



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2025 – 03:03 pm GMT

PDB ID : 9GO2  
Title : C1C2 Channelrhodopsin - SMX Light activated structure  
Authors : Mulder, M.; Weinert, T.; Skopintsev, P.; Bruenle, S.; Broser, M.; Hegemann, P.; Standfuss, J.  
Deposited on : 2024-09-04  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

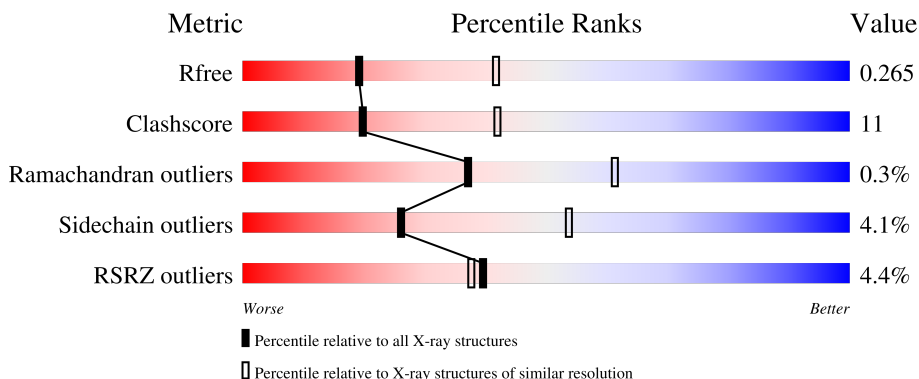
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	

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
2	OLC	A	701	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4776 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.

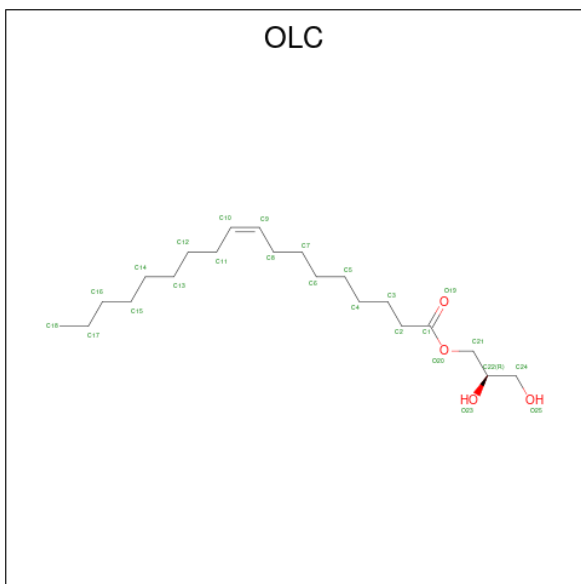
- Molecule 1 is a protein called Archaeal-type opsin 1, Archaeal-type opsin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	4603	3021	733	819	30	0	294	0

There are 8 discrepancies between the modelled and reference sequences:

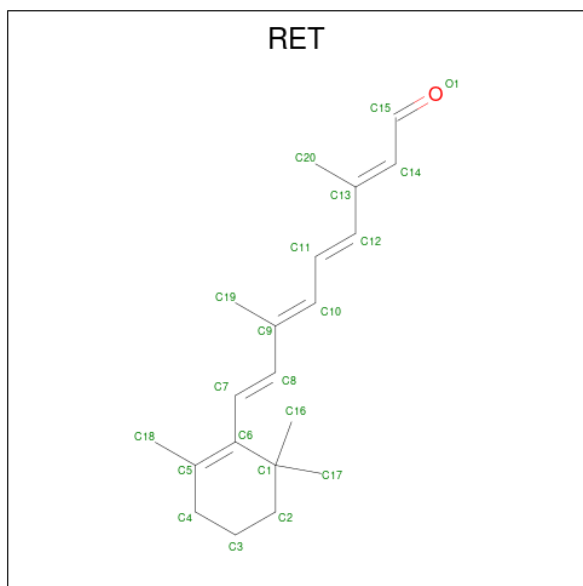
Chain	Residue	Modelled	Actual	Comment	Reference
A	656	SER	-	expression tag	UNP Q8RUT8
A	657	SER	-	expression tag	UNP Q8RUT8
A	658	GLU	-	expression tag	UNP Q8RUT8
A	659	ASP	-	expression tag	UNP Q8RUT8
A	660	LEU	-	expression tag	UNP Q8RUT8
A	661	TYR	-	expression tag	UNP Q8RUT8
A	662	PHE	-	expression tag	UNP Q8RUT8
A	663	GLN	-	expression tag	UNP Q8RUT8

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			25	21 4		
2	A	1	Total	C O	0	0
			16	14 2		
2	A	1	Total	C O	0	0
			14	10 4		
2	A	1	Total	C O	0	0
			16	12 4		
2	A	1	Total	C O	0	0
			18	14 4		
2	A	1	Total	C O	0	0
			10	8 2		
2	A	1	Total	C O	0	0
			10	8 2		
2	A	1	Total	C	0	0
			9	9		
2	A	1	Total	C	0	0
			8	8		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	1
			40	40		

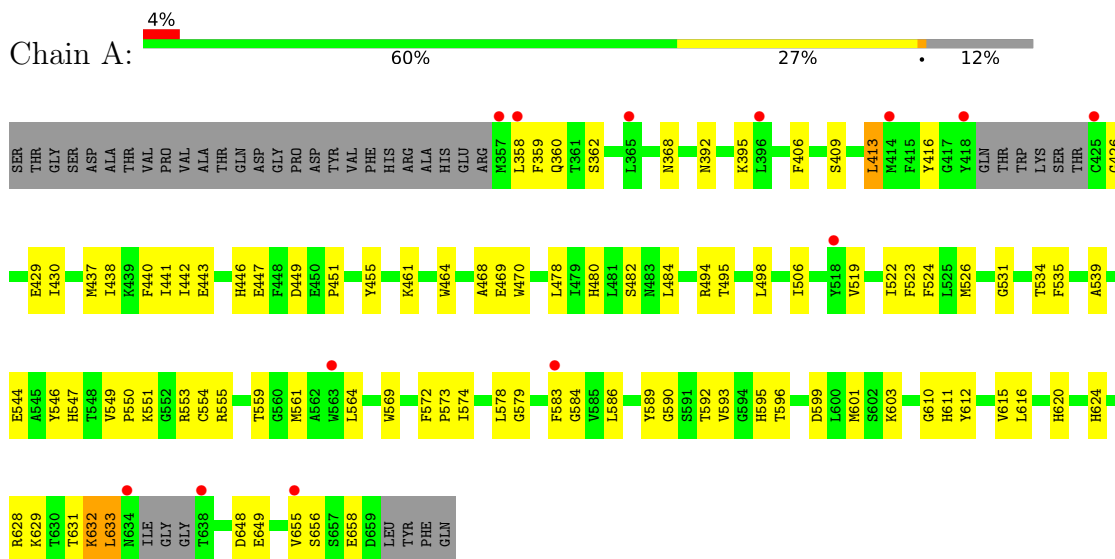
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0

### 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: Archaeal-type opsin 1, Archaeal-type opsin 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.40Å 141.70Å 94.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.85 – 2.70 70.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	62.9 (70.85-2.70) 62.7 (70.85-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	224.91 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.237 , 0.268 0.239 , 0.265	Depositor DCC
$R_{free}$ test set	10765 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 25.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: RET, OLC

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	0.36	2/4729 (0.0%)	0.67	8/6439 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	633[A]	LEU	CB-CG	-9.16	1.25	1.52
1	A	633[B]	LEU	CB-CG	-9.16	1.25	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633[A]	LEU	CB-CG-CD2	-12.60	89.58	111.00
1	A	633[B]	LEU	CB-CG-CD2	-12.60	89.58	111.00
1	A	633[A]	LEU	CB-CG-CD1	10.27	128.46	111.00
1	A	633[B]	LEU	CB-CG-CD1	10.27	128.46	111.00
1	A	358[A]	LEU	CB-CG-CD2	-9.06	95.60	111.00
1	A	358[B]	LEU	CB-CG-CD2	-9.06	95.60	111.00
1	A	633[A]	LEU	CA-CB-CG	8.36	134.53	115.30
1	A	633[B]	LEU	CA-CB-CG	8.36	134.53	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4603	0	4500	103	0
2	A	126	0	172	40	0
3	A	40	0	54	6	0
4	A	7	0	0	3	0
All	All	4776	0	4726	107	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 11.

