



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 09:01 AM JST

PDB ID : 7CRL
Title : Structure of Chloride ion pumping rhodopsin (ClR) with NTQ motif 50 ps after light activation
Authors : Yun, J.H.; Liu, H.; Lee, W.T.; Schmidt, M.
Deposited on : 2020-08-13
Resolution : 1.85 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 ⓘ](#)) 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 : 2.18
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) : 2.18

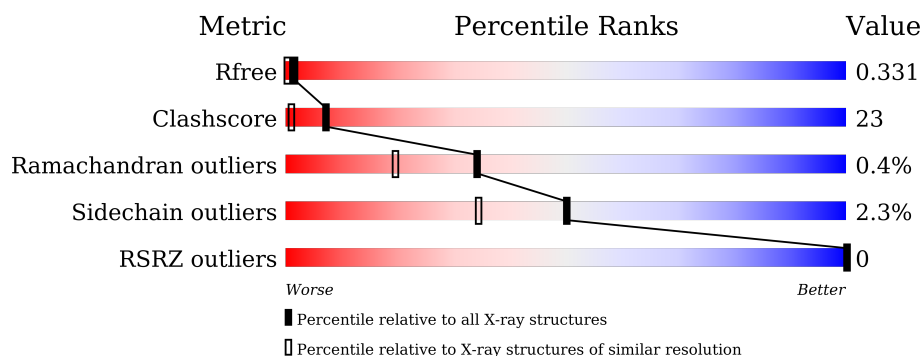
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	264	

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	RET	A	303	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2299 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.

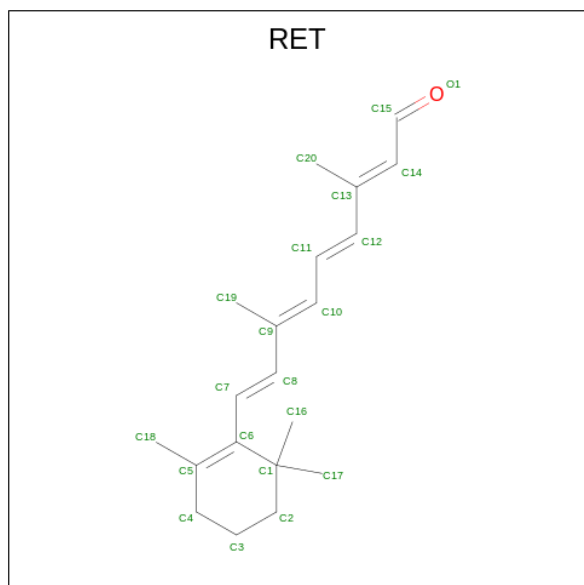
- Molecule 1 is a protein called Chloride pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2072	1378	321	359	14			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

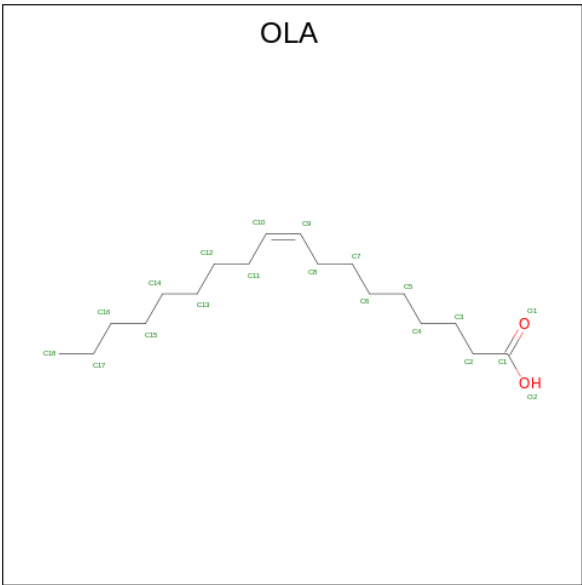
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			20	20		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	12	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			18	16	2		
4	A	1	Total	C	O	0	0
			12	10	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C		0	0
			6	6			
4	A	1	Total	C		0	0
			9	9			

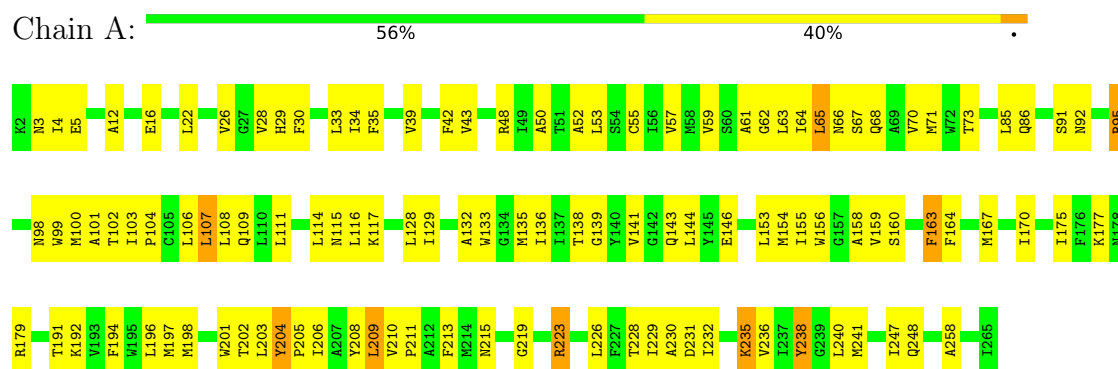
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total	O	0	0
			106	106		

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: Chloride pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.37Å 50.09Å 69.39Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	20.64 – 1.85 20.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.64-1.85) 92.6 (20.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.280 , 0.331 0.280 , 0.331	Depositor DCC
R_{free} test set	1720 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	1.8	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2299	wwPDB-VP
Average B, all atoms (Å ²)	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: RET, CL, 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	1.01	5/2124 (0.2%)	1.10	10/2896 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	CYS	CB-SG	9.20	1.97	1.82
1	A	238	TYR	CD1-CE1	-8.12	1.27	1.39
1	A	163	PHE	CB-CG	-6.81	1.39	1.51
1	A	204	TYR	CB-CG	-5.54	1.43	1.51
1	A	235	LYS	C-O	5.28	1.33	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	197	MET	CA-CB-CG	6.56	124.45	113.30
1	A	48	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	65	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	204	TYR	CB-CG-CD1	-5.62	117.63	121.00
1	A	204	TYR	CA-CB-CG	-5.33	103.27	113.40
1	A	107	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	209	LEU	CA-CB-CG	-5.17	103.42	115.30
1	A	95	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	65	LEU	CA-CB-CG	5.12	127.07	115.30

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	2072	0	2106	98	0
2	A	2	0	0	0	0
3	A	20	0	27	10	0
4	A	99	0	147	4	0
5	A	106	0	0	6	0
All	All	2299	0	2280	101	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 23.

