



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:02 PM BST

PDB ID : 6S0L
Title : Structure of the A2A adenosine receptor determined at SwissFEL using native-SAD at 4.57 keV from all available 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 : 2019-06-17
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references](#) 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

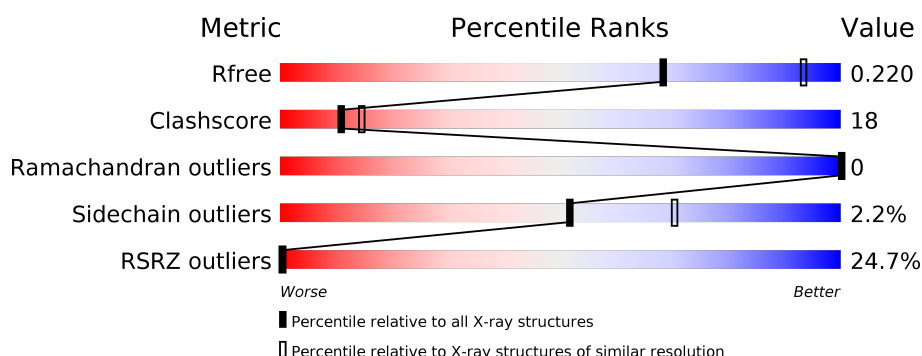
1 Overall quality at a glance

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 ≥ 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	1202	-	-	-	X
3	OLA	A	1205	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLB	A	1210	-	-	-	X
5	OLC	A	1211	-	-	-	X
6	CLR	A	1213	X	-	-	-
6	CLR	A	1214	X	-	-	-
6	CLR	A	1215	X	-	-	-

2 Entry composition [i](#)

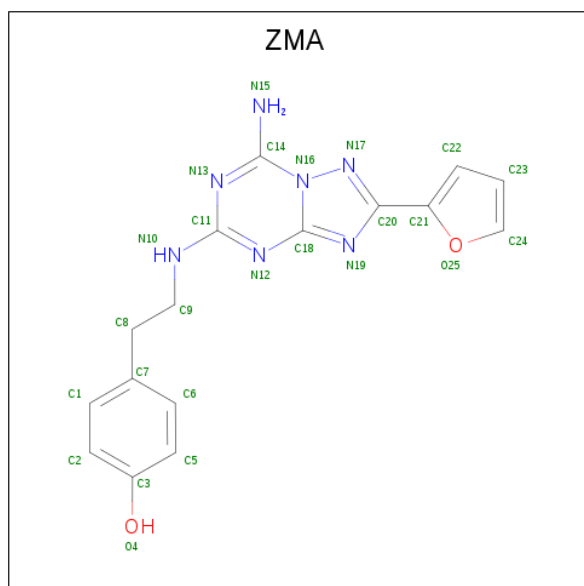
There are 6 unique types of molecules in this entry. The entry contains 3286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A2a adenosine receptor.

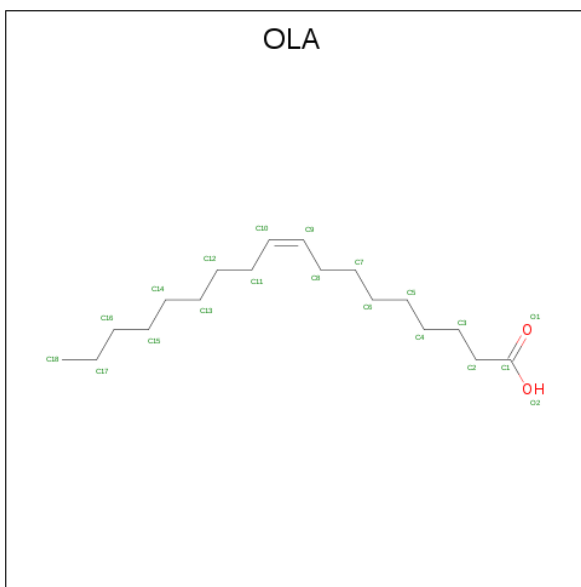
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2998	1953	506	517	22	0	0	0

- 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: C₁₆H₁₅N₇O₂).



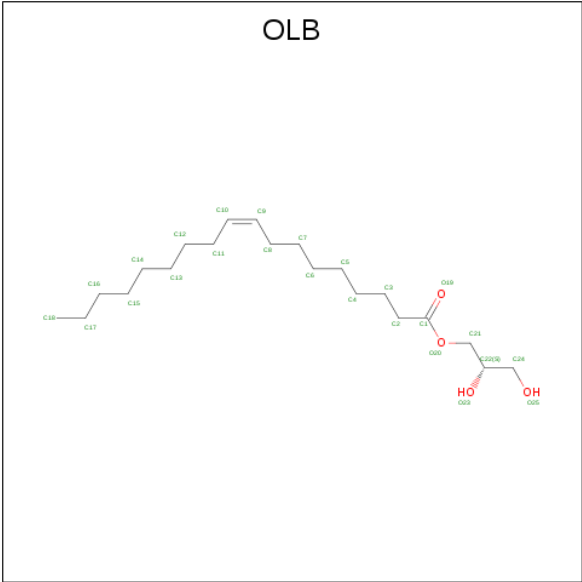
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	25	16	7	2	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



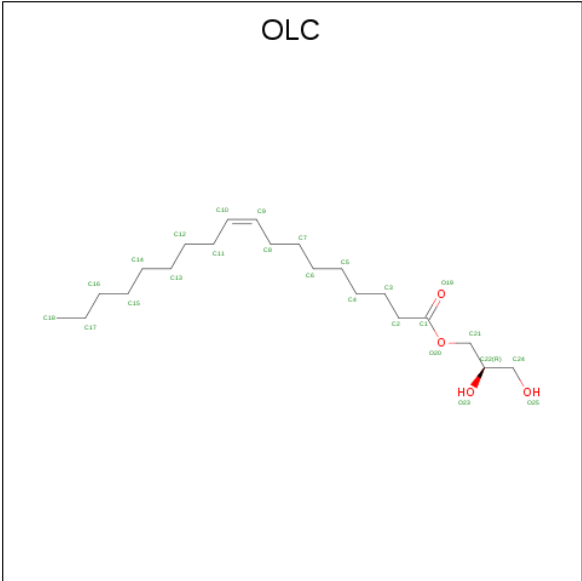
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			15	13	2		
3	A	1	Total	C	O	0	0
			9	7	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C		0	0
			10	10			
3	A	1	Total	C		0	0
			7	7			
3	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C₂₁H₄₀O₄).



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: C₂₁H₄₀O₄).



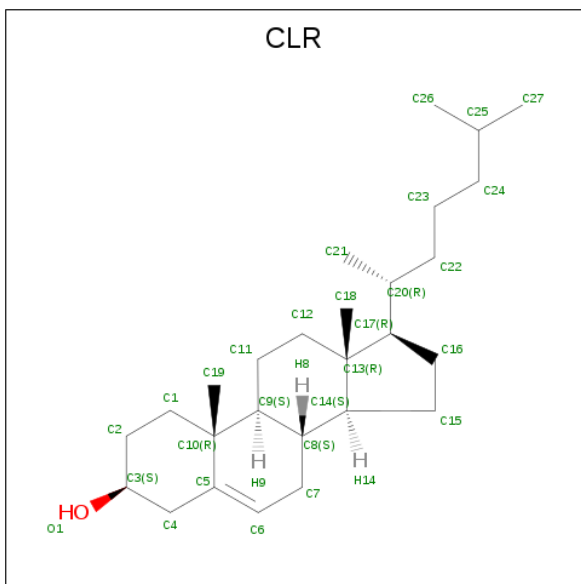
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		

Continued on next page...

Continued from previous page...

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		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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)	99.7 (34.49-2.65) 89.5 (35.76-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.197 , 0.220 0.197 , 0.220	Depositor DCC
R_{free} test set	785 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 110.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	119.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	2/3062 (0.1%)	0.67	3/4164 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	VAL	CB-CG1	-6.74	1.38	1.52
1	A	150	LYS	CE-NZ	6.10	1.64	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1074	ASP	CB-CG-OD1	-11.27	108.16	118.30
1	A	1074	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	1106	LEU	CB-CG-CD2	-6.29	100.31	111.00

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	81	1
2	A	25	0	15	2	0
3	A	96	0	141	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	39	0	52	3	0
5	A	44	0	65	2	0
6	A	84	0	117	40	0
All	All	3286	0	3458	123	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 18.

