



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:04 PM UTC

PDB ID : 7XJC / pdb_00007xjc
Title : Crystal structure of bacteriorhodopsin in the ground and K states after green laser irradiation
Authors : Taguchi, S.; Niwa, S.; Takeda, K.
Deposited on : 2022-04-16
Resolution : 1.33 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 ⓘ 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

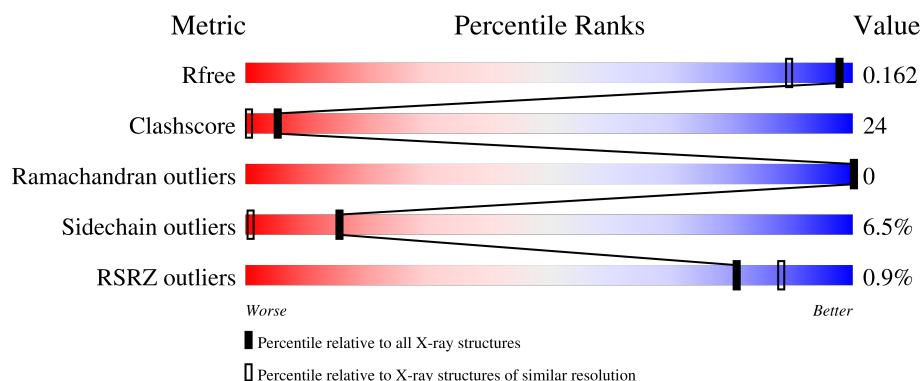
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	230	

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	L2P	A	302	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	L2P	A	303	X	-	-	-
3	L2P	A	304	X	-	X	-
3	L2P	A	305	X	-	-	-
3	L2P	A	306	X	-	X	-

2 Entry composition [i](#)

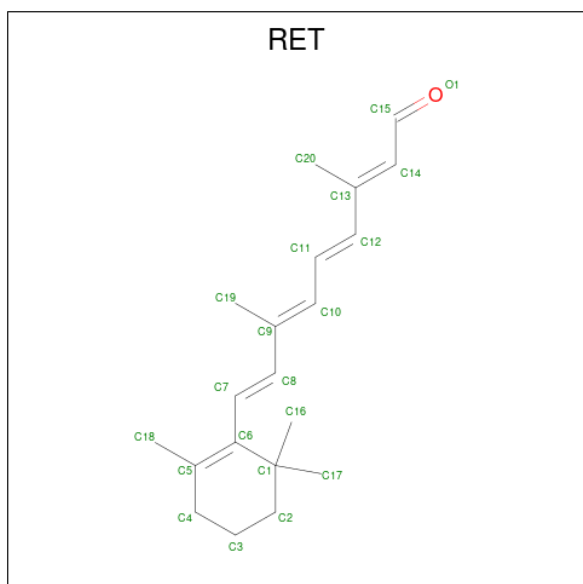
There are 5 unique types of molecules in this entry. The entry contains 4143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

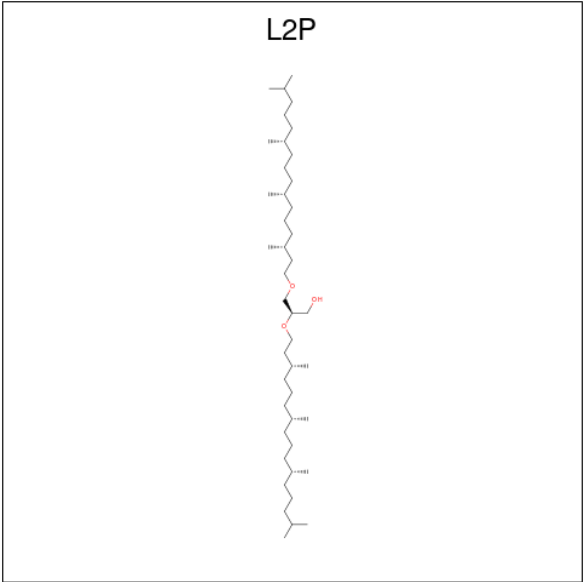
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	230	0
			3633	2432	553	629	19			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



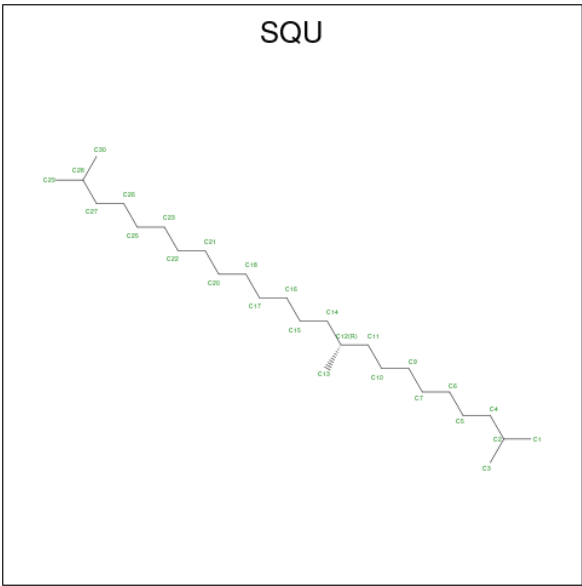
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	1
			40	40		

- Molecule 3 is 2,3-DI-PHYTANYL-GLYCEROL (CCD ID: L2P) (formula: $C_{43}H_{88}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			46	43	3		
3	A	1	Total	C	O	0	0
			40	37	3		
3	A	1	Total	C	O	0	0
			46	43	3		
3	A	1	Total	C	O	0	0
			46	43	3		
3	A	1	Total	C	O	0	0
			42	39	3		
3	A	1	Total	C	O	0	0
			17	15	2		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			26	23	3		
3	A	1	Total	C		0	0
			10	10			
3	A	1	Total	C	O	0	0
			10	7	3		
3	A	1	Total	C		0	0
			12	12			
3	A	1	Total	C		0	0
			10	10			
3	A	1	Total	C		0	0
			8	8			
3	A	1	Total	C	O	0	0
			18	17	1		

- Molecule 4 is 2,10,23-TRIMETHYL-TETRACOSANE (CCD ID: SQU) (formula: C₂₇H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			6	6		
4	A	1	Total	C	0	0
			11	11		
4	A	1	Total	C	0	0
			8	8		
4	A	1	Total	C	0	0
			8	8		

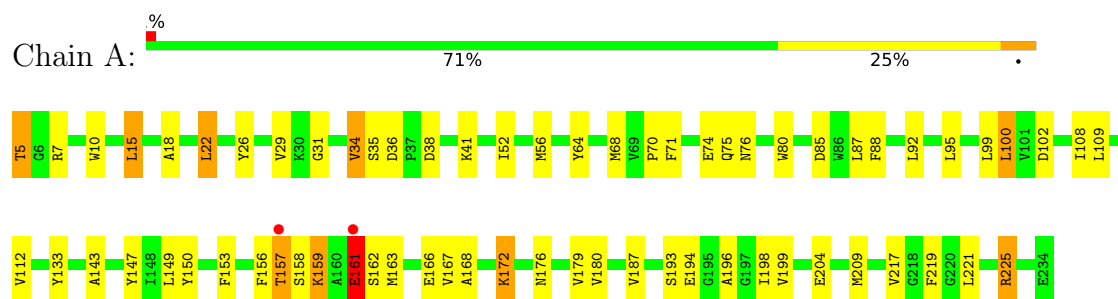
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	58
			96	96		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.57Å 60.57Å 110.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.33 50.00 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.33) 99.9 (50.00-1.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.33Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.131 , 0.172 0.125 , 0.162	Depositor DCC
R_{free} test set	2436 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 101.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.212 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4143	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, L2P, SQU