All (107) 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:583[B]:PHE:CZ	2:A:701:OLC:O20	1.98	1.16
1:A:583[B]:PHE:CE1	2:A:701:OLC:C24	2.29	1.15
1:A:583[B]:PHE:CD1	2:A:701:OLC:H24A	1.85	1.11
1:A:583[B]:PHE:CE1	2:A:701:OLC:C22	2.39	1.06
1:A:583[B]:PHE:HE1	2:A:701:OLC:H22	1.28	0.97
1:A:583[B]:PHE:HE1	2:A:701:OLC:C22	1.77	0.97
1:A:583[B]:PHE:CD1	2:A:701:OLC:C24	2.47	0.95
1:A:583[B]:PHE:CE1	2:A:701:OLC:H22	2.02	0.94
1:A:583[B]:PHE:CE1	2:A:701:OLC:H24A	2.01	0.92
1:A:583[B]:PHE:HE1	2:A:701:OLC:C24	1.86	0.87
1:A:583[B]:PHE:CE1	2:A:701:OLC:O20	2.29	0.85
1:A:535[B]:PHE:CE2	2:A:701:OLC:H17	2.16	0.81
1:A:535[B]:PHE:CD2	2:A:701:OLC:H17	2.18	0.78
1:A:574[B]:ILE:HD13	2:A:701:OLC:H11A	1.67	0.76
1:A:535[B]:PHE:HB3	2:A:707:OLC:H7A	1.68	0.74
1:A:583[B]:PHE:CE1	2:A:701:OLC:O25	2.41	0.73
1:A:595[B]:HIS:NE2	4:A:801:HOH:O	2.22	0.72
1:A:494[A]:ARG:NH2	4:A:802:HOH:O	2.24	0.69
1:A:531[B]:GLY:O	1:A:534[B]:THR:HG22	1.94	0.67
1:A:632[B]:LYS:HB3	1:A:656[B]:SER:HB3	1.76	0.67
1:A:519[A]:VAL:HG21	2:A:705:OLC:H2	1.79	0.65
1:A:574[B]:ILE:CD1	2:A:701:OLC:H11A	2.27	0.65
1:A:478[B]:LEU:HD13	1:A:498[B]:LEU:HG	1.79	0.65
1:A:583[B]:PHE:CD1	2:A:701:OLC:O25	2.49	0.65
1:A:551[A]:LYS:HA	1:A:555[A]:ARG:HH11	1.61	0.64
1:A:494[B]:ARG:NH2	1:A:544[B]:GLU:OE2	2.32	0.62
1:A:583[B]:PHE:CE1	2:A:701:OLC:C21	2.83	0.62
1:A:612[A]:TYR:O	1:A:615[A]:VAL:HG22	2.01	0.60
1:A:406[A]:PHE:HB2	1:A:440[A]:PHE:CD2	2.36	0.60
1:A:612[B]:TYR:O	1:A:615[B]:VAL:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648[B]:ASP:OD1	1:A:649[B]:GLU:N	2.35	0.59
1:A:583[B]:PHE:CZ	2:A:701:OLC:C1	2.86	0.59
1:A:443[A]:GLU:O	1:A:447[A]:GLU:HB2	2.03	0.58
1:A:535[B]:PHE:CE2	2:A:701:OLC:C17	2.88	0.57
1:A:658[B]:GLU:N	1:A:658[B]:GLU:OE1	2.38	0.57
1:A:478[A]:LEU:HD13	1:A:498[A]:LEU:HG	1.86	0.56
1:A:631[A]:THR:HA	1:A:655[A]:VAL:O	2.06	0.56
1:A:484[B]:LEU:HD22	1:A:561[B]:MET:HE1	1.87	0.55
1:A:539[B]:ALA:CB	2:A:707:OLC:H2A	2.37	0.55
1:A:561[A]:MET:HE1	1:A:610[A]:GLY:HA2	1.89	0.55
1:A:574[A]:ILE:O	1:A:578[A]:LEU:HD13	2.07	0.55
3:A:710[B]:RET:H171	3:A:710[B]:RET:H8	1.87	0.55
1:A:535[B]:PHE:CE2	2:A:701:OLC:C18	2.90	0.54
1:A:579[B]:GLY:HA2	1:A:586[B]:LEU:HB2	1.88	0.54
1:A:368[B]:ASN:O	1:A:368[B]:ASN:ND2	2.39	0.54
1:A:446[A]:HIS:HB3	1:A:449[A]:ASP:HB2	1.90	0.54
1:A:406[B]:PHE:HB2	1:A:440[B]:PHE:CG	2.44	0.53
1:A:443[B]:GLU:O	1:A:447[B]:GLU:HB2	2.09	0.53
1:A:620[B]:HIS:CE1	1:A:624[B]:HIS:HD2	2.26	0.52
1:A:632[A]:LYS:HE3	1:A:656[A]:SER:HB3	1.92	0.52
1:A:523[B]:PHE:CZ	2:A:705:OLC:H10	2.45	0.52
1:A:611[A]:HIS:O	1:A:615[A]:VAL:HG13	2.09	0.52
1:A:535[B]:PHE:HE2	2:A:701:OLC:H18	1.75	0.52
1:A:539[B]:ALA:HB1	2:A:707:OLC:H2A	1.93	0.51
1:A:360[A]:GLN:HE21	1:A:362[A]:SER:H	1.59	0.51
1:A:360[B]:GLN:HE21	1:A:362[B]:SER:H	1.58	0.51
1:A:395[B]:LYS:HG2	1:A:589[B]:TYR:CE1	2.46	0.50
1:A:583[B]:PHE:HE1	2:A:701:OLC:O25	1.86	0.50
1:A:551[A]:LYS:HA	1:A:555[A]:ARG:NH1	2.25	0.50
1:A:658[A]:GLU:OE1	1:A:658[A]:GLU:N	2.44	0.49
1:A:524[B]:PHE:HE2	2:A:701:OLC:H7A	1.77	0.49
1:A:446[B]:HIS:HB3	1:A:449[B]:ASP:HB2	1.95	0.49
1:A:573[B]:PRO:HG2	2:A:701:OLC:H12A	1.94	0.49
1:A:426[A]:GLY:O	1:A:430[A]:ILE:HD13	2.12	0.49
1:A:549[B]:VAL:HB	1:A:554[B]:CYS:HB3	1.95	0.49
1:A:564[B]:LEU:HD22	1:A:601[B]:MET:HB3	1.95	0.48
1:A:583[B]:PHE:HE1	2:A:701:OLC:HO25	1.52	0.48
1:A:590[A]:GLY:O	1:A:593[A]:VAL:HG22	2.12	0.48
1:A:592[B]:THR:O	1:A:596[B]:THR:HG23	2.14	0.48
1:A:583[B]:PHE:CE2	2:A:701:OLC:C1	2.97	0.48
1:A:359[B]:PHE:HA	4:A:803:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519[B]:VAL:HG21	2:A:705:OLC:H2	1.96	0.47
1:A:535[B]:PHE:HE2	2:A:701:OLC:C18	2.26	0.47
1:A:553[A]:ARG:HD2	1:A:616[A]:LEU:HD21	1.97	0.47
1:A:438[B]:ILE:O	1:A:441[B]:ILE:HG12	2.15	0.47
1:A:550[B]:PRO:O	1:A:555[B]:ARG:HG3	2.15	0.47
1:A:573[A]:PRO:HA	3:A:710[A]:RET:H172	1.98	0.46
1:A:416[A]:TYR:CE2	1:A:429[A]:GLU:HB3	2.50	0.46
1:A:531[A]:GLY:O	1:A:535[A]:PHE:HD1	2.00	0.45
1:A:416[B]:TYR:CE2	1:A:429[B]:GLU:HB3	2.52	0.45
1:A:470[A]:TRP:CD1	3:A:710[A]:RET:H14	2.51	0.45
1:A:583[B]:PHE:HD1	2:A:701:OLC:C24	2.22	0.44
1:A:583[B]:PHE:CE2	2:A:701:OLC:O20	2.60	0.44
3:A:710[A]:RET:H171	3:A:710[A]:RET:H8	2.00	0.44
1:A:559[A]:THR:HG21	2:A:709:OLC:H7	1.99	0.44
1:A:599[B]:ASP:OD1	1:A:603[B]:LYS:HE2	2.17	0.44
1:A:546[A]:TYR:CZ	1:A:555[A]:ARG:HD3	2.53	0.43
3:A:710[A]:RET:H181	3:A:710[A]:RET:H7	1.79	0.43
1:A:522[A]:ILE:O	1:A:526[A]:MET:HG3	2.19	0.43
1:A:632[B]:LYS:H	1:A:656[B]:SER:HA	1.84	0.43
1:A:441[A]:ILE:HG13	1:A:442[A]:ILE:N	2.33	0.42
2:A:703:OLC:H3	2:A:703:OLC:H6	1.75	0.42
1:A:464[A]:TRP:CE2	1:A:468[A]:ALA:HB2	2.54	0.42
1:A:547[A]:HIS:HA	1:A:555[A]:ARG:NH2	2.35	0.42
1:A:583[B]:PHE:HD1	2:A:701:OLC:O25	2.00	0.42
1:A:569[B]:TRP:CE2	3:A:710[B]:RET:H203	2.54	0.42
1:A:547[A]:HIS:HA	1:A:555[A]:ARG:HH21	1.85	0.41
1:A:395[B]:LYS:HG2	1:A:589[B]:TYR:CZ	2.56	0.41
1:A:413[A]:LEU:HD12	1:A:437[A]:MET:HE1	2.03	0.41
1:A:546[A]:TYR:HD2	1:A:547[A]:HIS:ND1	2.19	0.41
1:A:632[A]:LYS:HE3	1:A:656[A]:SER:CB	2.50	0.41
1:A:482[A]:SER:OG	1:A:495[A]:THR:HG23	2.21	0.41
1:A:470[B]:TRP:HE3	1:A:506[B]:ILE:HD12	1.86	0.40
1:A:564[B]:LEU:HD23	1:A:564[B]:LEU:HA	1.98	0.40
1:A:455[B]:TYR:HE1	1:A:461[B]:LYS:HE2	1.86	0.40
1:A:569[B]:TRP:HA	1:A:572[B]:PHE:HD2	1.85	0.40
1:A:574[B]:ILE:CD1	2:A:701:OLC:C11	2.99	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	576/333 (173%)	562 (98%)	12 (2%)	2 (0%)	37 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	584[A]	GLY
1	A	584[B]	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	484/282 (172%)	464 (96%)	20 (4%)	26 54