All (123) 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	1.79	1.61
6:A:1213:CLR:C7	6:A:1213:CLR:C8	1.76	1.59
6:A:1214:CLR:C7	6:A:1214:CLR:C8	1.76	1.57
6:A:1213:CLR:C8	6:A:1213:CLR:C14	1.78	1.57
6:A:1215:CLR:C7	6:A:1215:CLR:C8	1.76	1.56
6:A:1214:CLR:C8	6:A:1214:CLR:C14	1.80	1.54
6:A:1213:CLR:C17	6:A:1213:CLR:C13	1.81	1.39
6:A:1215:CLR:C13	6:A:1215:CLR:C17	1.81	1.37
6:A:1214:CLR:C13	6:A:1214:CLR:C17	1.82	1.36
1:A:1013:ASN:HD21	1:A:1032:LYS:HB2	1.14	1.12
1:A:150:LYS:HD2	1:A:153:LYS:HB2	1.48	0.94
6:A:1214:CLR:C8	6:A:1214:CLR:H14	1.98	0.93
6:A:1215:CLR:C8	6:A:1215:CLR:H14	1.98	0.93
6:A:1213:CLR:H14	6:A:1213:CLR:C8	1.99	0.91
6:A:1214:CLR:C17	6:A:1214:CLR:C18	2.47	0.91
6:A:1215:CLR:C17	6:A:1215:CLR:C18	2.49	0.91
6:A:1213:CLR:C17	6:A:1213:CLR:C18	2.50	0.89
1:A:42:ASN:HA	1:A:45:VAL:HG12	1.57	0.86
1:A:1013:ASN:ND2	1:A:1032:LYS:HB2	1.93	0.84
4:A:1210:OLB:H26	5:A:1212:OLC:H10	1.64	0.78
1:A:1013:ASN:HD21	1:A:1032:LYS:CB	1.97	0.76
1:A:1093:GLN:HG3	1:A:1096:THR:HB	1.67	0.76
1:A:45:VAL:HA	1:A:48:LEU:CD2	2.16	0.75
6:A:1213:CLR:C9	6:A:1213:CLR:C7	2.47	0.74
1:A:121:ALA:HA	1:A:124:ILE:HD12	1.72	0.72
6:A:1213:CLR:C6	6:A:1213:CLR:C8	2.38	0.71
1:A:1103:GLN:HA	1:A:1106:LEU:CD2	2.20	0.71
1:A:108:ILE:HD13	1:A:111:ARG:HB3	1.73	0.70
1:A:1021:ASP:OD2	1:A:1022:ASN:N	2.25	0.69
1:A:123:GLY:O	1:A:127:ILE:HD12	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD11	1:A:228:GLU:HB3	1.76	0.67
1:A:1103:GLN:HA	1:A:1106:LEU:HD23	1.76	0.67
1:A:1014:LEU:O	1:A:1017:ILE:HG13	1.97	0.65
6:A:1214:CLR:H181	6:A:1214:CLR:C16	2.24	0.64
1:A:42:ASN:HA	1:A:45:VAL:CG1	2.27	0.64
1:A:45:VAL:O	1:A:48:LEU:HD23	1.98	0.63
1:A:45:VAL:HA	1:A:48:LEU:HD22	1.80	0.63
1:A:1014:LEU:O	1:A:1018:GLU:HG2	2.01	0.61
1:A:1068:LEU:HD22	1:A:1102:ILE:HG21	1.82	0.60
1:A:61:PRO:O	1:A:65:THR:HG23	2.01	0.60
6:A:1213:CLR:C16	6:A:1213:CLR:H181	2.28	0.59
6:A:1214:CLR:C16	6:A:1214:CLR:C18	2.77	0.58
1:A:104:ILE:HG23	1:A:108:ILE:HD11	1.86	0.57
3:A:1202:OLA:H152	5:A:1211:OLC:H13	1.86	0.57
1:A:112:TYR:CZ	1:A:116:VAL:HG21	2.38	0.57
1:A:110:LEU:HD22	1:A:110:LEU:H	1.68	0.57
6:A:1214:CLR:C6	6:A:1214:CLR:C8	2.41	0.57
1:A:65:THR:HG22	3:A:1202:OLA:H71	1.85	0.57
1:A:117:THR:OG1	1:A:120:ARG:HG3	2.05	0.57
1:A:1103:GLN:NE2	1:A:1106:LEU:HD21	2.21	0.56
1:A:1101:TYR:O	1:A:1104:LYS:HG3	2.06	0.56
6:A:1214:CLR:C7	6:A:1214:CLR:C9	2.48	0.56
1:A:98:ILE:HD13	1:A:235:ALA:HB1	1.88	0.55
6:A:1215:CLR:C16	6:A:1215:CLR:C18	2.80	0.55
1:A:108:ILE:O	1:A:108:ILE:HD12	2.07	0.55
6:A:1215:CLR:H181	6:A:1215:CLR:C16	2.29	0.54
1:A:112:TYR:O	1:A:116:VAL:HG22	2.08	0.54
6:A:1213:CLR:C9	6:A:1213:CLR:C14	2.49	0.53
1:A:98:ILE:CD1	1:A:235:ALA:HB1	2.37	0.53
6:A:1213:CLR:C16	6:A:1213:CLR:C18	2.78	0.53
6:A:1215:CLR:C7	6:A:1215:CLR:C9	2.48	0.52
1:A:249:LEU:HD21	2:A:1201:ZMA:N17	2.24	0.52
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.45	0.52
6:A:1213:CLR:C7	6:A:1213:CLR:C14	2.87	0.51
1:A:227:LYS:O	1:A:227:LYS:HD2	2.10	0.51
6:A:1214:CLR:C9	6:A:1214:CLR:C14	2.48	0.51
1:A:50:ALA:O	1:A:54:LEU:HD12	2.11	0.50
1:A:112:TYR:CE1	1:A:116:VAL:HG21	2.46	0.50
1:A:289:ALA:O	1:A:296:ARG:HB2	2.12	0.50
1:A:63:ALA:HA	1:A:66:ILE:HG22	1.94	0.49
6:A:1215:CLR:C14	6:A:1215:CLR:C9	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LYS:CD	1:A:153:LYS:HB2	2.33	0.49
6:A:1215:CLR:C20	6:A:1215:CLR:C18	2.91	0.49
1:A:1013:ASN:HD22	1:A:1033:MET:HG3	1.78	0.48
1:A:293:ARG:HG2	1:A:296:ARG:NH1	2.28	0.48
1:A:249:LEU:HD22	2:A:1201:ZMA:O25	2.14	0.48
1:A:1063:HIS:CE1	1:A:1067:ILE:HD11	2.49	0.48
1:A:1032:LYS:N	1:A:1032:LYS:HE2	2.29	0.48
1:A:1034:ARG:NH2	1:A:1073:ASP:OD1	2.46	0.48
1:A:1074:ASP:O	1:A:1077:LYS:HG2	2.14	0.48
1:A:1004:GLU:OE2	1:A:222:ARG:NH2	2.47	0.48
1:A:95:LEU:HD21	1:A:238:ILE:HG22	1.94	0.48
1:A:1023:ALA:HB1	1:A:1079:ALA:O	2.13	0.47
1:A:1010:LEU:HD12	1:A:1033:MET:HG2	1.95	0.47
1:A:66:ILE:HD13	1:A:166:CYS:SG	2.55	0.47
6:A:1215:CLR:H181	6:A:1215:CLR:H152	1.64	0.46
1:A:46:VAL:HG11	4:A:1210:OLB:H2	1.98	0.46
1:A:1042:LYS:HB3	1:A:1042:LYS:HE2	1.63	0.46
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.81	0.46
1:A:1103:GLN:HA	1:A:1106:LEU:HD21	1.95	0.46
6:A:1215:CLR:C13	6:A:1215:CLR:C20	2.81	0.46
1:A:1067:ILE:O	1:A:1071:GLN:HG3	2.16	0.45
1:A:1103:GLN:CD	1:A:1106:LEU:HD21	2.36	0.45
6:A:1214:CLR:C18	6:A:1214:CLR:C20	2.95	0.45
6:A:1215:CLR:H273	6:A:1215:CLR:H231	1.73	0.45
1:A:1018:GLU:HB3	1:A:1019:LYS:NZ	2.32	0.45
1:A:201:PHE:CE1	1:A:233:LYS:HG3	2.52	0.45
1:A:65:THR:HG22	3:A:1202:OLA:C7	2.46	0.44
6:A:1215:CLR:C14	6:A:1215:CLR:C7	2.91	0.44
6:A:1214:CLR:H181	6:A:1214:CLR:H152	1.74	0.43
1:A:270:MET:O	1:A:274:ILE:HG13	2.18	0.43
1:A:1103:GLN:O	1:A:1103:GLN:HG3	2.18	0.43
1:A:3:ILE:O	1:A:3:ILE:HG13	2.19	0.43
1:A:1026:VAL:HG22	1:A:1030:LEU:CD2	2.49	0.43
1:A:185:CYS:O	1:A:189:PRO:HG2	2.19	0.42
1:A:1018:GLU:C	1:A:1019:LYS:HD3	2.39	0.42
1:A:21:ILE:HG13	1:A:22:LEU:N	2.34	0.42
1:A:96:LEU:O	1:A:100:ILE:HG13	2.19	0.42
1:A:293:ARG:HG2	1:A:296:ARG:HH12	1.84	0.42
1:A:238:ILE:HD11	1:A:287:ILE:HB	2.02	0.42
1:A:1017:ILE:HD13	1:A:1091:ALA:HB3	2.02	0.42
1:A:1034:ARG:HH21	1:A:1073:ASP:CG	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1213:CLR:C20	6:A:1213:CLR:C18	2.97	0.42
6:A:1214:CLR:C7	6:A:1214:CLR:C14	2.91	0.41
1:A:1065:PHE:O	1:A:1069:VAL:HG12	2.20	0.41
1:A:1022:ASN:HD21	1:A:1024:ALA:HB3	1.86	0.41
1:A:291:ARG:O	1:A:292:ILE:HD13	2.20	0.41
1:A:1067:ILE:HG22	1:A:1071:GLN:HG3	2.03	0.41
1:A:46:VAL:CG1	4:A:1210:OLB:H2	2.50	0.40
6:A:1215:CLR:H20	6:A:1215:CLR:C18	2.51	0.40
1:A:267:LEU:HA	1:A:267:LEU:HD12	1.88	0.40
1:A:21:ILE:HG13	1:A:22:LEU:H	1.86	0.40
1:A:201:PHE:CZ	1:A:233:LYS:HG3	2.56	0.40

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)
1:A:111:ARG:NH2	1:A:114:GLY:O[3_556]	2.15	0.05

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	384/433 (89%)	375 (98%)	9 (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	312/353 (88%)	305 (98%)	7 (2%)	52	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	39	ASN
1	A	48	LEU
1	A	111	ARG
1	A	156	SER
1	A	1073	ASP
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	1103	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
2	ZMA	A	1201	-	21,28,28	2.08	4 (19%)	22,39,39	3.12	9 (40%)
5	OLC	A	1211	-	24,24,24	0.79	2 (8%)	25,25,25	1.20	2 (8%)
5	OLC	A	1212	-	18,18,24	0.94	1 (5%)	18,19,25	1.15	1 (5%)
3	OLA	A	1204	-	5,8,19	0.32	0	4,8,19	0.74	0
3	OLA	A	1203	-	11,14,19	0.88	1 (9%)	10,14,19	0.57	0
4	OLB	A	1209	-	18,18,24	0.90	2 (11%)	18,19,25	1.29	1 (5%)
3	OLA	A	1207	-	6,6,19	0.35	0	5,5,19	0.35	0
6	CLR	A	1215	-	31,31,31	9.02	22 (70%)	48,48,48	3.73	19 (39%)
3	OLA	A	1202	-	16,19,19	0.74	1 (6%)	15,19,19	0.58	0
6	CLR	A	1213	-	31,31,31	9.12	21 (67%)	48,48,48	3.42	20 (41%)
3	OLA	A	1206	-	9,9,19	1.00	1 (11%)	8,8,19	0.77	0
3	OLA	A	1208	-	13,16,19	0.87	1 (7%)	12,16,19	0.43	0
3	OLA	A	1205	-	14,17,19	0.75	1 (7%)	13,17,19	0.62	0
4	OLB	A	1210	-	19,19,24	0.93	1 (5%)	20,20,25	1.19	1 (5%)
6	CLR	A	1214	-	31,31,31	9.10	21 (67%)	48,48,48	3.64	21 (43%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLR	A	1213	-	2/2/10/11	2/10/68/68	0/4/4/4
3	OLA	A	1206	-	-	3/7/7/17	-
3	OLA	A	1202	-	-	6/15/17/17	-
3	OLA	A	1205	-	-	12/13/15/17	-
4	OLB	A	1210	-	-	9/19/19/24	-

