



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:51 AM UTC

PDB ID : 8R97 / pdb_00008r97
Title : Crystal structure of the cryorhodopsin CryoR2 at pH 4.6, type B crystals, non-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 ⓘ 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

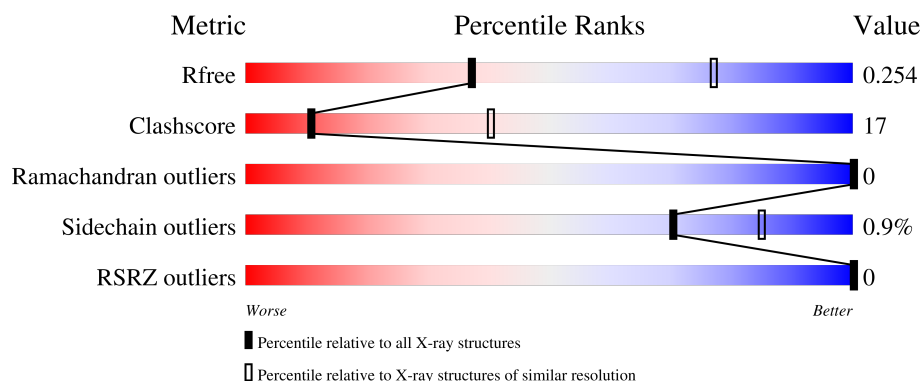
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	 66% 21% 12%
1	B	327	 63% 25% 12%
1	C	327	 62% 25% 12%
1	D	327	 61% 26% 12%
1	E	327	 61% 26% 13%

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Mol	Chain	Length	Quality of chain
1	F	327	 62%25%12%
1	G	327	 65%23%12%
1	H	327	 60%27%12%
1	I	327	 63%25%11%
1	K	327	 62%25%13%

2 Entry composition

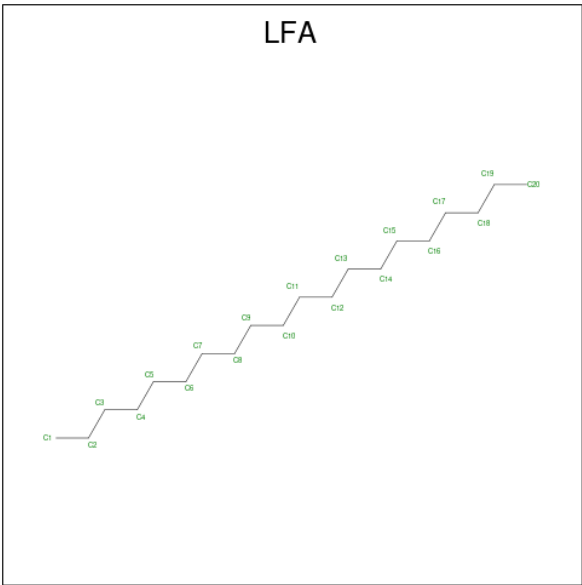
There are 5 unique types of molecules in this entry. The entry contains 21953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	287	Total	C	N	O	S	0	0	0
			2146	1411	346	383	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
			2138	1408	344	380	6			
1	D	288	Total	C	N	O	S	0	0	0
			2137	1407	342	382	6			
1	E	286	Total	C	N	O	S	0	0	0
			2132	1402	342	382	6			
1	H	287	Total	C	N	O	S	0	0	0
			2131	1402	344	379	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
			2153	1413	351	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
			2132	1402	342	382	6			

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



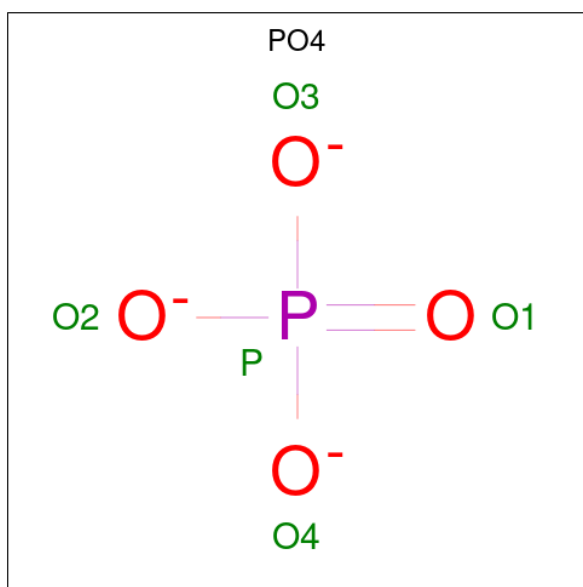
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 11 11	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total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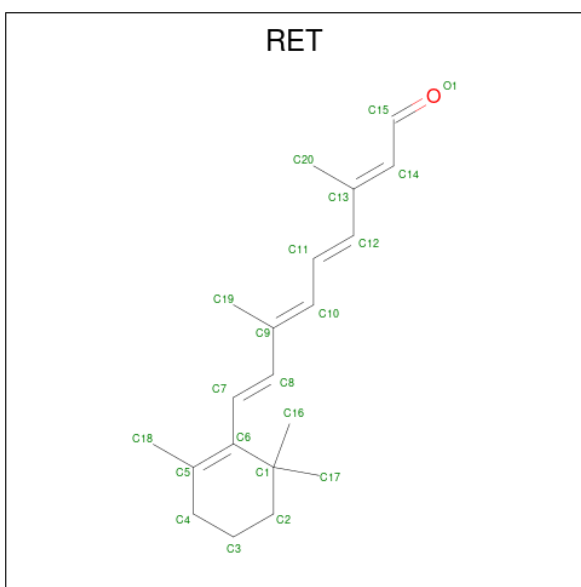
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C 6 6	0	0
2	H	1	Total C 6 6	0	0
2	G	1	Total C 11 11	0	0
2	G	1	Total C 7 7	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 7 7	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 12 12	0	0
2	I	1	Total C 10 10	0	0
2	K	1	Total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

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



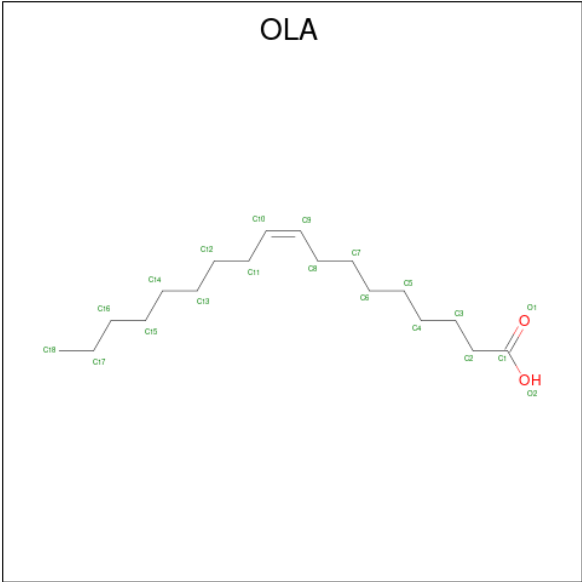
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	K	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
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 (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).

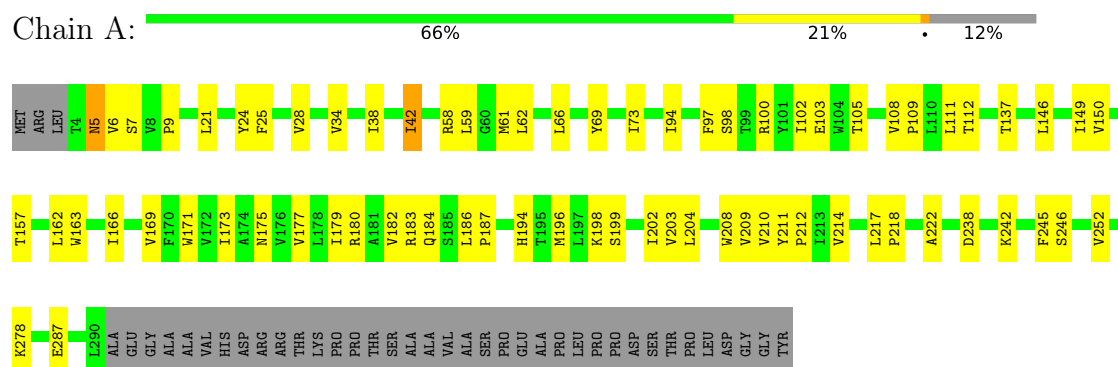


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			20	18	2		
5	I	1	Total	C	O	0	0
			20	18	2		

