



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:17 PM UTC

PDB ID : 6S0L / pdb_00006s0l
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)

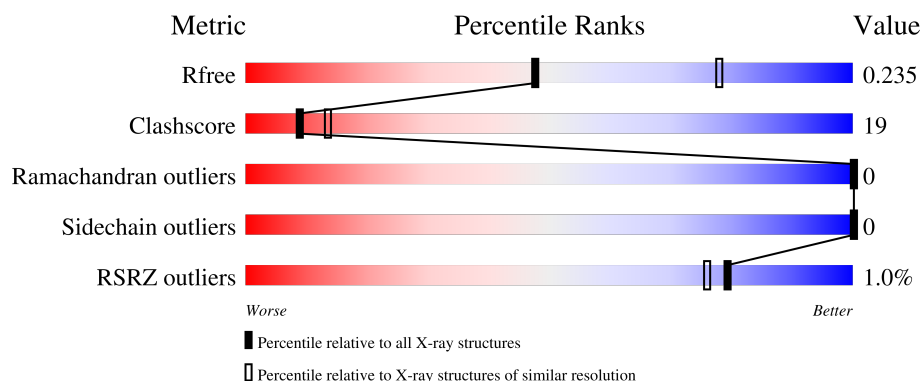
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	433	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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
6	CLR	A	1213	X	-	-	-
6	CLR	A	1214	X	-	-	-
6	CLR	A	1215	X	-	-	-

2 Entry composition [i](#)

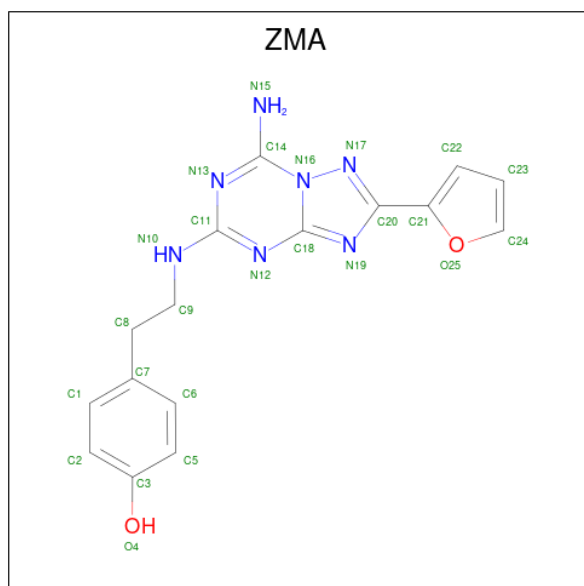
There are 6 unique types of molecules in this entry. The entry contains 3286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

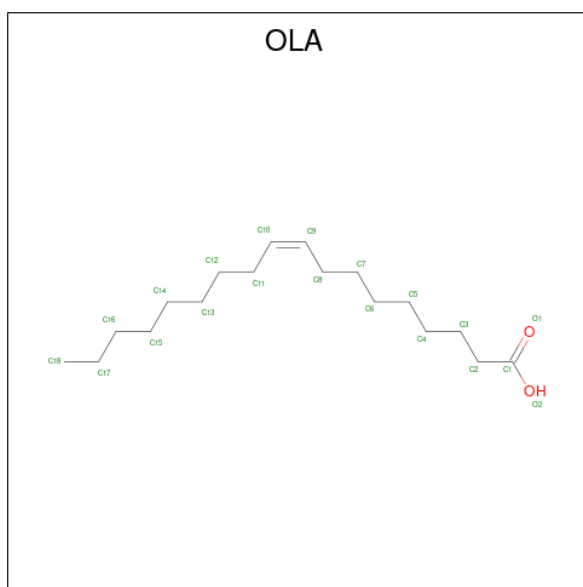
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	2998	1953	506	517	22	0	0	0

- 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 (CCD ID: ZMA) (formula: C₁₆H₁₅N₇O₂).



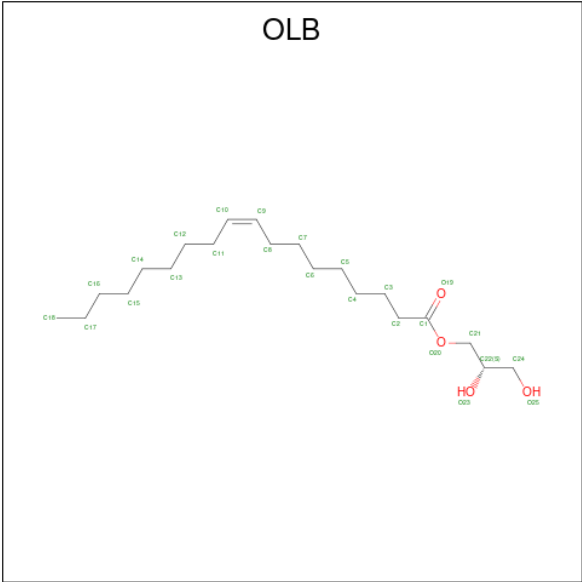
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	25	16	7	2	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



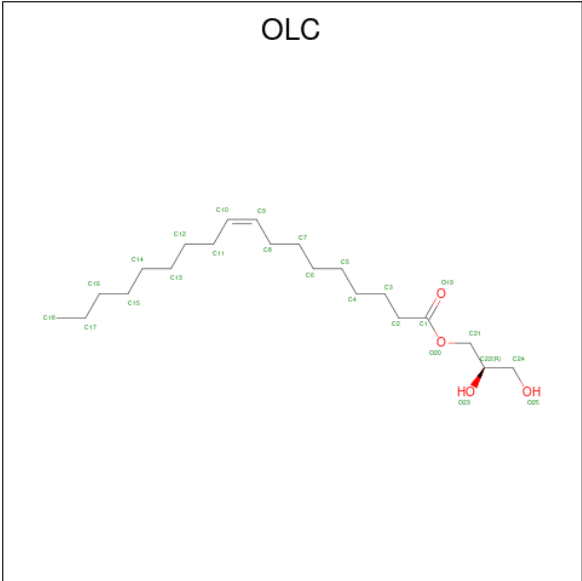
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			15	13	2		
3	A	1	Total	C	O	0	0
			9	7	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C		0	0
			10	10			
3	A	1	Total	C		0	0
			7	7			
3	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: $C_{21}H_{40}O_4$).



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 (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



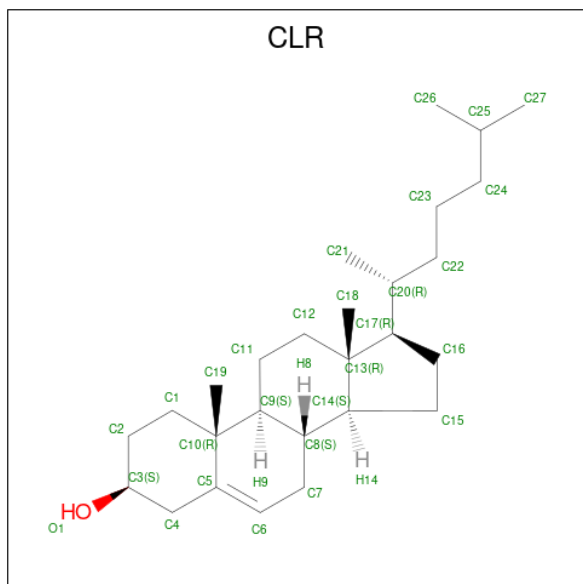
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		

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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 (CCD ID: CLR) (formula: $C_{27}H_{46}O$).

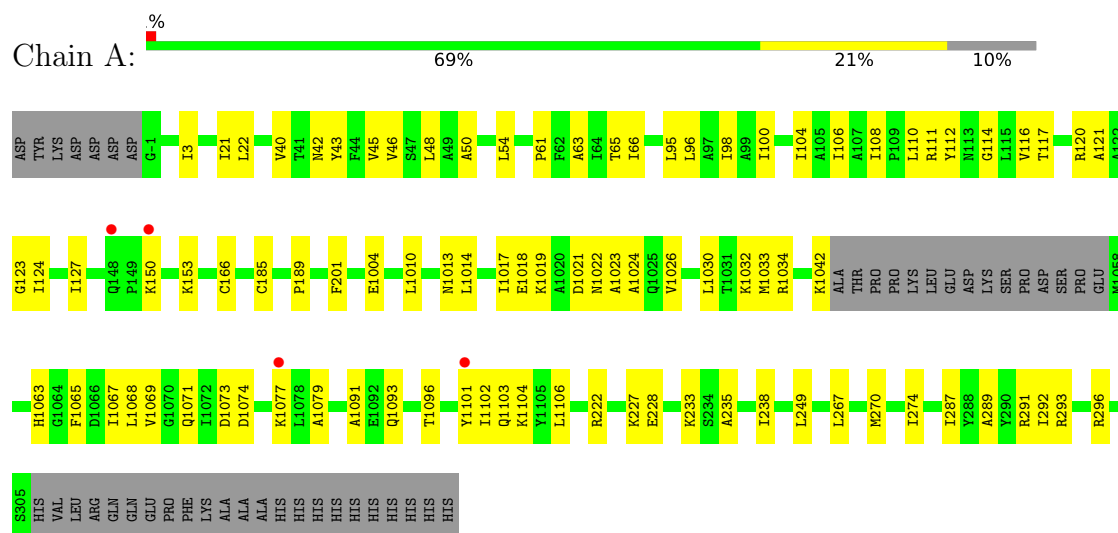


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	27	1		
6	A	1	Total	C	O	0	0
			28	27	1		
6	A	1	Total	C	O	0	0
			28	27	1		

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: A2a adenosine receptor



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 34.49 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.49-2.65) 89.4 (34.49-2.65)	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 0.214 , 0.235	Depositor DCC
R_{free} test set	787 reflections (2.69%)	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)	0.30 , 107.6	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	0.95	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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/3062	0.66	0/4164

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2998	0	3068	83	1
2	A	25	0	15	2	0
3	A	96	0	141	3	0
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	125	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 19.

