



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 8RLN / pdb_00008rln
Title : Crystal structure of human adenosine A2A receptor (construct A2A-PSB2-bRIL) complexed with the partial antagonist LUF5834 at the orthosteric pocket
Authors : Strater, N.; Claff, T.; Weisse, R.H.; Muller, C.E.
Deposited on : 2024-01-03
Resolution : 2.43 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)
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

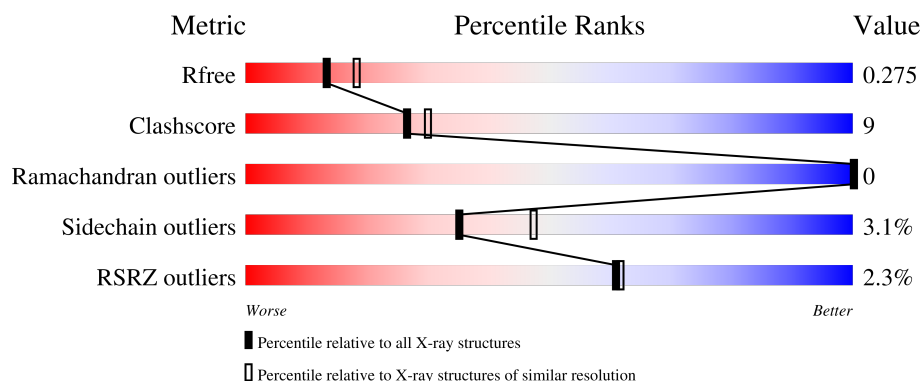
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

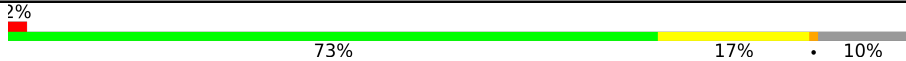
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	431	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6806 atoms, of which 3456 are hydrogens and 0 are deuteriums.

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

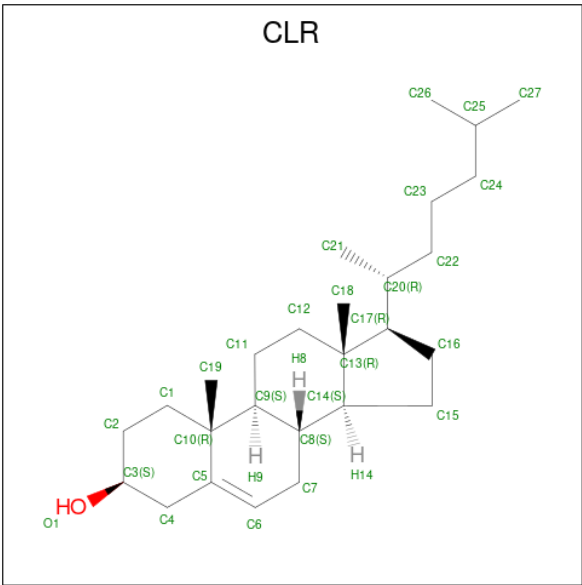
- Molecule 1 is a protein called Adenosine receptor A2a,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	388	6211	1995	3156	516	522	22	0	13	0

There are 25 discrepancies between the modelled and reference sequences:

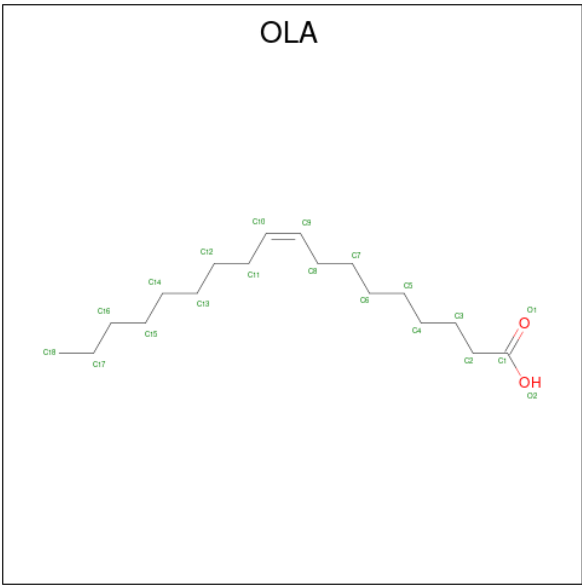
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	91	LYS	SER	conflict	UNP P29274
A	154	ALA	ASN	conflict	UNP P29274
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	GLY	conflict	UNP P29274
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

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



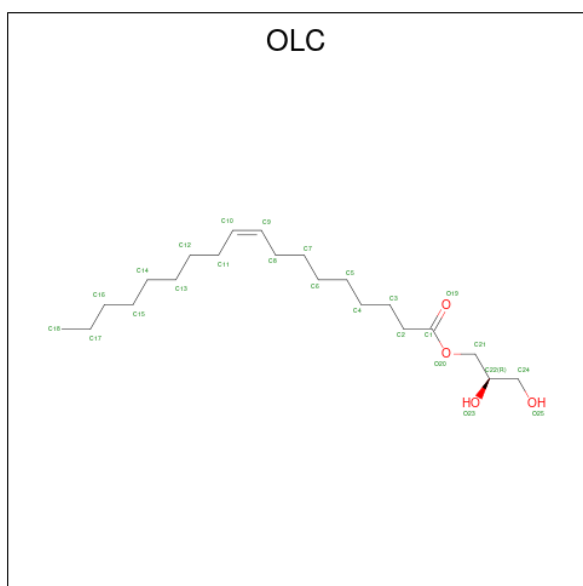
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			37	13	22	2		

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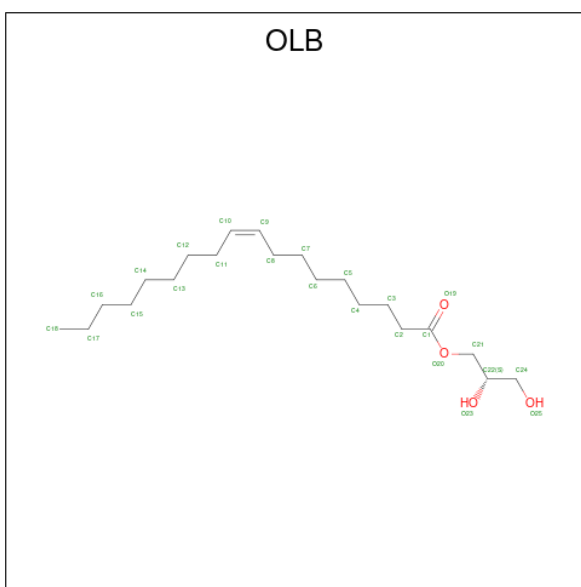
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			43	15	26	2		
3	A	1	Total	C	H	O	0	0
			21	7	12	2		
3	A	1	Total	C	O		0	0
			19	17	2			

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



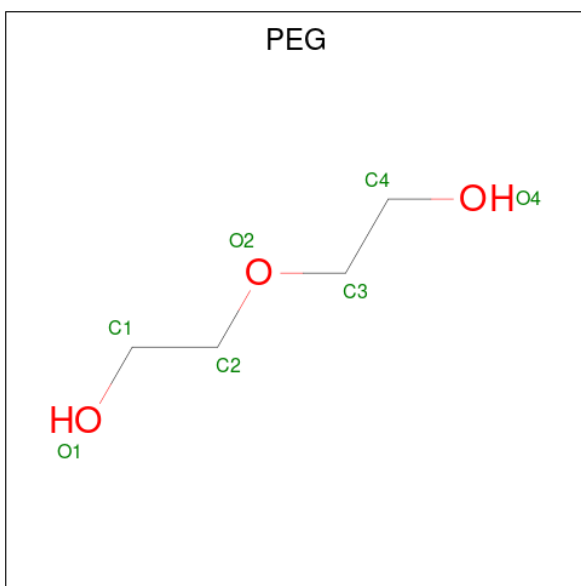
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			55	18	33	4		
4	A	1	Total	C	H	O	0	0
			38	12	22	4		
4	A	1	Total	C	O		0	0
			19	15	4			

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: $C_{21}H_{40}O_4$).