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1214	CLR	C8-C9	-21.25	1.13	1.53
6	A	1213	CLR	C8-C9	-21.24	1.13	1.53
6	A	1215	CLR	C8-C9	-20.84	1.13	1.53
6	A	1213	CLR	C13-C14	-19.20	1.18	1.55
6	A	1214	CLR	C13-C14	-18.53	1.19	1.55
6	A	1215	CLR	C13-C14	-18.02	1.20	1.55
6	A	1213	CLR	C7-C6	-17.01	1.13	1.50
6	A	1214	CLR	C7-C6	-16.89	1.13	1.50
6	A	1215	CLR	C7-C6	-16.54	1.14	1.50
6	A	1213	CLR	C12-C13	-16.45	1.24	1.54
6	A	1214	CLR	C12-C13	-16.12	1.25	1.54
6	A	1215	CLR	C12-C13	-15.60	1.26	1.54
6	A	1214	CLR	C11-C9	-14.49	1.29	1.53
6	A	1215	CLR	C11-C9	-14.38	1.29	1.53
6	A	1213	CLR	C11-C9	-14.20	1.30	1.53
6	A	1214	CLR	C13-C17	14.17	1.82	1.55
6	A	1215	CLR	C13-C17	14.13	1.81	1.55
6	A	1213	CLR	C13-C17	14.02	1.81	1.55
6	A	1215	CLR	C7-C8	13.87	1.76	1.53
6	A	1214	CLR	C7-C8	13.84	1.76	1.53
6	A	1214	CLR	C8-C14	13.83	1.80	1.53
6	A	1215	CLR	C10-C9	-13.75	1.33	1.56
6	A	1213	CLR	C7-C8	13.50	1.76	1.53
6	A	1215	CLR	C8-C14	13.41	1.79	1.53
6	A	1213	CLR	C8-C14	12.93	1.78	1.53
6	A	1213	CLR	C10-C9	-12.66	1.34	1.56
6	A	1214	CLR	C10-C9	-12.63	1.34	1.56
6	A	1215	CLR	C15-C14	8.58	1.72	1.54
6	A	1214	CLR	C15-C14	8.51	1.72	1.54
6	A	1213	CLR	C15-C14	8.40	1.71	1.54
6	A	1214	CLR	C12-C11	7.23	1.68	1.53
6	A	1213	CLR	C12-C11	7.08	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1215	CLR	C12-C11	6.94	1.68	1.53
2	A	1201	ZMA	C11-N10	6.66	1.44	1.34
6	A	1213	CLR	C20-C17	-6.41	1.43	1.54
6	A	1214	CLR	C20-C17	-6.14	1.43	1.54
6	A	1215	CLR	C20-C17	-5.91	1.44	1.54
6	A	1213	CLR	C4-C3	5.67	1.62	1.52
6	A	1215	CLR	C4-C3	5.61	1.62	1.52
6	A	1214	CLR	C4-C3	5.06	1.61	1.52
2	A	1201	ZMA	C14-N15	4.82	1.44	1.34
6	A	1213	CLR	C1-C10	4.67	1.63	1.54
6	A	1214	CLR	C16-C17	-4.34	1.45	1.54
6	A	1214	CLR	C1-C10	4.30	1.62	1.54
6	A	1215	CLR	C1-C10	4.26	1.62	1.54
6	A	1213	CLR	C16-C17	-4.03	1.46	1.54
6	A	1215	CLR	C16-C17	-3.99	1.46	1.54
6	A	1215	CLR	C19-C10	3.74	1.61	1.54
6	A	1213	CLR	C22-C20	3.66	1.63	1.54
6	A	1213	CLR	C19-C10	3.39	1.60	1.54
6	A	1215	CLR	C22-C20	3.08	1.62	1.54
2	A	1201	ZMA	C21-C20	-3.03	1.39	1.48
6	A	1214	CLR	C22-C20	3.03	1.62	1.54
3	A	1206	OLA	C9-C10	2.87	1.48	1.28
3	A	1208	OLA	C10-C9	2.85	1.48	1.31
5	A	1212	OLC	O20-C1	2.84	1.41	1.33
6	A	1214	CLR	C19-C10	2.83	1.59	1.54
6	A	1213	CLR	C10-C5	2.77	1.58	1.52
3	A	1203	OLA	C10-C9	2.77	1.47	1.31
4	A	1210	OLB	O20-C1	2.72	1.41	1.33
2	A	1201	ZMA	C14-N13	-2.71	1.31	1.34
3	A	1202	OLA	C10-C9	2.66	1.47	1.31
3	A	1205	OLA	C10-C9	2.65	1.47	1.31
6	A	1215	CLR	C10-C5	2.51	1.57	1.52
6	A	1215	CLR	O1-C3	-2.47	1.36	1.43
4	A	1209	OLB	O20-C1	2.45	1.40	1.33
6	A	1214	CLR	O1-C3	-2.37	1.36	1.43
5	A	1211	OLC	O20-C1	2.37	1.40	1.33
6	A	1213	CLR	O1-C3	-2.35	1.36	1.43
6	A	1213	CLR	C2-C3	2.34	1.57	1.51
6	A	1214	CLR	C10-C5	2.22	1.57	1.52
6	A	1215	CLR	C6-C5	2.15	1.37	1.33
6	A	1215	CLR	C18-C13	2.12	1.58	1.54
6	A	1214	CLR	C2-C3	2.10	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1215	CLR	C4-C5	2.09	1.56	1.51
5	A	1211	OLC	O20-C21	-2.08	1.40	1.45
6	A	1213	CLR	C4-C5	2.05	1.56	1.51
4	A	1209	OLB	O20-C21	-2.03	1.40	1.45
6	A	1214	CLR	C18-C13	2.01	1.57	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1215	CLR	C18-C13-C12	-13.34	89.52	110.59
6	A	1215	CLR	C12-C13-C14	11.96	125.84	107.27
6	A	1214	CLR	C18-C13-C12	-11.37	92.64	110.59
6	A	1213	CLR	C12-C13-C14	10.52	123.59	107.27
6	A	1214	CLR	C12-C13-C14	10.24	123.16	107.27
2	A	1201	ZMA	N17-C20-N19	-9.91	108.00	114.56
6	A	1214	CLR	C18-C13-C17	-9.82	93.40	111.71
6	A	1213	CLR	C18-C13-C12	-9.63	95.38	110.59
6	A	1215	CLR	C18-C13-C17	-9.41	94.16	111.71
6	A	1213	CLR	C18-C13-C17	-8.98	94.96	111.71
6	A	1214	CLR	C12-C13-C17	8.74	129.66	116.57
6	A	1215	CLR	C12-C13-C17	7.71	128.12	116.57
6	A	1213	CLR	C12-C13-C17	6.96	126.99	116.57
6	A	1214	CLR	C7-C8-C9	5.78	116.72	109.71
6	A	1213	CLR	C7-C8-C9	5.49	116.36	109.71
2	A	1201	ZMA	C9-C8-C7	-5.45	100.23	112.87
6	A	1215	CLR	C7-C8-C9	5.41	116.26	109.71
6	A	1213	CLR	C14-C8-C9	5.24	116.10	109.09
2	A	1201	ZMA	N15-C14-N16	5.00	121.34	117.97
6	A	1214	CLR	C7-C6-C5	-4.93	115.97	125.06
6	A	1215	CLR	C15-C14-C8	4.84	127.05	119.08
6	A	1214	CLR	C15-C14-C8	4.34	126.22	119.08
2	A	1201	ZMA	C9-N10-C11	-4.33	116.27	123.75
6	A	1213	CLR	C7-C6-C5	-4.28	117.17	125.06
6	A	1215	CLR	C7-C6-C5	-4.23	117.26	125.06
6	A	1215	CLR	C14-C8-C9	3.94	114.36	109.09
6	A	1213	CLR	C15-C14-C8	3.79	125.33	119.08
6	A	1213	CLR	C11-C9-C10	3.77	118.05	113.08
6	A	1213	CLR	C18-C13-C14	-3.74	104.74	111.71
6	A	1214	CLR	C19-C10-C1	-3.63	103.70	109.43
6	A	1215	CLR	C9-C10-C5	3.60	115.29	109.65
6	A	1213	CLR	C1-C10-C9	3.58	113.72	108.73
6	A	1214	CLR	C14-C8-C9	3.55	113.84	109.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1213	CLR	C19-C10-C1	-3.44	103.99	109.43
6	A	1214	CLR	C10-C9-C8	3.44	117.89	112.73
6	A	1215	CLR	C19-C10-C9	-3.42	107.60	111.68
6	A	1214	CLR	C1-C10-C9	3.37	113.43	108.73
2	A	1201	ZMA	N12-C11-N13	-3.37	120.90	126.23
6	A	1215	CLR	C18-C13-C14	-3.34	105.49	111.71
5	A	1211	OLC	O20-C1-C2	3.23	122.06	111.91
4	A	1209	OLB	O20-C1-C2	3.20	121.95	111.91
4	A	1210	OLB	O20-C1-C2	3.20	121.95	111.91
6	A	1214	CLR	C22-C20-C17	-3.12	103.85	110.28
6	A	1214	CLR	C11-C9-C10	3.12	117.18	113.08
6	A	1214	CLR	C9-C10-C5	3.06	114.45	109.65
6	A	1213	CLR	C16-C17-C13	-3.03	100.19	103.84
6	A	1214	CLR	C21-C20-C22	-2.93	105.78	110.36
6	A	1213	CLR	C9-C10-C5	2.91	114.21	109.65
6	A	1214	CLR	C19-C10-C5	-2.89	103.66	108.34
6	A	1213	CLR	C17-C13-C14	2.79	103.37	100.07
6	A	1213	CLR	C19-C10-C9	-2.76	108.39	111.68
6	A	1213	CLR	C22-C20-C17	-2.76	104.59	110.28
2	A	1201	ZMA	C21-C20-N17	2.76	128.26	123.44
6	A	1215	CLR	C10-C9-C8	2.75	116.86	112.73
6	A	1213	CLR	C8-C7-C6	-2.67	108.89	112.73
6	A	1215	CLR	C16-C17-C13	-2.67	100.62	103.84
5	A	1212	OLC	O20-C1-C2	2.54	119.87	111.91
6	A	1213	CLR	C16-C17-C20	-2.47	108.32	112.15
6	A	1215	CLR	C15-C16-C17	2.39	109.87	105.13
6	A	1215	CLR	C21-C20-C22	-2.35	106.68	110.36
6	A	1215	CLR	C22-C20-C17	-2.35	105.43	110.28
6	A	1215	CLR	C17-C13-C14	2.34	102.84	100.07
6	A	1213	CLR	C15-C16-C17	2.31	109.72	105.13
6	A	1215	CLR	C11-C9-C8	2.31	115.09	111.75
6	A	1214	CLR	C10-C5-C6	-2.31	119.37	122.90
2	A	1201	ZMA	N10-C11-N12	2.26	121.10	117.19
6	A	1214	CLR	C16-C17-C13	-2.26	101.12	103.84
5	A	1211	OLC	O20-C1-O19	-2.15	118.15	123.59
2	A	1201	ZMA	C5-C6-C7	-2.14	118.08	121.03
6	A	1214	CLR	C16-C17-C20	-2.12	108.86	112.15
6	A	1214	CLR	C18-C13-C14	-2.11	107.78	111.71
6	A	1215	CLR	C19-C10-C5	-2.10	104.95	108.34
2	A	1201	ZMA	C6-C7-C1	2.05	121.39	118.17
6	A	1214	CLR	C12-C11-C9	2.02	116.62	113.11

All (6) chirality outliers are listed below:

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

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1211	OLC	C21-C22-C24-O25
5	A	1211	OLC	O23-C22-C24-O25
3	A	1204	OLA	C1-C2-C3-C4
3	A	1203	OLA	C1-C2-C3-C4
4	A	1209	OLB	C21-C22-C24-O25
4	A	1209	OLB	O23-C22-C24-O25
3	A	1202	OLA	C1-C2-C3-C4
3	A	1208	OLA	C1-C2-C3-C4
3	A	1205	OLA	C1-C2-C3-C4
4	A	1210	OLB	O19-C1-O20-C21
4	A	1210	OLB	C2-C1-O20-C21
3	A	1208	OLA	C11-C10-C9-C8
3	A	1205	OLA	C11-C10-C9-C8
5	A	1212	OLC	C2-C1-O20-C21
6	A	1215	CLR	C22-C23-C24-C25
5	A	1212	OLC	O19-C1-O20-C21
3	A	1203	OLA	C5-C6-C7-C8
3	A	1202	OLA	C3-C4-C5-C6
6	A	1214	CLR	C23-C24-C25-C26
4	A	1210	OLB	C2-C3-C4-C5
5	A	1211	OLC	C4-C5-C6-C7
4	A	1210	OLB	C3-C4-C5-C6
4	A	1210	OLB	C5-C6-C7-C8
3	A	1208	OLA	C3-C4-C5-C6
3	A	1206	OLA	C12-C13-C14-C15
3	A	1208	OLA	C4-C5-C6-C7
6	A	1214	CLR	C23-C24-C25-C27
4	A	1209	OLB	C4-C5-C6-C7
3	A	1205	OLA	C4-C5-C6-C7
5	A	1211	OLC	C11-C12-C13-C14
5	A	1211	OLC	C3-C4-C5-C6
3	A	1205	OLA	C2-C3-C4-C5
3	A	1202	OLA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1203	OLA	C3-C4-C5-C6
5	A	1211	OLC	C6-C7-C8-C9
4	A	1210	OLB	C6-C7-C8-C9
6	A	1213	CLR	C23-C24-C25-C27
3	A	1202	OLA	C11-C12-C13-C14
3	A	1206	OLA	C11-C12-C13-C14
3	A	1208	OLA	C2-C3-C4-C5
6	A	1213	CLR	C23-C24-C25-C26
5	A	1211	OLC	C14-C15-C16-C17
5	A	1211	OLC	C10-C11-C12-C13
5	A	1212	OLC	C5-C6-C7-C8
5	A	1212	OLC	O20-C21-C22-C24
5	A	1211	OLC	C12-C13-C14-C15
6	A	1214	CLR	C21-C20-C22-C23
3	A	1205	OLA	C3-C4-C5-C6
4	A	1210	OLB	C7-C8-C9-C10
5	A	1212	OLC	O20-C21-C22-O23
3	A	1204	OLA	C3-C4-C5-C6
5	A	1212	OLC	C9-C10-C11-C12
5	A	1211	OLC	C5-C6-C7-C8
3	A	1205	OLA	C12-C13-C14-C15
3	A	1202	OLA	C14-C15-C16-C17
5	A	1212	OLC	C2-C3-C4-C5
4	A	1209	OLB	C3-C4-C5-C6
3	A	1207	OLA	C3-C4-C5-C6
3	A	1202	OLA	C11-C10-C9-C8
5	A	1211	OLC	C15-C16-C17-C18
3	A	1205	OLA	C10-C11-C12-C13
3	A	1203	OLA	C4-C5-C6-C7
3	A	1205	OLA	C6-C7-C8-C9
4	A	1210	OLB	C9-C10-C11-C12
3	A	1203	OLA	C11-C10-C9-C8
3	A	1205	OLA	C9-C10-C11-C12
3	A	1208	OLA	C7-C8-C9-C10
4	A	1209	OLB	C9-C10-C11-C12
3	A	1206	OLA	C9-C10-C11-C12
4	A	1209	OLB	O19-C1-O20-C21
3	A	1208	OLA	C9-C10-C11-C12
3	A	1205	OLA	C5-C6-C7-C8
4	A	1209	OLB	C2-C1-O20-C21
3	A	1208	OLA	C12-C13-C14-C15
5	A	1211	OLC	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