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	0.32	0/3730	0.71	0/5092

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161[A]	GLU	Sidechain
1	A	36[A]	ASP	Sidechain
1	A	7[C]	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3633	0	3726	152	0
2	A	40	0	54	5	0
3	A	341	0	556	126	0
4	A	33	0	54	9	0
5	A	96	0	0	5	0
All	All	4143	0	4390	205	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 24.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[C]:LEU:CG	1:A:22[C]:LEU:CD1	1.80	1.58
1:A:163[C]:MET:HE2	5:A:435[C]:HOH:O	1.32	1.27
1:A:22[C]:LEU:CD1	1:A:22[C]:LEU:CD2	2.21	1.18
1:A:22[C]:LEU:HD11	1:A:22[C]:LEU:HD21	1.43	1.00
1:A:22[C]:LEU:CD1	1:A:22[C]:LEU:HD21	1.91	0.99
1:A:158[C]:SER:O	1:A:161[C]:GLU:OE2	1.84	0.95
3:A:305:L2P:H491	3:A:305:L2P:H443	1.51	0.92
1:A:199[A]:VAL:HG22	3:A:306:L2P:H151	1.52	0.89
1:A:187[A]:VAL:HG11	3:A:306:L2P:H242	1.55	0.89
1:A:38[C]:ASP:O	1:A:41[C]:LYS:HG2	1.72	0.88
3:A:304:L2P:H521	3:A:304:L2P:H291	1.56	0.88
1:A:187[C]:VAL:HG11	3:A:306:L2P:H242	1.56	0.87
1:A:5[C]:THR:HA	1:A:10[C]:TRP:CD1	2.10	0.86
1:A:31[C]:GLY:O	1:A:34[C]:VAL:CG1	2.24	0.86
1:A:217[A]:VAL:HG11	3:A:316:L2P:H222	1.60	0.84
1:A:163[C]:MET:HG2	1:A:168[C]:ALA:HB2	1.60	0.83
1:A:38[A]:ASP:O	1:A:41[A]:LYS:HG2	1.83	0.79
1:A:153[C]:PHE:CE2	1:A:179[C]:VAL:HG21	2.18	0.78
1:A:80[C]:TRP:HH2	3:A:302:L2P:H122	1.49	0.78
3:A:305:L2P:H591	3:A:313:L2P:H571	1.64	0.78
1:A:217[C]:VAL:HG11	3:A:316:L2P:H222	1.65	0.77
3:A:305:L2P:H542	3:A:305:L2P:H201	1.66	0.77
3:A:304:L2P:H541	4:A:319:SQU:H232	1.67	0.77
1:A:176[A]:ASN:HD21	3:A:304:L2P:H12	1.50	0.75
1:A:80[A]:TRP:HH2	3:A:302:L2P:H122	1.51	0.74
1:A:95[C]:LEU:HD11	3:A:310:L2P:H32	1.68	0.74
1:A:163[C]:MET:CE	5:A:435[C]:HOH:O	2.04	0.74
1:A:109[C]:LEU:HD23	3:A:310:L2P:H121	1.70	0.72
3:A:304:L2P:H303	3:A:306:L2P:H243	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18[A]:ALA:O	1:A:22[A]:LEU:HD13	1.89	0.72
1:A:31[C]:GLY:O	1:A:34[C]:VAL:HG13	1.89	0.72
3:A:305:L2P:H291	3:A:315:L2P:H221	1.70	0.72
1:A:22[B]:LEU:HD11	4:A:317:SQU:H291	1.71	0.72
4:A:317:SQU:H28	4:A:318:SQU:H261	1.72	0.72
3:A:303:L2P:H593	3:A:305:L2P:H602	1.70	0.71
3:A:304:L2P:H602	3:A:306:L2P:H541	1.72	0.71
1:A:31[C]:GLY:O	1:A:34[C]:VAL:HG12	1.90	0.71
3:A:304:L2P:H511	4:A:319:SQU:H211	1.73	0.71
1:A:193[B]:SER:HB2	5:A:439[B]:HOH:O	1.90	0.71
1:A:199[C]:VAL:HG22	3:A:306:L2P:H151	1.71	0.70
3:A:310:L2P:H412	3:A:310:L2P:H122	1.74	0.70
1:A:41[C]:LYS:HD2	1:A:99[C]:LEU:HD13	1.74	0.70
1:A:109[B]:LEU:HD23	3:A:310:L2P:H121	1.74	0.68
3:A:304:L2P:H303	3:A:306:L2P:H251	1.74	0.68
1:A:176[C]:ASN:HD21	3:A:304:L2P:H12	1.58	0.68
1:A:68[C]:MET:CE	1:A:75[C]:GLN:O	2.43	0.67
1:A:198[A]:ILE:HG22	3:A:306:L2P:H421	1.77	0.66
1:A:15[B]:LEU:CD1	1:A:15[B]:LEU:N	2.59	0.65
1:A:31[A]:GLY:O	1:A:34[A]:VAL:HG13	1.96	0.65
1:A:166[C]:GLU:HG2	1:A:167[C]:VAL:N	2.11	0.65
3:A:304:L2P:H512	3:A:314:L2P:H271	1.77	0.65
3:A:304:L2P:H601	3:A:306:L2P:H193	1.79	0.65
1:A:68[C]:MET:HE1	1:A:75[C]:GLN:O	1.98	0.64
1:A:153[A]:PHE:CE2	1:A:179[A]:VAL:HG21	2.33	0.64
1:A:153[C]:PHE:HE2	1:A:179[C]:VAL:HG21	1.60	0.64
1:A:26[A]:TYR:HA	3:A:308:L2P:H422	1.80	0.62
1:A:95[A]:LEU:HD11	3:A:310:L2P:H32	1.80	0.62
3:A:302:L2P:H31	5:A:442[A]:HOH:O	1.97	0.62
1:A:194[C]:GLU:OE1	1:A:204[C]:GLU:OE2	2.18	0.62
1:A:38[A]:ASP:HA	1:A:41[A]:LYS:HE2	1.82	0.61
1:A:158[C]:SER:HB2	1:A:161[C]:GLU:OE2	2.00	0.61
1:A:52[C]:ILE:HD11	3:A:302:L2P:H301	1.83	0.61
1:A:15[B]:LEU:N	1:A:15[B]:LEU:HD13	2.16	0.60
1:A:68[C]:MET:HE3	1:A:75[C]:GLN:C	2.25	0.60
3:A:304:L2P:H493	4:A:319:SQU:H202	1.84	0.60
1:A:80[C]:TRP:CH2	3:A:302:L2P:H122	2.35	0.59
1:A:71[C]:PHE:O	1:A:74[C]:GLU:HG3	2.02	0.59
1:A:26[C]:TYR:HA	3:A:308:L2P:H422	1.83	0.59
1:A:38[C]:ASP:HA	1:A:41[C]:LYS:HE2	1.85	0.59
3:A:305:L2P:H293	3:A:315:L2P:H251	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52[A]:ILE:HD11	3:A:302:L2P:H301	1.84	0.58
1:A:71[A]:PHE:O	1:A:74[A]:GLU:HG2	2.03	0.58
3:A:304:L2P:H442	3:A:314:L2P:C18	2.33	0.58
1:A:102[C]:ASP:O	1:A:159[C]:LYS:HE2	2.03	0.58
1:A:161[C]:GLU:OE2	1:A:161[C]:GLU:CD	2.47	0.57
1:A:158[C]:SER:O	1:A:161[C]:GLU:HG3	2.04	0.57
1:A:149[A]:LEU:HD22	1:A:179[A]:VAL:HG22	1.86	0.57
1:A:176[A]:ASN:ND2	3:A:304:L2P:H12	2.16	0.57
1:A:221[A]:LEU:O	1:A:225[A]:ARG:HD3	2.05	0.56
3:A:306:L2P:H422	3:A:306:L2P:C13	2.36	0.56
1:A:64[A]:TYR:CE2	3:A:302:L2P:H112	2.40	0.56
1:A:150[A]:TYR:CZ	3:A:303:L2P:H192	2.40	0.56
3:A:303:L2P:H291	3:A:303:L2P:H511	1.88	0.55
1:A:153[A]:PHE:HE2	1:A:179[A]:VAL:HG21	1.71	0.55
1:A:166[A]:GLU:HG2	1:A:167[A]:VAL:N	2.20	0.55
1:A:158[C]:SER:O	1:A:161[C]:GLU:CD	2.49	0.55
1:A:41[A]:LYS:HD2	1:A:99[A]:LEU:HD13	1.87	0.55
1:A:108[A]:ILE:HG21	3:A:310:L2P:H2	1.88	0.55
1:A:26[C]:TYR:OH	3:A:316:L2P:H112	2.07	0.55
1:A:176[C]:ASN:ND2	3:A:304:L2P:H12	2.20	0.55
1:A:5[C]:THR:HA	1:A:10[C]:TRP:CG	2.42	0.55
1:A:64[C]:TYR:CE2	3:A:302:L2P:H112	2.42	0.54
1:A:158[C]:SER:O	1:A:161[C]:GLU:CG	2.55	0.54
3:A:306:L2P:H292	3:A:314:L2P:H293	1.89	0.54
3:A:304:L2P:C60	3:A:306:L2P:H193	2.37	0.54
1:A:198[C]:ILE:HG22	3:A:306:L2P:H421	1.89	0.54
1:A:29[C]:VAL:HG21	3:A:308:L2P:H421	1.89	0.54
1:A:29[A]:VAL:HG21	3:A:308:L2P:H421	1.88	0.53
3:A:305:L2P:H543	3:A:305:L2P:H572	1.90	0.53
1:A:179[C]:VAL:HG12	3:A:304:L2P:H211	1.90	0.53
1:A:92[A]:LEU:HD11	3:A:302:L2P:H302	1.89	0.53
1:A:225[A]:ARG:HH12	3:A:316:L2P:C1	2.22	0.53
1:A:180[A]:VAL:HG22	3:A:304:L2P:H202	1.91	0.53
3:A:304:L2P:C30	3:A:306:L2P:H243	2.39	0.53
1:A:179[A]:VAL:HG12	3:A:304:L2P:H211	1.89	0.52
3:A:303:L2P:C59	3:A:305:L2P:H602	2.38	0.52
1:A:92[C]:LEU:HD11	3:A:302:L2P:H302	1.90	0.52
1:A:108[C]:ILE:HG21	3:A:310:L2P:H2	1.90	0.52
1:A:179[A]:VAL:HG12	3:A:304:L2P:C21	2.40	0.52
3:A:305:L2P:H542	3:A:305:L2P:C20	2.38	0.52
3:A:303:L2P:H511	3:A:303:L2P:C29	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:L2P:H31	5:A:442[C]:HOH:O	2.05	0.51
1:A:112[A]:VAL:HG21	3:A:310:L2P:C42	2.41	0.51
1:A:147[A]:TYR:HE1	3:A:303:L2P:H111	1.76	0.51
3:A:304:L2P:H293	3:A:304:L2P:H551	1.92	0.51
1:A:26[A]:TYR:OH	3:A:316:L2P:H112	2.12	0.50
2:A:301[C]:RET:H171	2:A:301[C]:RET:H8	1.93	0.50
1:A:64[A]:TYR:HE2	3:A:302:L2P:H112	1.76	0.50
1:A:31[C]:GLY:C	1:A:34[C]:VAL:HG12	2.36	0.50
1:A:147[A]:TYR:CE1	3:A:303:L2P:H111	2.47	0.50
3:A:304:L2P:H571	3:A:306:L2P:H291	1.94	0.50
1:A:5[A]:THR:O	1:A:5[A]:THR:OG1	2.30	0.50
1:A:95[C]:LEU:CD1	3:A:310:L2P:H32	2.40	0.50
3:A:303:L2P:H201	3:A:303:L2P:H251	1.94	0.50
1:A:179[C]:VAL:HG12	3:A:304:L2P:C21	2.41	0.49
1:A:52[C]:ILE:HG12	3:A:302:L2P:H242	1.95	0.49
1:A:225[C]:ARG:HH12	3:A:316:L2P:C1	2.24	0.49
1:A:187[A]:VAL:CG1	3:A:306:L2P:H242	2.35	0.49
3:A:304:L2P:H541	4:A:319:SQU:C23	2.41	0.49
1:A:68[C]:MET:CE	1:A:75[C]:GLN:C	2.86	0.48
3:A:304:L2P:C30	3:A:306:L2P:H251	2.39	0.48
1:A:147[C]:TYR:CE1	3:A:303:L2P:H111	2.49	0.48
1:A:18[C]:ALA:O	1:A:22[C]:LEU:CD2	2.61	0.48
1:A:198[C]:ILE:HG21	3:A:306:L2P:H442	1.95	0.48
1:A:147[C]:TYR:HE1	3:A:303:L2P:H111	1.79	0.48
3:A:304:L2P:H542	3:A:314:L2P:C27	2.44	0.48
1:A:80[A]:TRP:CH2	3:A:302:L2P:H122	2.36	0.47
1:A:85[C]:ASP:C	1:A:85[C]:ASP:OD1	2.56	0.47
2:A:301[C]:RET:H181	2:A:301[C]:RET:H7	1.65	0.47
3:A:305:L2P:O1	3:A:305:L2P:H141	2.14	0.47
1:A:219[C]:PHE:C	1:A:219[C]:PHE:CD1	2.92	0.47
1:A:112[C]:VAL:HG21	3:A:310:L2P:C42	2.45	0.47
1:A:52[A]:ILE:HD11	3:A:302:L2P:C30	2.45	0.47
1:A:172[A]:LYS:HE2	3:A:304:L2P:H11	1.96	0.46
1:A:199[A]:VAL:CG2	3:A:306:L2P:H151	2.35	0.46
2:A:301[C]:RET:H171	2:A:301[C]:RET:C8	2.45	0.46
1:A:150[C]:TYR:CZ	3:A:303:L2P:H192	2.50	0.46
1:A:52[A]:ILE:CD1	3:A:302:L2P:H242	2.45	0.46
1:A:15[A]:LEU:HD13	1:A:209[A]:MET:HE1	1.98	0.46
1:A:88[C]:PHE:CD1	3:A:302:L2P:H271	2.50	0.46
1:A:52[A]:ILE:HG12	3:A:302:L2P:H242	1.97	0.46
2:A:301[A]:RET:H8	2:A:301[A]:RET:H161	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52[C]:ILE:HD11	3:A:302:L2P:C30	2.46	0.46
1:A:88[A]:PHE:CD1	3:A:302:L2P:H271	2.51	0.46
3:A:304:L2P:H543	4:A:319:SQU:H261	1.98	0.45
1:A:70[C]:PRO:HA	1:A:74[C]:GLU:O	2.17	0.45
1:A:22[B]:LEU:HD23	3:A:308:L2P:H462	1.98	0.45
3:A:304:L2P:H23	3:A:304:L2P:H201	1.42	0.45
1:A:56[A]:MET:HE3	3:A:302:L2P:H192	1.99	0.45
1:A:112[A]:VAL:HG21	3:A:310:L2P:H421	1.98	0.45
1:A:92[A]:LEU:HD11	3:A:302:L2P:C30	2.46	0.44
1:A:68[C]:MET:CE	1:A:75[C]:GLN:HB3	2.47	0.44
3:A:304:L2P:H552	3:A:306:L2P:H543	1.99	0.44
1:A:56[C]:MET:HA	1:A:56[C]:MET:HE2	2.00	0.44
1:A:87[C]:LEU:HD21	3:A:310:L2P:C57	2.47	0.44
1:A:92[C]:LEU:HD11	3:A:302:L2P:C30	2.47	0.44
1:A:18[C]:ALA:O	1:A:22[C]:LEU:HD23	2.18	0.44
1:A:74[C]:GLU:HG3	1:A:76[C]:ASN:HD21	1.82	0.44
1:A:52[C]:ILE:CD1	3:A:302:L2P:H242	2.47	0.43
1:A:95[A]:LEU:CD1	3:A:310:L2P:H32	2.43	0.43
1:A:157[C]:THR:C	1:A:159[C]:LYS:H	2.25	0.43
3:A:302:L2P:H53	3:A:302:L2P:H572	1.49	0.43
1:A:70[A]:PRO:HA	1:A:74[A]:GLU:O	2.18	0.43
1:A:163[C]:MET:HE3	1:A:163[C]:MET:HB2	1.73	0.43
3:A:311:L2P:H161	3:A:311:L2P:H122	1.74	0.43
2:A:301[C]:RET:H11	2:A:301[C]:RET:H191	1.70	0.43
1:A:156[C]:PHE:O	1:A:159[C]:LYS:HB2	2.18	0.43
1:A:64[A]:TYR:OH	3:A:302:L2P:H112	2.19	0.42
1:A:71[C]:PHE:O	1:A:74[C]:GLU:CG	2.66	0.42
1:A:100[C]:LEU:HD12	1:A:100[C]:LEU:HA	1.90	0.42
1:A:56[A]:MET:CE	3:A:302:L2P:H192	2.49	0.42
1:A:196[A]:ALA:HB3	1:A:198[A]:ILE:HD12	2.01	0.42
1:A:157[C]:THR:C	1:A:159[C]:LYS:N	2.78	0.42
1:A:133[A]:TYR:CE1	3:A:305:L2P:H122	2.54	0.42
3:A:304:L2P:H543	3:A:304:L2P:H562	1.68	0.42
1:A:64[C]:TYR:HE2	3:A:302:L2P:H112	1.80	0.42
1:A:74[A]:GLU:HG3	1:A:76[A]:ASN:OD1	2.19	0.42
1:A:180[A]:VAL:HG21	3:A:304:L2P:H471	2.02	0.41
1:A:180[C]:VAL:HG22	3:A:304:L2P:H202	2.01	0.41
4:A:317:SQU:C28	4:A:318:SQU:H261	2.45	0.41
1:A:159[C]:LYS:HZ2	1:A:159[C]:LYS:HG2	1.73	0.41
3:A:303:L2P:H112	3:A:303:L2P:H151	1.50	0.41
1:A:176[A]:ASN:HD21	3:A:304:L2P:C1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:L2P:H243	3:A:302:L2P:H262	1.78	0.41
4:A:317:SQU:H28	4:A:318:SQU:C26	2.46	0.41
1:A:221[C]:LEU:O	1:A:225[C]:ARG:HD3	2.20	0.41
3:A:305:L2P:C29	3:A:315:L2P:H251	2.50	0.41
1:A:194[A]:GLU:OE1	1:A:204[A]:GLU:OE2	2.38	0.41
1:A:194[C]:GLU:CD	1:A:204[C]:GLU:OE2	2.64	0.41
1:A:5[A]:THR:HA	1:A:10[A]:TRP:CD1	2.57	0.40
1:A:225[C]:ARG:HH22	3:A:316:L2P:C11	2.34	0.40
3:A:302:L2P:H301	3:A:302:L2P:H243	2.03	0.40
1:A:198[C]:ILE:CG2	3:A:306:L2P:H421	2.46	0.40
1:A:109[C]:LEU:CD2	3:A:310:L2P:H112	2.51	0.40
1:A:143[A]:ALA:HB2	3:A:305:L2P:H28	2.04	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	466/230 (203%)	456 (98%)	10 (2%)	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	378/184 (205%)	351 (93%)	27 (7%)	13 0