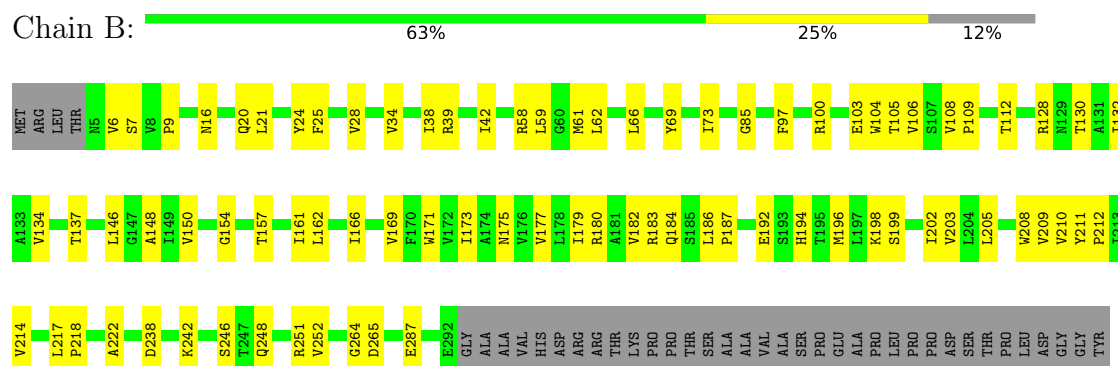
3 Residue-property plots

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

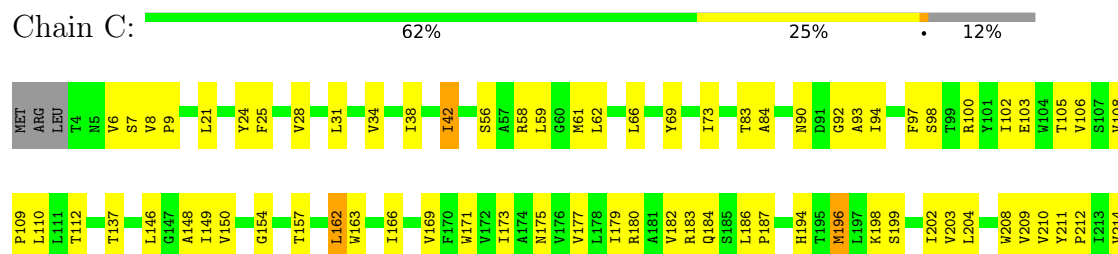
• Molecule 1: cryorhodopsin CryoR2



• Molecule 1: cryorhodopsin CryoR2



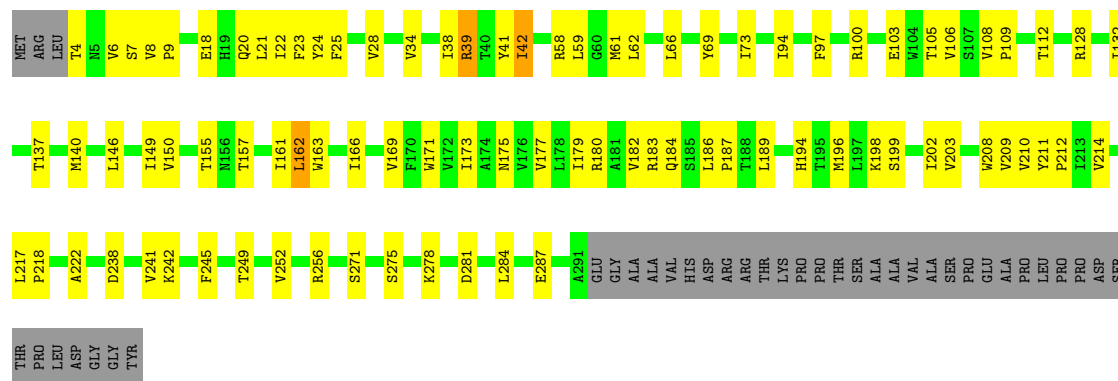
• Molecule 1: cryorhodopsin CryoR2





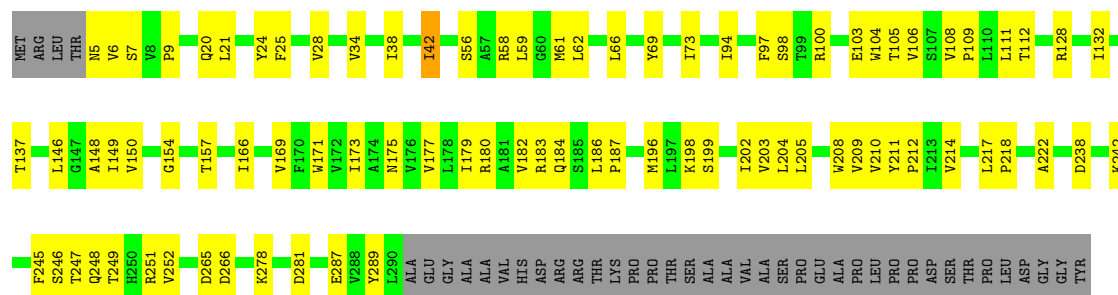
• Molecule 1: cryorhodopsin CryoR2

Chain D: 61% 26% 12%



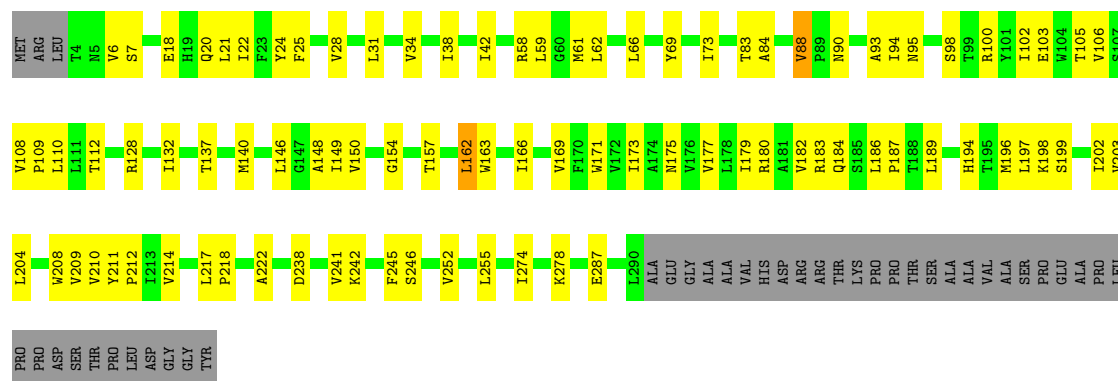
• Molecule 1: cryorhodopsin CryoR2

Chain E: 61% 26% 13%



• Molecule 1: cryorhodopsin CryoR2

Chain H: 60% 27% 12%



• Molecule 1: cryorhodopsin CryoR2

T249	L146	Met
V252	I149	Arg
E287	V150	Leu
L280	T157	T4
A291	T166	N5
GLY	V169	V6
ALA	F170	S7
ALA	V171	V8
VAL	I172	P9
HIS	I173	L21
ASP	A174	Y24
ARG	N175	F25
ARG	V176	V28
THR	V177	V34
LYS	L178	I38
PRO	I179	I42
PRO	R180	S56
THR	A181	A57
SER	V182	R58
ALA	L183	L59
ALA	K184	G60
VAL	S185	M61
ALA	L186	L62
SER	P187	L66
PRO	H194	A59
GLU	T195	Y69
ALA	M196	I73
PRO	L197	I94
LEU	K198	F97
PRO	S199	S98
ASP	I202	T99
THR	V203	R100
PRO	L204	Y101
LEU	W208	T102
ASP	V209	E103
GLY	V210	M104
GLY	Y211	T105
TYR	I213	V106
	V214	S107
	L217	P109
	P218	
	A222	T112
		I128
	D238	
	K242	I132
	F245	T137

Chain F: 62% 25% 12%

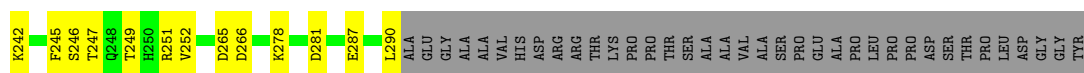
GLY TYR	V214	R128	R129	I132	T137	L146	G147	A148	I149	V150	G154	T157	L162	I166	V169	F170	W171	V172	I173	A174	N175	V176	L178	I179	R180	A181	V182	R183	Q184	S185	L186	P187	E192	M196	L197	K198	S199	L202	V203	L204	L205	W208	V209	V210	Y211	P212	T213			
	L217	P218	A222	D238	K242	S246	T247	Q248	R251	V252	T274	R286	E287	V288	Y289	L290	A291	GLU	GLY	ALA	ALA	VAL	HIS	ASP	ARG	ARG	THR	LYS	PRO	PRO	PRO	THR	ALA	ALA	VAL	ALA	SER	PRO	GLU	ALA	PRO	LEU	PRO	PRO	ASP	SER	THR	PRO	LEU	ASP
ARG	LEU	THR	N5	V6	S7	V8	P9	N16	A17	E18	H19	Q20	L21	T22	F23	V24	F25	L26	V27	V28	V34	I38	I42	R58	L59	G60	N61	L62	L66	L67	A68	V69	I73	G85	F97	R100	E103	W104	T105	V106	S107	V108	P109	T112	G125					

Chain I: 63% 25% 11%

[illegible]

Chain K: 62% 25% 13%

G147	G148	I149	V150	G154	T157	L162	V163	I166	V169	F170	H171	F172	I173	A174	V175	F176	V177	L178	I179	R180	A181	V182	R183	Q184	S185	L186	P187	M189	L197	K198	S199		I202	V203	L204	L205		V208	V209	V210	V211	P212	L213	V214		L217	P218		A222	D238		P241								
Met	Arg	Leu	Thr	N5	V6	S7	V8	P9		Q20	L21			Y24	F25	L26	V27	V28		V34		I38	R39		I42		R58	L59	G60	H61		L66		Y69		I73		N95	I96	F97		R100		E103	T104	T105	V106	S107	V108	P109	L110	L111		R128		I132		F142		L146



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.76Å 84.98Å 296.40Å 90.00° 96.83° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (20.00-3.00) 86.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.266 , 0.301 (Not available) , 0.254	Depositor DCC
R_{free} test set	3192 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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	0.94	EDS
Total number of atoms	21953	wwPDB-VP
Average B, all atoms (Å ²)	90.0	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 43.57 % 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 1.7304e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LFA, PO4, RET, OLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	0/2194	1.65	0/3013
1	B	1.00	0/2200	1.66	0/3022
1	C	1.02	0/2186	1.66	0/3003
1	D	1.01	0/2185	1.66	0/3004
1	E	1.00	0/2179	1.65	0/2994
1	F	1.00	0/2201	1.66	0/3022
1	G	1.01	0/2197	1.64	0/3018
1	H	1.02	0/2178	1.66	0/2992
1	I	1.01	0/2185	1.66	0/3004
1	K	1.01	0/2179	1.66	0/2994
All	All	1.01	0/21884	1.66	0/30066

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	2146	0	2186	69	0
1	B	2152	0	2192	75	0
1	C	2138	0	2176	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2137	0	2171	81	0
1	E	2132	0	2171	77	0
1	F	2153	0	2201	74	0
1	G	2149	0	2187	69	0
1	H	2131	0	2169	85	0
1	I	2138	0	2164	73	0
1	K	2132	0	2171	71	0
2	A	35	0	66	1	0
2	B	38	0	72	2	0
2	C	12	0	22	0	0
2	D	19	0	33	1	0
2	E	23	0	44	1	0
2	F	38	0	72	2	0
2	G	35	0	66	1	0
2	H	12	0	22	1	0
2	I	10	0	19	0	0
2	K	33	0	60	1	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	1	0
3	G	5	0	0	0	0
3	H	5	0	0	1	0
3	I	5	0	0	0	0
3	K	5	0	0	0	0
4	A	20	0	27	6	0
4	B	20	0	27	7	0
4	C	20	0	27	5	0
4	D	20	0	27	5	0
4	E	20	0	27	6	0
4	F	20	0	27	7	0
4	G	20	0	27	6	0
4	H	20	0	27	6	0
4	I	20	0	27	6	0
4	K	20	0	27	6	0
5	D	20	0	33	1	0
5	I	20	0	33	2	0
All	All	21953	0	22600	741	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 17.

The worst 5 of 741 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	1.60	1.01
1:H:31:LEU:O	1:H:34:VAL:HG12	1.58	0.99
1:E:5:ASN:HB2	1:E:157:THR:OG1	1.64	0.96
1:D:39:ARG:HG2	1:E:56:SER:HB2	1.49	0.94
1:K:5:ASN:HB2	1:K:157:THR:OG1	1.70	0.91

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	285/327 (87%)	271 (95%)	14 (5%)	0	100	100
1	B	286/327 (88%)	269 (94%)	17 (6%)	0	100	100
1	C	285/327 (87%)	269 (94%)	16 (6%)	0	100	100
1	D	286/327 (88%)	272 (95%)	14 (5%)	0	100	100
1	E	284/327 (87%)	268 (94%)	16 (6%)	0	100	100
1	F	285/327 (87%)	270 (95%)	15 (5%)	0	100	100
1	G	286/327 (88%)	273 (96%)	13 (4%)	0	100	100
1	H	285/327 (87%)	270 (95%)	15 (5%)	0	100	100
1	I	288/327 (88%)	274 (95%)	14 (5%)	0	100	100
1	K	284/327 (87%)	267 (94%)	17 (6%)	0	100	100
All	All	2854/3270 (87%)	2703 (95%)	151 (5%)	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	223/261 (85%)	221 (99%)	2 (1%)	70	85
1	B	224/261 (86%)	223 (100%)	1 (0%)	84	90
1	C	221/261 (85%)	218 (99%)	3 (1%)	59	80
1	D	221/261 (85%)	218 (99%)	3 (1%)	59	80
1	E	222/261 (85%)	221 (100%)	1 (0%)	81	89
1	F	225/261 (86%)	223 (99%)	2 (1%)	70	85
1	G	223/261 (85%)	219 (98%)	4 (2%)	51	77
1	H	220/261 (84%)	218 (99%)	2 (1%)	70	85
1	I	219/261 (84%)	217 (99%)	2 (1%)	70	85
1	K	222/261 (85%)	221 (100%)	1 (0%)	81	89
All	All	2220/2610 (85%)	2199 (99%)	21 (1%)	70	85

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

Mol	Chain	Res	Type
1	G	66	LEU
1	F	286	ARG
1	K	42	ILE
1	I	42	ILE
1	F	162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	19	HIS
1	K	20	GLN
1	K	175	ASN
1	K	19	HIS
1	H	20	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	403	-	9,9,19	0.09	0	8,8,18	0.09	0
4	RET	G	406	1	20,20,21	1.46	3 (15%)	27,27,28	1.00	2 (7%)
2	LFA	A	402	-	6,6,19	0.14	0	5,5,18	0.13	0
4	RET	B	406	1	20,20,21	1.51	4 (20%)	27,27,28	0.99	2 (7%)
2	LFA	B	404	-	7,7,19	0.10	0	6,6,18	0.08	0
2	LFA	D	403	-	8,8,19	0.09	0	7,7,18	0.12	0
4	RET	F	406	1	20,20,21	1.56	4 (20%)	27,27,28	1.01	2 (7%)
5	OLA	D	401	-	19,19,19	0.53	0	19,19,19	0.47	0
3	PO4	C	403	-	4,4,4	0.71	0	6,6,6	0.47	0
2	LFA	F	402	-	6,6,19	0.13	0	5,5,18	0.11	0
2	LFA	E	402	-	11,11,19	0.10	0	10,10,18	0.11	0
2	LFA	B	403	-	11,11,19	0.10	0	10,10,18	0.07	0
2	LFA	F	403	-	10,10,19	0.11	0	9,9,18	0.09	0
2	LFA	F	404	-	11,11,19	0.09	0	10,10,18	0.07	0
2	LFA	K	402	-	11,11,19	0.10	0	10,10,18	0.11	0
2	LFA	E	401	-	10,10,19	0.11	0	9,9,18	0.09	0
4	RET	C	404	1	20,20,21	1.51	3 (15%)	27,27,28	1.00	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	A	401	-	10,10,19	0.09	0	9,9,18	0.10	0
2	LFA	I	402	-	9,9,19	0.10	0	8,8,18	0.08	0
2	LFA	C	402	-	5,5,19	0.13	0	4,4,18	0.12	0
4	RET	D	405	1	20,20,21	1.57	3 (15%)	27,27,28	1.04	2 (7%)
4	RET	H	404	1	20,20,21	1.47	3 (15%)	27,27,28	1.07	2 (7%)
2	LFA	G	403	-	9,9,19	0.09	0	8,8,18	0.07	0
3	PO4	G	405	-	4,4,4	0.70	0	6,6,6	0.45	0
3	PO4	F	405	-	4,4,4	0.66	0	6,6,6	0.47	0
2	LFA	A	404	-	6,6,19	0.12	0	5,5,18	0.11	0
4	RET	A	406	1	20,20,21	1.53	3 (15%)	27,27,28	1.03	2 (7%)
2	LFA	B	401	-	6,6,19	0.14	0	5,5,18	0.09	0
2	LFA	D	402	-	9,9,19	0.09	0	8,8,18	0.10	0
2	LFA	K	401	-	10,10,19	0.10	0	9,9,18	0.09	0
5	OLA	I	401	-	19,19,19	0.53	0	19,19,19	0.46	0
2	LFA	B	402	-	10,10,19	0.11	0	9,9,18	0.10	0
4	RET	E	404	1	20,20,21	1.51	4 (20%)	27,27,28	1.00	1 (3%)
2	LFA	C	401	-	5,5,19	0.15	0	4,4,18	0.12	0
2	LFA	H	401	-	5,5,19	0.16	0	4,4,18	0.13	0
3	PO4	K	404	-	4,4,4	0.69	0	6,6,6	0.48	0
4	RET	K	405	1	20,20,21	1.57	3 (15%)	27,27,28	0.99	1 (3%)
2	LFA	G	402	-	6,6,19	0.13	0	5,5,18	0.11	0
2	LFA	G	404	-	6,6,19	0.10	0	5,5,18	0.09	0
2	LFA	K	403	-	9,9,19	0.07	0	8,8,18	0.10	0
3	PO4	A	405	-	4,4,4	0.69	0	6,6,6	0.47	0
3	PO4	I	403	-	4,4,4	0.69	0	6,6,6	0.47	0
3	PO4	B	405	-	4,4,4	0.72	0	6,6,6	0.46	0
3	PO4	H	403	-	4,4,4	0.68	0	6,6,6	0.46	0
2	LFA	H	402	-	5,5,19	0.16	0	4,4,18	0.13	0
4	RET	I	404	1	20,20,21	1.60	3 (15%)	27,27,28	1.07	2 (7%)
3	PO4	E	403	-	4,4,4	0.72	0	6,6,6	0.44	0
2	LFA	G	401	-	10,10,19	0.09	0	9,9,18	0.09	0
3	PO4	D	404	-	4,4,4	0.74	0	6,6,6	0.46	0
2	LFA	F	401	-	7,7,19	0.13	0	6,6,18	0.11	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	A	403	-	-	1/7/7/17	-