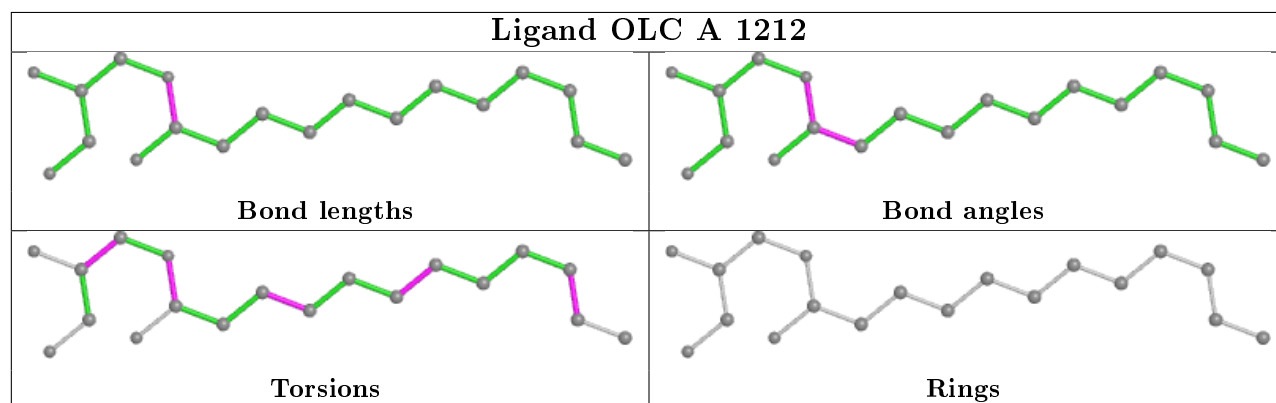
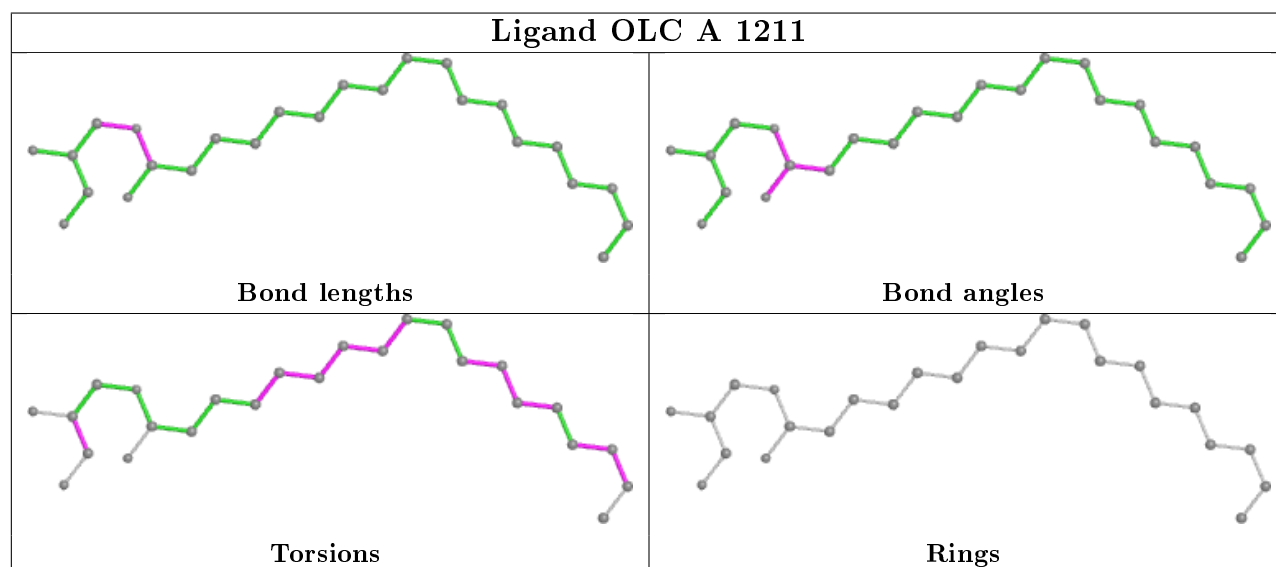
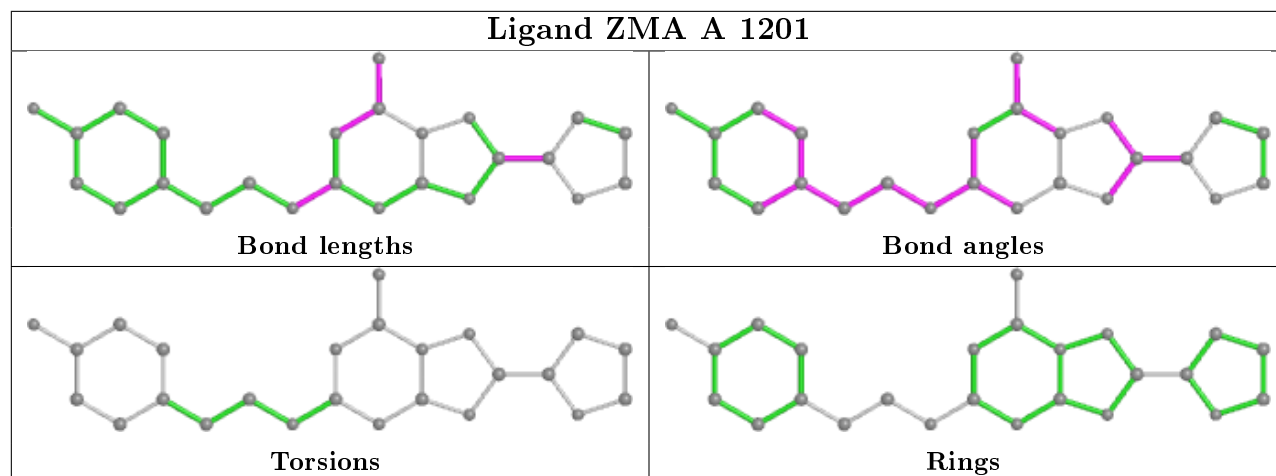
Mol	Chain	Res	Type	Atoms
3	A	1203	OLA	C9-C10-C11-C12
3	A	1207	OLA	C6-C7-C8-C9
4	A	1210	OLB	O20-C21-C22-O23
3	A	1205	OLA	C13-C14-C15-C16
3	A	1205	OLA	C7-C8-C9-C10

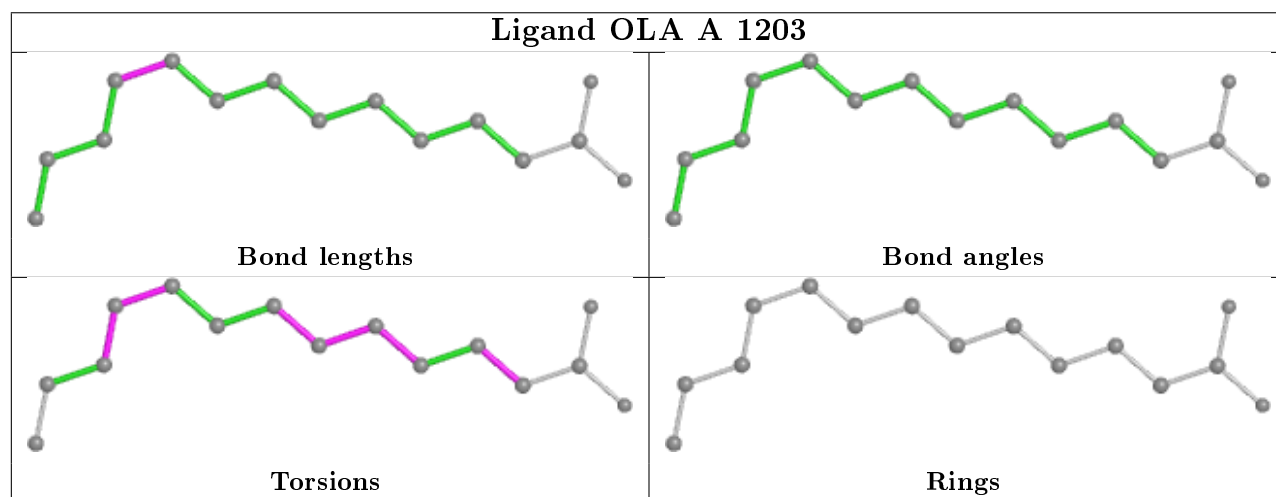
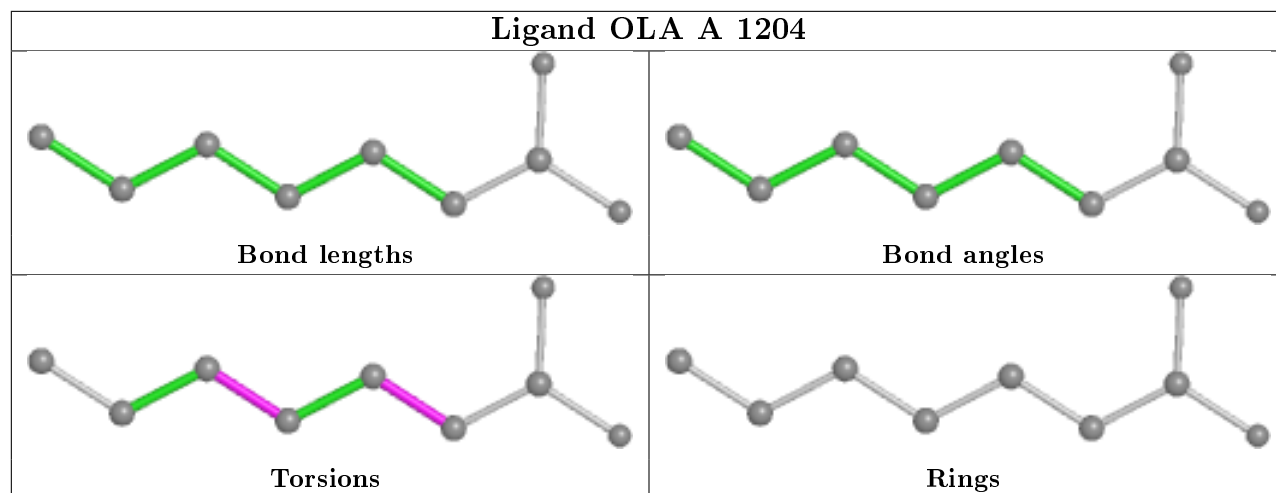
There are no ring outliers.