All (125) 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:C8	6:A:1215:CLR:C7	1.76	1.56
6:A:1214:CLR:C8	6:A:1214:CLR:C14	1.80	1.54
6:A:1213:CLR:C13	6:A:1213:CLR:C17	1.81	1.39
6:A:1215:CLR:C13	6:A:1215:CLR:C17	1.81	1.37
6:A:1214:CLR:C17	6:A:1214:CLR:C13	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:C8	6:A:1213:CLR:H14	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:C7	6:A:1213:CLR:C9	2.47	0.74
1:A:121:ALA:HA	1:A:124:ILE:HD12	1.72	0.72
6:A:1213:CLR:C8	6:A:1213:CLR:C6	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
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:H181	6:A:1213:CLR:C16	2.28	0.59
6:A:1214:CLR:C18	6:A:1214:CLR:C16	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:110:LEU:HD22	1.68	0.57
6:A:1214:CLR:C8	6:A:1214:CLR:C6	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:C18	6:A:1215:CLR:C16	2.80	0.55
1:A:108:ILE:HD12	1:A:108:ILE:O	2.07	0.55
6:A:1215:CLR:C16	6:A:1215:CLR:H181	2.29	0.54
1:A:112:TYR:O	1:A:116:VAL:HG22	2.08	0.54
1:A:98:ILE:CD1	1:A:235:ALA:HB1	2.37	0.53
6:A:1213:CLR:C14	6:A:1213:CLR:C9	2.49	0.53
6:A:1213:CLR:C18	6:A:1213:CLR:C16	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:C14	6:A:1214:CLR:C9	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:1103:GLN:CD	1:A:1106:LEU:HD21	2.36	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
1:A:150:LYS:CD	1:A:153:LYS:HB2	2.33	0.49
6:A:1215:CLR:C18	6:A:1215:CLR:C20	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:95:LEU:HD21	1:A:238:ILE:HG22	1.94	0.48
1:A:1004:GLU:OE2	1:A:222:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1018:GLU:C	1:A:1019:LYS:HD3	2.39	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:1034:ARG:HH21	1:A:1073:ASP:CG	2.23	0.46
1:A:104:ILE:HG22	1:A:112:TYR:HD1	1.81	0.46
1:A:1042:LYS:HE2	1:A:1042:LYS:HB3	1.63	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
6:A:1214:CLR:C18	6:A:1214:CLR:C20	2.95	0.45
6:A:1215:CLR:H231	6:A:1215:CLR:H273	1.73	0.45
1:A:201:PHE:CE1	1:A:233:LYS:HG3	2.52	0.45
1:A:1018:GLU:HB3	1:A:1019:LYS:NZ	2.32	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:HG13	1:A:3:ILE:O	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: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
6:A:1213:CLR:C18	6:A:1213:CLR:C20	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:1102:ILE:C	1:A:1102:ILE:HD12	2.46	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:C18	6:A:1215:CLR:H20	2.51	0.40
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.88	0.40
1:A:21:ILE:HG13	1:A:22:LEU:H	1.86	0.40
1:A:117:THR:HG1	1:A:120:ARG:HG3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	312 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	1013	ASN
1	A	1063	HIS
1	A	1103	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	OLA	A	1202	-	19,19,19	0.82	1 (5%)	19,19,19	0.94	1 (5%)
4	OLB	A	1209	-	18,18,24	0.90	2 (11%)	19,19,25	1.29	1 (5%)
3	OLA	A	1203	-	14,14,19	0.95	1 (7%)	14,14,19	0.90	0
3	OLA	A	1207	-	6,6,19	0.36	0	5,5,19	0.37	0
3	OLA	A	1208	-	16,16,19	0.89	1 (6%)	16,16,19	1.05	2 (12%)
4	OLB	A	1210	-	19,19,24	0.94	1 (5%)	20,20,25	1.20	1 (5%)
5	OLC	A	1212	-	18,18,24	0.94	1 (5%)	19,19,25	1.15	1 (5%)
6	CLR	A	1213	-	31,31,31	9.43	21 (67%)	48,48,48	3.56	20 (41%)
6	CLR	A	1215	-	31,31,31	9.32	22 (70%)	48,48,48	3.90	20 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLA	A	1205	-	17,17,19	0.84	1 (5%)	17,17,19	1.02	1 (5%)
6	CLR	A	1214	-	31,31,31	9.40	21 (67%)	48,48,48	3.79	22 (45%)
2	ZMA	A	1201	-	26,28,28	1.81	3 (11%)	30,39,39	2.67	12 (40%)
5	OLC	A	1211	-	24,24,24	0.80	2 (8%)	25,25,25	1.22	2 (8%)
3	OLA	A	1204	-	8,8,19	0.81	0	8,8,19	1.15	0
3	OLA	A	1206	-	9,9,19	1.02	1 (11%)	8,8,19	0.72	0

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

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

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1214	CLR	C8-C9	-21.60	1.13	1.53
6	A	1213	CLR	C8-C9	-21.60	1.13	1.53
6	A	1215	CLR	C8-C9	-21.18	1.13	1.53
6	A	1213	CLR	C13-C14	-19.88	1.18	1.55
6	A	1214	CLR	C13-C14	-19.19	1.19	1.55
6	A	1215	CLR	C13-C14	-18.66	1.20	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1213	CLR	C7-C6	-17.97	1.13	1.50
6	A	1214	CLR	C7-C6	-17.84	1.13	1.50
6	A	1215	CLR	C7-C6	-17.47	1.14	1.50
6	A	1213	CLR	C12-C13	-16.96	1.24	1.54
6	A	1214	CLR	C12-C13	-16.62	1.25	1.54
6	A	1215	CLR	C12-C13	-16.08	1.26	1.54
6	A	1214	CLR	C11-C9	-14.74	1.29	1.53
6	A	1214	CLR	C13-C17	14.68	1.82	1.55
6	A	1215	CLR	C13-C17	14.65	1.81	1.55
6	A	1215	CLR	C11-C9	-14.63	1.29	1.53
6	A	1215	CLR	C7-C8	14.54	1.76	1.53
6	A	1213	CLR	C13-C17	14.53	1.81	1.55
6	A	1215	CLR	C10-C9	-14.51	1.33	1.56
6	A	1214	CLR	C7-C8	14.50	1.76	1.53
6	A	1213	CLR	C11-C9	-14.45	1.30	1.53
6	A	1213	CLR	C7-C8	14.15	1.76	1.53
6	A	1214	CLR	C8-C14	14.06	1.80	1.53
6	A	1215	CLR	C8-C14	13.62	1.79	1.53
6	A	1213	CLR	C10-C9	-13.36	1.34	1.56
6	A	1214	CLR	C10-C9	-13.33	1.34	1.56
6	A	1213	CLR	C8-C14	13.14	1.78	1.53
6	A	1215	CLR	C15-C14	8.72	1.72	1.54
6	A	1214	CLR	C15-C14	8.65	1.72	1.54
6	A	1213	CLR	C15-C14	8.54	1.71	1.54
6	A	1214	CLR	C12-C11	7.72	1.68	1.53
6	A	1213	CLR	C12-C11	7.56	1.68	1.53
6	A	1215	CLR	C12-C11	7.41	1.68	1.53
6	A	1213	CLR	C20-C17	-6.54	1.43	1.54
6	A	1214	CLR	C20-C17	-6.27	1.43	1.54
6	A	1215	CLR	C20-C17	-6.03	1.44	1.54
2	A	1201	ZMA	C14-N15	5.71	1.44	1.34
6	A	1213	CLR	C4-C3	5.62	1.62	1.52
6	A	1215	CLR	C4-C3	5.55	1.62	1.52
6	A	1214	CLR	C4-C3	5.01	1.61	1.52
2	A	1201	ZMA	C18-N16	-4.90	1.31	1.38
6	A	1213	CLR	C1-C10	4.84	1.63	1.54
6	A	1214	CLR	C1-C10	4.46	1.62	1.54
6	A	1215	CLR	C1-C10	4.42	1.62	1.54
6	A	1214	CLR	C16-C17	-4.42	1.45	1.54
6	A	1213	CLR	C16-C17	-4.10	1.46	1.54
6	A	1215	CLR	C16-C17	-4.06	1.46	1.54
6	A	1215	CLR	C19-C10	3.94	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1213	CLR	C22-C20	3.82	1.63	1.54
6	A	1213	CLR	C19-C10	3.57	1.60	1.54
6	A	1215	CLR	C22-C20	3.21	1.62	1.54
6	A	1214	CLR	C22-C20	3.16	1.62	1.54
6	A	1214	CLR	C19-C10	2.98	1.59	1.54
3	A	1206	OLA	C9-C10	2.93	1.48	1.29
3	A	1208	OLA	C10-C9	2.92	1.48	1.31
6	A	1213	CLR	C10-C5	2.87	1.58	1.52
3	A	1203	OLA	C10-C9	2.84	1.47	1.31
5	A	1212	OLC	O20-C1	2.84	1.41	1.33
3	A	1202	OLA	C10-C9	2.73	1.47	1.31
4	A	1210	OLB	O20-C1	2.72	1.41	1.33
3	A	1205	OLA	C10-C9	2.71	1.47	1.31
2	A	1201	ZMA	C14-N16	-2.71	1.34	1.37
6	A	1215	CLR	C10-C5	2.60	1.57	1.52
6	A	1215	CLR	O1-C3	-2.52	1.36	1.43
4	A	1209	OLB	O20-C1	2.45	1.40	1.33
6	A	1214	CLR	O1-C3	-2.43	1.36	1.43
6	A	1213	CLR	C2-C3	2.42	1.57	1.51
6	A	1213	CLR	O1-C3	-2.41	1.36	1.43
5	A	1211	OLC	O20-C1	2.36	1.40	1.33
6	A	1214	CLR	C10-C5	2.31	1.57	1.52
6	A	1215	CLR	C6-C5	2.29	1.37	1.33
6	A	1215	CLR	C4-C5	2.26	1.56	1.51
6	A	1215	CLR	C18-C13	2.25	1.58	1.54
6	A	1213	CLR	C4-C5	2.21	1.56	1.51
6	A	1214	CLR	C2-C3	2.17	1.56	1.51
6	A	1214	CLR	C18-C13	2.13	1.57	1.54
5	A	1211	OLC	O20-C21	-2.13	1.40	1.45
4	A	1209	OLB	O20-C21	-2.08	1.40	1.45