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

Mol	Chain	Res	Type
1	A	5[A]	THR
1	A	5[C]	THR
1	A	15[A]	LEU
1	A	15[B]	LEU
1	A	15[C]	LEU
1	A	22[A]	LEU
1	A	22[B]	LEU
1	A	22[C]	LEU
1	A	34[A]	VAL
1	A	34[C]	VAL
1	A	35[A]	SER
1	A	35[B]	SER
1	A	35[C]	SER
1	A	100[A]	LEU
1	A	100[C]	LEU
1	A	157[A]	THR
1	A	157[C]	THR
1	A	159[A]	LYS
1	A	159[C]	LYS
1	A	161[A]	GLU
1	A	161[C]	GLU
1	A	162[A]	SER
1	A	162[C]	SER
1	A	172[A]	LYS
1	A	172[C]	LYS
1	A	225[A]	ARG
1	A	225[C]	ARG

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

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 ⓘ

20 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	L2P	A	306	-	41,41,45	0.51	0	46,48,53	2.17	9 (19%)
3	L2P	A	310	-	25,25,45	0.69	0	25,25,53	2.06	8 (32%)
3	L2P	A	309	-	9,9,45	0.49	0	8,8,53	1.79	2 (25%)
3	L2P	A	314	-	9,9,45	0.34	0	8,8,53	0.25	0
3	L2P	A	308	-	16,16,45	0.58	0	15,16,53	1.85	7 (46%)
3	L2P	A	315	-	7,7,45	0.40	0	6,6,53	0.28	0
3	L2P	A	302	-	45,45,45	0.49	0	51,53,53	2.15	14 (27%)
3	L2P	A	312	-	9,9,45	0.63	0	9,9,53	2.71	1 (11%)
3	L2P	A	313	-	11,11,45	0.34	0	10,10,53	0.16	0
3	L2P	A	303	-	39,39,45	0.71	0	41,41,53	1.41	5 (12%)
3	L2P	A	316	-	17,17,45	0.34	0	16,16,53	0.33	0
2	RET	A	301[C]	1	20,20,21	2.19	4 (20%)	27,27,28	2.75	13 (48%)
3	L2P	A	311	-	9,9,45	0.41	0	9,9,53	0.21	0
4	SQU	A	317	-	10,10,26	0.31	0	10,10,28	0.40	0
4	SQU	A	318	-	7,7,26	1.32	1 (14%)	6,6,28	0.32	0
3	L2P	A	304	-	45,45,45	0.49	0	51,53,53	2.01	8 (15%)
4	SQU	A	319	-	7,7,26	0.32	0	6,6,28	0.27	0
2	RET	A	301[A]	1	20,20,21	2.10	2 (10%)	27,27,28	2.46	15 (55%)
4	SQU	A	307	-	5,5,26	0.39	0	4,4,28	0.42	0
3	L2P	A	305	-	45,45,45	0.47	0	51,53,53	2.00	10 (19%)

