



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:23 AM UTC

PDB ID : 8R96 / pdb_00008r96
Title : Crystal structure of the cryorhodopsin CryoR2 at pH 4.6, type A crystals
Authors : Kovalev, K.; Lamm, G.H.U.; Marin, E.
Deposited on : 2023-11-30
Resolution : 2.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

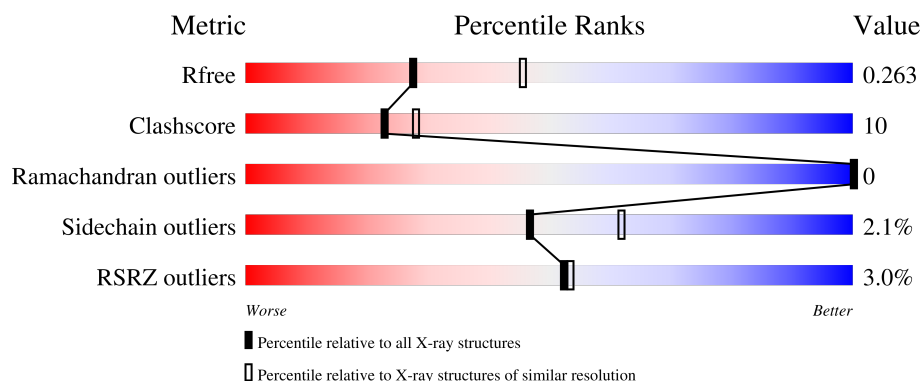
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	327	3% 72% 15% • 12%
1	B	327	3% 72% 15% • 11%
1	C	327	0% 69% 18% • 12%
1	D	327	2% 71% 17% • 12%
1	E	327	3% 69% 17% • 13%

2 Entry composition [i](#)

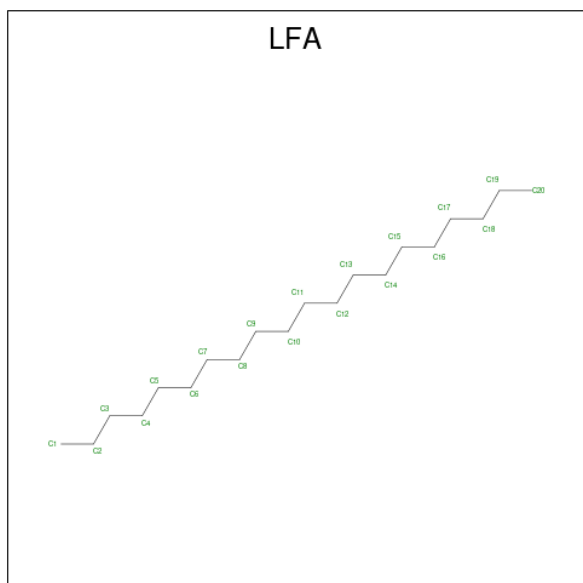
There are 6 unique types of molecules in this entry. The entry contains 11044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cryorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2155	1415	350	384	6			
1	B	290	Total	C	N	O	S	0	0	0
			2162	1419	349	388	6			
1	C	287	Total	C	N	O	S	0	0	0
			2138	1408	344	380	6			
1	D	289	Total	C	N	O	S	0	0	0
			2140	1409	341	384	6			
1	E	286	Total	C	N	O	S	0	0	0
			2143	1408	347	382	6			

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			11	11		

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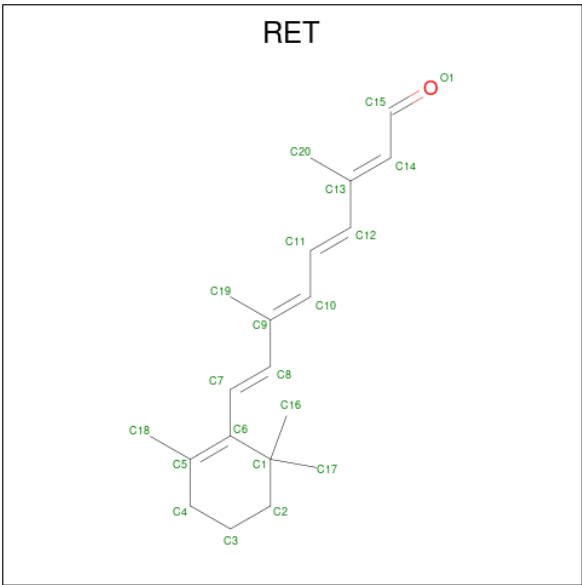
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 7 7	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 12 12	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 11 11	0	0
2	D	1	Total C 8 8	0	0
2	E	1	Total C 11 11	0	0
2	E	1	Total C 13 13	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



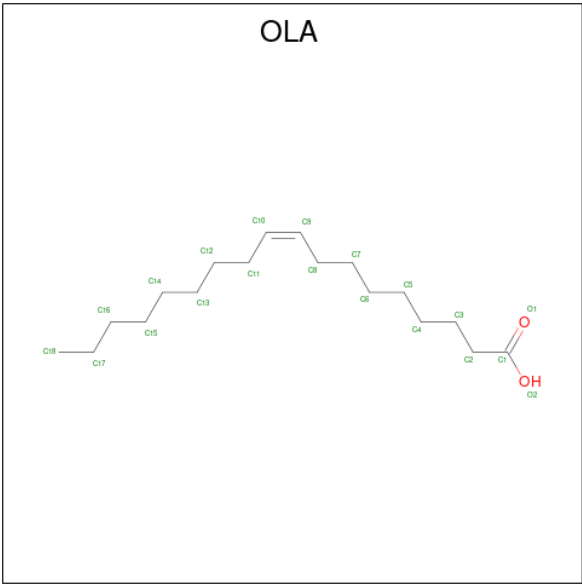
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 20 20	0	0
4	B	1	Total C 20 20	0	0
4	C	1	Total C 20 20	0	0
4	D	1	Total C 20 20	0	0
4	E	1	Total C 20 20	0	0

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			20	18	2		

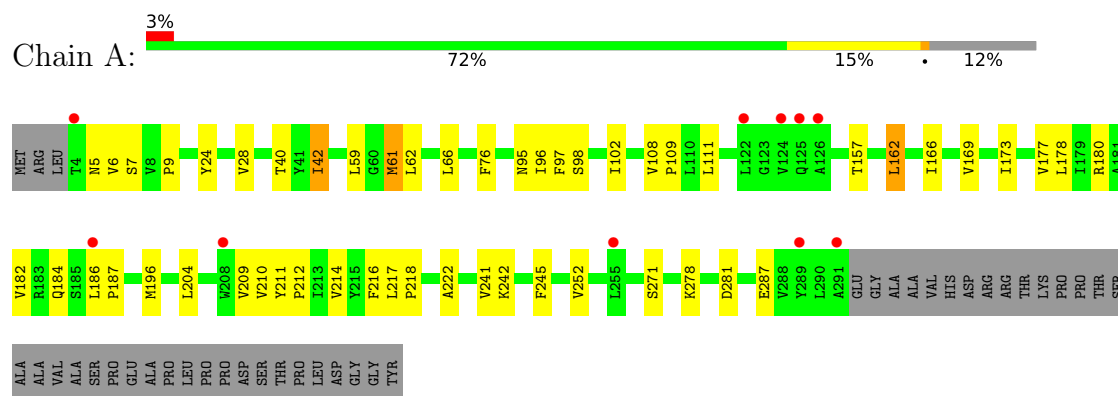
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	9	Total	O	0	0
			9	9		
6	C	6	Total	O	0	0
			6	6		
6	D	7	Total	O	0	0
			7	7		
6	E	5	Total	O	0	0
			5	5		

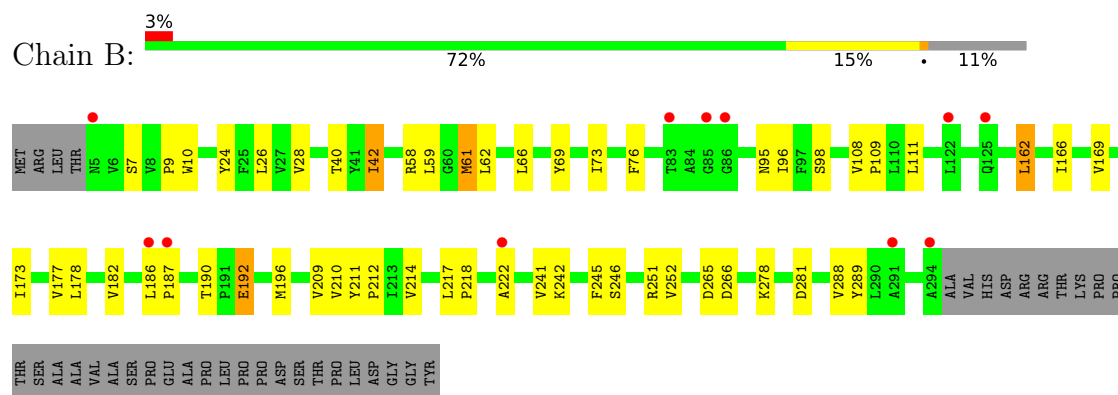
3 Residue-property plots [i](#)

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.

