Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 11:49 PM EDT

PDB ID	:	3T45
Title	:	Crystal structure of bacteriorhodopsin mutant A215T, a phototaxis signaling mutant at 3.0 A resolution
Authors	:	Ozorowski, G.; Luecke, H.
Deposited on	:	2011-07-25
Resolution	:	3.01 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

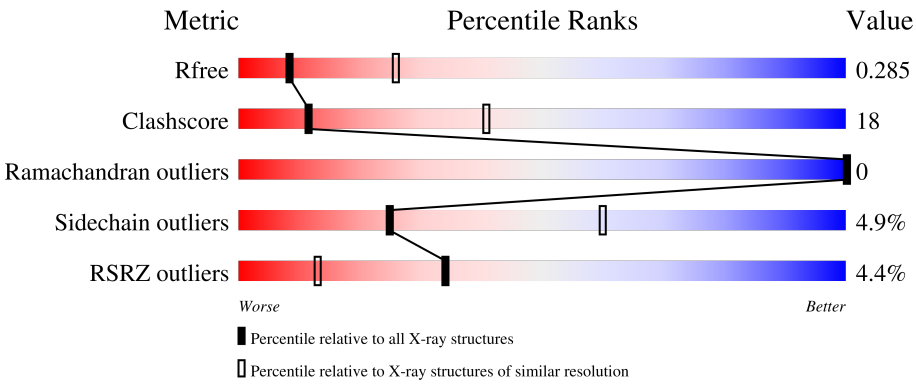
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	225	3% 72% 24% •
1	B	225	5% 68% 28% •
1	C	225	5% 69% 28% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LI1	B	603	-	-	-	X
3	LI1	C	613	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5664 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.

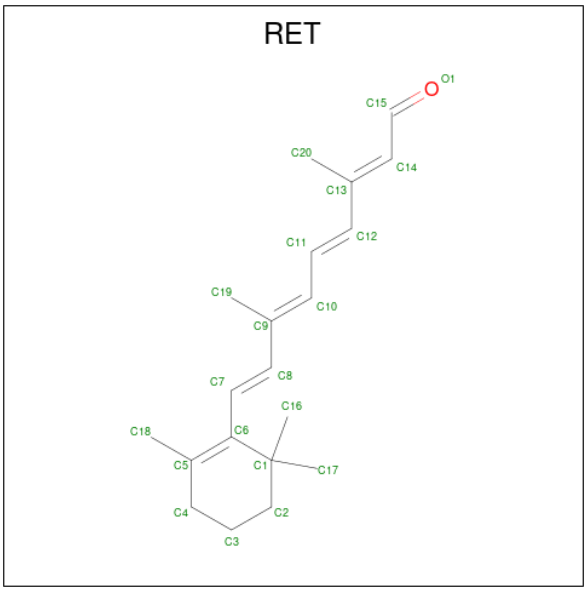
- Molecule 1 is a protein called Bacteriorhodopsin (GROUND STATE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1747	1175	266	297	9	0	0	0
1	B	225	1747	1175	266	297	9	0	0	0
1	C	225	1747	1175	266	297	9	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

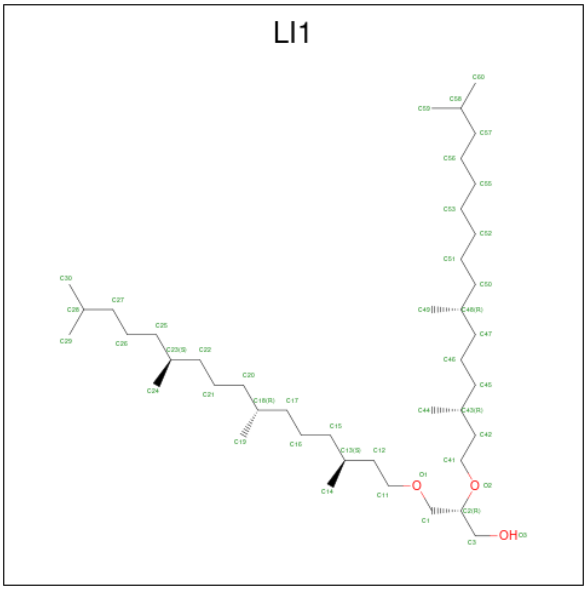
Chain	Residue	Modelled	Actual	Comment	Reference
A	215	THR	ALA	engineered mutation	UNP P02945
B	215	THR	ALA	engineered mutation	UNP P02945
C	215	THR	ALA	engineered mutation	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 3 is 1-[2,6,10.14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: $C_{42}H_{86}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 45 42 3	0	0
3	A	1	Total C O 24 21 3	0	0
3	B	1	Total C O 26 23 3	0	0
3	B	1	Total C O 37 34 3	0	0
3	B	1	Total C O 40 37 3	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C O 41 38 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 20 20	0	0
3	C	1	Total C O 45 42 3	0	0
3	C	1	Total C O 25 23 2	0	0

- Molecule 4 is water.

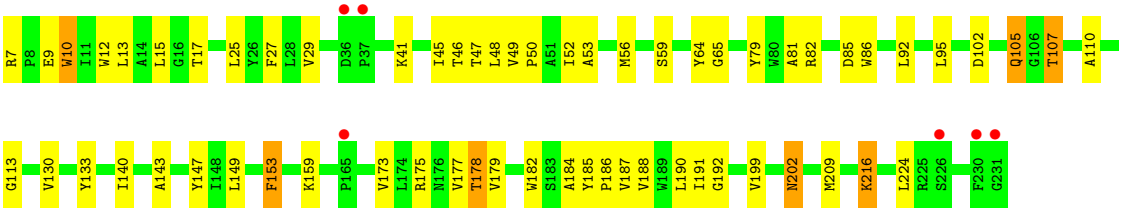
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	14	Total O 14 14	0	0
4	C	13	Total O 13 13	0	0

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.

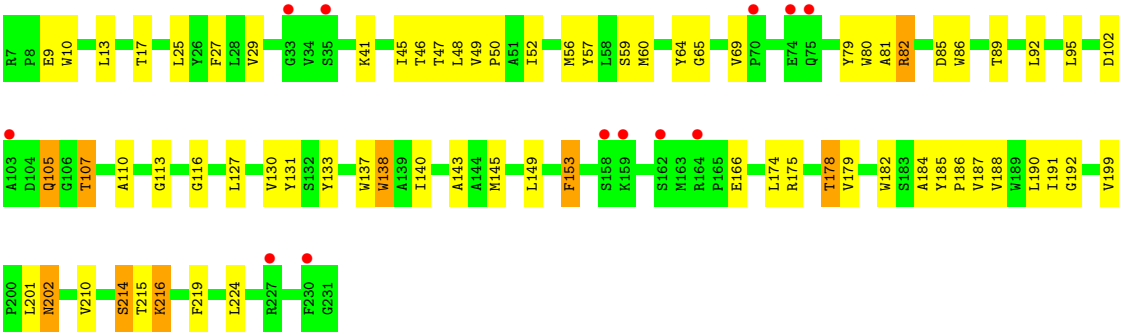
• Molecule 1: Bacteriorhodopsin (GROUND STATE)

Chain A:



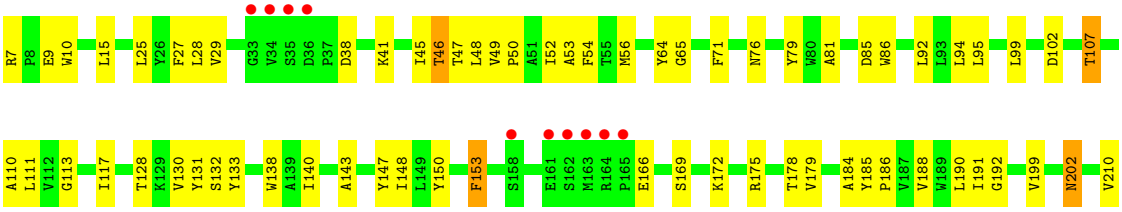
• Molecule 1: Bacteriorhodopsin (GROUND STATE)

Chain B:



• Molecule 1: Bacteriorhodopsin (GROUND STATE)

Chain C:



S214
T215
K216
L224
F230
G231

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	61.45Å 106.14Å 124.84Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	32.67 – 3.01 32.67 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.67-3.01) 97.3 (32.67-3.01)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.288 0.236 , 0.285	Depositor DCC
R_{free} test set	780 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 83.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5664	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: RET, LI1

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	0.63	1/1795 (0.1%)	0.69	1/2452 (0.0%)
1	B	0.65	3/1795 (0.2%)	0.70	1/2452 (0.0%)
1	C	0.64	0/1795	0.71	1/2452 (0.0%)
All	All	0.64	4/5385 (0.1%)	0.70	3/7356 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	TRP	CD2-CE2	5.88	1.48	1.41
1	B	10	TRP	CD2-CE2	5.31	1.47	1.41
1	B	138	TRP	CD2-CE2	5.19	1.47	1.41
1	A	10	TRP	CD2-CE2	5.14	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	216	LYS	CD-CE-NZ	-5.32	99.47	111.70
1	C	216	LYS	CD-CE-NZ	-5.30	99.51	111.70
1	A	216	LYS	CD-CE-NZ	-5.26	99.61	111.70

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	1747	0	1805	49	0
1	B	1747	0	1805	57	0
1	C	1747	0	1805	59	0
2	A	20	0	27	4	0
2	B	20	0	27	5	0
2	C	20	0	27	5	0
3	A	69	0	123	12	0
3	B	186	0	330	32	0
3	C	70	0	132	9	0
4	A	11	0	0	3	0
4	B	14	0	0	1	0
4	C	13	0	0	4	0
All	All	5664	0	6081	206	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 18.