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392[A]	ASN
1	A	392[B]	ASN
1	A	409[A]	SER
1	A	409[B]	SER
1	A	413[A]	LEU
1	A	413[B]	LEU
1	A	451[A]	PRO
1	A	451[B]	PRO
1	A	469[A]	GLU

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Mol	Chain	Res	Type
1	A	469[B]	GLU
1	A	480[A]	HIS
1	A	480[B]	HIS
1	A	628[A]	ARG
1	A	628[B]	ARG
1	A	629[A]	LYS
1	A	629[B]	LYS
1	A	632[A]	LYS
1	A	632[B]	LYS
1	A	633[A]	LEU
1	A	633[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

11 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	OLC	A	702	-	15,15,24	1.27	1 (6%)	15,15,25	1.47	1 (6%)
2	OLC	A	707	-	9,9,24	1.46	1 (11%)	9,9,25	1.20	0
3	RET	A	710[A]	1	20,20,21	0.73	1 (5%)	27,27,28	0.59	1 (3%)
2	OLC	A	706	-	9,9,24	1.47	1 (11%)	9,9,25	1.19	0
2	OLC	A	701	-	24,24,24	1.06	1 (4%)	25,25,25	1.24	2 (8%)
2	OLC	A	703	-	13,13,24	1.21	1 (7%)	14,14,25	1.08	1 (7%)
2	OLC	A	705	-	17,17,24	1.20	1 (5%)	18,18,25	1.18	2 (11%)
2	OLC	A	708	-	8,8,24	0.91	0	7,7,25	1.62	1 (14%)
3	RET	A	710[B]	1	20,20,21	0.70	1 (5%)	27,27,28	0.62	1 (3%)
2	OLC	A	709	-	7,7,24	0.72	0	6,6,25	0.72	0
2	OLC	A	704	-	15,15,24	1.19	1 (6%)	16,16,25	1.08	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	OLC	A	702	-	-	7/13/13/24	-
2	OLC	A	707	-	-	5/7/7/24	-
3	RET	A	710[A]	1	-	0/13/30/31	0/1/1/1
2	OLC	A	706	-	-	5/7/7/24	-
2	OLC	A	701	-	-	13/24/24/24	-
2	OLC	A	703	-	-	9/13/13/24	-
2	OLC	A	705	-	-	10/17/17/24	-
2	OLC	A	708	-	-	3/6/6/24	-
3	RET	A	710[B]	1	-	0/13/30/31	0/1/1/1
2	OLC	A	709	-	-	3/5/5/24	-
2	OLC	A	704	-	-	9/15/15/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	OLC	O20-C1	3.36	1.42	1.30
2	A	707	OLC	O20-C1	3.33	1.41	1.30
2	A	706	OLC	O20-C1	3.33	1.41	1.30
2	A	704	OLC	O20-C1	3.10	1.42	1.33
2	A	701	OLC	O20-C1	3.04	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	705	OLC	O20-C1	2.96	1.42	1.33
2	A	703	OLC	O20-C1	2.93	1.41	1.33
3	A	710[A]	RET	C14-C13	2.82	1.36	1.33
3	A	710[B]	RET	C14-C13	2.59	1.35	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	708	OLC	C8-C9-C10	3.81	152.77	126.84
2	A	702	OLC	C8-C9-C10	3.70	153.14	124.73
2	A	701	OLC	C8-C9-C10	3.69	153.02	124.73
2	A	705	OLC	C8-C9-C10	2.72	152.67	131.07
2	A	704	OLC	O20-C1-C2	2.71	120.41	111.91
2	A	703	OLC	O20-C1-C2	2.64	120.19	111.91
2	A	701	OLC	O20-C1-C2	2.57	119.96	111.91
2	A	705	OLC	O20-C1-C2	2.55	119.91	111.91
3	A	710[B]	RET	C8-C7-C6	2.12	133.15	127.20
3	A	710[A]	RET	C8-C7-C6	2.03	132.91	127.20

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	704	OLC	C21-C22-C24-O25
2	A	704	OLC	O20-C21-C22-C24
2	A	701	OLC	O19-C1-O20-C21
2	A	701	OLC	C2-C1-O20-C21
2	A	704	OLC	O20-C21-C22-O23
2	A	703	OLC	O23-C22-C24-O25
2	A	701	OLC	C1-C2-C3-C4
2	A	707	OLC	C1-C2-C3-C4
2	A	701	OLC	C11-C12-C13-C14
2	A	702	OLC	C5-C6-C7-C8
2	A	702	OLC	C3-C4-C5-C6
2	A	701	OLC	C14-C15-C16-C17
2	A	703	OLC	C21-C22-C24-O25
2	A	704	OLC	C3-C4-C5-C6
2	A	709	OLC	C4-C5-C6-C7
2	A	701	OLC	C13-C14-C15-C16
2	A	701	OLC	C3-C4-C5-C6
2	A	705	OLC	C2-C3-C4-C5
2	A	706	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	704	OLC	O23-C22-C24-O25
2	A	707	OLC	C4-C5-C6-C7
2	A	701	OLC	C6-C7-C8-C9
2	A	705	OLC	C6-C7-C8-C9
2	A	705	OLC	C1-C2-C3-C4
2	A	703	OLC	C1-C2-C3-C4
2	A	706	OLC	C1-C2-C3-C4
2	A	707	OLC	C3-C4-C5-C6
2	A	701	OLC	C2-C3-C4-C5
2	A	701	OLC	C10-C11-C12-C13
2	A	702	OLC	C6-C7-C8-C9
2	A	708	OLC	C6-C7-C8-C9
2	A	703	OLC	C4-C5-C6-C7
2	A	705	OLC	C7-C8-C9-C10
2	A	705	OLC	C4-C5-C6-C7
2	A	708	OLC	C3-C4-C5-C6
2	A	705	OLC	C5-C6-C7-C8
2	A	703	OLC	O20-C21-C22-O23
2	A	704	OLC	C6-C7-C8-C9
2	A	709	OLC	C3-C4-C5-C6
2	A	703	OLC	O20-C21-C22-C24
2	A	703	OLC	C2-C1-O20-C21
2	A	706	OLC	C4-C5-C6-C7
2	A	703	OLC	O19-C1-O20-C21
2	A	701	OLC	C21-C22-C24-O25
2	A	702	OLC	C4-C5-C6-C7
2	A	702	OLC	C2-C3-C4-C5
2	A	703	OLC	O20-C1-C2-C3
2	A	701	OLC	O23-C22-C24-O25
2	A	709	OLC	C5-C6-C7-C8
2	A	701	OLC	C7-C8-C9-C10
2	A	708	OLC	C7-C8-C9-C10
2	A	704	OLC	C5-C6-C7-C8
2	A	706	OLC	O20-C1-C2-C3
2	A	702	OLC	C9-C10-C11-C12
2	A	706	OLC	O19-C1-C2-C3
2	A	707	OLC	C5-C6-C7-C8
2	A	705	OLC	O20-C1-C2-C3
2	A	705	OLC	O23-C22-C24-O25
2	A	704	OLC	C2-C1-O20-C21
2	A	705	OLC	C3-C4-C5-C6
2	A	704	OLC	O19-C1-O20-C21

