wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2024 – 12:08 am GMT

PDB ID	:	8R98
Title	:	Crystal structure of the cryorhodopsin CryoR2 at pH 4.6, type B crystals, illuminated state
Authors	:	Kovalev, K.; Lamm, G.H.U.; Marin, E.
Deposited on	:	2023-11-30
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

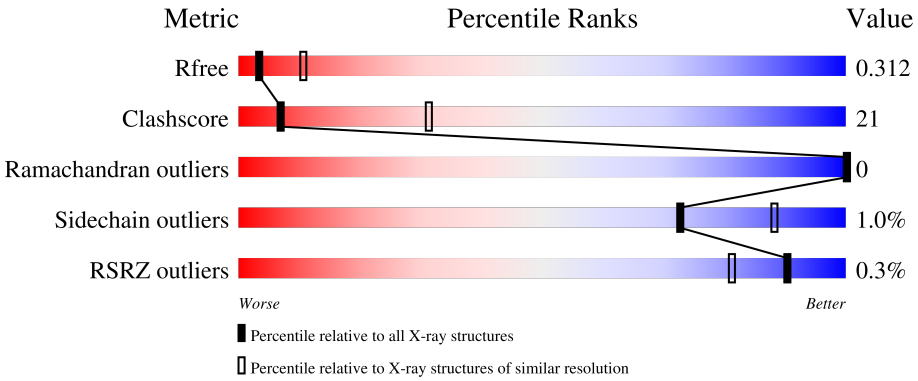
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 <=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	56% 31% 13%
1	B	327	% 57% 31% 12%
1	C	327	52% 35% • 12%
1	D	327	56% 31% 12%
1	E	327	56% 31% 13%

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Mol	Chain	Length	Quality of chain
1	F	327	58% 29% 12%
1	G	327	% 55% 33% 12%
1	H	327	54% 34% 12%
1	I	327	57% 31% 11%
1	K	327	56% 31% 13%

2 Entry composition (i)

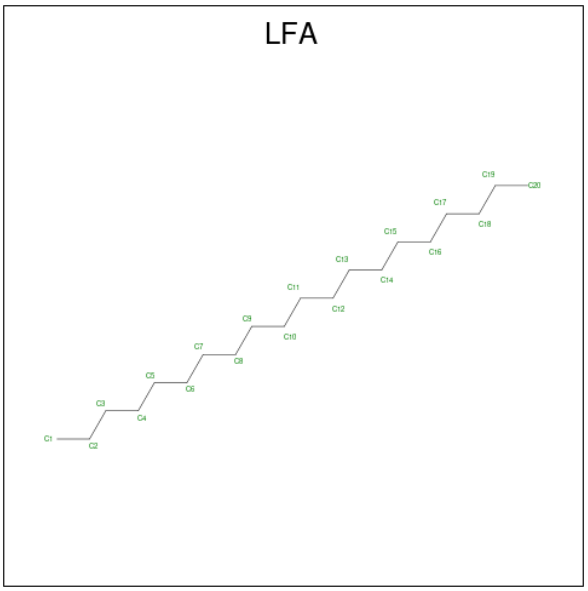
There are 5 unique types of molecules in this entry. The entry contains 21848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CryoR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2118	1393	341	378	6			
1	B	288	Total	C	N	O	S	0	0	0
			2152	1413	349	384	6			
1	C	287	Total	C	N	O	S	0	0	0
			2128	1403	341	378	6			
1	D	288	Total	C	N	O	S	0	0	0
			2134	1404	342	382	6			
1	E	286	Total	C	N	O	S	0	0	0
			2118	1393	339	380	6			
1	H	287	Total	C	N	O	S	0	0	0
			2119	1395	340	378	6			
1	G	288	Total	C	N	O	S	0	0	0
			2149	1412	347	384	6			
1	F	287	Total	C	N	O	S	0	0	0
			2144	1407	348	383	6			
1	I	290	Total	C	N	O	S	0	0	0
			2138	1408	339	385	6			
1	K	286	Total	C	N	O	S	0	0	0
			2122	1395	342	380	5			

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 11 11	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 7 7	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 8 8	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 9 9	0	0
2	E	1	Total C 11 11	0	0
2	E	1	Total C 12 12	0	0

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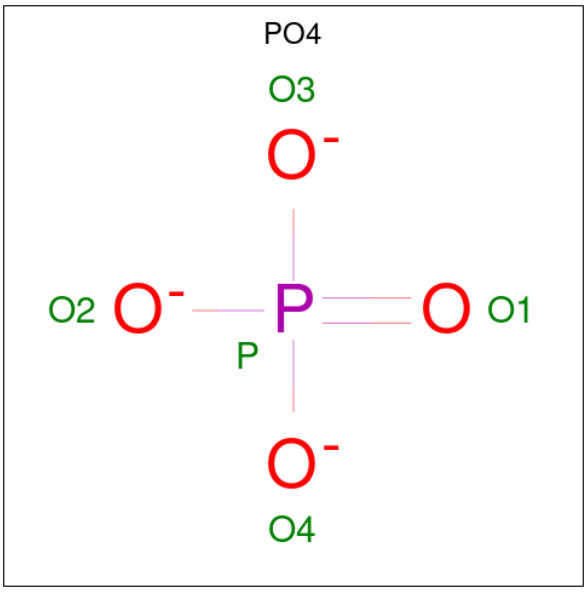
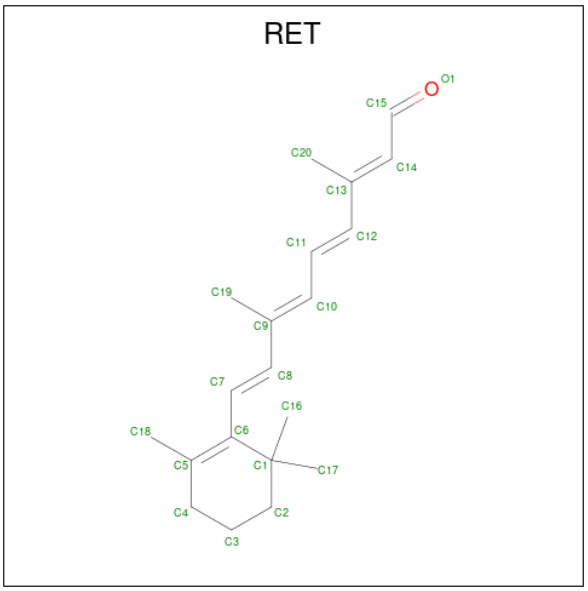
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C 6 6	0	0
2	H	1	Total C 6 6	0	0
2	G	1	Total C 11 11	0	0
2	G	1	Total C 7 7	0	0
2	G	1	Total C 7 7	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 7 7	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 12 12	0	0
2	I	1	Total C 10 10	0	0
2	K	1	Total C 11 11	0	0
2	K	1	Total C 10 10	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



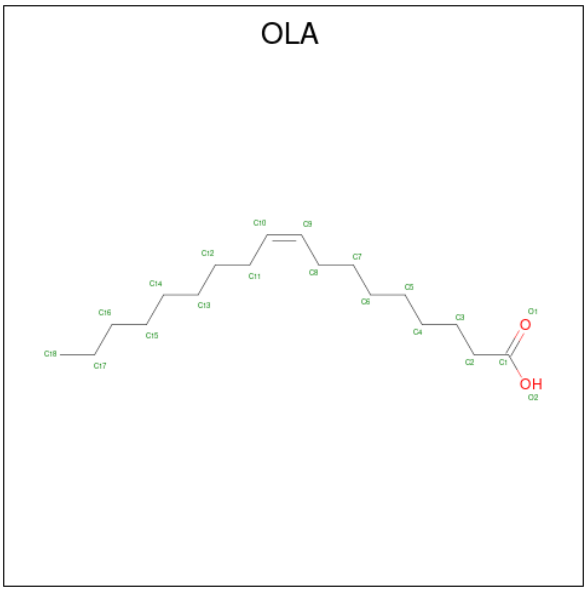
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	K	1	Total O P 5 4 1	0	0

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (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
4	H	1	Total C 20 20	0	0
4	G	1	Total C 20 20	0	0
4	F	1	Total C 20 20	0	0
4	I	1	Total C 20 20	0	0
4	K	1	Total C 20 20	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



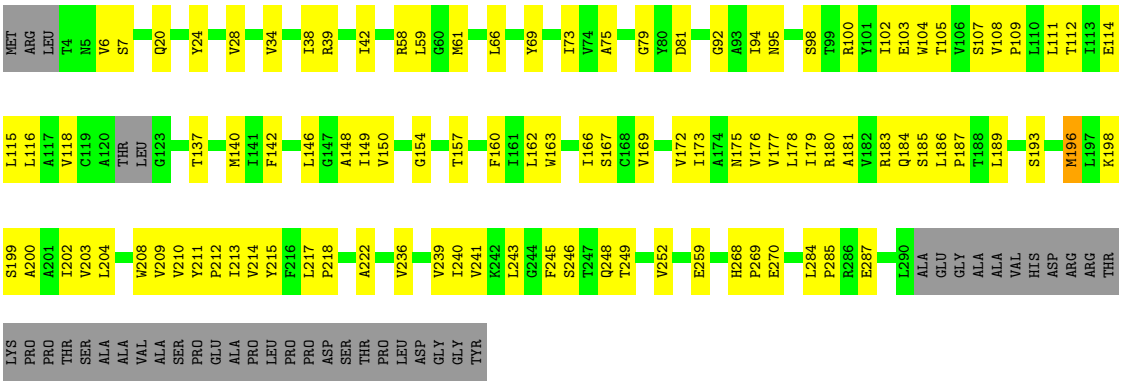
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C 11 11	0	0
5	I	1	Total C 12 12	0	0

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.

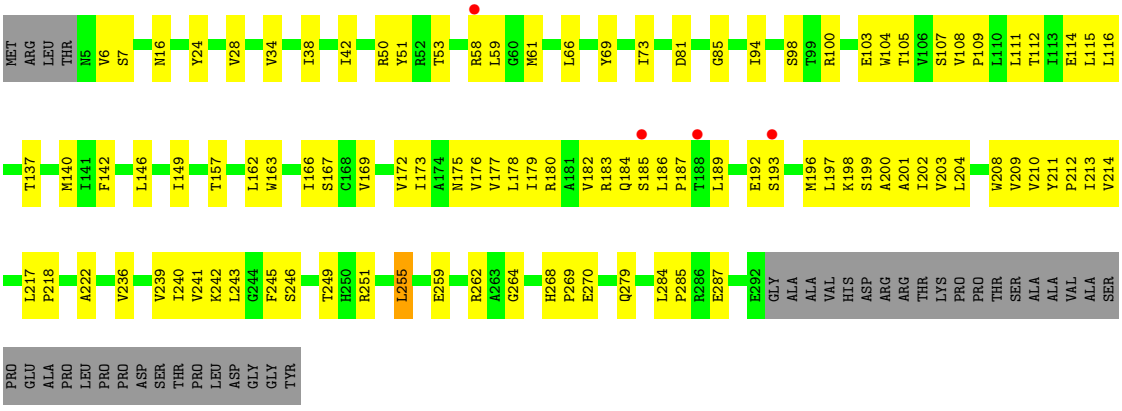
• Molecule 1: cryorhodopsin CryoR2

Chain A:



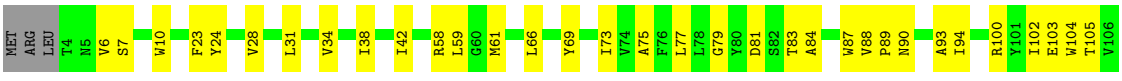
• Molecule 1: cryorhodopsin CryoR2

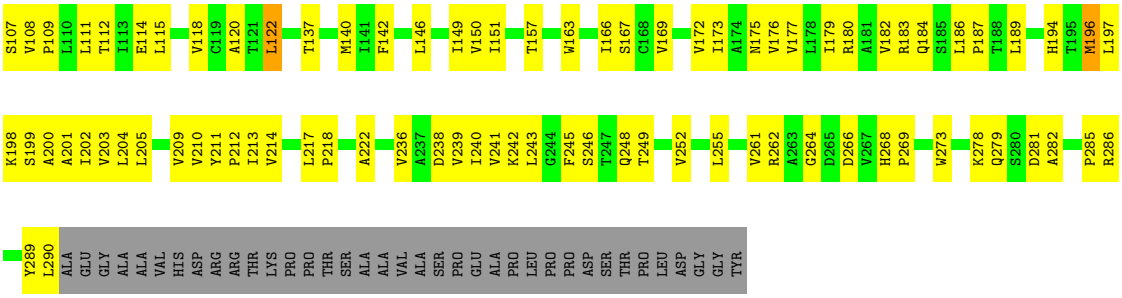
Chain B:



• Molecule 1: cryorhodopsin CryoR2

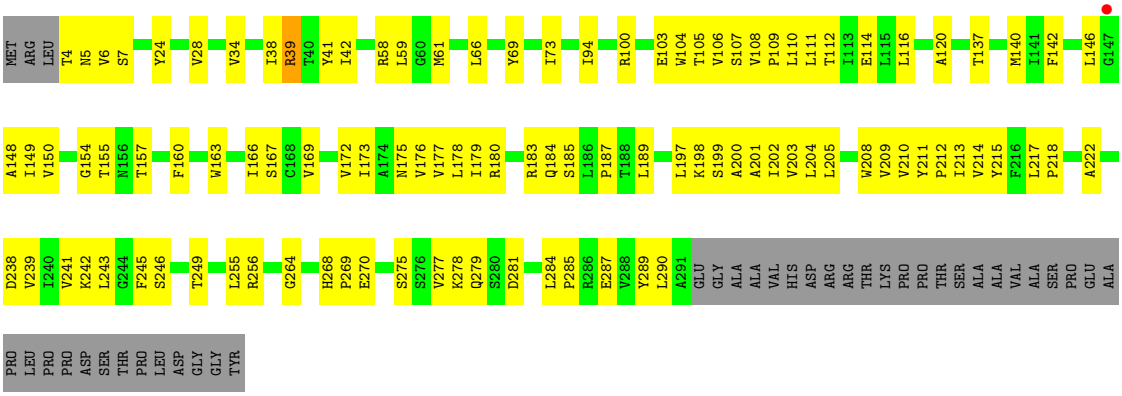
Chain C:





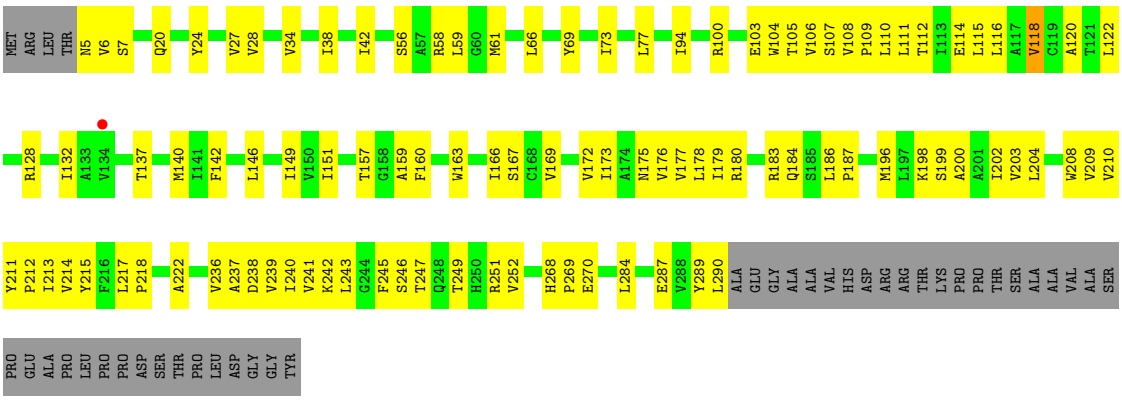
• Molecule 1: cryorhodopsin CryoR2

Chain D:



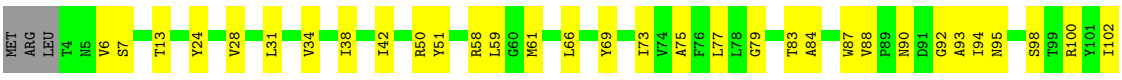
• Molecule 1: cryorhodopsin CryoR2

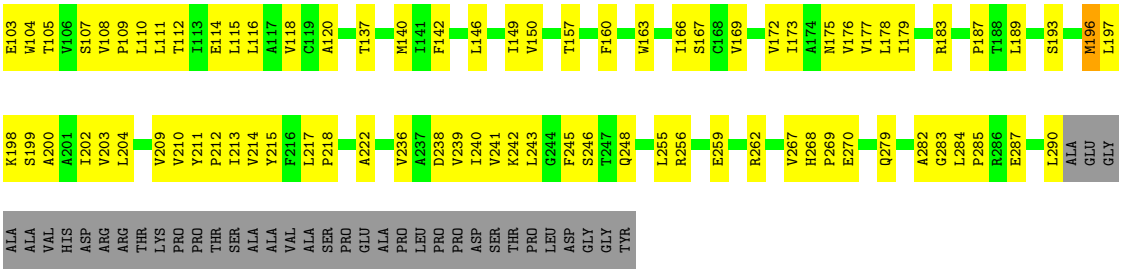
Chain E:



• Molecule 1: cryorhodopsin CryoR2

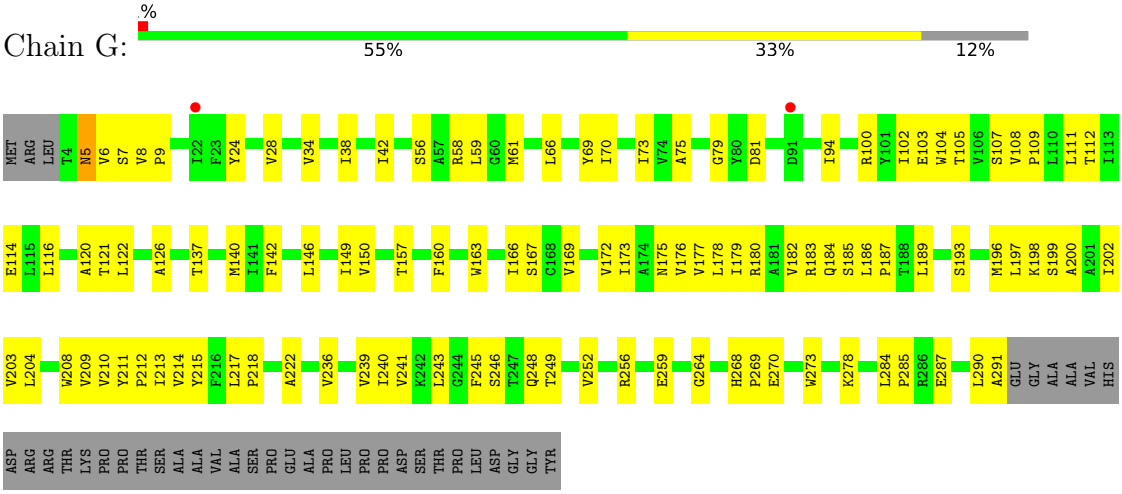
Chain H:





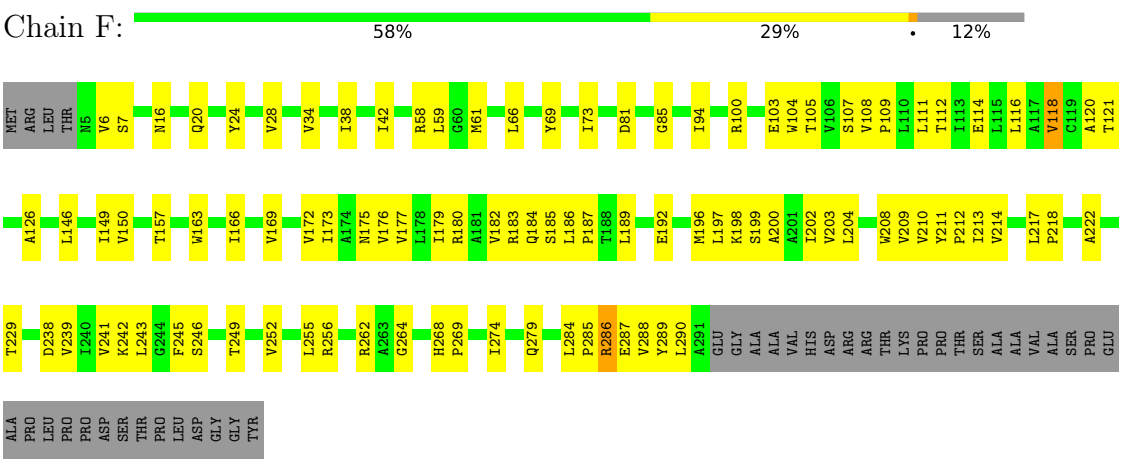
• Molecule 1: cryorhodopsin CryoR2

Chain G:



• Molecule 1: cryorhodopsin CryoR2

Chain F:



• Molecule 1: cryorhodopsin CryoR2

Chain I:

• Molecule 1: cryorhodopsin CryoR2

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.11Å 84.96Å 296.94Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.2 (20.00-3.00) 77.2 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.287 , 0.309 0.290 , 0.312	Depositor DCC
R_{free} test set	3642 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	91.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21848	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9541e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LFA, RET, OLA, PO4

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	0.68	0/2165	0.66	0/2973
1	B	0.67	0/2200	0.67	0/3022
1	C	0.67	0/2176	0.65	0/2991
1	D	0.67	0/2182	0.66	0/3000
1	E	0.67	0/2165	0.66	0/2976
1	F	0.67	0/2192	0.66	0/3011
1	G	0.68	0/2197	0.65	0/3018
1	H	0.67	0/2166	0.66	0/2977
1	I	0.68	0/2185	0.66	0/3004
1	K	0.67	0/2169	0.67	0/2982
All	All	0.67	0/21797	0.66	0/29954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2118	0	2143	93	0
1	B	2152	0	2192	93	0
1	C	2128	0	2161	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2134	0	2162	91	0
1	E	2118	0	2142	94	0
1	F	2144	0	2181	84	0
1	G	2149	0	2187	105	0
1	H	2119	0	2145	97	0
1	I	2138	0	2164	99	0
1	K	2122	0	2151	93	0
2	A	35	0	66	1	0
2	B	38	0	72	1	0
2	C	12	0	22	0	0
2	D	19	0	33	0	0
2	E	23	0	44	1	0
2	F	31	0	59	3	0
2	G	52	0	95	1	0
2	H	12	0	22	0	0
2	I	10	0	19	0	0
2	K	21	0	37	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	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	K	5	0	0	0	0
4	A	20	0	27	4	0
4	B	20	0	27	5	0
4	C	20	0	27	6	0
4	D	20	0	27	6	0
4	E	20	0	27	4	0
4	F	20	0	27	4	0
4	G	20	0	27	6	0
4	H	20	0	27	4	0
4	I	20	0	27	6	0
4	K	20	0	27	6	0
5	D	11	0	19	0	0
5	I	12	0	21	0	0
All	All	21848	0	22407	922	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 21.

The worst 5 of 922 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	1.46	1.14
1:H:31:LEU:O	1:H:34:VAL:HG12	1.46	1.10
1:C:94:ILE:HD11	1:C:149:ILE:HG23	1.44	0.99
1:D:39:ARG:HG2	1:E:56:SER:HB2	1.56	0.87
1:E:247:THR:HG22	1:E:251:ARG:HD2	1.59	0.85

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	281/327 (86%)	273 (97%)	8 (3%)	0	100	100
1	B	286/327 (88%)	277 (97%)	9 (3%)	0	100	100
1	C	285/327 (87%)	277 (97%)	8 (3%)	0	100	100
1	D	286/327 (88%)	278 (97%)	8 (3%)	0	100	100
1	E	284/327 (87%)	275 (97%)	9 (3%)	0	100	100
1	F	285/327 (87%)	276 (97%)	9 (3%)	0	100	100
1	G	286/327 (88%)	278 (97%)	8 (3%)	0	100	100
1	H	285/327 (87%)	275 (96%)	10 (4%)	0	100	100
1	I	288/327 (88%)	277 (96%)	11 (4%)	0	100	100
1	K	284/327 (87%)	277 (98%)	7 (2%)	0	100	100
All	All	2850/3270 (87%)	2763 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	218/261 (84%)	216 (99%)	2 (1%)	75 89
1	B	224/261 (86%)	221 (99%)	3 (1%)	65 85
1	C	219/261 (84%)	216 (99%)	3 (1%)	62 83
1	D	220/261 (84%)	218 (99%)	2 (1%)	75 89
1	E	218/261 (84%)	217 (100%)	1 (0%)	86 94
1	F	223/261 (85%)	220 (99%)	3 (1%)	65 85
1	G	223/261 (85%)	221 (99%)	2 (1%)	75 89
1	H	217/261 (83%)	215 (99%)	2 (1%)	75 89
1	I	219/261 (84%)	216 (99%)	3 (1%)	62 83
1	K	219/261 (84%)	219 (100%)	0	100 100
All	All	2200/2610 (84%)	2179 (99%)	21 (1%)	73 88

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	81	ASP
1	F	286	ARG
1	I	255	LEU
1	I	118	VAL
1	F	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	5	ASN
1	G	250	HIS
1	G	184	GLN
1	F	20	GLN
1	C	250	HIS

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)

50 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	LFA	F	402	-	10,10,19	0.10	0	9,9,18	0.07	0
3	PO4	H	403	-	4,4,4	0.65	0	6,6,6	0.43	0
2	LFA	I	402	-	9,9,19	0.09	0	8,8,18	0.07	0
2	LFA	H	402	-	5,5,19	0.14	0	4,4,18	0.10	0
2	LFA	C	402	-	5,5,19	0.13	0	4,4,18	0.10	0
3	PO4	F	404	-	4,4,4	0.67	0	6,6,6	0.43	0
2	LFA	D	402	-	9,9,19	0.09	0	8,8,18	0.08	0
4	RET	F	405	1	20,20,21	1.69	3 (15%)	27,27,28	1.10	2 (7%)
2	LFA	A	401	-	10,10,19	0.09	0	9,9,18	0.08	0
3	PO4	E	403	-	4,4,4	0.66	0	6,6,6	0.43	0
4	RET	G	408	1	20,20,21	1.64	3 (15%)	27,27,28	1.04	1 (3%)
5	OLA	I	401	-	11,11,19	0.18	0	9,10,19	0.12	0
2	LFA	B	402	-	10,10,19	0.10	0	9,9,18	0.07	0
2	LFA	K	401	-	10,10,19	0.09	0	9,9,18	0.06	0
2	LFA	G	404	-	9,9,19	0.09	0	8,8,18	0.08	0
2	LFA	C	401	-	5,5,19	0.13	0	4,4,18	0.09	0
4	RET	D	405	1	20,20,21	1.64	3 (15%)	27,27,28	1.04	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	B	405	-	4,4,4	0.65	0	6,6,6	0.43	0
2	LFA	A	403	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	A	404	-	6,6,19	0.12	0	5,5,18	0.09	0
2	LFA	B	401	-	6,6,19	0.14	0	5,5,18	0.08	0
3	PO4	D	404	-	4,4,4	0.65	0	6,6,6	0.44	0
2	LFA	G	405	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	E	402	-	11,11,19	0.09	0	10,10,18	0.07	0
4	RET	B	406	1	20,20,21	1.59	4 (20%)	27,27,28	1.10	2 (7%)
4	RET	C	404	1	20,20,21	1.66	3 (15%)	27,27,28	1.08	2 (7%)
2	LFA	B	403	-	11,11,19	0.08	0	10,10,18	0.06	0
3	PO4	K	403	-	4,4,4	0.65	0	6,6,6	0.42	0
2	LFA	F	401	-	7,7,19	0.12	0	6,6,18	0.08	0
3	PO4	I	403	-	4,4,4	0.67	0	6,6,6	0.42	0
4	RET	E	404	1	20,20,21	1.69	3 (15%)	27,27,28	1.10	2 (7%)
4	RET	H	404	1	20,20,21	1.66	3 (15%)	27,27,28	1.10	2 (7%)
2	LFA	G	406	-	6,6,19	0.12	0	5,5,18	0.08	0
2	LFA	K	402	-	9,9,19	0.08	0	8,8,18	0.09	0
4	RET	K	404	1	20,20,21	1.71	3 (15%)	27,27,28	1.08	2 (7%)
2	LFA	G	402	-	6,6,19	0.13	0	5,5,18	0.07	0
2	LFA	D	403	-	8,8,19	0.09	0	7,7,18	0.09	0
2	LFA	H	401	-	5,5,19	0.14	0	4,4,18	0.11	0
5	OLA	D	401	-	10,10,19	0.20	0	9,9,19	0.25	0
2	LFA	A	402	-	6,6,19	0.13	0	5,5,18	0.13	0
3	PO4	G	407	-	4,4,4	0.66	0	6,6,6	0.43	0
2	LFA	B	404	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	F	403	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	E	401	-	10,10,19	0.10	0	9,9,18	0.06	0
2	LFA	G	403	-	6,6,19	0.12	0	5,5,18	0.10	0
4	RET	A	406	1	20,20,21	1.67	3 (15%)	27,27,28	1.03	1 (3%)
3	PO4	A	405	-	4,4,4	0.66	0	6,6,6	0.43	0
4	RET	I	404	1	20,20,21	1.61	3 (15%)	27,27,28	1.03	2 (7%)
3	PO4	C	403	-	4,4,4	0.65	0	6,6,6	0.43	0
2	LFA	G	401	-	10,10,19	0.09	0	9,9,18	0.07	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
2	LFA	F	402	-	-	3/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	I	402	-	-	0/7/7/17	-
2	LFA	H	402	-	-	0/3/3/17	-
2	LFA	C	402	-	-	0/3/3/17	-
2	LFA	D	402	-	-	0/7/7/17	-
4	RET	F	405	1	-	0/13/30/31	0/1/1/1
2	LFA	A	401	-	-	3/8/8/17	-
4	RET	G	408	1	-	0/13/30/31	0/1/1/1
5	OLA	I	401	-	-	1/9/9/17	-
2	LFA	B	402	-	-	4/8/8/17	-
2	LFA	K	401	-	-	0/8/8/17	-
2	LFA	G	404	-	-	1/7/7/17	-
2	LFA	C	401	-	-	1/3/3/17	-
4	RET	D	405	1	-	0/13/30/31	0/1/1/1
2	LFA	A	403	-	-	1/7/7/17	-
2	LFA	A	404	-	-	3/4/4/17	-
2	LFA	B	401	-	-	0/4/4/17	-
2	LFA	G	405	-	-	0/7/7/17	-
2	LFA	E	402	-	-	1/9/9/17	-
4	RET	B	406	1	-	0/13/30/31	0/1/1/1
4	RET	C	404	1	-	0/13/30/31	0/1/1/1
2	LFA	B	403	-	-	2/9/9/17	-
2	LFA	F	401	-	-	1/5/5/17	-
4	RET	E	404	1	-	0/13/30/31	0/1/1/1
4	RET	H	404	1	-	0/13/30/31	0/1/1/1
2	LFA	G	406	-	-	0/4/4/17	-
2	LFA	K	402	-	-	0/7/7/17	-
4	RET	K	404	1	-	0/13/30/31	0/1/1/1
2	LFA	G	402	-	-	0/4/4/17	-
2	LFA	D	403	-	-	0/6/6/17	-
2	LFA	H	401	-	-	1/3/3/17	-
5	OLA	D	401	-	-	0/8/8/17	-
2	LFA	A	402	-	-	0/4/4/17	-
2	LFA	B	404	-	-	1/5/5/17	-
2	LFA	F	403	-	-	8/9/9/17	-
2	LFA	E	401	-	-	1/8/8/17	-
2	LFA	G	403	-	-	1/4/4/17	-
4	RET	A	406	1	-	0/13/30/31	0/1/1/1
4	RET	I	404	1	-	0/13/30/31	0/1/1/1
2	LFA	G	401	-	-	3/8/8/17	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	404	RET	C14-C13	4.39	1.37	1.33
4	G	408	RET	C10-C9	4.20	1.41	1.35
4	C	404	RET	C10-C9	4.19	1.41	1.35
4	I	404	RET	C10-C9	4.18	1.41	1.35
4	E	404	RET	C10-C9	4.15	1.41	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	406	RET	C19-C9-C10	-4.11	117.16	122.92
4	E	404	RET	C19-C9-C10	-4.09	117.19	122.92
4	F	405	RET	C19-C9-C10	-4.02	117.30	122.92
4	K	404	RET	C19-C9-C10	-4.01	117.31	122.92
4	H	404	RET	C19-C9-C10	-3.98	117.35	122.92