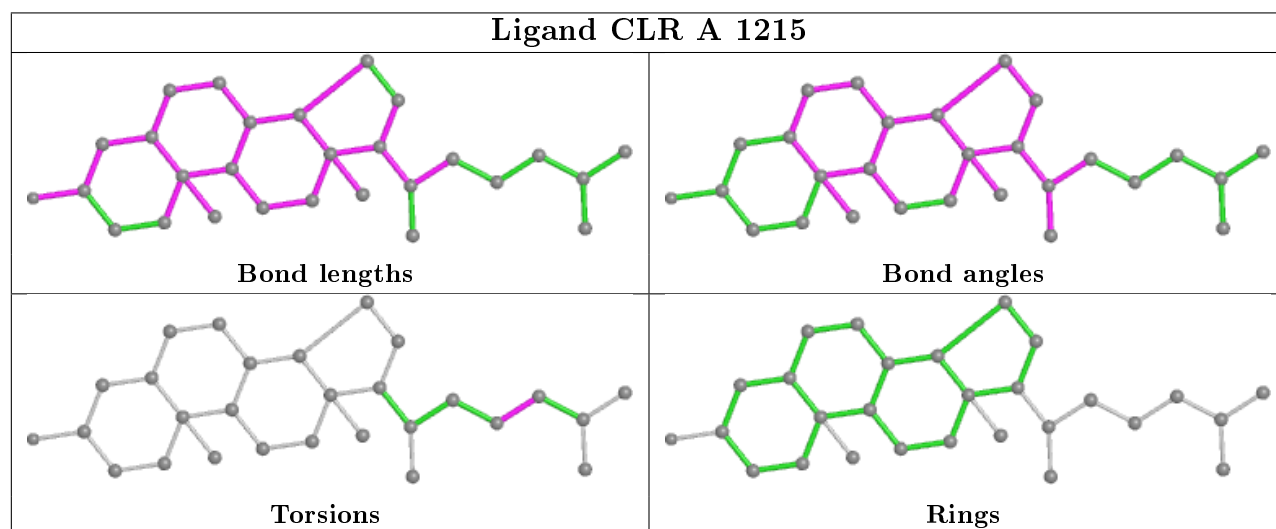
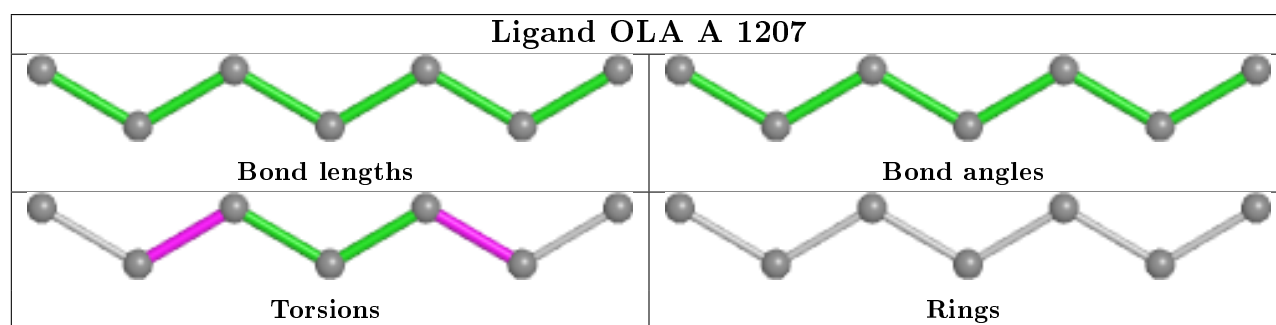
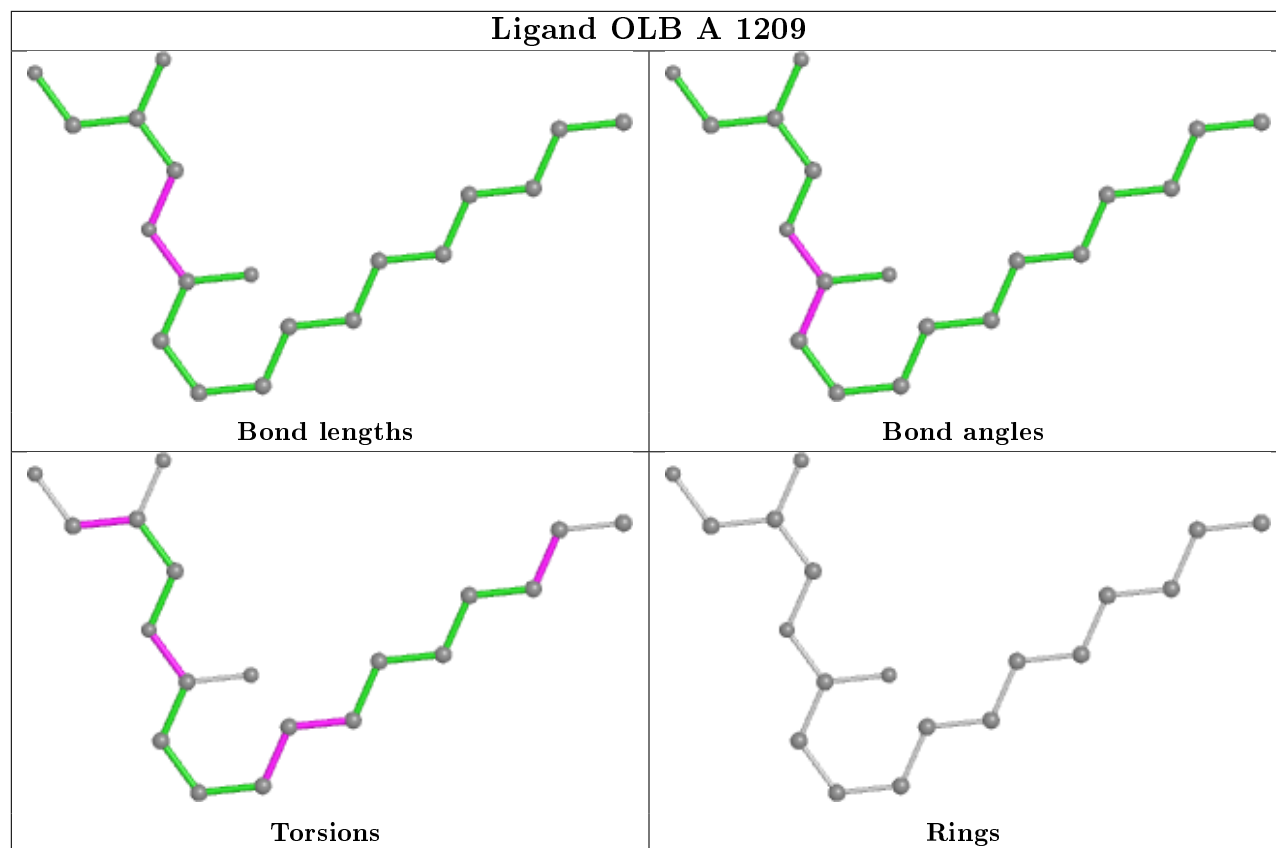
8 monomers are involved in 48 short contacts:

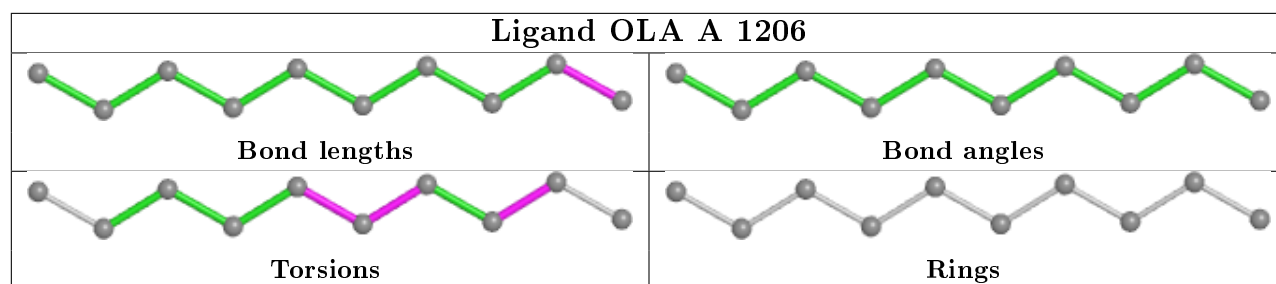
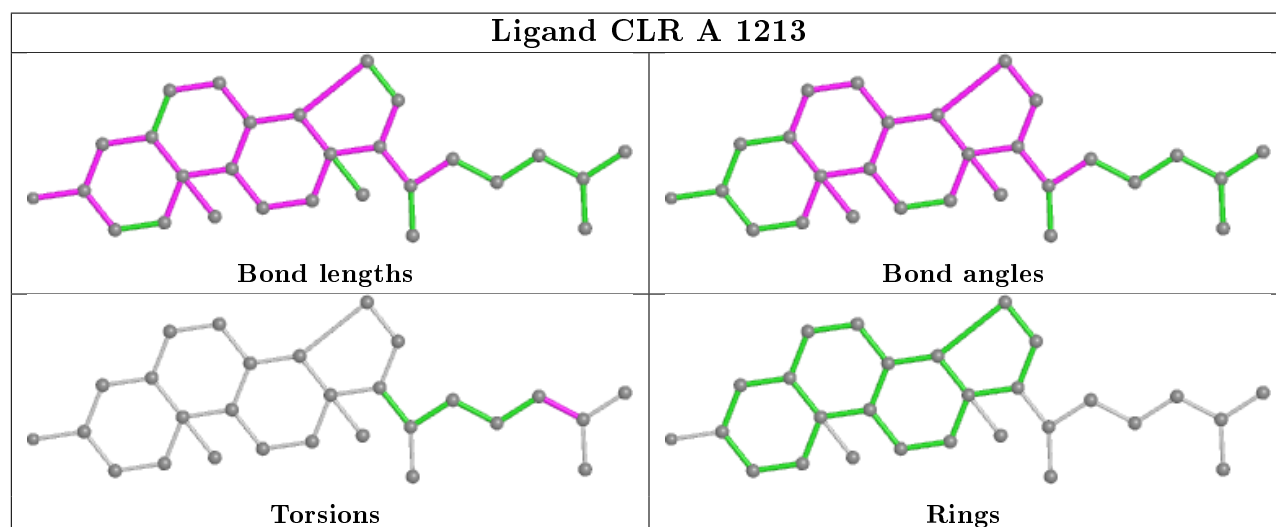
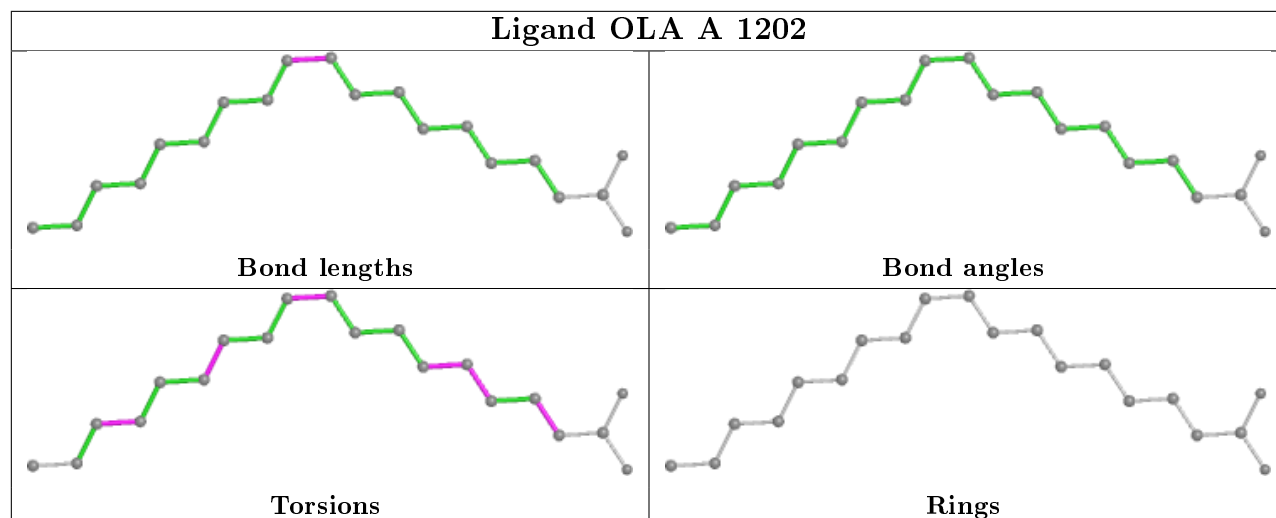
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ZMA	2	0
5	A	1211	OLC	1	0
5	A	1212	OLC	1	0
6	A	1215	CLR	15	0
3	A	1202	OLA	3	0
6	A	1213	CLR	12	0
4	A	1210	OLB	3	0
6	A	1214	CLR	13	0