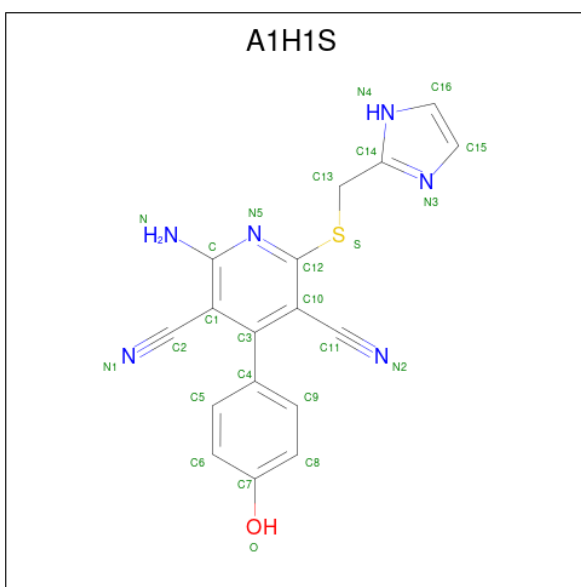
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			43	14	25	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is 2-azanyl-4-(4-hydroxyphenyl)-6-(1 {H}-imidazol-2-ylmethylsulfanyl)pyridine-3,5-dicarbonitrile (CCD ID: A1H1S) (formula: $C_{17}H_{12}N_6OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	S	0	0
			37	17	12	6	1	1		

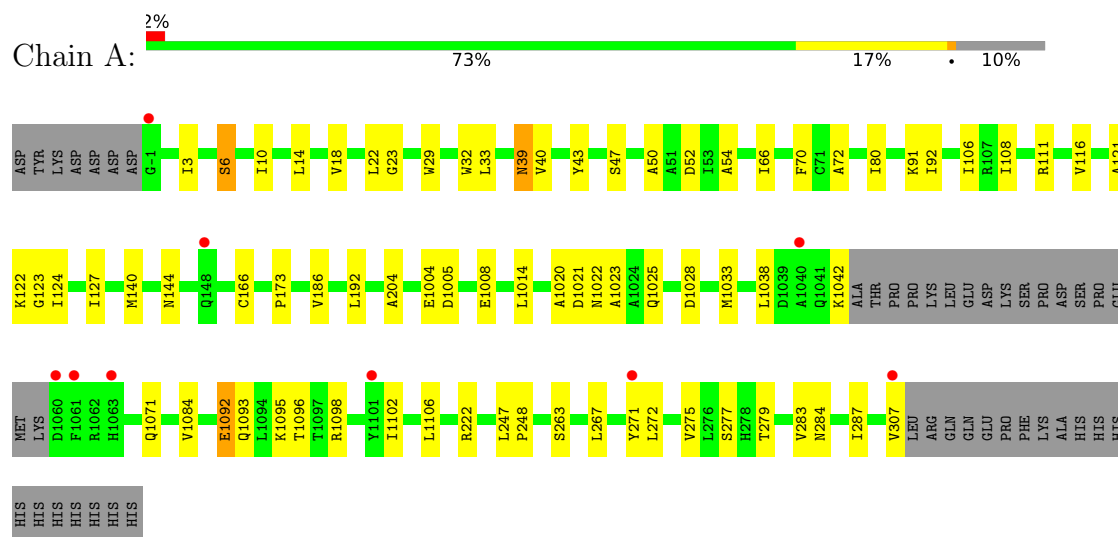
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	4
			44	44		

3 Residue-property plots

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

- Molecule 1: Adenosine receptor A2a,Soluble cytochrome b562



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.56Å 179.69Å 140.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.23 – 2.43 70.23 – 2.43	Depositor EDS
% Data completeness (in resolution range)	86.3 (70.23-2.43) 86.4 (70.23-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.281 0.207 , 0.275	Depositor DCC
R_{free} test set	866 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6806	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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: OLC, CLR, A1H1S, OLA, OLB, PEG

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	0.61	0/3183	0.74	0/4329

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 [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	3055	3156	3090	57	0
2	A	84	138	138	3	0
3	A	60	60	82	4	0
4	A	57	55	77	3	0
5	A	18	25	23	2	0
6	A	7	10	10	0	0
7	A	25	12	0	4	0
8	A	44	0	0	4	0
All	All	3350	3456	3420	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:LEU:HD11	1:A:222:ARG:HH21	1.41	0.84
1:A:1092:GLU:OE1	8:A:1301:HOH:O	2.14	0.64
1:A:1004:GLU:OE1	1:A:222:ARG:NH2	2.33	0.61
1:A:29:TRP:CD1	1:A:33:LEU:HD11	2.35	0.61
1:A:1023:ALA:HB2	1:A:1084:VAL:HG22	1.82	0.61
1:A:124:ILE:HD13	3:A:1206:OLA:H31	1.83	0.60
1:A:47:SER:HA	4:A:1213:OLC:H2A	1.83	0.60
1:A:92[B]:ILE:HD11	1:A:186:VAL:HG22	1.84	0.59
1:A:263:SER:O	2:A:1202:CLR:O1	2.21	0.58
7:A:1211:A1H1S:C5	7:A:1211:A1H1S:C11	2.80	0.57
1:A:50:ALA:HB1	5:A:1208:OLB:H18	1.88	0.56
1:A:29:TRP:NE1	1:A:33:LEU:HD11	2.22	0.55
7:A:1211:A1H1S:C2	7:A:1211:A1H1S:C9	2.83	0.55
1:A:1106:LEU:HD11	1:A:222:ARG:NH2	2.17	0.54
1:A:70:PHE:CE2	1:A:72:ALA:HB2	2.43	0.54
1:A:275[B]:VAL:O	1:A:279:THR:HG23	2.08	0.54
1:A:14:LEU:O	1:A:18:VAL:HG23	2.09	0.53
1:A:40:VAL:HG13	1:A:121:ALA:HB2	1.92	0.51
1:A:267:LEU:HD11	1:A:271:TYR:CE1	2.45	0.51
1:A:32:TRP:HD1	1:A:33:LEU:HD23	1.75	0.51
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.93	0.51
1:A:92[B]:ILE:HD13	1:A:186:VAL:HA	1.93	0.51
1:A:54:ALA:HB2	5:A:1208:OLB:H23	1.94	0.49
1:A:39:ASN:HB2	8:A:1323:HOH:O	2.11	0.49
1:A:80:ILE:HG22	2:A:1201:CLR:H182	1.94	0.49
7:A:1211:A1H1S:C2	8:A:1303[B]:HOH:O	2.61	0.48
1:A:66:ILE:HG13	1:A:166:CYS:SG	2.54	0.48
1:A:108:ILE:HD12	1:A:111:ARG:HB2	1.95	0.48
1:A:106:ILE:CD1	1:A:204:ALA:HB2	2.44	0.48
1:A:122:LYS:HE2	4:A:1213:OLC:C24	2.44	0.47
1:A:271:TYR:HD2	3:A:1212:OLA:H62	1.80	0.47
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.44	0.47
1:A:267:LEU:HD12	1:A:267:LEU:O	2.14	0.47
1:A:272:LEU:HA	1:A:275[B]:VAL:HG22	1.96	0.46
7:A:1211:A1H1S:N2	8:A:1302[A]:HOH:O	2.36	0.45
1:A:287:ILE:HD12	1:A:287:ILE:HG23	1.68	0.45
3:A:1212:OLA:H112	3:A:1212:OLA:H82	1.39	0.44
1:A:1020:ALA:HB1	1:A:1025:GLN:OE1	2.18	0.44
1:A:271:TYR:CD2	3:A:1212:OLA:H62	2.52	0.44
1:A:1014:LEU:CD2	1:A:1033:MET:HE1	2.48	0.43
1:A:1098:ARG:HA	1:A:1102:ILE:HB	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:N	1:A:248:PRO:CD	2.81	0.43
1:A:1014:LEU:HD13	1:A:1095:LYS:HG2	1.99	0.43
1:A:1023:ALA:CB	1:A:1084:VAL:HG22	2.49	0.43
1:A:108:ILE:O	1:A:108:ILE:HG13	2.18	0.43
1:A:123:GLY:O	1:A:127:ILE:HD12	2.19	0.42
1:A:22:LEU:O	1:A:23:GLY:C	2.63	0.41
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.86	0.41
1:A:275[A]:VAL:O	1:A:279:THR:HG23	2.20	0.41
1:A:144:ASN:HA	1:A:173:PRO:HD3	2.02	0.41
2:A:1203:CLR:H211	2:A:1203:CLR:H232	1.84	0.41
1:A:6:SER:O	1:A:10:ILE:HG13	2.20	0.41
1:A:52:ASP:OD1	1:A:91:LYS:HD3	2.21	0.41
1:A:40:VAL:HA	1:A:43:TYR:CD2	2.55	0.41
1:A:1005:ASP:O	1:A:1008:GLU:N	2.49	0.41
1:A:3:ILE:O	1:A:3:ILE:HG12	2.20	0.41
1:A:267:LEU:HD12	1:A:267:LEU:C	2.45	0.41
1:A:283:VAL:O	1:A:284:ASN:C	2.62	0.41
1:A:1038:LEU:N	1:A:1038:LEU:HD23	2.35	0.40
1:A:122:LYS:HE2	4:A:1213:OLC:O25	2.21	0.40
1:A:1071:GLN:NE2	1:A:1093:GLN:HB3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	397/431 (92%)	385 (97%)	12 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	329/359 (92%)	319 (97%)	10 (3%)	36 48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	39	ASN
1	A	1021	ASP
1	A	1022	ASN
1	A	1028	ASP
1	A	1042	LYS
1	A	1092	GLU
1	A	1096	THR
1	A	277	SER
1	A	307	VAL