All (206) 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:B:49:VAL:CG1	1:B:216:LYS:HG2	1.90	0.99
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.26	0.98
1:A:49:VAL:CG1	1:A:216:LYS:HG2	1.94	0.97
1:B:116:GLY:HA3	3:B:602:LI1:H593	1.48	0.95
1:C:49:VAL:CG1	1:C:216:LYS:HG2	1.97	0.94
3:A:600:LI1:H241	3:A:600:LI1:C27	2.01	0.91
3:A:600:LI1:H241	3:A:600:LI1:H272	1.54	0.90
1:B:49:VAL:HG12	1:B:216:LYS:HG2	1.56	0.84
1:C:184:ALA:O	1:C:188:VAL:HG23	1.76	0.84
1:B:202:ASN:HD22	1:B:202:ASN:H	1.24	0.81
1:A:49:VAL:HG12	1:A:216:LYS:HG2	1.60	0.81
1:A:202:ASN:HD22	1:A:202:ASN:H	1.29	0.80
1:A:25:LEU:O	1:A:29:VAL:HG23	1.85	0.76
1:C:202:ASN:HD22	1:C:202:ASN:H	1.31	0.76
1:A:184:ALA:O	1:A:188:VAL:HG23	1.86	0.75
1:C:25:LEU:O	1:C:29:VAL:HG23	1.88	0.73
1:C:49:VAL:HG12	1:C:216:LYS:HG2	1.68	0.73
1:B:25:LEU:O	1:B:29:VAL:HG23	1.88	0.73
3:A:600:LI1:H441	3:A:600:LI1:H211	1.72	0.72
1:C:41:LYS:O	1:C:45:ILE:HG13	1.89	0.72
1:B:202:ASN:H	1:B:202:ASN:ND2	1.89	0.70
3:B:603:LI1:H162	3:B:603:LI1:H11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASN:H	1:A:202:ASN:ND2	1.89	0.69
1:B:82:ARG:HH11	1:B:82:ARG:CG	2.02	0.68
1:A:49:VAL:HG11	1:A:216:LYS:HG2	1.74	0.68
1:B:49:VAL:HG11	1:B:216:LYS:HG2	1.75	0.68
1:C:86:TRP:CD1	2:C:301:RET:H14	2.29	0.67
1:B:48:LEU:HD11	1:C:113:GLY:HA3	1.77	0.66
1:B:45:ILE:HG23	1:B:92:LEU:HD22	1.77	0.66
1:A:86:TRP:CD1	2:A:301:RET:H14	2.30	0.66
3:B:611:LI1:C14	3:B:612:LI1:H13	2.26	0.66
1:C:202:ASN:H	1:C:202:ASN:ND2	1.92	0.65
1:C:85:ASP:OD2	4:C:402:HOH:O	2.13	0.65
1:B:131:TYR:OH	3:B:611:LI1:H152	1.95	0.65
1:C:49:VAL:HG11	1:C:216:LYS:HG2	1.78	0.64
3:B:604:LI1:H112	3:B:604:LI1:H162	1.78	0.64
1:B:153:PHE:HD1	1:B:175:ARG:HD2	1.63	0.64
3:B:604:LI1:H441	3:B:615:LI1:H172	1.79	0.63
3:A:600:LI1:C27	3:A:600:LI1:C24	2.76	0.62
1:A:82:ARG:NH1	4:A:406:HOH:O	2.32	0.61
2:C:301:RET:H171	2:C:301:RET:H8	1.83	0.61
1:C:48:LEU:O	1:C:52:ILE:HG13	2.01	0.60
1:C:131:TYR:HB3	4:C:419:HOH:O	2.01	0.60
1:B:47:THR:O	1:B:50:PRO:HD2	2.00	0.60
1:B:47:THR:C	1:B:50:PRO:HD2	2.22	0.59
1:B:56:MET:HG3	1:B:85:ASP:HB2	1.83	0.59
3:B:611:LI1:H13	3:B:612:LI1:H13	1.85	0.59
1:A:178:THR:HG23	4:A:501:HOH:O	2.03	0.58
3:B:603:LI1:H442	3:B:603:LI1:C19	2.33	0.58
1:B:86:TRP:CD1	2:B:301:RET:H14	2.39	0.58
1:A:47:THR:C	1:A:50:PRO:HD2	2.24	0.58
3:A:600:LI1:H241	3:A:600:LI1:H271	1.82	0.58
1:B:107:THR:O	1:B:110:ALA:HB3	2.03	0.58
3:B:611:LI1:H48	3:B:611:LI1:H172	1.85	0.57
3:B:603:LI1:H442	3:B:603:LI1:H191	1.86	0.57
1:C:113:GLY:O	1:C:117:ILE:HG13	2.04	0.57
1:A:41:LYS:O	1:A:45:ILE:HG13	2.05	0.57
1:B:27:PHE:CD1	1:B:224:LEU:HD12	2.40	0.56
1:C:27:PHE:CD1	1:C:224:LEU:HD12	2.40	0.56
1:C:185:TYR:N	1:C:186:PRO:HD2	2.20	0.56
1:A:85:ASP:OD1	1:A:85:ASP:C	2.43	0.56
1:A:153:PHE:HD1	1:A:175:ARG:HD2	1.70	0.56
1:A:187:VAL:O	1:A:191:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:OH	3:B:602:LI1:H452	2.05	0.56
1:A:45:ILE:HG23	1:A:92:LEU:HD22	1.88	0.56
1:A:130:VAL:O	1:A:133:TYR:HB2	2.05	0.56
3:C:606:LI1:H202	3:C:606:LI1:H443	1.89	0.55
1:B:41:LYS:O	1:B:45:ILE:HG13	2.07	0.55
1:A:27:PHE:CD1	1:A:224:LEU:HD12	2.42	0.55
1:C:107:THR:O	1:C:110:ALA:HB3	2.07	0.54
1:C:45:ILE:HG23	1:C:92:LEU:HD22	1.90	0.54
1:B:13:LEU:O	1:B:17:THR:OG1	2.24	0.54
1:C:85:ASP:OD1	1:C:85:ASP:C	2.46	0.54
1:A:47:THR:O	1:A:50:PRO:HD2	2.09	0.53
1:C:9:GLU:HB3	1:C:202:ASN:HA	1.91	0.52
1:A:159:LYS:HE3	4:A:514:HOH:O	2.08	0.52
3:B:611:LI1:H492	3:B:611:LI1:H421	1.92	0.52
1:C:138:TRP:CE2	1:C:190:LEU:HD13	2.45	0.52
1:B:190:LEU:HD21	3:B:611:LI1:H252	1.92	0.52
1:C:175:ARG:O	1:C:179:VAL:HG23	2.10	0.52
1:C:28:LEU:CD1	3:C:613:LI1:H193	2.39	0.52
3:B:611:LI1:H13	3:B:612:LI1:H162	1.92	0.52
1:A:9:GLU:HB3	1:A:202:ASN:HA	1.92	0.52
2:A:301:RET:H8	2:A:301:RET:H171	1.93	0.51
1:B:130:VAL:O	1:B:133:TYR:HB2	2.11	0.51
1:C:128:THR:HG23	4:C:412:HOH:O	2.10	0.51
3:A:600:LI1:C24	3:A:600:LI1:H271	2.41	0.51
1:C:7:ARG:O	1:C:10:TRP:HB3	2.11	0.51
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.93	0.51
1:B:105:GLN:NE2	1:B:105:GLN:H	2.09	0.51
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.93	0.50
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.76	0.50
1:A:86:TRP:NE1	2:A:301:RET:H14	2.26	0.50
1:B:192:GLY:HA2	1:B:199:VAL:HG22	1.93	0.50
1:A:48:LEU:O	1:A:52:ILE:HG13	2.12	0.50
1:C:192:GLY:HA2	1:C:199:VAL:HG22	1.93	0.50
1:C:65:GLY:HA3	1:C:81:ALA:HB2	1.93	0.49
1:A:147:TYR:CZ	3:C:613:LI1:H192	2.47	0.49
1:C:132:SER:N	4:C:419:HOH:O	2.09	0.49
1:A:107:THR:O	1:A:110:ALA:HB3	2.13	0.49
1:C:28:LEU:HD11	3:C:613:LI1:H193	1.94	0.49
1:B:201:LEU:N	4:B:418:HOH:O	2.44	0.49
1:C:130:VAL:O	1:C:133:TYR:HB2	2.12	0.49
1:A:185:TYR:N	1:A:186:PRO:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:O	1:B:191:ILE:HG12	2.13	0.49
3:B:611:LI1:C13	3:B:612:LI1:H13	2.42	0.48
3:B:611:LI1:H191	3:B:612:LI1:H212	1.95	0.48
1:B:48:LEU:O	1:B:52:ILE:HG13	2.14	0.48
1:B:145:MET:CE	1:B:186:PRO:HG3	2.44	0.48
1:C:71:PHE:O	1:C:76:ASN:ND2	2.42	0.47
3:B:603:LI1:H451	3:C:606:LI1:H602	1.96	0.47
1:A:192:GLY:HA2	1:A:199:VAL:HG22	1.96	0.47
1:A:105:GLN:H	1:A:105:GLN:NE2	2.12	0.47
1:B:9:GLU:HB3	1:B:202:ASN:HA	1.96	0.47
3:A:600:LI1:C44	3:A:600:LI1:H161	2.45	0.47
1:B:175:ARG:O	1:B:179:VAL:HG23	2.15	0.47
1:C:47:THR:C	1:C:50:PRO:HD2	2.35	0.47
1:A:48:LEU:HD11	1:B:113:GLY:HA3	1.97	0.47
2:A:301:RET:H7	2:A:301:RET:H181	1.55	0.47
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.96	0.47
1:C:56:MET:HG3	1:C:85:ASP:HB2	1.97	0.46
1:B:80:TRP:CH2	3:B:604:LI1:H471	2.49	0.46
1:B:178:THR:O	1:B:182:TRP:HB2	2.15	0.46
1:A:7:ARG:NH1	1:A:79:TYR:OH	2.49	0.46
3:B:611:LI1:H143	3:B:612:LI1:H13	1.97	0.46
1:A:140:ILE:O	1:A:143:ALA:HB3	2.15	0.46
1:C:54:PHE:CD2	3:C:613:LI1:H303	2.51	0.46
1:B:80:TRP:HH2	3:B:604:LI1:H471	1.81	0.46
3:B:603:LI1:H31	3:B:603:LI1:H411	1.51	0.46
3:B:602:LI1:H592	3:B:602:LI1:H561	1.83	0.45
1:A:59:SER:O	1:A:64:TYR:N	2.49	0.45
1:A:178:THR:O	1:A:182:TRP:HB2	2.15	0.45
2:B:301:RET:H8	2:B:301:RET:H171	1.97	0.45
1:C:186:PRO:HB3	2:C:301:RET:H42	1.97	0.45
1:A:175:ARG:O	1:A:179:VAL:HG23	2.17	0.45
1:A:190:LEU:HD21	3:A:600:LI1:H303	1.97	0.45
1:B:59:SER:O	1:B:64:TYR:N	2.50	0.45
3:B:604:LI1:H493	3:B:604:LI1:H461	1.80	0.45
3:B:611:LI1:C19	3:B:612:LI1:H212	2.47	0.45
1:A:113:GLY:HA3	1:C:48:LEU:HD11	1.99	0.45
1:B:57:TYR:HA	1:B:60:MET:CE	2.47	0.45
1:C:7:ARG:NH1	1:C:79:TYR:OH	2.49	0.45
3:B:603:LI1:H492	1:C:140:ILE:HG12	1.99	0.45
1:C:111:LEU:HD22	1:C:148:ILE:HG23	1.98	0.45
1:B:174:LEU:O	1:B:178:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:O	1:B:214:SER:OG	2.34	0.44
1:C:46:THR:HB	1:C:224:LEU:HD11	1.99	0.44
1:C:48:LEU:HD23	1:C:48:LEU:HA	1.86	0.44
1:B:149:LEU:O	1:B:153:PHE:HB2	2.17	0.44
1:C:94:LEU:HD13	1:C:111:LEU:HB3	2.00	0.44
1:C:53:ALA:HB2	1:C:216:LYS:HE2	1.98	0.44
3:B:602:LI1:H12	3:B:602:LI1:H411	1.74	0.44
1:B:86:TRP:HA	1:B:89:THR:OG1	2.18	0.44
1:B:219:PHE:C	1:B:219:PHE:CD1	2.90	0.44
1:C:210:VAL:O	1:C:214:SER:OG	2.36	0.44
1:B:82:ARG:CG	1:B:82:ARG:NH1	2.71	0.43
1:B:185:TYR:N	1:B:186:PRO:HD2	2.33	0.43
1:B:85:ASP:C	1:B:85:ASP:OD1	2.56	0.43
1:C:38:ASP:HA	1:C:41:LYS:HE3	2.00	0.43
1:A:7:ARG:O	1:A:10:TRP:HB3	2.18	0.43
1:A:12:TRP:O	1:A:209:MET:HG3	2.19	0.43
1:B:184:ALA:O	1:B:188:VAL:HG23	2.18	0.43
1:A:173:VAL:O	1:A:177:VAL:HG23	2.19	0.43
1:A:53:ALA:HB2	1:A:216:LYS:HE2	2.01	0.43
3:B:611:LI1:H143	3:B:611:LI1:H111	1.81	0.43
2:C:301:RET:H181	2:C:301:RET:H7	1.58	0.43
3:B:603:LI1:H191	3:B:603:LI1:H211	1.80	0.42
3:C:613:LI1:H243	3:C:613:LI1:H212	1.73	0.42
1:C:202:ASN:ND2	1:C:202:ASN:N	2.65	0.42
3:B:604:LI1:H162	3:B:604:LI1:C11	2.42	0.42
1:C:153:PHE:HD1	1:C:175:ARG:HD2	1.84	0.42
3:A:600:LI1:H603	3:A:600:LI1:H562	1.81	0.42
1:B:138:TRP:CD1	2:B:301:RET:H32	2.55	0.42
1:C:140:ILE:O	1:C:143:ALA:HB3	2.19	0.42
1:B:25:LEU:HD11	3:B:603:LI1:C29	2.50	0.42
1:B:86:TRP:NE1	2:B:301:RET:H14	2.35	0.42
3:A:600:LI1:H452	3:A:600:LI1:H411	1.48	0.42
1:B:69:VAL:HG21	1:B:127:LEU:HA	2.02	0.42
1:B:140:ILE:O	1:B:143:ALA:HB3	2.20	0.42
1:C:147:TYR:O	1:C:150:TYR:HB3	2.20	0.41
1:B:60:MET:HG2	1:B:79:TYR:HD1	1.85	0.41
1:C:191:ILE:H	1:C:191:ILE:HG12	1.72	0.41
1:C:54:PHE:CE2	3:C:613:LI1:H303	2.55	0.41
1:A:50:PRO:HA	1:A:53:ALA:HB3	2.01	0.41
1:A:149:LEU:O	1:A:153:PHE:HB2	2.20	0.41
3:A:608:LI1:H31	1:C:64:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:RET:H171	2:C:301:RET:C8	2.48	0.41
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.76	0.41
1:B:57:TYR:HA	1:B:60:MET:HE2	2.01	0.41
1:C:47:THR:O	1:C:50:PRO:HD2	2.20	0.41
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.92	0.41
1:B:215:THR:O	1:B:219:PHE:HB3	2.20	0.41
1:A:13:LEU:O	1:A:17:THR:OG1	2.33	0.41
1:A:15:LEU:O	1:A:15:LEU:HD23	2.21	0.41
1:A:202:ASN:ND2	1:A:202:ASN:N	2.60	0.41
2:B:301:RET:H181	2:B:301:RET:H7	1.61	0.41
1:C:27:PHE:HB2	1:C:47:THR:HG23	2.03	0.41
1:C:172:LYS:HG2	1:C:175:ARG:HH12	1.85	0.41
1:C:15:LEU:HD23	1:C:15:LEU:O	2.20	0.40
1:C:41:LYS:HD2	1:C:99:LEU:HD13	2.02	0.40
3:C:613:LI1:H243	3:C:613:LI1:H191	2.04	0.40
1:B:166:GLU:H	1:B:166:GLU:HG2	1.66	0.40
3:B:605:LI1:H492	3:B:605:LI1:H461	1.94	0.40
3:A:600:LI1:H2	3:A:600:LI1:H422	1.72	0.40
3:B:604:LI1:H192	3:B:604:LI1:H161	1.75	0.40
1:C:166:GLU:H	1:C:166:GLU:HG2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/225 (99%)	208 (93%)	15 (7%)	0	100	100
1	B	223/225 (99%)	206 (92%)	17 (8%)	0	100	100
1	C	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
All	All	669/675 (99%)	624 (93%)	45 (7%)	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	182/182 (100%)	174 (96%)	8 (4%)	28	64
1	B	182/182 (100%)	172 (94%)	10 (6%)	21	55
1	C	182/182 (100%)	173 (95%)	9 (5%)	25	60
All	All	546/546 (100%)	519 (95%)	27 (5%)	25	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	95	LEU
1	A	102	ASP
1	A	105	GLN
1	A	107	THR
1	A	153	PHE
1	A	178	THR
1	A	202	ASN
1	B	46	THR
1	B	82	ARG
1	B	95	LEU
1	B	102	ASP
1	B	105	GLN
1	B	107	THR
1	B	153	PHE
1	B	178	THR
1	B	202	ASN
1	B	214	SER
1	C	46	THR
1	C	95	LEU
1	C	102	ASP
1	C	107	THR
1	C	153	PHE