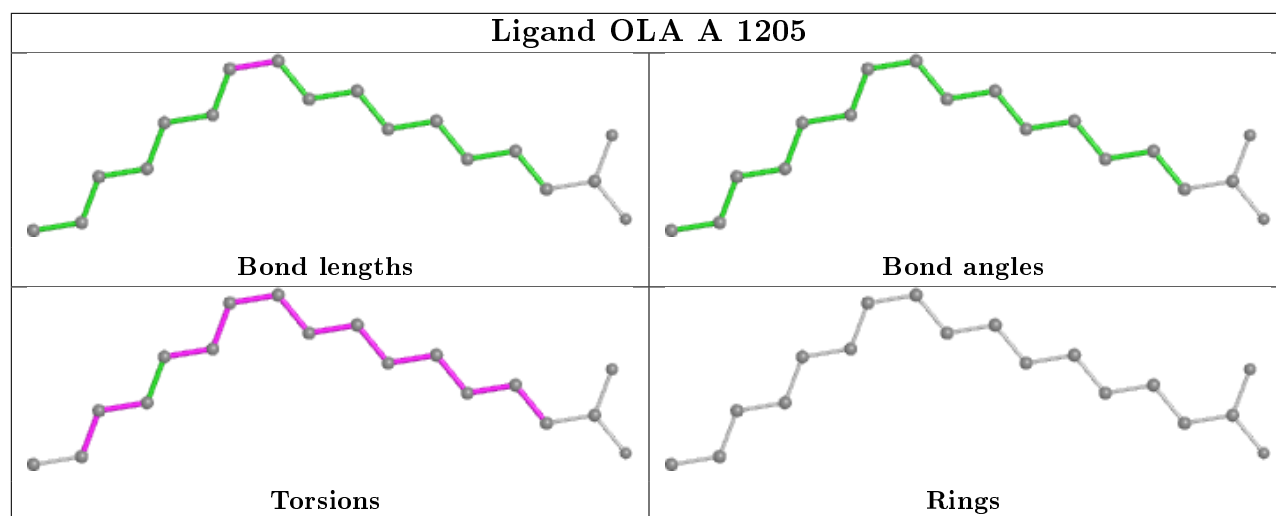
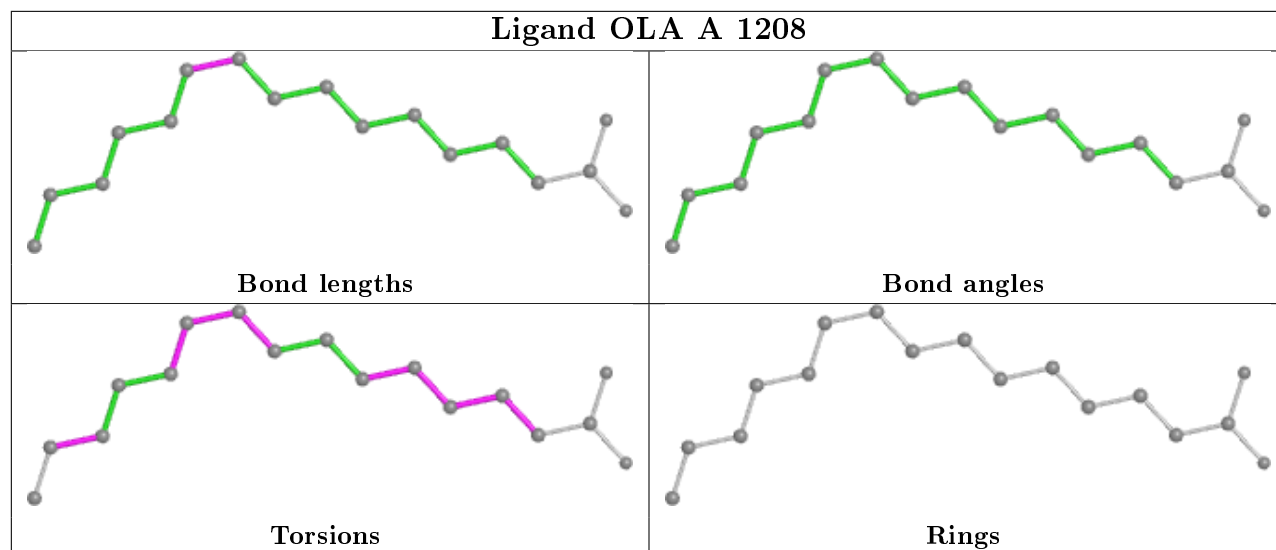
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

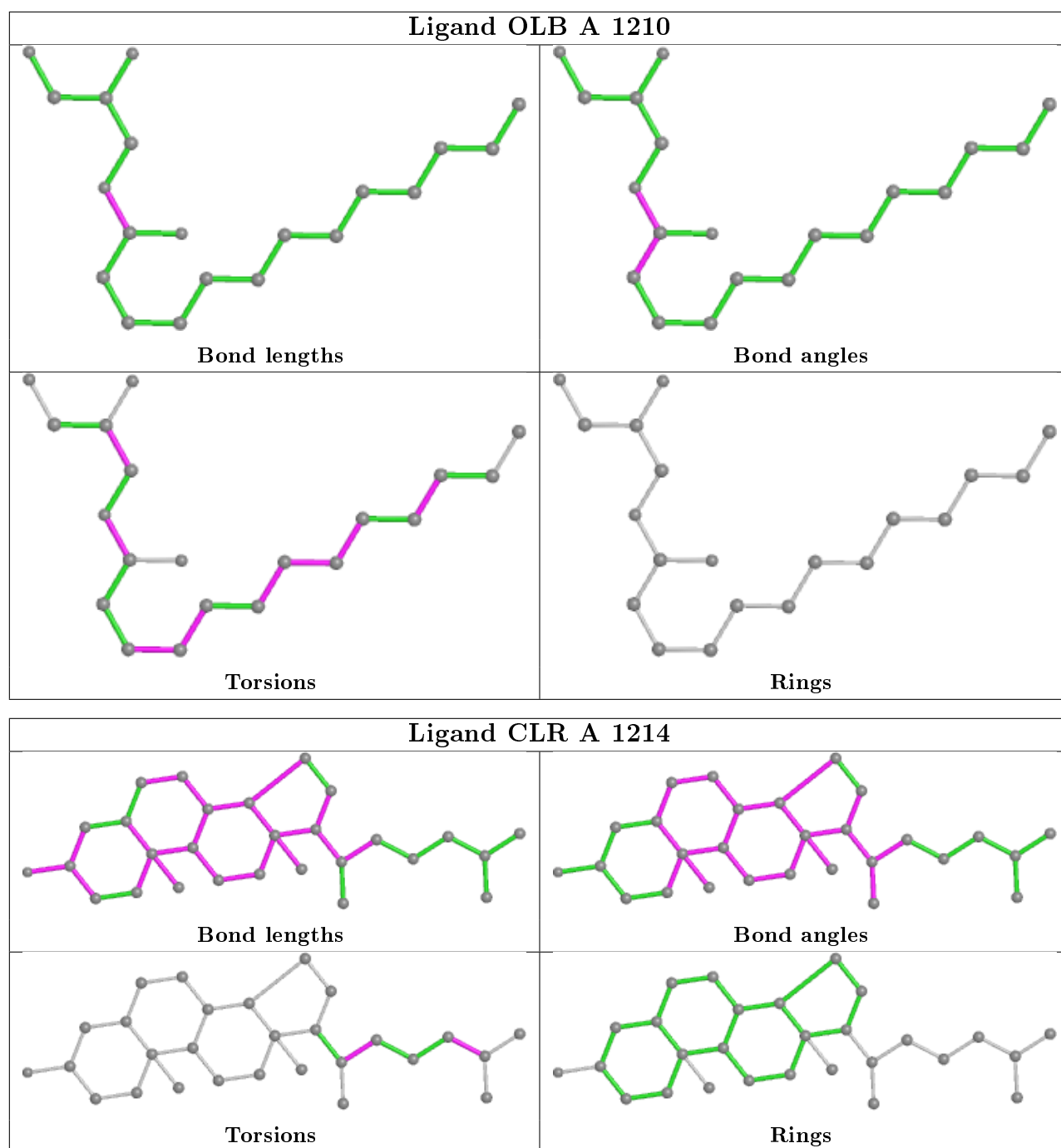












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/433 (89%)	1.43	96 (24%) 0 0	85, 112, 154, 192	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1091	ALA	9.5
1	A	1062	ARG	9.1
1	A	1060	ASP	8.5
1	A	1087	ALA	7.8
1	A	1061	PHE	7.1
1	A	111	ARG	7.0
1	A	1101	TYR	6.5
1	A	1090	ALA	6.4
1	A	1020	ALA	5.9
1	A	-1	GLY	5.8
1	A	1030	LEU	5.6
1	A	1092	GLU	5.6
1	A	1059	LYS	5.5
1	A	1063	HIS	5.4
1	A	1058	MET	5.3
1	A	1016	VAL	5.2
1	A	1029	ALA	5.1
1	A	154	ALA	4.8
1	A	1021	ASP	4.7
1	A	1085	LYS	4.7
1	A	225	LEU	4.6
1	A	1094	LEU	4.6
1	A	1105	TYR	4.6
1	A	1026	VAL	4.5
1	A	1095	LYS	4.3
1	A	156	SER	4.0
1	A	1106	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1006	ASN	3.9
1	A	1013	ASN	3.7
1	A	134	ALA	3.6
1	A	282	VAL	3.6
1	A	1099	ASN	3.6
1	A	150	LYS	3.6
1	A	1066	ASP	3.6
1	A	304	ARG	3.5
1	A	1019	LYS	3.5
1	A	1007	TRP	3.4
1	A	1064	GLY	3.4
1	A	1074	ASP	3.3
1	A	1024	ALA	3.3
1	A	1015	LYS	3.3
1	A	1003	LEU	3.3
1	A	197	TYR	3.2
1	A	263	SER	3.2
1	A	138	THR	3.2
1	A	1023	ALA	3.2
1	A	135	ILE	3.1
1	A	1011	ASN	3.1
1	A	112	TYR	3.1
1	A	1100	ALA	3.0
1	A	1033	MET	3.0
1	A	1102	ILE	3.0
1	A	1077	LYS	3.0
1	A	143	TRP	2.9
1	A	82	CYS	2.9
1	A	38	GLN	2.9
1	A	139	PRO	2.8
1	A	262	CYS	2.8
1	A	283	VAL	2.7
1	A	144	ASN	2.7
1	A	1093	GLN	2.7
1	A	176	TYR	2.7
1	A	1032	LYS	2.7
1	A	292	ILE	2.7
1	A	222	ARG	2.6
1	A	1097	THR	2.6
1	A	1022	ASN	2.6
1	A	1009	THR	2.6
1	A	137	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1084	VAL	2.5
1	A	107	ALA	2.5
1	A	110	LEU	2.5
1	A	5	GLY	2.4
1	A	108	ILE	2.4
1	A	226	GLN	2.3
1	A	35	SER	2.3
1	A	32	TRP	2.3
1	A	136	GLY	2.3
1	A	1089	ALA	2.3
1	A	264	HIS	2.3
1	A	116	VAL	2.2
1	A	1067	ILE	2.2
1	A	1018	GLU	2.2
1	A	85	LEU	2.2
1	A	153	LYS	2.2
1	A	1017	ILE	2.2
1	A	281	SER	2.2
1	A	220	ARG	2.2
1	A	9	TYR	2.2
1	A	1088	GLN	2.1
1	A	1025	GLN	2.1
1	A	300	ARG	2.1
1	A	8	VAL	2.0
1	A	33	LEU	2.0
1	A	12	VAL	2.0
1	A	115	LEU	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,

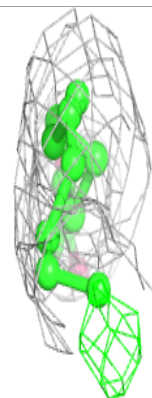
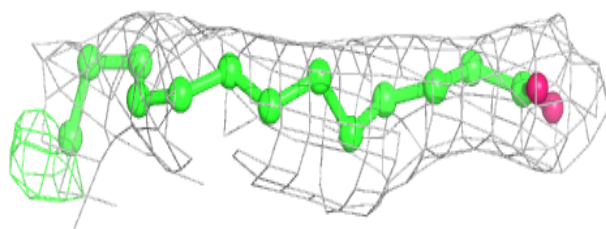
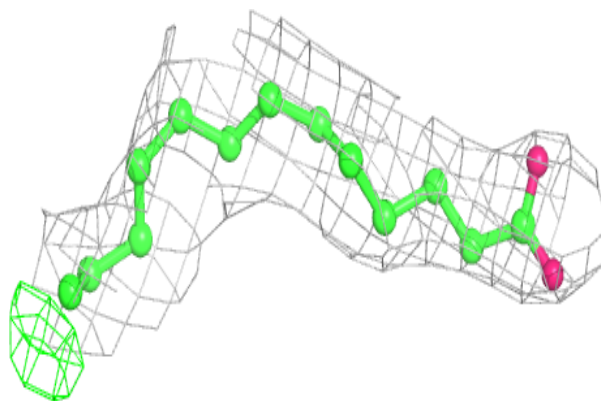
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OLA	A	1203	15/20	0.56	0.21	121,125,137,142	0
3	OLA	A	1205	18/20	0.57	0.61	108,117,135,135	0
3	OLA	A	1204	9/20	0.63	0.38	111,118,124,131	0
5	OLC	A	1212	19/25	0.66	0.40	106,123,140,141	0
3	OLA	A	1202	20/20	0.72	0.41	108,124,139,142	0
4	OLB	A	1210	20/25	0.72	0.43	116,131,139,147	0
3	OLA	A	1208	17/20	0.74	0.38	109,120,129,134	0
5	OLC	A	1211	25/25	0.75	0.58	110,126,143,145	0
4	OLB	A	1209	19/25	0.80	0.26	109,122,132,133	0
3	OLA	A	1207	7/20	0.81	0.41	108,114,119,120	0
3	OLA	A	1206	10/20	0.84	0.45	102,109,116,117	0
6	CLR	A	1213	28/28	0.85	0.30	107,118,125,132	0
6	CLR	A	1215	28/28	0.86	0.27	104,115,128,129	0
2	ZMA	A	1201	25/25	0.92	0.32	86,93,111,119	0
6	CLR	A	1214	28/28	0.93	0.23	106,116,119,128	0