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	402	LFA	C6-C7-C8-C9
2	A	404	LFA	C15-C16-C17-C18
2	B	402	LFA	C6-C7-C8-C9
2	F	402	LFA	C7-C8-C9-C10
2	F	403	LFA	C6-C7-C8-C9

There are no ring outliers.

19 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	402	LFA	1	0
4	F	405	RET	4	0
4	G	408	RET	6	0
2	G	404	LFA	1	0
4	D	405	RET	6	0
2	A	404	LFA	1	0
3	D	404	PO4	1	0
2	E	402	LFA	1	0
4	B	406	RET	5	0
4	C	404	RET	6	0
2	F	401	LFA	1	0
4	E	404	RET	4	0
4	H	404	RET	4	0

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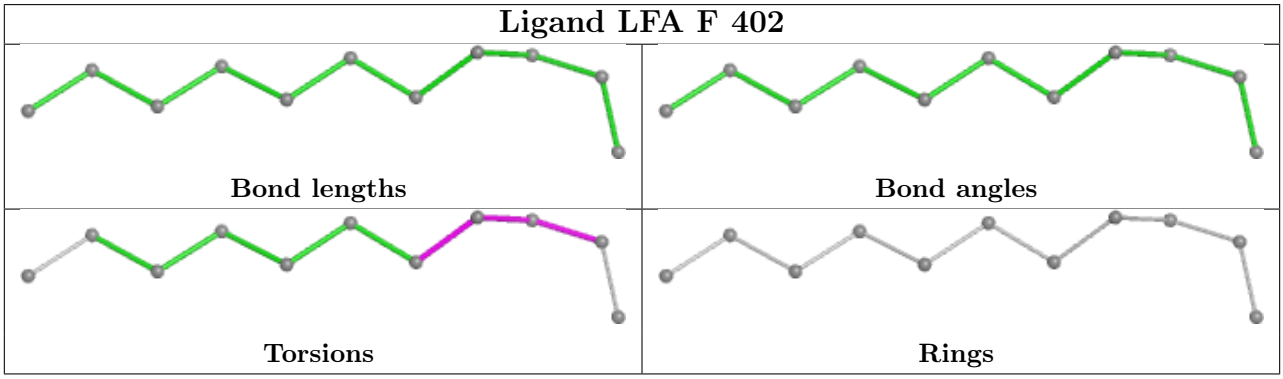
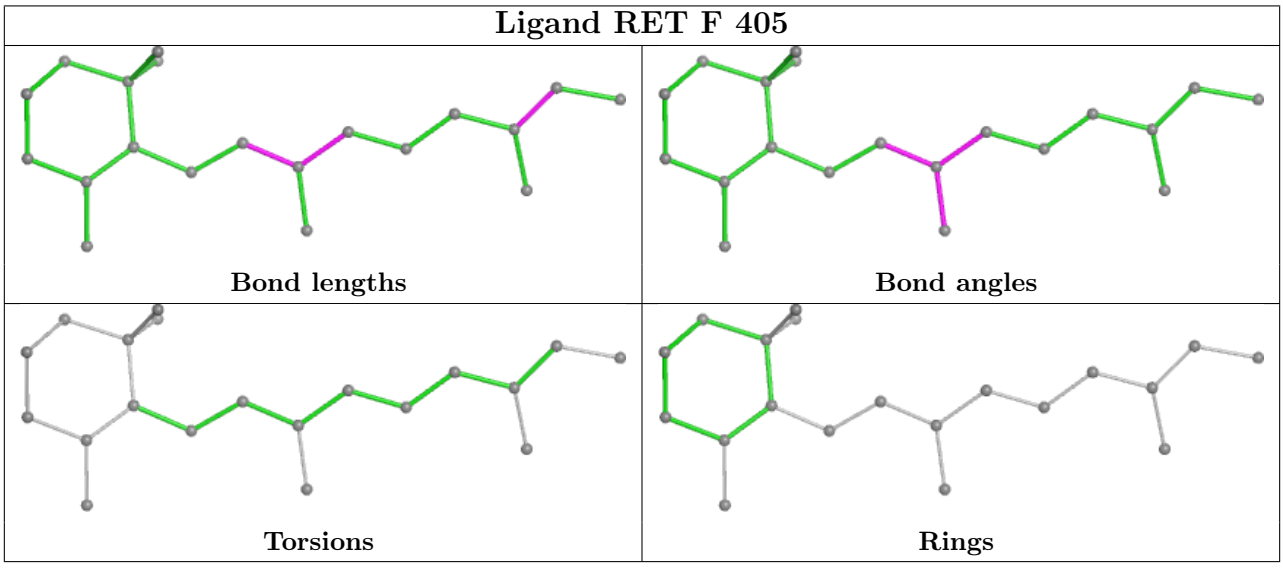
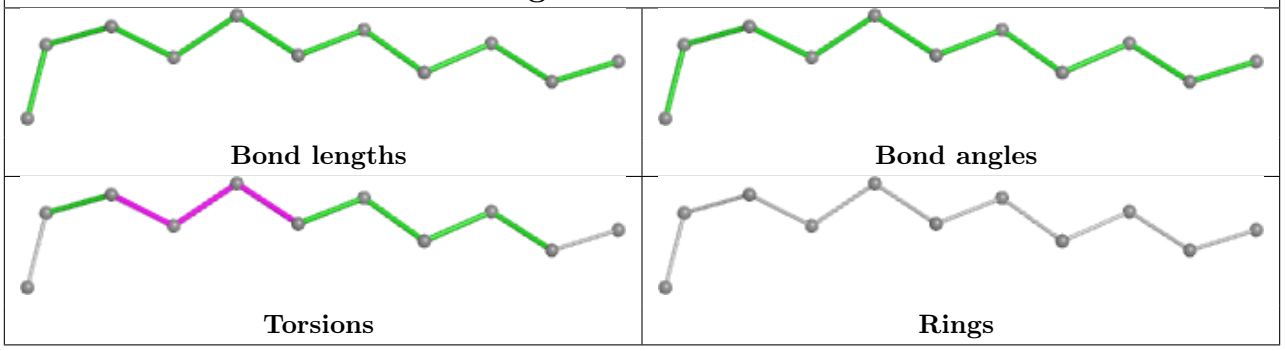
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	406	LFA	1	0
4	K	404	RET	6	0
2	B	404	LFA	1	0
2	F	403	LFA	1	0
4	A	406	RET	4	0
4	I	404	RET	6	0

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 then 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.