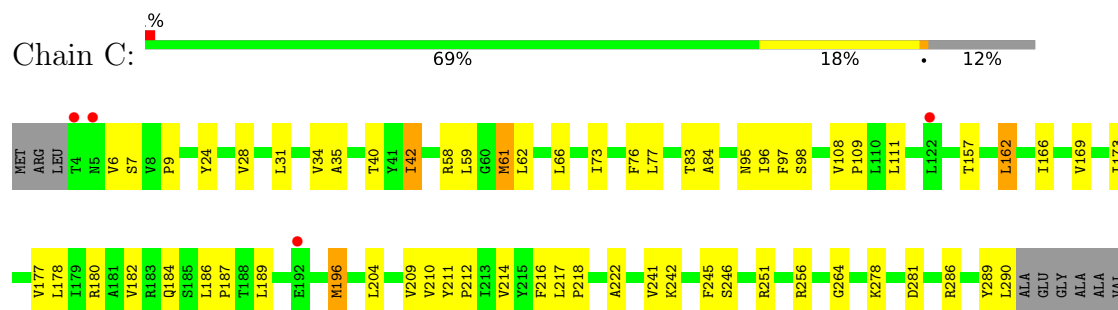
• Molecule 1: cryorhodopsin



• Molecule 1: cryorhodopsin



• Molecule 1: cryorhodopsin



HIS
ASP
ARG
ARG
ARG
THR
LYS
PRO
PRO
THR
SER
ALA
ALA
VAL
ALA
SER
PRO
GLU
ALA
PRO
LEU
PRO
PRO
ASP
SER
THR
PRO
LEU
ASP
GLY
GLY
TYR

● Molecule 1: cryorhodopsin

Chain D:  2% 71% 17% 12%

MET ARG L3 T4 N5 V6 S7 V8 P9 W10 Y24 Y28 T40 Y41 I42 R58 L59 G60 M61 L62 L66 Y69 I73 F76 A84 N95 I96 F97 S98 V108 P109 L110 L111 T121 T157 L162 I166 V169 I173 V177 L178 I179

R180 A191 V182 R183 P187 S185 L186 P187 T188 L189 M196 V209 V210 Y211 P212 P213 V214 V215 F216 L217 P218 A222 V241 K242 L243 G244 F245 S246 V252 R256 Y289 L290 A291 GLY ALA VAL HIS ASP ARG THR LYS PRO THR SER ALA VAL ALA

SER PRO GLU ALA THR LEU PRO PRO ASP THR PRO LEU ASP GLY TYR

● Molecule 1: cryorhodopsin

Chain E:  3% 69% 17% 13%

MET ARG LEU THR N5 V6 S7 P8 W9 Y24 Y27 V28 T40 Y41 I42 R58 L59 G60 M61 L62 L66 F76 A84 G85 G86 N95 I96 F97 S98 V108 P109 L110 L111 L122 G123 V124 Q125 T157 L162 I166 V169 I173 V177 L178

V182 L186 P187 T188 L189 E192 M196 V209 V210 Y211 P212 L213 V215 F216 L217 P218 L219 F220 G221 A222 V239 L240 K242 L243 G244 F245 S246 R251 V252 L255 R256 V261 K278 D281 R286 E287 V288 Y289 L290 ALA GLY GLY ALA VAL HIS

ASP ARG ARG THR LYS PRO PRO THR SER SER ALA VAL ALA SER PRO GLU ALA PRO PRO LEU PRO PRO ASP SER THR PRO LEU ASP GLY TYR

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 295.67Å 185.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.46 20.00 – 2.46	Depositor EDS
% Data completeness (in resolution range)	65.4 (20.00-2.46) 65.6 (20.00-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.47Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.239 , 0.254 0.246 , 0.263	Depositor DCC
R_{free} test set	2746 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11044	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: PO4, LFA, OLA, RET

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	1.00	0/2203	1.61	0/3025
1	B	0.99	0/2210	1.62	0/3035
1	C	0.99	0/2186	1.62	0/3003
1	D	1.00	0/2188	1.62	0/3009
1	E	0.99	0/2191	1.62	0/3009
All	All	0.99	0/10978	1.62	0/15081

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	2155	0	2198	40	0
1	B	2162	0	2199	43	0
1	C	2138	0	2176	51	0
1	D	2140	0	2168	49	0
1	E	2143	0	2187	49	0
2	A	42	0	79	0	0
2	B	23	0	44	0	0
2	C	12	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	29	0	55	1	0
2	E	24	0	46	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	20	0	27	5	0
4	B	20	0	27	4	0
4	C	20	0	27	4	0
4	D	20	0	27	5	0
4	E	20	0	27	4	0
5	D	20	0	33	1	0
6	A	4	0	0	0	0
6	B	9	0	0	0	0
6	C	6	0	0	0	0
6	D	7	0	0	0	0
6	E	5	0	0	0	0
All	All	11044	0	11342	233	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 10.

The worst 5 of 233 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:C:31:LEU:O	1:C:34:VAL:HG12	1.49	1.09
1:E:5:ASN:HB2	1:E:157:THR:OG1	1.53	1.07
1:D:196:MET:HE2	1:D:196:MET:HA	1.46	0.98
1:E:289:TYR:O	1:E:290:LEU:HD23	1.73	0.88
1:D:58:ARG:HD2	1:D:246:SER:HB2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	286/327 (88%)	276 (96%)	10 (4%)	0	100	100
1	B	288/327 (88%)	272 (94%)	16 (6%)	0	100	100
1	C	285/327 (87%)	272 (95%)	13 (5%)	0	100	100
1	D	287/327 (88%)	273 (95%)	14 (5%)	0	100	100
1	E	284/327 (87%)	272 (96%)	12 (4%)	0	100	100
All	All	1430/1635 (88%)	1365 (96%)	65 (4%)	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	224/261 (86%)	219 (98%)	5 (2%)	45	60
1	B	224/261 (86%)	220 (98%)	4 (2%)	51	65
1	C	221/261 (85%)	217 (98%)	4 (2%)	51	65
1	D	221/261 (85%)	217 (98%)	4 (2%)	51	65
1	E	224/261 (86%)	218 (97%)	6 (3%)	39	54
All	All	1114/1305 (85%)	1091 (98%)	23 (2%)	47	62