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1215	CLR	C18-C13-C12	-14.30	89.52	110.61
6	A	1215	CLR	C12-C13-C14	12.42	125.84	107.25
6	A	1214	CLR	C18-C13-C12	-12.19	92.64	110.61
6	A	1213	CLR	C12-C13-C14	10.92	123.59	107.25
6	A	1214	CLR	C12-C13-C14	10.64	123.16	107.25
6	A	1213	CLR	C18-C13-C12	-10.33	95.38	110.61
6	A	1214	CLR	C18-C13-C17	-10.08	93.40	111.68
6	A	1215	CLR	C18-C13-C17	-9.66	94.16	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1213	CLR	C18-C13-C17	-9.22	94.96	111.68
6	A	1214	CLR	C12-C13-C17	8.87	129.66	116.60
6	A	1215	CLR	C12-C13-C17	7.82	128.12	116.60
6	A	1213	CLR	C12-C13-C17	7.05	126.99	116.60
2	A	1201	ZMA	C20-N17-N16	6.81	108.44	101.39
2	A	1201	ZMA	N17-C20-N19	-6.53	108.00	115.38
6	A	1214	CLR	C7-C8-C9	6.05	116.72	109.72
6	A	1213	CLR	C7-C8-C9	5.74	116.36	109.72
6	A	1215	CLR	C7-C8-C9	5.66	116.26	109.72
2	A	1201	ZMA	C9-C8-C7	-5.59	100.23	112.83
6	A	1213	CLR	C14-C8-C9	5.37	116.10	109.09
6	A	1214	CLR	C7-C6-C5	-5.36	115.97	125.02
6	A	1215	CLR	C15-C14-C8	4.98	127.05	119.10
6	A	1213	CLR	C7-C6-C5	-4.65	117.17	125.02
6	A	1215	CLR	C7-C6-C5	-4.59	117.26	125.02
6	A	1214	CLR	C15-C14-C8	4.47	126.22	119.10
2	A	1201	ZMA	N10-C11-N12	4.08	121.10	116.95
6	A	1215	CLR	C14-C8-C9	4.04	114.36	109.09
6	A	1213	CLR	C11-C9-C10	4.02	118.05	113.08
6	A	1213	CLR	C15-C14-C8	3.90	125.33	119.10
6	A	1215	CLR	C9-C10-C5	3.85	115.29	109.65
6	A	1213	CLR	C18-C13-C14	-3.82	104.74	111.68
6	A	1213	CLR	C1-C10-C9	3.77	113.72	108.74
6	A	1214	CLR	C19-C10-C1	-3.77	103.70	109.43
6	A	1214	CLR	C14-C8-C9	3.64	113.84	109.09
6	A	1215	CLR	C19-C10-C9	-3.62	107.60	111.66
6	A	1213	CLR	C19-C10-C1	-3.57	103.99	109.43
2	A	1201	ZMA	N16-C18-N12	-3.55	119.52	122.61
6	A	1214	CLR	C1-C10-C9	3.55	113.43	108.74
6	A	1214	CLR	C10-C9-C8	3.54	117.89	112.71
6	A	1215	CLR	C18-C13-C14	-3.41	105.49	111.68
2	A	1201	ZMA	N13-C11-N12	-3.40	120.90	126.79
5	A	1211	OLC	O20-C1-C2	3.35	122.06	111.83
6	A	1214	CLR	C11-C9-C10	3.32	117.18	113.08
4	A	1209	OLB	O20-C1-C2	3.32	121.95	111.83
4	A	1210	OLB	O20-C1-C2	3.32	121.95	111.83
6	A	1214	CLR	C9-C10-C5	3.28	114.45	109.65
2	A	1201	ZMA	C18-N16-N17	-3.17	108.05	110.41
6	A	1214	CLR	C22-C20-C17	-3.13	103.85	110.33
6	A	1213	CLR	C9-C10-C5	3.11	114.21	109.65
6	A	1213	CLR	C16-C17-C13	-3.11	100.19	103.84
6	A	1214	CLR	C19-C10-C5	-3.09	103.66	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1214	CLR	C21-C20-C22	-2.95	105.78	110.34
6	A	1213	CLR	C19-C10-C9	-2.91	108.39	111.66
6	A	1213	CLR	C17-C13-C14	2.85	103.37	100.10
6	A	1215	CLR	C10-C9-C8	2.84	116.86	112.71
6	A	1213	CLR	C8-C7-C6	-2.80	108.89	112.76
6	A	1213	CLR	C22-C20-C17	-2.77	104.59	110.33
3	A	1202	OLA	C3-C2-C1	-2.74	107.36	114.51
6	A	1215	CLR	C16-C17-C13	-2.74	100.62	103.84
2	A	1201	ZMA	C9-N10-C11	-2.71	116.27	122.35
2	A	1201	ZMA	N12-C18-N19	2.66	131.95	127.73
5	A	1212	OLC	O20-C1-C2	2.64	119.87	111.83
6	A	1213	CLR	C16-C17-C20	-2.55	108.32	112.18
3	A	1208	OLA	O2-C1-C2	2.52	121.97	114.00
6	A	1214	CLR	C10-C5-C6	-2.44	119.37	122.93
6	A	1215	CLR	C15-C16-C17	2.41	109.87	105.14
2	A	1201	ZMA	N15-C14-N16	2.41	121.34	118.32
6	A	1215	CLR	C17-C13-C14	2.39	102.84	100.10
6	A	1215	CLR	C11-C9-C8	2.37	115.09	111.78
6	A	1215	CLR	C21-C20-C22	-2.37	106.68	110.34
6	A	1215	CLR	C22-C20-C17	-2.36	105.43	110.33
6	A	1213	CLR	C15-C16-C17	2.34	109.72	105.14
6	A	1214	CLR	C16-C17-C13	-2.31	101.12	103.84
3	A	1205	OLA	O2-C1-C2	2.27	121.16	114.00
6	A	1215	CLR	C19-C10-C5	-2.25	104.95	108.38
2	A	1201	ZMA	C5-C6-C7	-2.22	118.08	121.00
3	A	1208	OLA	C3-C2-C1	-2.22	108.73	114.51
6	A	1214	CLR	C16-C17-C20	-2.19	108.86	112.18
5	A	1211	OLC	O20-C1-O19	-2.19	118.15	123.63
6	A	1214	CLR	C18-C13-C14	-2.15	107.78	111.68
2	A	1201	ZMA	C6-C7-C1	2.12	121.39	118.23
6	A	1215	CLR	C4-C5-C6	2.11	123.43	120.57
6	A	1214	CLR	C12-C11-C9	2.05	116.62	113.14
6	A	1214	CLR	C23-C22-C20	-2.04	109.38	115.08