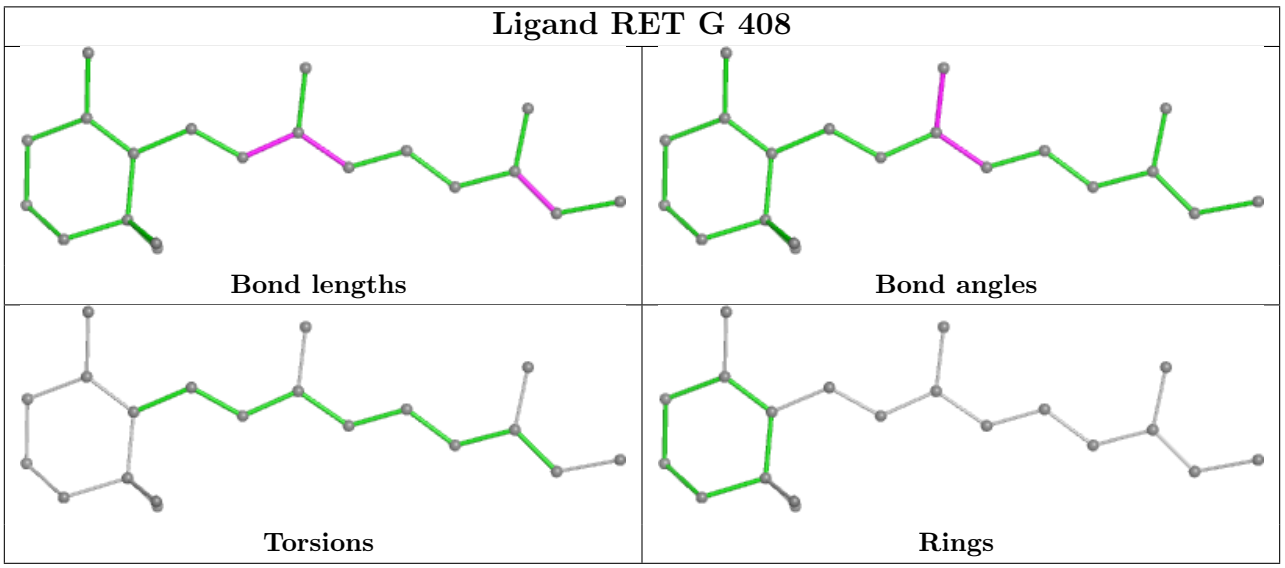




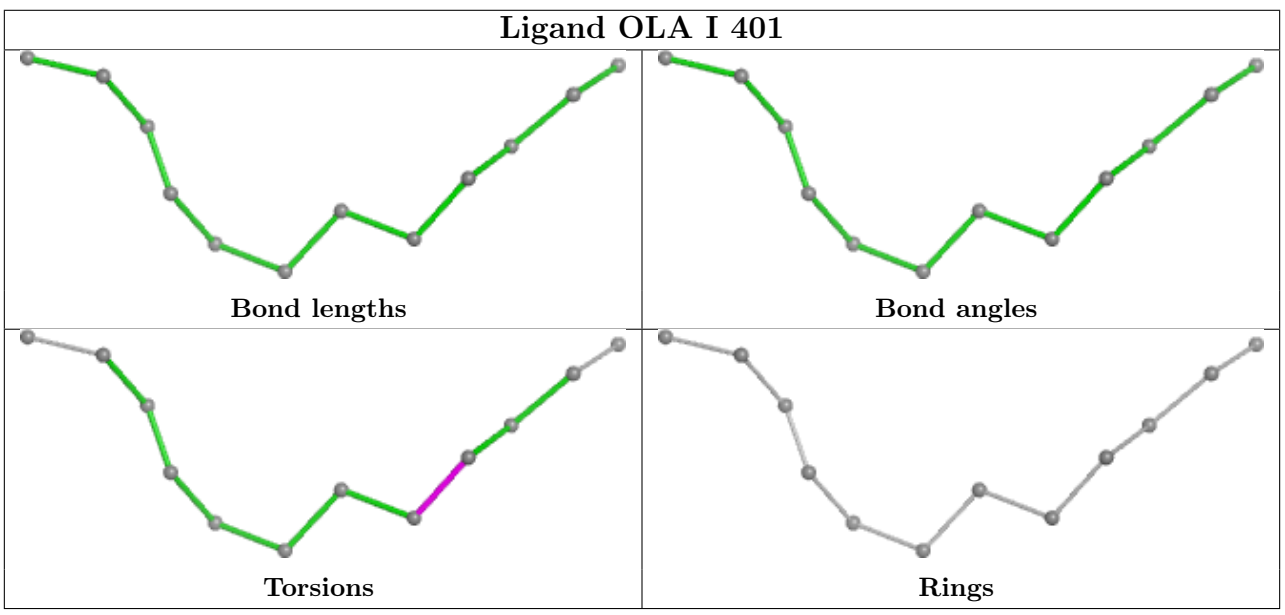
Ligand LFA A 401



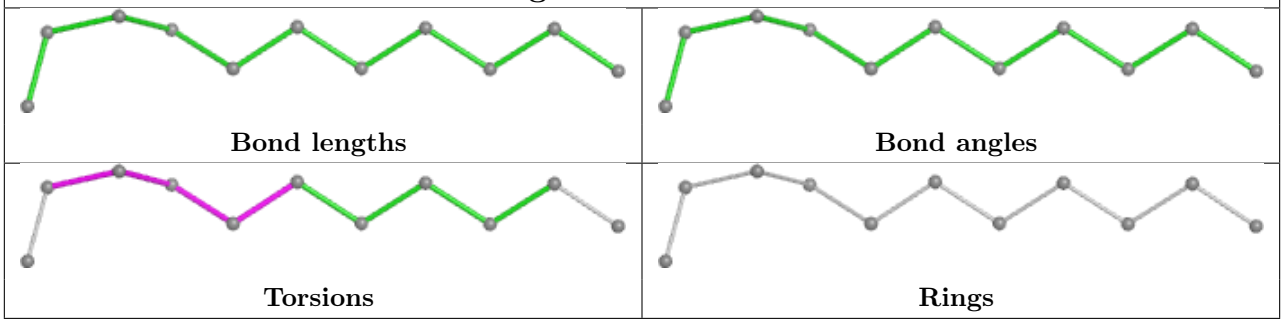
Ligand RET G 408



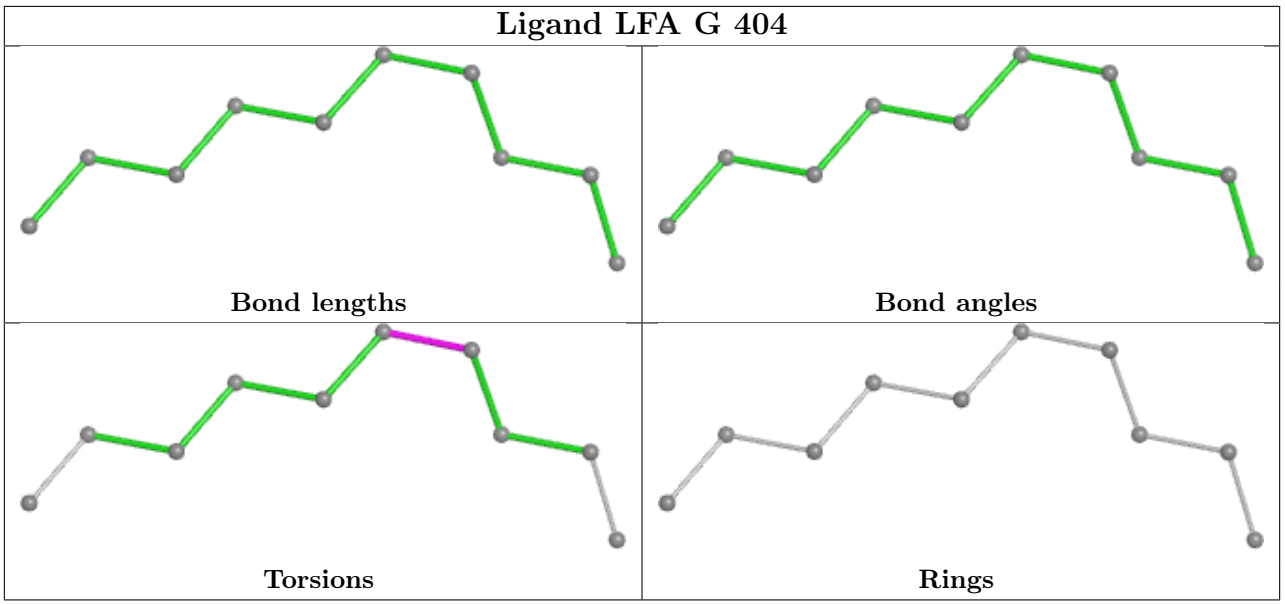
Ligand OLA I 401



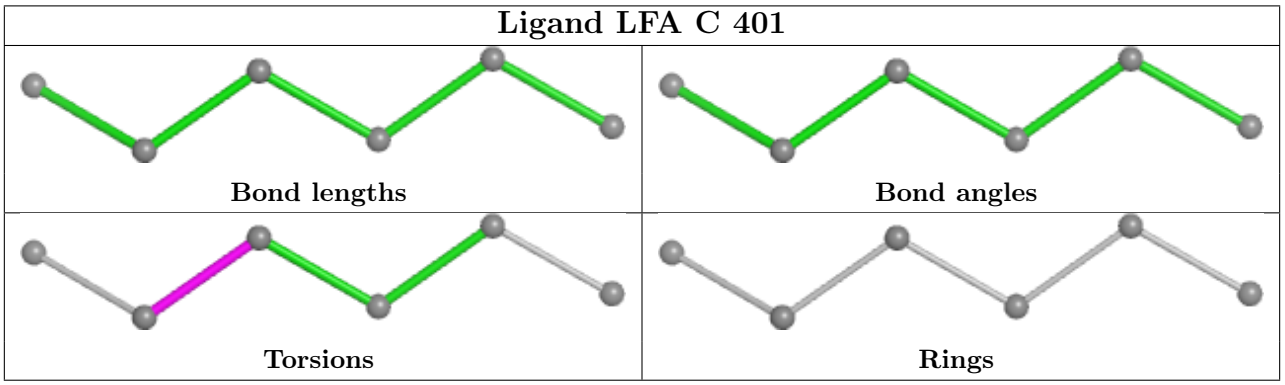
Ligand LFA B 402



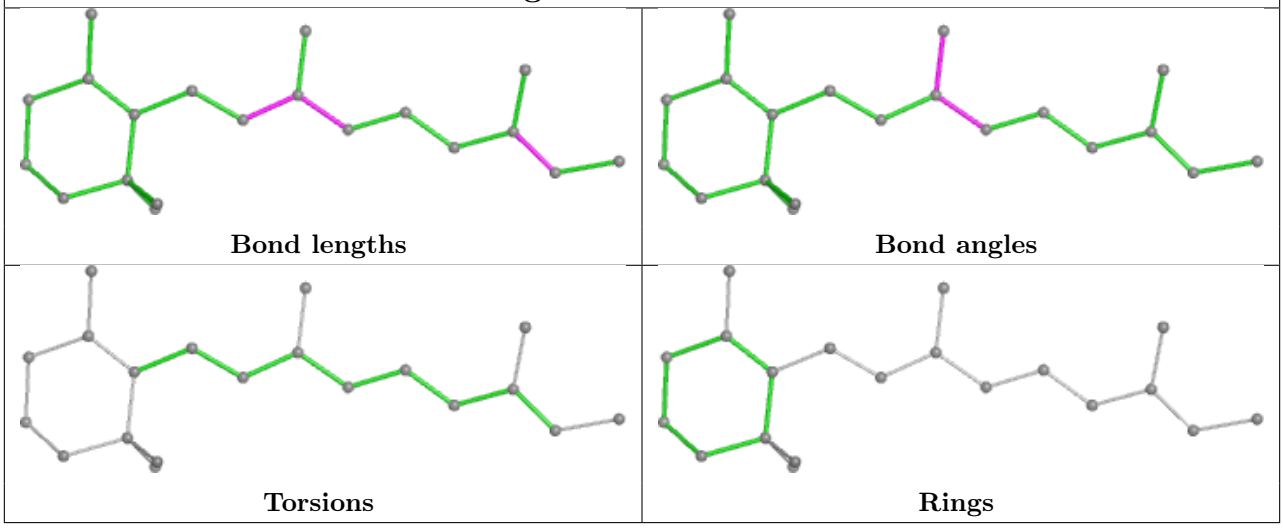
Ligand LFA G 404



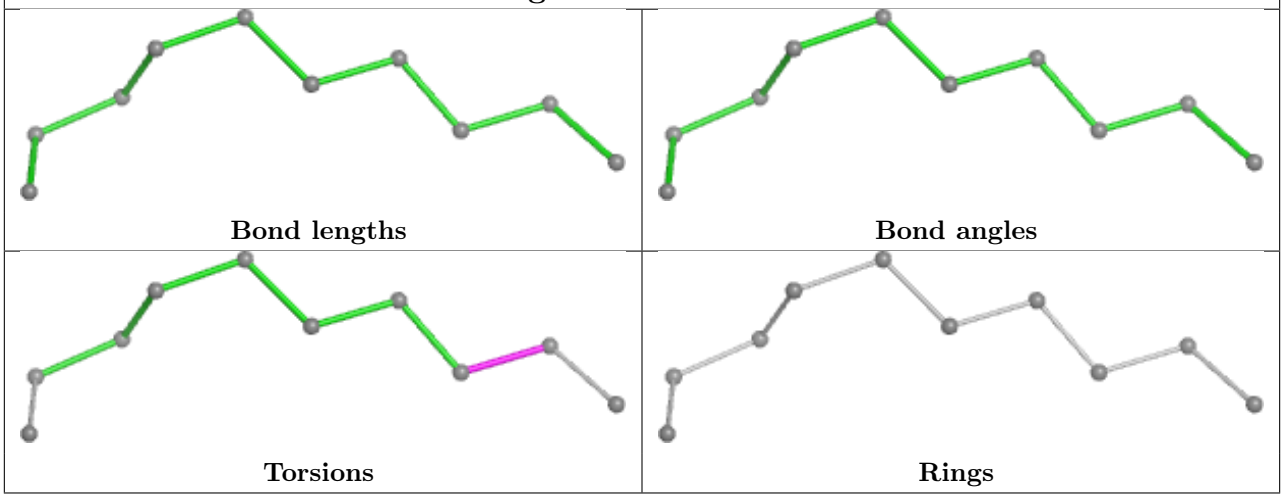
Ligand LFA C 401



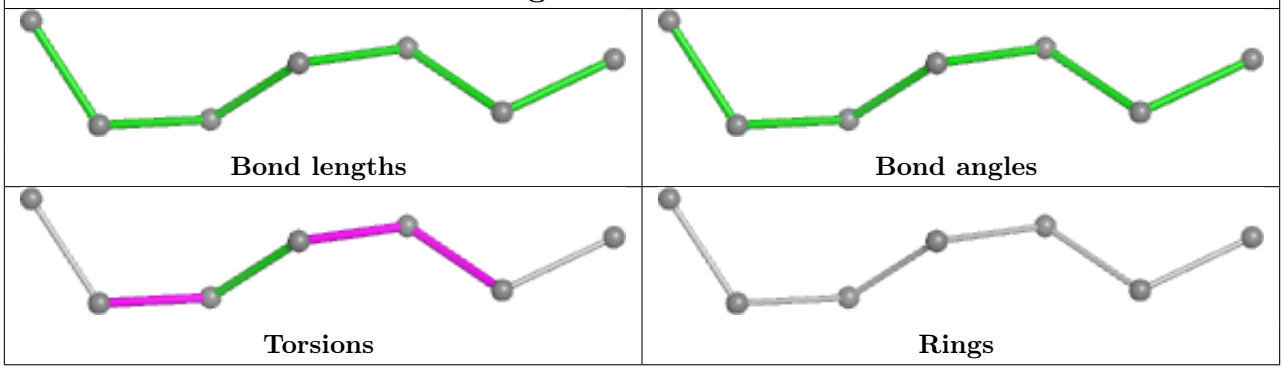