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Mol	Chain	Res	Type
1	C	169	SER
1	C	178	THR
1	C	202	ASN
1	C	214	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	202	ASN
1	B	105	GLN
1	B	202	ASN
1	C	202	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
3	LI1	B	602	-	25,25,44	0.62	0	27,28,51	1.02	2 (7%)
3	LI1	B	611	-	40,40,44	0.49	0	44,46,51	0.73	0
3	LI1	B	605	-	13,13,44	0.51	0	13,14,51	0.52	0
2	RET	A	301	1	20,20,21	0.99	0	27,27,28	1.85	7 (25%)
3	LI1	B	615	-	7,7,44	0.39	0	7,7,51	0.33	0
3	LI1	B	612	-	19,19,44	0.34	0	22,22,51	0.82	1 (4%)
3	LI1	C	613	-	24,24,44	0.46	0	26,27,51	0.58	0
3	LI1	B	604	-	39,39,44	0.60	0	43,45,51	0.85	1 (2%)
3	LI1	C	606	-	44,44,44	0.44	0	49,51,51	0.53	0
2	RET	B	301	1	20,20,21	1.03	0	27,27,28	1.70	6 (22%)
2	RET	C	301	1	20,20,21	1.01	1 (5%)	27,27,28	1.75	7 (25%)
3	LI1	A	600	-	44,44,44	0.58	0	49,51,51	1.00	3 (6%)
3	LI1	A	608	-	23,23,44	0.59	0	23,24,51	0.95	2 (8%)
3	LI1	B	603	-	36,36,44	0.68	1 (2%)	40,42,51	0.80	2 (5%)

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
3	LI1	B	602	-	-	16/27/27/49	-
3	LI1	B	611	-	-	22/45/45/49	-
3	LI1	B	605	-	-	4/12/12/49	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	LI1	B	615	-	-	4/5/5/49	-
3	LI1	B	612	-	-	12/20/20/49	-
3	LI1	C	613	-	-	18/25/25/49	-
3	LI1	B	604	-	-	24/43/43/49	-
3	LI1	C	606	-	-	30/49/49/49	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
3	LI1	A	600	-	-	23/49/49/49	-
3	LI1	A	608	-	-	9/24/24/49	-
3	LI1	B	603	-	-	21/41/41/49	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	RET	C14-C13	2.74	1.35	1.33
3	B	603	LI1	C3-C2	2.17	1.56	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	LI1	O2-C41-C42	4.24	117.67	108.77
2	B	301	RET	C10-C11-C12	-4.13	111.23	123.20
2	A	301	RET	C10-C11-C12	-3.78	112.23	123.20
2	C	301	RET	C7-C8-C9	-3.75	120.69	126.23
3	B	603	LI1	O1-C1-C2	3.58	117.63	109.42
2	A	301	RET	C18-C5-C6	-3.47	120.70	124.48
2	C	301	RET	C10-C11-C12	-3.41	113.31	123.20
2	B	301	RET	C19-C9-C8	3.36	123.22	118.09
2	A	301	RET	C19-C9-C8	3.35	123.21	118.09
2	C	301	RET	C18-C5-C6	-3.35	120.83	124.48
2	A	301	RET	C7-C8-C9	-3.32	121.32	126.23
3	B	604	LI1	O2-C41-C42	3.19	115.47	108.77
2	C	301	RET	C1-C6-C7	3.15	124.19	115.65
3	B	602	LI1	O2-C2-C1	3.04	118.77	109.06
2	A	301	RET	C1-C6-C7	3.02	123.85	115.65
2	C	301	RET	C7-C6-C5	-3.02	114.60	121.56
2	C	301	RET	C3-C4-C5	-3.00	108.71	114.06
2	B	301	RET	C7-C8-C9	-2.91	121.93	126.23
2	B	301	RET	C1-C6-C7	2.91	123.55	115.65
2	A	301	RET	C7-C6-C5	-2.86	114.96	121.56
2	B	301	RET	C7-C6-C5	-2.80	115.10	121.56
3	A	600	LI1	C21-C20-C18	-2.58	107.41	115.97
3	B	602	LI1	C41-O2-C2	2.40	122.16	115.53
3	B	612	LI1	C21-C20-C18	-2.33	108.22	115.97
2	B	301	RET	C17-C1-C2	-2.20	100.49	108.95
3	A	608	LI1	O2-C2-C1	2.18	116.01	109.06
2	C	301	RET	C19-C9-C8	2.14	121.36	118.09
2	A	301	RET	C19-C9-C10	-2.13	119.36	122.82
3	B	603	LI1	O2-C2-C3	2.13	114.30	108.64
3	A	600	LI1	O3-C3-C2	-2.07	106.44	111.77
3	A	608	LI1	O2-C41-C42	2.06	113.10	108.77

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	LI1	C42-C41-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	600	LI1	C41-C42-C43-C44
3	A	600	LI1	C41-C42-C43-C45
3	A	608	LI1	C42-C41-O2-C2
3	A	608	LI1	C44-C43-C45-C46
3	B	602	LI1	C1-C2-C3-O3
3	B	602	LI1	O2-C2-C3-O3
3	B	602	LI1	C1-C2-O2-C41
3	B	602	LI1	C42-C41-O2-C2
3	B	602	LI1	O2-C41-C42-C43
3	B	603	LI1	C1-C2-C3-O3
3	B	603	LI1	O2-C2-C3-O3
3	B	603	LI1	C42-C41-O2-C2
3	B	603	LI1	C41-C42-C43-C44
3	B	603	LI1	C11-C12-C13-C14
3	B	604	LI1	C41-C42-C43-C44
3	B	604	LI1	C41-C42-C43-C45
3	B	611	LI1	C1-C2-C3-O3
3	B	611	LI1	O2-C2-C3-O3
3	C	606	LI1	C1-C2-C3-O3
3	C	606	LI1	O2-C2-C3-O3
3	C	606	LI1	C11-C12-C13-C14
3	C	606	LI1	C24-C23-C25-C26
3	C	613	LI1	C1-C2-C3-O3
3	C	613	LI1	C11-C12-C13-C14
3	B	611	LI1	O2-C41-C42-C43
3	B	611	LI1	O1-C11-C12-C13
3	B	603	LI1	C19-C18-C20-C21
3	B	604	LI1	C46-C47-C48-C49
3	B	604	LI1	C16-C17-C18-C19
3	B	611	LI1	C14-C13-C15-C16
3	C	613	LI1	C16-C17-C18-C19
3	C	613	LI1	C21-C22-C23-C24
3	B	604	LI1	C12-C13-C15-C16
3	B	605	LI1	C45-C46-C47-C48
3	C	613	LI1	C20-C21-C22-C23
3	B	603	LI1	C43-C45-C46-C47
3	B	612	LI1	C15-C16-C17-C18
3	A	600	LI1	C43-C45-C46-C47
3	A	600	LI1	C48-C50-C51-C52
3	B	612	LI1	C23-C25-C26-C27
3	C	606	LI1	C13-C15-C16-C17
3	B	604	LI1	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	C	606	LI1	C55-C56-C57-C58
3	A	600	LI1	C55-C56-C57-C58
3	A	600	LI1	C15-C16-C17-C18
3	B	603	LI1	C18-C20-C21-C22
3	B	604	LI1	C45-C46-C47-C48
3	C	606	LI1	C43-C45-C46-C47
3	C	606	LI1	C15-C16-C17-C18
3	B	602	LI1	C55-C56-C57-C58
3	B	611	LI1	C15-C16-C17-C18
3	C	613	LI1	C15-C16-C17-C18
3	B	615	LI1	C16-C17-C18-C19
3	C	606	LI1	C26-C27-C28-C30
3	A	600	LI1	C20-C21-C22-C23
3	B	615	LI1	C13-C15-C16-C17
3	C	606	LI1	C26-C27-C28-C29
3	A	600	LI1	C17-C18-C20-C21
3	A	608	LI1	C52-C53-C55-C56
3	B	604	LI1	C56-C57-C58-C59
3	A	608	LI1	C47-C48-C50-C51
3	B	602	LI1	C45-C46-C47-C48
3	A	608	LI1	C51-C52-C53-C55
3	A	600	LI1	C13-C15-C16-C17
3	C	613	LI1	C26-C27-C28-C29
3	B	611	LI1	C48-C50-C51-C52
3	B	604	LI1	C56-C57-C58-C60
3	B	615	LI1	C16-C17-C18-C20
3	C	606	LI1	C56-C57-C58-C59
3	C	606	LI1	C52-C53-C55-C56
3	B	612	LI1	C26-C27-C28-C30
3	B	602	LI1	C51-C52-C53-C55
3	B	611	LI1	C18-C20-C21-C22
3	B	602	LI1	C50-C51-C52-C53
3	B	611	LI1	C52-C53-C55-C56
3	A	600	LI1	C42-C43-C45-C46
3	B	611	LI1	C42-C43-C45-C46
3	B	611	LI1	C46-C47-C48-C50
3	C	606	LI1	C47-C48-C50-C51
3	A	600	LI1	C56-C57-C58-C59
3	C	606	LI1	C23-C25-C26-C27
3	B	602	LI1	O1-C1-C2-C3
3	B	604	LI1	O1-C1-C2-C3
3	B	611	LI1	C51-C52-C53-C55

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Mol	Chain	Res	Type	Atoms
3	B	602	LI1	C48-C50-C51-C52
3	C	606	LI1	C56-C57-C58-C60
3	C	613	LI1	C26-C27-C28-C30
3	C	613	LI1	C25-C26-C27-C28
3	C	606	LI1	C50-C51-C52-C53
3	C	606	LI1	C18-C20-C21-C22
3	B	604	LI1	C53-C55-C56-C57
3	A	608	LI1	C45-C46-C47-C48
3	B	602	LI1	C43-C45-C46-C47
3	A	600	LI1	O1-C11-C12-C13
3	B	604	LI1	O2-C41-C42-C43
3	B	605	LI1	O2-C41-C42-C43
3	B	603	LI1	C15-C16-C17-C18
3	A	600	LI1	C44-C43-C45-C46
3	A	600	LI1	C19-C18-C20-C21
3	B	611	LI1	C44-C43-C45-C46
3	B	611	LI1	C46-C47-C48-C49
3	B	615	LI1	C14-C13-C15-C16
3	B	604	LI1	C2-C1-O1-C11
3	C	606	LI1	C53-C55-C56-C57
3	A	608	LI1	C42-C43-C45-C46
3	B	611	LI1	C12-C13-C15-C16
3	C	606	LI1	C22-C23-C25-C26
3	A	600	LI1	C53-C55-C56-C57
3	B	603	LI1	C3-C2-O2-C41
3	C	606	LI1	O1-C1-C2-C3
3	B	603	LI1	C45-C46-C47-C48
3	B	611	LI1	C56-C57-C58-C60
3	A	600	LI1	C56-C57-C58-C60
3	B	602	LI1	C52-C53-C55-C56
3	B	604	LI1	C42-C41-O2-C2
3	C	606	LI1	C20-C21-C22-C23
3	B	612	LI1	C17-C18-C20-C21
3	C	606	LI1	C42-C43-C45-C46
3	C	613	LI1	C16-C17-C18-C20
3	B	611	LI1	C13-C15-C16-C17
3	B	605	LI1	C46-C47-C48-C49
3	B	612	LI1	C26-C27-C28-C29
3	B	611	LI1	O1-C1-C2-O2
3	C	606	LI1	O1-C1-C2-O2
3	C	606	LI1	C49-C48-C50-C51
3	B	604	LI1	C52-C53-C55-C56