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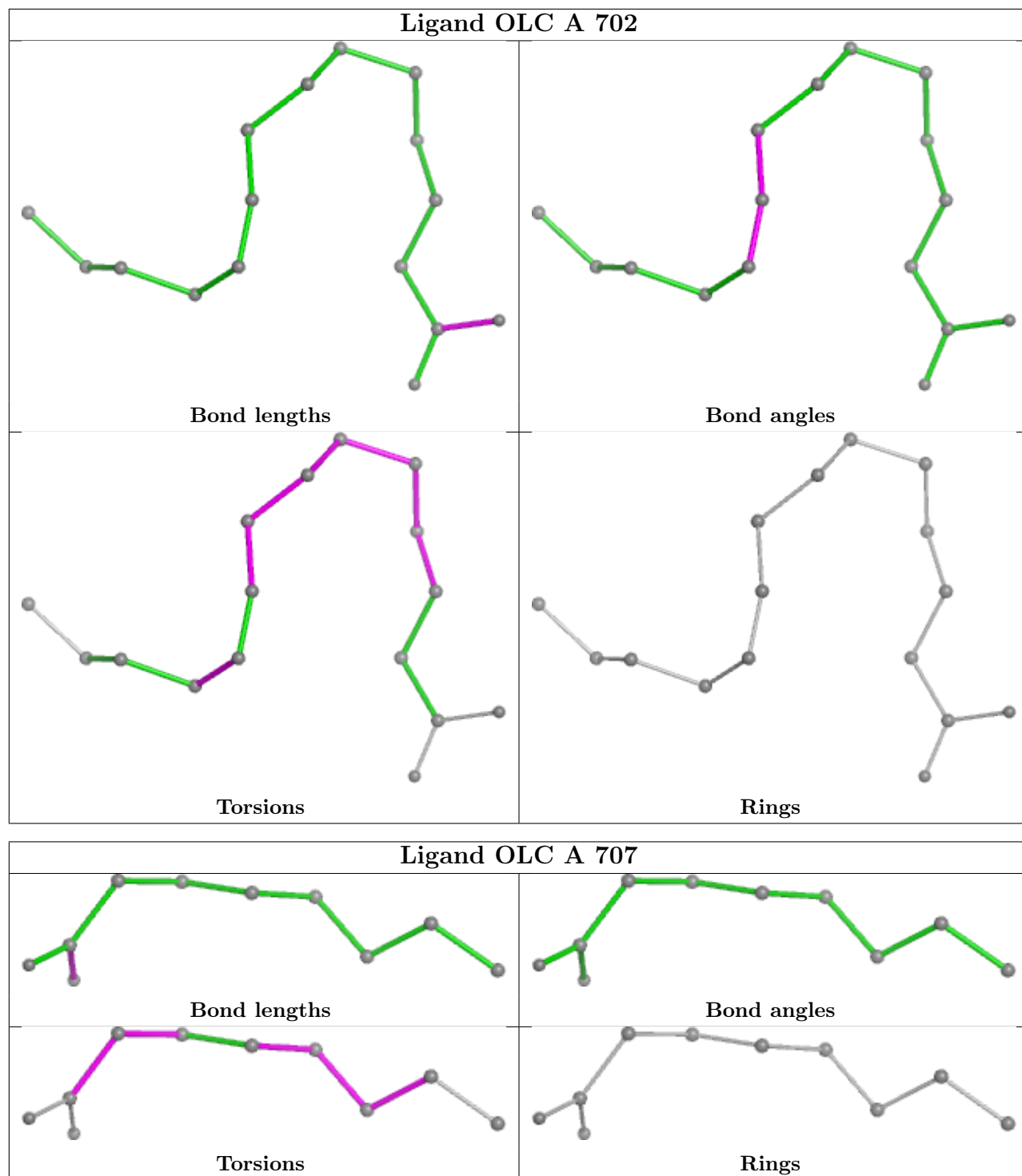
Mol	Chain	Res	Type	Atoms
2	A	705	OLC	O19-C1-C2-C3
2	A	702	OLC	C7-C8-C9-C10
2	A	707	OLC	O20-C1-C2-C3

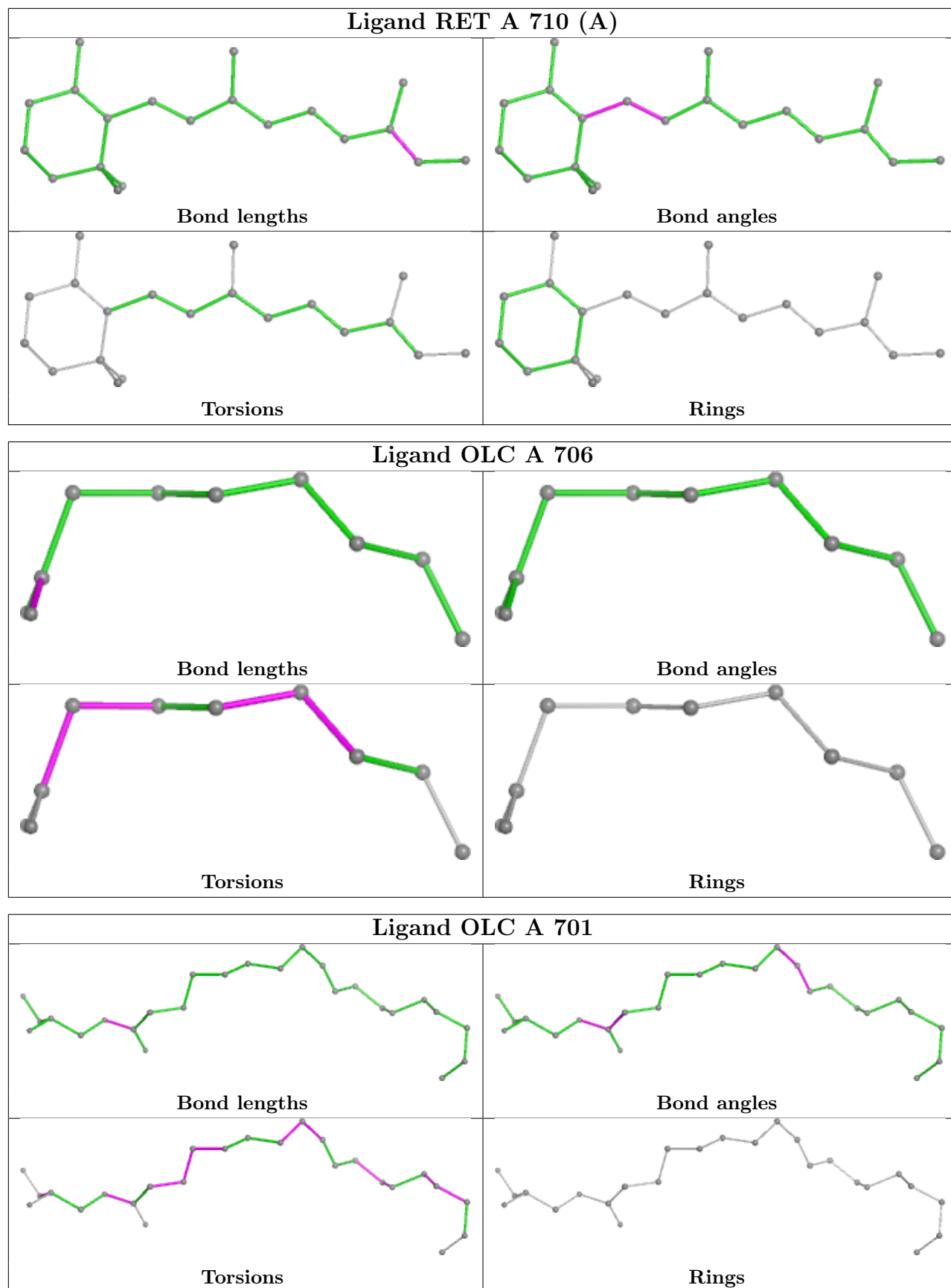
There are no ring outliers.