Ligand RET D 405



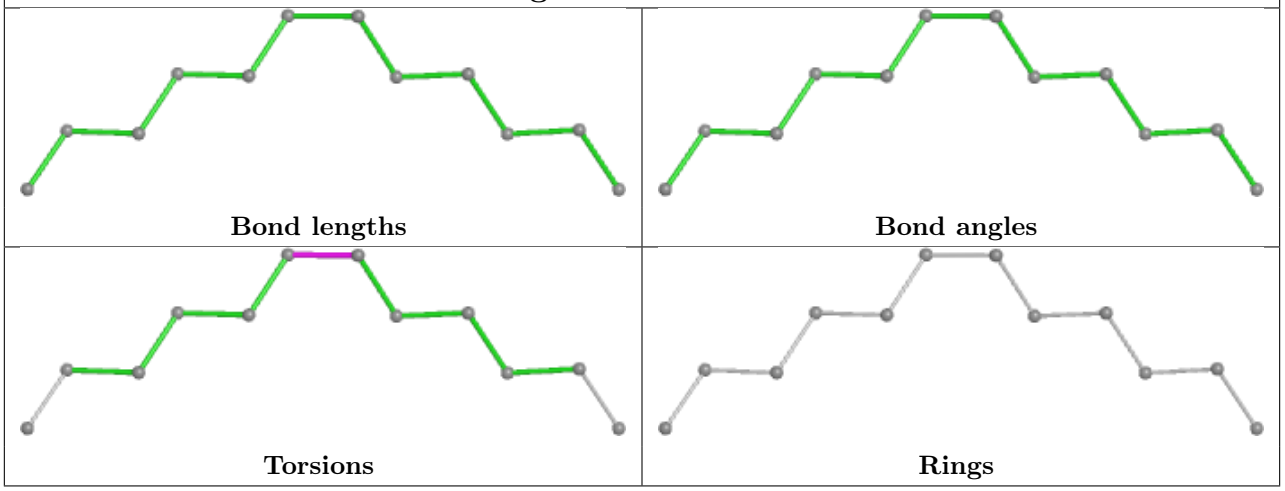
Ligand LFA A 403



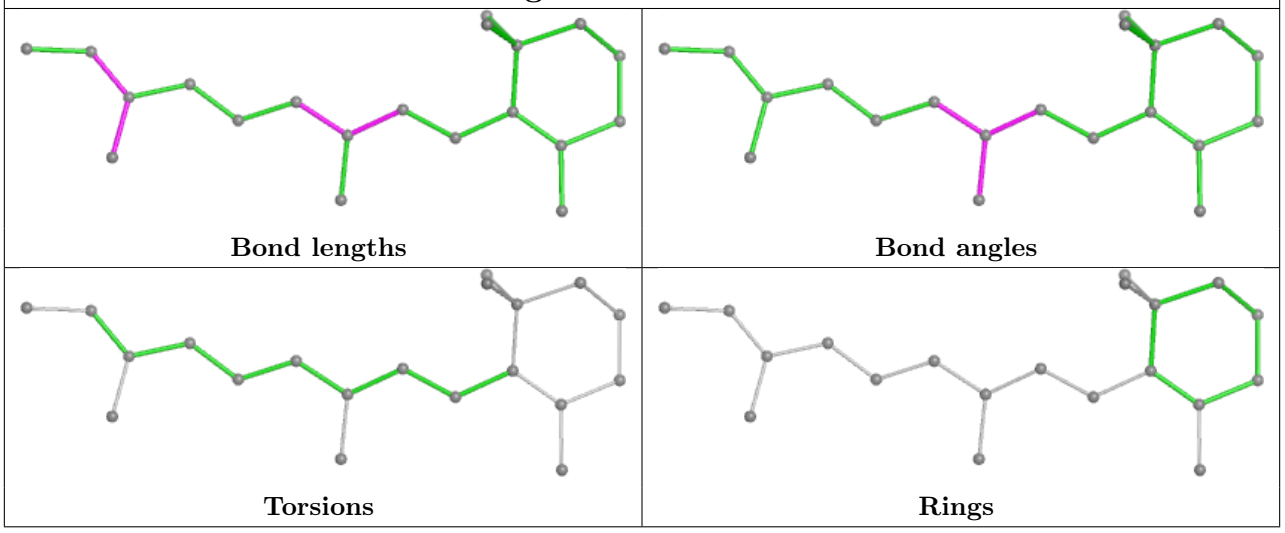
Ligand LFA A 404



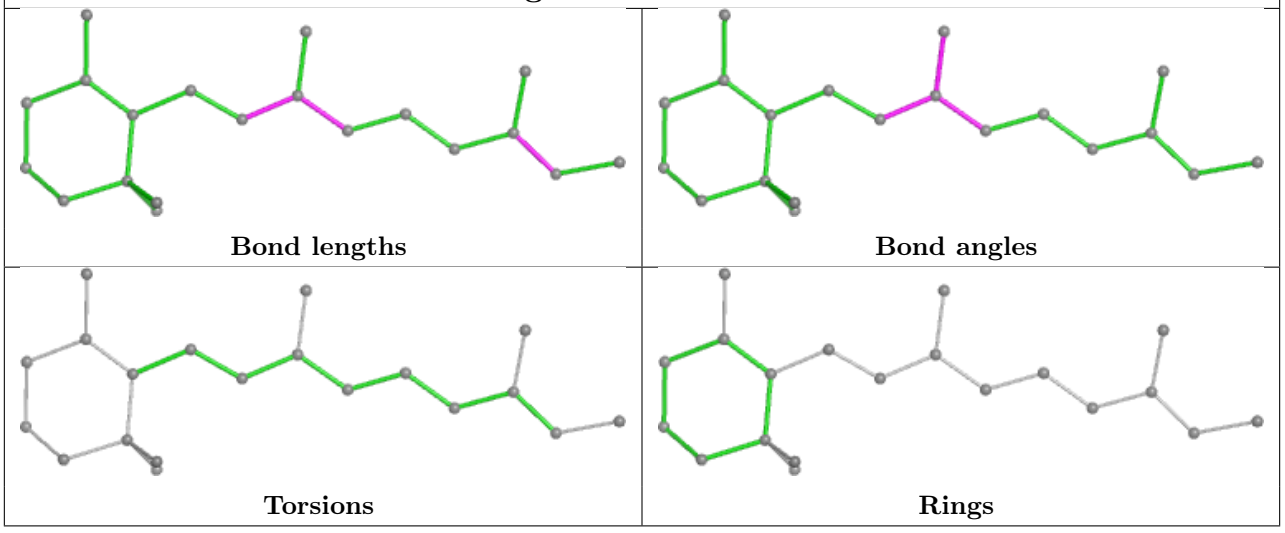
Ligand LFA E 402



Ligand RET B 406



Ligand RET C 404



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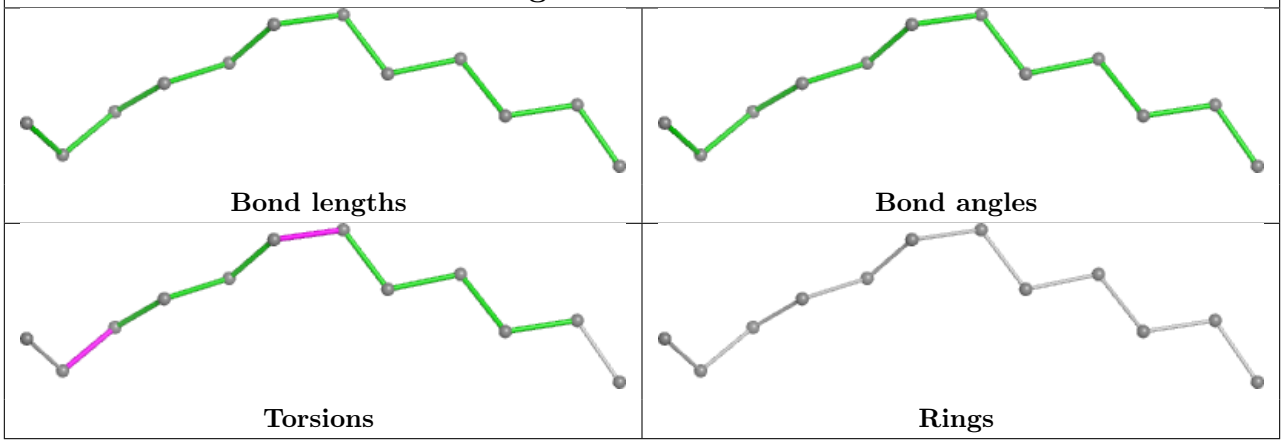
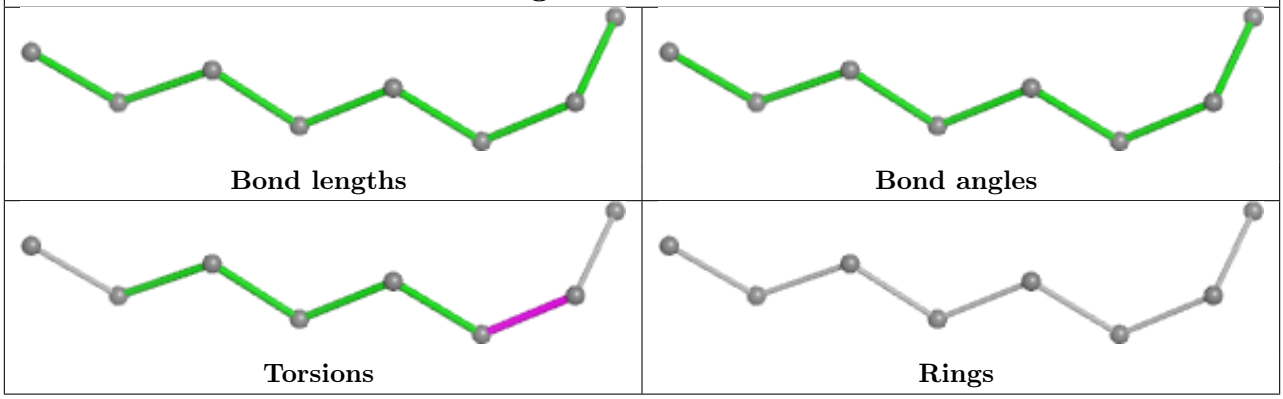
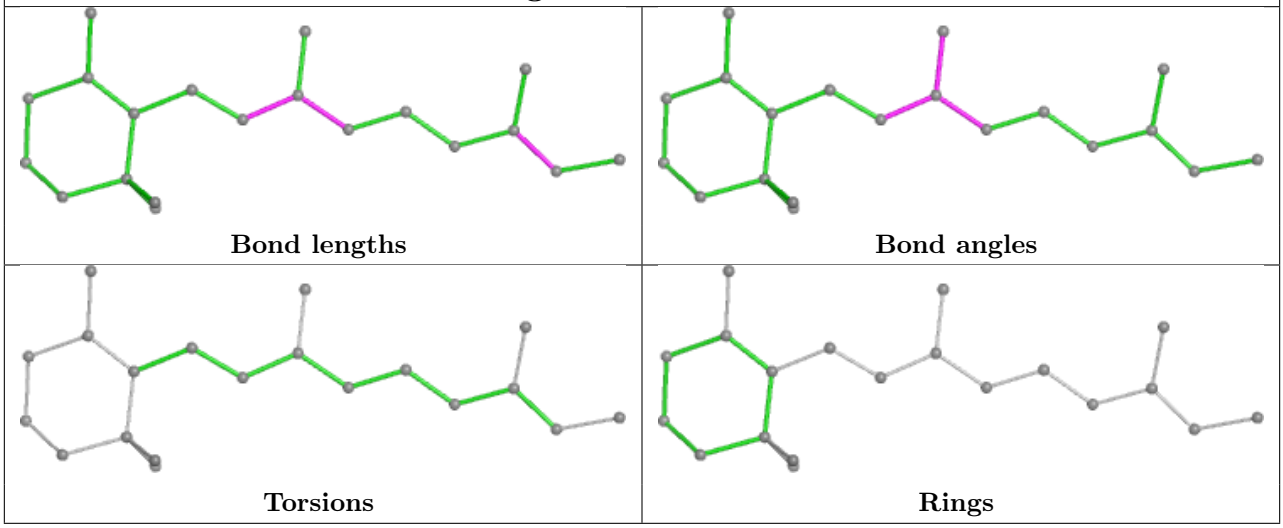