All (6) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
6	A	1215	CLR	C8

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1209	OLB	C21-C22-C24-O25
4	A	1209	OLB	O23-C22-C24-O25
5	A	1211	OLC	C21-C22-C24-O25
5	A	1211	OLC	O23-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
3	A	1202	OLA	C1-C2-C3-C4
6	A	1215	CLR	C22-C23-C24-C25
5	A	1212	OLC	O19-C1-O20-C21
6	A	1214	CLR	C23-C24-C25-C26
6	A	1214	CLR	C23-C24-C25-C27
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	C3-C4-C5-C6
4	A	1210	OLB	C5-C6-C7-C8
5	A	1211	OLC	C4-C5-C6-C7
3	A	1206	OLA	C12-C13-C14-C15
3	A	1208	OLA	C3-C4-C5-C6
3	A	1208	OLA	C4-C5-C6-C7
3	A	1205	OLA	C2-C3-C4-C5
6	A	1213	CLR	C23-C24-C25-C26
6	A	1213	CLR	C23-C24-C25-C27
3	A	1203	OLA	C3-C4-C5-C6
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
4	A	1210	OLB	C6-C7-C8-C9
3	A	1202	OLA	C4-C5-C6-C7
3	A	1205	OLA	C1-C2-C3-C4
5	A	1211	OLC	C10-C11-C12-C13
5	A	1211	OLC	C6-C7-C8-C9
3	A	1202	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	1206	OLA	C11-C12-C13-C14
3	A	1208	OLA	C2-C3-C4-C5
5	A	1211	OLC	C14-C15-C16-C17
5	A	1212	OLC	C5-C6-C7-C8
5	A	1212	OLC	O20-C21-C22-O23
5	A	1211	OLC	C12-C13-C14-C15
5	A	1212	OLC	O20-C21-C22-C24
6	A	1214	CLR	C21-C20-C22-C23
3	A	1208	OLA	C1-C2-C3-C4
4	A	1210	OLB	C7-C8-C9-C10
3	A	1204	OLA	C1-C2-C3-C4
3	A	1205	OLA	C3-C4-C5-C6
3	A	1204	OLA	C3-C4-C5-C6
3	A	1203	OLA	C1-C2-C3-C4
3	A	1205	OLA	C12-C13-C14-C15
3	A	1202	OLA	C11-C10-C9-C8
5	A	1211	OLC	C5-C6-C7-C8
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	1205	OLA	C10-C11-C12-C13
3	A	1207	OLA	C3-C4-C5-C6
5	A	1211	OLC	C15-C16-C17-C18
5	A	1212	OLC	C9-C10-C11-C12
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
4	A	1209	OLB	C9-C10-C11-C12
3	A	1208	OLA	O2-C1-C2-C3
3	A	1206	OLA	C9-C10-C11-C12
3	A	1208	OLA	C7-C8-C9-C10
3	A	1205	OLA	O2-C1-C2-C3
3	A	1208	OLA	O1-C1-C2-C3
3	A	1208	OLA	C9-C10-C11-C12
4	A	1209	OLB	O19-C1-O20-C21
3	A	1205	OLA	O1-C1-C2-C3
3	A	1203	OLA	C9-C10-C11-C12
5	A	1211	OLC	C7-C8-C9-C10
3	A	1205	OLA	C5-C6-C7-C8
3	A	1208	OLA	C12-C13-C14-C15

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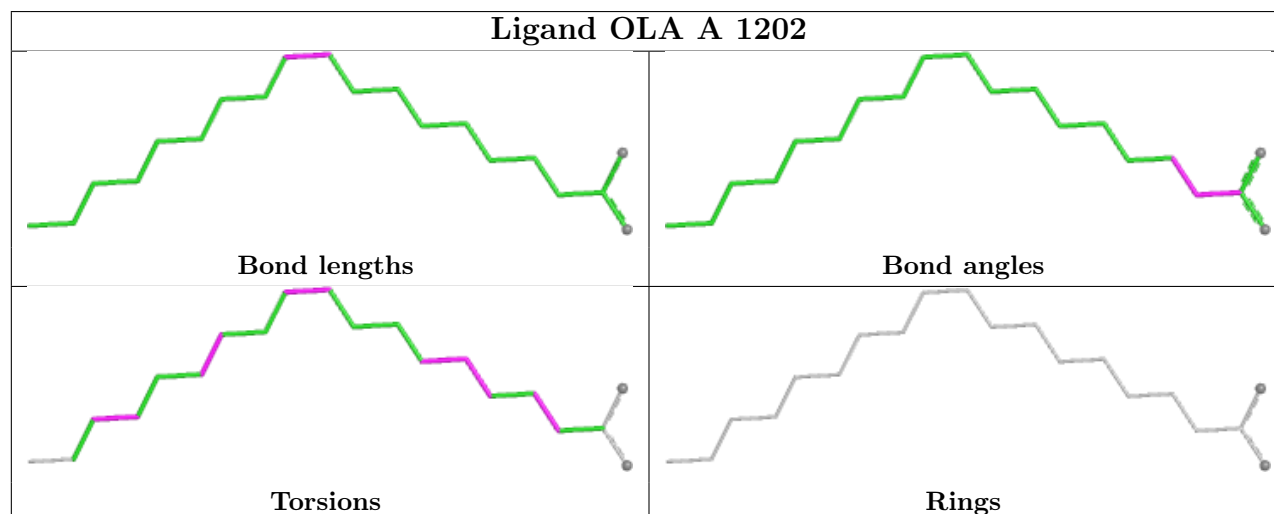
Mol	Chain	Res	Type	Atoms
4	A	1209	OLB	C2-C1-O20-C21
3	A	1207	OLA	C6-C7-C8-C9
3	A	1205	OLA	C13-C14-C15-C16

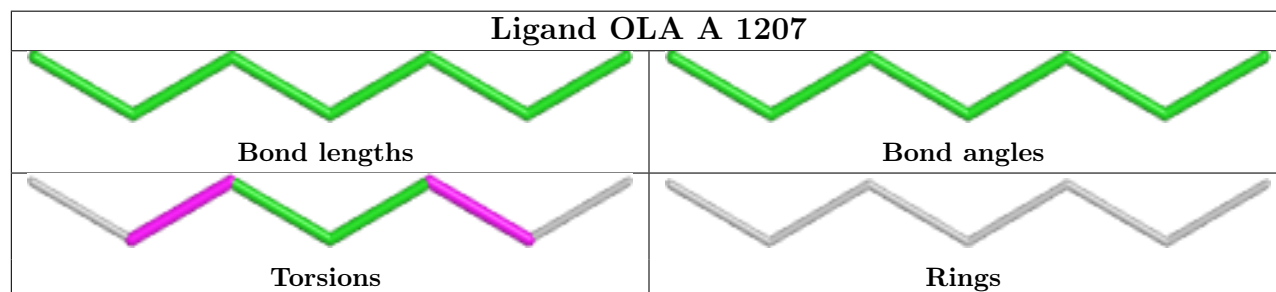
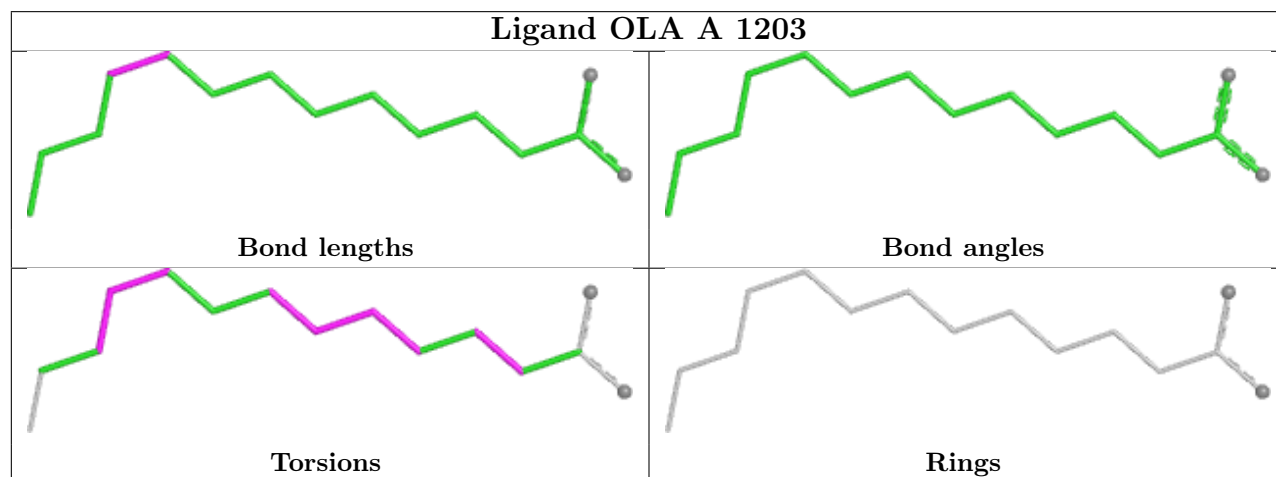
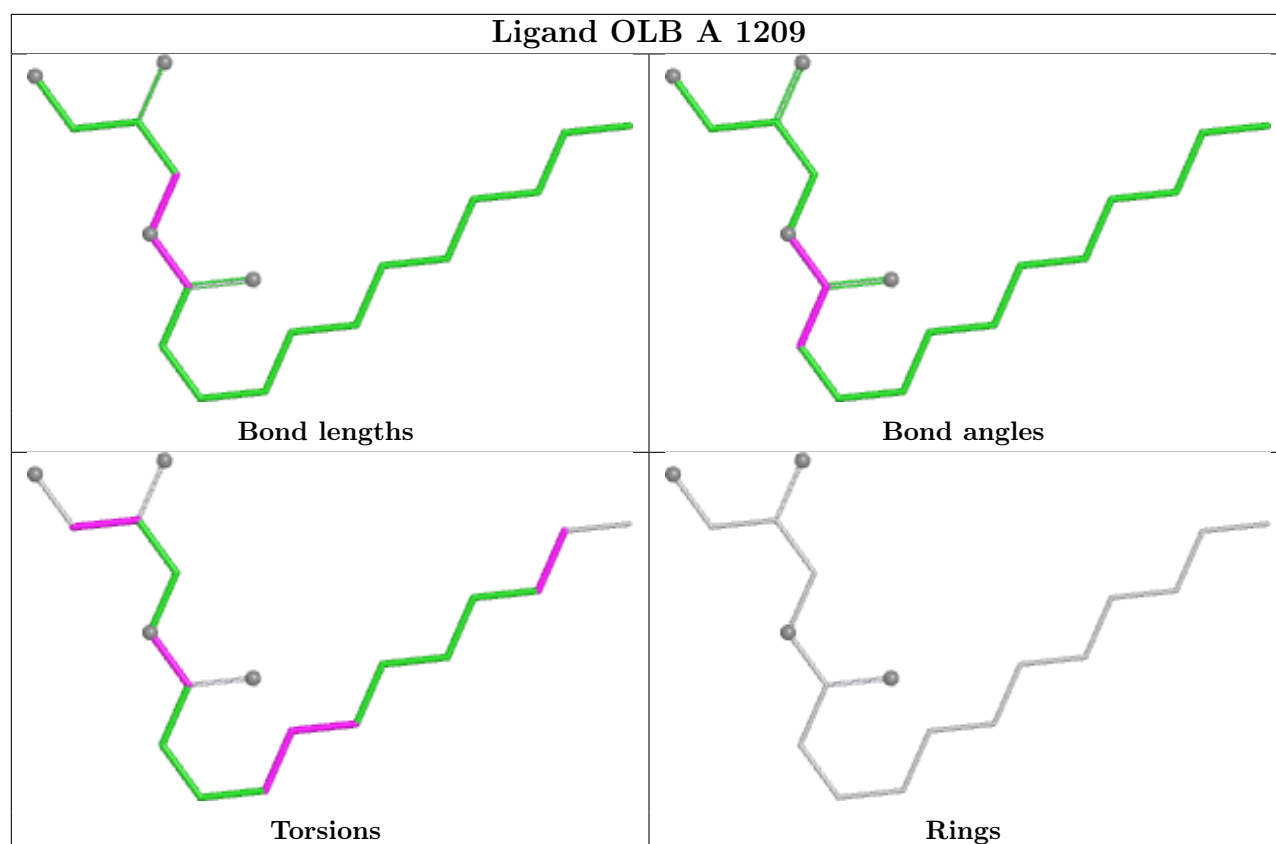
There are no ring outliers.