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Mol	Chain	Res	Type	Atoms
3	C	613	LI1	C18-C20-C21-C22
3	B	603	LI1	O2-C41-C42-C43
3	B	612	LI1	C25-C26-C27-C28
3	B	602	LI1	C46-C47-C48-C50
3	B	604	LI1	C16-C17-C18-C20
3	B	604	LI1	C17-C18-C20-C21
3	B	612	LI1	C12-C13-C15-C16
3	B	612	LI1	C21-C22-C23-C25
3	C	613	LI1	C22-C23-C25-C26
3	C	606	LI1	C51-C52-C53-C55
3	B	604	LI1	O1-C11-C12-C13
3	B	603	LI1	C14-C13-C15-C16
3	C	606	LI1	C12-C11-O1-C1
3	B	604	LI1	O1-C1-C2-O2
3	C	613	LI1	C23-C25-C26-C27
3	B	603	LI1	O1-C1-C2-C3
3	B	603	LI1	C11-C12-C13-C15
3	C	606	LI1	C41-C42-C43-C45
3	A	600	LI1	O2-C41-C42-C43
3	C	606	LI1	O2-C41-C42-C43
3	C	613	LI1	O1-C11-C12-C13
3	B	603	LI1	C16-C17-C18-C19
3	B	612	LI1	C19-C18-C20-C21
3	C	613	LI1	C21-C22-C23-C25
3	B	612	LI1	C20-C21-C22-C23
3	B	603	LI1	C26-C27-C28-C29
3	B	603	LI1	C26-C27-C28-C30
3	C	613	LI1	C2-C1-O1-C11
3	B	602	LI1	O1-C1-C2-O2
3	B	611	LI1	O1-C1-C2-C3
3	A	608	LI1	C2-C1-O1-C11
3	B	611	LI1	C56-C57-C58-C59
3	B	602	LI1	C46-C47-C48-C49
3	B	611	LI1	C20-C21-C22-C23
3	A	600	LI1	C51-C52-C53-C55
3	B	604	LI1	C43-C45-C46-C47
3	A	600	LI1	C14-C13-C15-C16
3	C	606	LI1	C19-C18-C20-C21
3	A	600	LI1	C47-C48-C50-C51
3	B	603	LI1	C12-C13-C15-C16
3	C	613	LI1	C12-C11-O1-C1
3	B	611	LI1	C12-C11-O1-C1

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Mol	Chain	Res	Type	Atoms
3	A	608	LI1	C56-C57-C58-C60
3	B	605	LI1	C42-C41-O2-C2
3	B	603	LI1	O1-C11-C12-C13
3	C	606	LI1	C44-C43-C45-C46
3	C	613	LI1	C24-C23-C25-C26
3	B	604	LI1	C46-C47-C48-C50
3	B	604	LI1	C12-C11-O1-C1
3	A	600	LI1	C23-C25-C26-C27
3	B	604	LI1	C19-C18-C20-C21
3	B	612	LI1	C14-C13-C15-C16
3	A	600	LI1	C46-C47-C48-C50
3	B	603	LI1	C16-C17-C18-C20
3	B	612	LI1	C21-C22-C23-C24
3	B	604	LI1	C1-C2-C3-O3

There are no ring outliers.

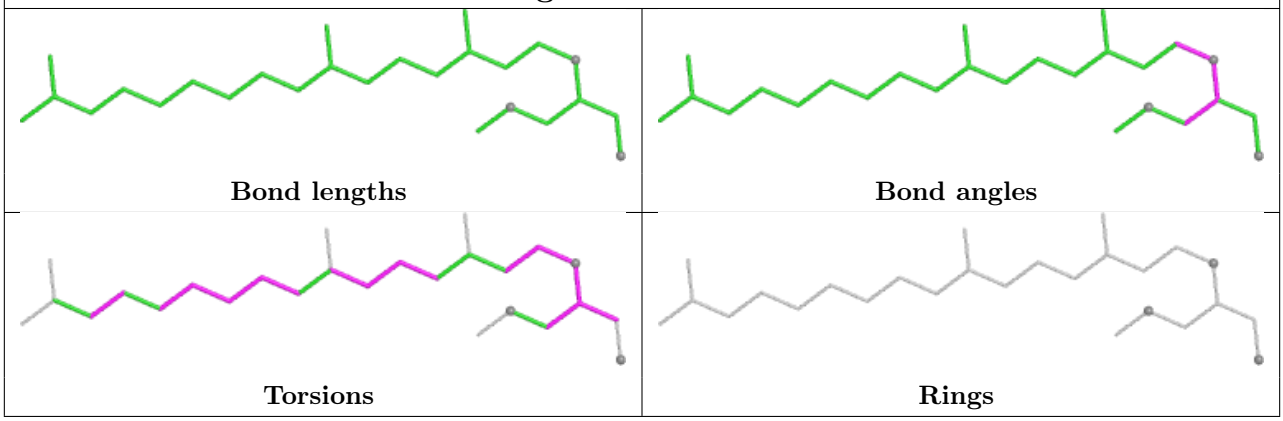
14 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	LI1	4	0
3	B	611	LI1	12	0
3	B	605	LI1	1	0
2	A	301	RET	4	0
3	B	615	LI1	1	0
3	B	612	LI1	7	0
3	C	613	LI1	7	0
3	B	604	LI1	7	0
3	C	606	LI1	2	0
2	B	301	RET	5	0
2	C	301	RET	5	0
3	A	600	LI1	11	0
3	A	608	LI1	1	0
3	B	603	LI1	8	0

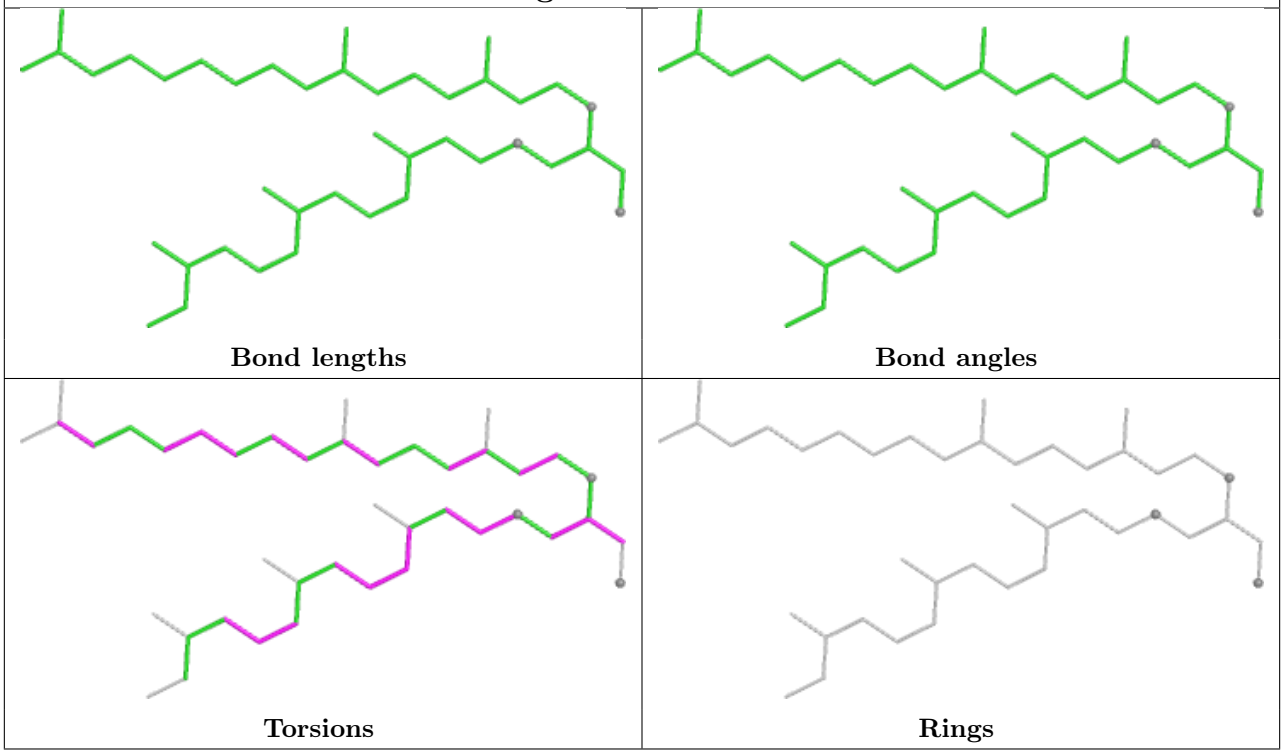
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 LI1 B 602



Ligand LI1 B 611



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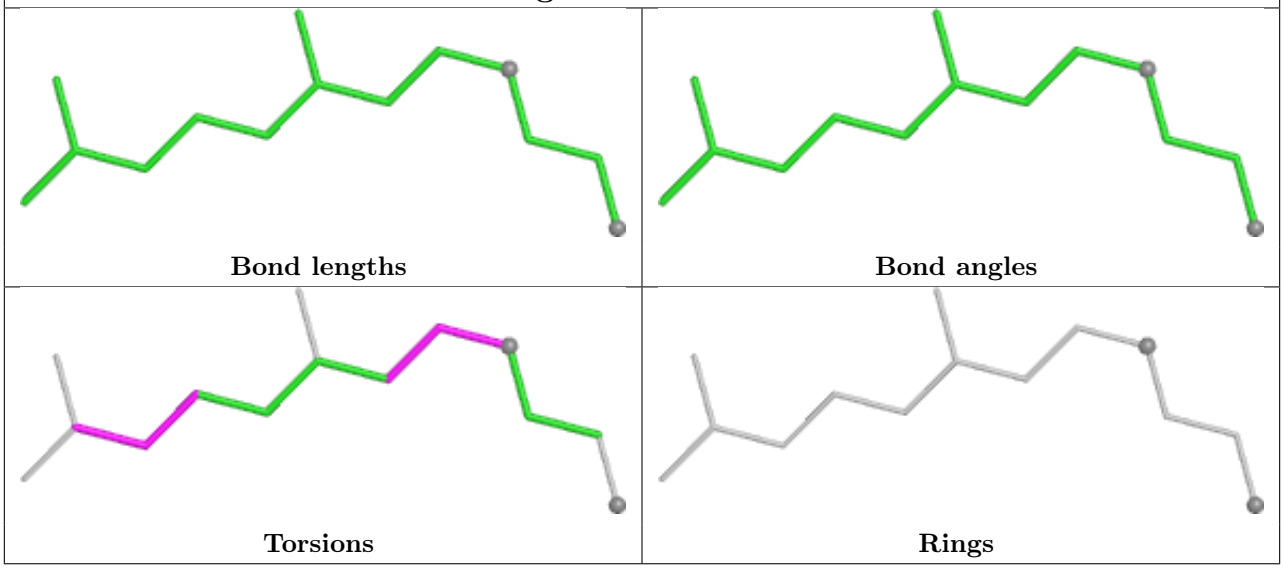
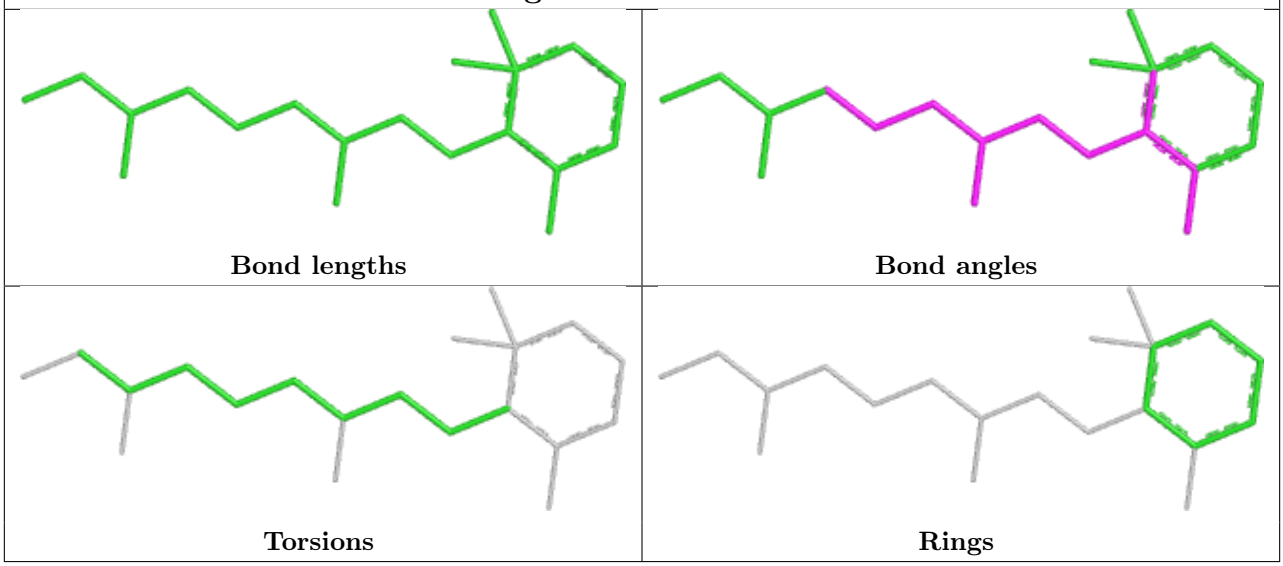
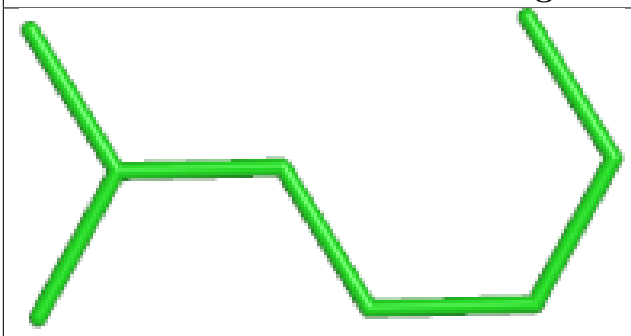