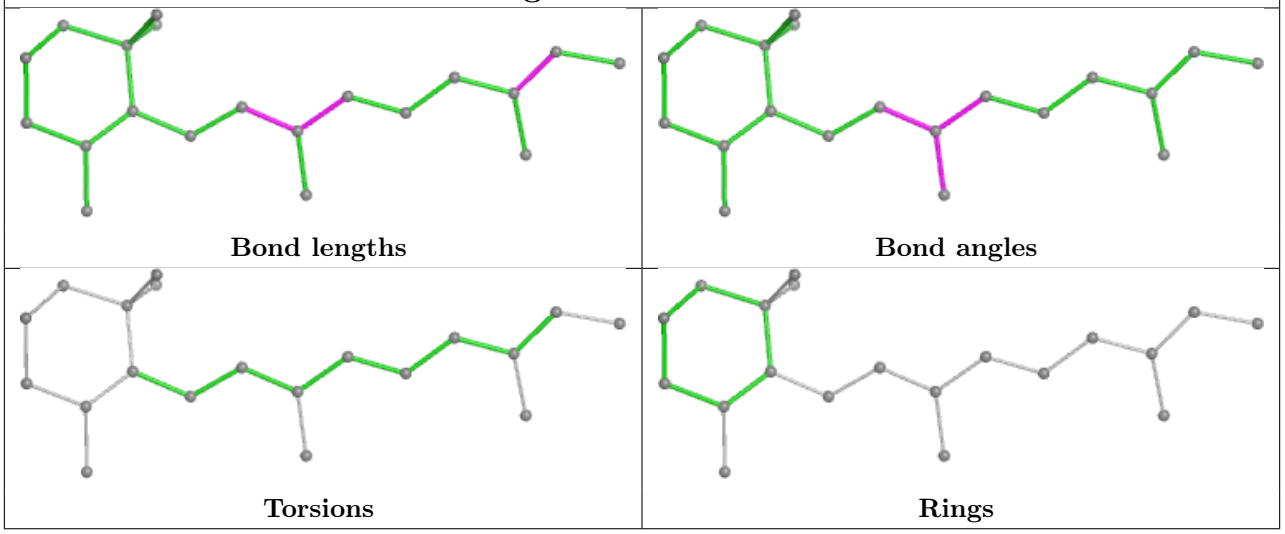
Ligand LFA F 401



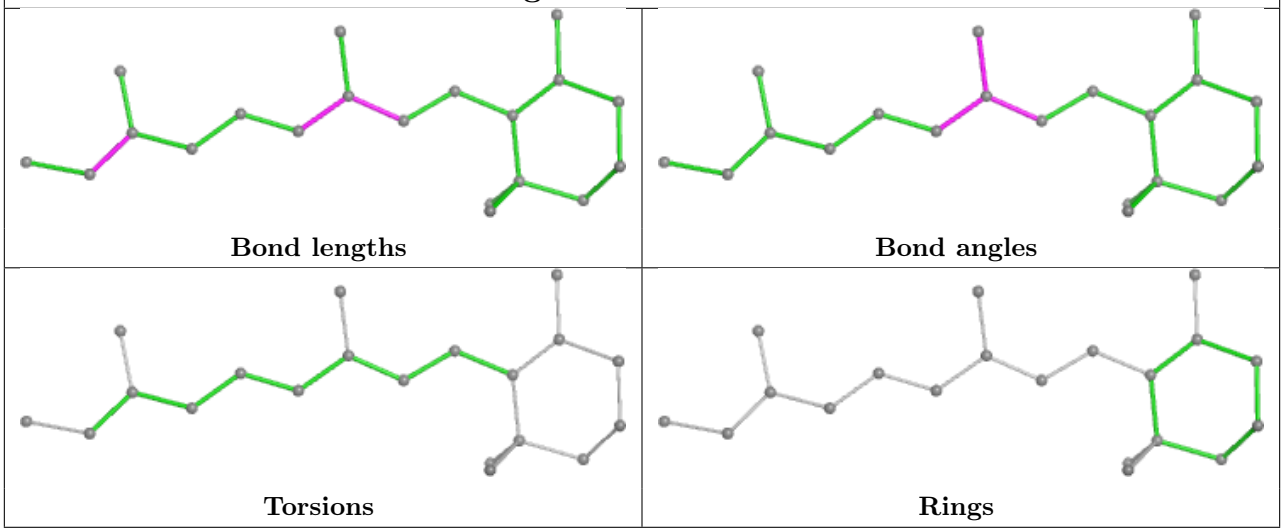
Ligand RET E 404



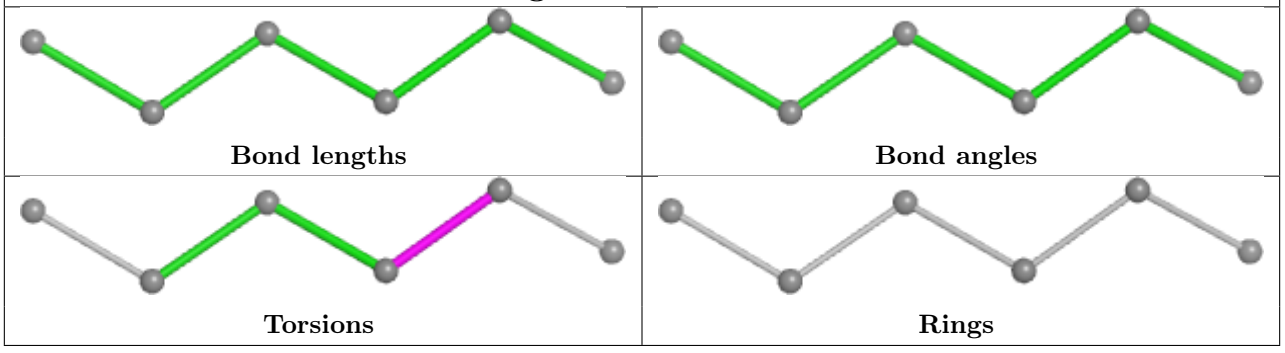
Ligand RET H 404

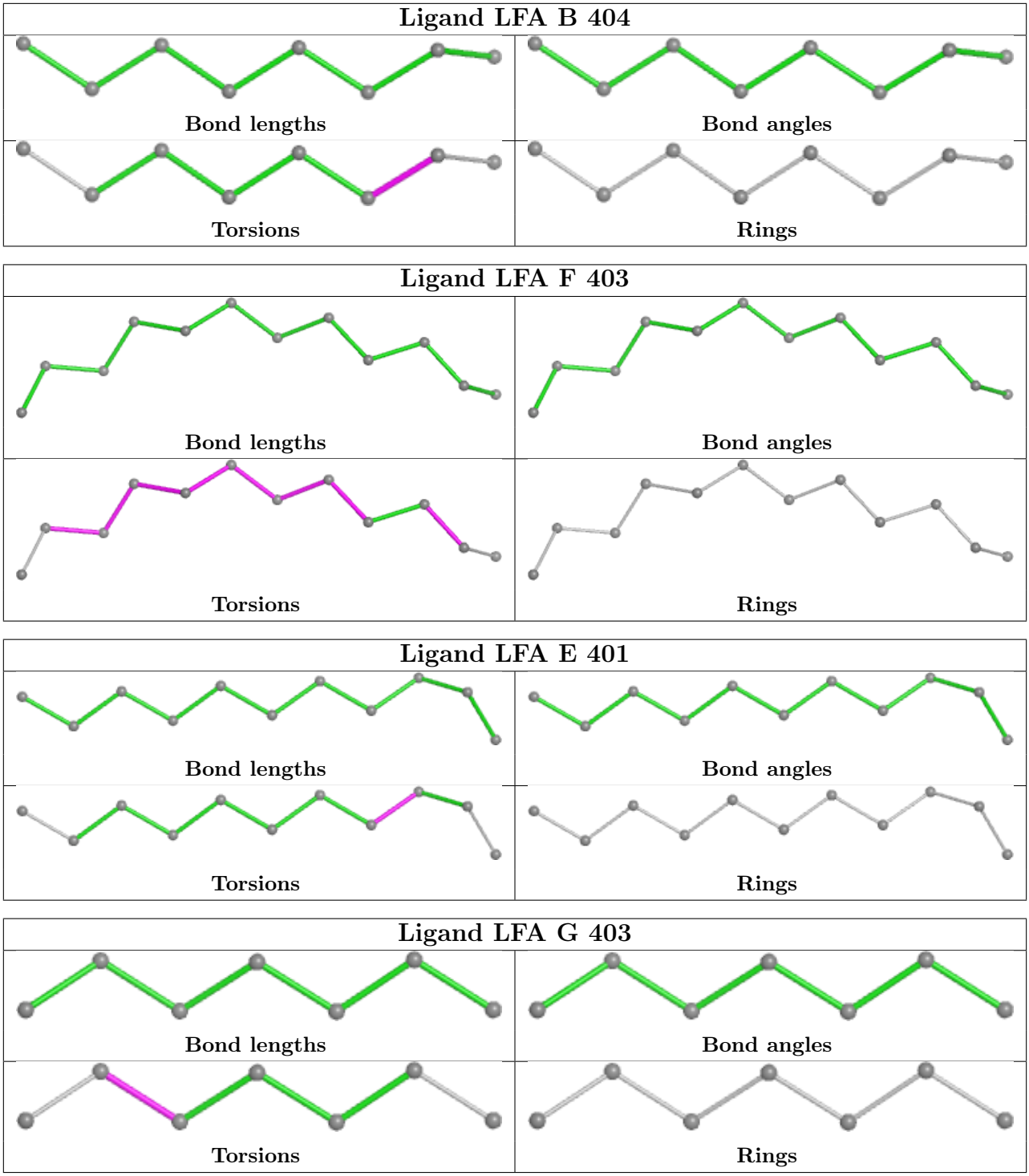


Ligand RET K 404



Ligand LFA H 401




Ligand LFA B 404
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA F 403
Bond lengths
Bond angles
Torsions
Rings
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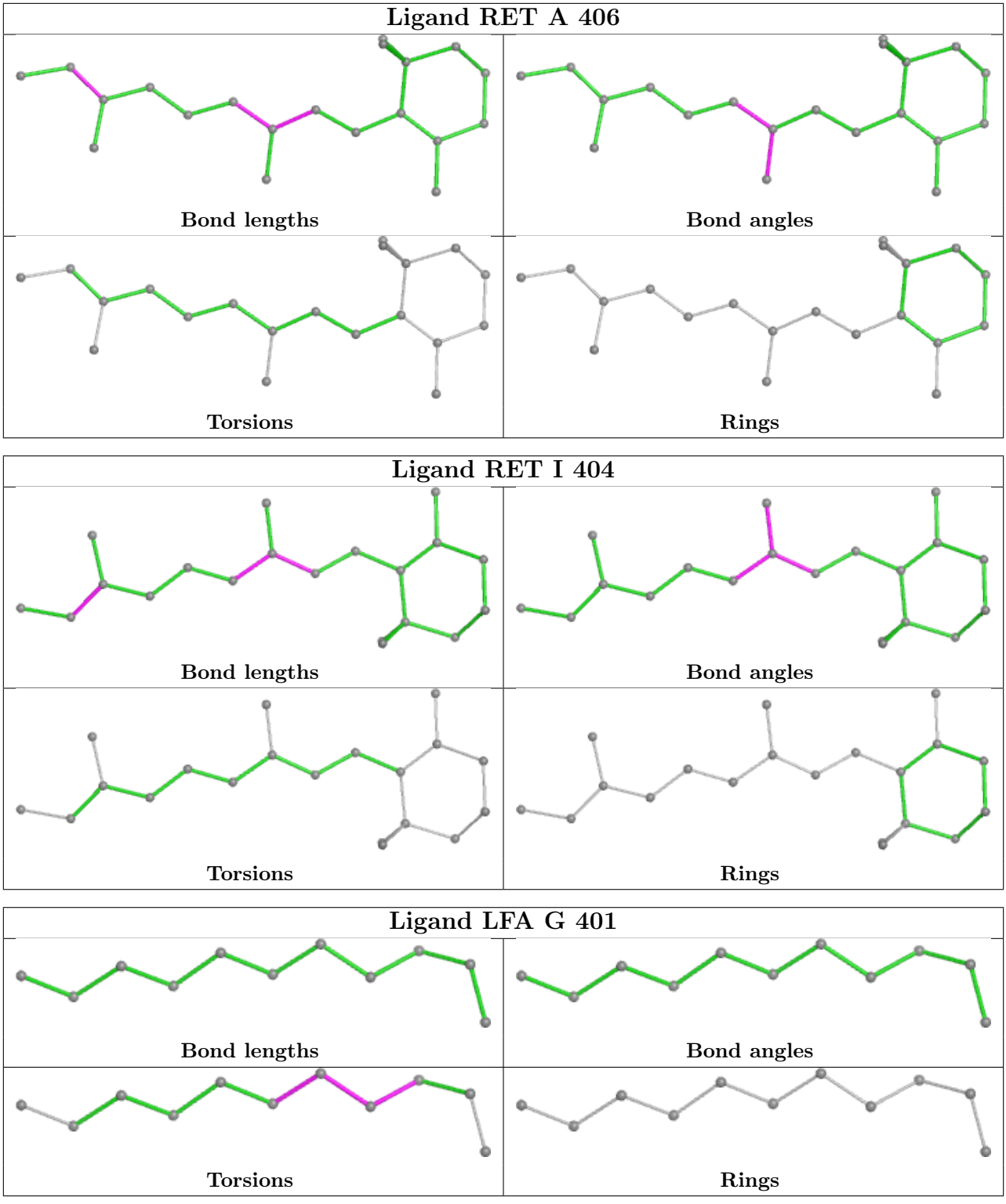
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA G 403
Bond lengths
Bond angles
Torsions
Rings



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

6.1 Protein, DNA and RNA chains

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^{th} 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	285/327 (87%)	-0.24	0 100 100	50, 85, 118, 152	0
1	B	288/327 (88%)	-0.14	4 (1%) 73 52	53, 85, 145, 191	0
1	C	287/327 (87%)	-0.19	0 100 100	49, 93, 131, 172	0
1	D	288/327 (88%)	-0.18	1 (0%) 90 81	56, 99, 133, 167	0
1	E	286/327 (87%)	-0.22	1 (0%) 90 81	54, 91, 132, 159	0
1	F	287/327 (87%)	-0.28	0 100 100	52, 85, 130, 171	0
1	G	288/327 (88%)	-0.21	2 (0%) 84 68	54, 88, 127, 187	0
1	H	287/327 (87%)	-0.20	0 100 100	57, 92, 127, 153	0
1	I	290/327 (88%)	-0.19	0 100 100	56, 100, 131, 168	0
1	K	286/327 (87%)	-0.21	0 100 100	50, 91, 129, 149	0
All	All	2872/3270 (87%)	-0.21	8 (0%) 90 81	49, 91, 132, 191	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	SER	2.9
1	B	188	THR	2.8
1	B	185	SER	2.6
1	G	22	ILE	2.5
1	G	91	ASP	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	I	403	5/5	0.50	0.09	138,149,151,154	0
3	PO4	G	407	5/5	0.56	0.11	147,155,158,162	0
3	PO4	A	405	5/5	0.56	0.10	133,137,147,148	0
3	PO4	D	404	5/5	0.58	0.08	137,137,145,148	0
3	PO4	B	405	5/5	0.63	0.10	109,121,126,128	0
2	LFA	H	401	6/20	0.63	0.20	22,34,54,55	0
2	LFA	F	402	11/20	0.71	0.11	19,47,65,65	0
2	LFA	H	402	6/20	0.71	0.12	18,24,40,41	0
2	LFA	C	401	6/20	0.72	0.18	33,52,67,70	0
2	LFA	A	404	7/20	0.74	0.10	67,80,92,95	0
2	LFA	G	406	7/20	0.74	0.11	78,90,97,98	0
3	PO4	F	404	5/5	0.75	0.09	104,109,119,127	0
3	PO4	E	403	5/5	0.75	0.07	118,121,129,130	0
2	LFA	B	404	8/20	0.76	0.13	17,38,42,43	0
2	LFA	K	402	10/20	0.77	0.12	31,73,87,90	0
2	LFA	D	403	9/20	0.78	0.11	34,69,91,92	0
2	LFA	F	401	8/20	0.79	0.12	18,36,45,45	0
2	LFA	B	402	11/20	0.79	0.11	20,45,69,70	0
2	LFA	A	403	10/20	0.79	0.22	30,57,74,75	0
2	LFA	G	405	10/20	0.79	0.19	33,56,62,63	0
2	LFA	E	401	11/20	0.79	0.12	18,44,62,63	0
3	PO4	K	403	5/5	0.80	0.08	131,134,137,143	0
5	OLA	I	401	12/20	0.80	0.18	19,75,85,87	0
3	PO4	H	403	5/5	0.81	0.09	129,134,137,139	0
5	OLA	D	401	11/20	0.81	0.15	32,86,99,102	0
2	LFA	E	402	12/20	0.81	0.12	80,86,119,121	0
2	LFA	K	401	11/20	0.83	0.12	18,44,66,66	0
2	LFA	G	403	7/20	0.84	0.11	20,28,49,51	0
3	PO4	C	403	5/5	0.85	0.08	120,125,128,128	0
2	LFA	A	402	7/20	0.85	0.13	18,25,46,47	0
2	LFA	F	403	12/20	0.86	0.18	32,76,89,89	0
2	LFA	C	402	6/20	0.87	0.07	15,21,34,36	0

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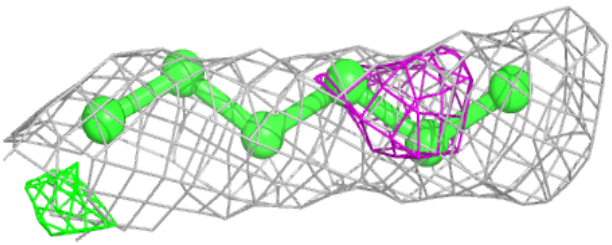
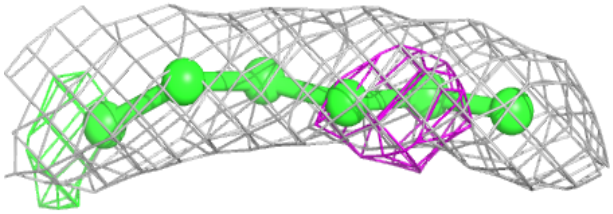
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	D	402	10/20	0.87	0.10	20,68,92,96	0
2	LFA	B	401	7/20	0.87	0.10	16,25,47,47	0
2	LFA	G	404	10/20	0.89	0.11	18,60,87,87	0
2	LFA	B	403	12/20	0.89	0.16	29,74,79,79	0
2	LFA	G	402	7/20	0.91	0.10	19,32,61,62	0
4	RET	I	404	20/21	0.91	0.21	109,119,129,130	0
4	RET	H	404	20/21	0.92	0.19	85,98,110,112	0
4	RET	G	408	20/21	0.92	0.22	90,97,130,132	0
2	LFA	G	401	11/20	0.92	0.12	16,46,86,89	0
4	RET	B	406	20/21	0.92	0.16	85,96,101,104	0
4	RET	C	404	20/21	0.92	0.20	91,100,111,112	0
4	RET	A	406	20/21	0.93	0.17	89,100,120,122	0
4	RET	D	405	20/21	0.93	0.21	113,119,127,131	0
4	RET	K	404	20/21	0.93	0.18	92,108,115,116	0
4	RET	E	404	20/21	0.93	0.18	93,106,114,122	0
2	LFA	I	402	10/20	0.93	0.08	21,62,89,90	0
2	LFA	A	401	11/20	0.94	0.09	19,57,85,88	0
4	RET	F	405	20/21	0.94	0.14	69,84,99,100	0

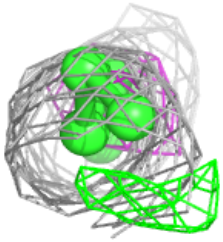
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA H 401:

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

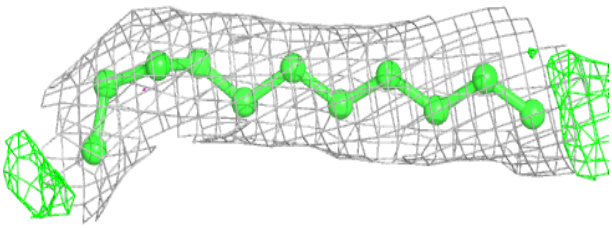


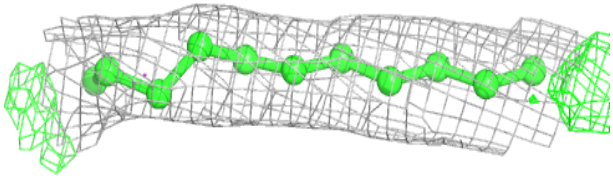


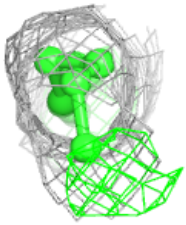


Electron density around LFA F 402:

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

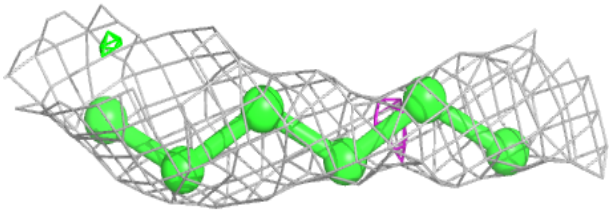


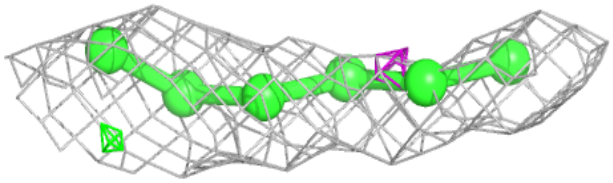


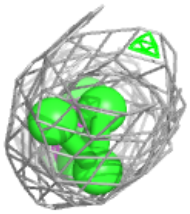


Electron density around LFA C 401:

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

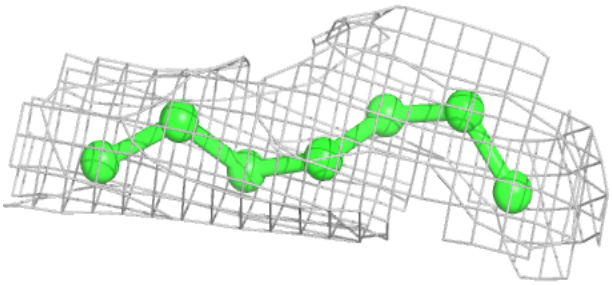


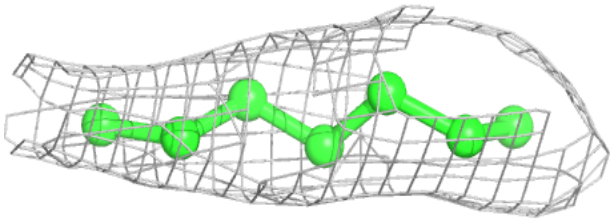


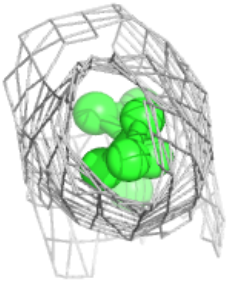


Electron density around LFA A 404:

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

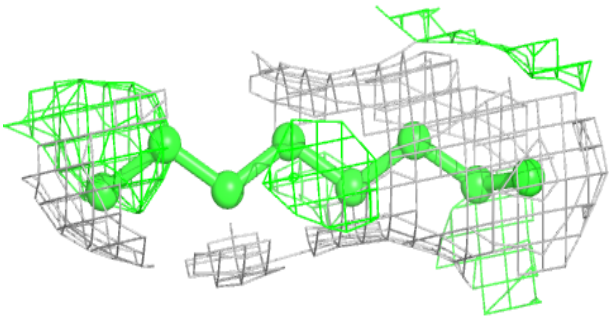


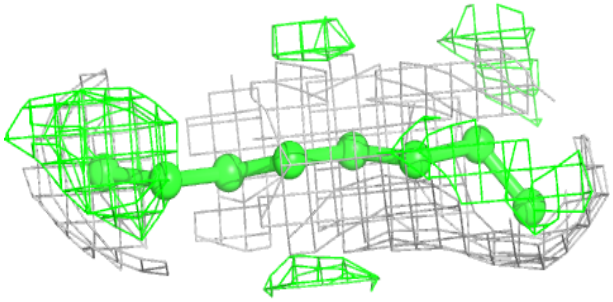


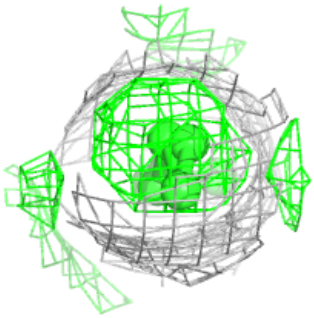


Electron density around LFA B 404:

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

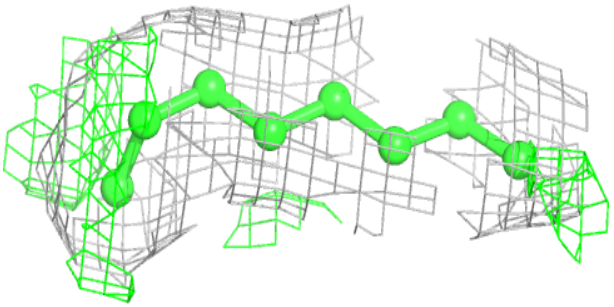


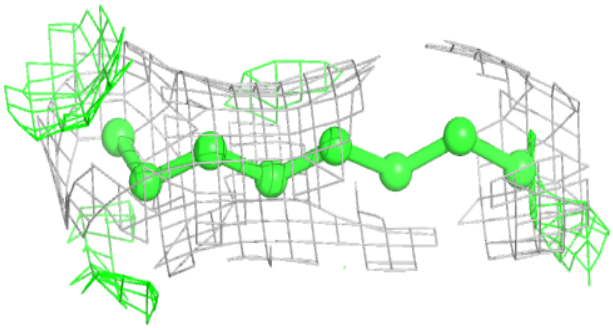


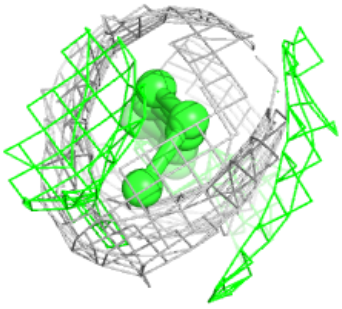


Electron density around LFA F 401:

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

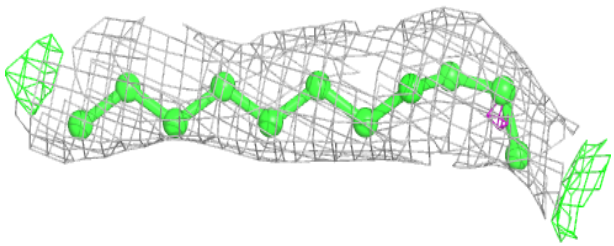


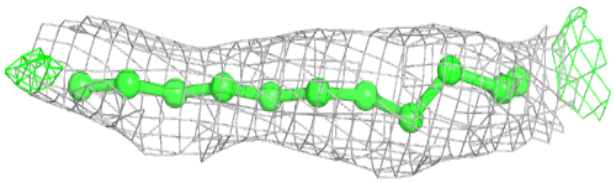


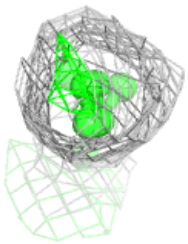


Electron density around LFA B 402:

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

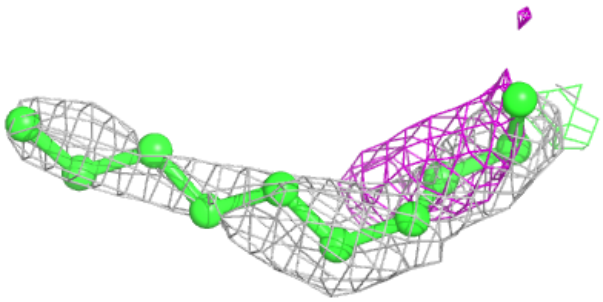


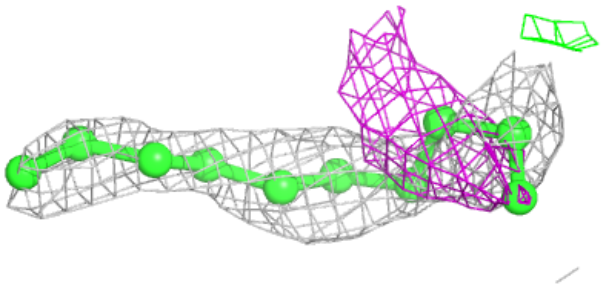


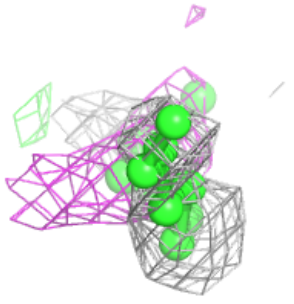


Electron density around LFA A 403:

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

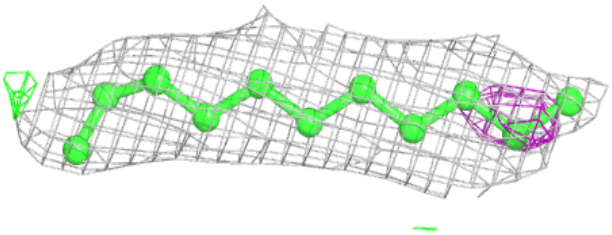


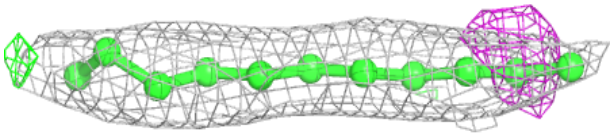


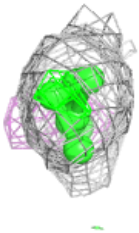


Electron density around LFA E 401:

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

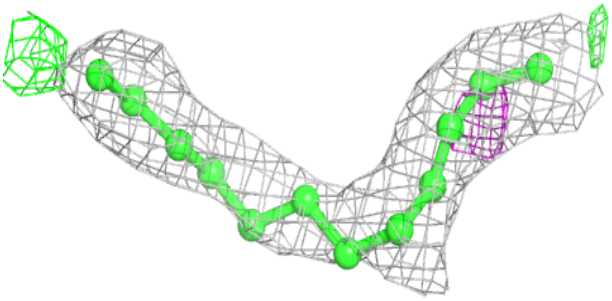


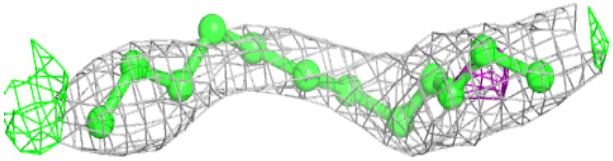


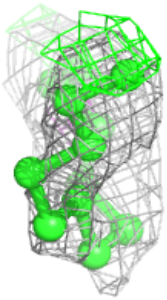


Electron density around OLA I 401:

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

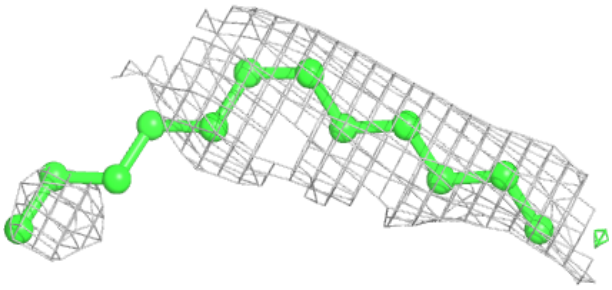


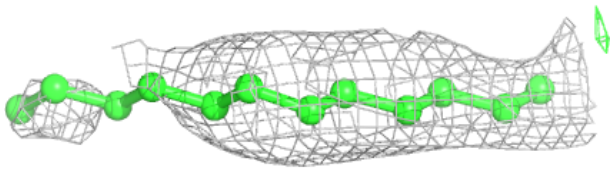


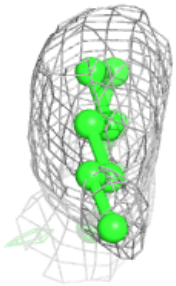


Electron density around LFA E 402:

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

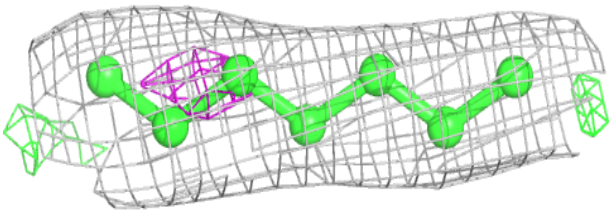


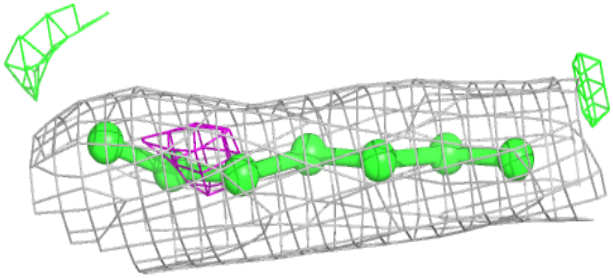


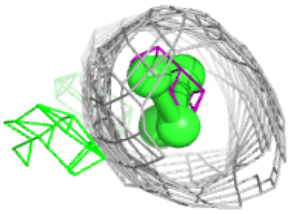


Electron density around LFA G 403:

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

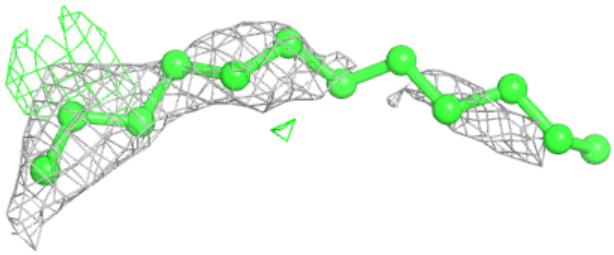


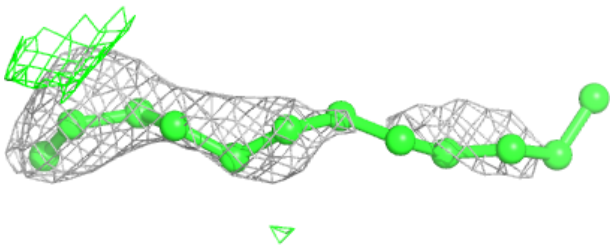


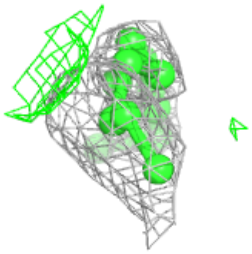


Electron density around LFA F 403:

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

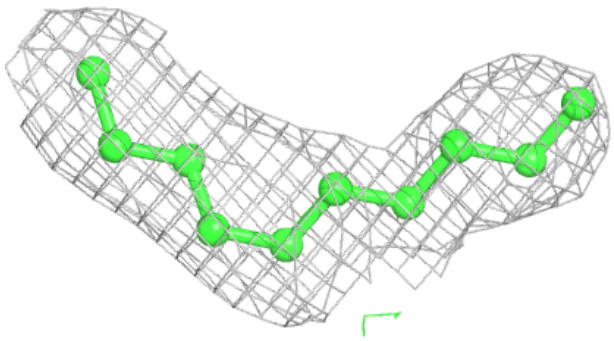


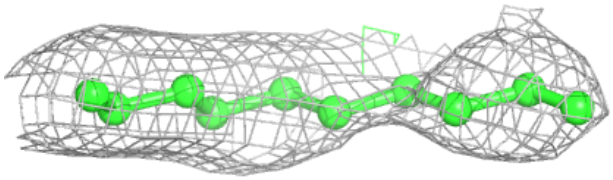


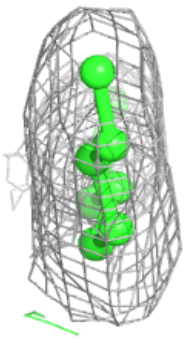


Electron density around LFA G 404:

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

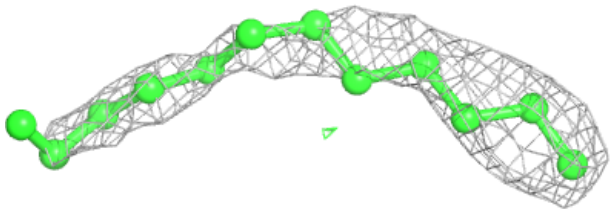


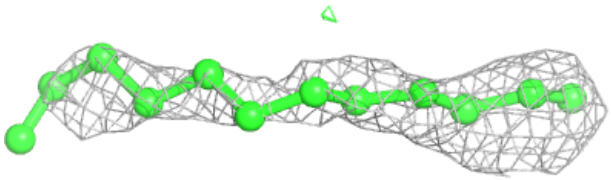


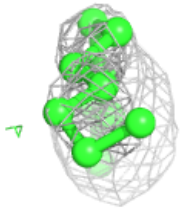


Electron density around LFA B 403:

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

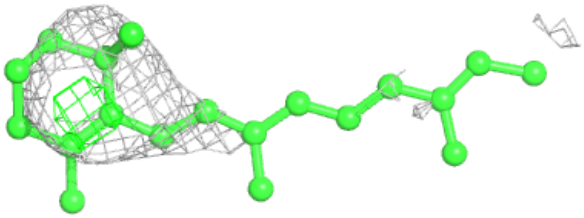


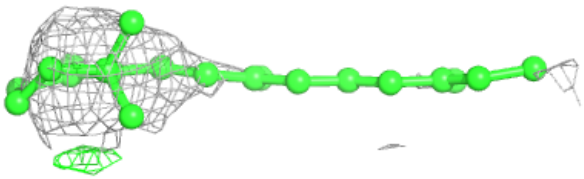


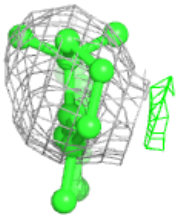


Electron density around RET I 404:

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

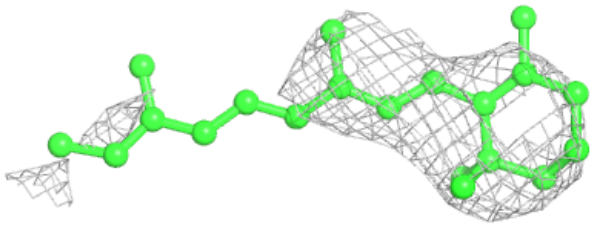


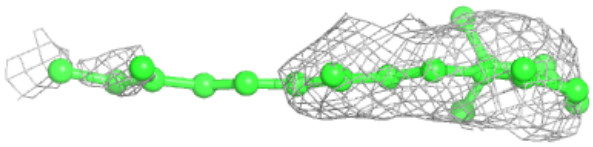


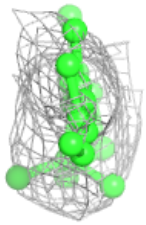


Electron density around RET H 404:

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

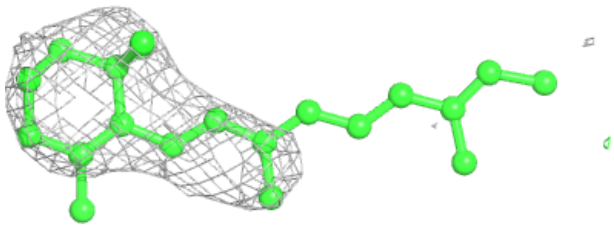


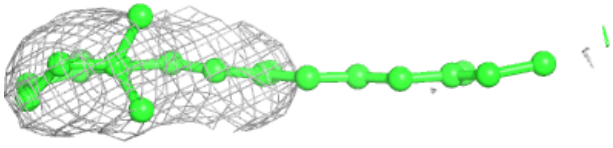


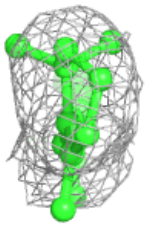


Electron density around RET G 408:

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

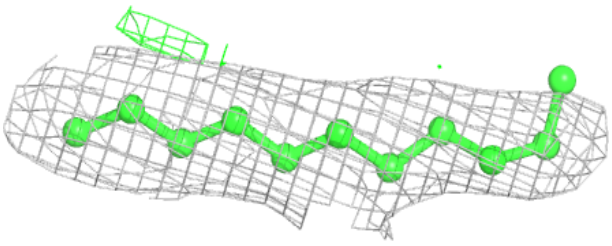


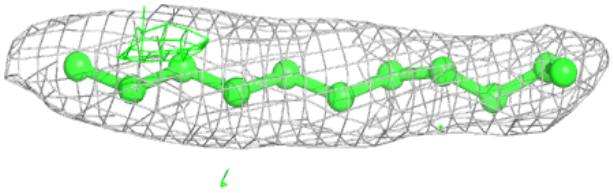


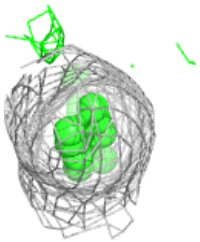


Electron density around LFA G 401:

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

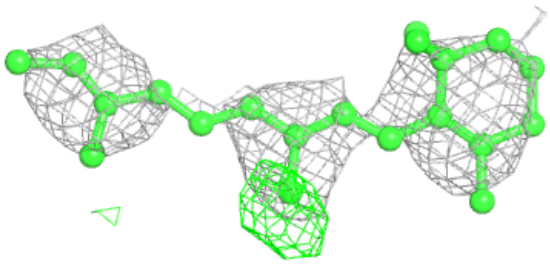


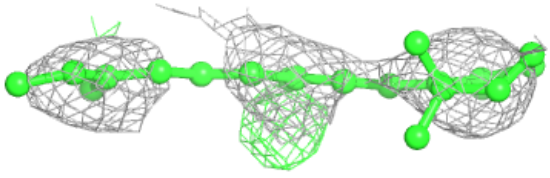


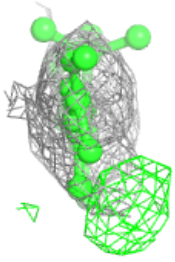


Electron density around RET B 406:

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

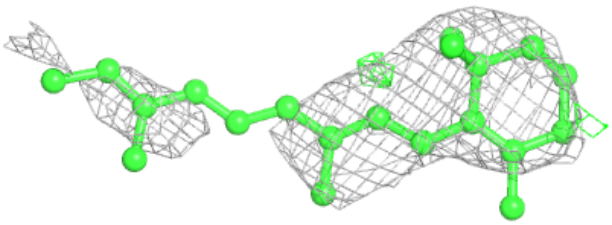


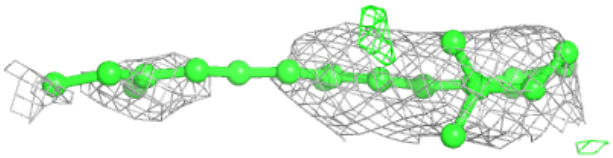


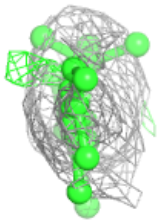


Electron density around RET C 404:

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

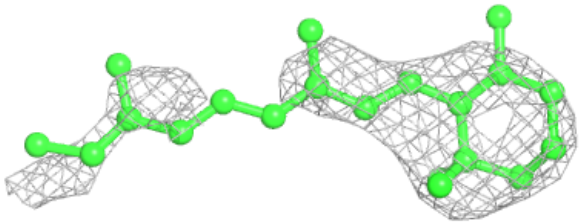


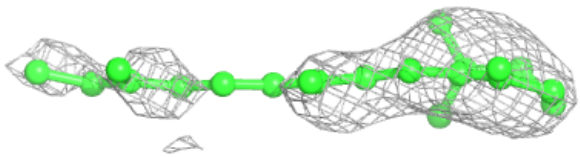


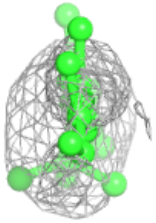


Electron density around RET A 406:

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

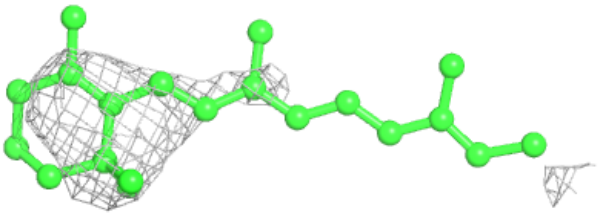


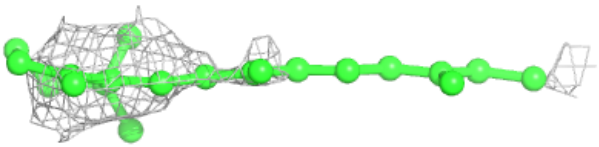


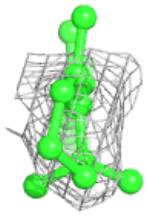


Electron density around RET D 405:

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

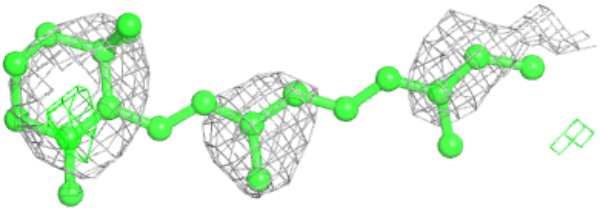


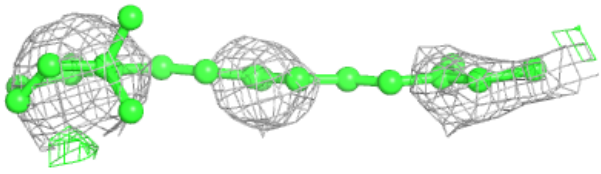


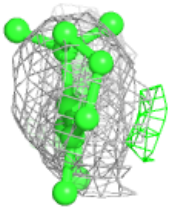


Electron density around RET K 404:

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

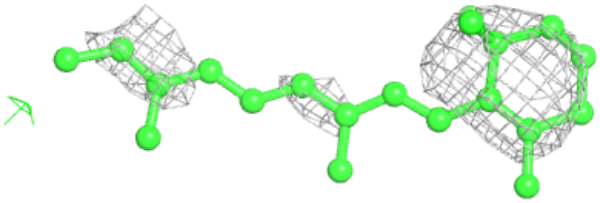


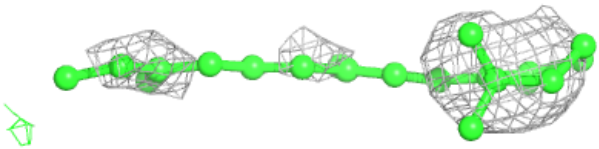


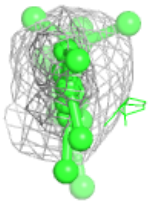


Electron density around RET E 404:

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

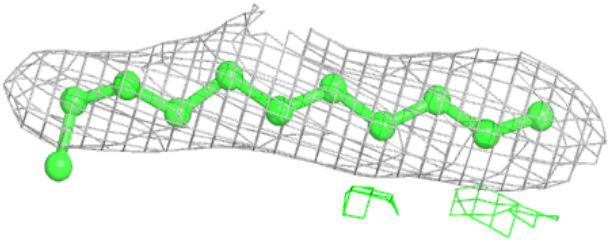


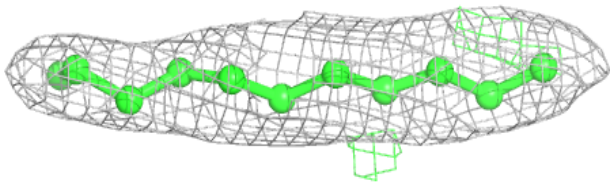


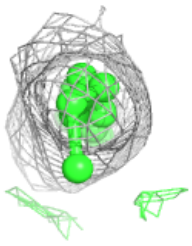


Electron density around LFA A 401:

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

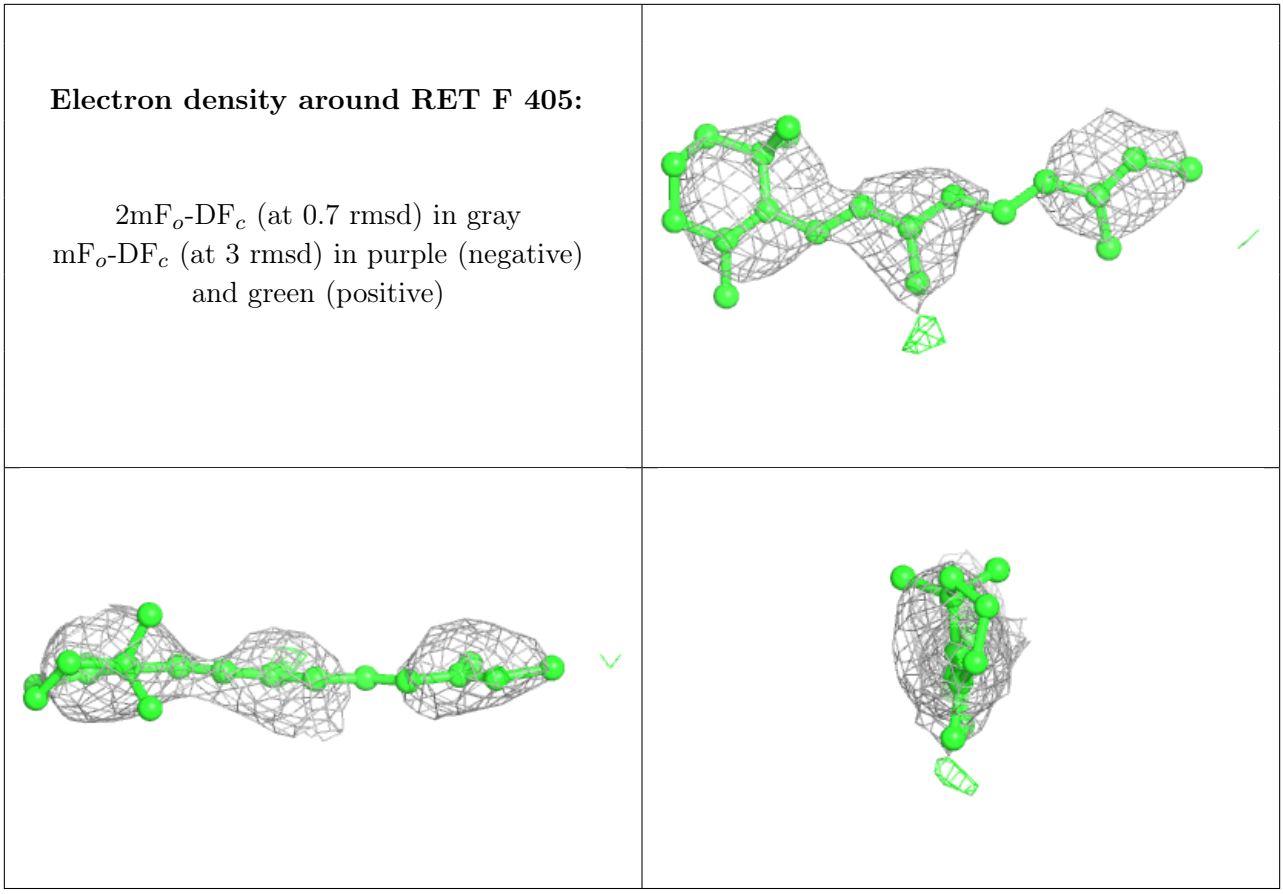






Electron density around RET F 405:

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



6.5 Other polymers

There are no such residues in this entry.