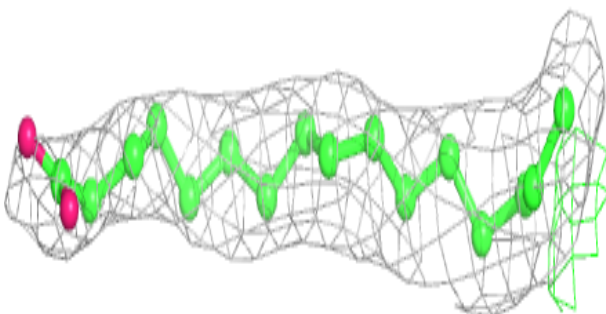
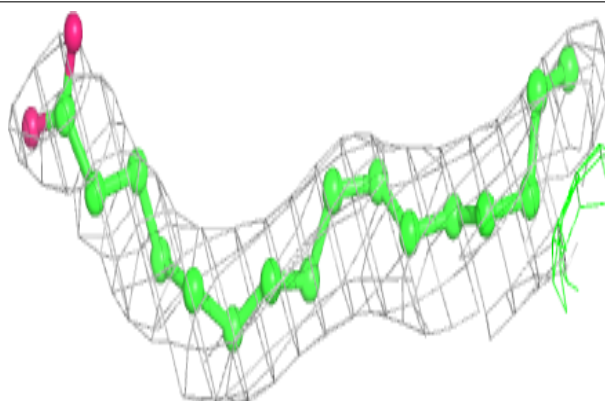
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

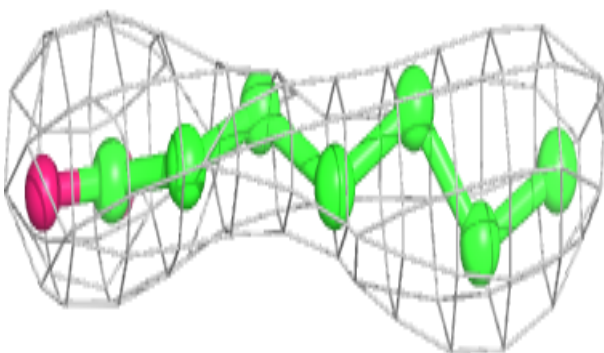
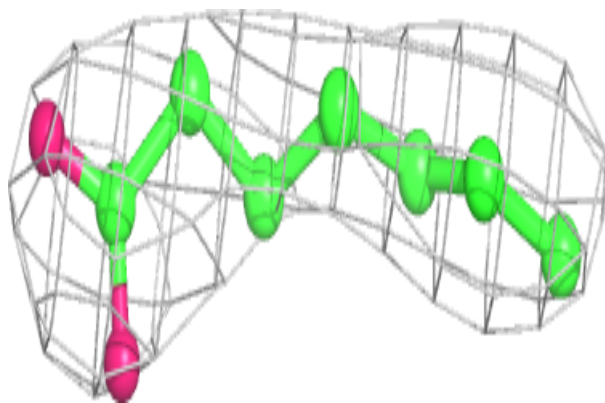
**Electron density around OLA A 1205:**

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

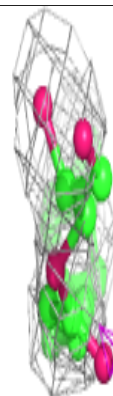
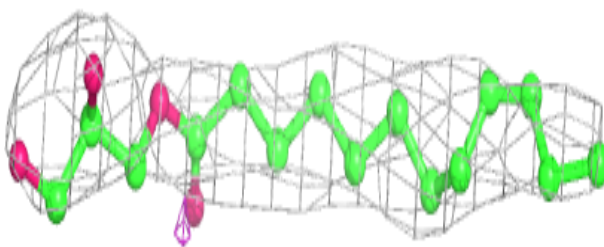
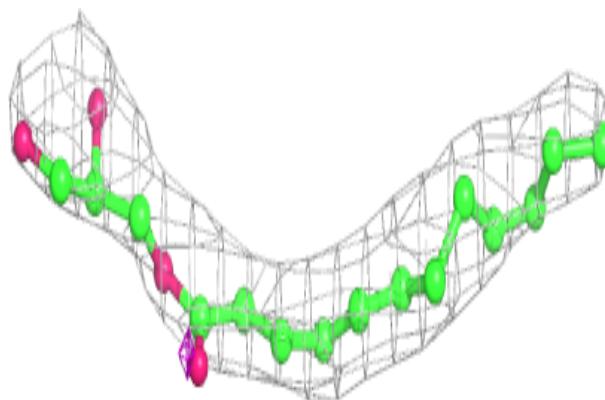


Electron density around OLA A 1204:

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

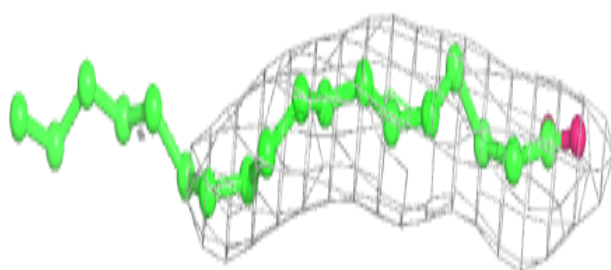
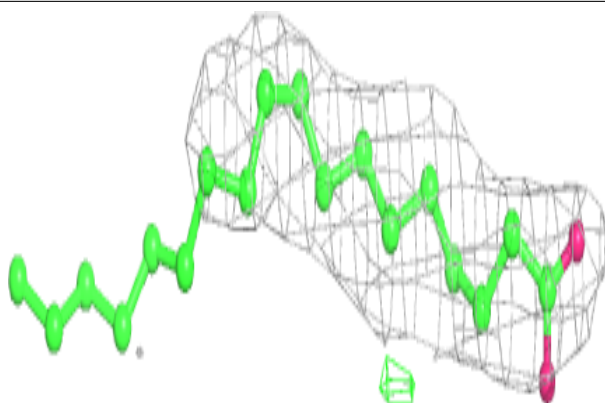
**Electron density around OLC A 1212:**

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

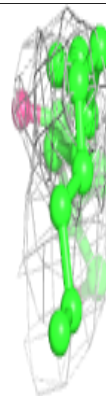
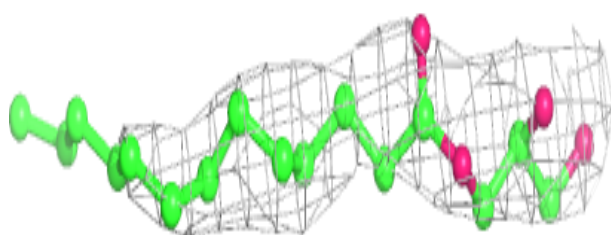
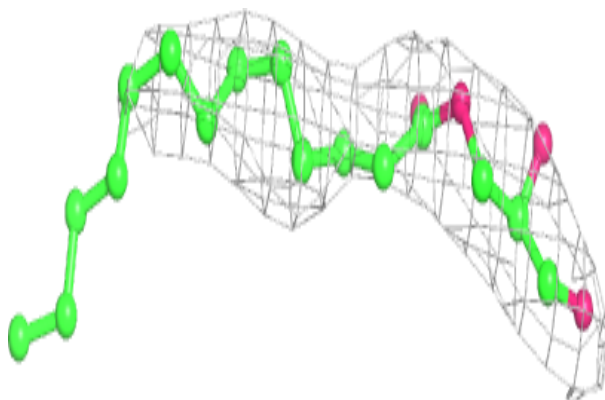


Electron density around OLA A 1202:

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

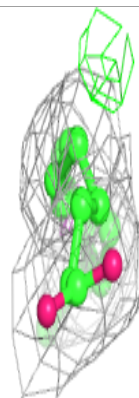
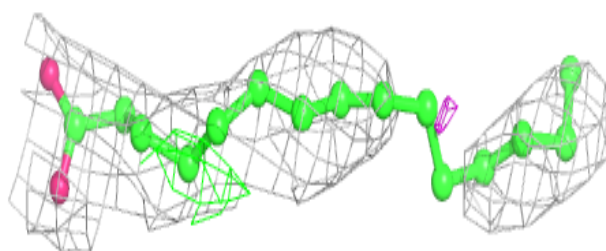
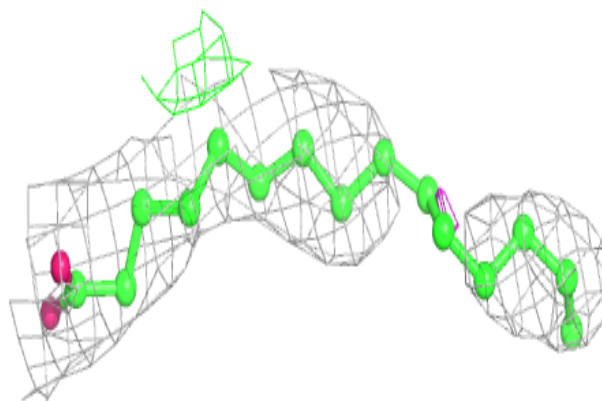
**Electron density around OLB A 1210:**

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

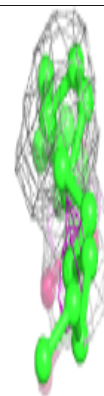
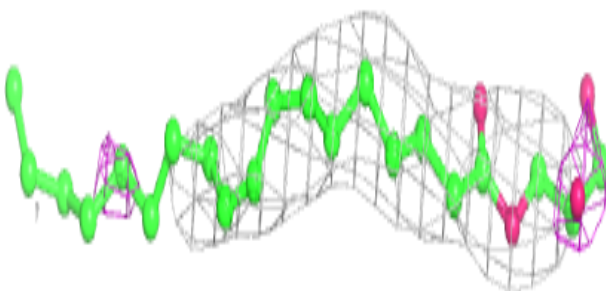
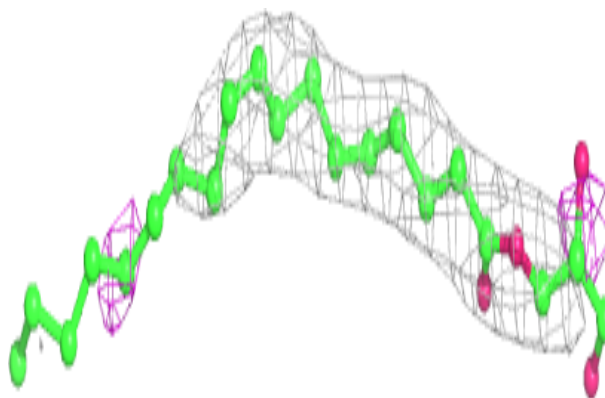


Electron density around OLA A 1208:

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

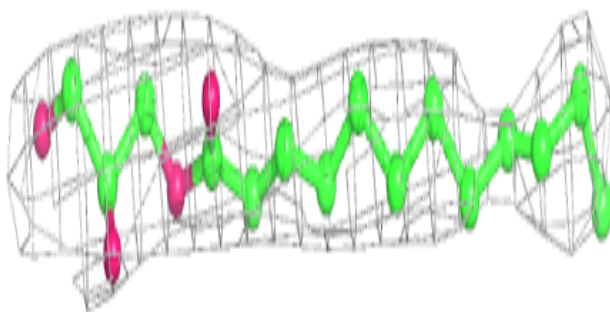
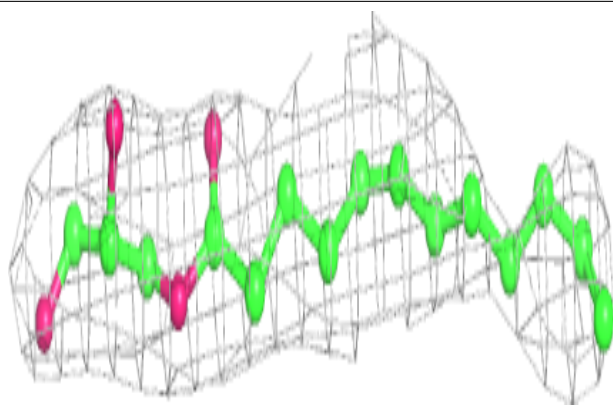
**Electron density around OLC A 1211:**