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	61	MET
1	E	5	ASN
1	D	243	LEU
1	E	42	ILE
1	B	61	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	268	HIS
1	E	5	ASN
1	E	268	HIS
1	E	19	HIS
1	C	268	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 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	$\# Z > 2$
5	OLA	D	401	-	19,19,19	0.53	0	19,19,19	0.47	0
4	RET	B	404	1	20,20,21	1.58	3 (15%)	27,27,28	1.00	1 (3%)
2	LFA	A	406	-	6,6,19	0.11	0	5,5,18	0.11	0
2	LFA	A	405	-	9,9,19	0.11	0	8,8,18	0.08	0
2	LFA	A	404	-	6,6,19	0.12	0	5,5,18	0.13	0
3	PO4	A	403	-	4,4,4	0.70	0	6,6,6	0.47	0
3	PO4	E	402	-	4,4,4	0.74	0	6,6,6	0.44	0
2	LFA	B	402	-	11,11,19	0.10	0	10,10,18	0.08	0
2	LFA	C	401	-	5,5,19	0.14	0	4,4,18	0.13	0
2	LFA	A	401	-	10,10,19	0.10	0	9,9,18	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	RET	E	404	1	20,20,21	1.58	3 (15%)	27,27,28	1.01	1 (3%)
4	RET	A	407	1	20,20,21	1.54	3 (15%)	27,27,28	1.03	1 (3%)
2	LFA	D	403	-	9,9,19	0.11	0	8,8,18	0.09	0
2	LFA	D	405	-	7,7,19	0.12	0	6,6,18	0.10	0
3	PO4	D	402	-	4,4,4	0.76	0	6,6,6	0.45	0
2	LFA	B	401	-	10,10,19	0.11	0	9,9,18	0.10	0
2	LFA	D	404	-	10,10,19	0.10	0	9,9,18	0.07	0
4	RET	D	406	1	20,20,21	1.59	3 (15%)	27,27,28	1.00	1 (3%)
2	LFA	E	401	-	10,10,19	0.11	0	9,9,18	0.09	0
4	RET	C	404	1	20,20,21	1.62	3 (15%)	27,27,28	1.01	1 (3%)
2	LFA	E	403	-	12,12,19	0.08	0	11,11,18	0.09	0
2	LFA	C	403	-	5,5,19	0.15	0	4,4,18	0.12	0
3	PO4	C	402	-	4,4,4	0.71	0	6,6,6	0.47	0
3	PO4	B	403	-	4,4,4	0.74	0	6,6,6	0.45	0
2	LFA	A	402	-	6,6,19	0.13	0	5,5,18	0.10	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
5	OLA	D	401	-	-	7/17/17/17	-
4	RET	B	404	1	-	0/13/30/31	0/1/1/1
2	LFA	A	406	-	-	2/4/4/17	-
2	LFA	A	405	-	-	1/7/7/17	-
2	LFA	A	404	-	-	0/4/4/17	-
2	LFA	B	402	-	-	8/9/9/17	-
2	LFA	C	401	-	-	1/3/3/17	-
2	LFA	A	401	-	-	3/8/8/17	-
4	RET	E	404	1	-	0/13/30/31	0/1/1/1
4	RET	A	407	1	-	0/13/30/31	0/1/1/1
2	LFA	D	403	-	-	0/7/7/17	-
2	LFA	D	405	-	-	1/5/5/17	-
2	LFA	B	401	-	-	4/8/8/17	-
2	LFA	D	404	-	-	1/8/8/17	-
4	RET	D	406	1	-	0/13/30/31	0/1/1/1
2	LFA	E	401	-	-	1/8/8/17	-
4	RET	C	404	1	-	0/13/30/31	0/1/1/1
2	LFA	E	403	-	-	2/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	403	-	-	0/3/3/17	-
2	LFA	A	402	-	-	0/4/4/17	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	406	RET	C14-C13	4.46	1.36	1.33
4	C	404	RET	C14-C13	4.44	1.36	1.33
4	B	404	RET	C14-C13	4.42	1.36	1.33
4	E	404	RET	C14-C13	4.40	1.36	1.33
4	A	407	RET	C14-C13	4.03	1.36	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404	RET	C19-C9-C10	-3.37	117.36	122.82
4	A	407	RET	C19-C9-C10	-3.31	117.46	122.82
4	B	404	RET	C19-C9-C10	-3.29	117.48	122.82
4	D	406	RET	C19-C9-C10	-3.27	117.52	122.82
4	C	404	RET	C19-C9-C10	-3.13	117.75	122.82

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	LFA	C5-C6-C7-C8
5	D	401	OLA	C13-C14-C15-C16
2	A	406	LFA	C15-C16-C17-C18
2	B	402	LFA	C7-C8-C9-C10
5	D	401	OLA	C6-C7-C8-C9

There are no ring outliers.

7 monomers are involved in 24 short contacts:

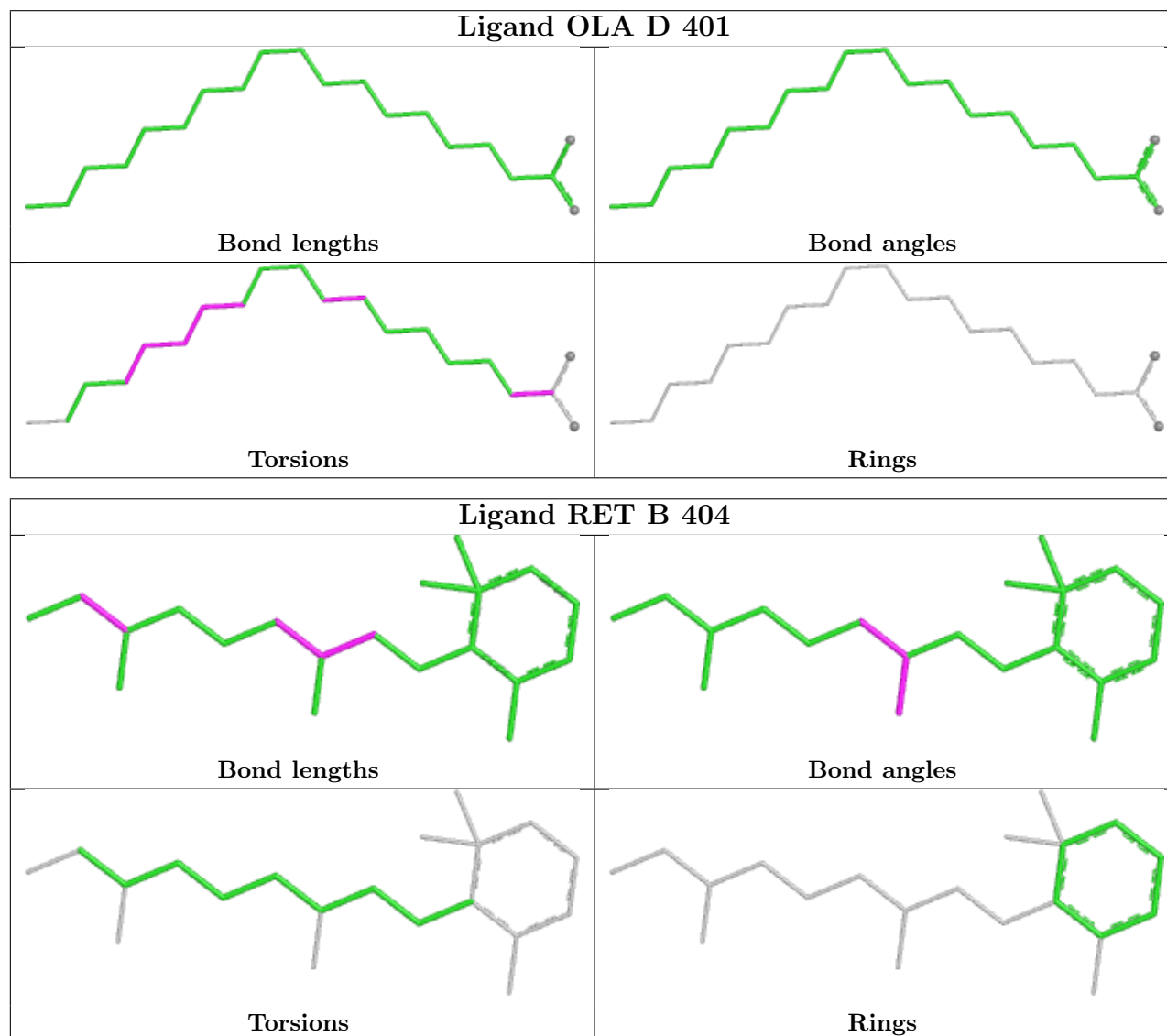
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	OLA	1	0
4	B	404	RET	4	0
4	E	404	RET	4	0
4	A	407	RET	5	0
2	D	405	LFA	1	0
4	D	406	RET	5	0