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	L2P	A	306	-	3/3/8/9	23/47/47/51	-
3	L2P	A	310	-	-	14/25/25/51	-
3	L2P	A	309	-	-	3/7/7/51	-
3	L2P	A	314	-	-	3/7/7/51	-
3	L2P	A	308	-	-	11/15/15/51	-
3	L2P	A	315	-	-	4/5/5/51	-
3	L2P	A	302	-	5/5/9/9	30/51/51/51	-
3	L2P	A	312	-	-	5/8/8/51	-
3	L2P	A	313	-	-	5/9/9/51	-
3	L2P	A	303	-	1/1/3/9	27/40/40/51	-
3	L2P	A	316	-	-	10/15/15/51	-
2	RET	A	301[C]	1	-	3/13/30/31	0/1/1/1
3	L2P	A	311	-	-	1/8/8/51	-
4	SQU	A	317	-	-	6/8/8/25	-
4	SQU	A	318	-	-	2/5/5/25	-
3	L2P	A	304	-	2/2/9/9	28/51/51/51	-
4	SQU	A	319	-	-	3/5/5/25	-
2	RET	A	301[A]	1	-	2/13/30/31	0/1/1/1
4	SQU	A	307	-	-	1/3/3/25	-
3	L2P	A	305	-	4/4/9/9	26/51/51/51	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[C]	RET	C14-C13	8.24	1.39	1.33
2	A	301[A]	RET	C14-C13	8.08	1.39	1.33
4	A	318	SQU	C30-C28	-3.40	1.26	1.50
2	A	301[C]	RET	C5-C6	2.55	1.38	1.34
2	A	301[C]	RET	C20-C13	-2.47	1.45	1.50
2	A	301[C]	RET	C19-C9	-2.26	1.46	1.50
2	A	301[A]	RET	C5-C6	2.24	1.38	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	312	L2P	O2-C2-C1	8.05	137.50	109.70
3	A	306	L2P	O2-C41-C42	7.69	124.93	108.77
3	A	302	L2P	O2-C41-C42	7.47	124.46	108.77
3	A	304	L2P	O2-C41-C42	6.78	123.00	108.77
2	A	301[A]	RET	C11-C10-C9	-6.59	118.03	127.28
2	A	301[C]	RET	C19-C9-C8	5.88	127.06	118.09
3	A	310	L2P	O1-C1-C2	5.75	122.60	109.42
2	A	301[C]	RET	C11-C10-C9	-5.66	119.34	127.28
3	A	305	L2P	O2-C41-C42	5.46	120.24	108.77
3	A	306	L2P	C41-O2-C2	5.41	130.48	115.53
3	A	305	L2P	O1-C1-C2	5.41	121.82	109.42
3	A	304	L2P	C41-O2-C2	5.39	130.41	115.53
3	A	303	L2P	O2-C2-C3	5.25	122.60	108.64
3	A	305	L2P	O2-C2-C3	5.23	122.56	108.64
3	A	302	L2P	C41-O2-C2	5.23	129.97	115.53
3	A	302	L2P	O2-C2-C3	4.96	121.85	108.64
2	A	301[C]	RET	C16-C1-C6	4.85	117.85	110.24
3	A	304	L2P	O1-C1-C2	4.79	120.40	109.42
3	A	306	L2P	O1-C1-C2	4.78	120.38	109.42
3	A	304	L2P	O3-C3-C2	4.48	123.30	111.77
2	A	301[A]	RET	C8-C9-C10	-4.36	112.15	119.01
3	A	305	L2P	O3-C3-C2	4.33	122.91	111.77
3	A	302	L2P	O1-C1-C2	4.25	119.16	109.42
3	A	304	L2P	O2-C2-C3	4.21	119.84	108.64
3	A	310	L2P	O2-C2-C3	4.14	119.66	108.64
2	A	301[C]	RET	C7-C8-C9	-4.13	120.12	126.23
2	A	301[A]	RET	C16-C1-C6	-4.07	103.87	110.24
3	A	306	L2P	O2-C2-C3	4.01	119.32	108.64
3	A	309	L2P	O1-C11-C12	3.95	125.30	109.79
3	A	302	L2P	O3-C3-C2	3.91	121.83	111.77
3	A	306	L2P	O3-C3-C2	3.83	121.62	111.77
2	A	301[C]	RET	C7-C6-C5	-3.77	112.86	121.56
2	A	301[A]	RET	C19-C9-C10	3.75	128.90	122.82
2	A	301[C]	RET	C8-C9-C10	-3.70	113.19	119.01
3	A	308	L2P	C11-O1-C1	3.67	129.34	113.26
3	A	310	L2P	C11-O1-C1	3.67	129.74	113.58
2	A	301[C]	RET	C2-C3-C4	3.57	119.12	111.28
3	A	305	L2P	O2-C2-C1	3.52	120.29	109.06
3	A	306	L2P	O2-C2-C1	3.42	119.97	109.06
3	A	305	L2P	C41-O2-C2	3.36	124.81	115.53
3	A	302	L2P	O2-C2-C1	3.35	119.76	109.06
3	A	303	L2P	C11-O1-C1	3.34	128.27	113.58
3	A	304	L2P	O2-C2-C1	3.24	119.39	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	L2P	C11-O1-C1	3.19	127.63	113.58
3	A	310	L2P	O2-C2-C1	3.17	119.17	109.06
3	A	304	L2P	C11-O1-C1	3.16	127.50	113.58
3	A	310	L2P	O3-C3-C2	3.15	119.87	111.77
3	A	302	L2P	C11-O1-C1	2.87	126.21	113.58
3	A	309	L2P	C1-O1-C11	2.85	130.09	112.90
2	A	301[C]	RET	C1-C6-C7	2.85	123.37	115.65
2	A	301[A]	RET	C20-C13-C14	2.84	131.48	123.63
3	A	303	L2P	O1-C1-C2	2.79	115.82	109.42
2	A	301[C]	RET	C2-C1-C6	2.79	114.49	110.44
3	A	305	L2P	C44-C43-C45	2.79	121.21	111.27
3	A	308	L2P	C41-O2-C2	2.76	125.35	113.26
2	A	301[C]	RET	C12-C13-C14	2.70	125.72	118.55
3	A	310	L2P	C41-O2-C2	2.64	122.84	115.53
3	A	310	L2P	O2-C41-C42	2.62	118.26	109.37
2	A	301[C]	RET	C17-C1-C2	-2.60	98.95	108.95
2	A	301[A]	RET	C10-C11-C12	-2.60	115.66	123.20
3	A	302	L2P	C44-C43-C45	2.59	120.52	111.27
2	A	301[A]	RET	C12-C13-C14	-2.57	111.73	118.55
3	A	302	L2P	C54-C53-C55	2.53	120.30	111.27
2	A	301[A]	RET	C17-C1-C6	2.44	114.07	110.24
3	A	306	L2P	C11-O1-C1	2.40	124.14	113.58
3	A	303	L2P	O1-C11-C12	2.40	122.91	110.32
3	A	308	L2P	C44-C43-C45	2.39	119.78	111.27
2	A	301[A]	RET	C4-C5-C6	2.34	125.87	122.70
2	A	301[C]	RET	C20-C13-C14	-2.29	117.30	123.63
3	A	302	L2P	C19-C18-C17	2.26	119.33	111.27
2	A	301[A]	RET	C17-C1-C2	-2.24	100.36	108.95
2	A	301[A]	RET	C17-C1-C16	2.23	115.00	108.63
3	A	305	L2P	C1-C2-C3	2.22	116.93	111.80
2	A	301[A]	RET	C1-C6-C7	2.21	121.66	115.65
3	A	302	L2P	C1-C2-C3	2.18	116.84	111.80
3	A	308	L2P	O1-C11-C12	2.18	121.76	110.32
3	A	302	L2P	C19-C18-C20	2.17	119.01	111.27
3	A	305	L2P	C19-C18-C20	2.16	118.98	111.27
2	A	301[A]	RET	C1-C6-C5	-2.16	119.68	122.64
2	A	301[C]	RET	C3-C4-C5	-2.14	110.24	114.06
3	A	302	L2P	C44-C43-C42	2.11	118.80	111.27
2	A	301[A]	RET	C15-C14-C13	-2.10	116.46	127.72
3	A	306	L2P	C14-C13-C12	2.09	118.72	111.27
3	A	308	L2P	C44-C43-C42	2.09	118.72	111.27
2	A	301[A]	RET	C18-C5-C4	-2.09	109.15	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	L2P	O2-C2-C1	2.08	115.71	109.06
3	A	306	L2P	C50-C48-C47	2.06	122.49	112.07
3	A	308	L2P	O2-C41-C42	2.04	123.22	110.29
3	A	310	L2P	O1-C11-C12	2.02	120.94	110.32
3	A	302	L2P	C49-C48-C47	2.02	118.48	111.27
3	A	308	L2P	O1-C1-C2	2.02	119.56	110.35
3	A	304	L2P	C54-C53-C52	2.01	118.44	111.27

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	302	L2P	C18
3	A	302	L2P	C43
3	A	302	L2P	C2
3	A	302	L2P	C48
3	A	302	L2P	C23
3	A	303	L2P	C2
3	A	304	L2P	C43
3	A	304	L2P	C18
3	A	305	L2P	C43
3	A	305	L2P	C13
3	A	305	L2P	C2
3	A	305	L2P	C23
3	A	306	L2P	C43
3	A	306	L2P	C53
3	A	306	L2P	C23

All (207) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	RET	C20-C13-C14-C15
2	A	301[C]	RET	C12-C13-C14-C15
2	A	301[C]	RET	C20-C13-C14-C15
3	A	302	L2P	C1-C2-C3-O3
3	A	302	L2P	O2-C2-C3-O3
3	A	302	L2P	C41-C42-C43-C44
3	A	303	L2P	O1-C1-C2-O2
3	A	303	L2P	C16-C17-C18-C19
3	A	304	L2P	C11-C12-C13-C14
3	A	304	L2P	C16-C17-C18-C19
3	A	305	L2P	O2-C2-C3-O3
3	A	305	L2P	C42-C41-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	305	L2P	C16-C17-C18-C19
3	A	305	L2P	C41-C42-C43-C44
3	A	305	L2P	C41-C42-C43-C45
3	A	306	L2P	C2-C1-O1-C11
3	A	306	L2P	C11-C12-C13-C14
3	A	310	L2P	C1-C2-C3-O3
3	A	310	L2P	C42-C41-O2-C2
3	A	304	L2P	C20-C21-C22-C23
3	A	308	L2P	C1-C2-O2-C41
3	A	303	L2P	C11-C12-C13-C15
3	A	304	L2P	O2-C41-C42-C43
3	A	305	L2P	O2-C41-C42-C43
3	A	302	L2P	C53-C55-C56-C57
3	A	310	L2P	C45-C46-C47-C48
3	A	303	L2P	C12-C11-O1-C1
3	A	303	L2P	C21-C22-C23-C25
3	A	302	L2P	C16-C17-C18-C19
3	A	302	L2P	C46-C47-C48-C49
3	A	302	L2P	C51-C52-C53-C54
3	A	304	L2P	C46-C47-C48-C49
3	A	304	L2P	C51-C52-C53-C54
3	A	304	L2P	C54-C53-C55-C56
3	A	305	L2P	C24-C23-C25-C26
3	A	305	L2P	C46-C47-C48-C49
3	A	306	L2P	C14-C13-C15-C16
3	A	306	L2P	C44-C43-C45-C46
3	A	306	L2P	C46-C47-C48-C49
3	A	308	L2P	C44-C43-C45-C46
3	A	308	L2P	C11-C12-C13-C14
3	A	304	L2P	C25-C26-C27-C28
3	A	305	L2P	C50-C51-C52-C53
3	A	310	L2P	O1-C11-C12-C13
3	A	316	L2P	O1-C11-C12-C13
3	A	302	L2P	C23-C25-C26-C27
3	A	306	L2P	C50-C51-C52-C53
3	A	312	L2P	O1-C1-C2-C3
3	A	302	L2P	C42-C41-O2-C2
3	A	304	L2P	C42-C41-O2-C2
3	A	302	L2P	C26-C27-C28-C29
3	A	303	L2P	C26-C27-C28-C29
3	A	304	L2P	C56-C57-C58-C60
3	A	312	L2P	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	312	L2P	C1-C2-C3-O3
3	A	305	L2P	C26-C27-C28-C30
3	A	305	L2P	C43-C45-C46-C47
4	A	317	SQU	C25-C26-C27-C28
3	A	302	L2P	O2-C41-C42-C43
3	A	302	L2P	C56-C57-C58-C59
3	A	304	L2P	C18-C20-C21-C22
3	A	302	L2P	C25-C26-C27-C28
3	A	316	L2P	C20-C21-C22-C23
3	A	302	L2P	C42-C43-C45-C46
3	A	302	L2P	C48-C50-C51-C52
3	A	305	L2P	C20-C21-C22-C23
3	A	305	L2P	C23-C25-C26-C27
3	A	303	L2P	C13-C15-C16-C17
3	A	316	L2P	C17-C18-C20-C21
3	A	303	L2P	C23-C25-C26-C27
4	A	317	SQU	C22-C23-C25-C26
3	A	302	L2P	C24-C23-C25-C26
3	A	303	L2P	C46-C47-C48-C50
3	A	303	L2P	O2-C41-C42-C43
3	A	309	L2P	C15-C16-C17-C18
3	A	303	L2P	C53-C55-C56-C57
4	A	317	SQU	C23-C25-C26-C27
3	A	305	L2P	C15-C16-C17-C18
3	A	304	L2P	O1-C11-C12-C13
3	A	303	L2P	C52-C53-C55-C56
3	A	316	L2P	C12-C13-C15-C16
3	A	310	L2P	C43-C45-C46-C47
3	A	304	L2P	C56-C57-C58-C59
3	A	310	L2P	C51-C52-C53-C55
3	A	303	L2P	C43-C45-C46-C47
3	A	308	L2P	C45-C46-C47-C48
3	A	313	L2P	C52-C53-C55-C56
3	A	316	L2P	C21-C22-C23-C25
3	A	303	L2P	C25-C26-C27-C28
3	A	313	L2P	C50-C51-C52-C53
3	A	306	L2P	C45-C46-C47-C48
3	A	316	L2P	C13-C15-C16-C17
3	A	305	L2P	C21-C22-C23-C24
3	A	303	L2P	O1-C1-C2-C3
3	A	304	L2P	O1-C1-C2-C3
2	A	301[C]	RET	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
3	A	313	L2P	C51-C52-C53-C55
4	A	307	SQU	C6-C7-C9-C10
3	A	313	L2P	C53-C55-C56-C57
3	A	303	L2P	C51-C52-C53-C55
3	A	312	L2P	C2-C1-O1-C11
2	A	301[A]	RET	C12-C13-C14-C15
3	A	316	L2P	C18-C20-C21-C22
4	A	317	SQU	C18-C20-C21-C22
3	A	315	L2P	C23-C25-C26-C27
3	A	308	L2P	C46-C47-C48-C49
3	A	316	L2P	C25-C26-C27-C28
4	A	319	SQU	C18-C20-C21-C22
3	A	302	L2P	C54-C53-C55-C56
3	A	305	L2P	C14-C13-C15-C16
3	A	306	L2P	C24-C23-C25-C26
3	A	306	L2P	C51-C52-C53-C54
3	A	304	L2P	C12-C13-C15-C16
3	A	305	L2P	C47-C48-C50-C51
3	A	306	L2P	C21-C22-C23-C25
3	A	303	L2P	C20-C21-C22-C23
3	A	306	L2P	O1-C1-C2-C3
3	A	310	L2P	O1-C1-C2-C3
3	A	305	L2P	C1-C2-C3-O3
3	A	315	L2P	C20-C21-C22-C23
3	A	310	L2P	C53-C55-C56-C57
3	A	306	L2P	C12-C11-O1-C1
3	A	303	L2P	C12-C13-C15-C16
3	A	305	L2P	C26-C27-C28-C29
3	A	314	L2P	C22-C23-C25-C26
3	A	316	L2P	C22-C23-C25-C26
3	A	313	L2P	C55-C56-C57-C58
3	A	309	L2P	O1-C11-C12-C13
3	A	306	L2P	C15-C16-C17-C18
3	A	304	L2P	C26-C27-C28-C29
3	A	302	L2P	C51-C52-C53-C55
3	A	303	L2P	C16-C17-C18-C20
3	A	304	L2P	C16-C17-C18-C20
3	A	304	L2P	C47-C48-C50-C51
3	A	305	L2P	C42-C43-C45-C46
3	A	305	L2P	C46-C47-C48-C50
3	A	306	L2P	C47-C48-C50-C51
3	A	304	L2P	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	A	306	L2P	C26-C27-C28-C29
3	A	302	L2P	O1-C1-C2-C3
3	A	305	L2P	O1-C1-C2-C3
4	A	317	SQU	C21-C22-C23-C25
3	A	304	L2P	O1-C1-C2-O2
3	A	303	L2P	O1-C11-C12-C13
3	A	303	L2P	C22-C23-C25-C26
3	A	304	L2P	C52-C53-C55-C56
3	A	306	L2P	C16-C17-C18-C20
4	A	317	SQU	C26-C27-C28-C30
3	A	314	L2P	C18-C20-C21-C22
3	A	310	L2P	C12-C13-C15-C16
3	A	304	L2P	C12-C11-O1-C1
3	A	303	L2P	C45-C46-C47-C48
3	A	306	L2P	C42-C41-O2-C2
3	A	308	L2P	C12-C11-O1-C1
3	A	309	L2P	C12-C11-O1-C1
3	A	306	L2P	C41-C42-C43-C45
3	A	303	L2P	C18-C20-C21-C22
3	A	306	L2P	C52-C53-C55-C56
4	A	318	SQU	C23-C25-C26-C27
3	A	302	L2P	C13-C15-C16-C17
3	A	305	L2P	C21-C22-C23-C25
3	A	310	L2P	C13-C15-C16-C17
3	A	310	L2P	C12-C11-O1-C1
3	A	314	L2P	C26-C27-C28-C29
3	A	302	L2P	C18-C20-C21-C22
3	A	310	L2P	C2-C1-O1-C11
3	A	302	L2P	C26-C27-C28-C30
3	A	311	L2P	C12-C13-C15-C16
3	A	302	L2P	C19-C18-C20-C21
3	A	303	L2P	C42-C43-C45-C46
4	A	319	SQU	C23-C25-C26-C27
3	A	305	L2P	C12-C13-C15-C16
3	A	302	L2P	C56-C57-C58-C60
3	A	306	L2P	C23-C25-C26-C27
3	A	302	L2P	C21-C22-C23-C24
3	A	304	L2P	C21-C22-C23-C24
3	A	305	L2P	C49-C48-C50-C51
3	A	304	L2P	C1-C2-C3-O3
3	A	310	L2P	C47-C48-C50-C51
3	A	303	L2P	C26-C27-C28-C30

