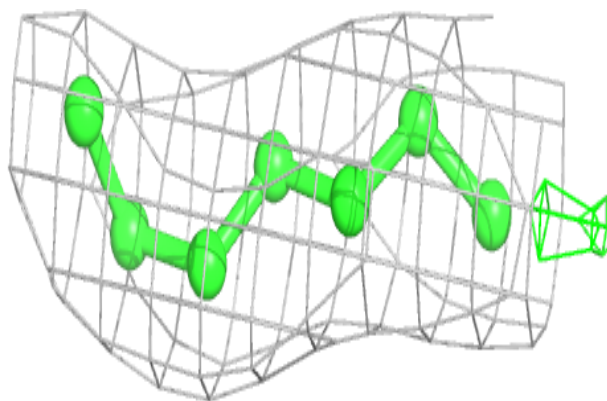
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



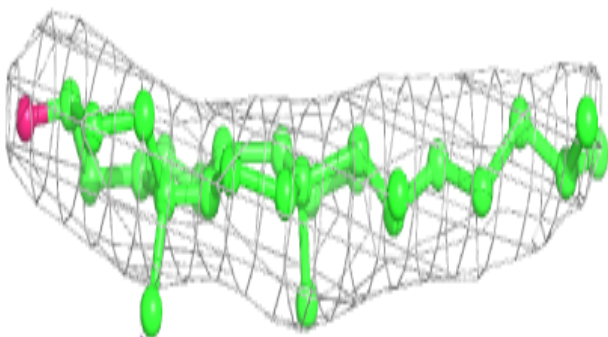
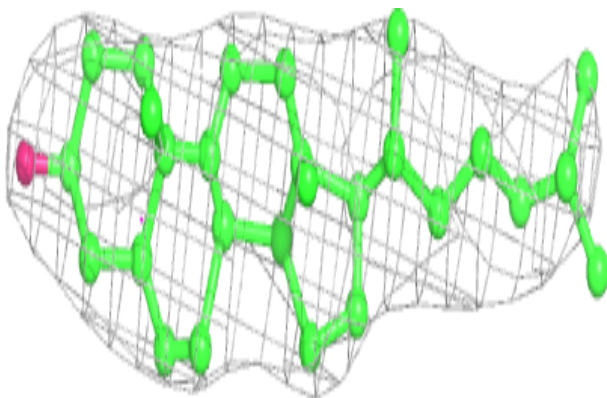


**Electron density around OLA A 1207:**

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

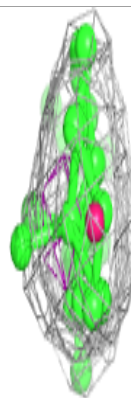
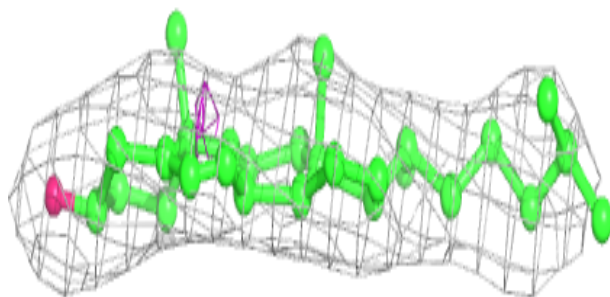
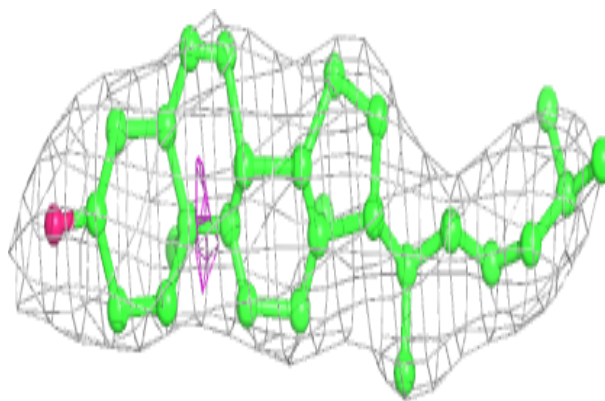
**Electron density around CLR A 1213:**

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

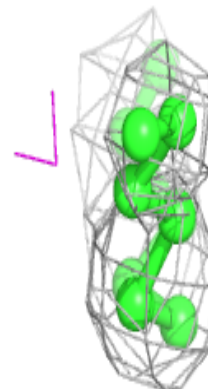
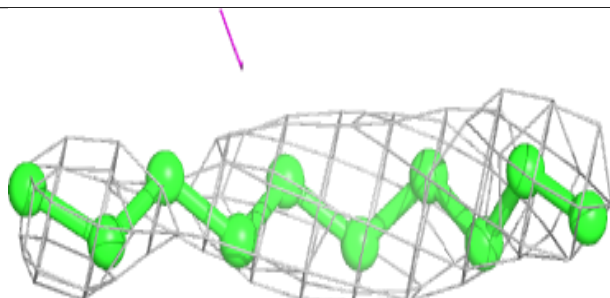
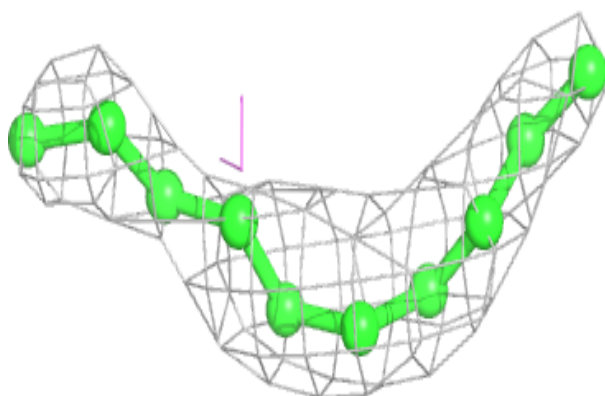