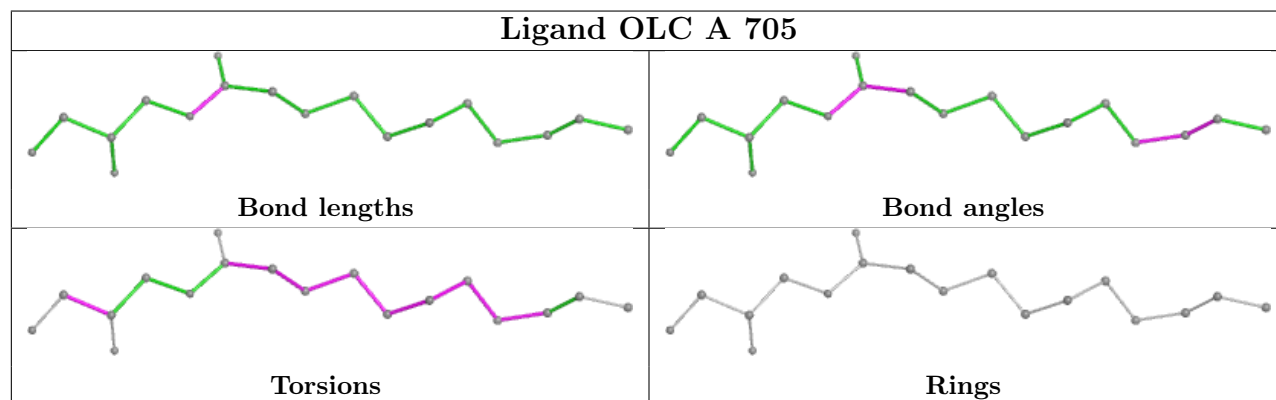
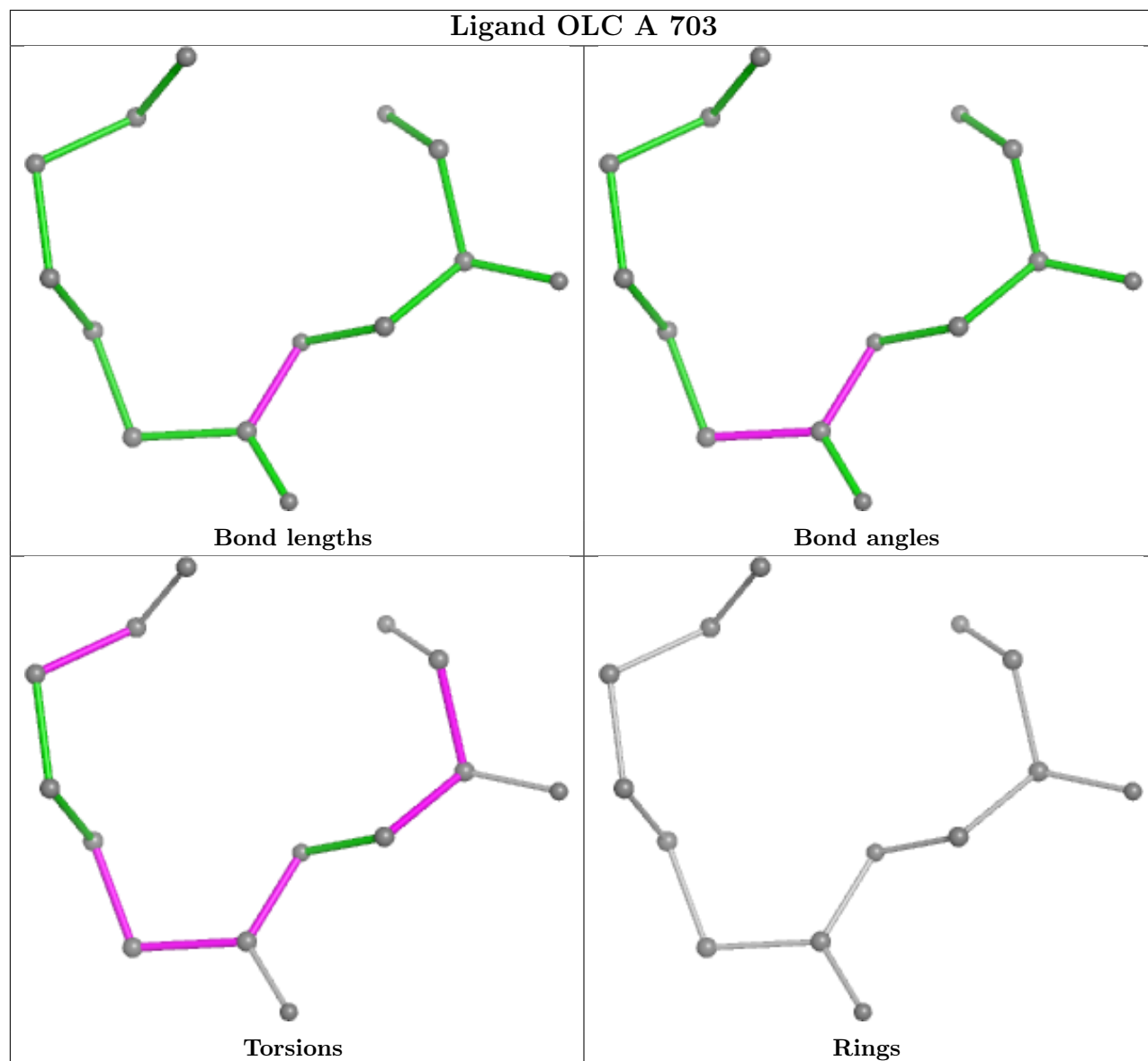
7 monomers are involved in 46 short contacts:

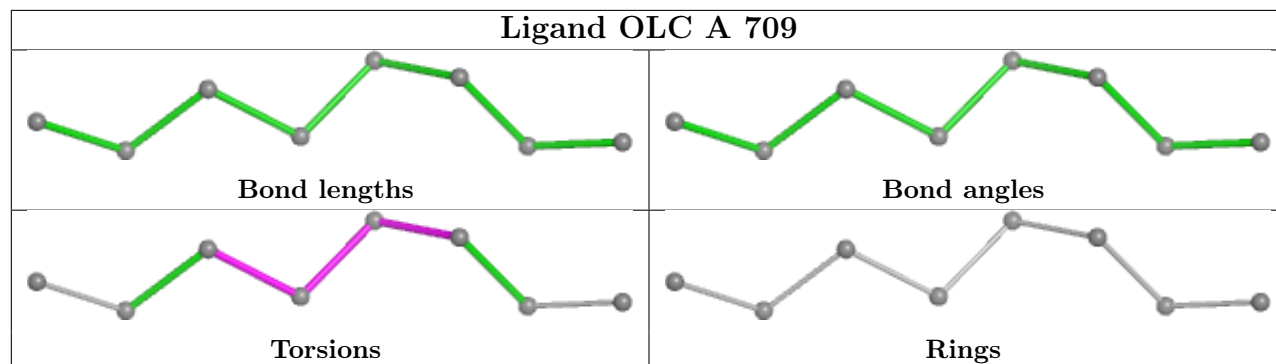
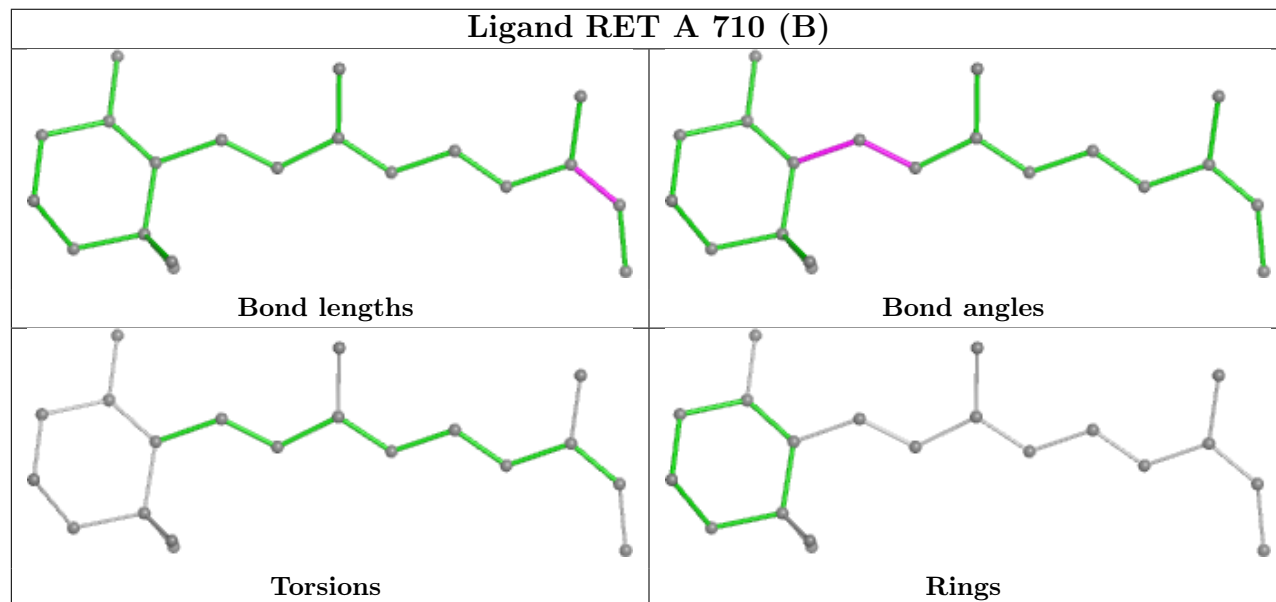
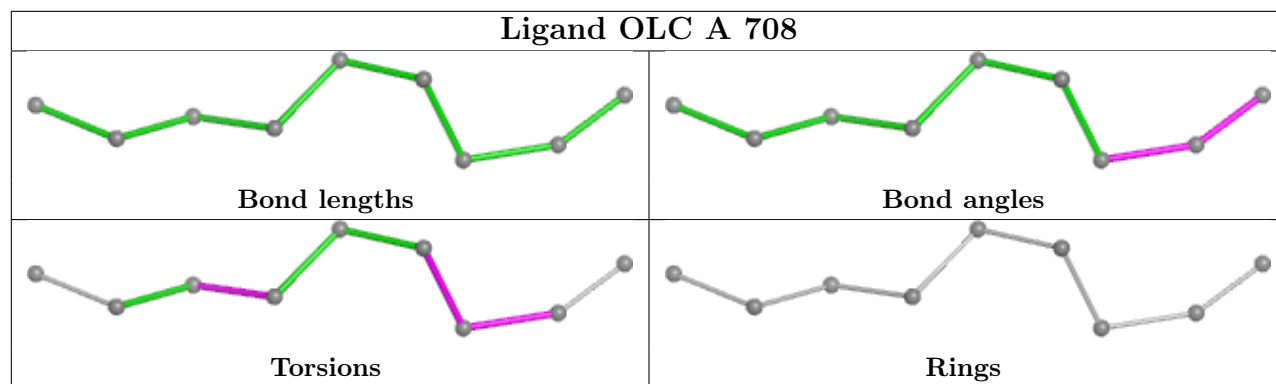
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	707	OLC	3	0
3	A	710[A]	RET	4	0
2	A	701	OLC	32	0
2	A	703	OLC	1	0
2	A	705	OLC	3	0
3	A	710[B]	RET	2	0
2	A	709	OLC	1	0

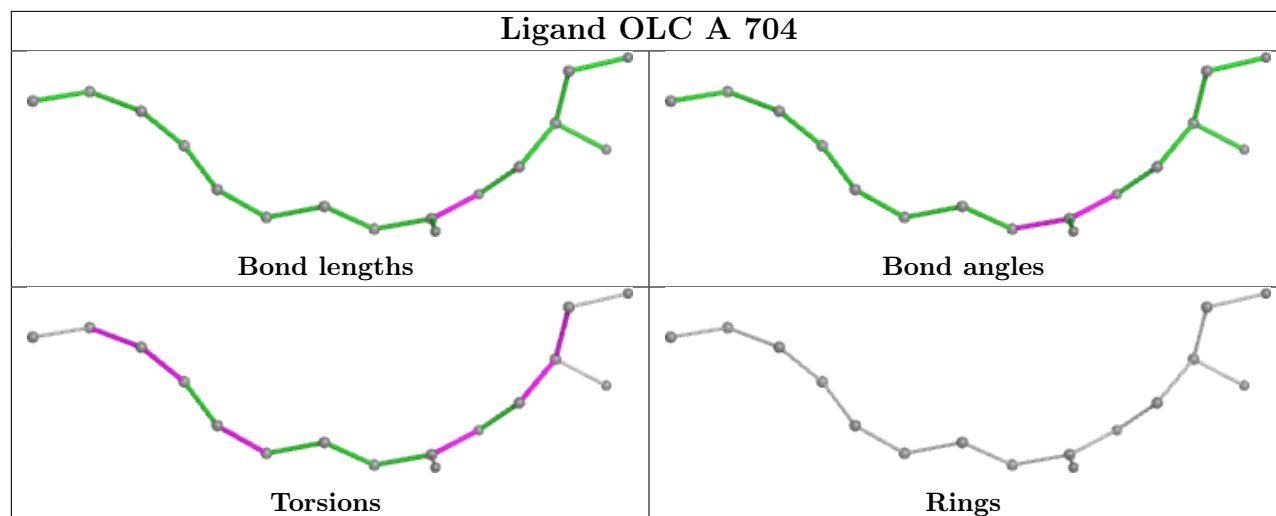
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	294/333 (88%)	0.17	13 (4%) 39 38	14, 27, 47, 111	294 (100%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583[A]	PHE	10.0
1	A	518[A]	TYR	3.8
1	A	634[A]	ASN	3.6
1	A	358[A]	LEU	3.5
1	A	563[A]	TRP	3.3
1	A	655[A]	VAL	3.0
1	A	357[A]	MET	2.9
1	A	638[A]	THR	2.7
1	A	425[A]	CYS	2.5
1	A	396[A]	LEU	2.4
1	A	418[A]	TYR	2.4
1	A	365[A]	LEU	2.4
1	A	414[A]	MET	2.2