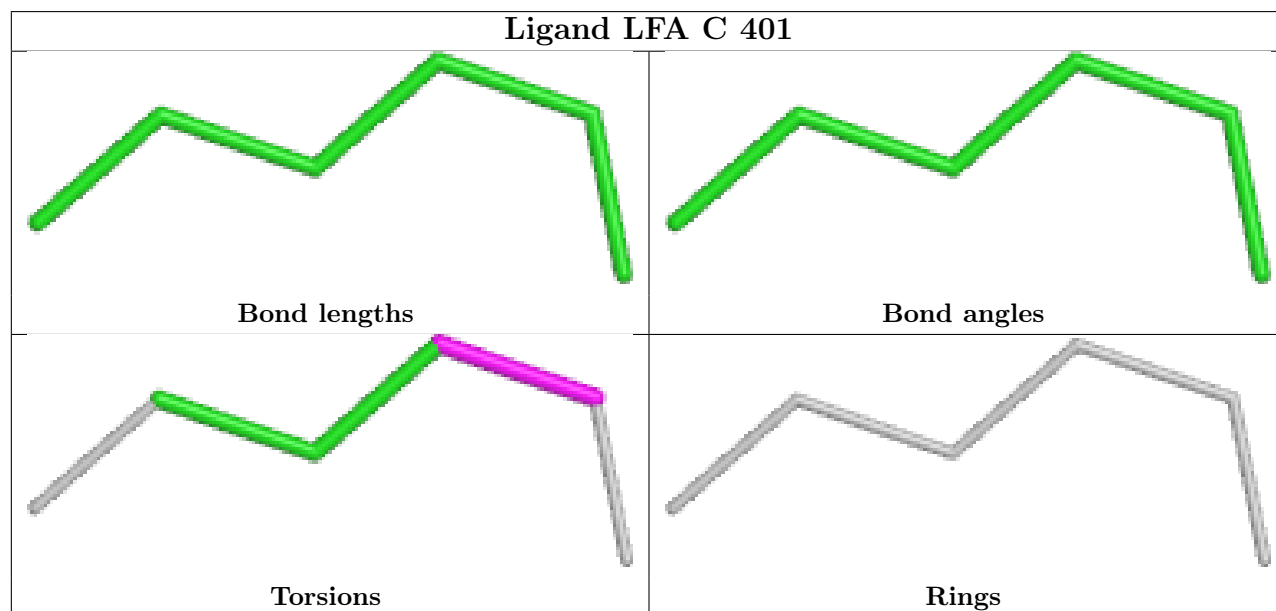
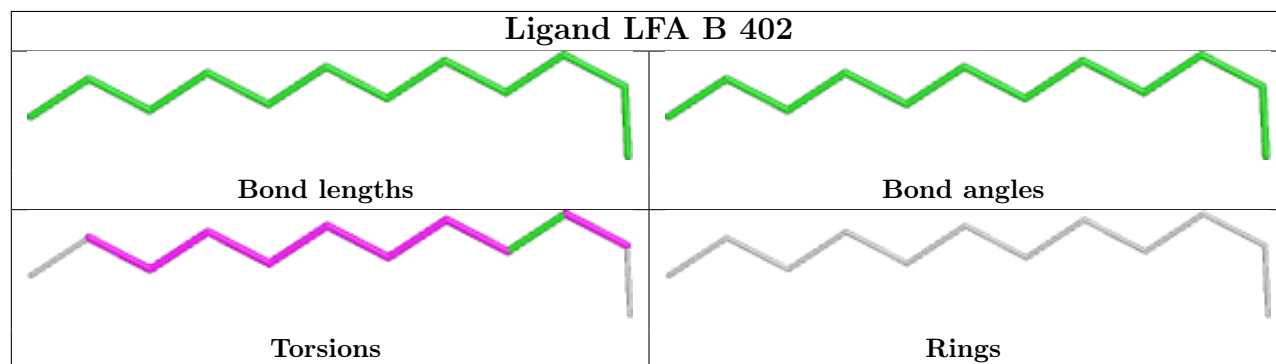
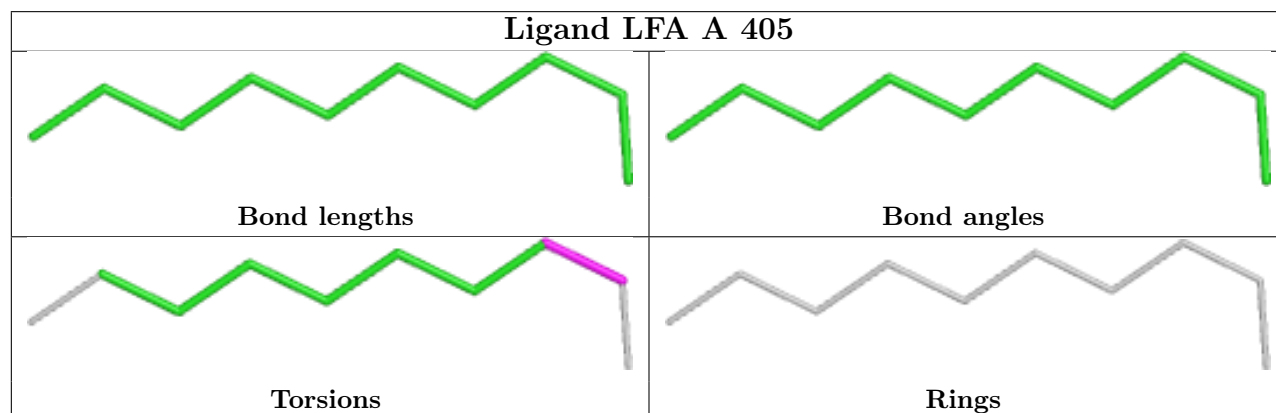
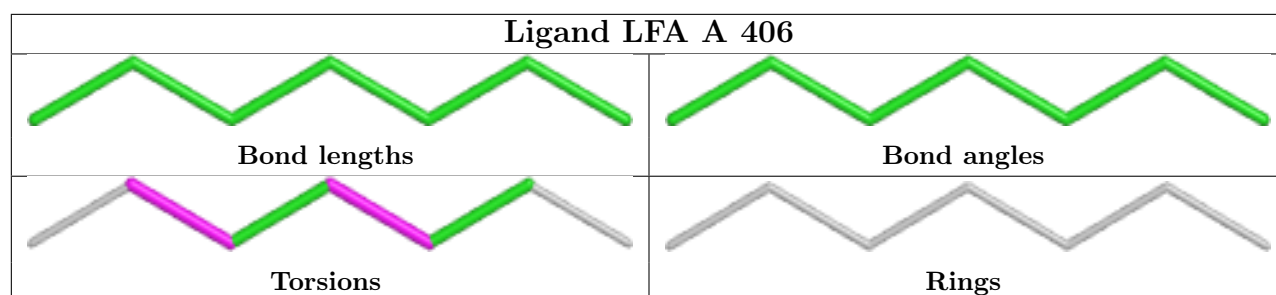
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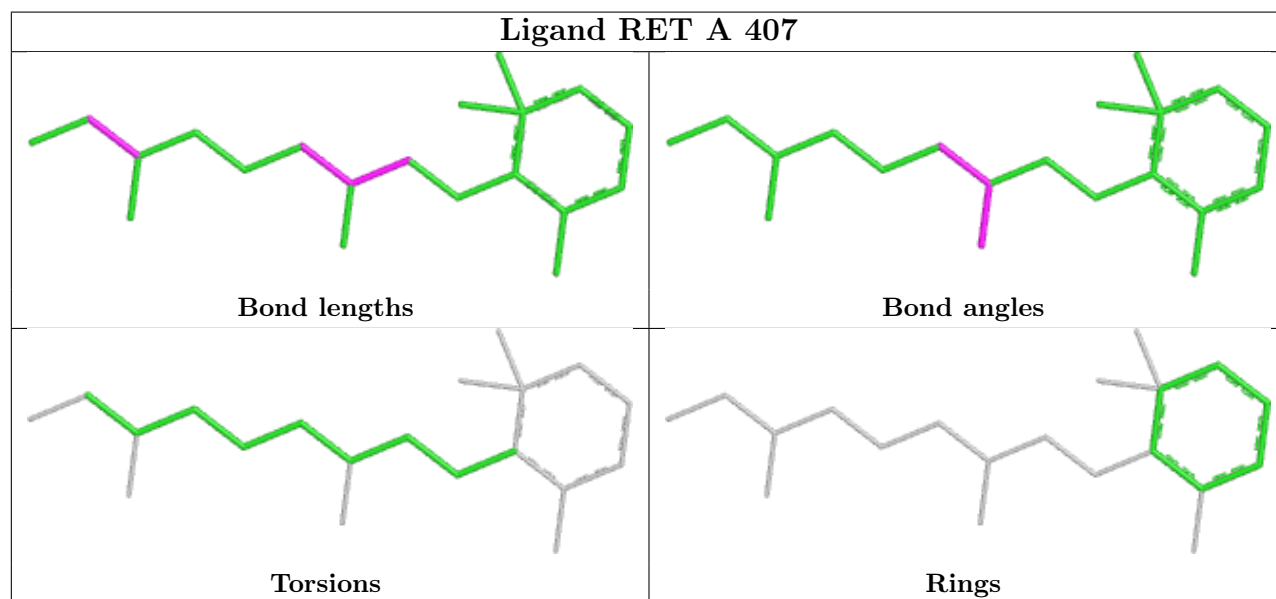
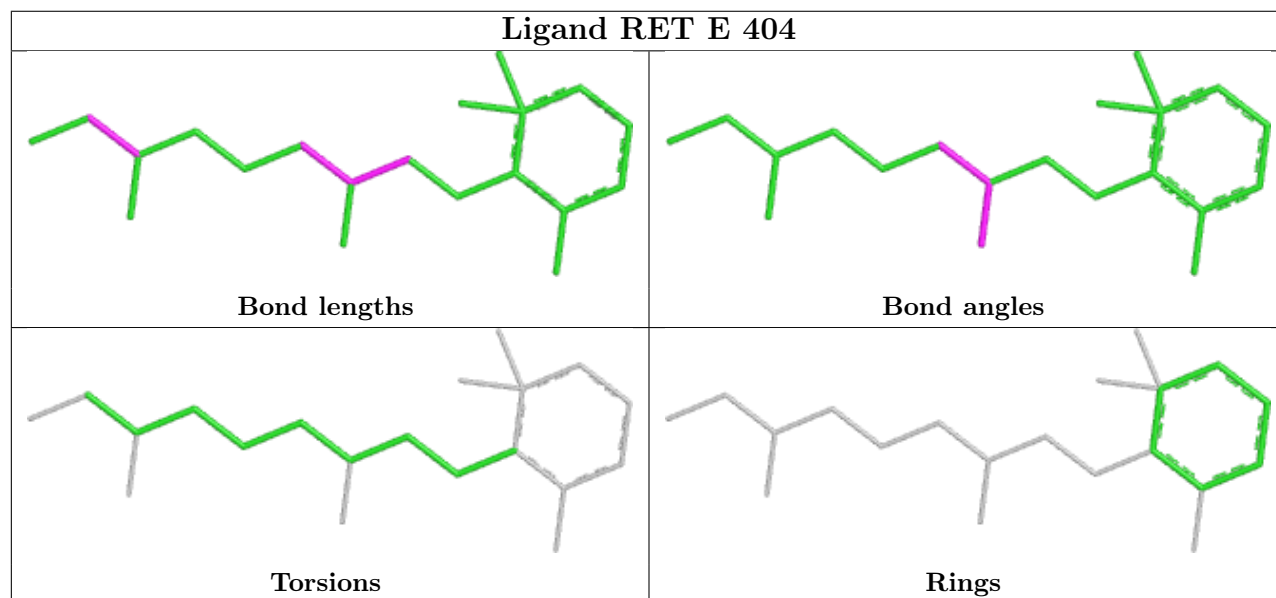
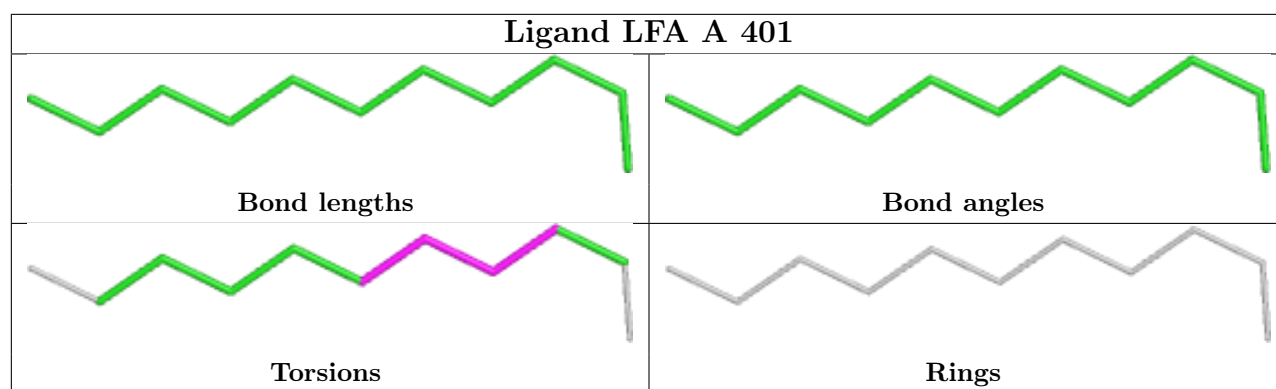
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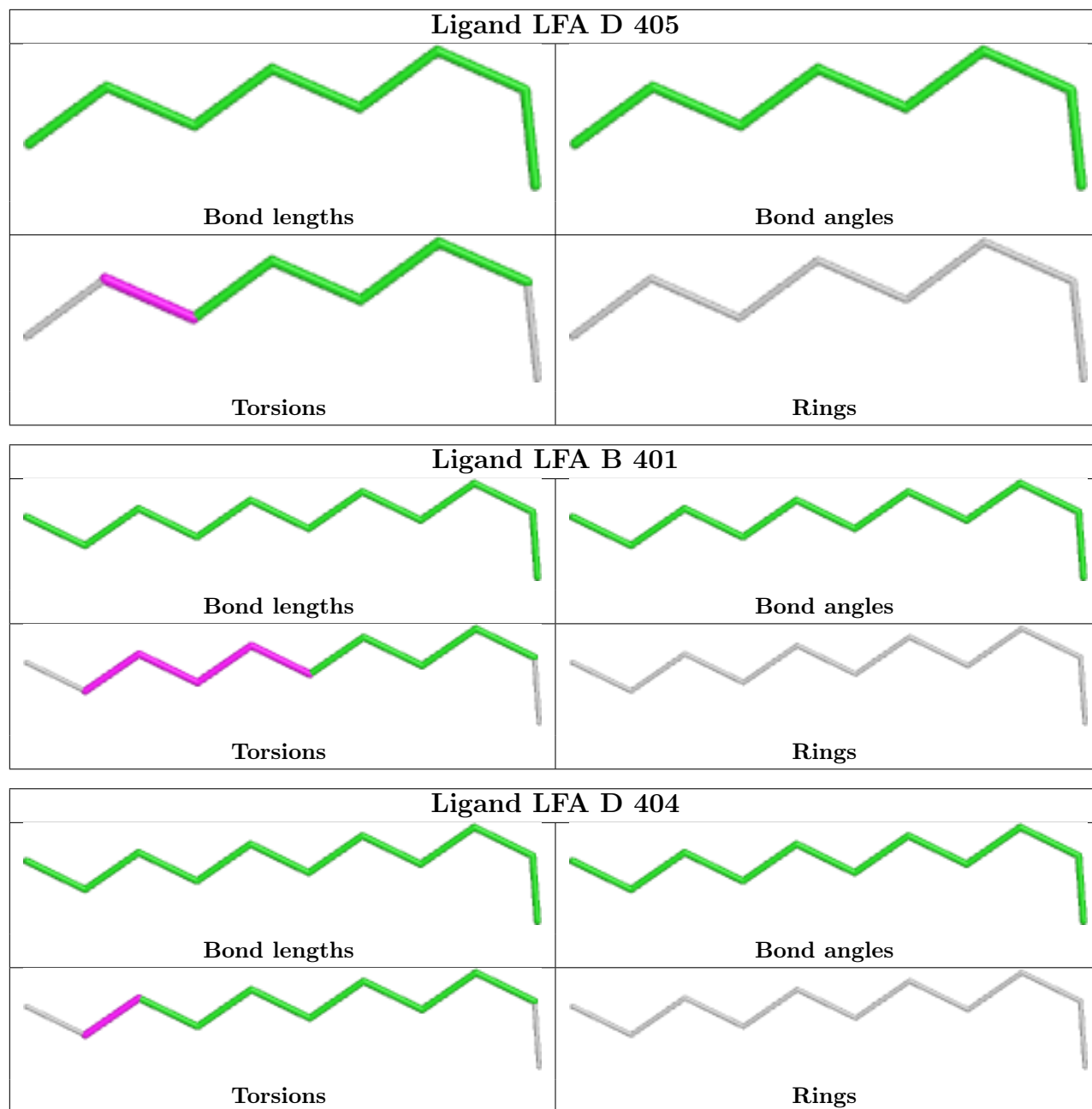
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	RET	4	0