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Mol	Chain	Res	Type	Atoms
3	A	306	L2P	O1-C1-C2-O2
3	A	310	L2P	C52-C53-C55-C56
3	A	303	L2P	C48-C50-C51-C52
3	A	315	L2P	C22-C23-C25-C26
3	A	306	L2P	C54-C53-C55-C56
3	A	312	L2P	O2-C2-C3-O3
3	A	308	L2P	C42-C41-O2-C2
3	A	315	L2P	C21-C22-C23-C25
3	A	308	L2P	C43-C45-C46-C47
3	A	316	L2P	C16-C17-C18-C20
3	A	304	L2P	C14-C13-C15-C16
4	A	318	SQU	C21-C22-C23-C25
3	A	302	L2P	C2-C1-O1-C11
3	A	304	L2P	C2-C1-O1-C11
3	A	302	L2P	C52-C53-C55-C56
3	A	306	L2P	C51-C52-C53-C55
3	A	308	L2P	O2-C41-C42-C43
3	A	302	L2P	C12-C11-O1-C1
3	A	302	L2P	C17-C18-C20-C21
3	A	302	L2P	C47-C48-C50-C51
3	A	308	L2P	C2-C1-O1-C11
3	A	305	L2P	C53-C55-C56-C57
3	A	304	L2P	C24-C23-C25-C26
4	A	319	SQU	C20-C21-C22-C23
3	A	308	L2P	C41-C42-C43-C44
3	A	304	L2P	C23-C25-C26-C27
3	A	303	L2P	C1-C2-C3-O3

There are no ring outliers.

17 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	L2P	21	0
3	A	310	L2P	14	0
3	A	314	L2P	4	0
3	A	308	L2P	5	0
3	A	315	L2P	3	0
3	A	302	L2P	30	0
3	A	313	L2P	1	0
3	A	303	L2P	12	0
3	A	316	L2P	7	0
2	A	301[C]	RET	4	0

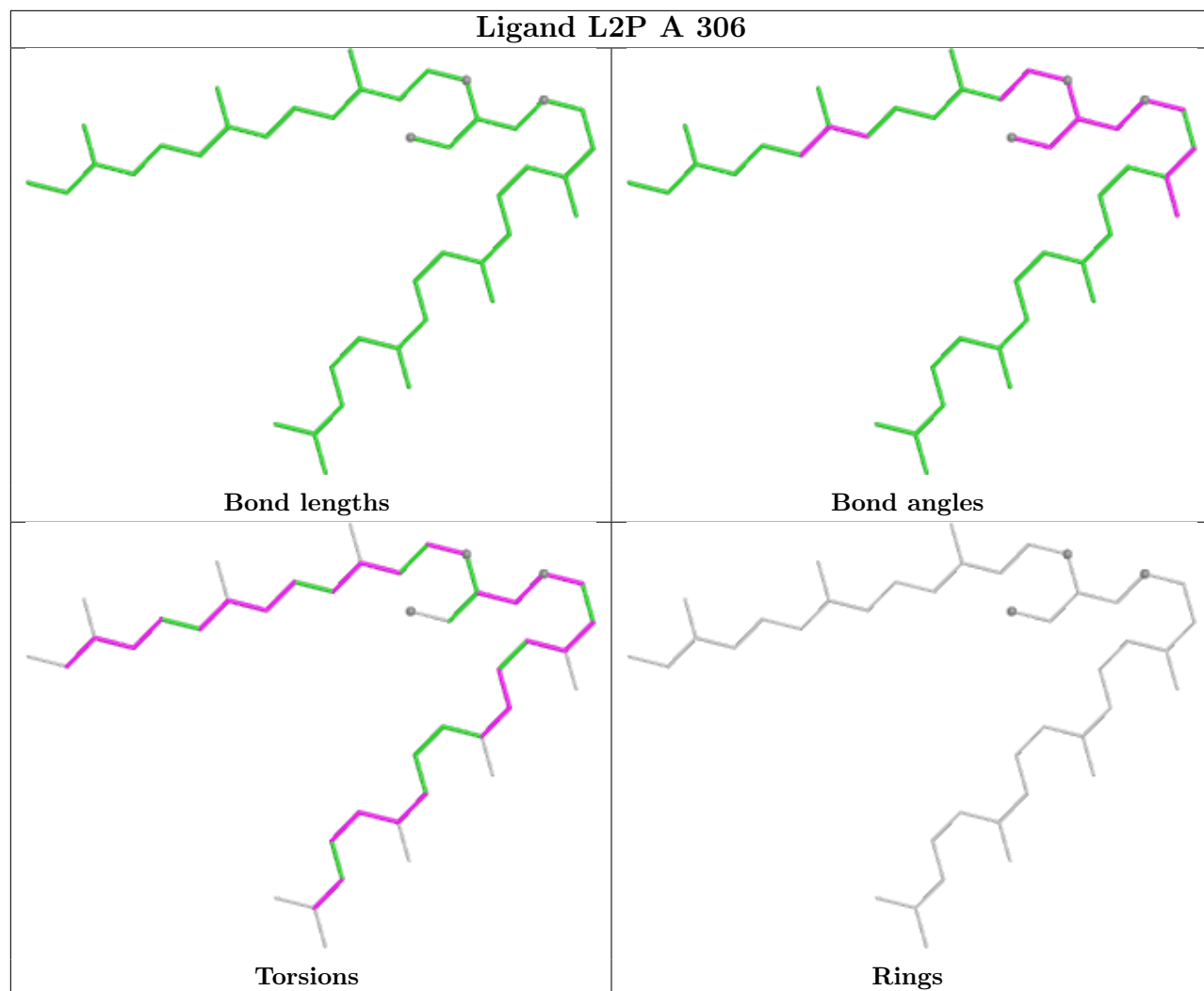
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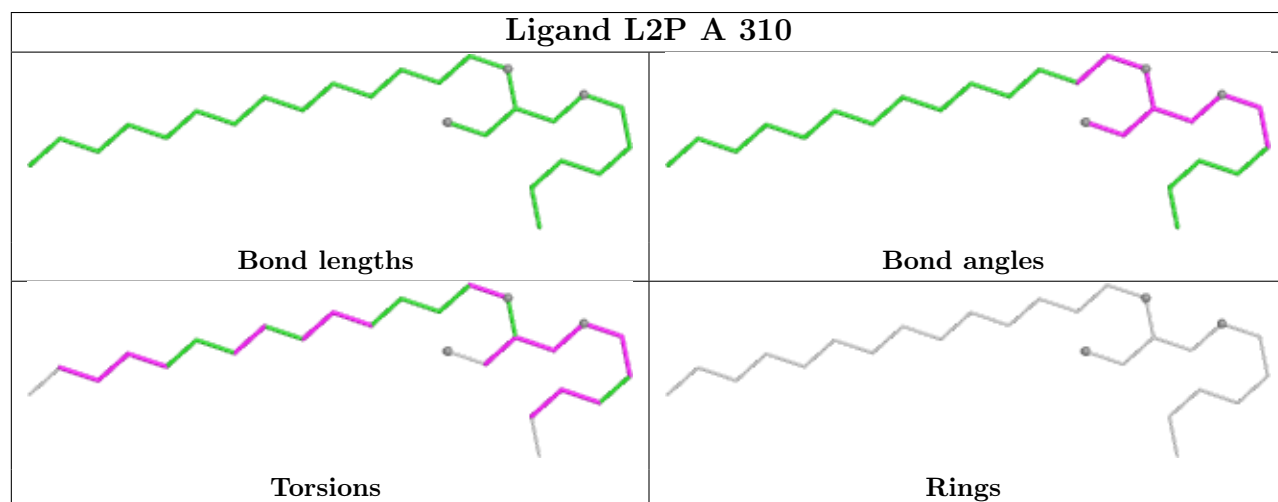
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	311	L2P	1	0
4	A	317	SQU	4	0
4	A	318	SQU	3	0
3	A	304	L2P	34	0
4	A	319	SQU	5	0
2	A	301[A]	RET	1	0
3	A	305	L2P	13	0