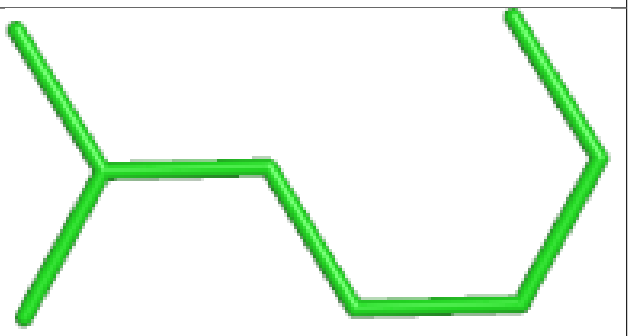
Ligand RET A 301



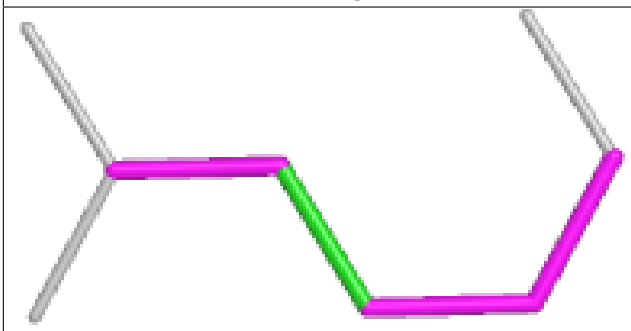
Ligand LI1 B 615



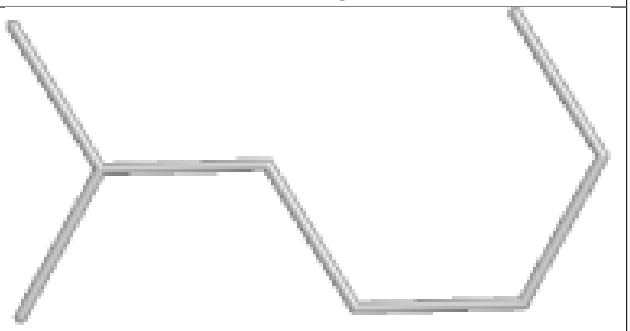
Bond lengths



Bond angles

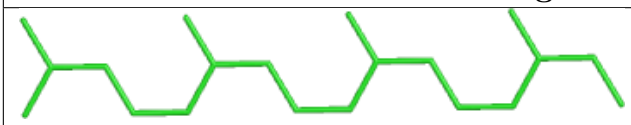


Torsions

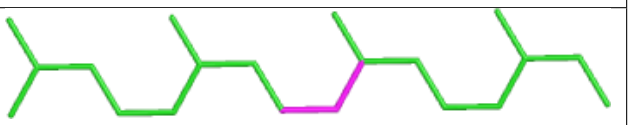


Rings

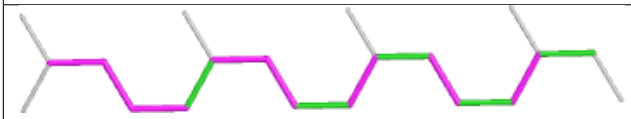
Ligand LI1 B 612



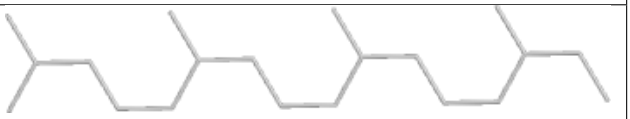
Bond lengths



Bond angles

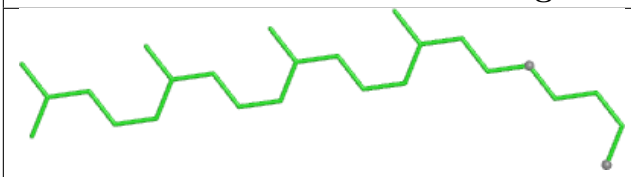


Torsions

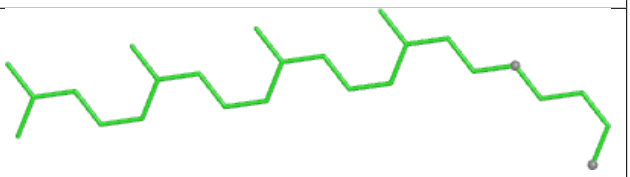


Rings

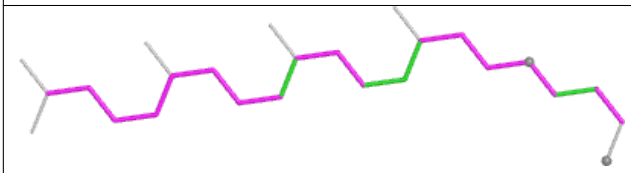
Ligand LI1 C 613



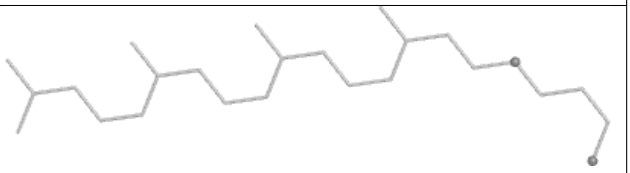
Bond lengths



Bond angles

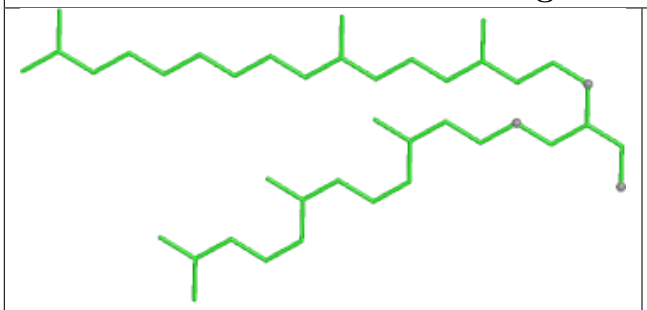


Torsions

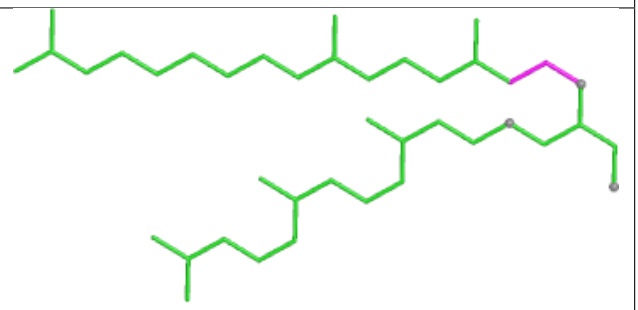


Rings

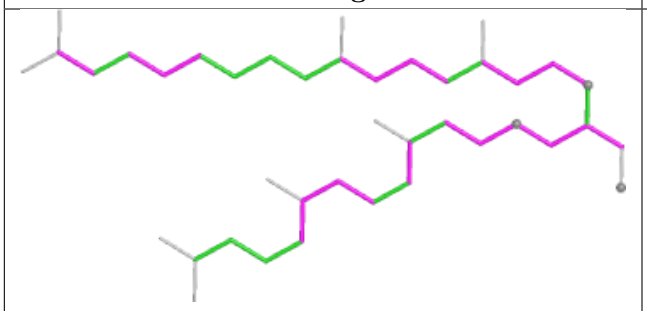
Ligand LI1 B 604



Bond lengths



Bond angles



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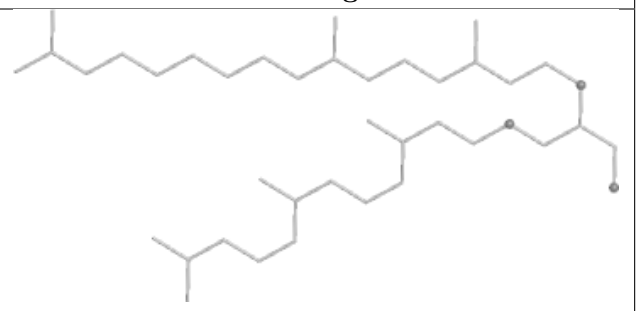

Rings

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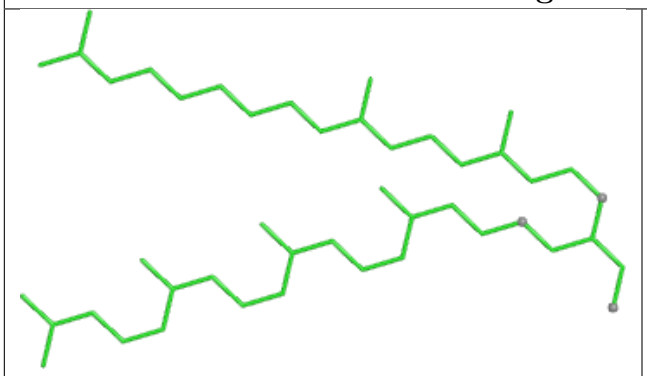
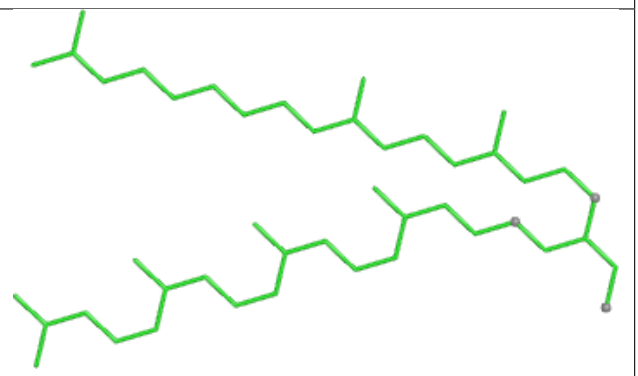
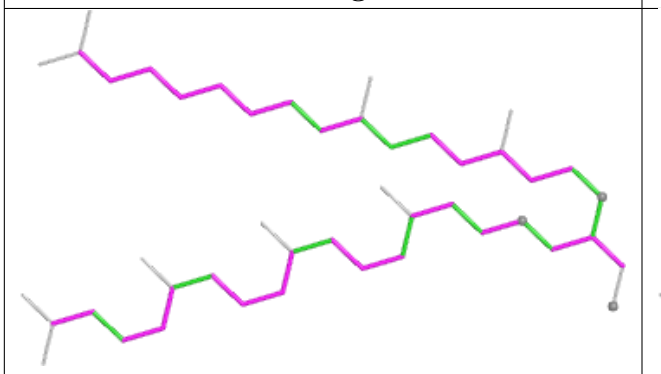