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	181	ASN
1	A	1071	GLN
1	A	226	GLN
1	A	253	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	CLR	A	1203	-	31,31,31	0.28	0	48,48,48	0.53	0
4	OLC	A	1209	-	15,15,24	0.64	0	16,16,25	0.53	0
6	PEG	A	1210	-	6,6,6	0.09	0	5,5,5	0.22	0
7	A1H1S	A	1211	-	25,27,27	0.54	0	33,37,37	0.68	1 (3%)
2	CLR	A	1202	-	31,31,31	0.24	0	48,48,48	0.49	0
3	OLA	A	1212	-	18,18,19	0.91	1 (5%)	18,18,19	1.16	2 (11%)
5	OLB	A	1208	-	17,17,24	0.48	0	18,18,25	0.55	0
3	OLA	A	1204	-	14,14,19	1.21	1 (7%)	14,14,19	1.16	2 (14%)
3	OLA	A	1206	-	8,8,19	0.63	0	8,8,19	1.45	2 (25%)
4	OLC	A	1213	-	18,18,24	0.36	0	19,19,25	0.39	0
4	OLC	A	1207	-	21,21,24	0.47	0	22,22,25	0.53	0
2	CLR	A	1201	-	31,31,31	0.21	0	48,48,48	0.51	0
3	OLA	A	1205	-	16,16,19	0.96	1 (6%)	16,16,19	0.93	1 (6%)

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	CLR	A	1203	-	-	1/10/68/68	0/4/4/4
4	OLC	A	1209	-	-	3/15/15/24	-
6	PEG	A	1210	-	-	2/4/4/4	-
7	A1H1S	A	1211	-	-	4/11/13/13	0/3/3/3
2	CLR	A	1202	-	-	1/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	1212	-	-	4/16/16/17	-
5	OLB	A	1208	-	-	5/17/17/24	-
3	OLA	A	1204	-	-	6/12/12/17	-
3	OLA	A	1206	-	-	4/6/6/17	-
4	OLC	A	1213	-	-	10/18/18/24	-
4	OLC	A	1207	-	-	7/21/21/24	-
2	CLR	A	1201	-	-	1/10/68/68	0/4/4/4
3	OLA	A	1205	-	-	4/14/14/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	OLA	C10-C9	3.29	1.50	1.31
3	A	1205	OLA	C10-C9	3.10	1.49	1.31
3	A	1212	OLA	C10-C9	2.78	1.47	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1204	OLA	O2-C1-C2	2.87	123.05	114.00
3	A	1212	OLA	O2-C1-O1	-2.78	116.19	123.33
3	A	1204	OLA	O2-C1-O1	-2.74	116.28	123.33
3	A	1212	OLA	O2-C1-C2	2.63	122.32	114.00
3	A	1206	OLA	C3-C2-C1	-2.50	107.98	114.51
3	A	1205	OLA	O2-C1-C2	2.30	121.28	114.00
3	A	1206	OLA	O2-C1-C2	2.15	120.81	114.00
7	A	1211	A1H1S	C14-C13-S	-2.10	105.54	111.09

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1213	OLC	C21-C22-C24-O25
7	A	1211	A1H1S	C10-C3-C4-C5
2	A	1202	CLR	C21-C20-C22-C23
7	A	1211	A1H1S	C1-C3-C4-C5
4	A	1213	OLC	O23-C22-C24-O25
5	A	1208	OLB	C1-C2-C3-C4
4	A	1213	OLC	C1-C2-C3-C4
7	A	1211	A1H1S	C10-C3-C4-C9

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Mol	Chain	Res	Type	Atoms
4	A	1209	OLC	O20-C21-C22-O23
4	A	1209	OLC	O20-C21-C22-C24
7	A	1211	A1H1S	C1-C3-C4-C9
3	A	1204	OLA	C1-C2-C3-C4
4	A	1213	OLC	O20-C21-C22-O23
4	A	1207	OLC	C11-C12-C13-C14
3	A	1204	OLA	C3-C4-C5-C6
3	A	1204	OLA	C2-C3-C4-C5
4	A	1213	OLC	C6-C7-C8-C9
6	A	1210	PEG	O2-C3-C4-O4
3	A	1206	OLA	C3-C4-C5-C6
5	A	1208	OLB	C2-C1-O20-C21
6	A	1210	PEG	O1-C1-C2-O2
3	A	1205	OLA	C5-C6-C7-C8
3	A	1212	OLA	C14-C15-C16-C17
3	A	1212	OLA	C4-C5-C6-C7
5	A	1208	OLB	C3-C4-C5-C6
4	A	1207	OLC	C12-C13-C14-C15
4	A	1213	OLC	C2-C1-O20-C21
5	A	1208	OLB	O19-C1-O20-C21
4	A	1207	OLC	C5-C6-C7-C8
4	A	1213	OLC	C3-C4-C5-C6
4	A	1213	OLC	O20-C21-C22-C24
3	A	1204	OLA	C4-C5-C6-C7
4	A	1209	OLC	O23-C22-C24-O25
4	A	1207	OLC	C4-C5-C6-C7
3	A	1212	OLA	C13-C14-C15-C16
4	A	1207	OLC	C21-C22-C24-O25
2	A	1201	CLR	C21-C20-C22-C23
4	A	1213	OLC	O19-C1-O20-C21
3	A	1205	OLA	C6-C7-C8-C9
3	A	1206	OLA	C2-C3-C4-C5
5	A	1208	OLB	C6-C7-C8-C9
4	A	1213	OLC	C7-C8-C9-C10
4	A	1207	OLC	C7-C8-C9-C10
4	A	1207	OLC	C10-C11-C12-C13
3	A	1206	OLA	O2-C1-C2-C3
3	A	1212	OLA	C5-C6-C7-C8
3	A	1206	OLA	O1-C1-C2-C3
3	A	1204	OLA	C9-C10-C11-C12
3	A	1205	OLA	C7-C8-C9-C10
3	A	1204	OLA	C7-C8-C9-C10

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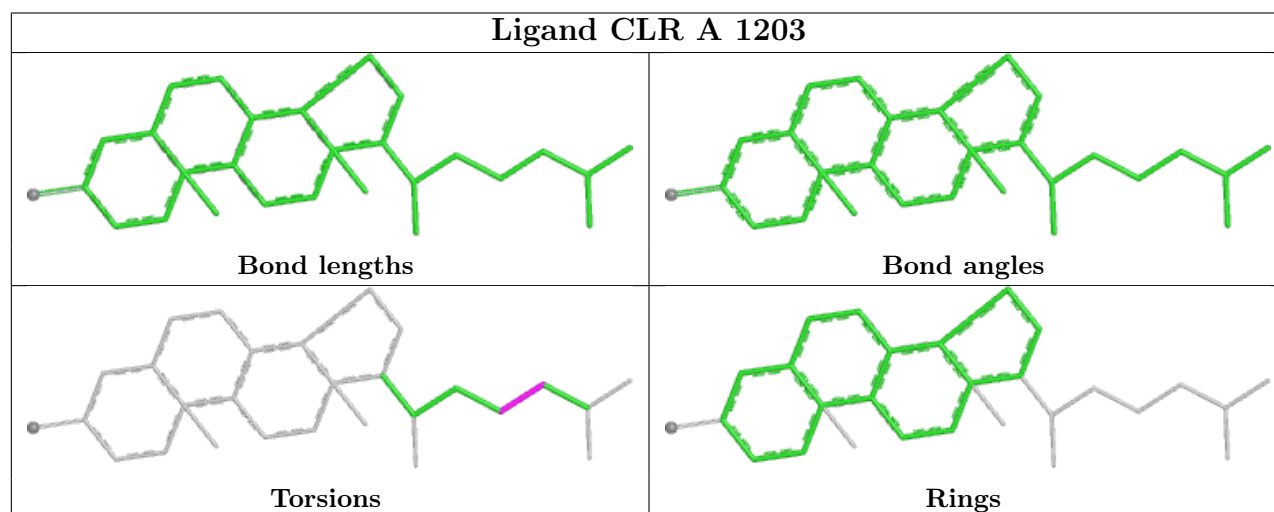
Mol	Chain	Res	Type	Atoms
2	A	1203	CLR	C22-C23-C24-C25
3	A	1205	OLA	C2-C3-C4-C5