All (101) 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:139:GLY:HA2	3:A:303:RET:H21	1.59	0.83
1:A:104:PRO:HB3	1:A:129:ILE:HG12	1.63	0.80
1:A:109:GLN:OE1	5:A:401:HOH:O	2.02	0.76
1:A:223:ARG:NH1	5:A:403:HOH:O	2.20	0.74
1:A:141:VAL:HA	1:A:144:LEU:HD12	1.69	0.74
1:A:203:LEU:HB2	1:A:230:ALA:HB2	1.71	0.73
1:A:107:LEU:HD13	1:A:128:LEU:HB3	1.70	0.73
1:A:4:ILE:HG21	1:A:211:PRO:HB3	1.71	0.72
3:A:303:RET:H8	3:A:303:RET:H171	1.72	0.71
1:A:73:THR:O	5:A:402:HOH:O	2.12	0.66
1:A:204:TYR:HB2	1:A:205:PRO:HD3	1.77	0.66
1:A:138:THR:HG22	1:A:156:TRP:HZ3	1.61	0.66
1:A:210:VAL:HG21	1:A:223:ARG:HB2	1.78	0.65
1:A:65:LEU:HD21	1:A:231:ASP:OD2	1.97	0.65
1:A:139:GLY:HA3	3:A:303:RET:H162	1.78	0.65
1:A:201:TRP:HA	1:A:204:TYR:HD2	1.61	0.64
1:A:52:ALA:HB2	5:A:432:HOH:O	1.99	0.62
1:A:67:SER:O	1:A:71:MET:HG3	1.99	0.61
1:A:98:ASN:O	1:A:101:ALA:N	2.30	0.60
1:A:104:PRO:O	1:A:108:LEU:N	2.30	0.60
1:A:132:ALA:HB2	1:A:167:MET:SD	2.42	0.60
1:A:208:TYR:CD1	3:A:303:RET:H22	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:O	1:A:16:GLU:HG3	2.02	0.58
1:A:179:ARG:HE	1:A:191:THR:CG2	2.17	0.57
1:A:175:ILE:HD13	1:A:194:PHE:HB2	1.87	0.57
1:A:42:PHE:O	1:A:258:ALA:HB2	2.05	0.56
1:A:59:VAL:O	1:A:63:LEU:HG	2.05	0.56
1:A:164:PHE:CE1	1:A:201:TRP:HE3	2.24	0.56
1:A:196:LEU:HD23	1:A:241:MET:SD	2.46	0.55
1:A:103:ILE:HD12	1:A:136:ILE:HD11	1.88	0.55
1:A:202:THR:O	1:A:206:ILE:HD12	2.06	0.55
1:A:205:PRO:HG3	3:A:303:RET:C5	2.37	0.55
1:A:139:GLY:HA3	3:A:303:RET:C16	2.39	0.53
1:A:138:THR:HG22	1:A:156:TRP:CZ3	2.42	0.53
1:A:29:HIS:CD2	1:A:61:ALA:HB3	2.44	0.52
1:A:35:PHE:O	1:A:39:VAL:HG22	2.10	0.52
1:A:143:GLN:HA	1:A:146:GLU:HB3	1.92	0.51
1:A:64:ILE:O	1:A:68:GLN:HG2	2.11	0.50
1:A:61:ALA:HB2	1:A:235:LYS:HD3	1.94	0.50
1:A:100:MET:HA	1:A:136:ILE:HD13	1.94	0.49
1:A:155:ILE:O	1:A:159:VAL:HG23	2.12	0.49
1:A:194:PHE:O	1:A:198:MET:HG2	2.12	0.49
1:A:22:LEU:O	1:A:26:VAL:HG23	2.12	0.49
1:A:135:MET:HB2	1:A:163:PHE:HB3	1.93	0.49
1:A:201:TRP:CD1	1:A:201:TRP:N	2.79	0.49
1:A:43:VAL:HG22	1:A:247:ILE:HG12	1.95	0.48
1:A:103:ILE:HA	1:A:106:LEU:HD12	1.95	0.48
1:A:53:LEU:O	1:A:57:VAL:HG23	2.13	0.48
1:A:248:GLN:NE2	1:A:248:GLN:HA	2.28	0.48
1:A:50:ALA:O	1:A:109:GLN:NE2	2.46	0.48
1:A:92:ASN:HD22	1:A:223:ARG:HH11	1.60	0.48
1:A:247:ILE:HD12	4:A:310:OLA:H31	1.95	0.47
1:A:63:LEU:HD12	5:A:496:HOH:O	2.14	0.47
1:A:201:TRP:HA	1:A:204:TYR:CD2	2.46	0.46
1:A:204:TYR:CE2	1:A:230:ALA:HB1	2.50	0.46
1:A:204:TYR:CZ	1:A:230:ALA:HB1	2.51	0.46
1:A:34:ILE:HD12	4:A:307:OLA:H9	1.98	0.46
1:A:111:LEU:HD22	1:A:116:LEU:HD12	1.97	0.46
1:A:85:LEU:HG	1:A:86:GLN:N	2.31	0.46
1:A:204:TYR:CB	1:A:205:PRO:HD3	2.43	0.46
1:A:135:MET:HE2	1:A:136:ILE:HG13	1.96	0.45
1:A:206:ILE:HG22	1:A:226:LEU:HD13	1.97	0.45
1:A:106:LEU:HD22	1:A:238:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:O	1:A:232:ILE:HG13	2.16	0.45
1:A:114:LEU:HA	1:A:114:LEU:HD23	1.82	0.45
1:A:143:GLN:HB2	5:A:429:HOH:O	2.16	0.45
1:A:204:TYR:HB3	3:A:303:RET:H8	1.98	0.45
1:A:30:PHE:O	1:A:33:LEU:HB3	2.17	0.45
3:A:303:RET:H7	3:A:303:RET:H181	1.89	0.45
1:A:211:PRO:O	1:A:215:ASN:HB2	2.18	0.44
1:A:28:VAL:HG12	1:A:236:VAL:HG21	2.00	0.44
1:A:139:GLY:CA	3:A:303:RET:H21	2.39	0.44
1:A:26:VAL:HG13	1:A:30:PHE:CE2	2.53	0.44
1:A:114:LEU:O	1:A:115:ASN:HB2	2.18	0.43
1:A:154:MET:O	1:A:158:ALA:N	2.28	0.43
1:A:71:MET:HB2	1:A:71:MET:HE2	1.89	0.43
1:A:107:LEU:O	1:A:111:LEU:HG	2.18	0.43
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.83	0.43
1:A:66:ASN:O	1:A:70:VAL:HG23	2.19	0.43
1:A:92:ASN:HB3	1:A:95:ARG:HD2	2.01	0.42
1:A:146:GLU:HB2	1:A:211:PRO:HG3	2.01	0.42
1:A:164:PHE:HE1	1:A:201:TRP:CE3	2.37	0.42
1:A:3:ASN:OD1	1:A:5:GLU:HB2	2.19	0.42
1:A:138:THR:OG1	1:A:160:SER:HB2	2.19	0.42
1:A:128:LEU:HG	1:A:170:ILE:HG21	2.01	0.42
1:A:229:ILE:HG12	4:A:305:OLA:H162	2.01	0.42
1:A:92:ASN:HB3	1:A:95:ARG:HG3	2.01	0.42
1:A:203:LEU:N	1:A:203:LEU:HD23	2.34	0.42
1:A:210:VAL:HG11	1:A:219:GLY:O	2.19	0.41
1:A:100:MET:HE3	1:A:133:TRP:CD2	2.54	0.41
1:A:35:PHE:CG	4:A:308:OLA:H21	2.56	0.41
1:A:99:TRP:HA	1:A:102:THR:OG1	2.21	0.41
1:A:203:LEU:CB	1:A:230:ALA:HB2	2.44	0.41
3:A:303:RET:H11	3:A:303:RET:H191	1.87	0.41
1:A:198:MET:O	1:A:202:THR:OG1	2.19	0.41
1:A:57:VAL:HG11	1:A:106:LEU:HD21	2.03	0.41
1:A:164:PHE:HE1	1:A:201:TRP:HE3	1.67	0.41
1:A:209:LEU:HA	1:A:209:LEU:HD23	1.79	0.40
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.71	0.40
1:A:153:LEU:HD21	1:A:209:LEU:HD23	2.03	0.40
1:A:208:TYR:CD2	1:A:208:TYR:O	2.74	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	262/264 (99%)	244 (93%)	17 (6%)	1 (0%)	34	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLY