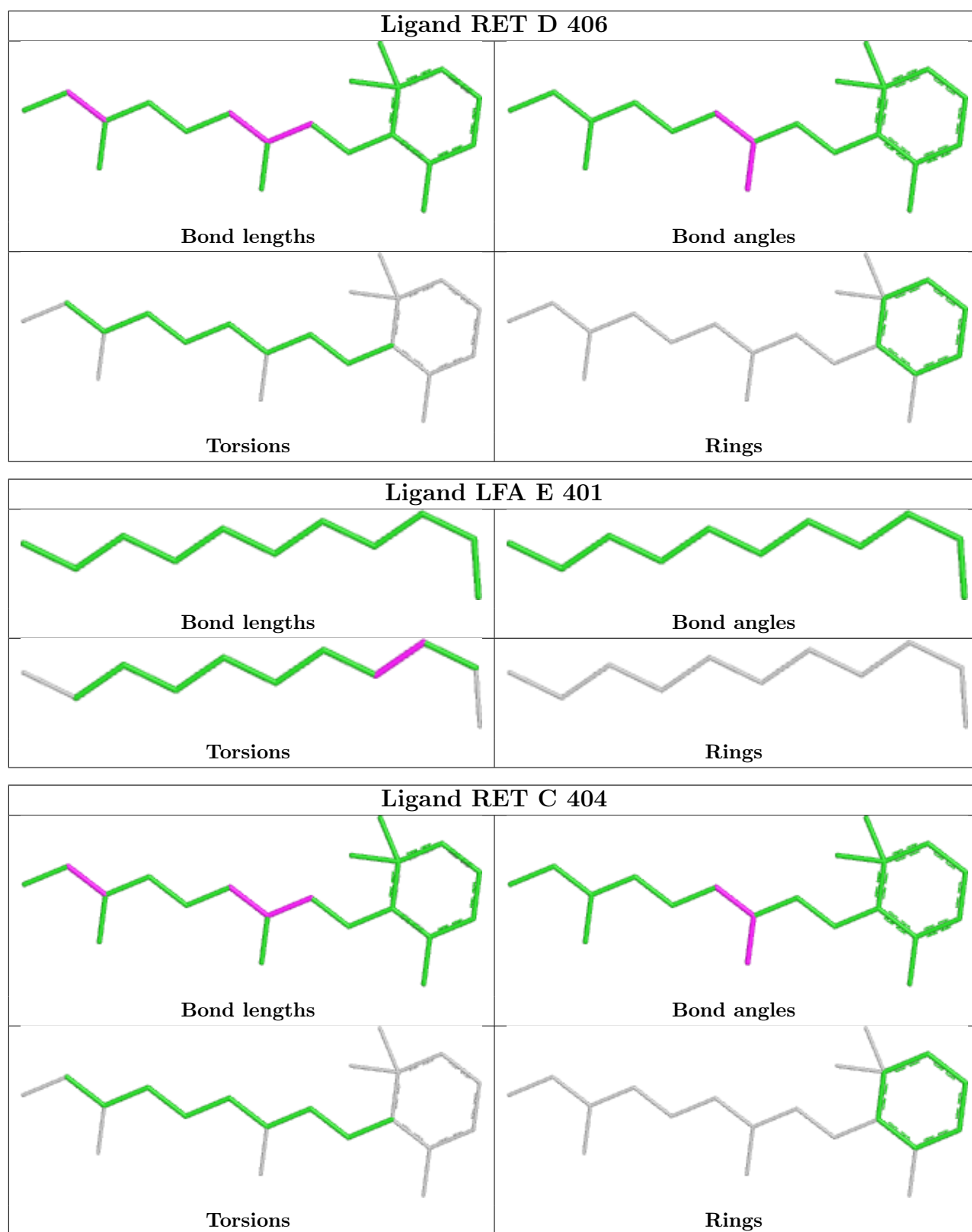
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