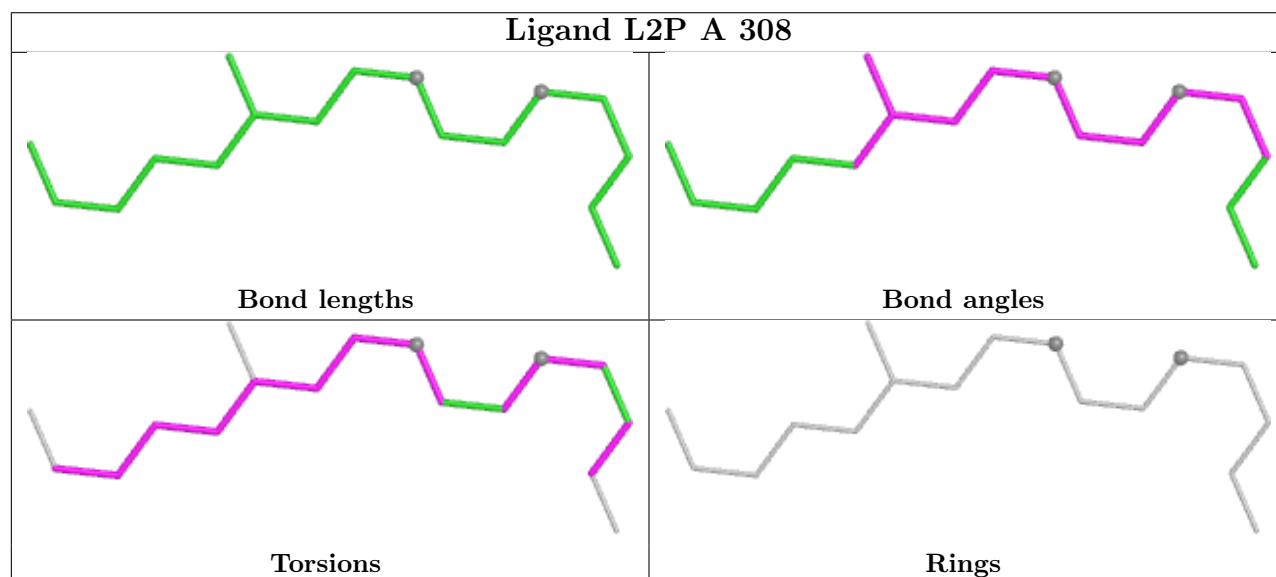
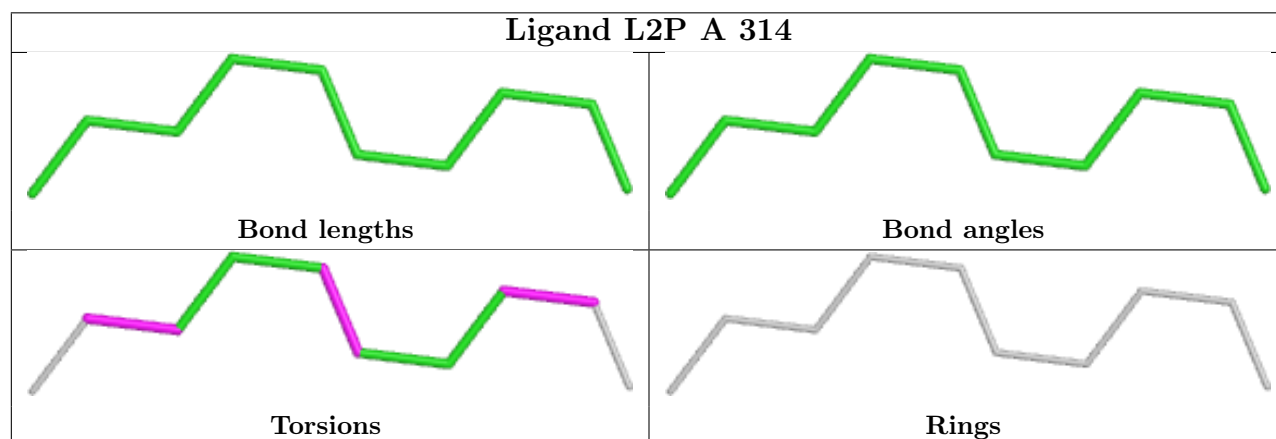
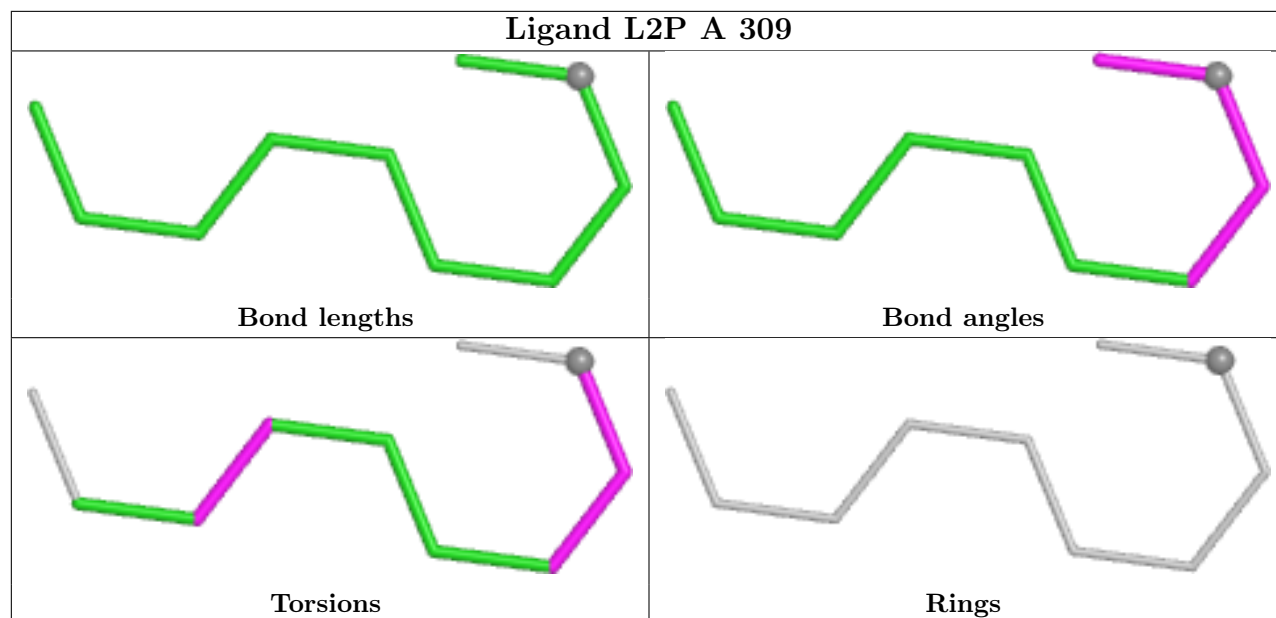
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

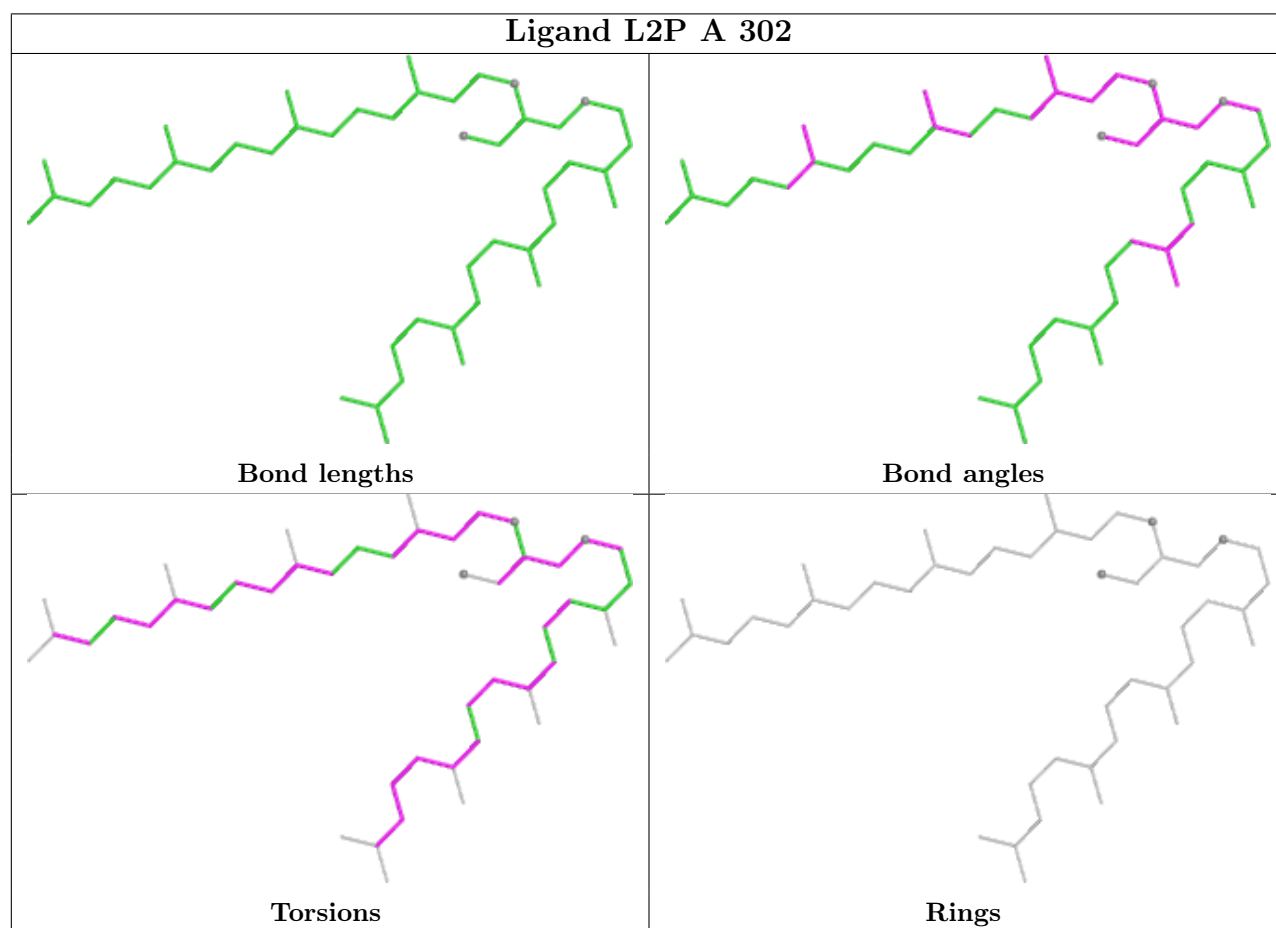
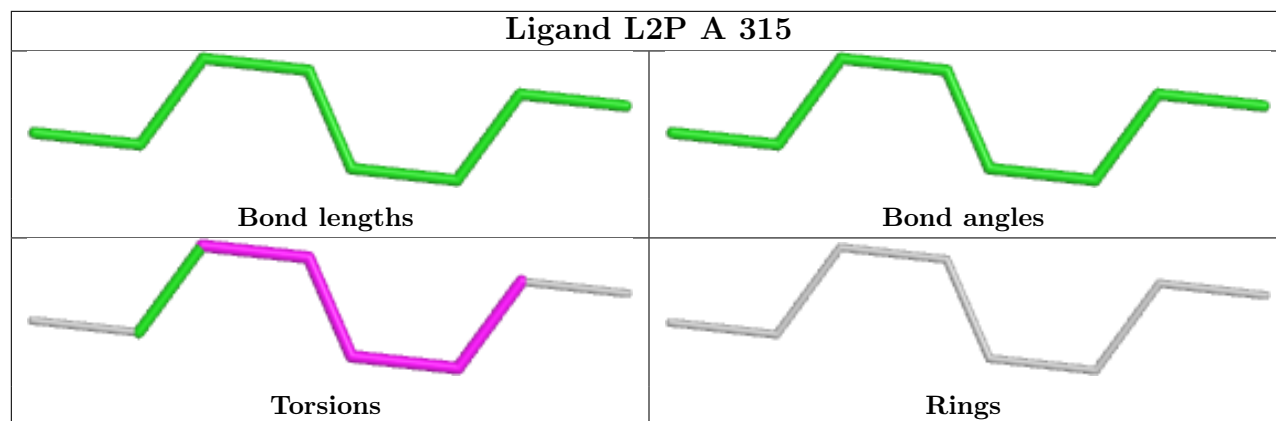
Ligand L2P A 306