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

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	404	RET	C14-C13	4.46	1.36	1.33
4	D	405	RET	C14-C13	4.38	1.36	1.33
4	K	405	RET	C14-C13	4.22	1.36	1.33
4	A	406	RET	C14-C13	4.16	1.36	1.33
4	F	406	RET	C14-C13	4.12	1.36	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	404	RET	C19-C9-C10	-3.55	117.07	122.82
4	D	405	RET	C19-C9-C10	-3.41	117.30	122.82
4	F	406	RET	C19-C9-C10	-3.38	117.34	122.82
4	E	404	RET	C19-C9-C10	-3.30	117.46	122.82
4	H	404	RET	C19-C9-C10	-3.30	117.47	122.82

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	404	LFA	C15-C16-C17-C18
2	F	403	LFA	C6-C7-C8-C9
2	B	403	LFA	C5-C6-C7-C8
2	B	402	LFA	C6-C7-C8-C9
5	I	401	OLA	C13-C14-C15-C16

There are no ring outliers.

26 monomers are involved in 74 short contacts:

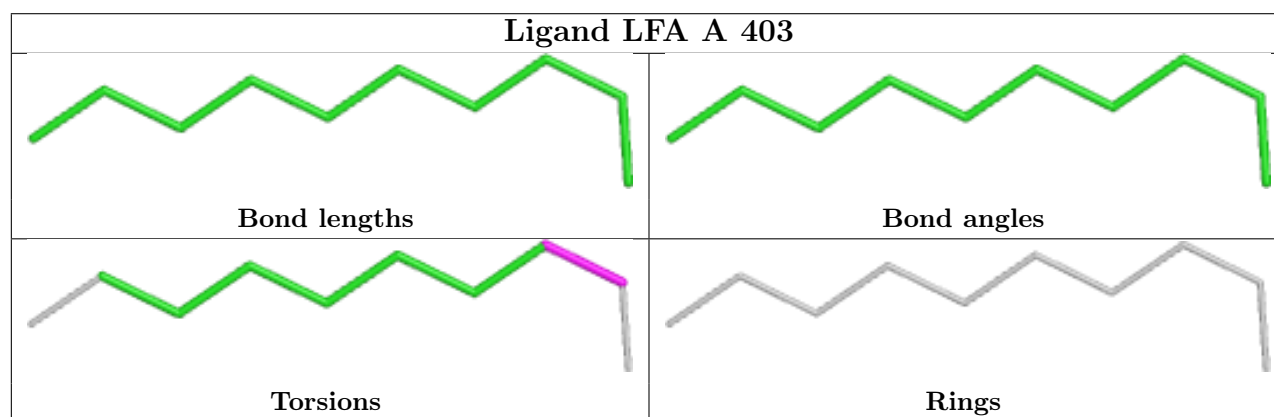
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	406	RET	6	0
4	B	406	RET	7	0
2	B	404	LFA	1	0
2	D	403	LFA	1	0
4	F	406	RET	7	0
5	D	401	OLA	1	0
2	E	402	LFA	1	0
2	B	403	LFA	1	0
2	F	404	LFA	1	0
2	K	402	LFA	1	0
4	C	404	RET	5	0
4	D	405	RET	5	0
4	H	404	RET	6	0

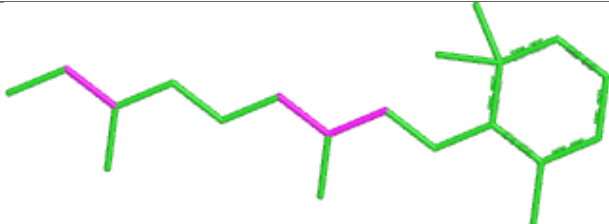
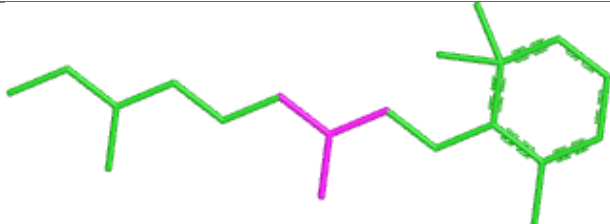
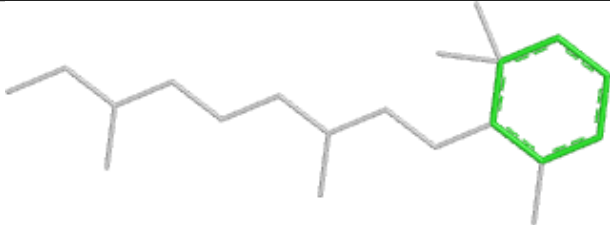
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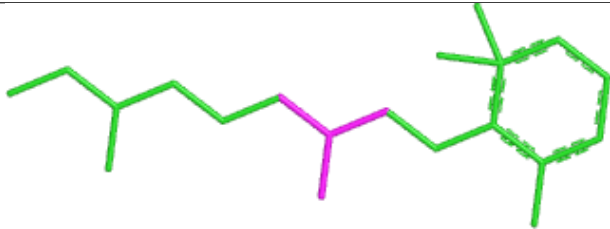
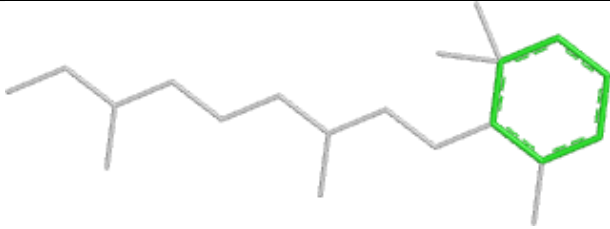
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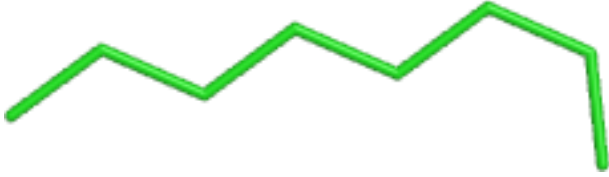
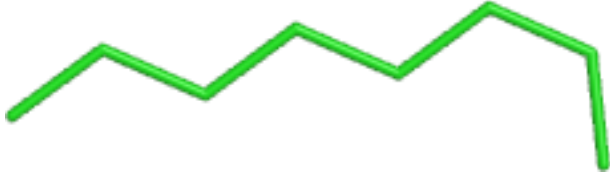
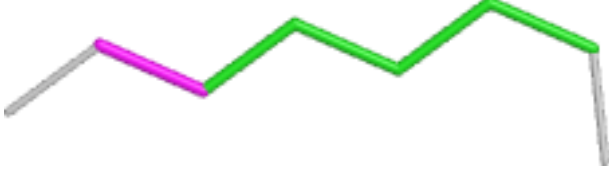
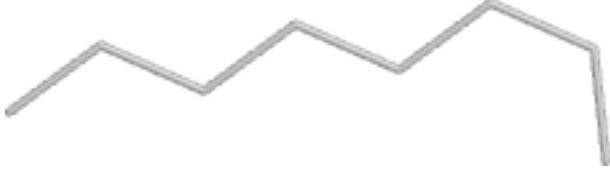
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	405	PO4	1	0
2	A	404	LFA	1	0
4	A	406	RET	6	0
2	D	402	LFA	1	0
5	I	401	OLA	2	0
4	E	404	RET	6	0
2	H	401	LFA	1	0
4	K	405	RET	6	0
2	G	404	LFA	1	0
3	H	403	PO4	1	0
4	I	404	RET	6	0
3	D	404	PO4	1	0
2	F	401	LFA	1	0

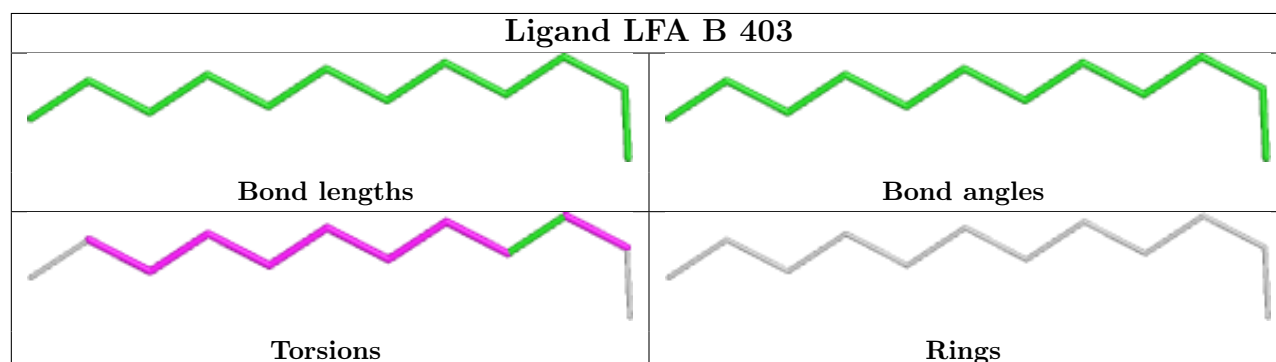
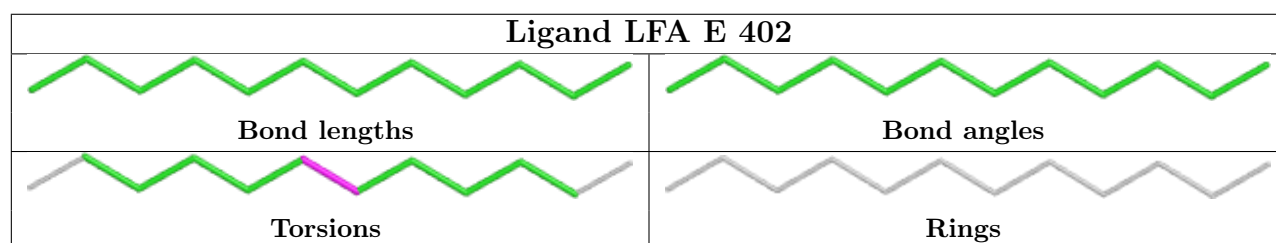
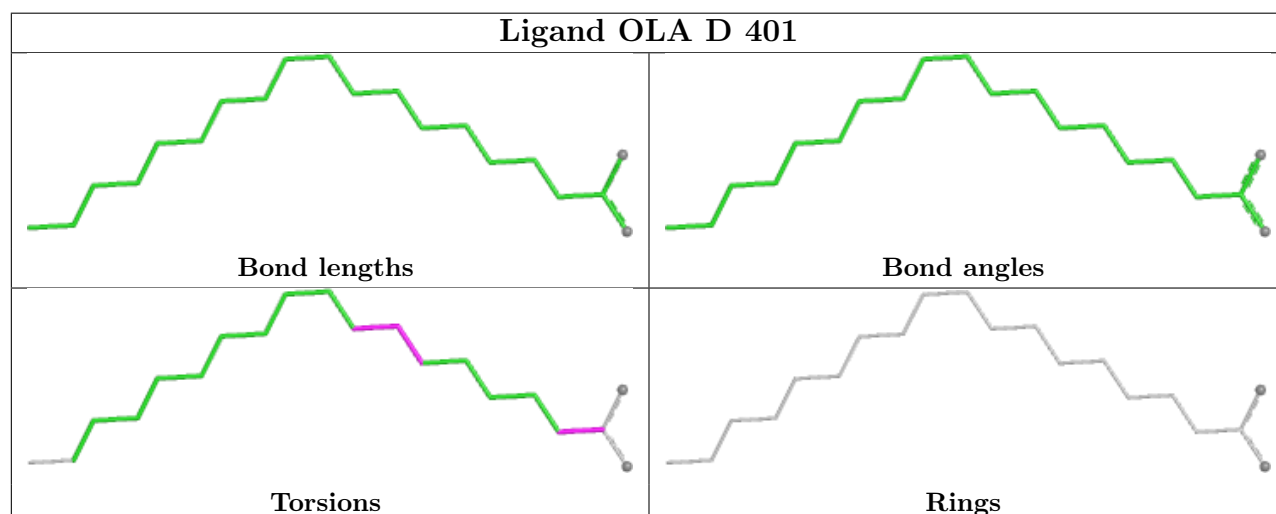
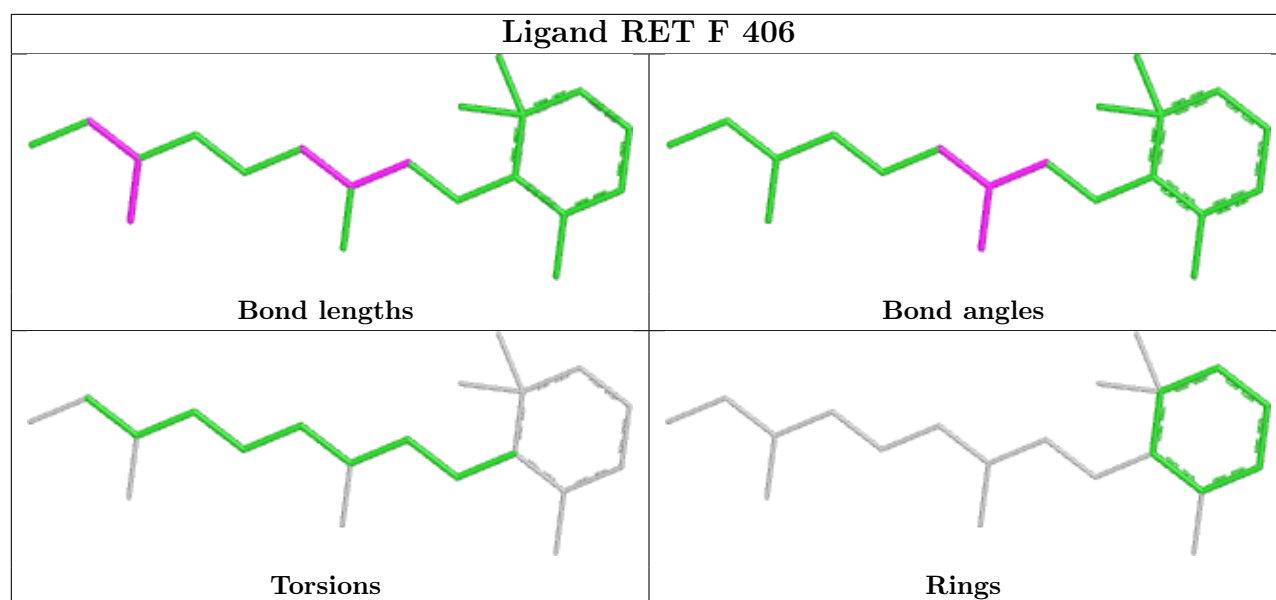
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