Ligand LFA E 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	288/327 (88%)	0.29	10 (3%) 47 47	33, 62, 101, 134	0
1	B	290/327 (88%)	0.16	11 (3%) 44 44	30, 56, 96, 132	0
1	C	287/327 (87%)	0.19	4 (1%) 73 75	37, 60, 98, 119	0
1	D	289/327 (88%)	0.31	8 (2%) 55 56	38, 60, 98, 117	0
1	E	286/327 (87%)	0.28	10 (3%) 47 47	35, 61, 97, 117	0
All	All	1440/1635 (88%)	0.25	43 (2%) 52 53	30, 60, 99, 134	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	5.1
1	E	85	GLY	4.4
1	E	84	ALA	3.6
1	C	4	THR	3.5
1	D	291	ALA	3.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

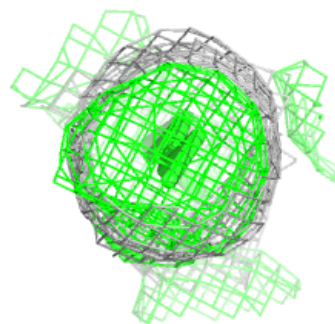
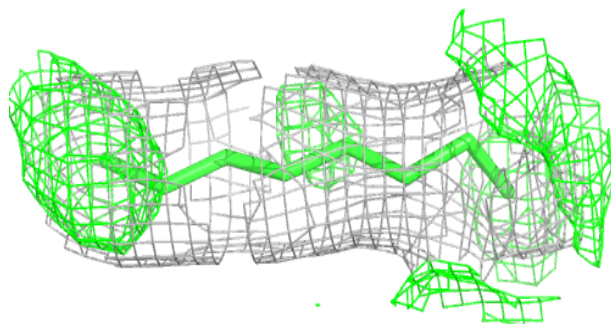
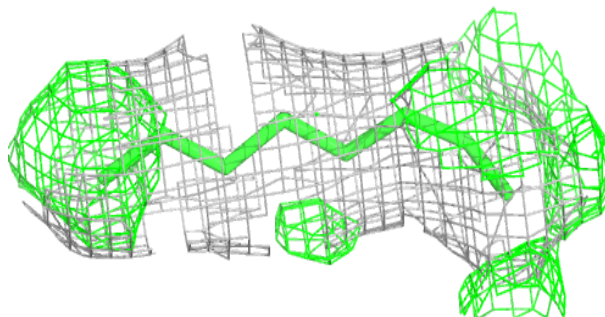
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LFA	D	403	10/20	0.56	0.13	44,85,89,89	0
2	LFA	D	405	8/20	0.56	0.22	44,56,65,66	0
2	LFA	C	403	6/20	0.72	0.10	37,54,60,62	0
2	LFA	D	404	11/20	0.75	0.13	45,75,86,86	0
2	LFA	A	402	7/20	0.78	0.14	40,58,65,68	0
2	LFA	A	406	7/20	0.78	0.12	61,66,73,78	0
3	PO4	C	402	5/5	0.80	0.10	102,106,117,124	0
3	PO4	A	403	5/5	0.82	0.11	88,100,108,114	0
2	LFA	E	401	11/20	0.82	0.12	33,47,52,53	0
2	LFA	E	403	13/20	0.83	0.11	70,79,96,98	0
2	LFA	A	404	7/20	0.83	0.11	34,41,50,52	0
2	LFA	A	405	10/20	0.83	0.13	40,67,69,71	0
3	PO4	E	402	5/5	0.83	0.11	88,91,104,105	0
2	LFA	B	401	11/20	0.84	0.11	34,46,55,56	0
3	PO4	D	402	5/5	0.84	0.10	92,92,99,99	0
2	LFA	A	401	11/20	0.84	0.14	44,70,72,73	0
3	PO4	B	403	5/5	0.85	0.08	90,92,102,103	0
2	LFA	C	401	6/20	0.87	0.12	30,40,55,57	0
5	OLA	D	401	20/20	0.87	0.15	71,78,95,98	0
2	LFA	B	402	12/20	0.88	0.15	44,68,80,81	0
4	RET	E	404	20/21	0.92	0.15	61,72,78,78	0
4	RET	A	407	20/21	0.93	0.15	58,72,86,87	0
4	RET	B	404	20/21	0.94	0.11	50,58,62,65	0
4	RET	D	406	20/21	0.94	0.12	58,63,73,75	0
4	RET	C	404	20/21	0.95	0.11	54,63,67,68	0