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

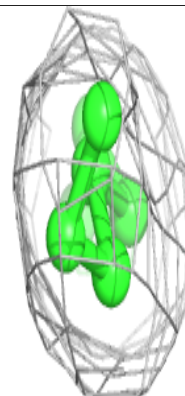
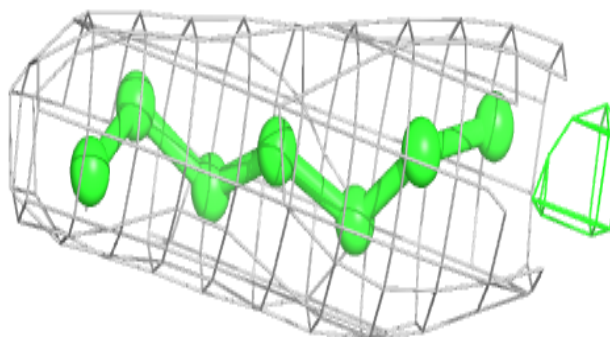
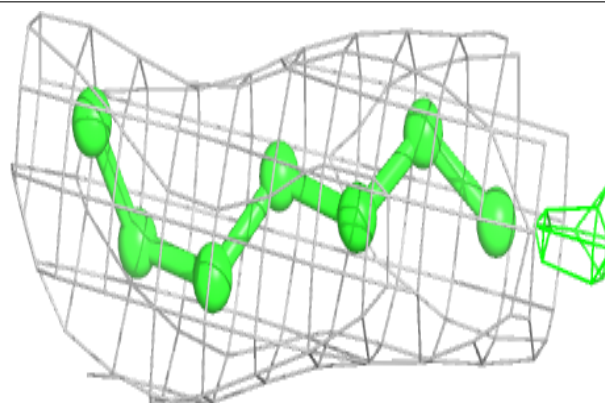


Electron density around OLB A 1209:

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

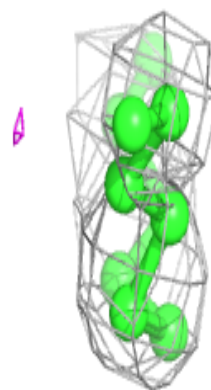
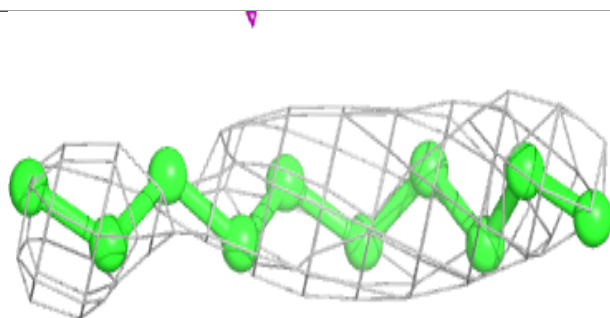
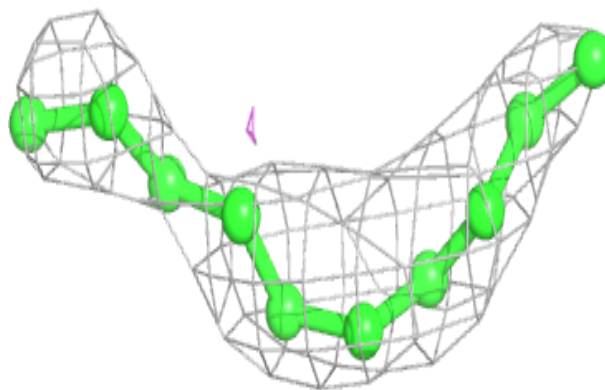
**Electron density around OLA A 1207:**

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

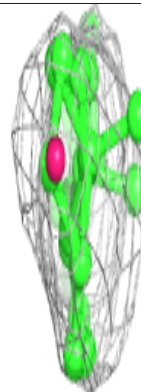
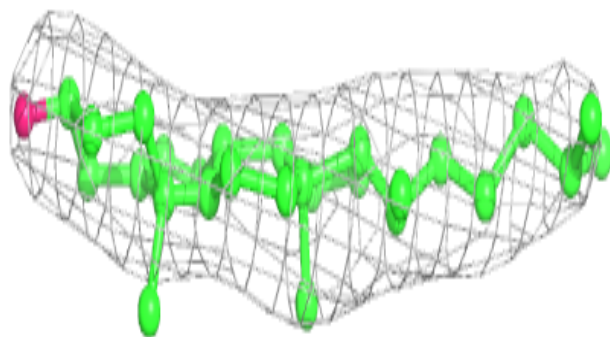
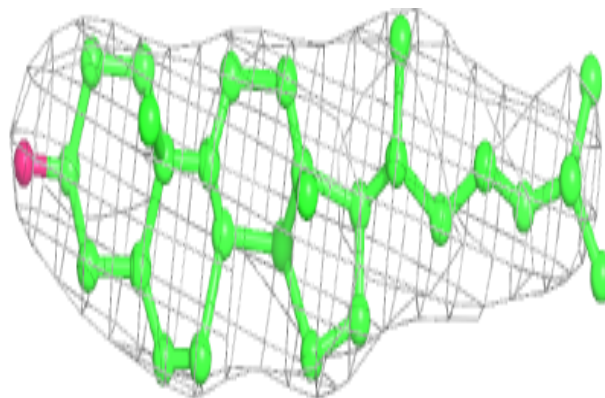


Electron density around OLA A 1206:

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

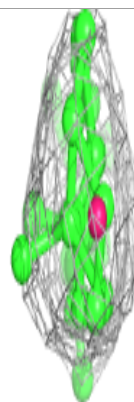
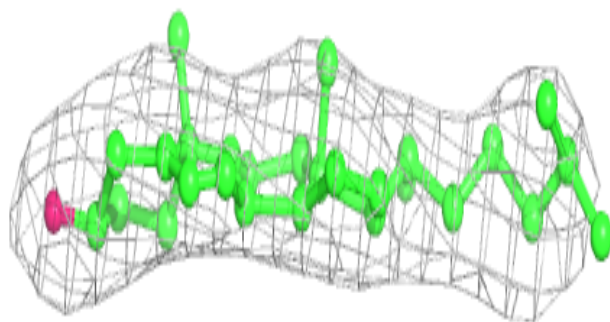
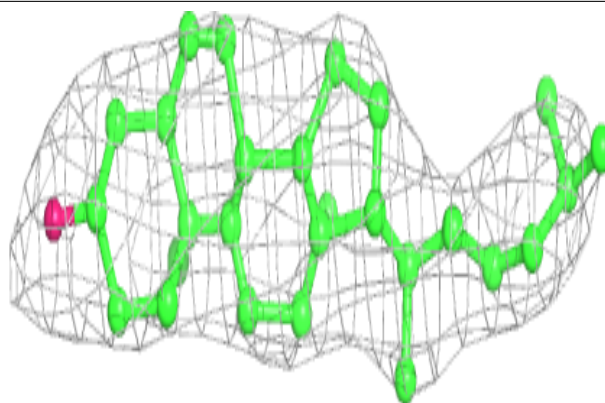
**Electron density around CLR A 1213:**

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

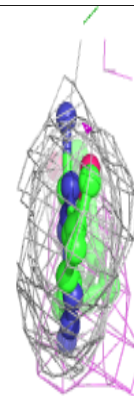
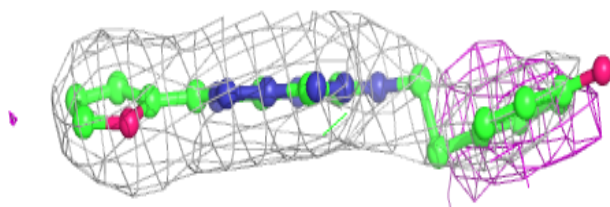
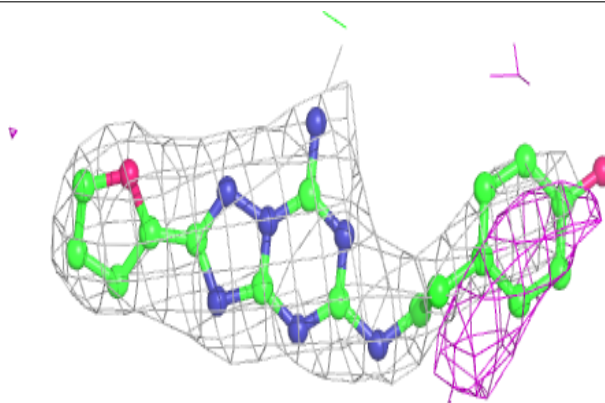


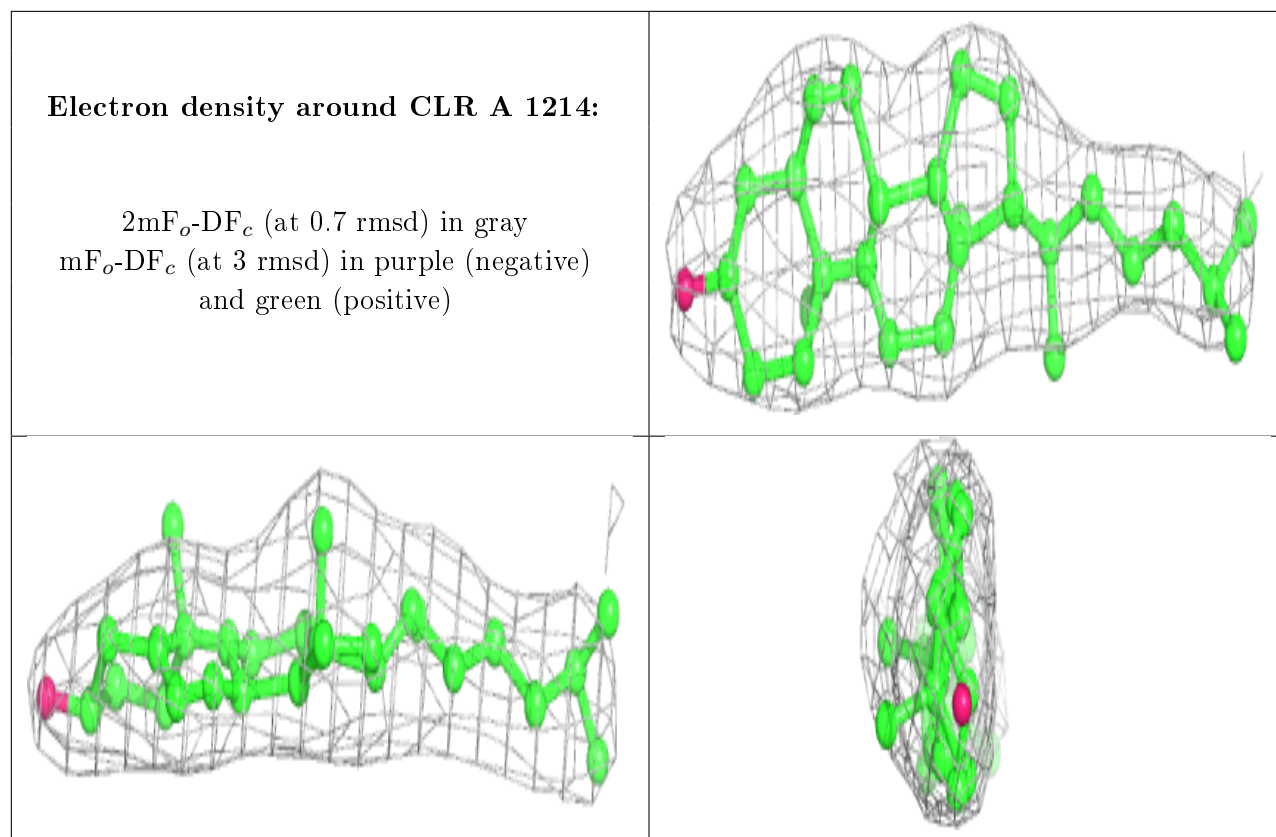
Electron density around CLR A 1215:

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

**Electron density around 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.