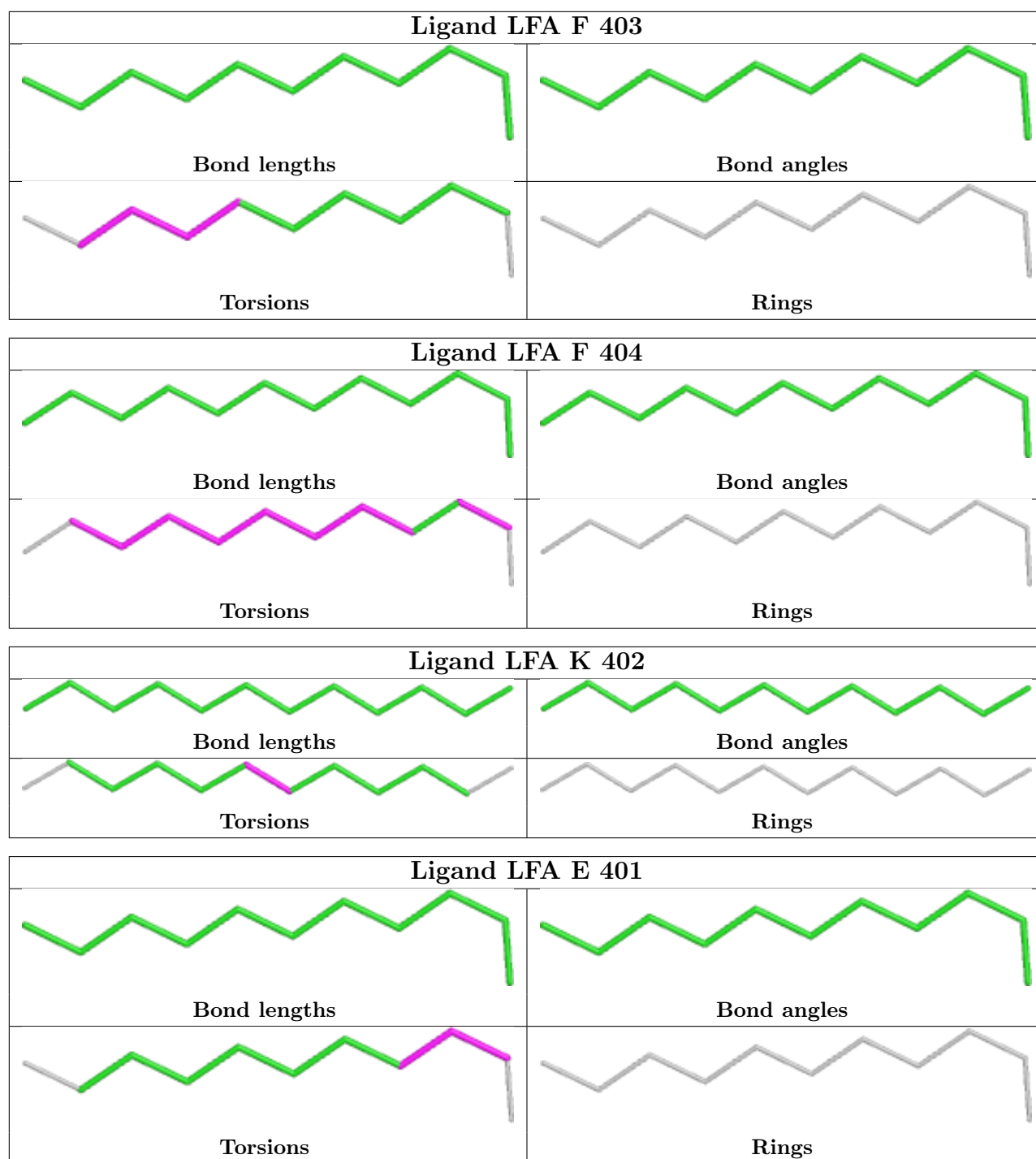


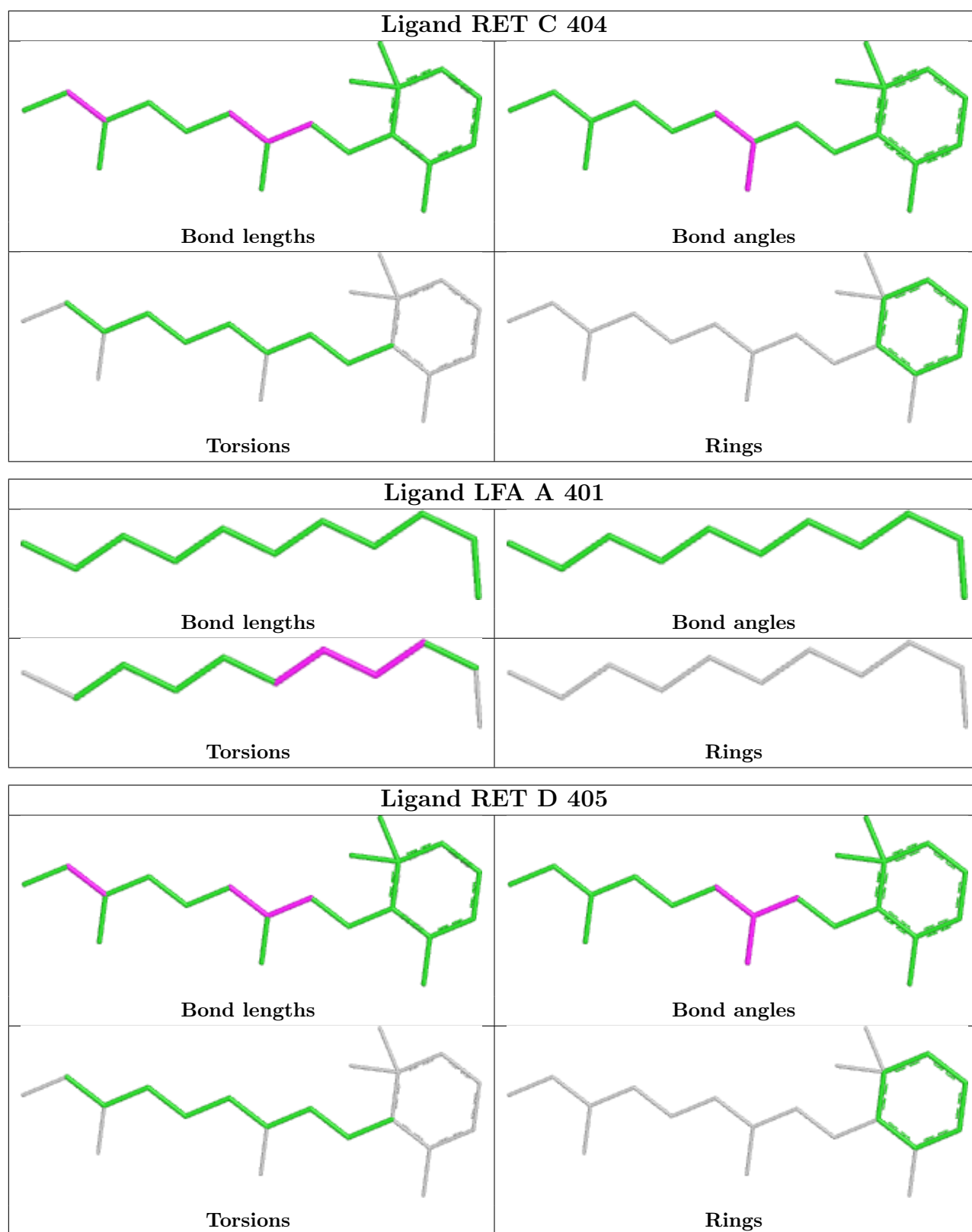
Ligand RET G 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