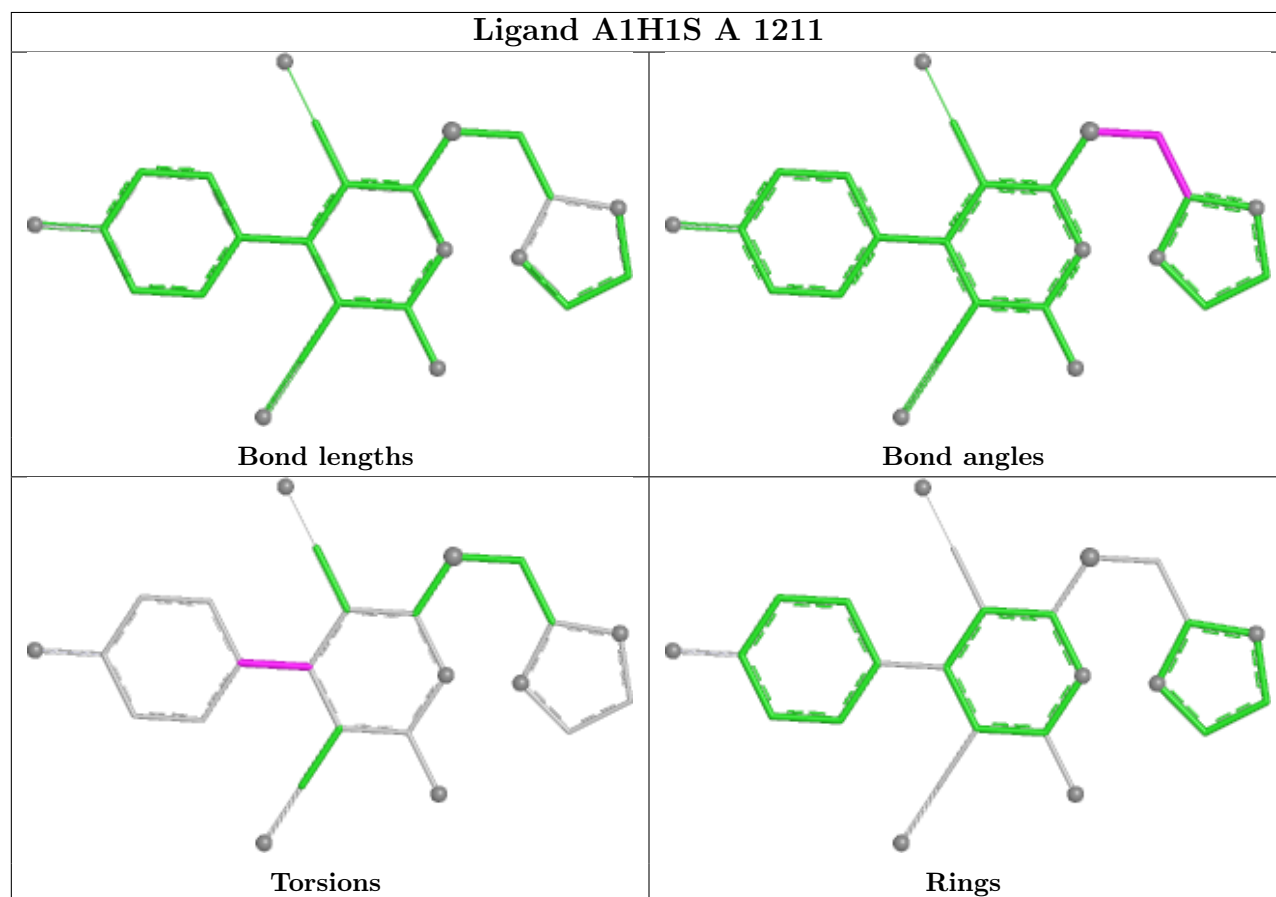
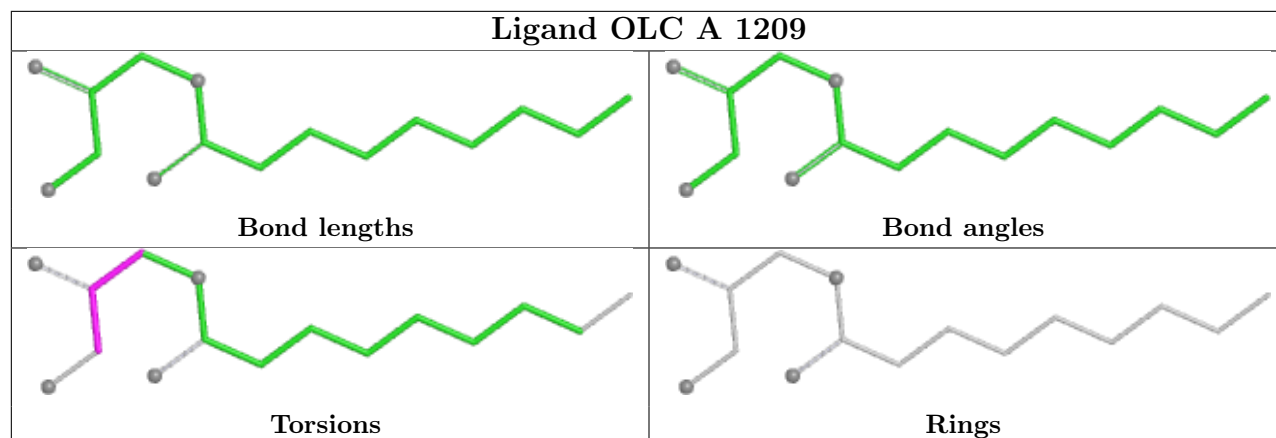
There are no ring outliers.

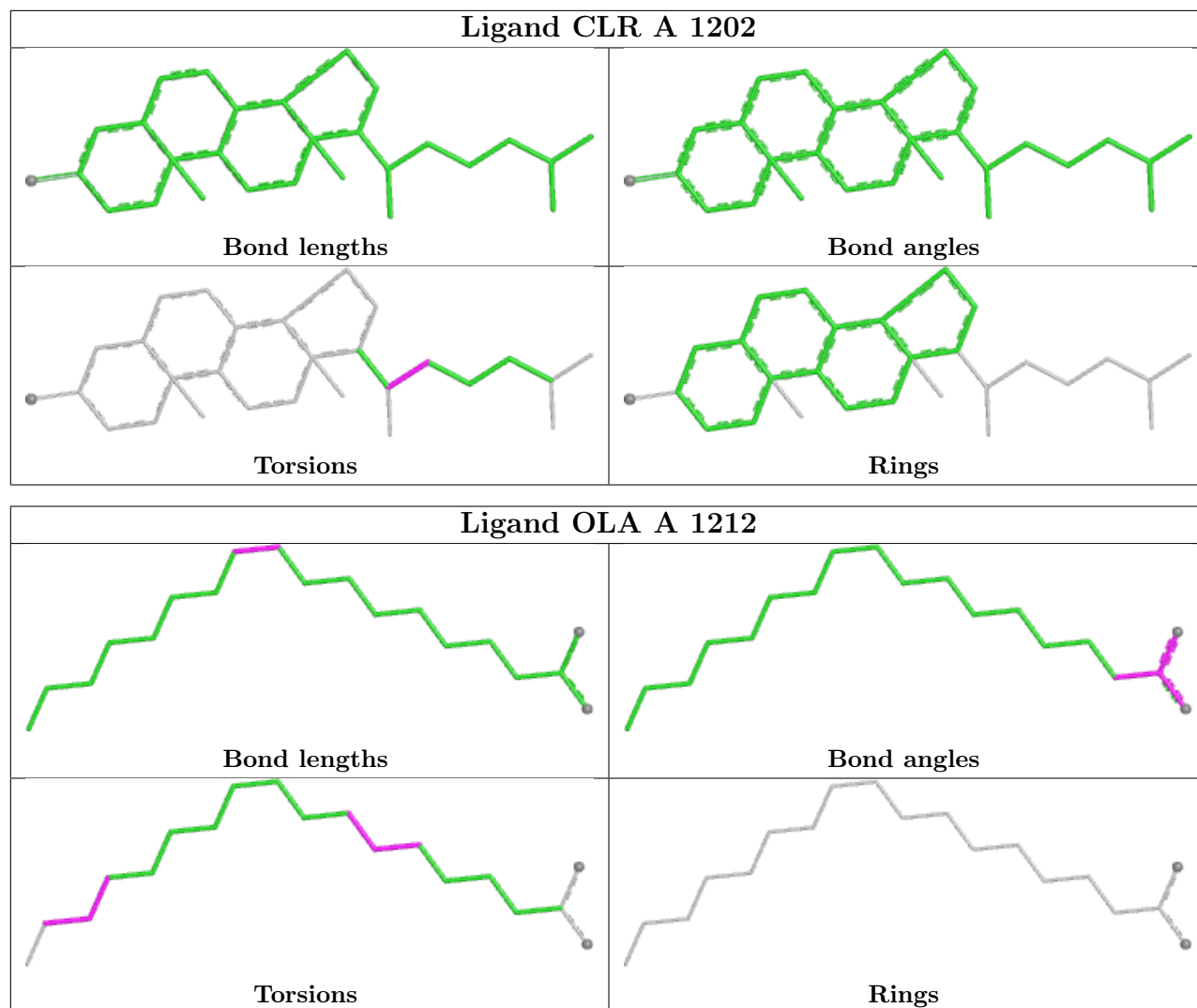
8 monomers are involved in 16 short contacts:

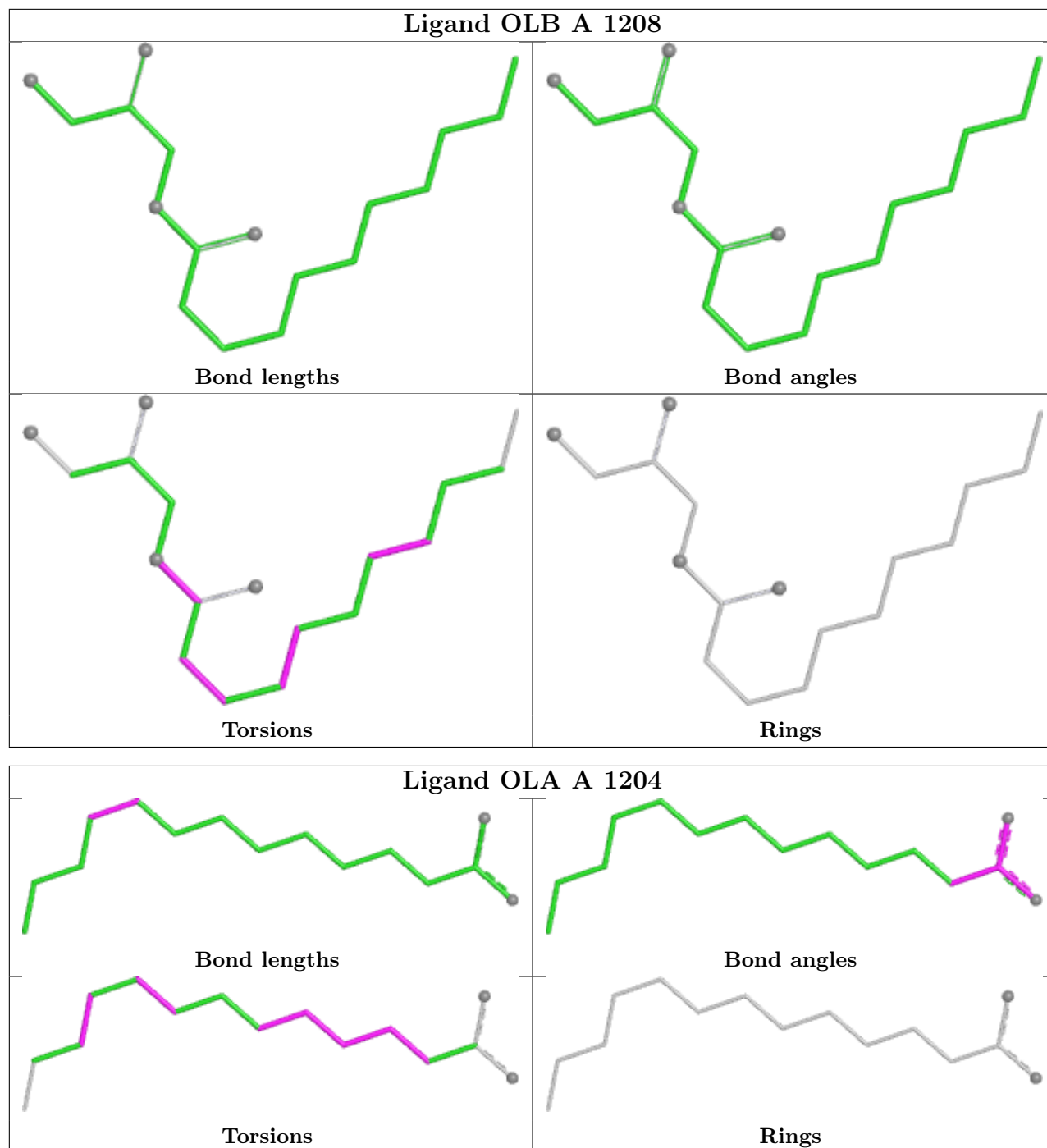
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1203	CLR	1	0
7	A	1211	A1H1S	4	0
2	A	1202	CLR	1	0
3	A	1212	OLA	3	0
5	A	1208	OLB	2	0
3	A	1206	OLA	1	0
4	A	1213	OLC	3	0
2	A	1201	CLR	1	0