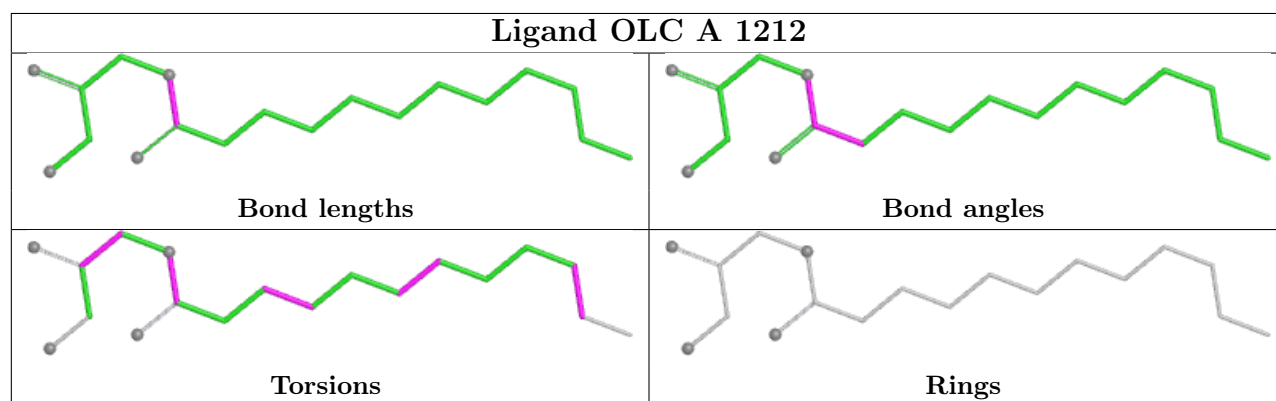
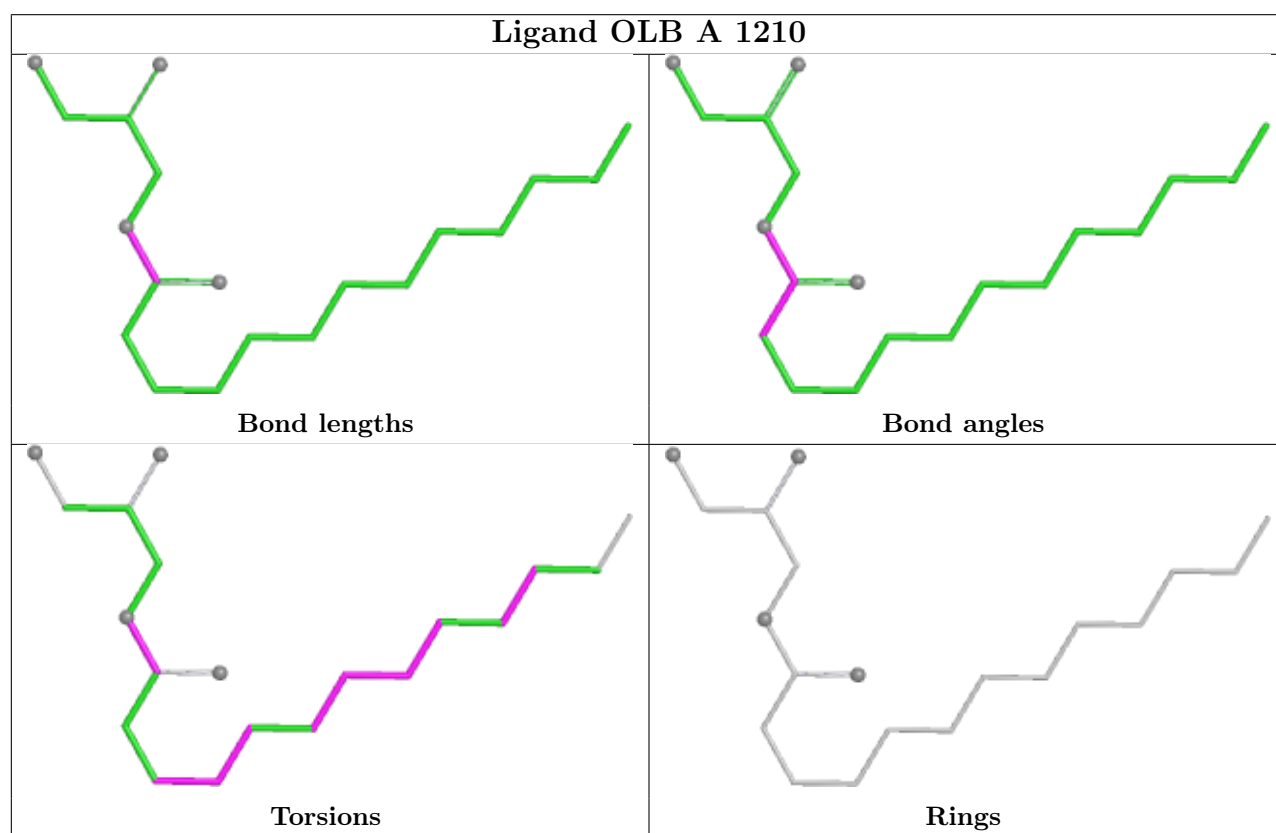
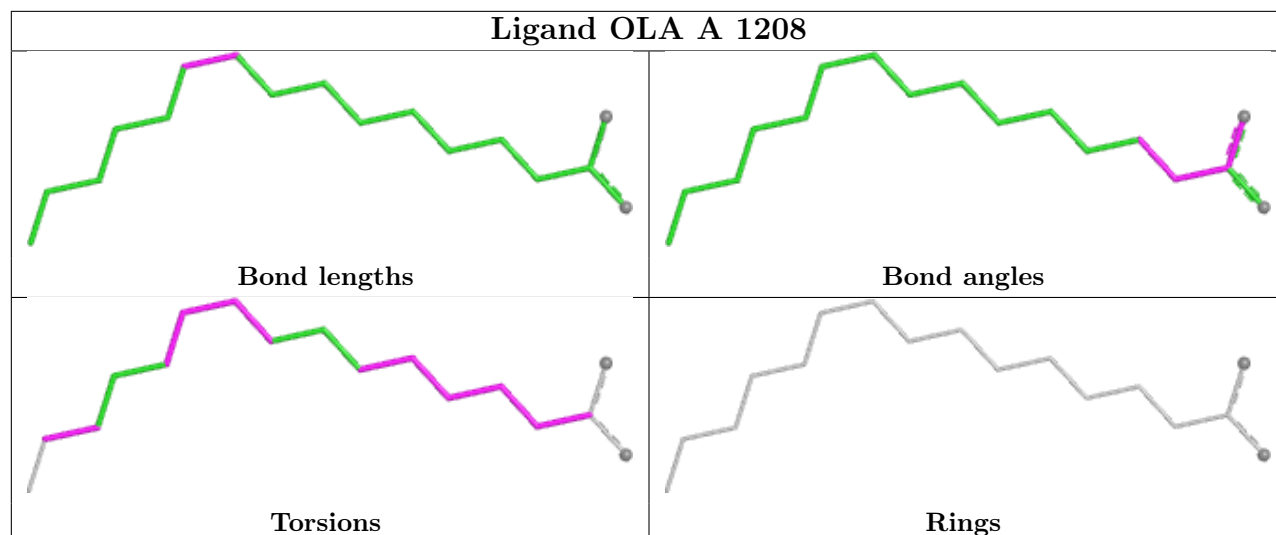
8 monomers are involved in 48 short contacts:

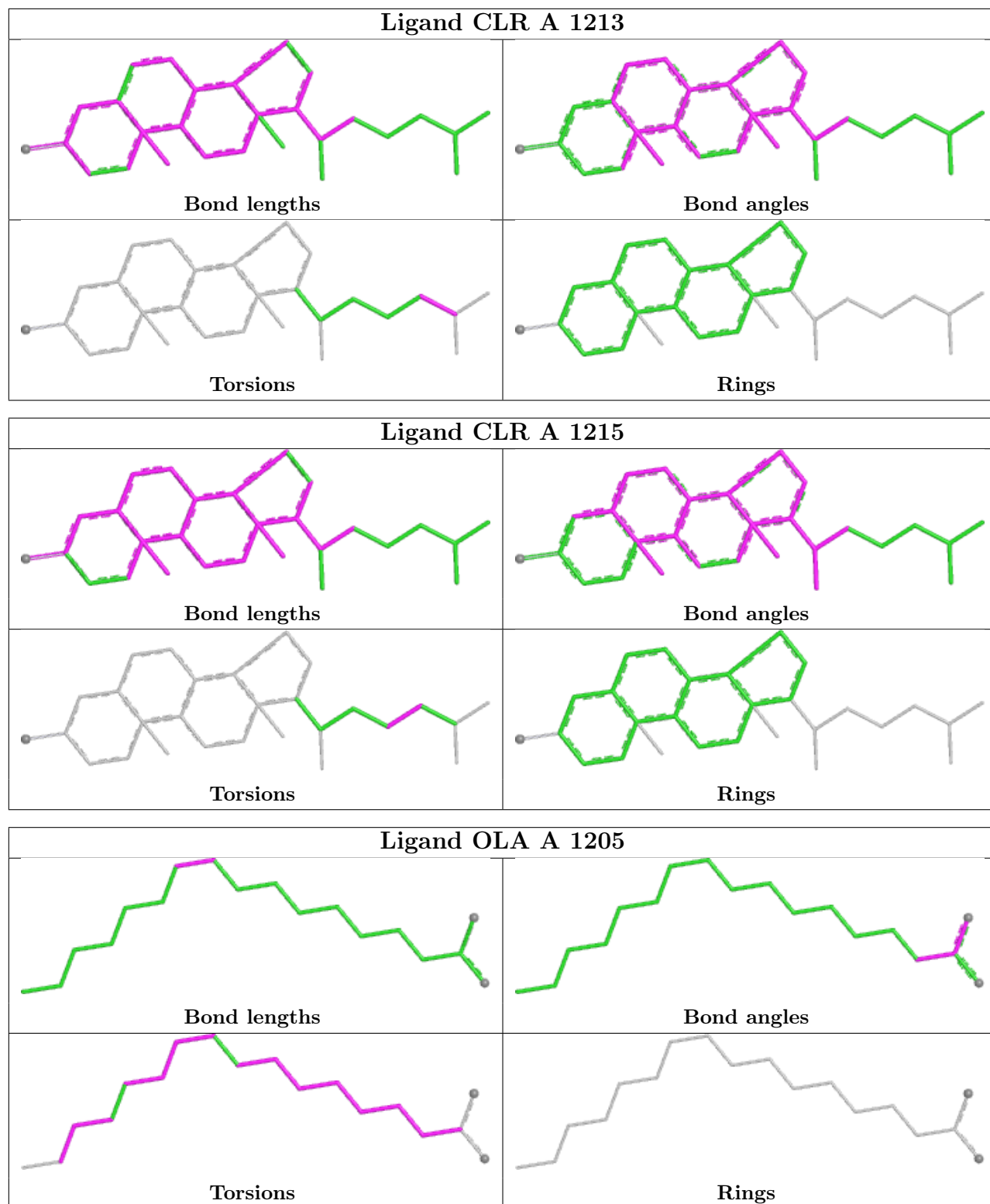
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	OLA	3	0
4	A	1210	OLB	3	0
5	A	1212	OLC	1	0
6	A	1213	CLR	12	0
6	A	1215	CLR	15	0
6	A	1214	CLR	13	0
2	A	1201	ZMA	2	0
5	A	1211	OLC	1	0

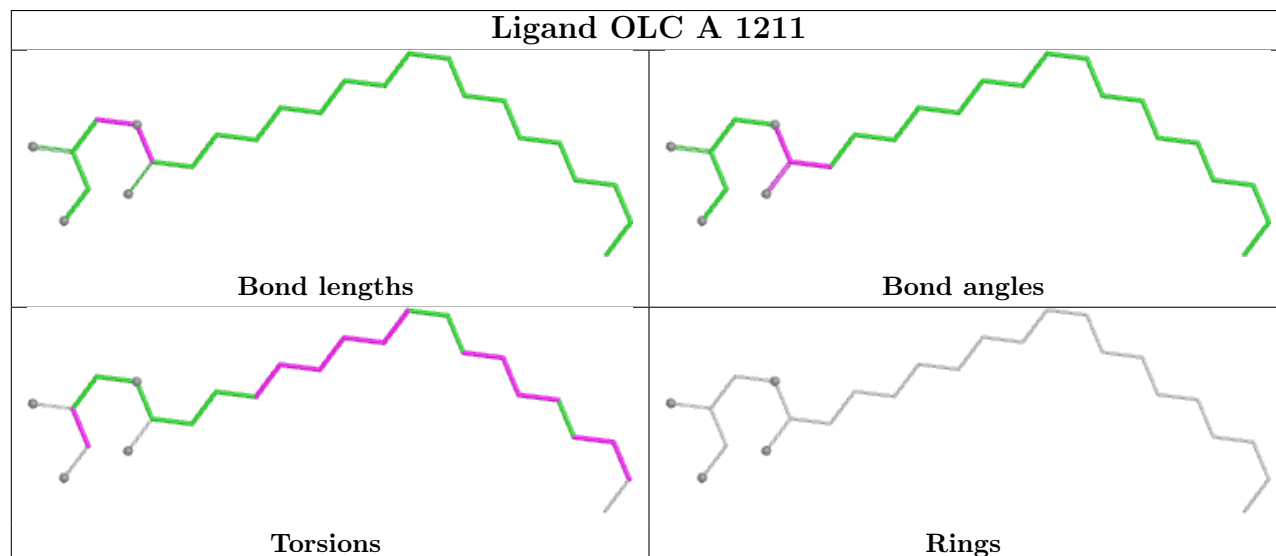
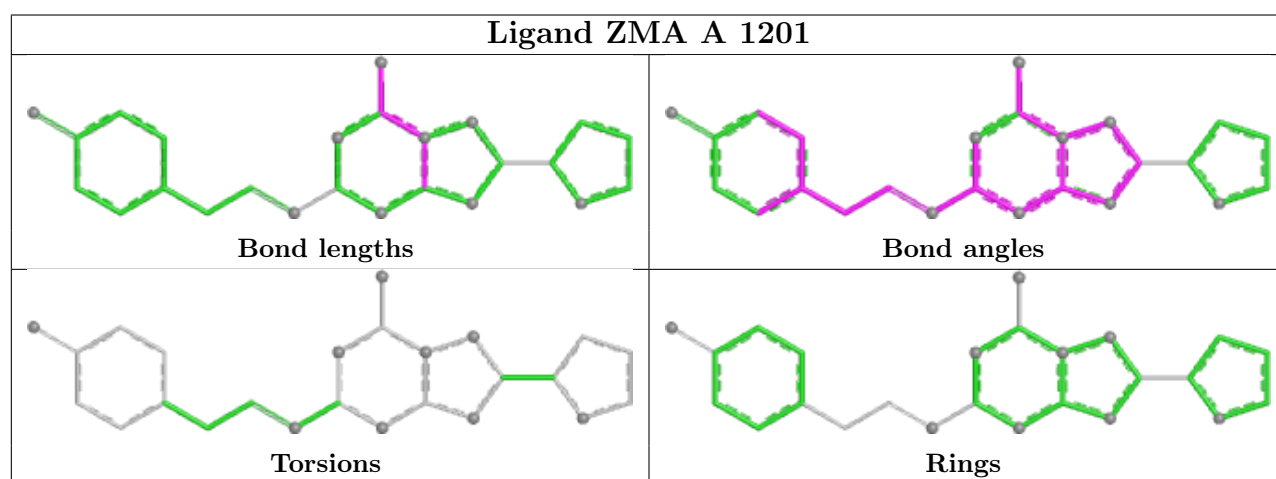
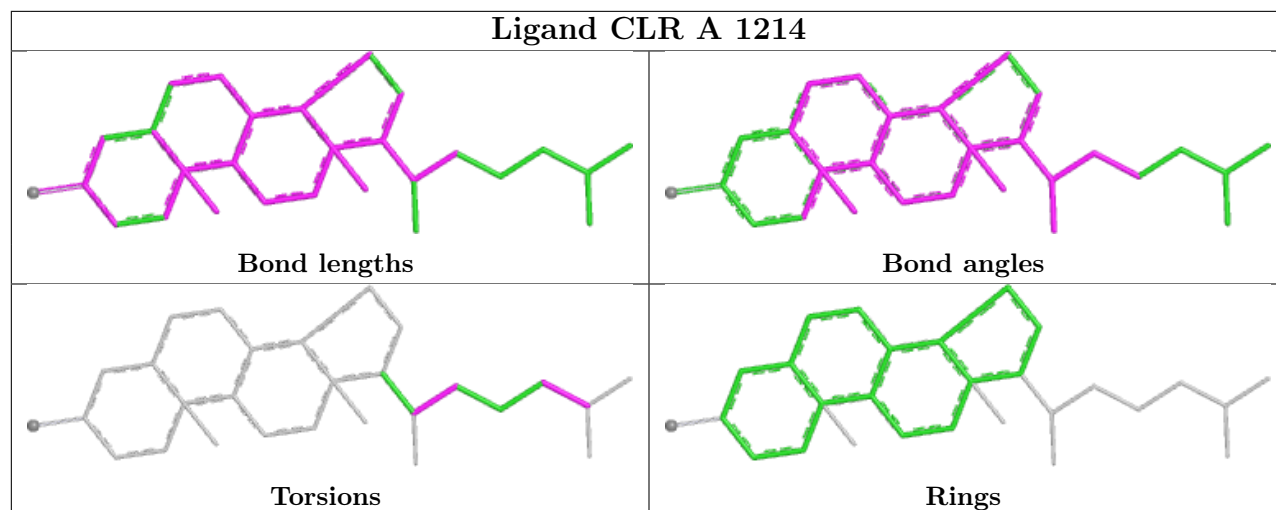
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