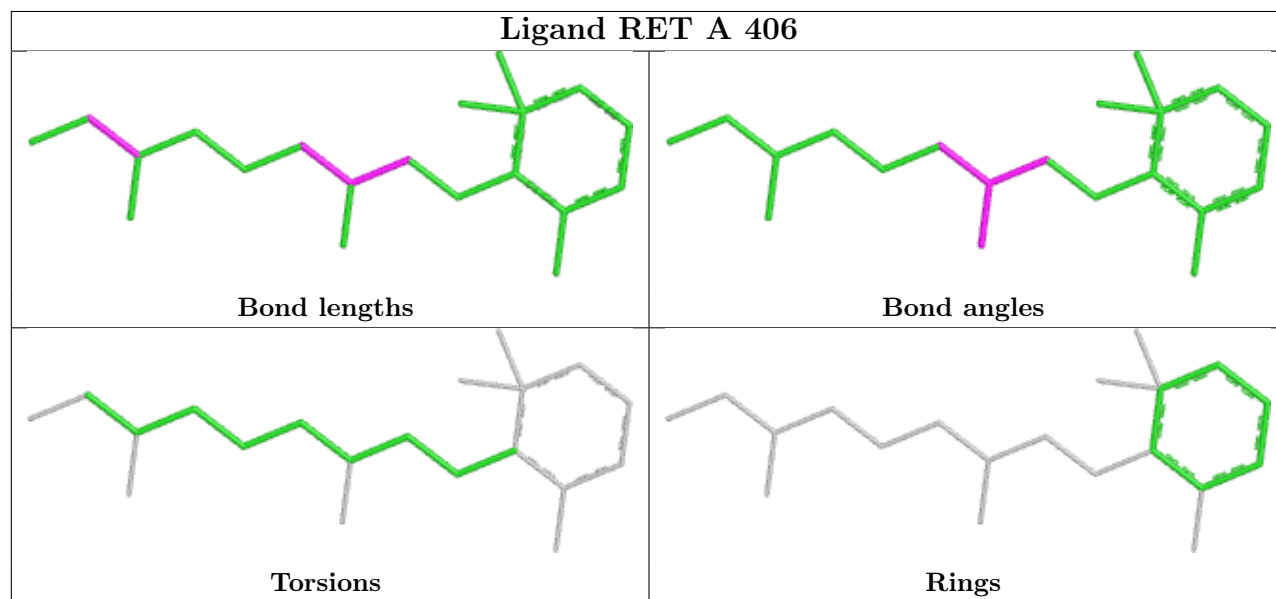
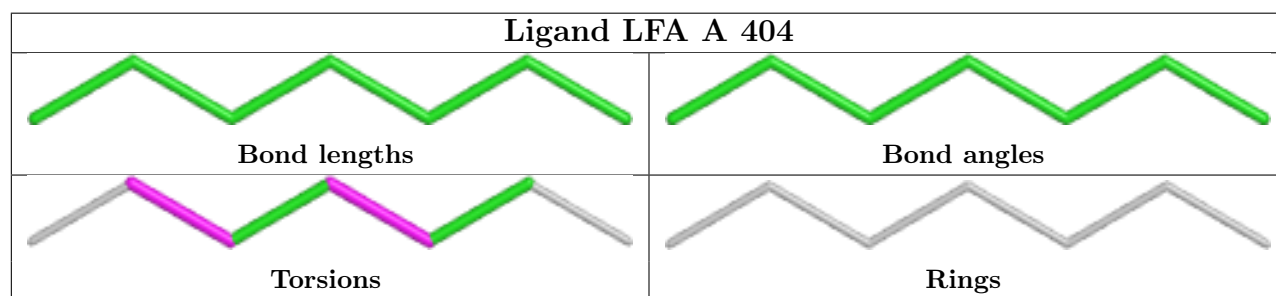
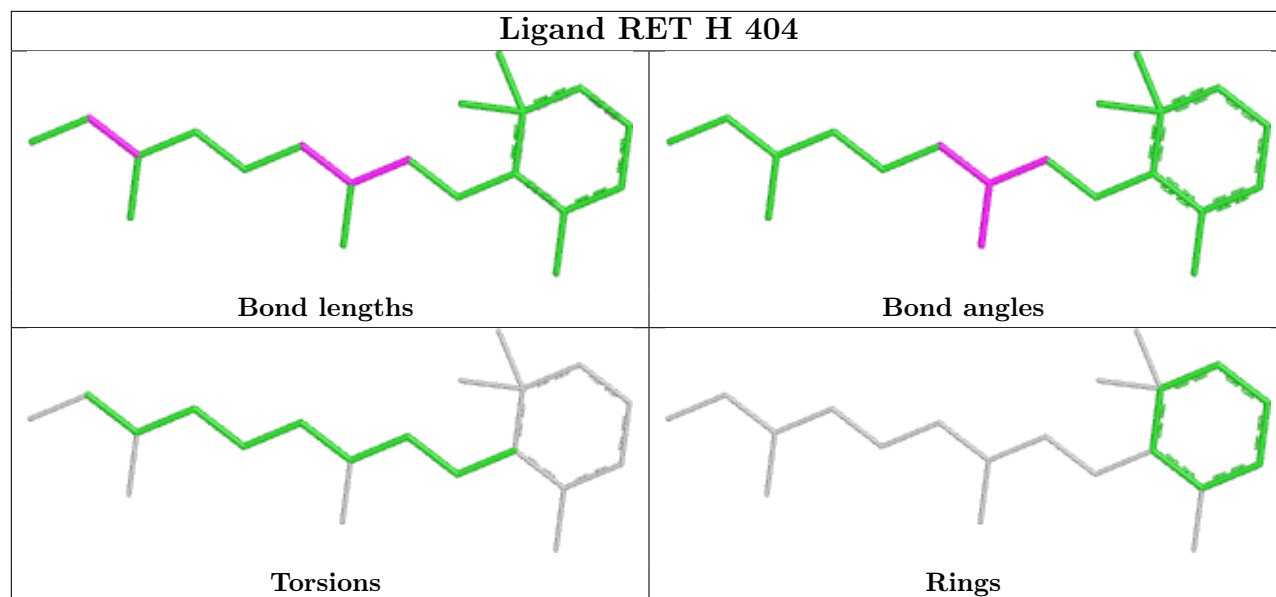
Ligand RET B 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

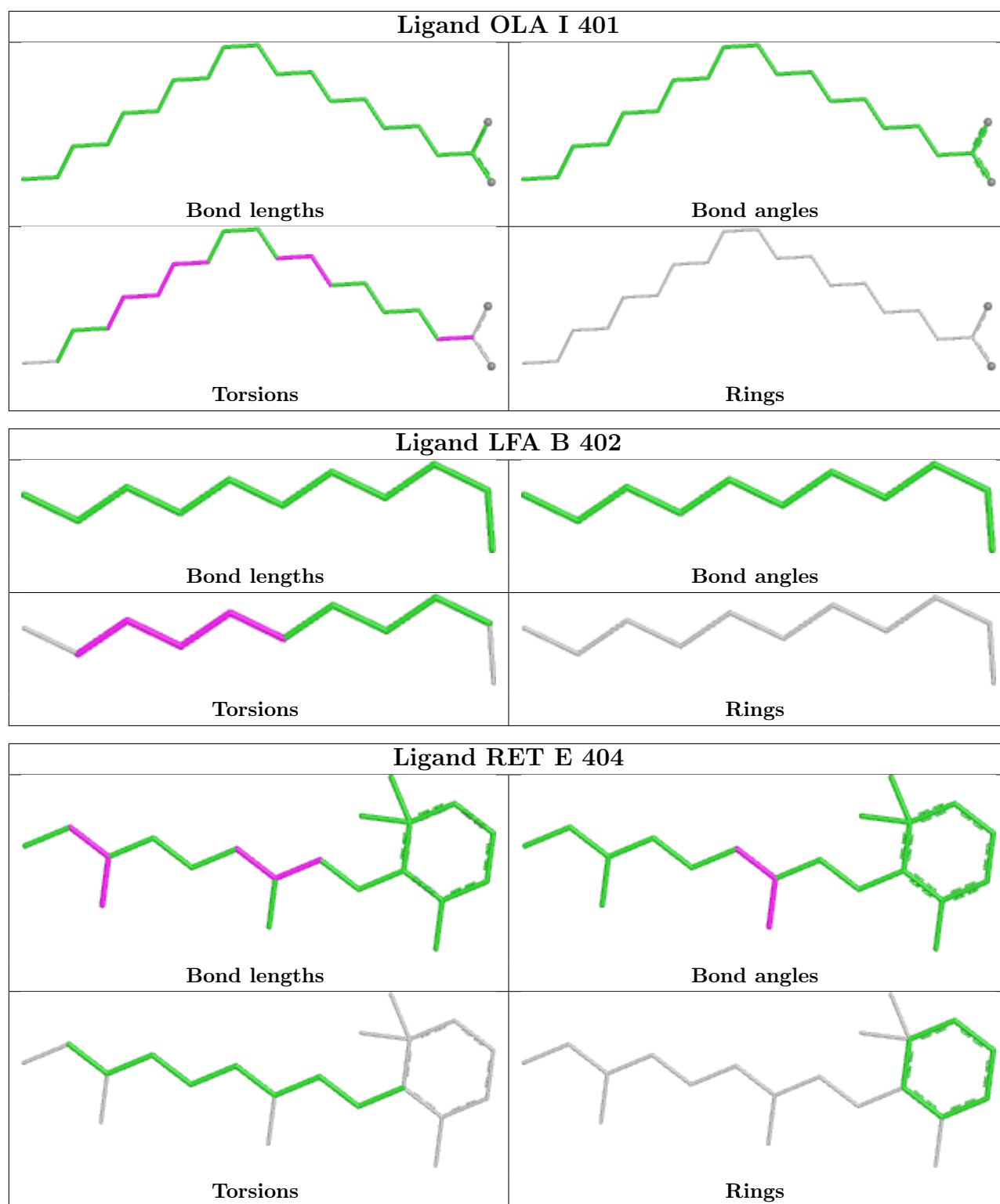
Ligand LFA B 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

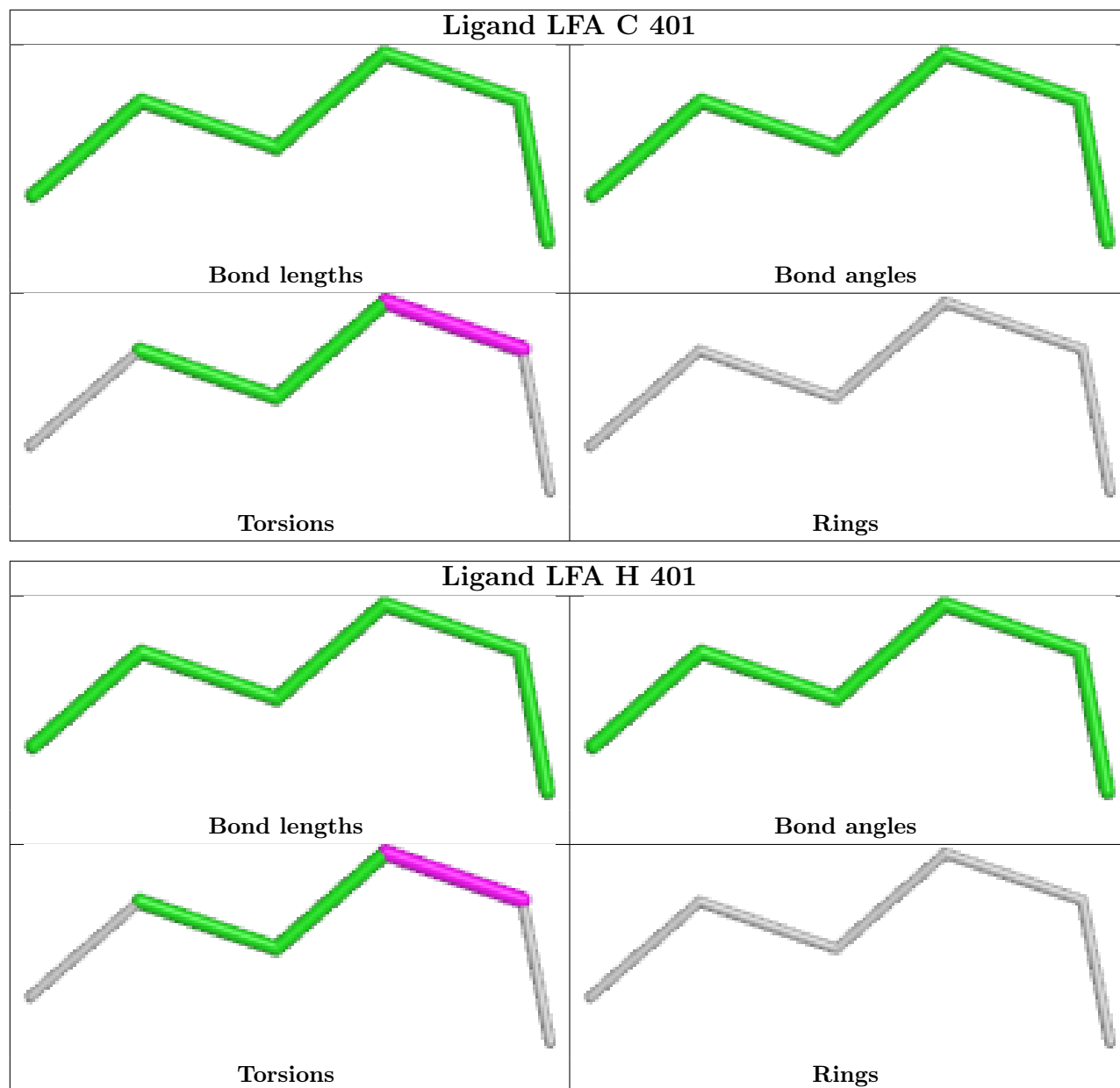


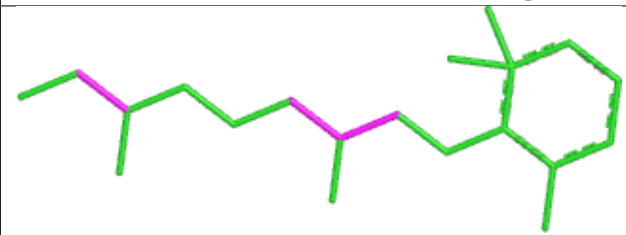
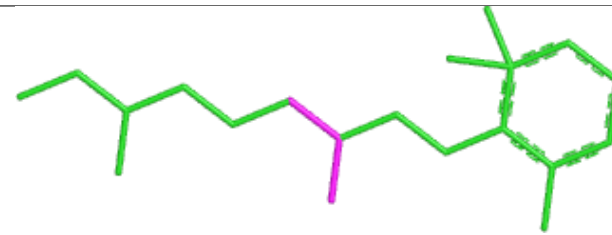
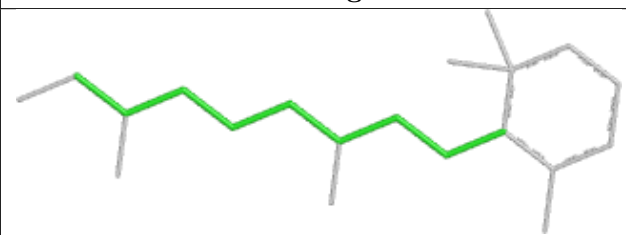
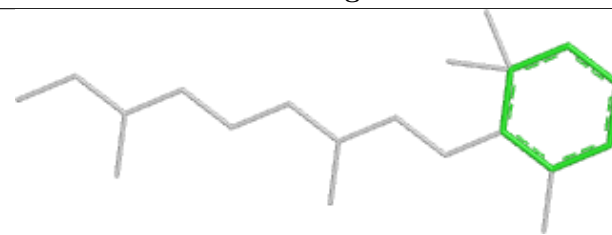