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	217/217 (100%)	212 (98%)	5 (2%)	50	34

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

Mol	Chain	Res	Type
1	A	91	SER
1	A	177	LYS
1	A	192	LYS
1	A	213	PHE
1	A	223	ARG

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

Mol	Chain	Res	Type
1	A	98	ASN
1	A	109	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 ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OLA	A	308	-	16,19,19	0.81	1 (6%)	15,19,19	0.61	0
4	OLA	A	307	-	8,11,19	1.09	1 (12%)	7,11,19	0.67	0
4	OLA	A	305	-	16,19,19	0.80	1 (6%)	15,19,19	0.90	0
4	OLA	A	304	-	10,13,19	0.90	1 (10%)	8,13,19	1.25	1 (12%)
4	OLA	A	309	-	5,5,19	0.40	0	4,4,19	0.59	0
4	OLA	A	310	-	8,8,19	0.34	0	7,7,19	1.32	1 (14%)
3	RET	A	303	1	20,20,21	4.08	13 (65%)	27,27,28	3.95	13 (48%)
4	OLA	A	306	-	14,17,19	0.77	1 (7%)	13,17,19	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
4	OLA	A	308	-	-	9/15/17/17	-
4	OLA	A	307	-	-	5/7/9/17	-
4	OLA	A	305	-	-	10/15/17/17	-
4	OLA	A	304	-	-	7/9/11/17	-
4	OLA	A	309	-	-	1/3/3/17	-
4	OLA	A	310	-	-	5/6/6/17	-
3	RET	A	303	1	-	4/13/30/31	0/1/1/1
4	OLA	A	306	-	-	7/13/15/17	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	RET	C1-C6	7.60	1.64	1.53
3	A	303	RET	C5-C6	-7.45	1.21	1.34
3	A	303	RET	C2-C1	7.32	1.71	1.54
3	A	303	RET	C4-C5	-6.16	1.38	1.51
3	A	303	RET	C12-C13	5.17	1.57	1.45
3	A	303	RET	C11-C10	4.42	1.57	1.43
3	A	303	RET	C10-C9	4.24	1.41	1.35
3	A	303	RET	C14-C13	4.19	1.37	1.33
3	A	303	RET	C7-C6	3.85	1.58	1.45
3	A	303	RET	C2-C3	2.94	1.59	1.52
4	A	308	OLA	C10-C9	2.92	1.48	1.31
4	A	307	OLA	C10-C9	2.88	1.48	1.28
3	A	303	RET	C17-C1	2.71	1.59	1.53
4	A	305	OLA	C10-C9	2.71	1.47	1.31
4	A	304	OLA	C10-C9	2.65	1.47	1.31
4	A	306	OLA	C10-C9	2.56	1.46	1.31
3	A	303	RET	C11-C12	2.44	1.40	1.34
3	A	303	RET	C19-C9	2.24	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	RET	C18-C5-C6	-13.38	109.51	124.53
3	A	303	RET	C11-C10-C9	-7.27	116.93	127.31
3	A	303	RET	C20-C13-C14	-6.19	105.43	123.71
3	A	303	RET	C11-C12-C13	-5.80	110.11	126.42
3	A	303	RET	C16-C1-C6	-4.88	102.38	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	RET	C12-C13-C14	4.59	133.35	118.80
3	A	303	RET	C18-C5-C4	3.97	121.24	113.62
3	A	303	RET	C8-C7-C6	-3.06	118.59	127.20
3	A	303	RET	C4-C5-C6	-2.81	118.65	122.73
3	A	303	RET	C8-C9-C10	-2.76	114.71	118.94
3	A	303	RET	C3-C2-C1	-2.58	105.36	114.60
4	A	304	OLA	C4-C3-C2	-2.45	104.21	113.76
4	A	310	OLA	C7-C6-C5	-2.45	101.99	114.42
3	A	303	RET	C7-C6-C5	-2.25	116.00	121.46
3	A	303	RET	C10-C11-C12	2.09	129.74	123.22