**Electron density around CLR A 1215:**

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

**Electron density around OLA A 1206:**

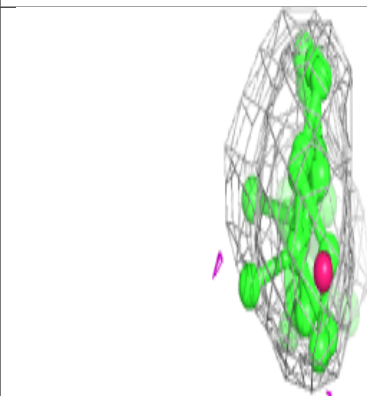
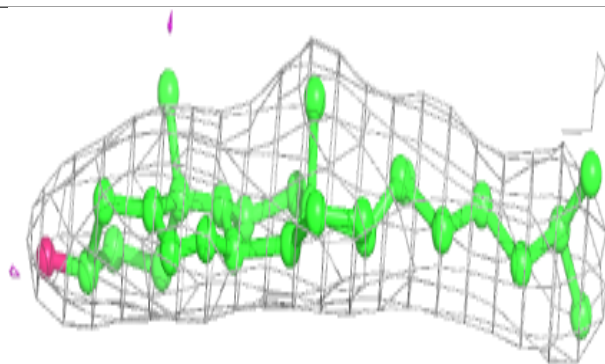
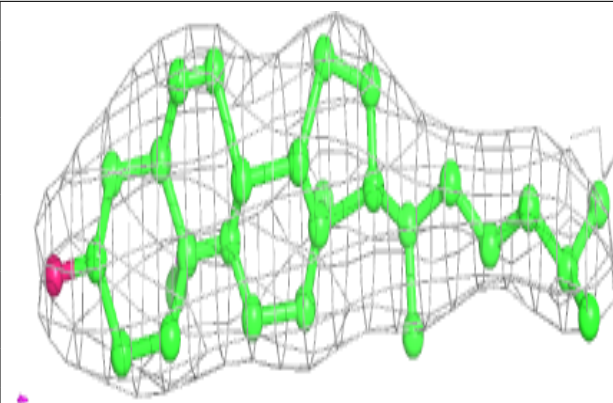
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



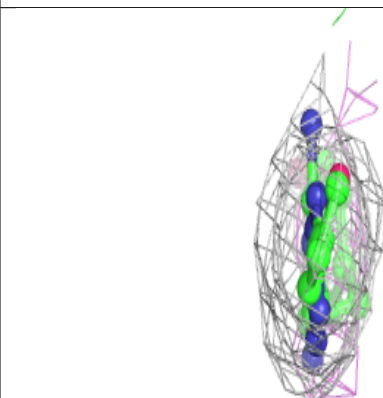
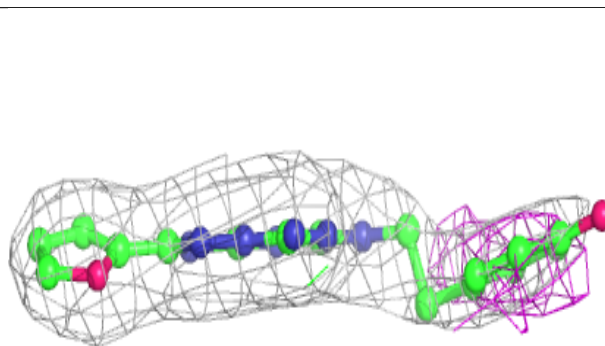
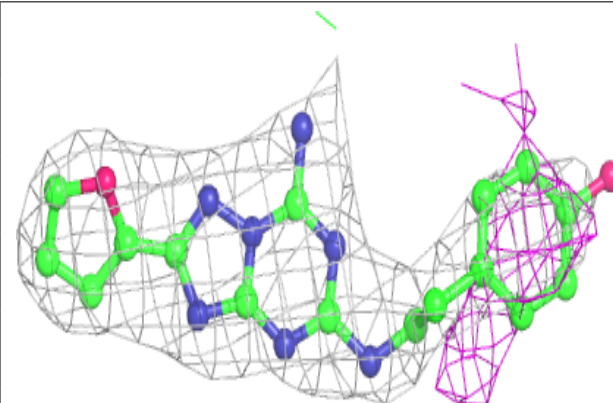


**Electron density around CLR A 1214:**

$2mF_o-DF_c$  (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

There are no such residues in this entry.