### 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.

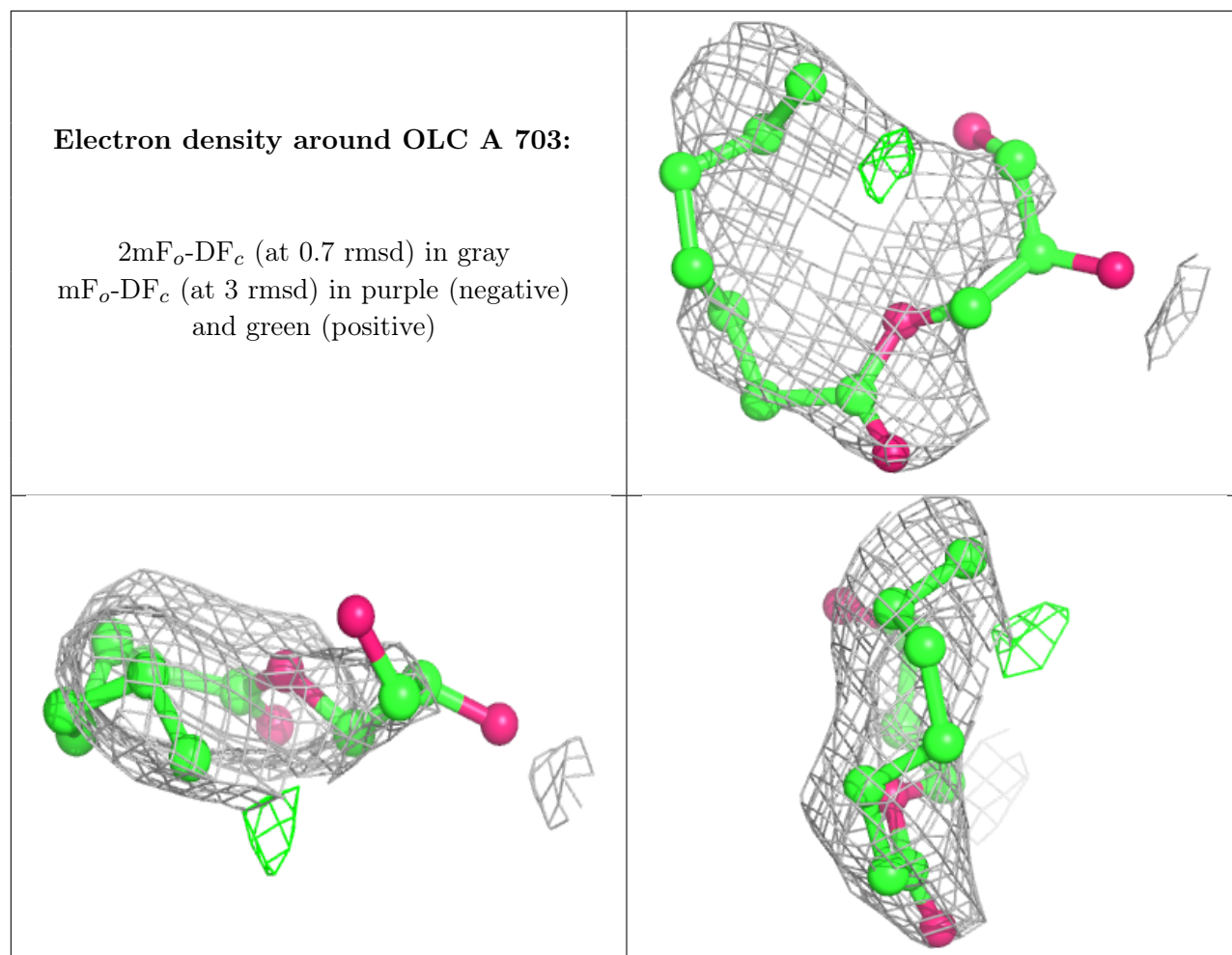
## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OLC	A	703	14/25	0.56	0.17	76,103,127,127	0
2	OLC	A	706	10/25	0.66	0.16	43,80,100,111	0
2	OLC	A	705	18/25	0.68	0.20	48,82,104,111	0
2	OLC	A	702	16/25	0.72	0.18	46,90,106,112	0
2	OLC	A	701	25/25	0.72	0.17	56,78,154,199	0
2	OLC	A	709	8/25	0.74	0.17	64,75,91,92	0
2	OLC	A	704	16/25	0.76	0.16	38,59,87,91	0
2	OLC	A	707	10/25	0.83	0.15	62,75,101,103	0
2	OLC	A	708	9/25	0.88	0.14	58,66,74,77	0
3	RET	A	710[A]	20/21	0.88	0.11	36,52,57,57	20
3	RET	A	710[B]	20/21	0.88	0.11	37,49,55,55	20

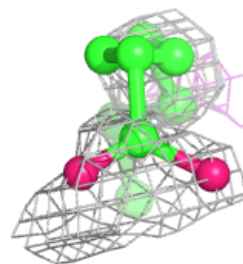
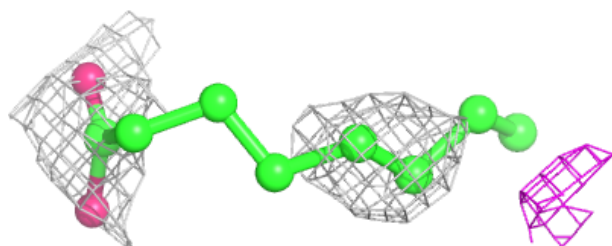
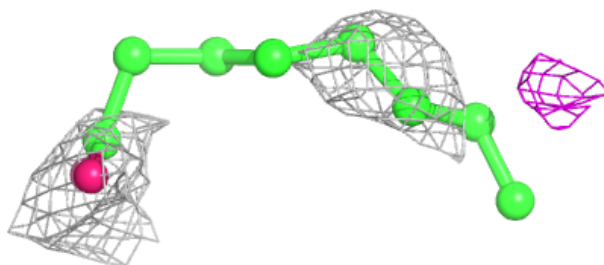
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



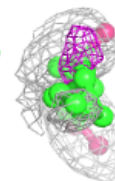
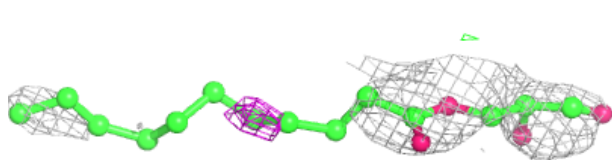
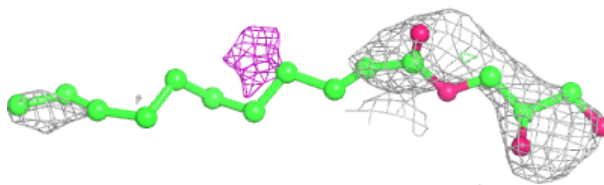


**Electron density around OLC A 706:**

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

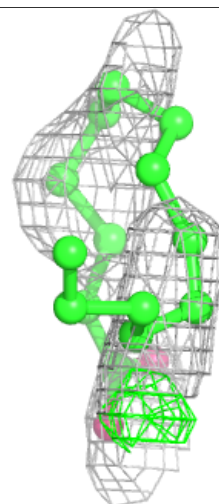
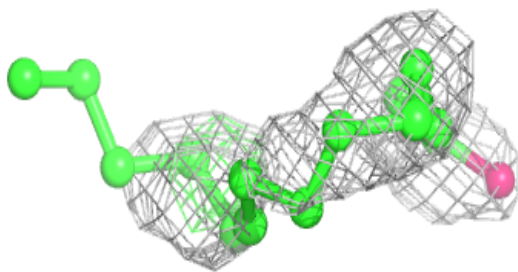
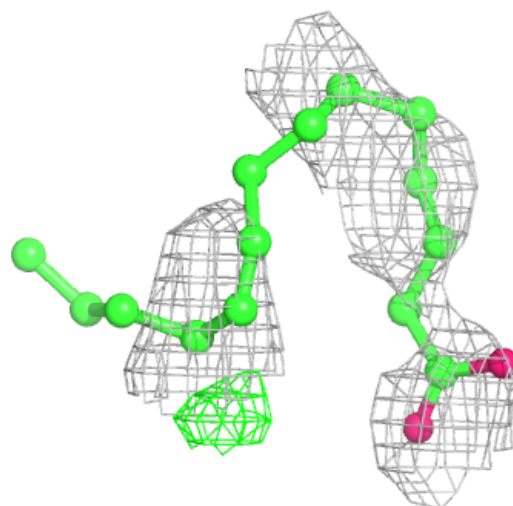
**Electron density around OLC A 705:**

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



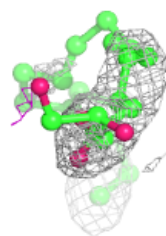
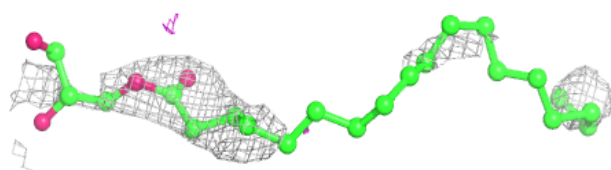
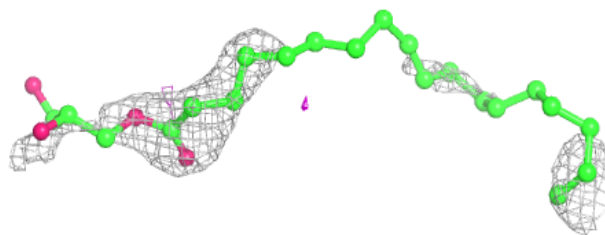
**Electron density around OLC A 702:**