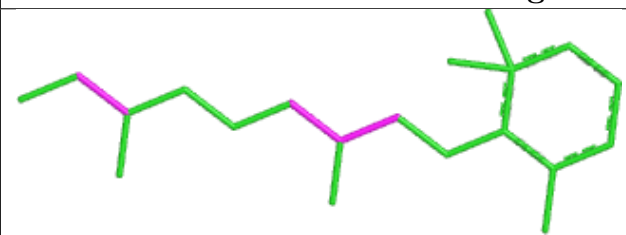
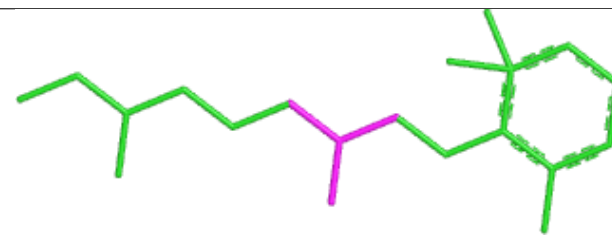
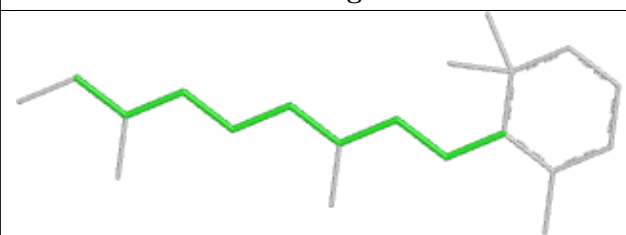
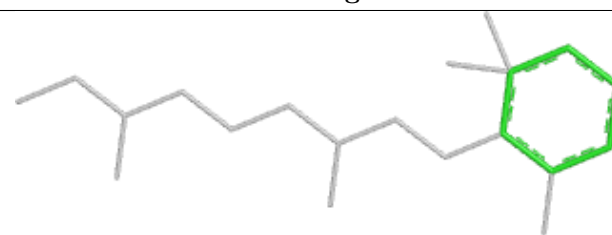


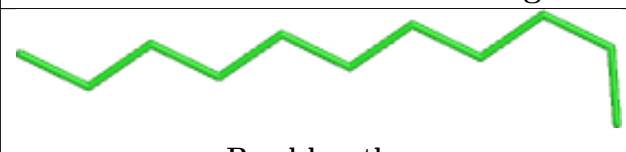
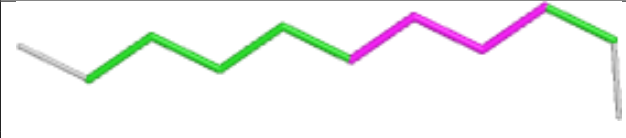
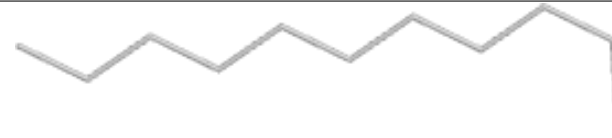


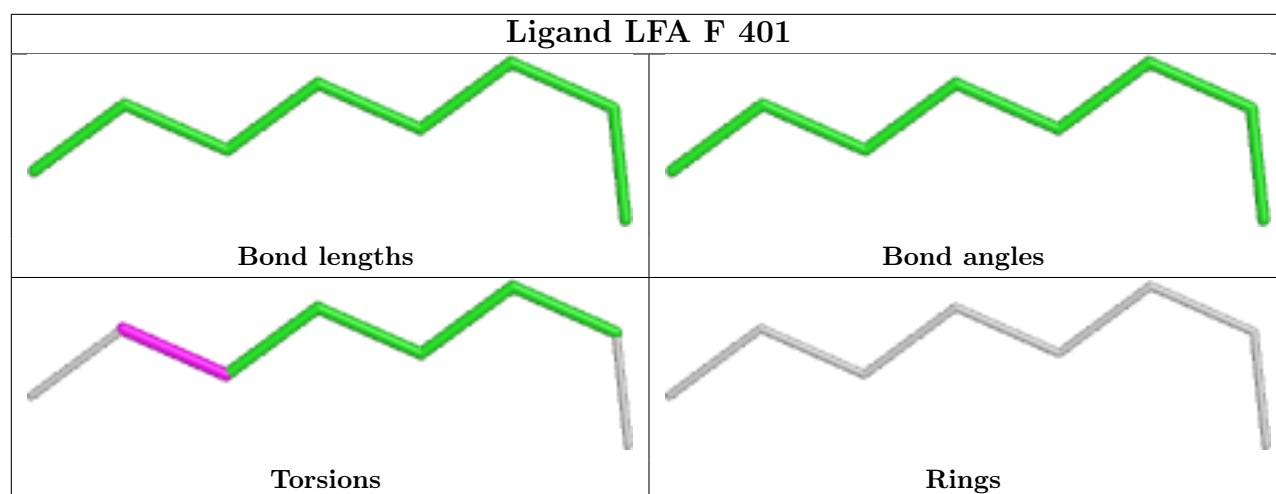




Ligand RET K 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand RET I 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA G 401	
	
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	287/327 (87%)	-0.28	0 100 100	58, 85, 131, 174	0
1	B	288/327 (88%)	-0.38	0 100 100	50, 81, 119, 178	0
1	C	287/327 (87%)	-0.27	0 100 100	59, 91, 135, 185	0
1	D	288/327 (88%)	-0.28	0 100 100	56, 93, 130, 164	0
1	E	286/327 (87%)	-0.32	0 100 100	57, 85, 124, 173	0
1	F	287/327 (87%)	-0.38	0 100 100	56, 81, 120, 161	0
1	G	288/327 (88%)	-0.33	0 100 100	54, 86, 130, 157	0
1	H	287/327 (87%)	-0.33	0 100 100	59, 90, 130, 178	0
1	I	290/327 (88%)	-0.30	0 100 100	54, 92, 128, 157	0
1	K	286/327 (87%)	-0.35	0 100 100	52, 86, 122, 158	0
All	All	2874/3270 (87%)	-0.32	0 100 100	50, 87, 129, 185	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no 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	F	401	8/20	0.44	0.26	55,65,82,84	0
2	LFA	F	403	11/20	0.58	0.17	58,83,97,97	0
2	LFA	G	402	7/20	0.61	0.12	60,72,85,90	0
2	LFA	B	404	8/20	0.64	0.26	56,73,89,94	0
3	PO4	A	405	5/5	0.66	0.10	107,137,151,157	0
3	PO4	G	405	5/5	0.67	0.11	97,113,131,142	0
2	LFA	A	402	7/20	0.69	0.14	53,73,98,103	0
2	LFA	H	401	6/20	0.71	0.20	68,90,99,99	0
5	OLA	I	401	20/20	0.72	0.18	71,105,119,122	0
2	LFA	C	401	6/20	0.73	0.20	72,93,103,106	0
2	LFA	D	403	9/20	0.75	0.11	68,93,105,114	0
2	LFA	G	404	7/20	0.76	0.10	69,105,110,110	0
2	LFA	B	402	11/20	0.76	0.14	67,84,94,96	0
2	LFA	K	403	10/20	0.77	0.10	78,103,121,124	0
2	LFA	H	402	6/20	0.77	0.09	49,57,58,61	0
2	LFA	B	401	7/20	0.79	0.16	55,82,91,97	0
3	PO4	E	403	5/5	0.79	0.09	114,122,138,139	0
2	LFA	E	402	12/20	0.80	0.10	77,85,100,107	0
2	LFA	D	402	10/20	0.80	0.08	66,90,91,94	0
2	LFA	F	402	7/20	0.80	0.17	63,95,101,110	0
3	PO4	I	403	5/5	0.81	0.06	113,126,135,137	0
5	OLA	D	401	20/20	0.81	0.15	80,109,120,126	0
3	PO4	H	403	5/5	0.81	0.08	133,135,142,168	0
2	LFA	A	404	7/20	0.82	0.09	63,82,98,101	0
2	LFA	C	402	6/20	0.82	0.09	53,61,70,71	0
3	PO4	C	403	5/5	0.83	0.07	110,113,133,139	0
3	PO4	D	404	5/5	0.85	0.06	115,119,123,125	0
3	PO4	B	405	5/5	0.86	0.08	97,101,111,122	0
2	LFA	A	403	10/20	0.86	0.14	74,84,95,100	0
3	PO4	F	405	5/5	0.86	0.07	89,105,115,125	0
2	LFA	G	403	10/20	0.87	0.13	67,86,99,99	0
2	LFA	K	402	12/20	0.87	0.08	85,88,93,99	0
3	PO4	K	404	5/5	0.88	0.08	114,122,128,130	0
2	LFA	I	402	10/20	0.88	0.07	58,83,101,102	0
2	LFA	F	404	12/20	0.88	0.22	75,94,107,107	0
2	LFA	A	401	11/20	0.90	0.13	66,95,116,118	0
2	LFA	K	401	11/20	0.90	0.09	60,70,80,84	0
2	LFA	G	401	11/20	0.90	0.18	50,76,111,111	0
2	LFA	E	401	11/20	0.90	0.09	53,58,62,63	0
4	RET	G	406	20/21	0.92	0.19	73,91,120,122	0
4	RET	I	404	20/21	0.92	0.17	89,114,132,134	0

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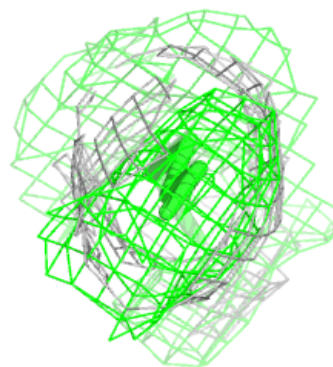
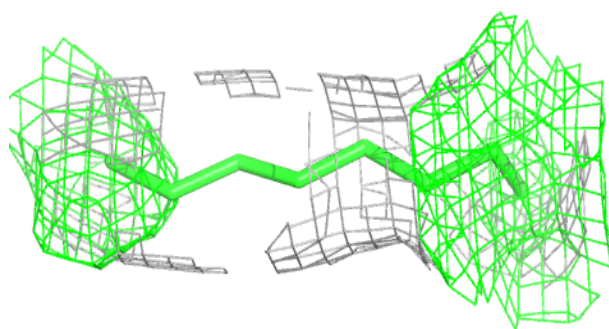
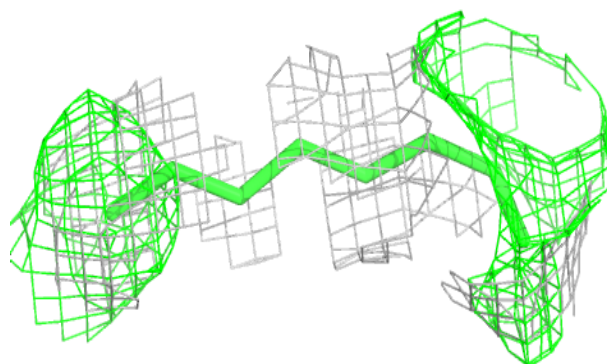
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	RET	D	405	20/21	0.93	0.18	86,101,118,126	0
4	RET	H	404	20/21	0.93	0.15	80,91,105,106	0
2	LFA	B	403	12/20	0.94	0.14	60,87,96,100	0
4	RET	A	406	20/21	0.94	0.15	76,92,103,103	0
4	RET	C	404	20/21	0.94	0.15	76,91,110,114	0
4	RET	B	406	20/21	0.95	0.13	70,87,97,99	0
4	RET	K	405	20/21	0.95	0.14	80,95,112,114	0
4	RET	E	404	20/21	0.95	0.12	79,88,101,102	0
4	RET	F	406	20/21	0.95	0.11	59,73,87,96	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.