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	RET	C1-C6-C7-C8
3	A	303	RET	C5-C6-C7-C8
4	A	304	OLA	C1-C2-C3-C4
4	A	304	OLA	C11-C10-C9-C8
4	A	304	OLA	C9-C10-C11-C12
4	A	305	OLA	C1-C2-C3-C4
4	A	305	OLA	C11-C10-C9-C8
4	A	306	OLA	C1-C2-C3-C4
4	A	308	OLA	C1-C2-C3-C4
3	A	303	RET	C7-C8-C9-C19
3	A	303	RET	C7-C8-C9-C10
4	A	308	OLA	C11-C12-C13-C14
4	A	310	OLA	C4-C5-C6-C7
4	A	308	OLA	C13-C14-C15-C16
4	A	308	OLA	C4-C5-C6-C7
4	A	308	OLA	C12-C13-C14-C15
4	A	306	OLA	C6-C7-C8-C9
4	A	305	OLA	C5-C6-C7-C8
4	A	305	OLA	C13-C14-C15-C16
4	A	304	OLA	C4-C5-C6-C7
4	A	305	OLA	C10-C11-C12-C13
4	A	308	OLA	C3-C4-C5-C6
4	A	305	OLA	C12-C13-C14-C15
4	A	308	OLA	C6-C7-C8-C9
4	A	306	OLA	C11-C10-C9-C8
4	A	305	OLA	C2-C3-C4-C5
4	A	304	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	306	OLA	C4-C5-C6-C7
4	A	307	OLA	C5-C6-C7-C8
4	A	306	OLA	C13-C14-C15-C16
4	A	310	OLA	C6-C7-C8-C9
4	A	309	OLA	C3-C4-C5-C6
4	A	307	OLA	C3-C4-C5-C6
4	A	308	OLA	C2-C3-C4-C5
4	A	306	OLA	C3-C4-C5-C6
4	A	307	OLA	C1-C2-C3-C4
4	A	310	OLA	C3-C4-C5-C6
4	A	308	OLA	C14-C15-C16-C17
4	A	305	OLA	C15-C16-C17-C18
4	A	310	OLA	C5-C6-C7-C8
4	A	310	OLA	C2-C3-C4-C5
4	A	307	OLA	C4-C5-C6-C7
4	A	305	OLA	C9-C10-C11-C12
4	A	306	OLA	C12-C13-C14-C15
4	A	307	OLA	C7-C8-C9-C10
4	A	304	OLA	C6-C7-C8-C9
4	A	305	OLA	C7-C8-C9-C10
4	A	304	OLA	C7-C8-C9-C10

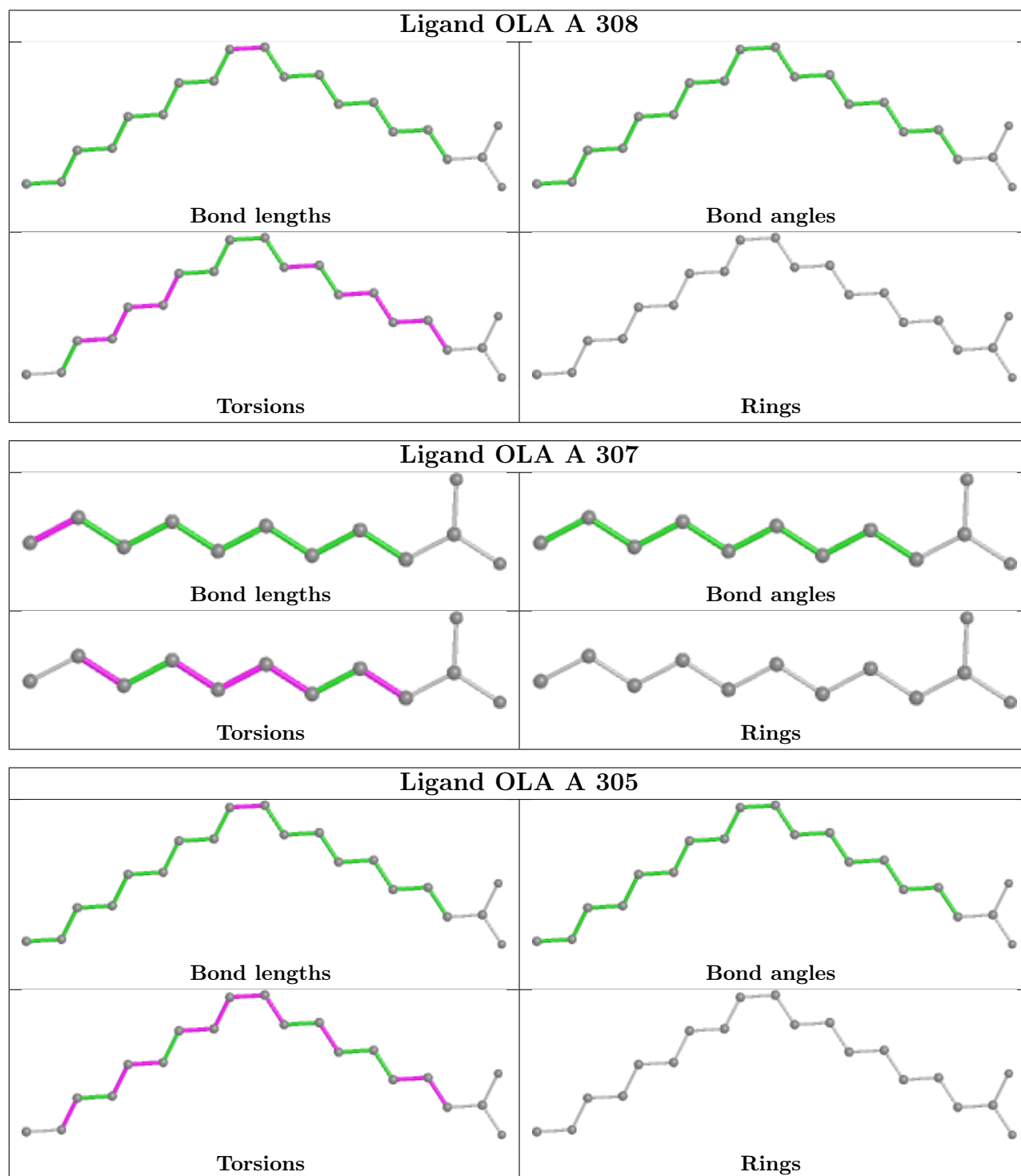
There are no ring outliers.