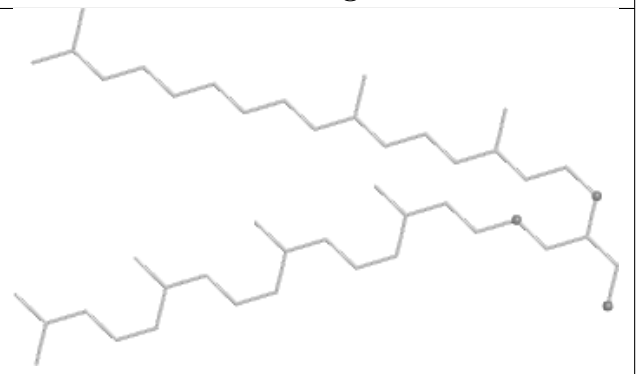
Bond lengths



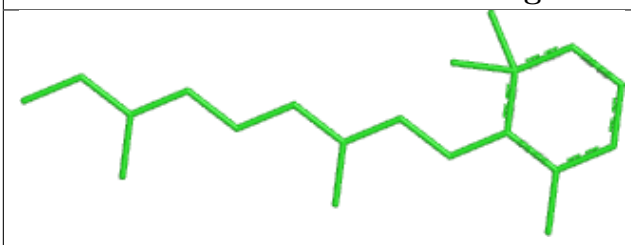
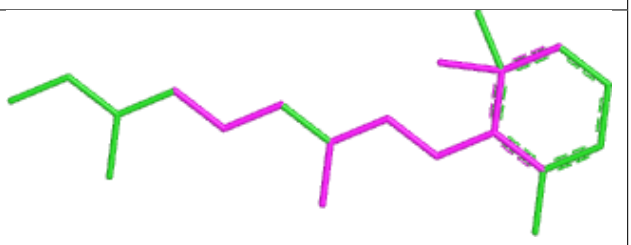
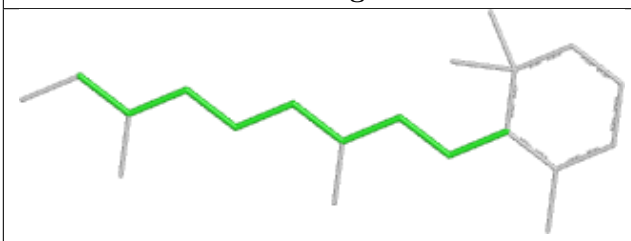
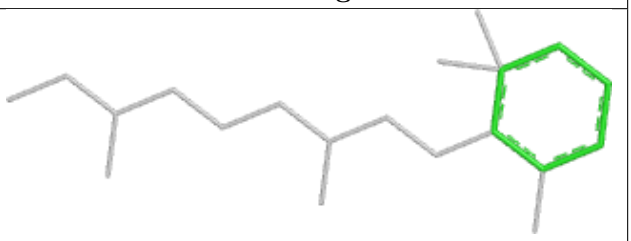
Bond angles

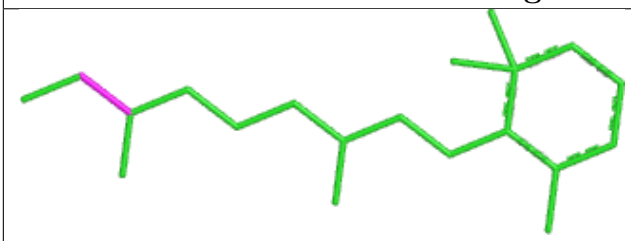
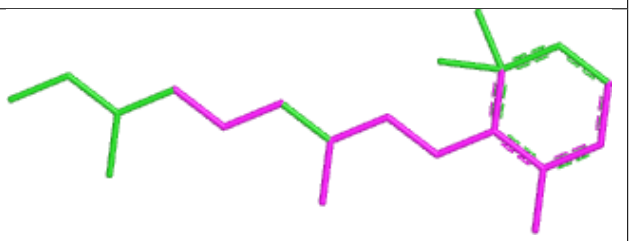
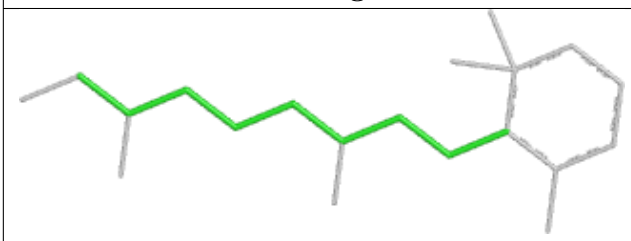
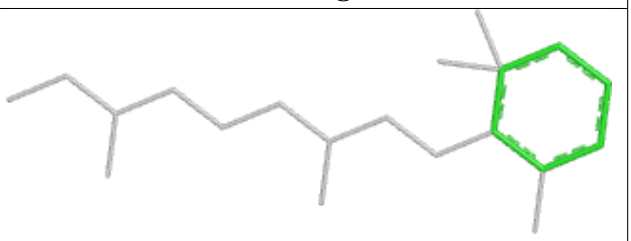


Torsions

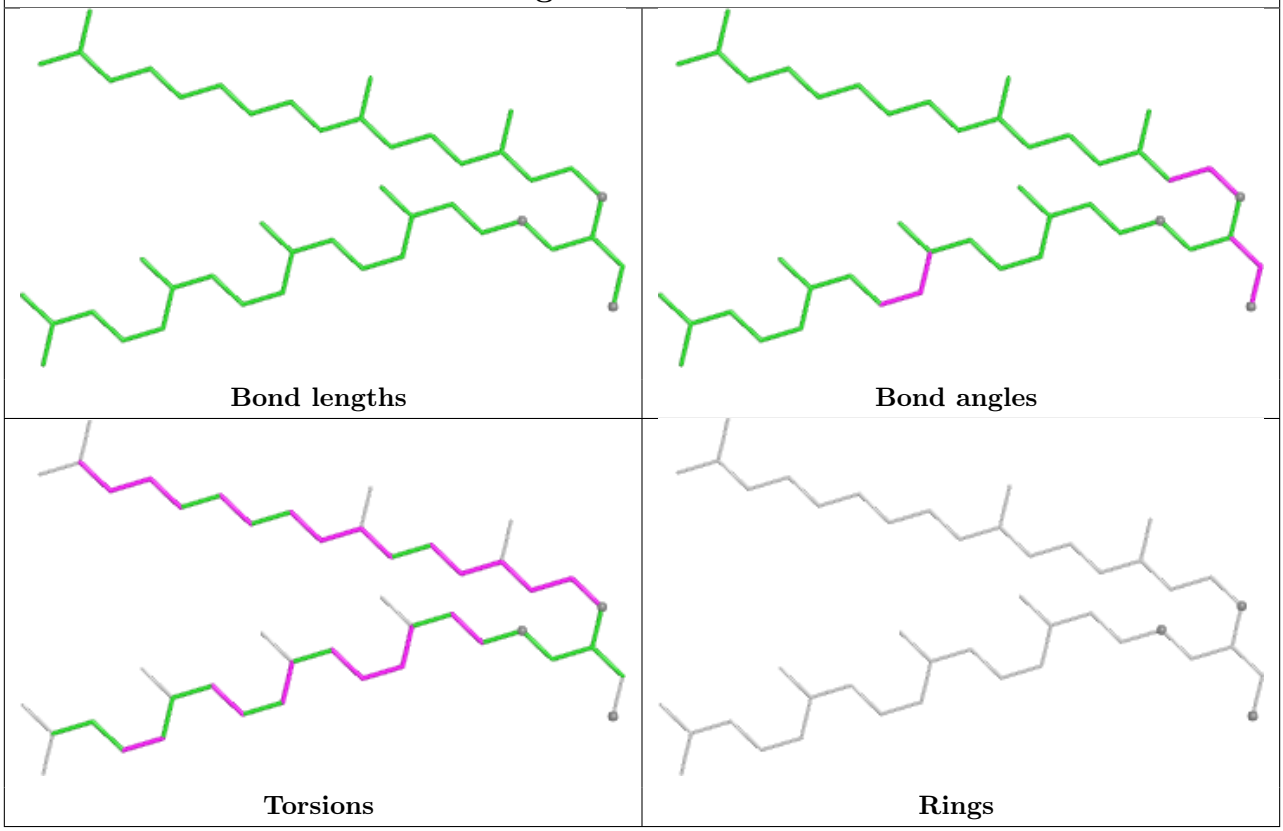


Rings

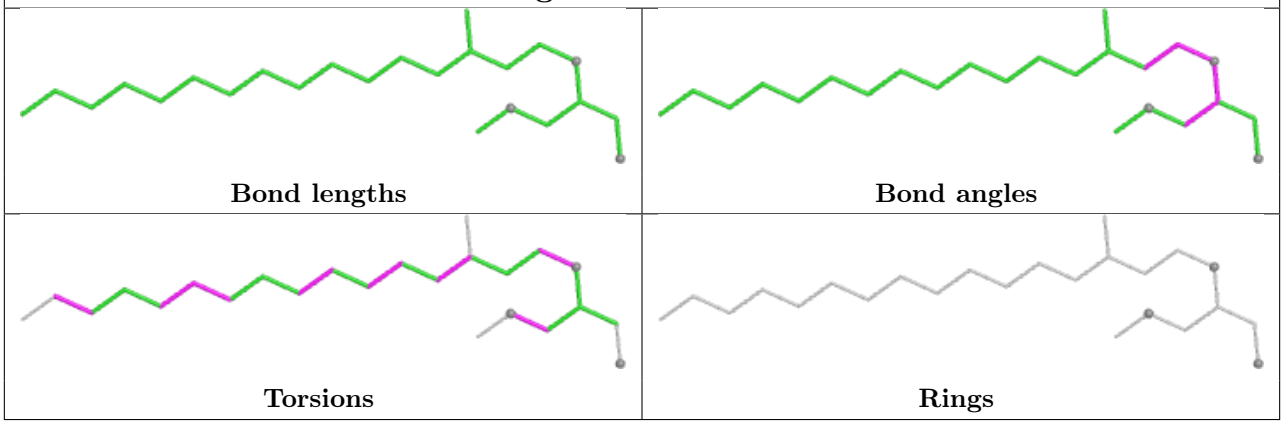
Ligand RET B 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RET C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

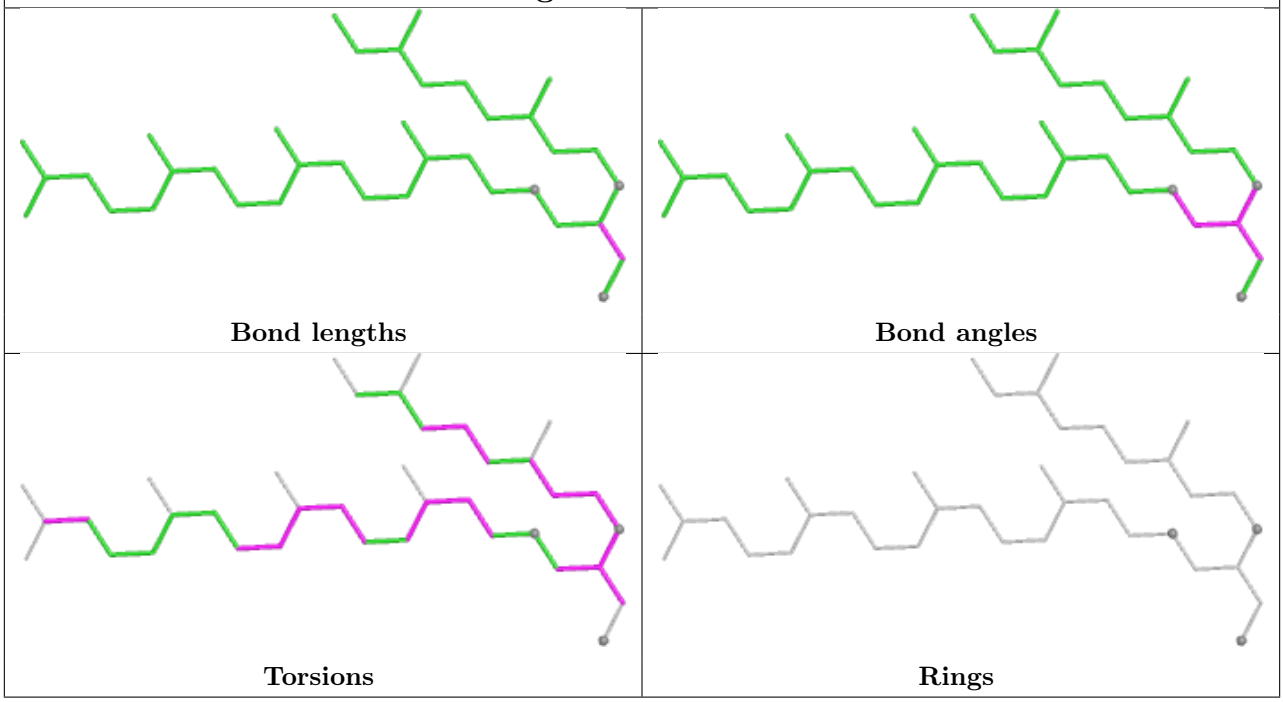
Ligand LI1 A 600



Ligand LI1 A 608



Ligand LI1 B 603



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	225/225 (100%)	-0.27	6 (2%)	54	26	28, 42, 75, 97	0
1	B	225/225 (100%)	-0.14	12 (5%)	26	9	31, 43, 75, 95	0
1	C	225/225 (100%)	-0.23	12 (5%)	26	9	30, 43, 75, 111	0
All	All	675/675 (100%)	-0.22	30 (4%)	34	13	28, 43, 76, 111	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	GLN	5.5
1	A	231	GLY	4.1
1	C	165	PRO	3.7
1	C	35	SER	3.7
1	B	162	SER	3.2
1	C	33	GLY	3.2
1	B	227	ARG	3.0
1	B	35	SER	3.0
1	C	158	SER	3.0
1	C	36	ASP	3.0
1	B	74	GLU	2.9
1	C	162	SER	2.9
1	C	34	VAL	2.8
1	C	231	GLY	2.8
1	B	158	SER	2.7
1	A	165	PRO	2.6
1	A	230	PHE	2.5
1	C	161	GLU	2.5
1	B	70	PRO	2.5
1	A	37	PRO	2.4
1	B	230	PHE	2.4
1	B	33	GLY	2.4
1	C	164	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	159	LYS	2.3
1	A	36	ASP	2.3
1	B	164	ARG	2.2
1	C	230	PHE	2.1
1	B	103	ALA	2.0
1	A	226	SER	2.0
1	C	163	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