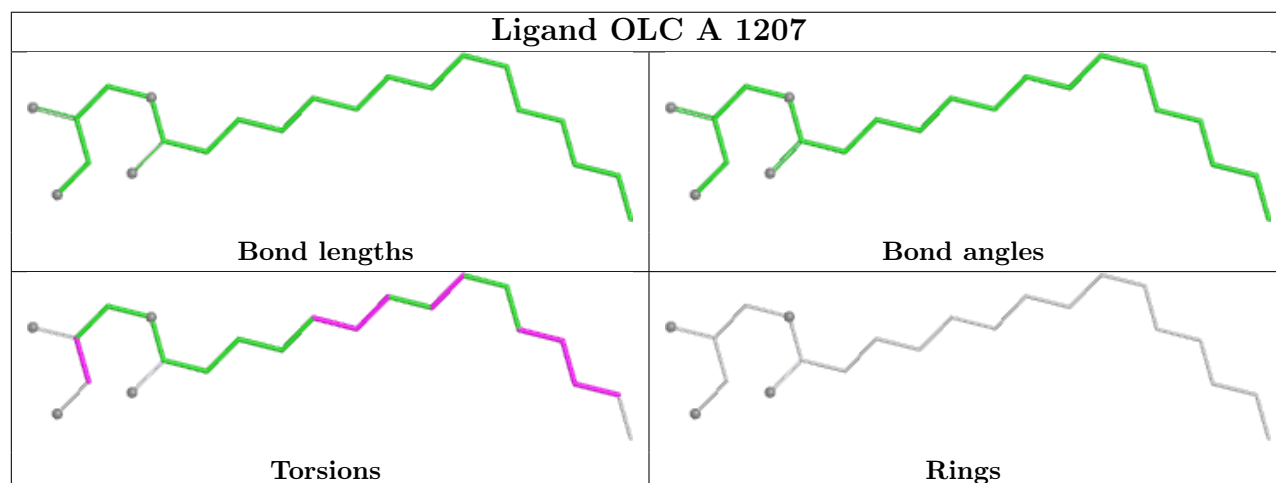
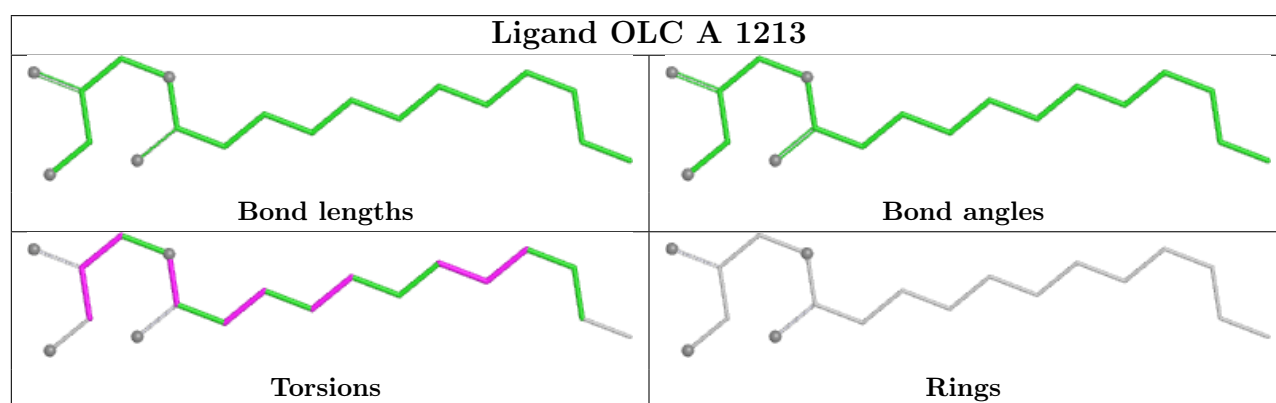
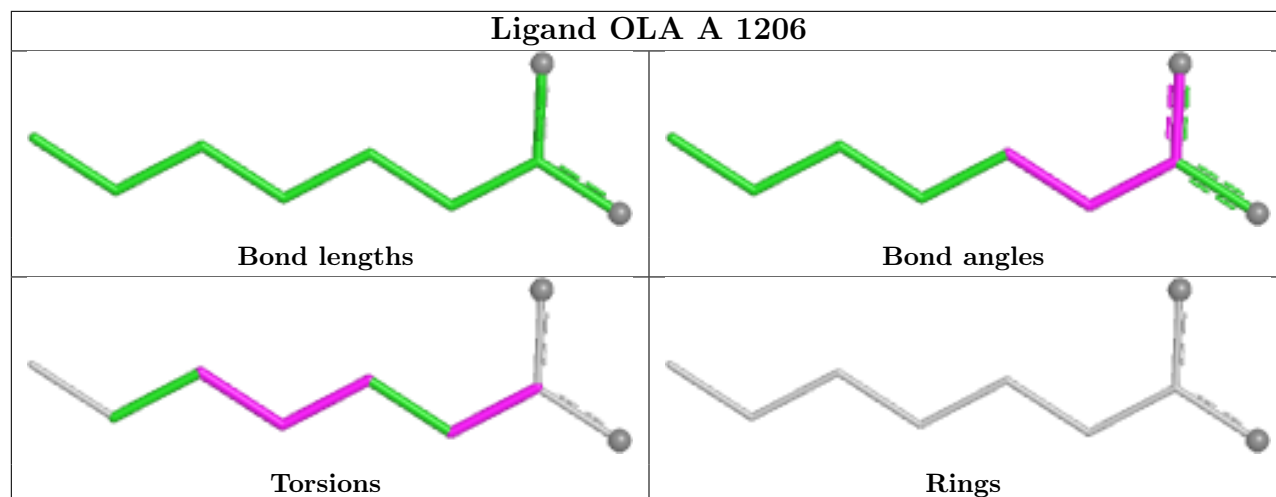
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

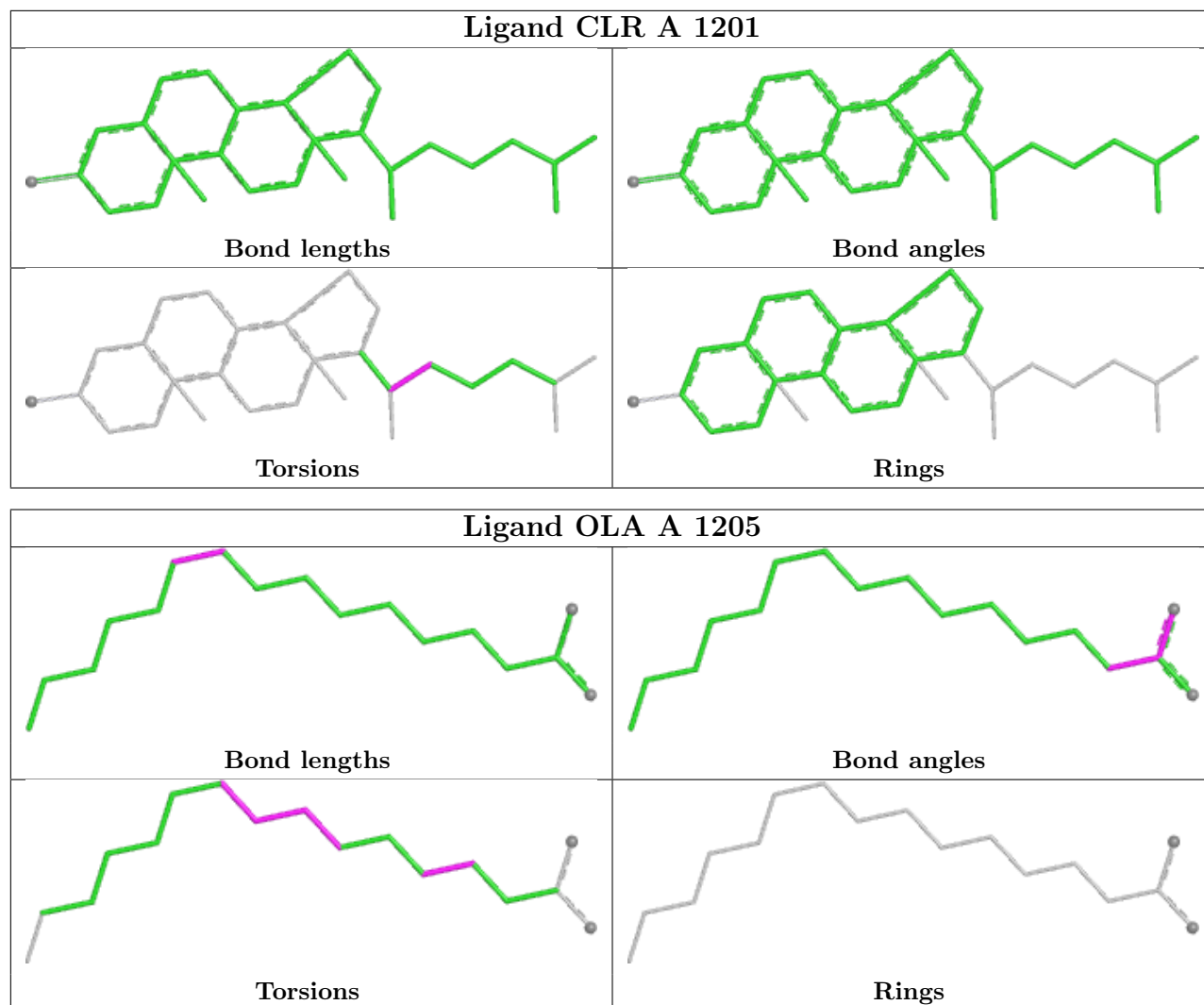












5.7 Other polymers [i](#)

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	388/431 (90%)	0.01	9 (2%) 61 62	17, 47, 92, 146	5 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	3.0
1	A	1063	HIS	3.0
1	A	-1	GLY	3.0
1	A	1061	PHE	2.9
1	A	271	TYR	2.4
1	A	148	GLN	2.3
1	A	1101	TYR	2.3
1	A	1040	ALA	2.1
1	A	1060	ASP	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](#)