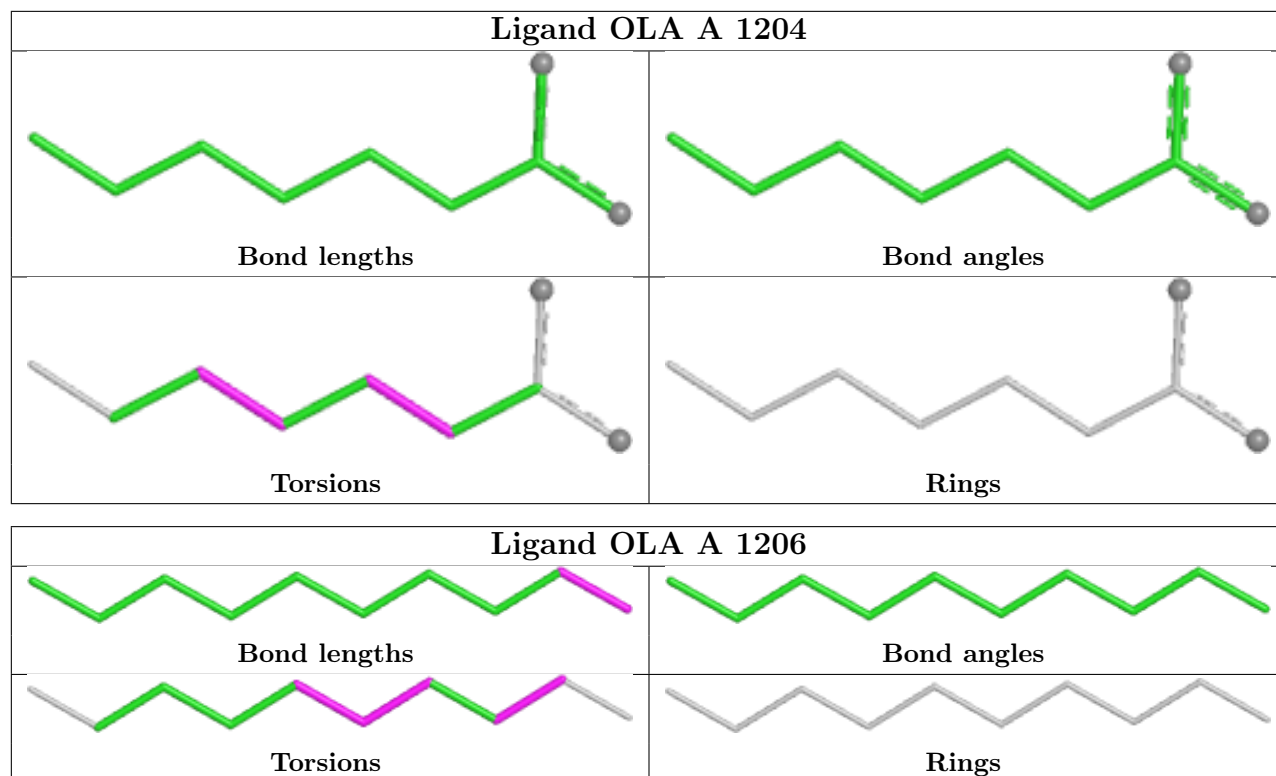












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/433 (89%)	0.03	4 (1%) 79 76	85, 112, 154, 192	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLN	3.5
1	A	1101	TYR	2.9
1	A	150	LYS	2.8
1	A	1077	LYS	2.1

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 oligosaccharides 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(Å ²)	Q<0.9
3	OLA	A	1203	15/20	0.85	0.13	121,125,137,142	0
4	OLB	A	1210	20/25	0.85	0.17	116,131,139,147	0
3	OLA	A	1208	17/20	0.88	0.15	109,120,129,134	0

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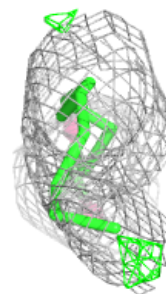
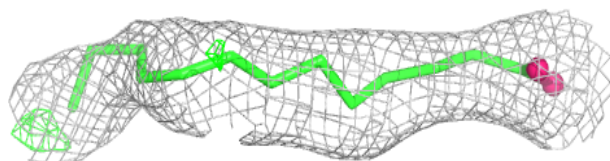
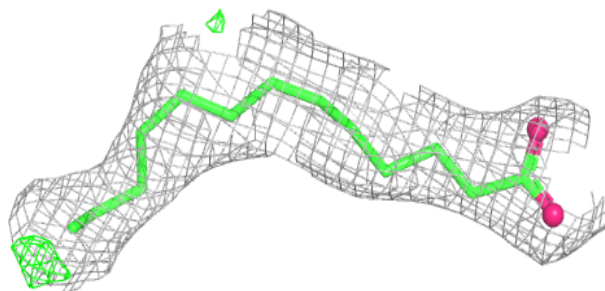
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLB	A	1209	19/25	0.88	0.13	109,122,132,133	0
3	OLA	A	1202	20/20	0.88	0.15	108,124,139,142	0
3	OLA	A	1207	7/20	0.90	0.15	108,114,119,120	0
3	OLA	A	1205	18/20	0.91	0.17	108,117,135,135	0
5	OLC	A	1212	19/25	0.91	0.14	106,123,140,141	0
5	OLC	A	1211	25/25	0.92	0.14	110,126,143,145	0
6	CLR	A	1213	28/28	0.93	0.13	107,118,125,132	0
6	CLR	A	1214	28/28	0.93	0.11	106,116,119,128	0
3	OLA	A	1204	9/20	0.95	0.12	111,118,124,131	0
3	OLA	A	1206	10/20	0.96	0.16	102,109,116,117	0
6	CLR	A	1215	28/28	0.96	0.11	104,115,128,129	0
2	ZMA	A	1201	25/25	0.97	0.07	86,93,111,119	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.

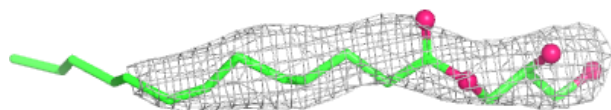
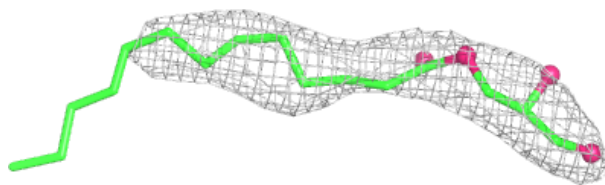
Electron density around OLA A 1203:

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

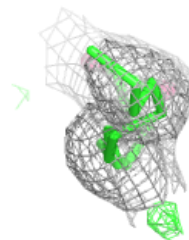
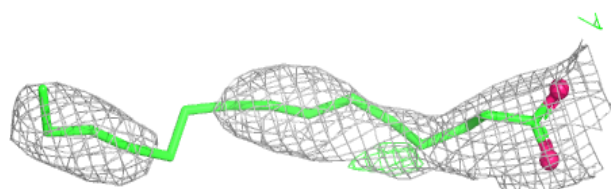
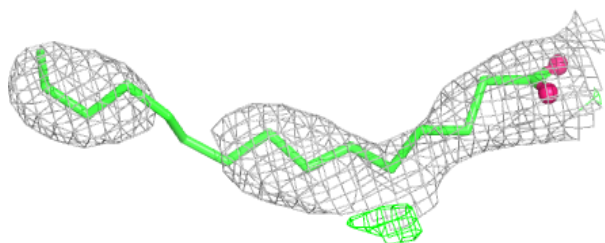


Electron density around OLB A 1210:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

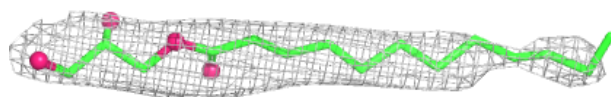
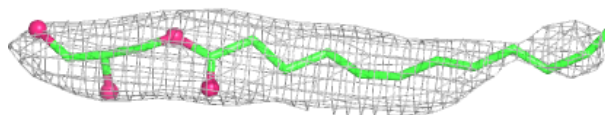
**Electron density around OLA A 1208:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

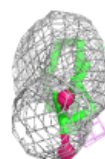
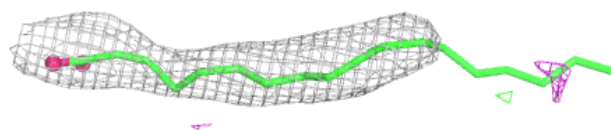
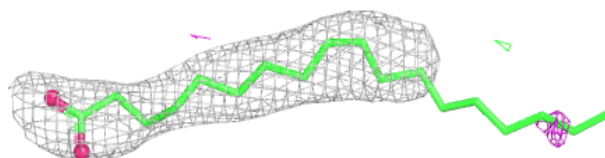