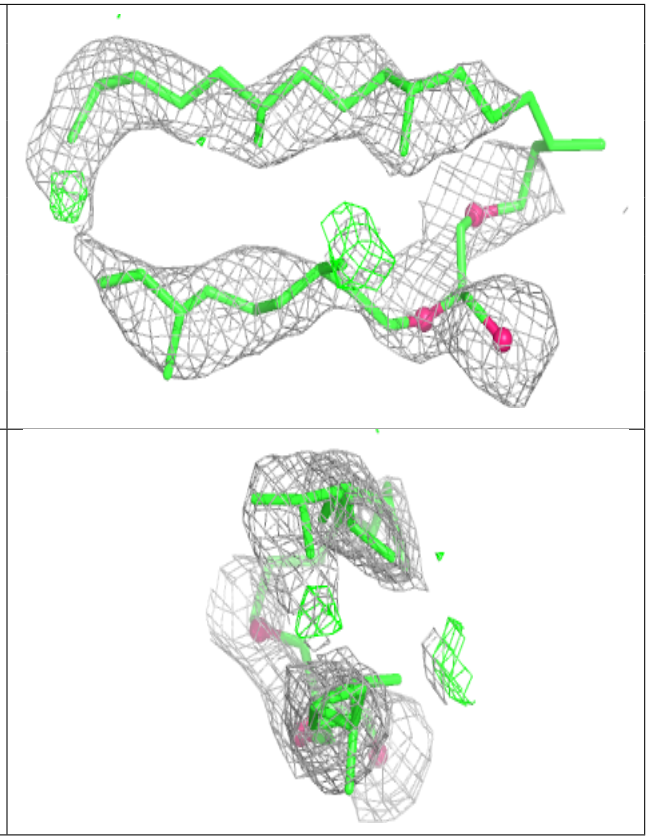
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LI1	B	603	37/45	0.64	0.41	48,59,71,76	0
3	LI1	C	613	25/45	0.70	0.40	61,67,102,111	0
3	LI1	B	612	20/45	0.78	0.32	48,56,63,64	0
3	LI1	C	606	45/45	0.78	0.31	47,68,95,96	0
3	LI1	A	600	45/45	0.78	0.30	30,44,64,66	0
3	LI1	A	608	24/45	0.84	0.29	33,40,63,67	0
3	LI1	B	602	26/45	0.84	0.30	34,41,53,55	0
3	LI1	B	611	41/45	0.85	0.25	32,56,73,77	0
3	LI1	B	605	14/45	0.88	0.26	44,49,54,55	0
3	LI1	B	604	40/45	0.90	0.22	35,41,54,58	0
3	LI1	B	615	8/45	0.91	0.22	36,39,41,42	0
2	RET	B	301	20/21	0.92	0.21	27,31,34,35	0
2	RET	A	301	20/21	0.92	0.25	34,37,42,43	0
2	RET	C	301	20/21	0.94	0.20	31,33,36,38	0

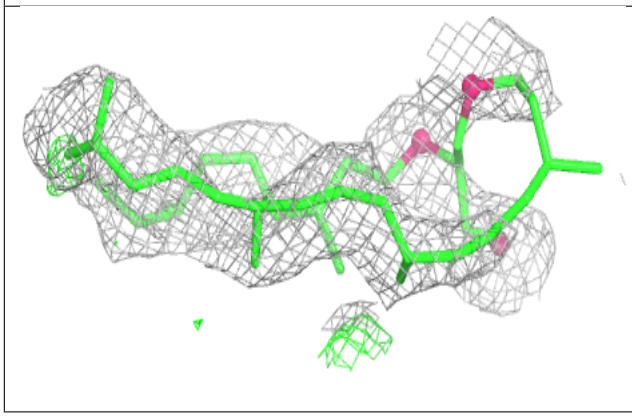
The following is a graphical depiction of the model fit to experimental electron density of all

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 LI1 B 603:

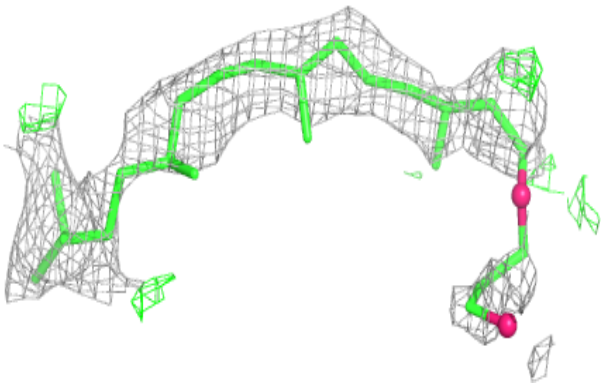
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

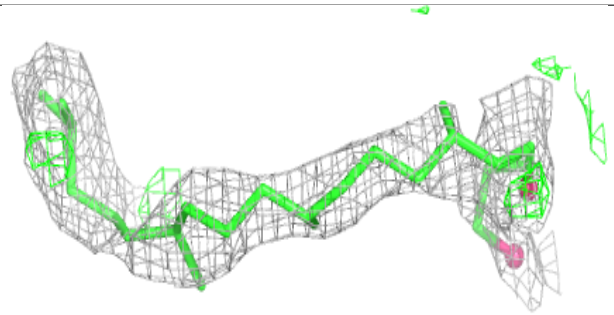


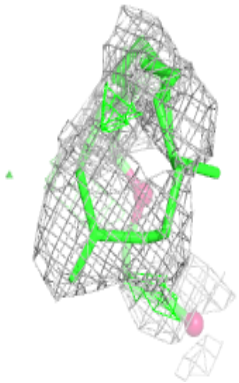


Electron density around LI1 C 613:

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







Electron density around LI1 B 612:

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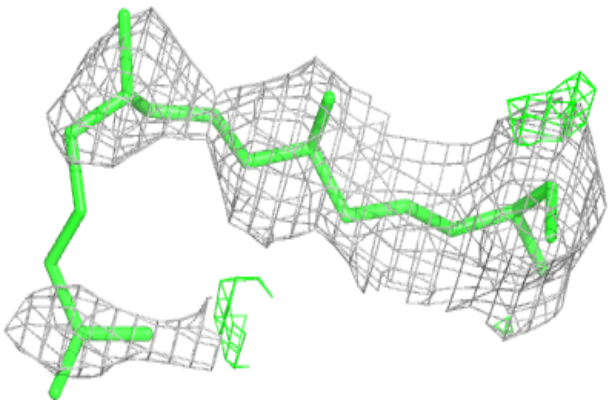
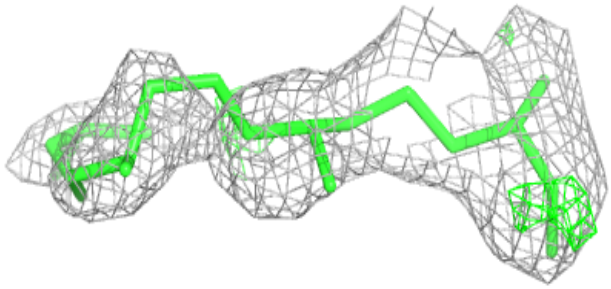
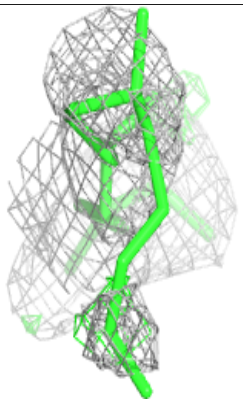
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around LI1 C 606:

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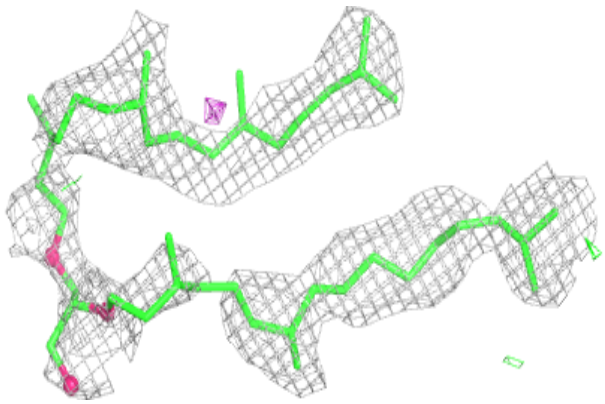
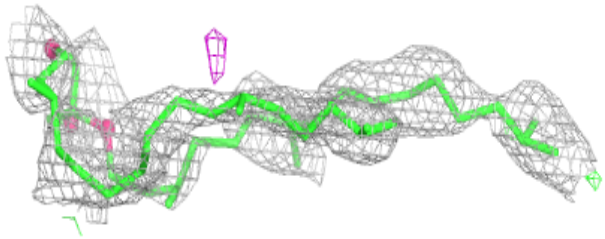
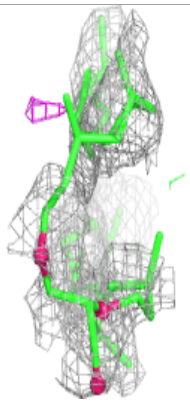
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

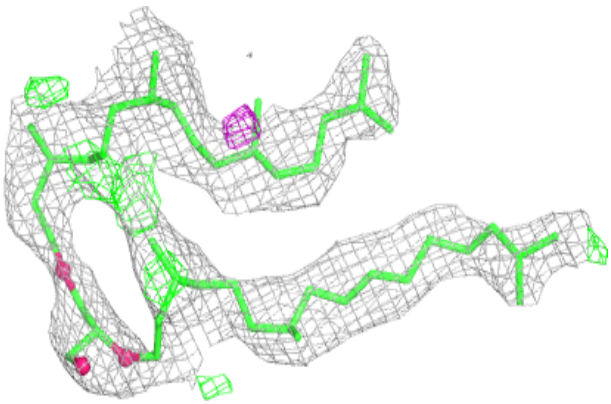


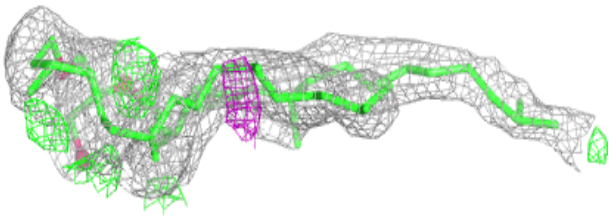


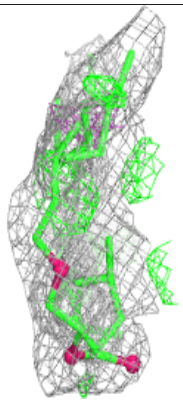


Electron density around LI1 A 600:

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

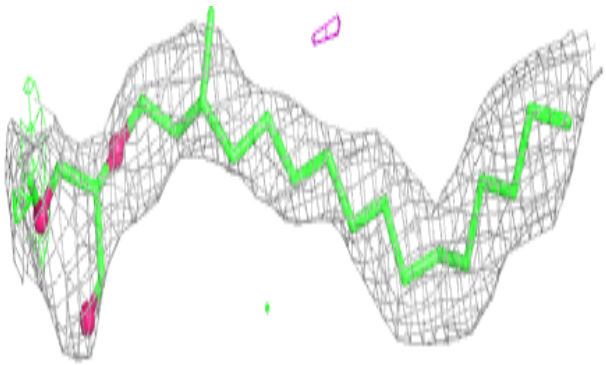


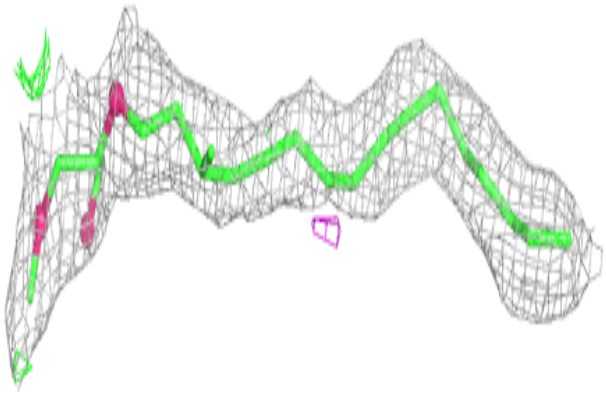


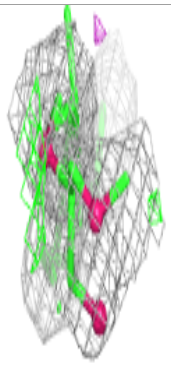


Electron density around LI1 A 608:

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

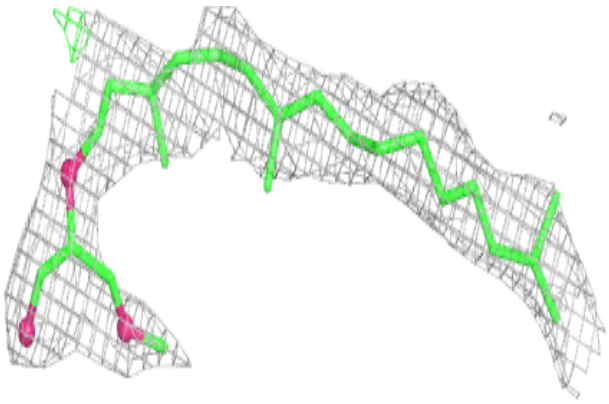


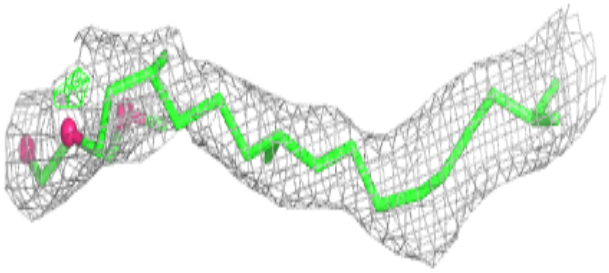


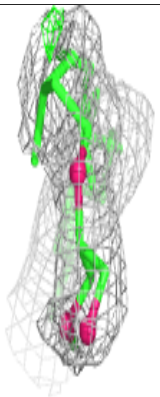


Electron density around LI1 B 602:

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

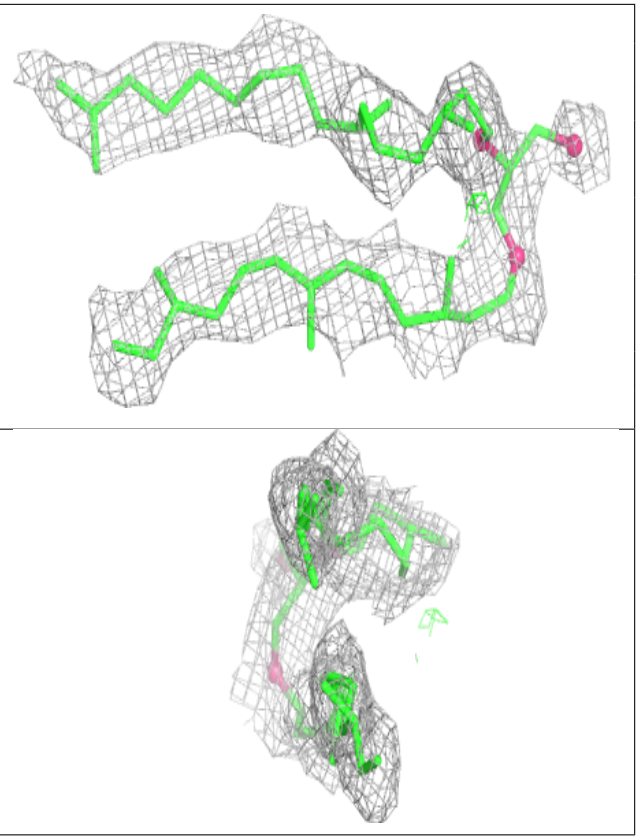






Electron density around LI1 B 611:

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



Electron density around LI1 B 605:

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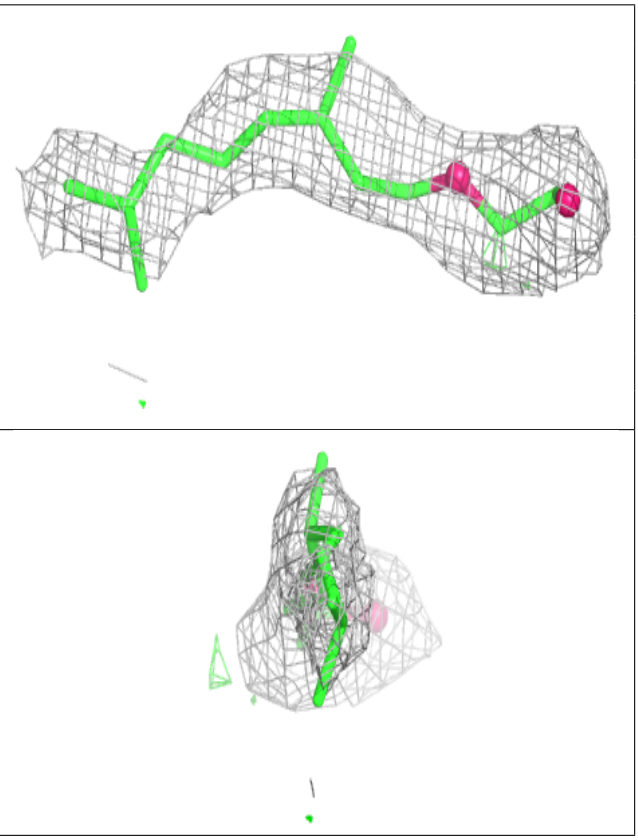
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LI1 B 604:

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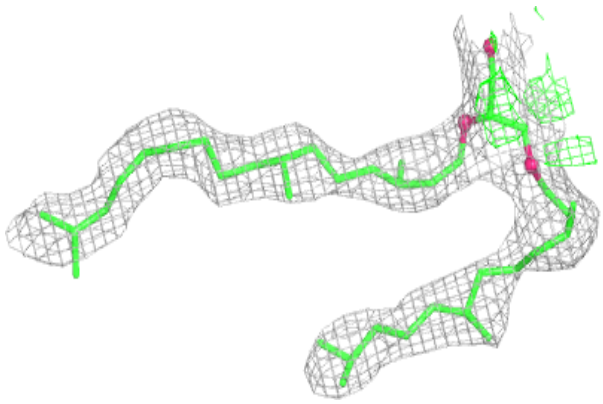
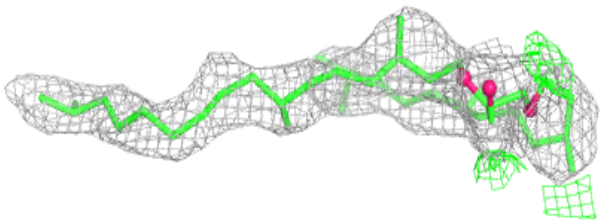
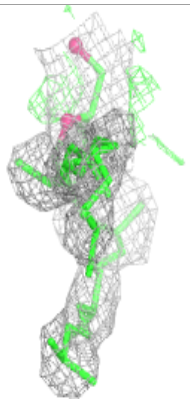
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around LI1 B 615:

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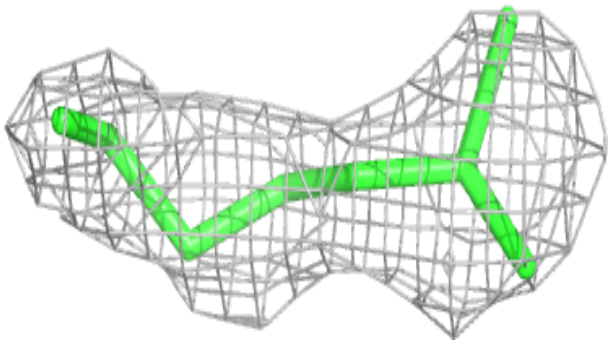
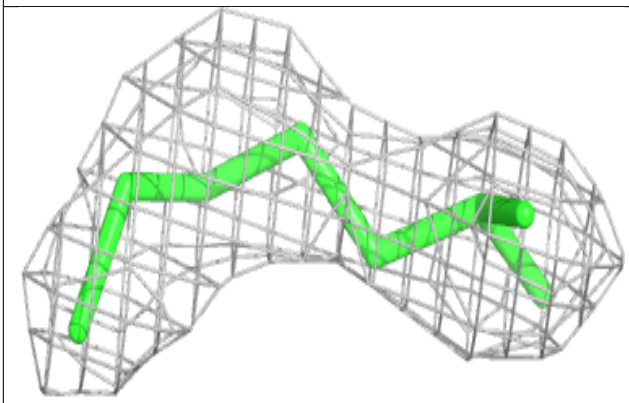
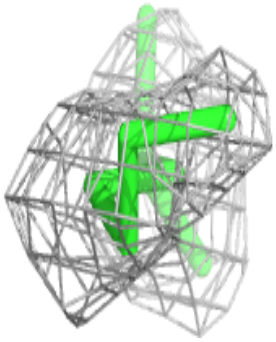
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around RET B 301:

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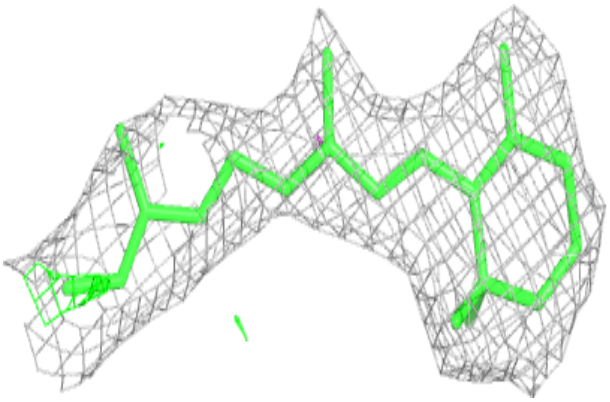
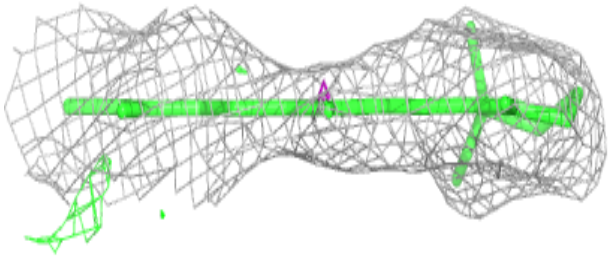
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around RET A 301:

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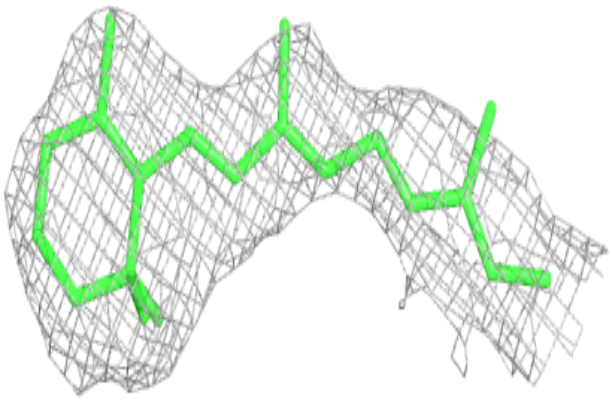
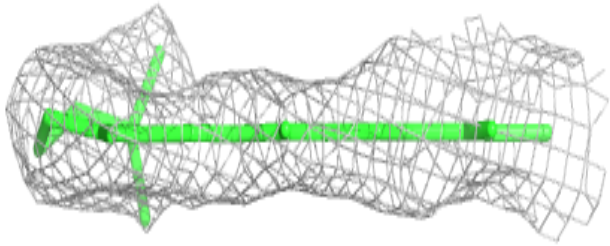
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around RET C 301:

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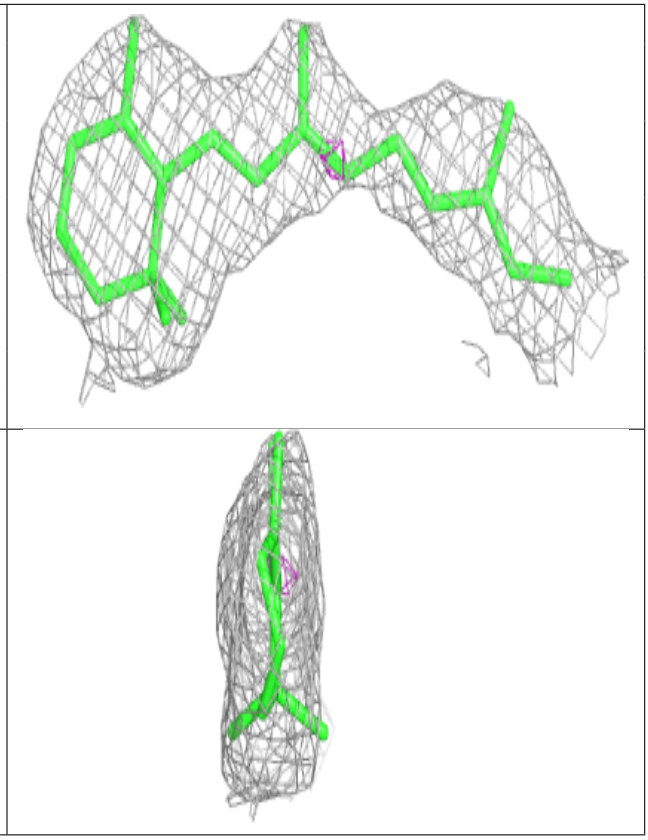
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.