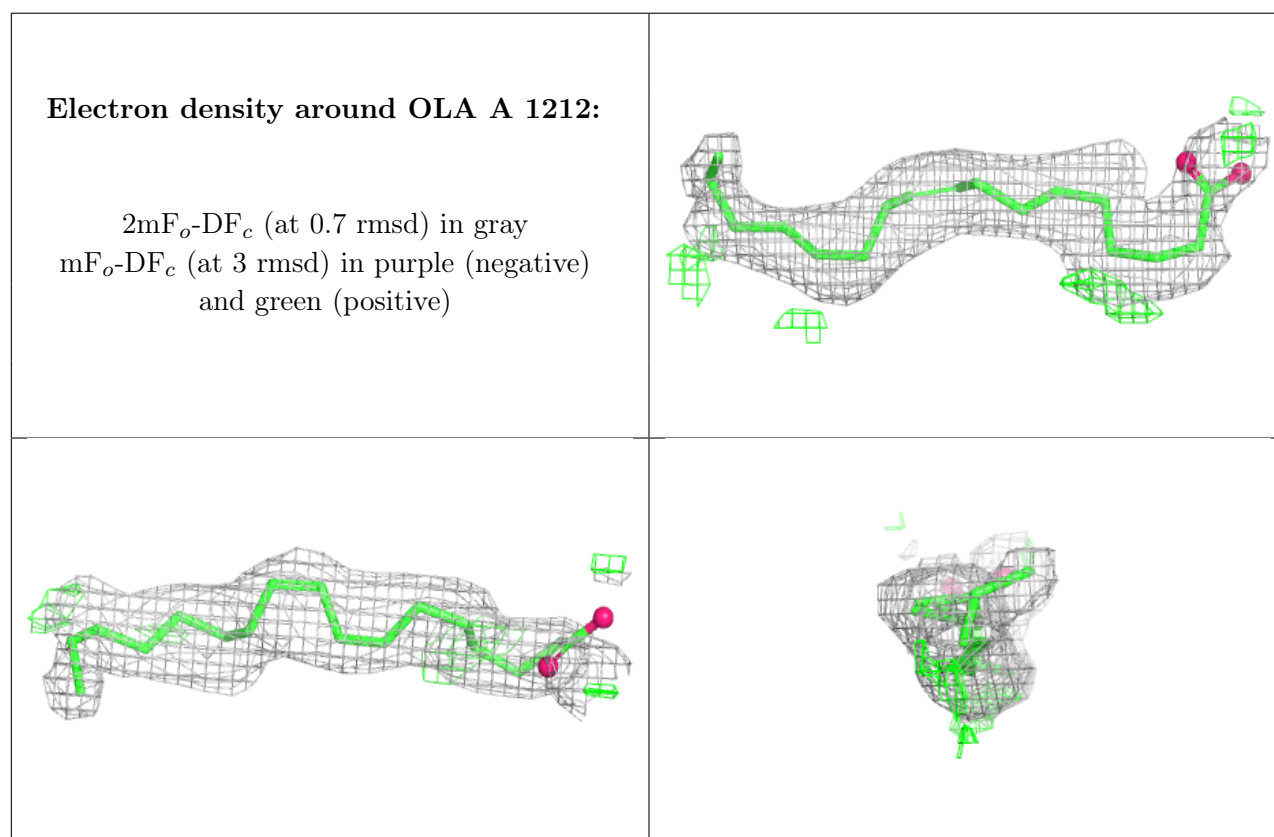
There are no oligosaccharides in this entry.

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.

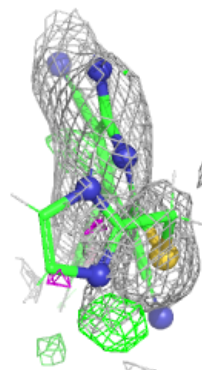
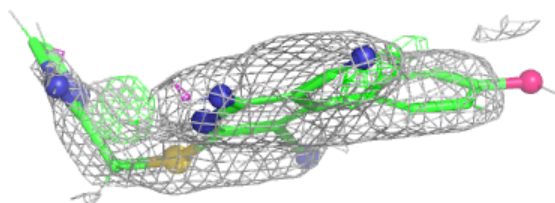
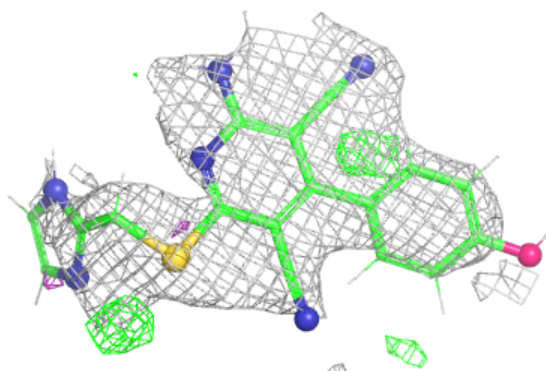
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLA	A	1212	19/20	0.84	0.19	33,53,104,127	0
7	A1H1S	A	1211	25/25	0.86	0.21	16,46,80,84	37
4	OLC	A	1213	19/25	0.87	0.20	44,63,93,95	0
6	PEG	A	1210	7/7	0.87	0.12	56,71,86,93	0
4	OLC	A	1209	16/25	0.87	0.14	24,54,86,91	0
5	OLB	A	1208	18/25	0.88	0.13	34,63,83,100	0
4	OLC	A	1207	22/25	0.89	0.13	32,60,90,109	0
3	OLA	A	1204	15/20	0.89	0.12	40,64,73,77	0
2	CLR	A	1202	28/28	0.90	0.11	30,55,75,82	0
3	OLA	A	1206	9/20	0.91	0.12	34,50,60,74	0
3	OLA	A	1205	17/20	0.92	0.12	38,59,87,90	0
2	CLR	A	1203	28/28	0.94	0.09	33,47,68,84	0
2	CLR	A	1201	28/28	0.95	0.09	32,50,77,93	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.

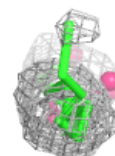
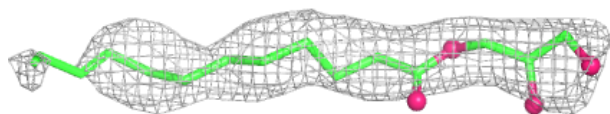
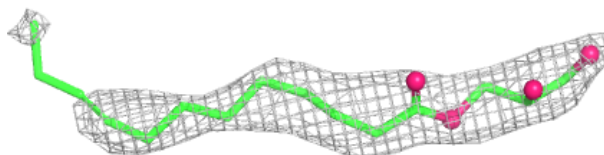


Electron density around A1H1S A 1211:

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

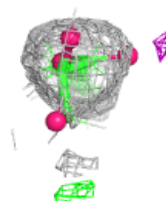
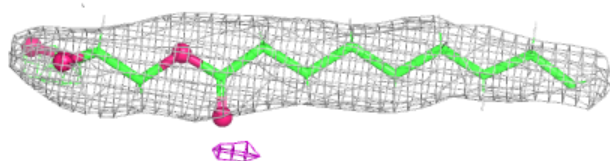
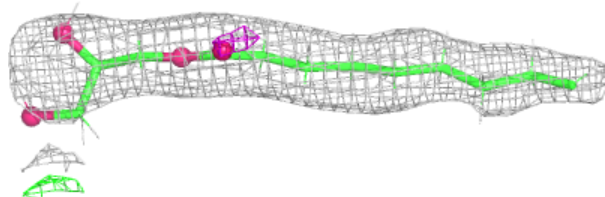
**Electron density around OLC A 1213:**

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

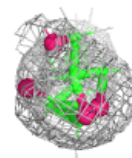
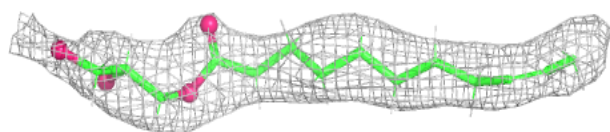
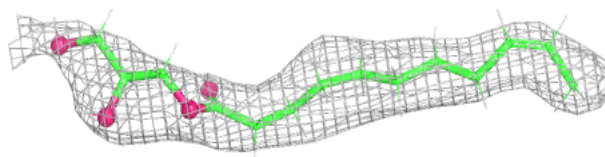


Electron density around OLC A 1209:

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

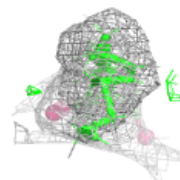
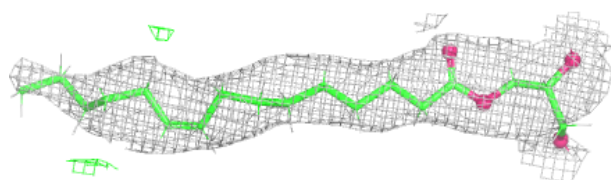
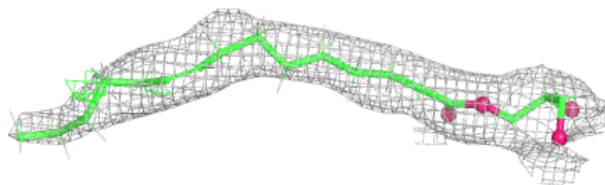
**Electron density around OLB A 1208:**