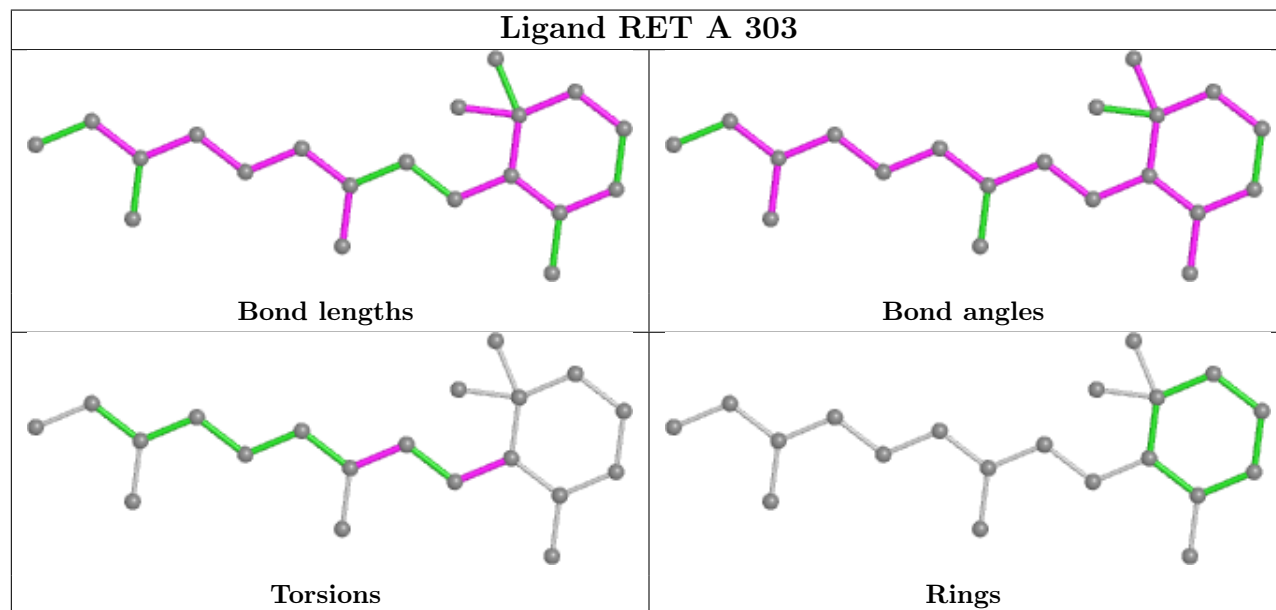
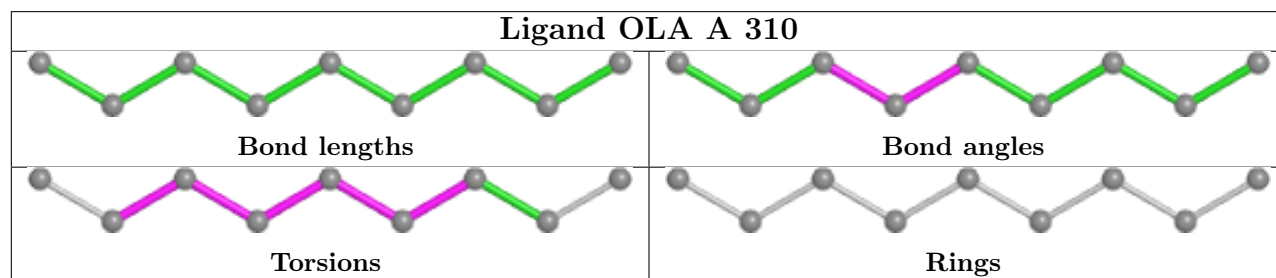
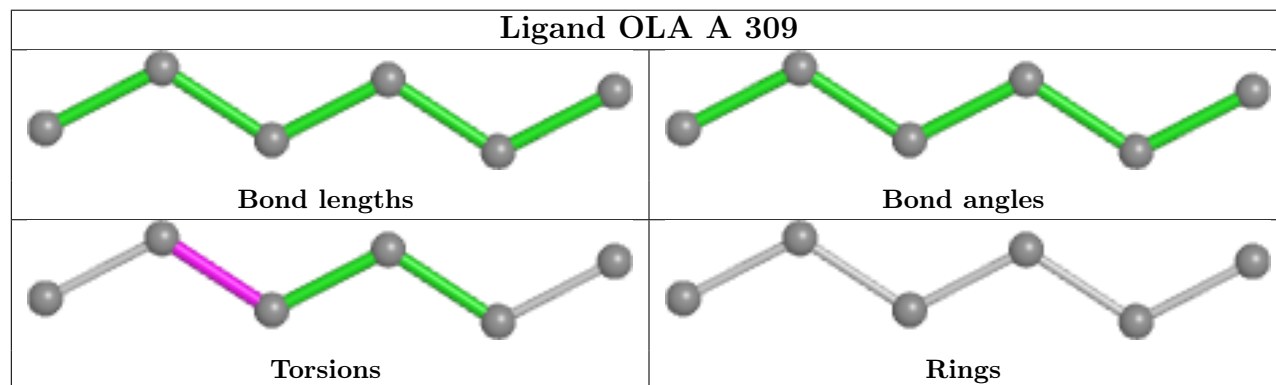
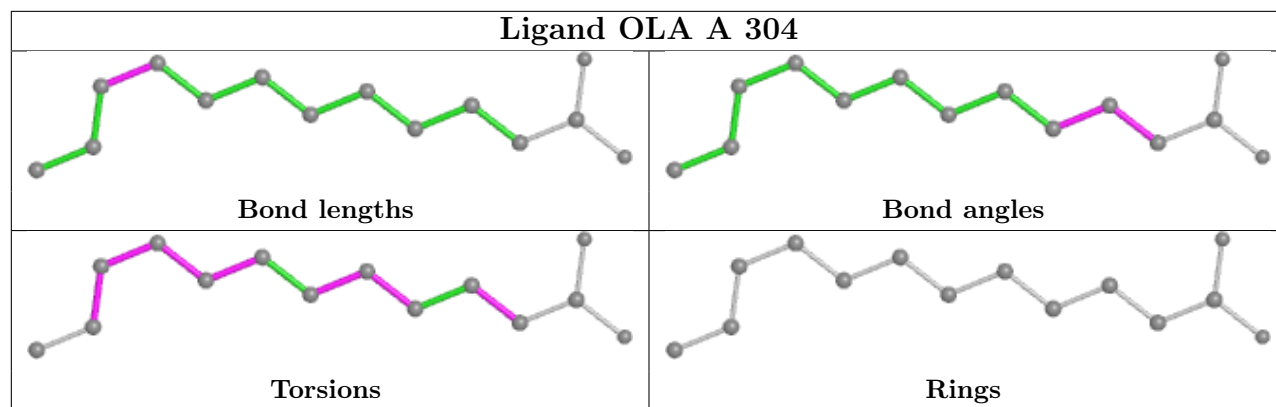
5 monomers are involved in 14 short contacts:

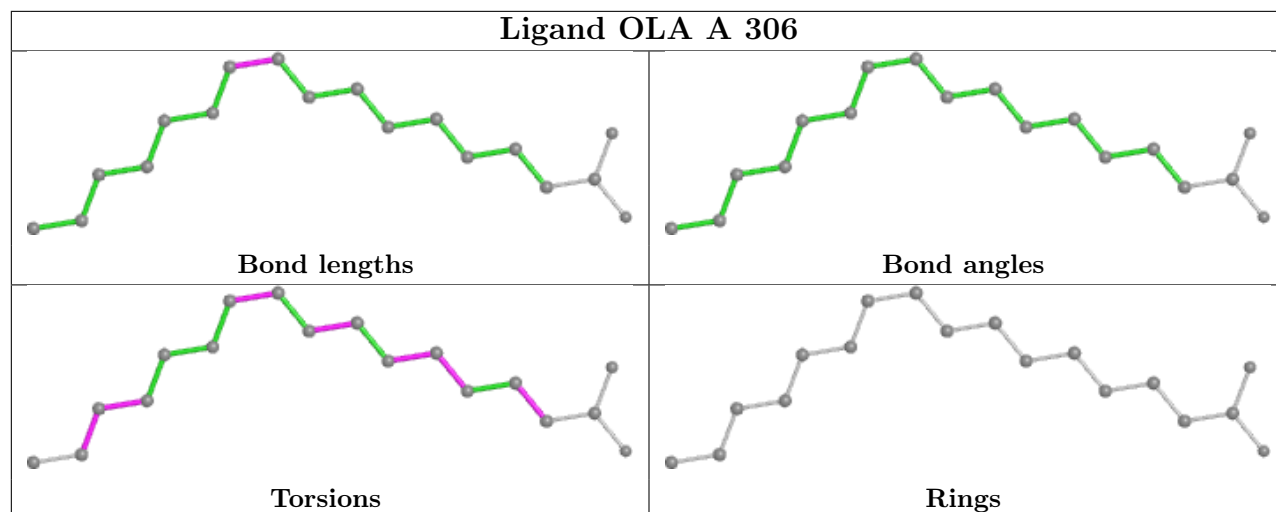
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	308	OLA	1	0
4	A	307	OLA	1	0
4	A	305	OLA	1	0
4	A	310	OLA	1	0
3	A	303	RET	10	0

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	264/264 (100%)	0.11	0 100 100	3, 3, 7, 19	0

There are no RSRZ outliers to report.

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](#)

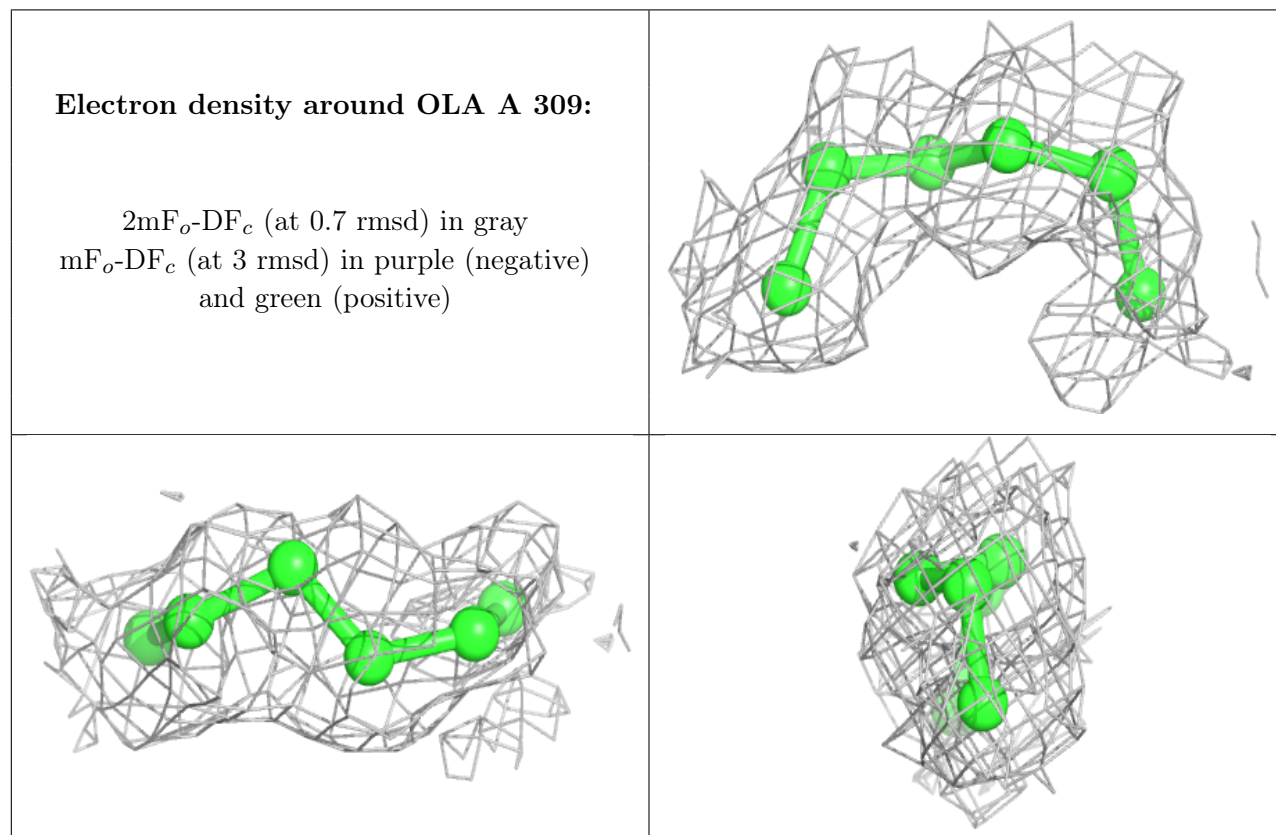
There are no monosaccharides in this entry.

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.