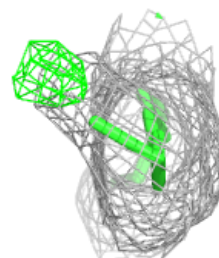
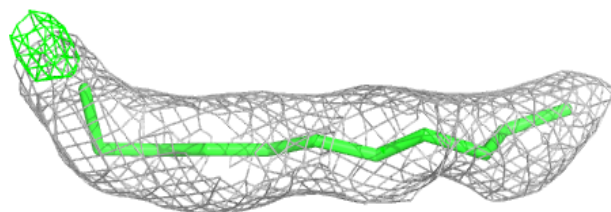
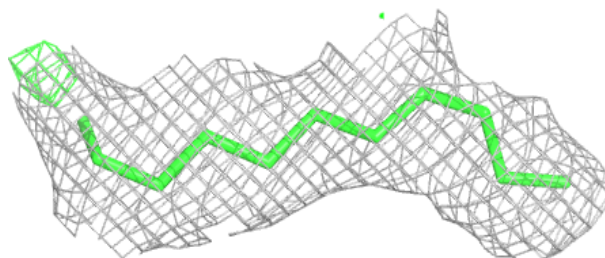
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA D 405:

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

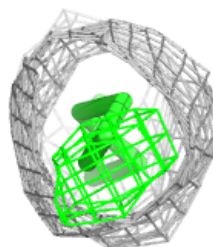
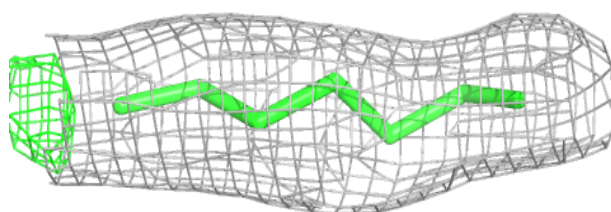
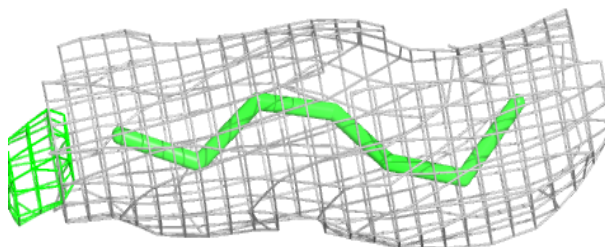
**Electron density around LFA D 404:**

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

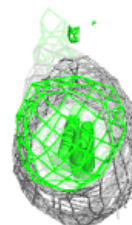
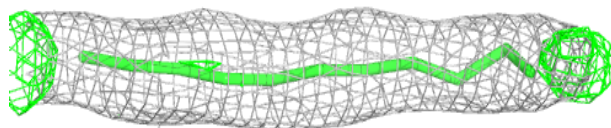
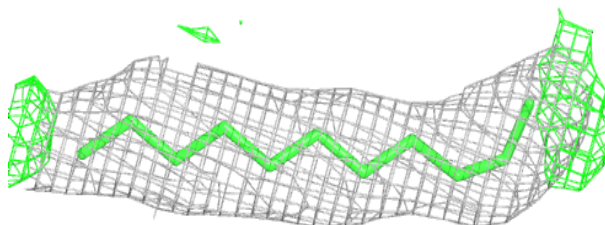


Electron density around LFA A 406:

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

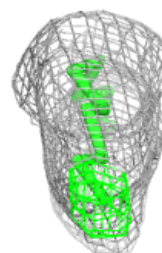
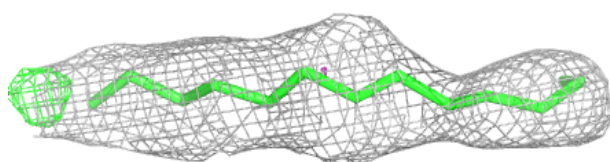
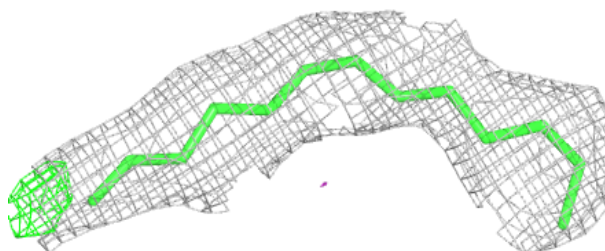
**Electron density around LFA E 401:**

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

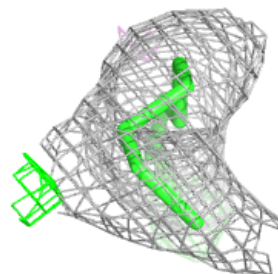
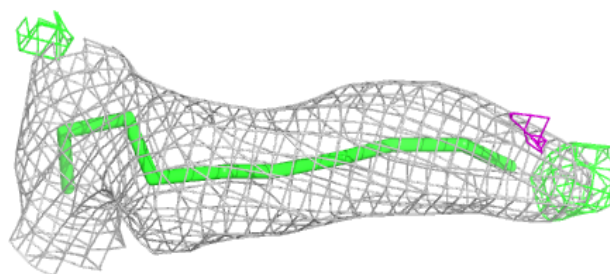
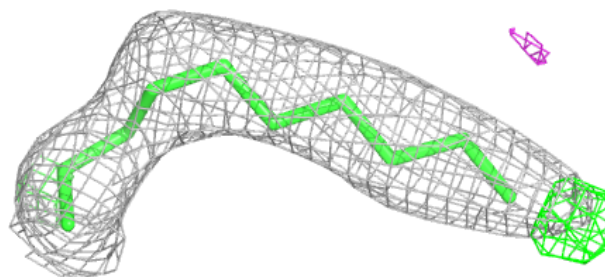


Electron density around LFA E 403:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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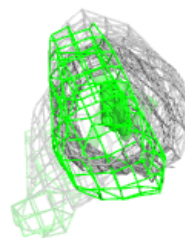
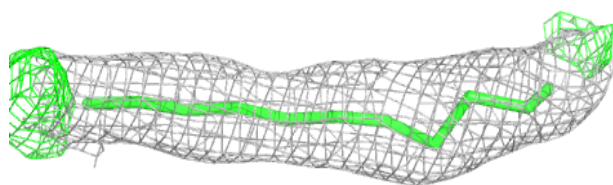
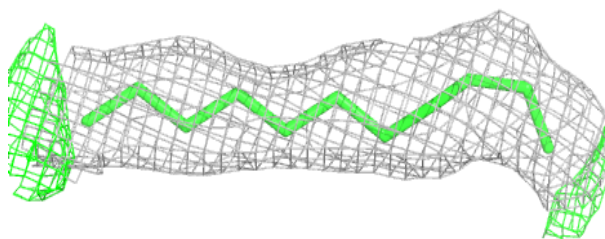
**Electron density around LFA A 405:**

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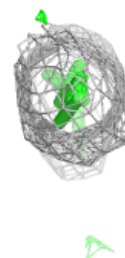
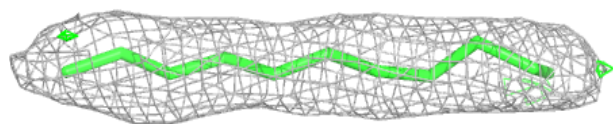
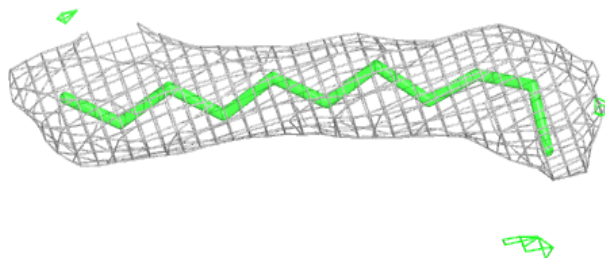


Electron density around LFA B 401:

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and green (positive)

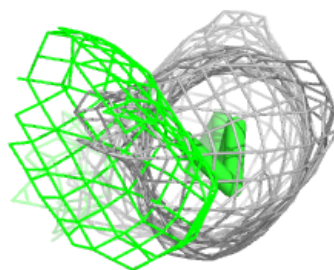
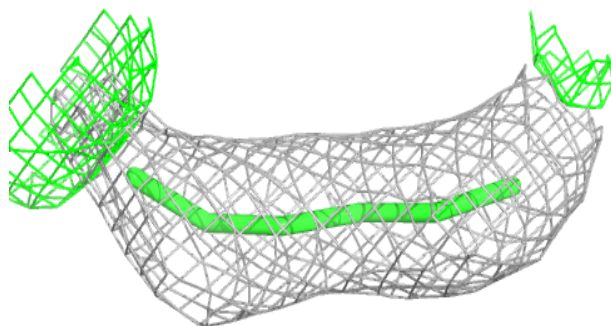
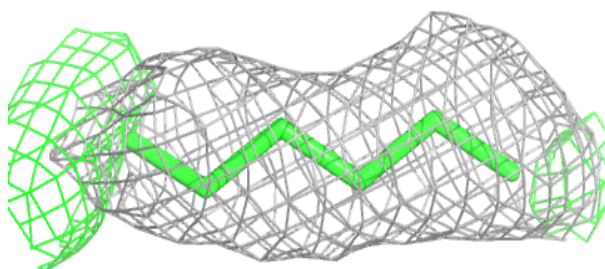
**Electron density around LFA A 401:**