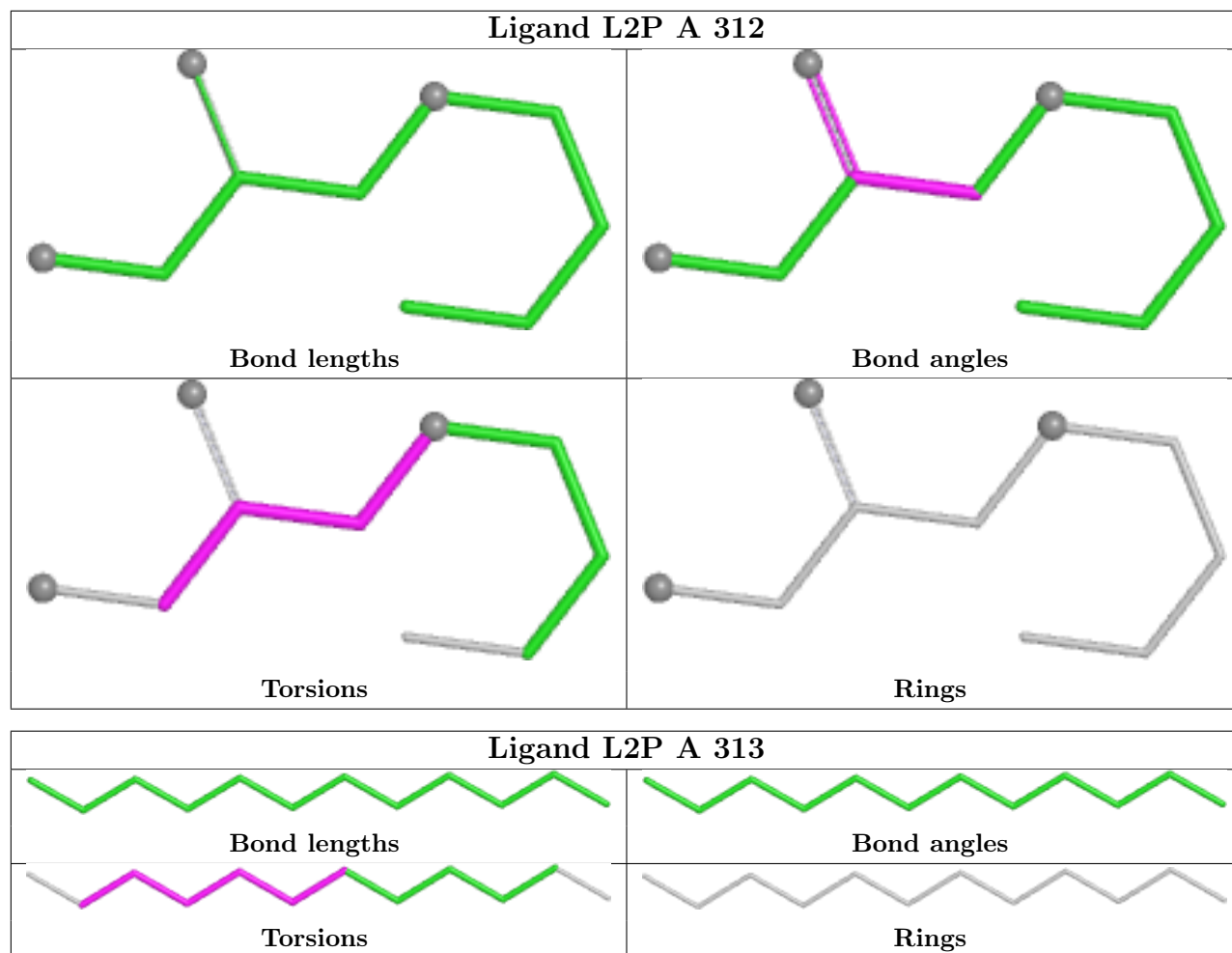


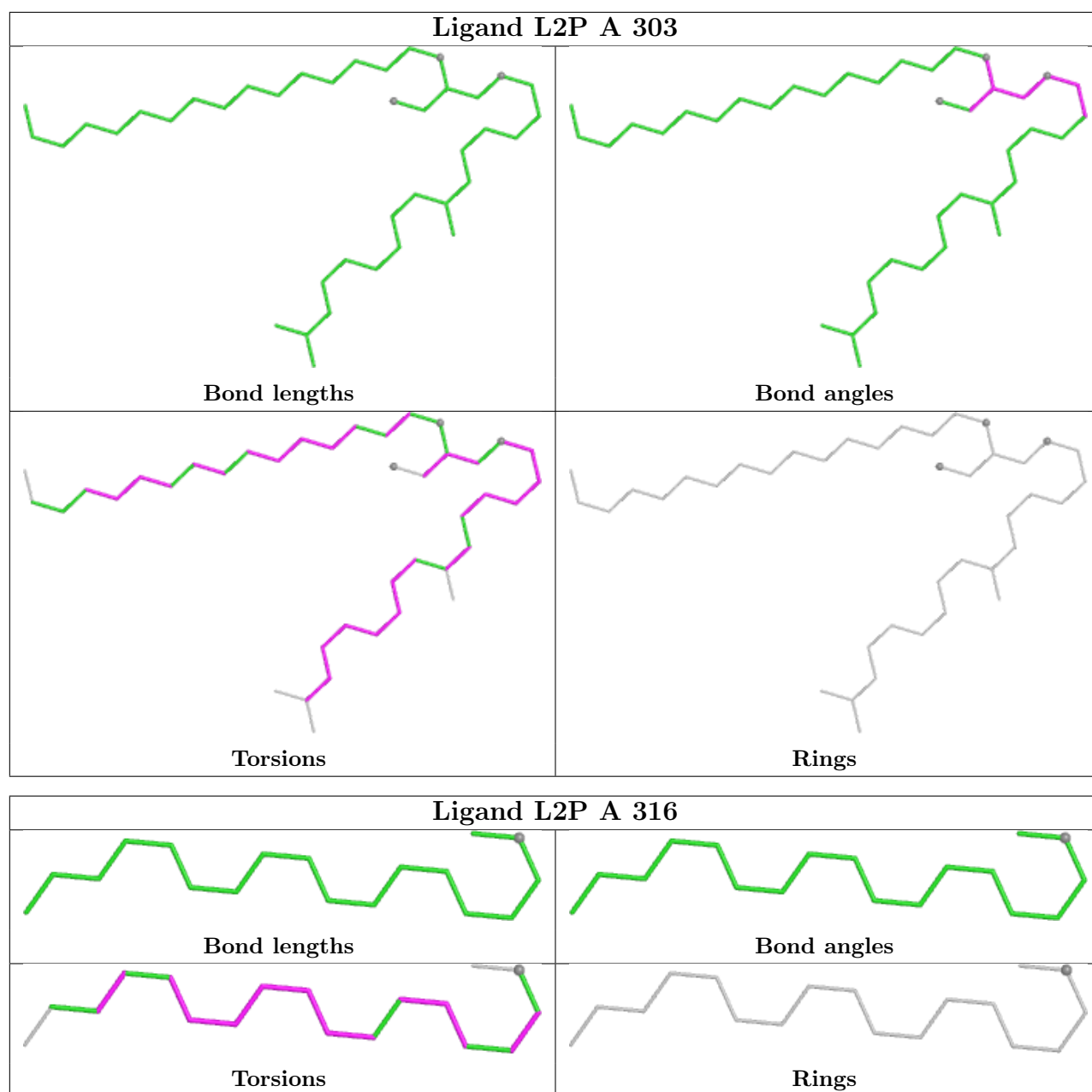
Ligand L2P A 310

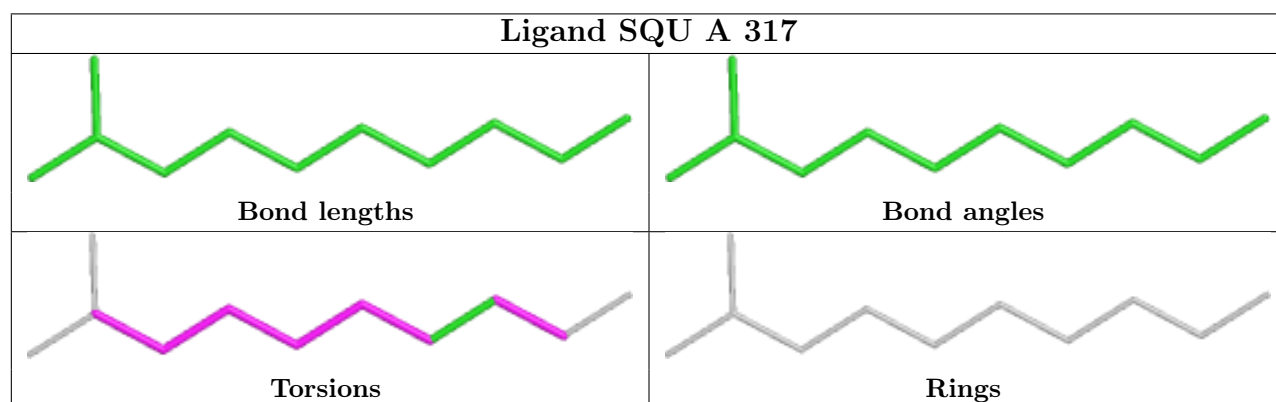
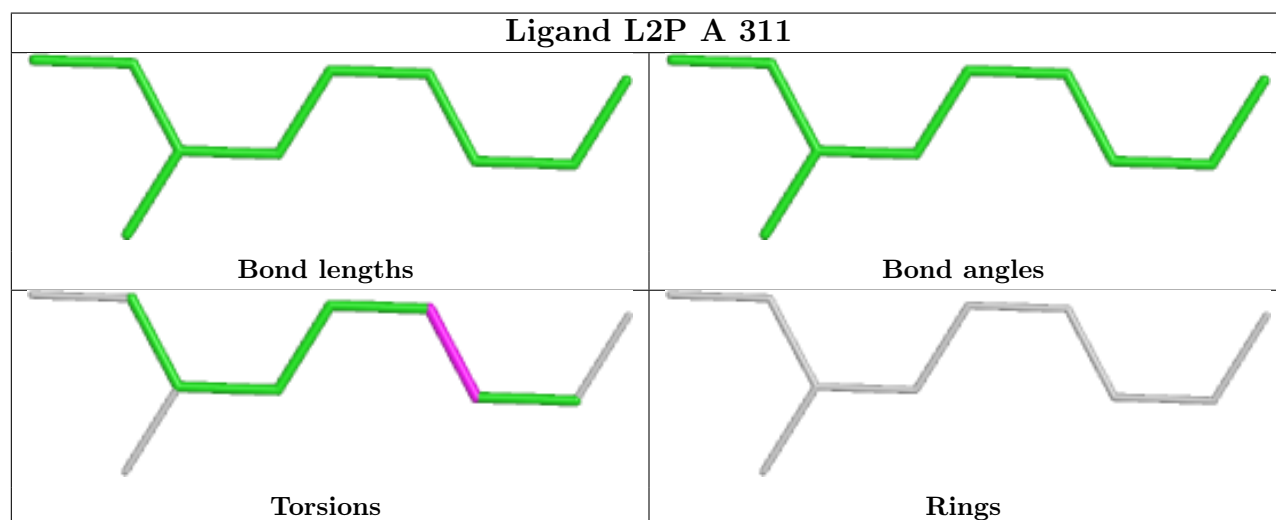