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

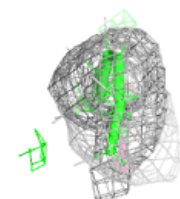
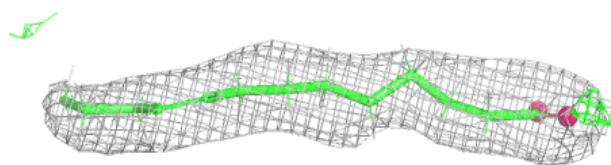
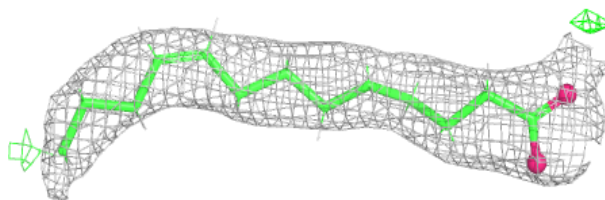


Electron density around OLC A 1207:

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

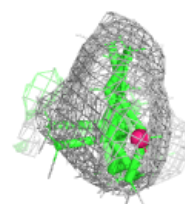
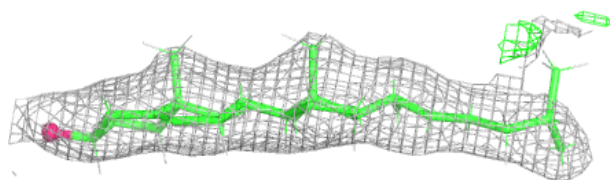
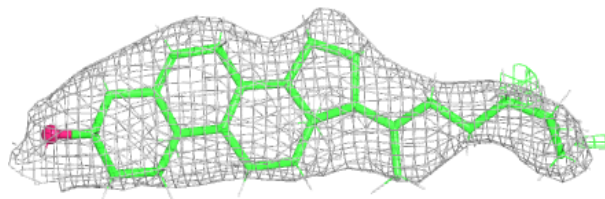
**Electron density around OLA A 1204:**

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

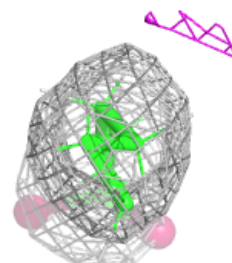
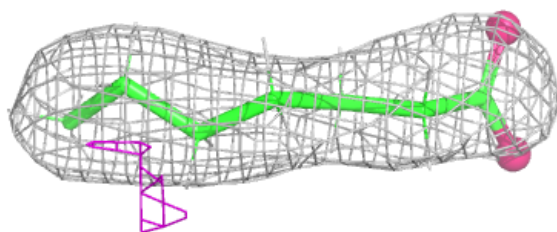
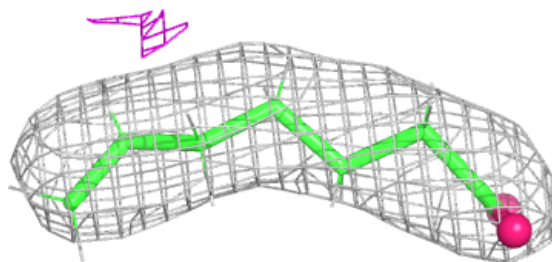


Electron density around CLR A 1202:

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

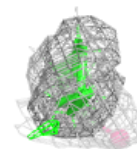
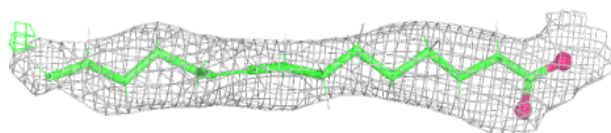
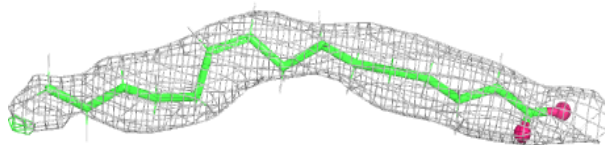
**Electron density around OLA A 1206:**

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and green (positive)

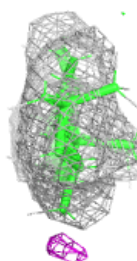
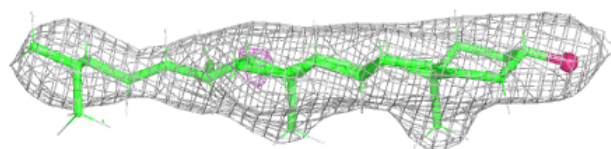
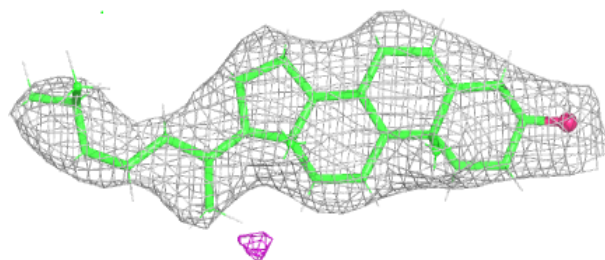


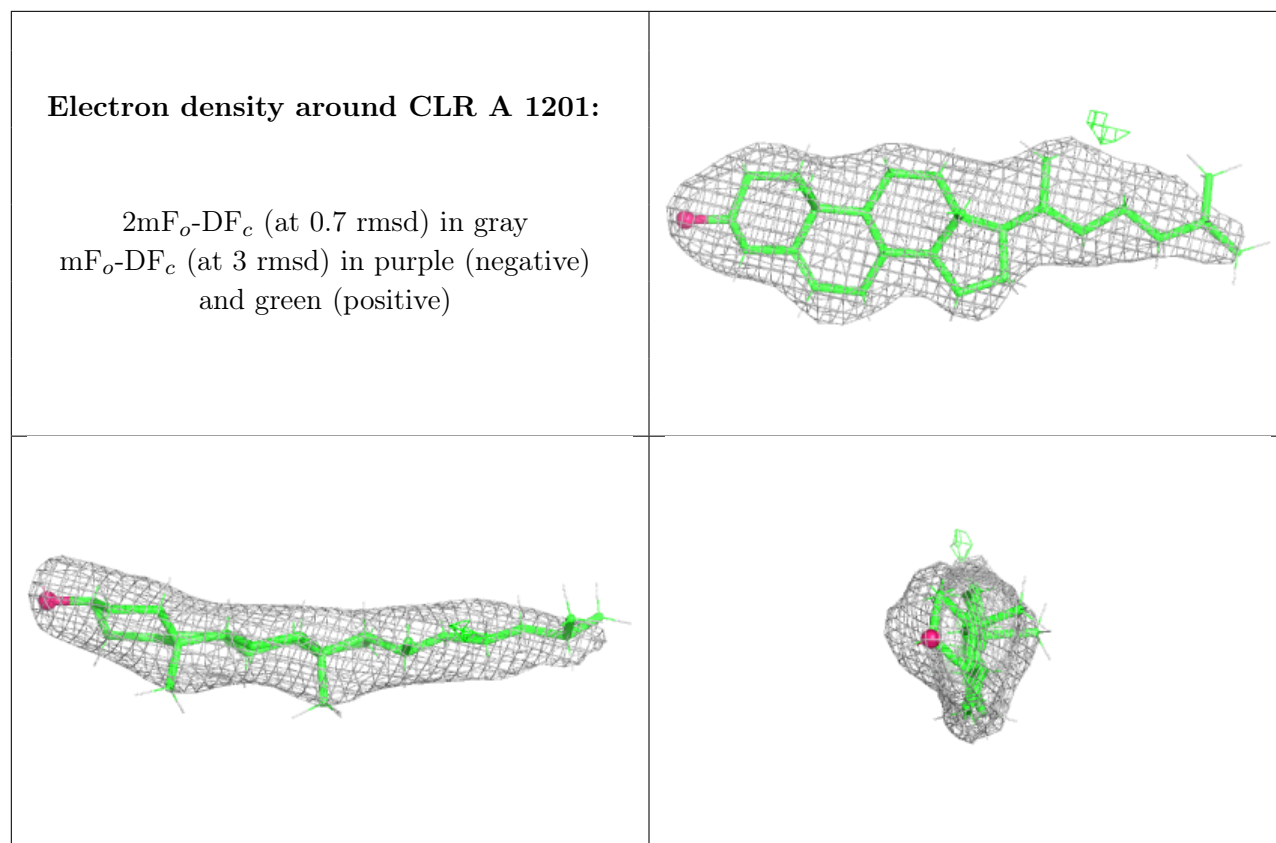
Electron density around OLA A 1205:

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

**Electron density around CLR A 1203:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.