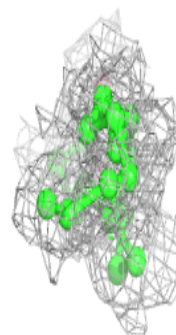
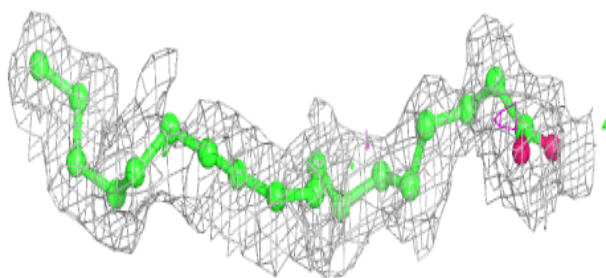
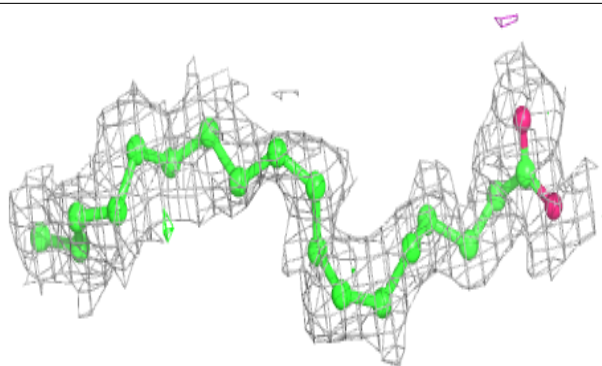
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLA	A	309	6/20	0.77	0.19	5,7,8,8	4
4	OLA	A	308	20/20	0.80	0.14	5,7,15,17	16
4	OLA	A	306	18/20	0.80	0.17	3,3,5,8	15
4	OLA	A	310	9/20	0.81	0.17	4,5,5,6	7
4	OLA	A	307	12/20	0.82	0.15	3,3,4,4	11
4	OLA	A	304	14/20	0.86	0.12	4,4,7,8	10
3	RET	A	303	20/21	0.87	0.17	2,2,2,2	0
4	OLA	A	305	20/20	0.88	0.13	2,2,3,3	13
2	CL	A	302	1/1	0.94	0.09	4,4,4,4	1
2	CL	A	301	1/1	0.98	0.07	2,2,2,2	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.

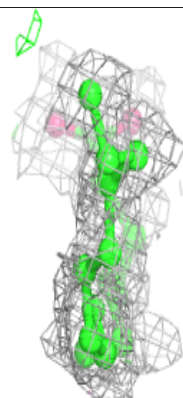
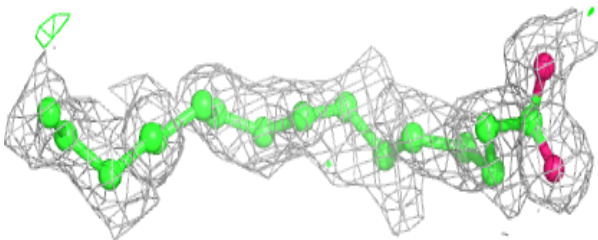
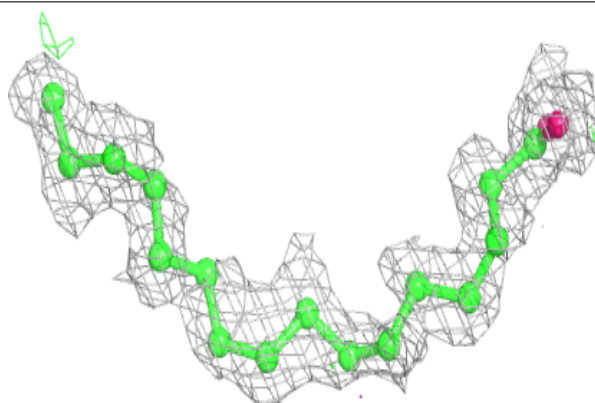


Electron density around OLA A 308:

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

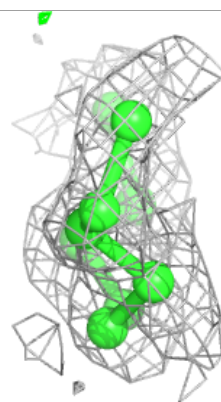
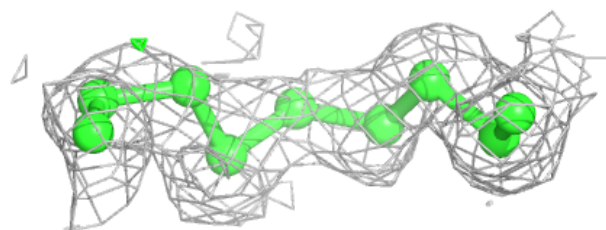
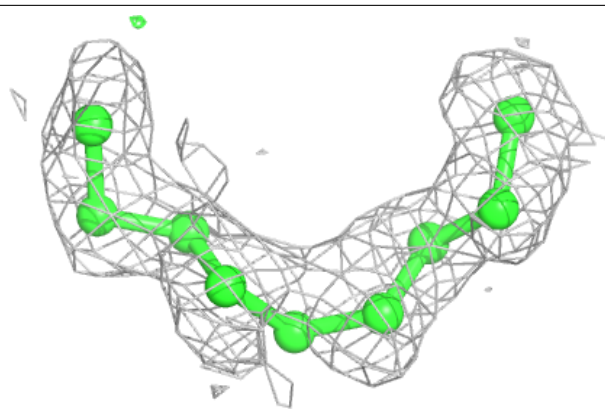
**Electron density around OLA A 306:**

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

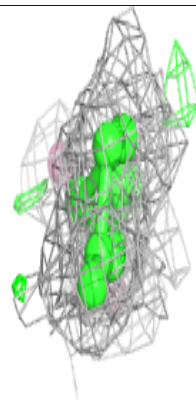
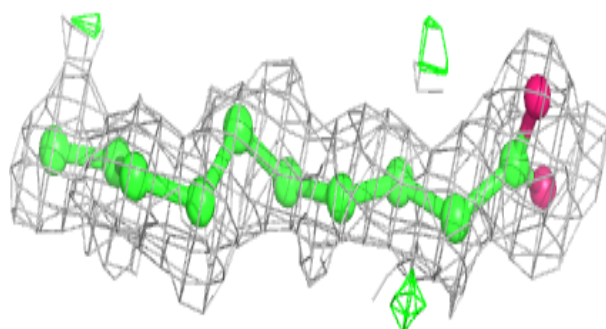
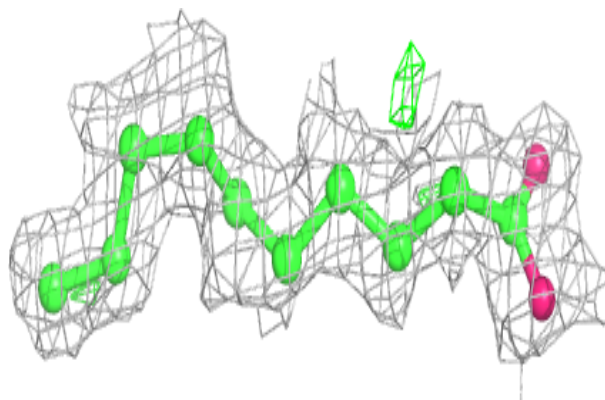


Electron density around OLA A 310:

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

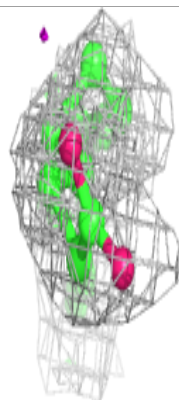
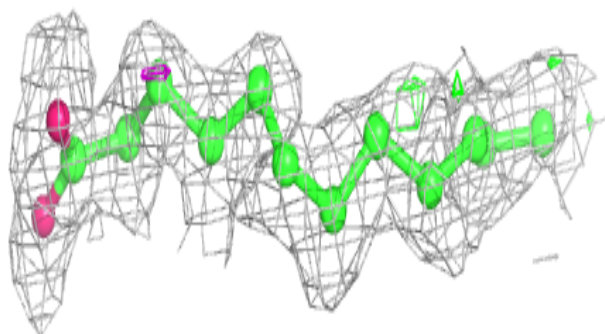
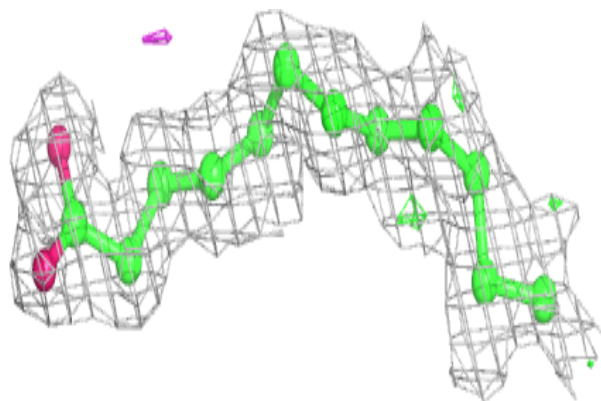
**Electron density around OLA A 307:**

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

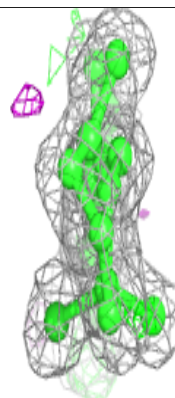
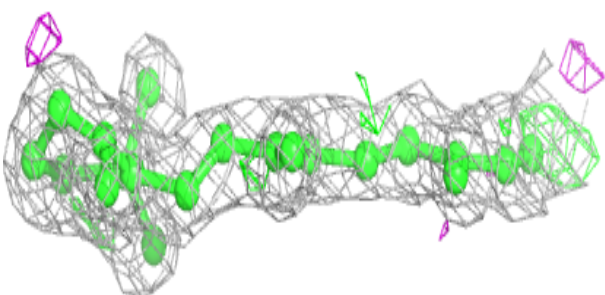
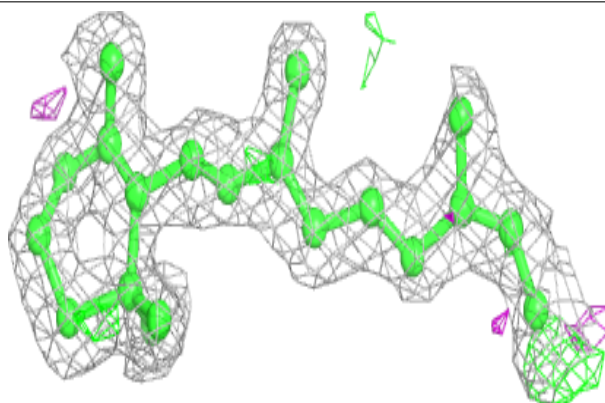


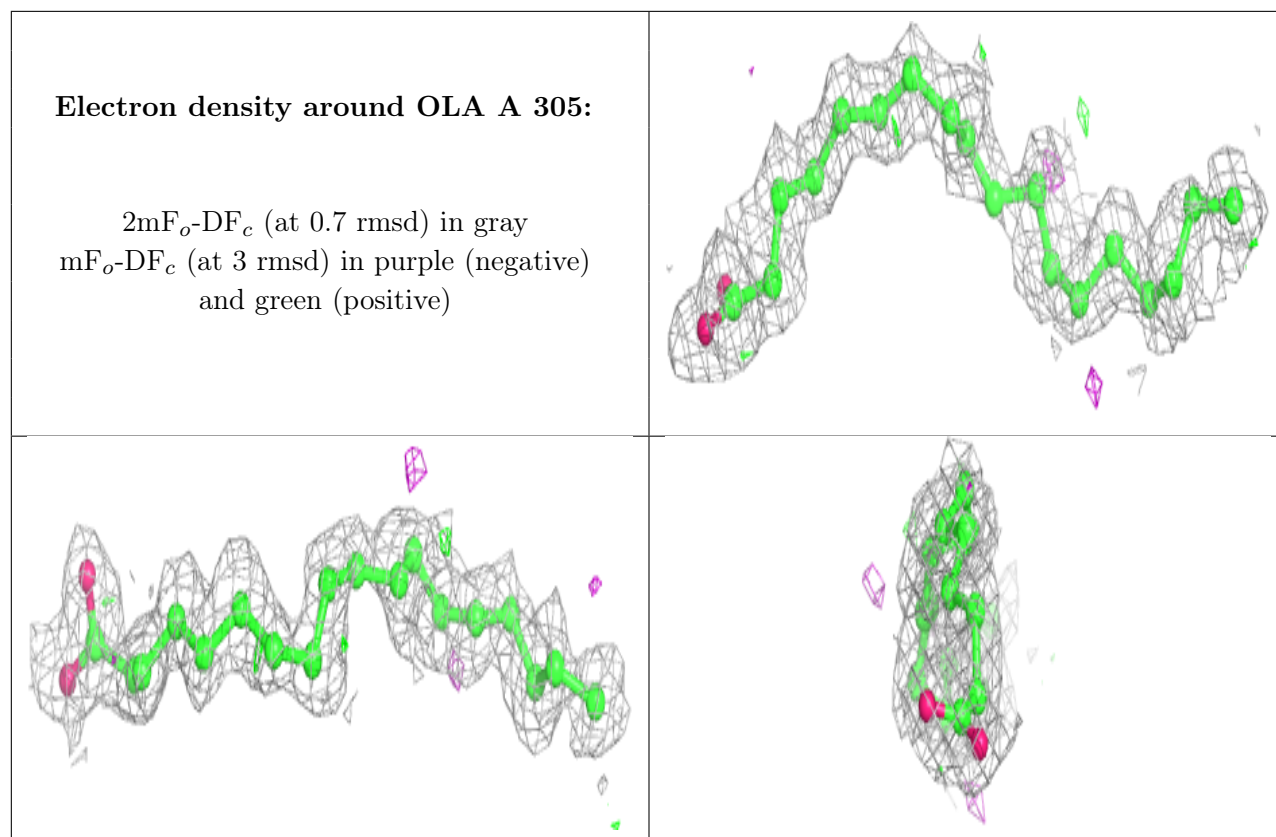
Electron density around OLA A 304:

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

**Electron density around RET A 303:**

$2mF_o-DF_c$ (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.