Electron density around OLB A 1209:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

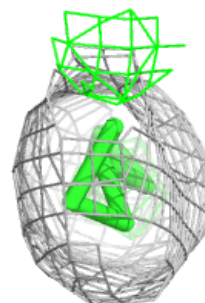
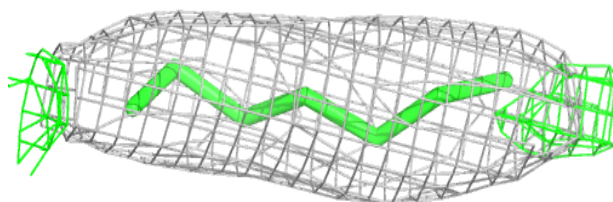
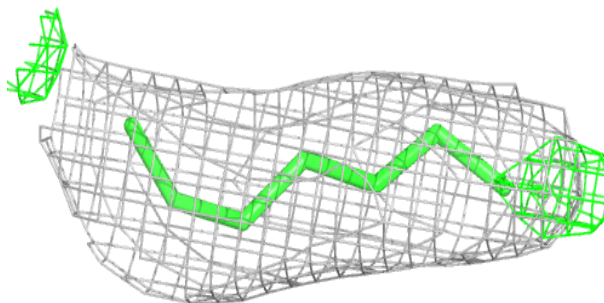
**Electron density around OLA A 1202:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

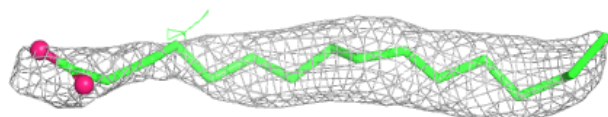
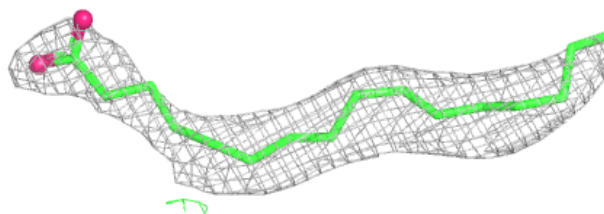


Electron density around OLA A 1207:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

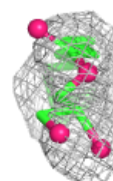
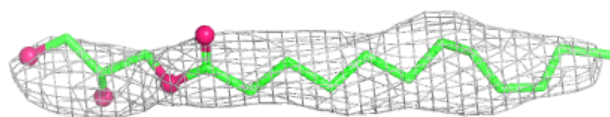
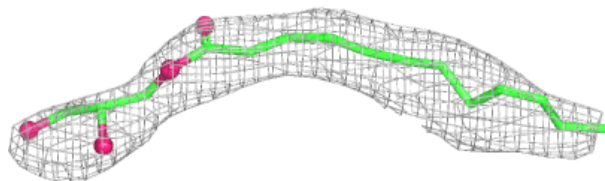
**Electron density around OLA A 1205:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

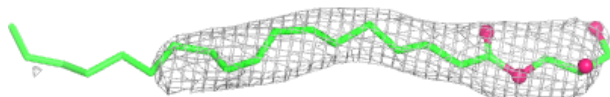
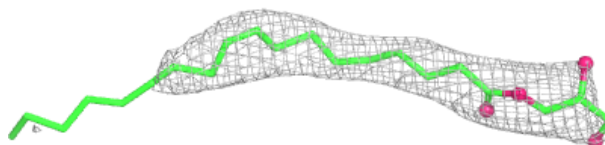


Electron density around OLC A 1212:

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and green (positive)

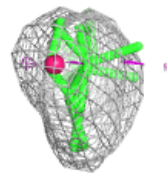
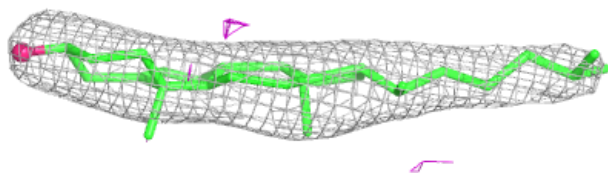
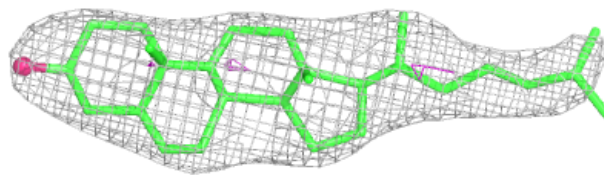
**Electron density around OLC A 1211:**

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and green (positive)

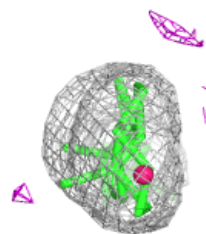
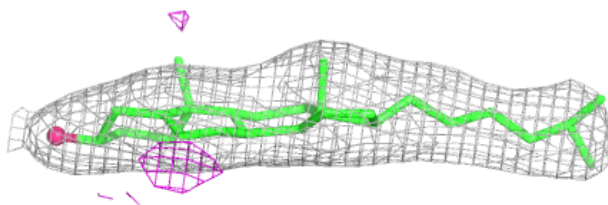
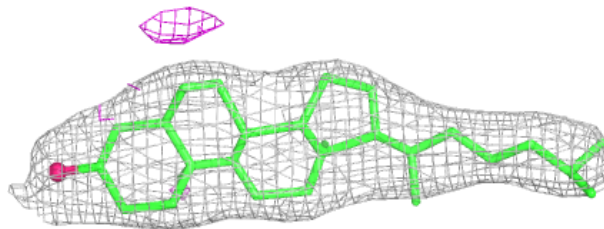


Electron density around CLR A 1213:

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and green (positive)

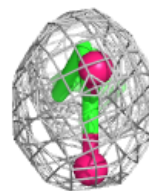
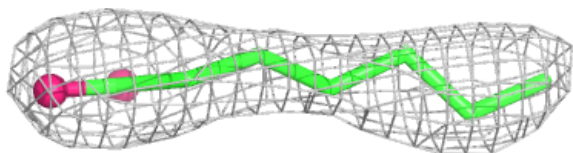
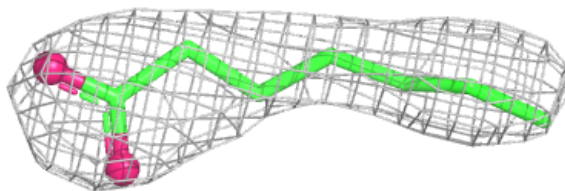
**Electron density around CLR A 1214:**

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and green (positive)

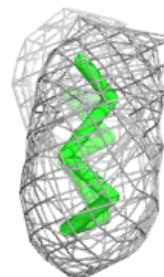
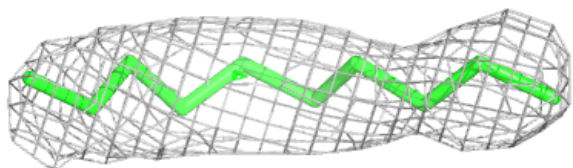
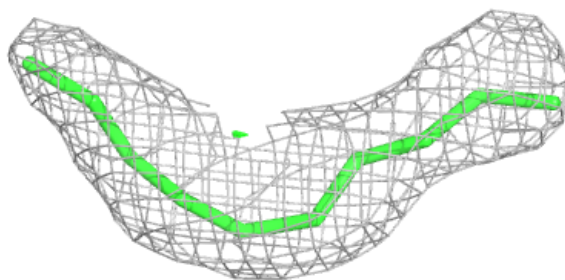


Electron density around OLA A 1204:

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and green (positive)

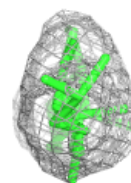
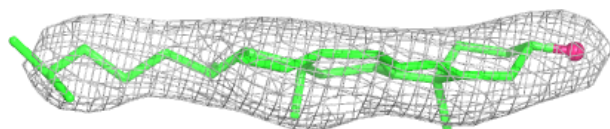
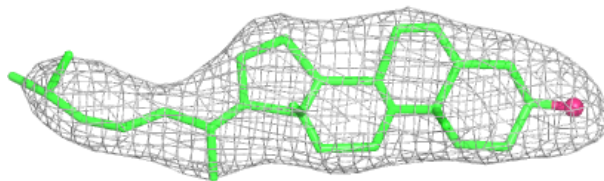
**Electron density around OLA A 1206:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

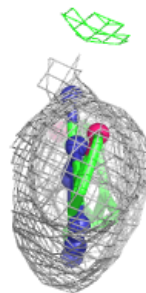
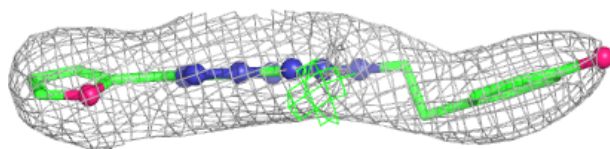
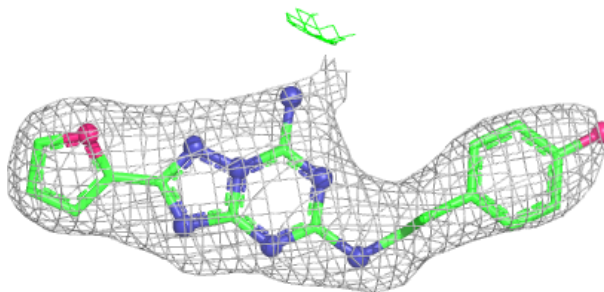


Electron density around CLR A 1215:

$2mF_o-DF_c$ (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.