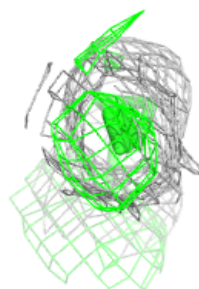
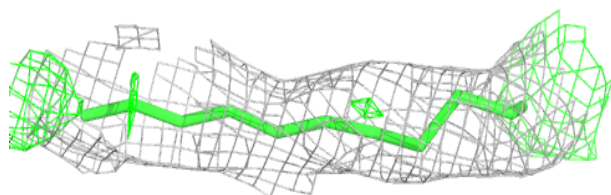
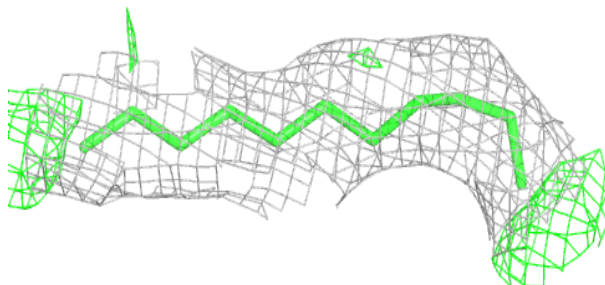
Electron density around LFA F 401:

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

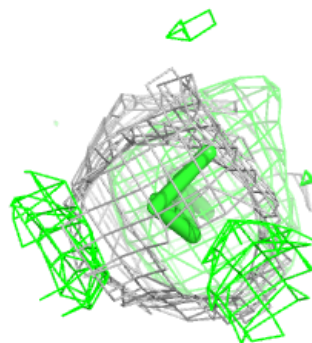
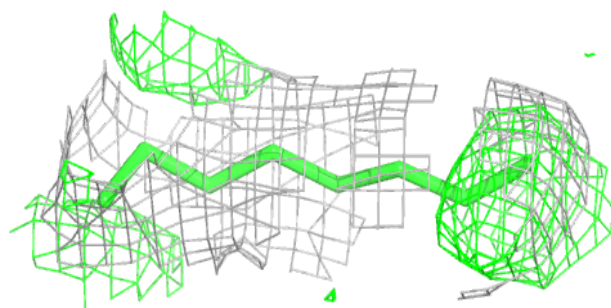
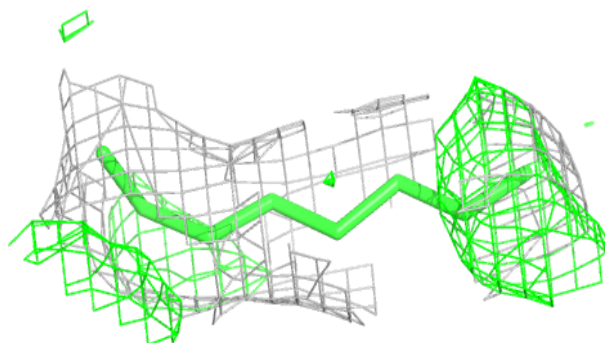


Electron density around LFA F 403:

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and green (positive)

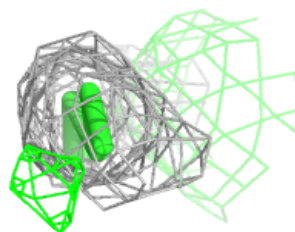
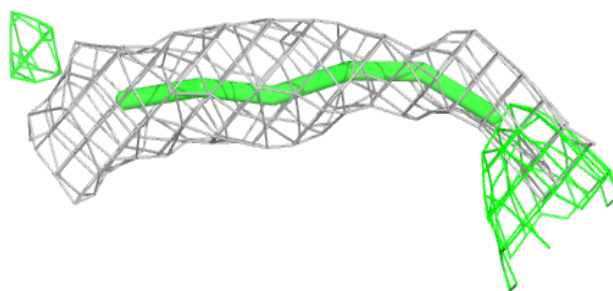
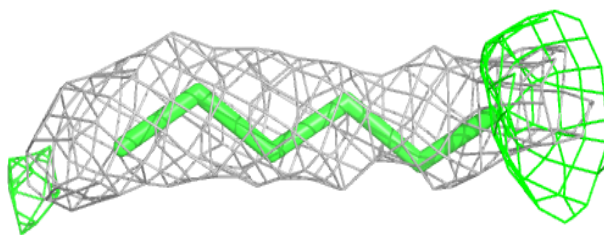
**Electron density around LFA B 404:**

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and green (positive)

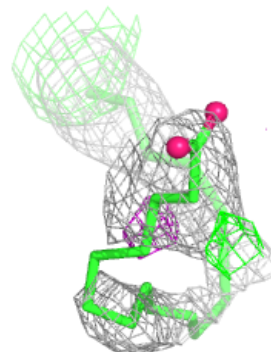
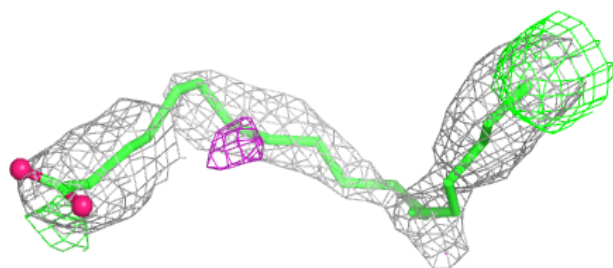
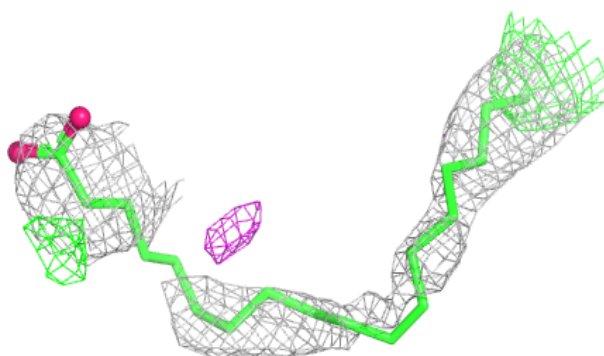


Electron density around LFA H 401:

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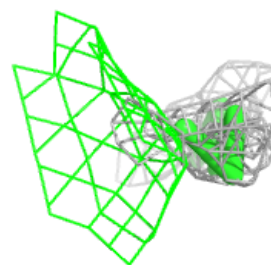
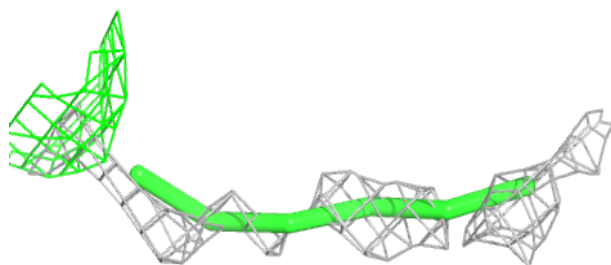
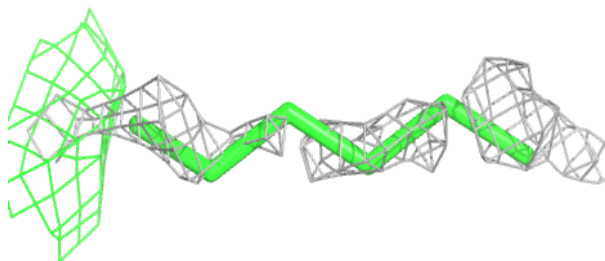
**Electron density around OLA I 401:**

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

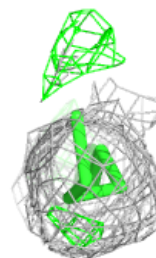
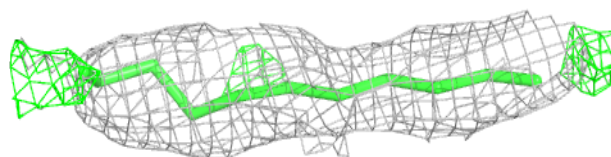
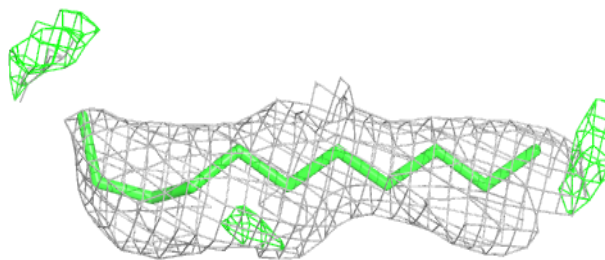


Electron density around LFA C 401:

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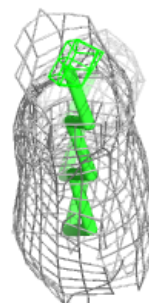
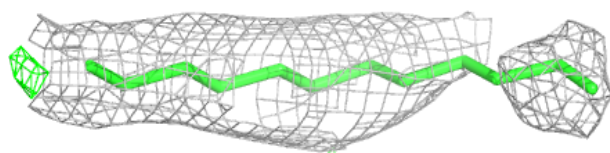
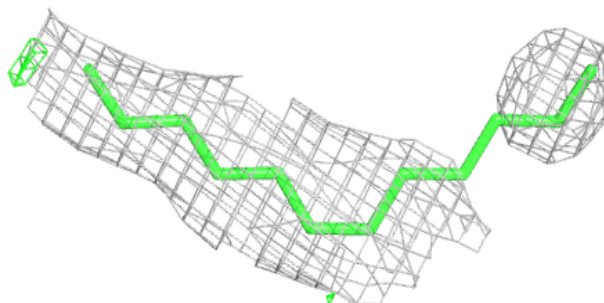
**Electron density around LFA B 402:**

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

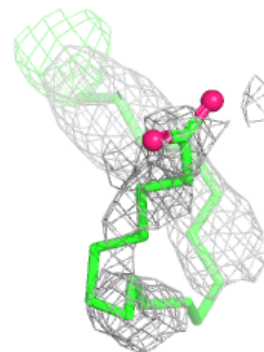
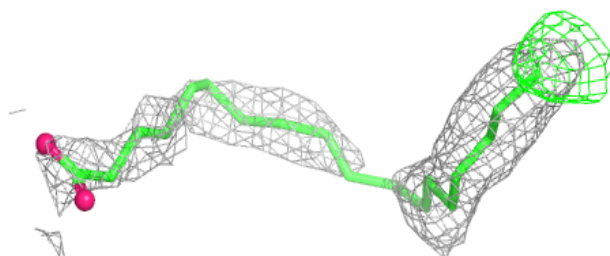
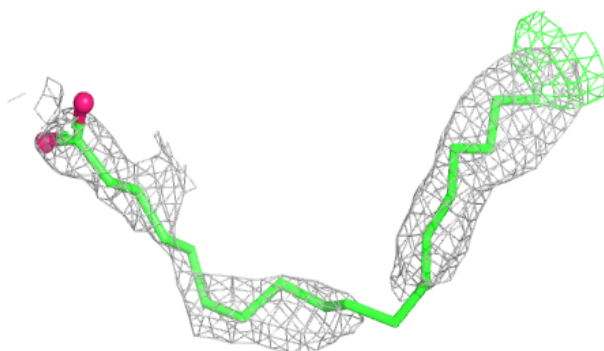


Electron density around LFA E 402:

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and green (positive)

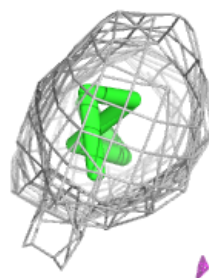
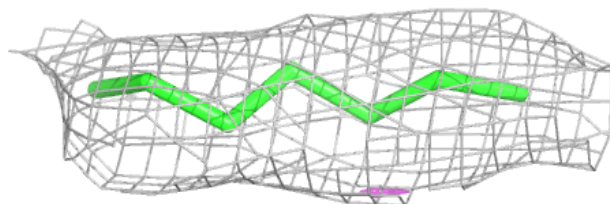
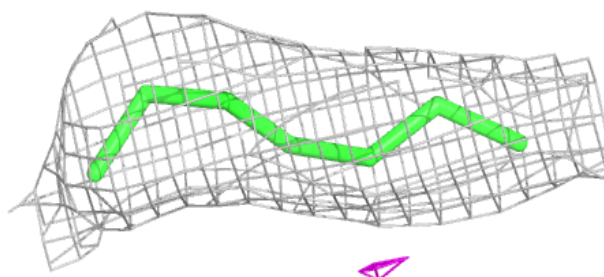
**Electron density around OLA D 401:**

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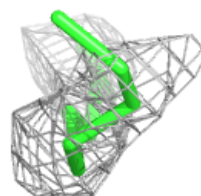
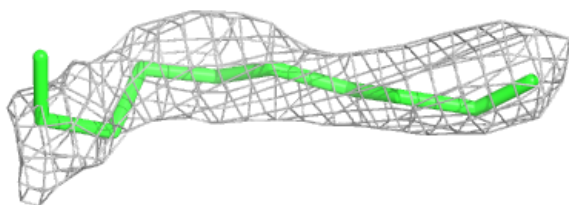
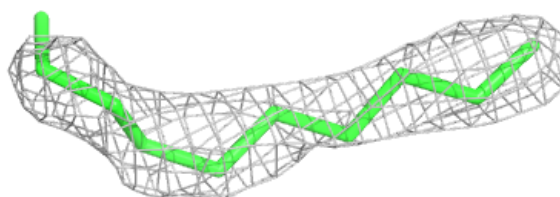


Electron density around LFA A 404:

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and green (positive)

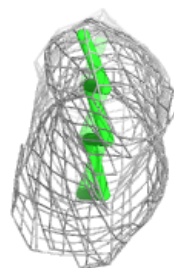
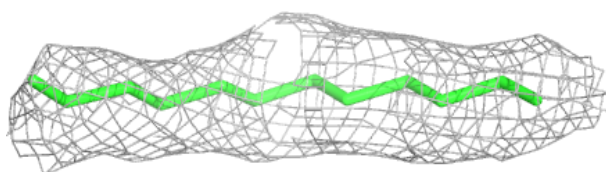
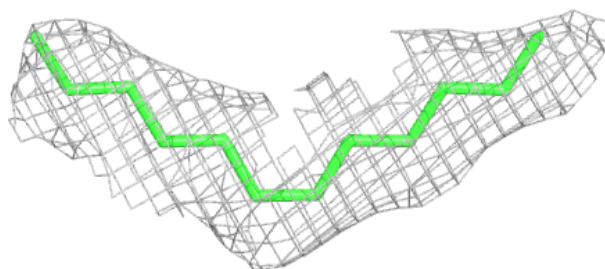
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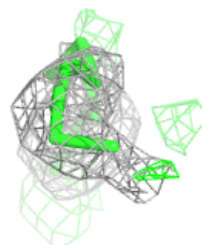
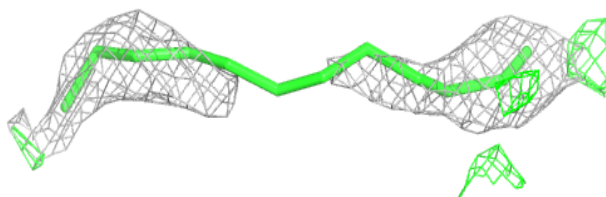
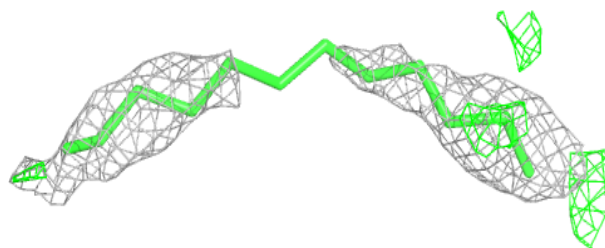