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

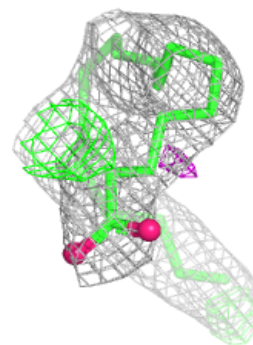
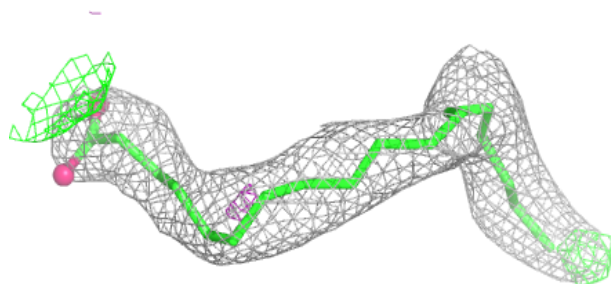
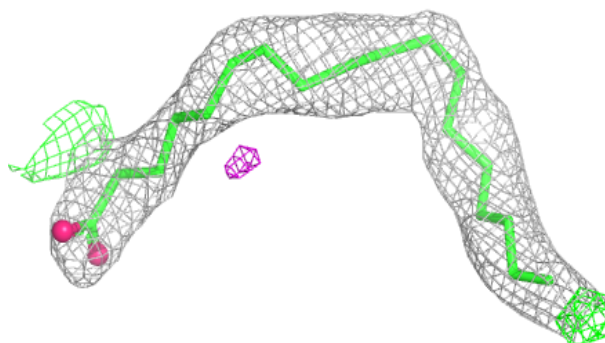


Electron density around LFA C 401:

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and green (positive)

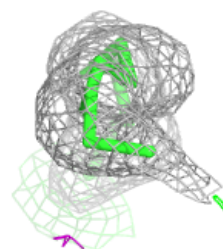
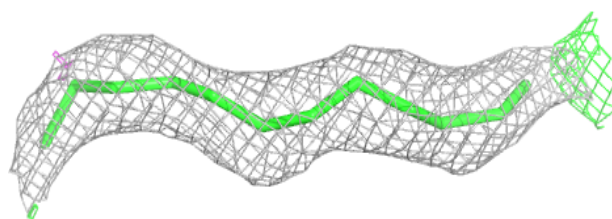
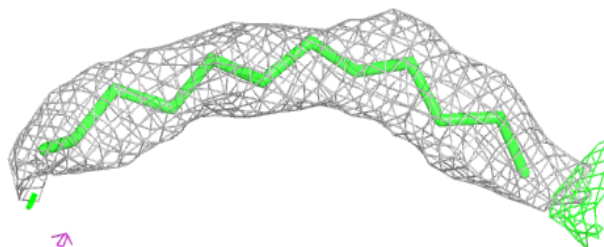
**Electron density around OLA D 401:**

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

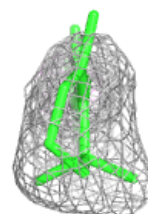
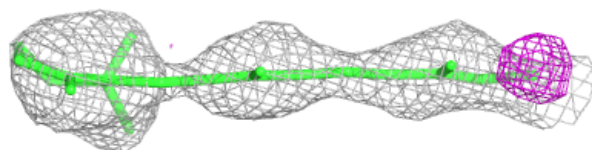
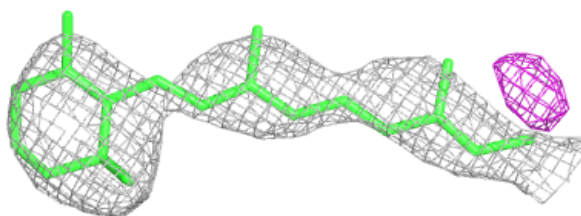


Electron density around LFA B 402:

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

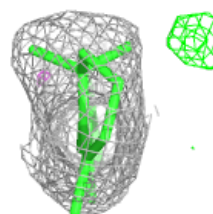
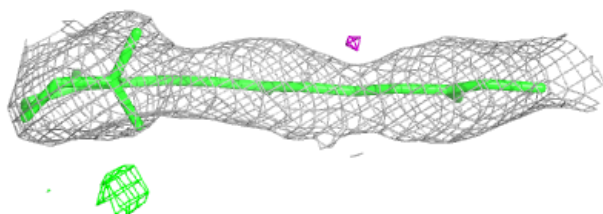
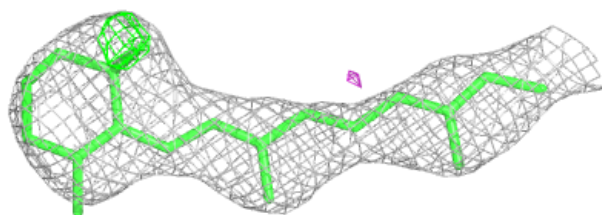
**Electron density around RET E 404:**

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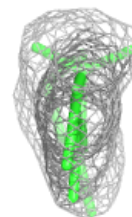
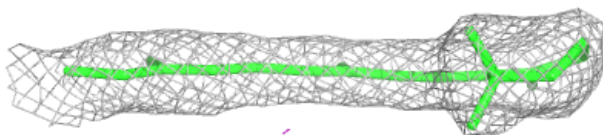
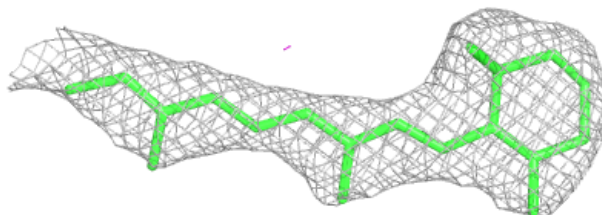


Electron density around RET A 407:

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

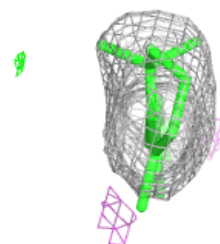
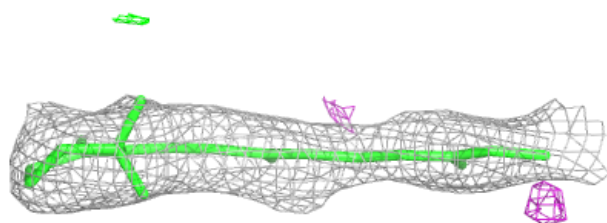
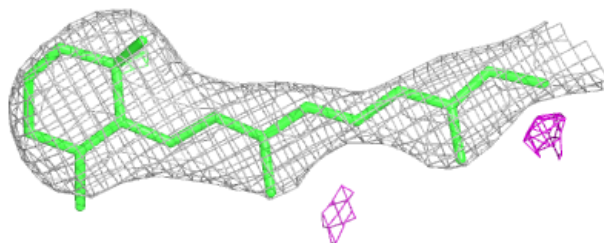
**Electron density around RET B 404:**

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

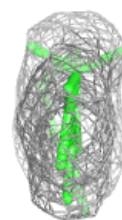
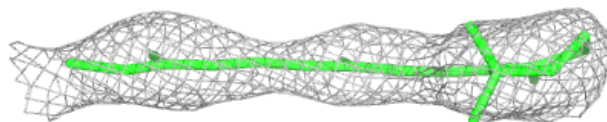
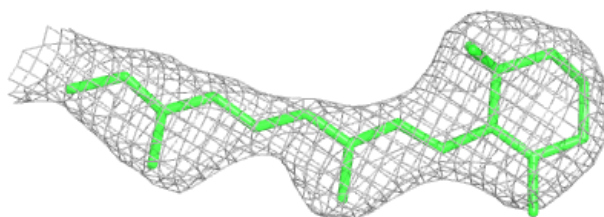


Electron density around RET D 406:

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

**Electron density around RET C 404:**

$2mF_o-DF_c$ (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.