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

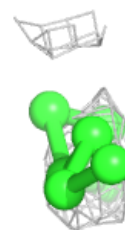
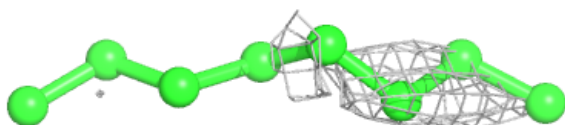
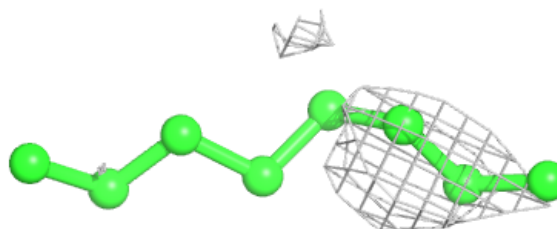


**Electron density around OLC A 701:**

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

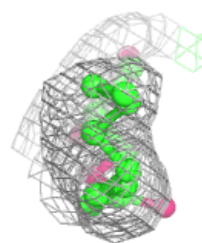
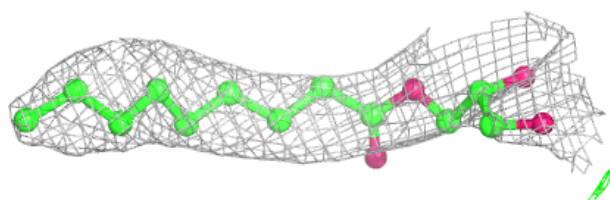
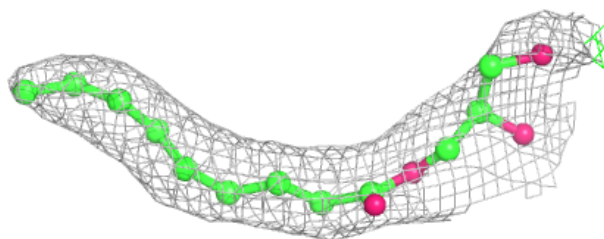
**Electron density around OLC A 709:**

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

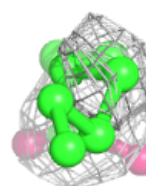
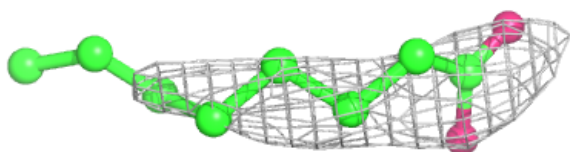
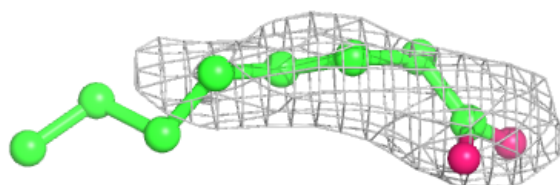


**Electron density around OLC A 704:**

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

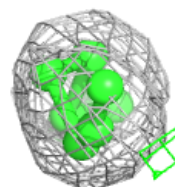
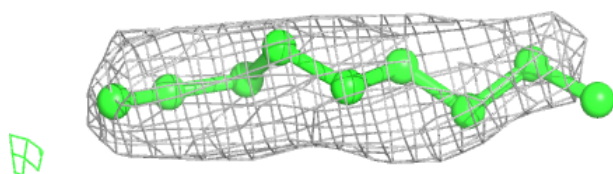
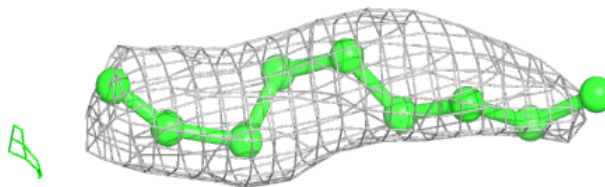
**Electron density around OLC A 707:**

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

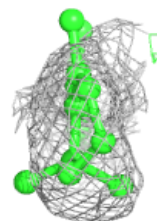
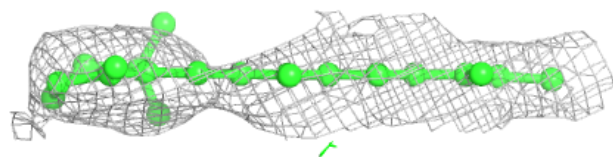
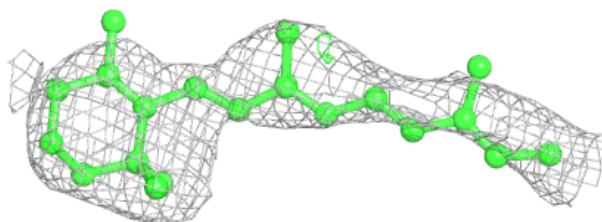


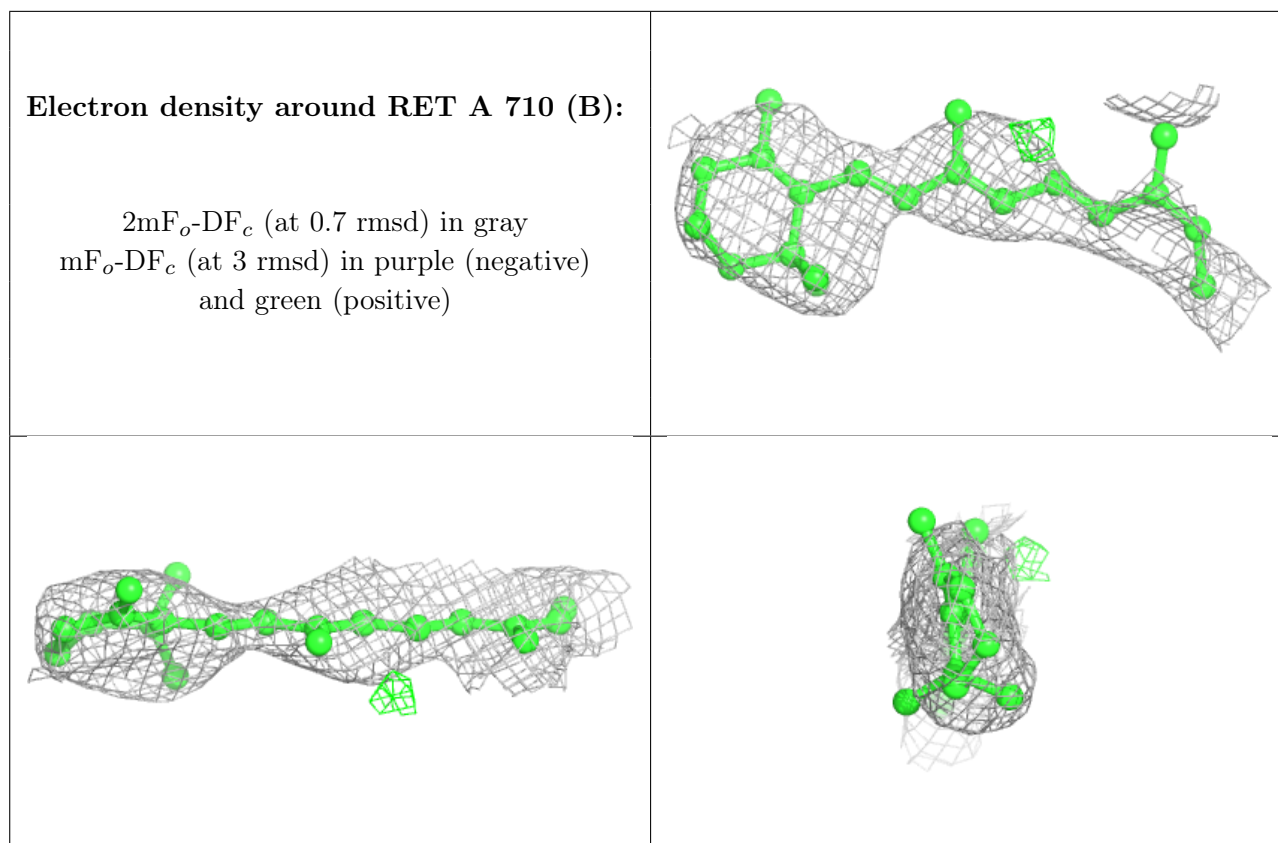
**Electron density around OLC A 708:**

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

**Electron density around RET A 710 (A):**

$2mF_o-DF_c$  (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.