Electron density around LFA K 402:

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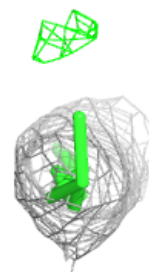
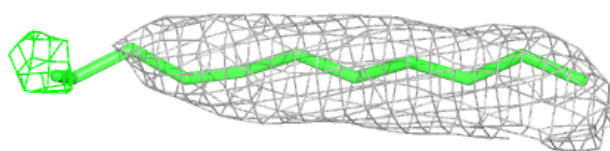
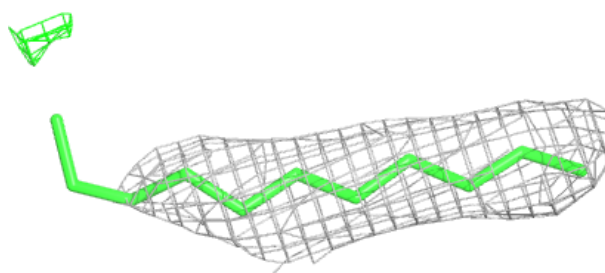
**Electron density around LFA F 404:**

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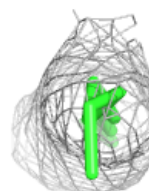
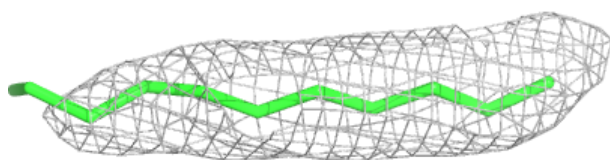
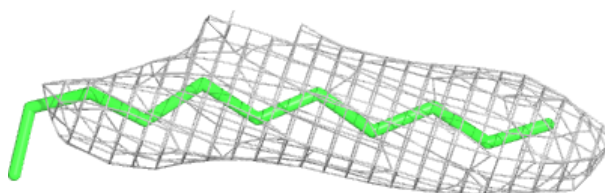


Electron density around LFA A 401:

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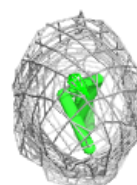
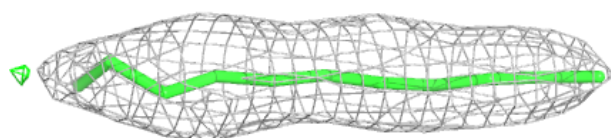
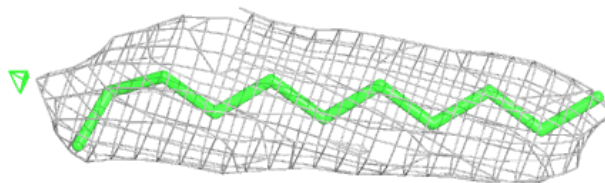
**Electron density around LFA G 401:**

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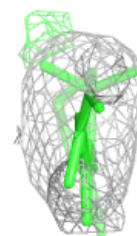
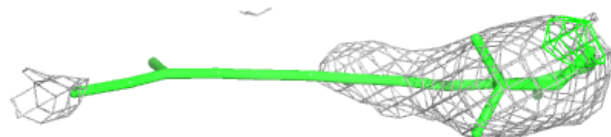
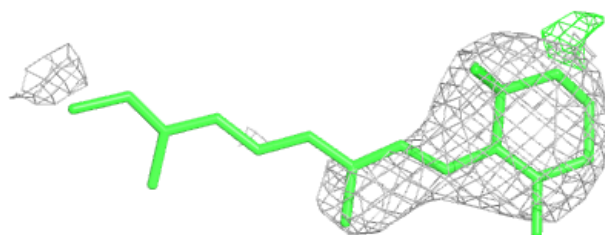


Electron density around LFA E 401:

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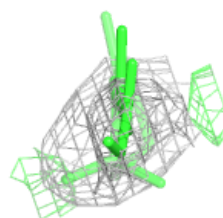
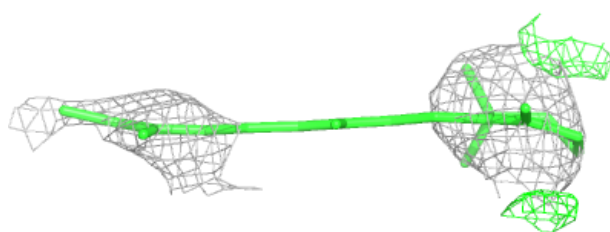
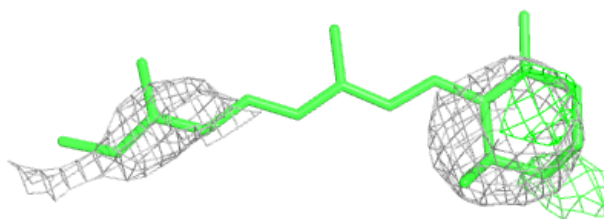
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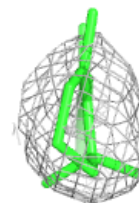
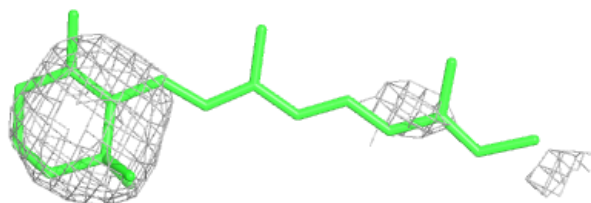


Electron density around RET I 404:

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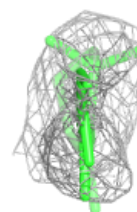
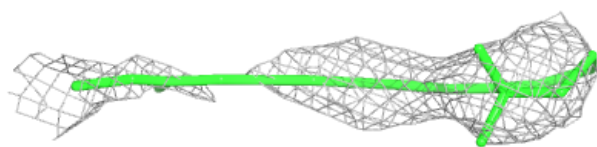
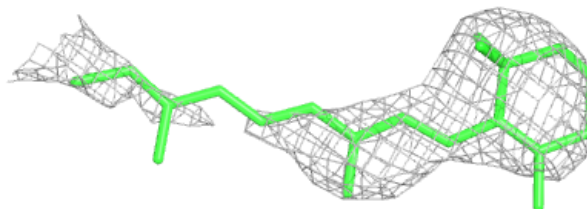
**Electron density around RET D 405:**

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

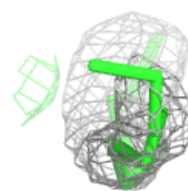
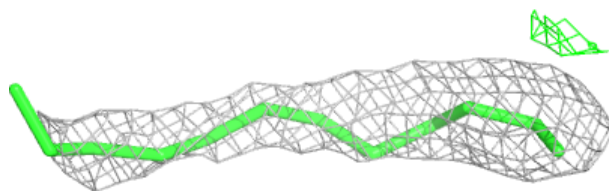
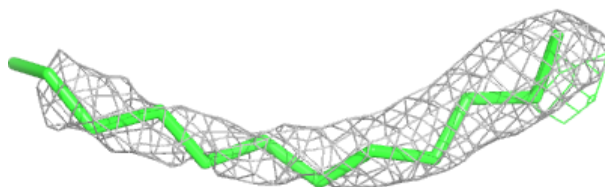


Electron density around RET H 404:

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

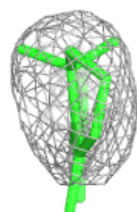
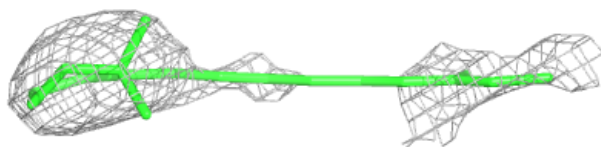
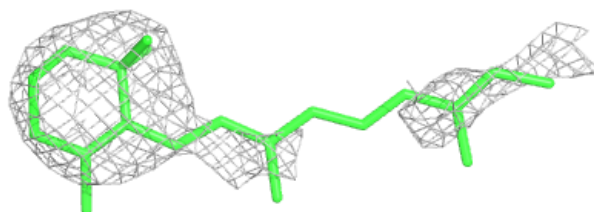
**Electron density around LFA B 403:**

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

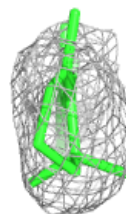
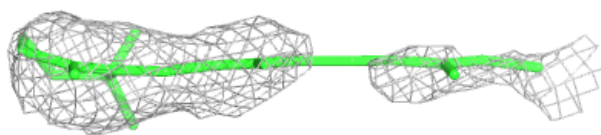
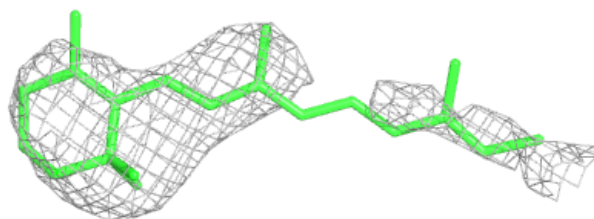


Electron density around RET A 406:

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

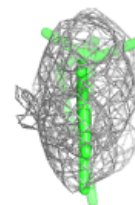
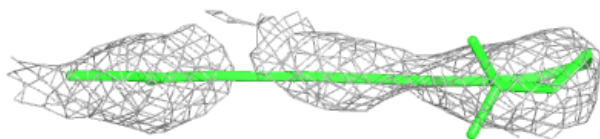
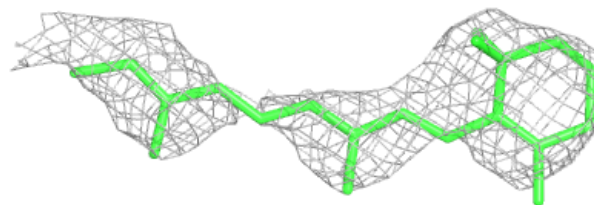
**Electron density around RET C 404:**

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

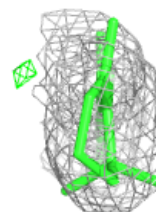
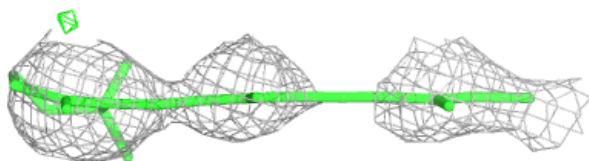
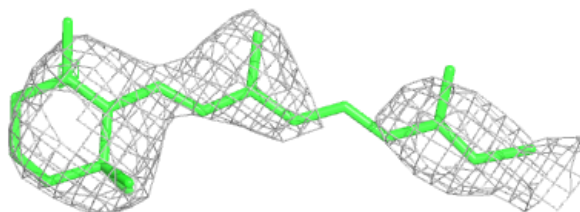


Electron density around RET B 406:

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

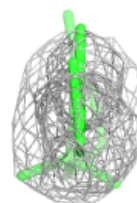
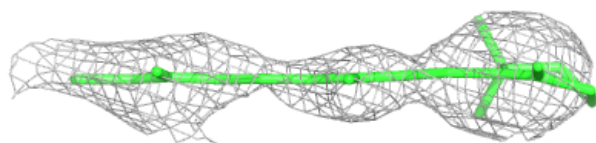
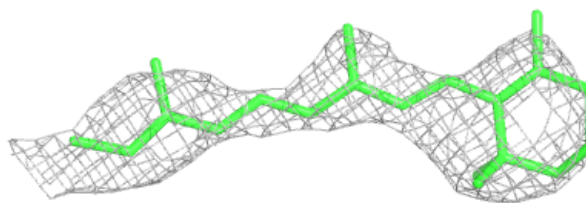
**Electron density around RET K 405:**

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

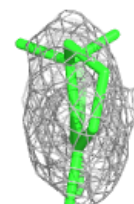
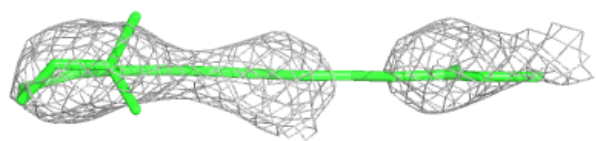
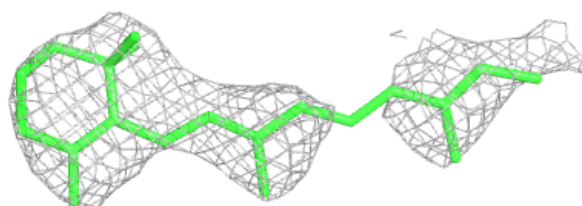


Electron density around RET E 404:

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

**Electron density around RET F 406:**

$2mF_o-DF_c$ (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.