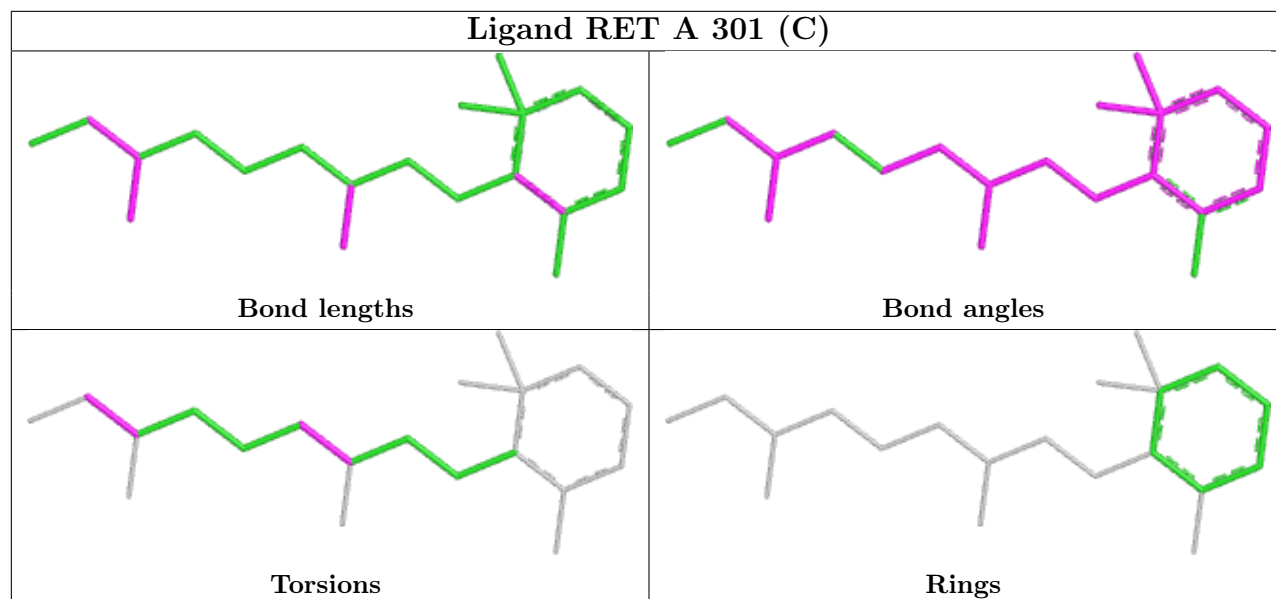


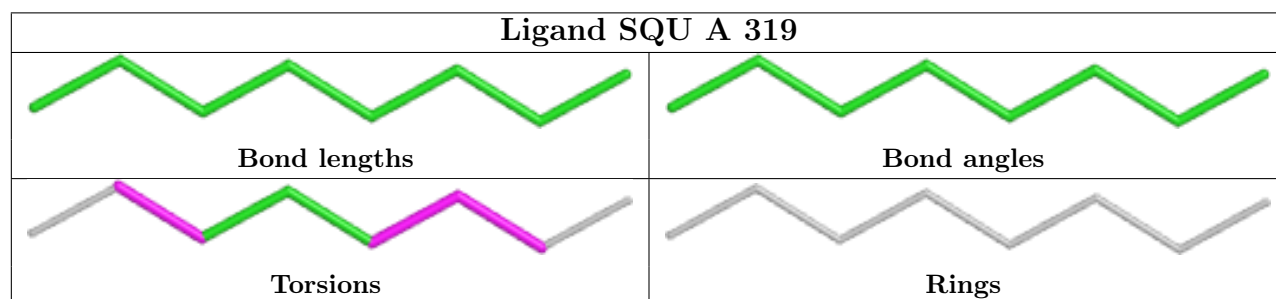
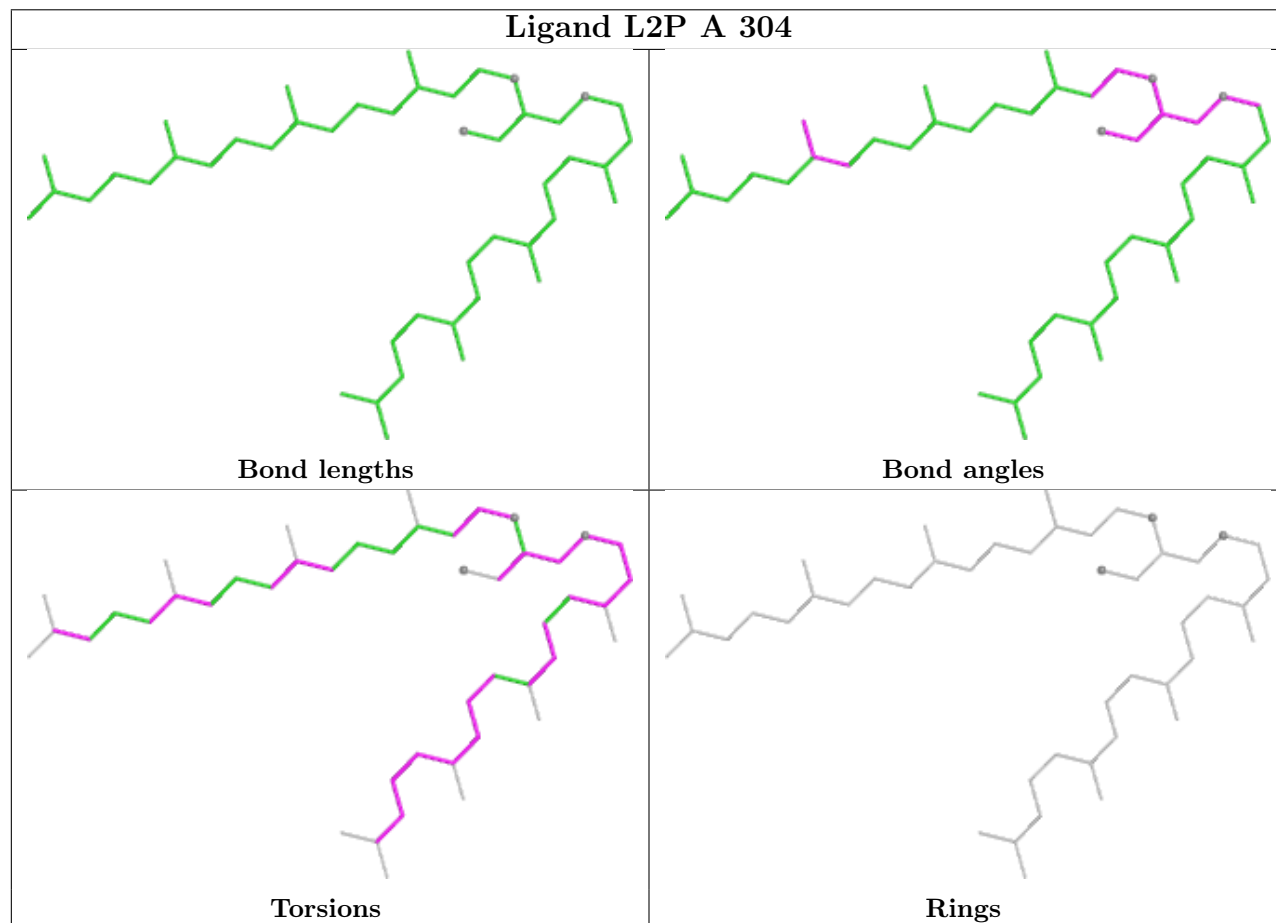
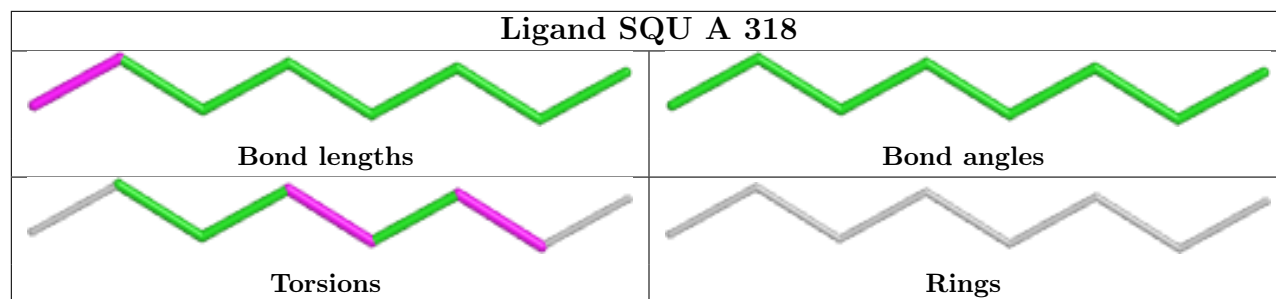


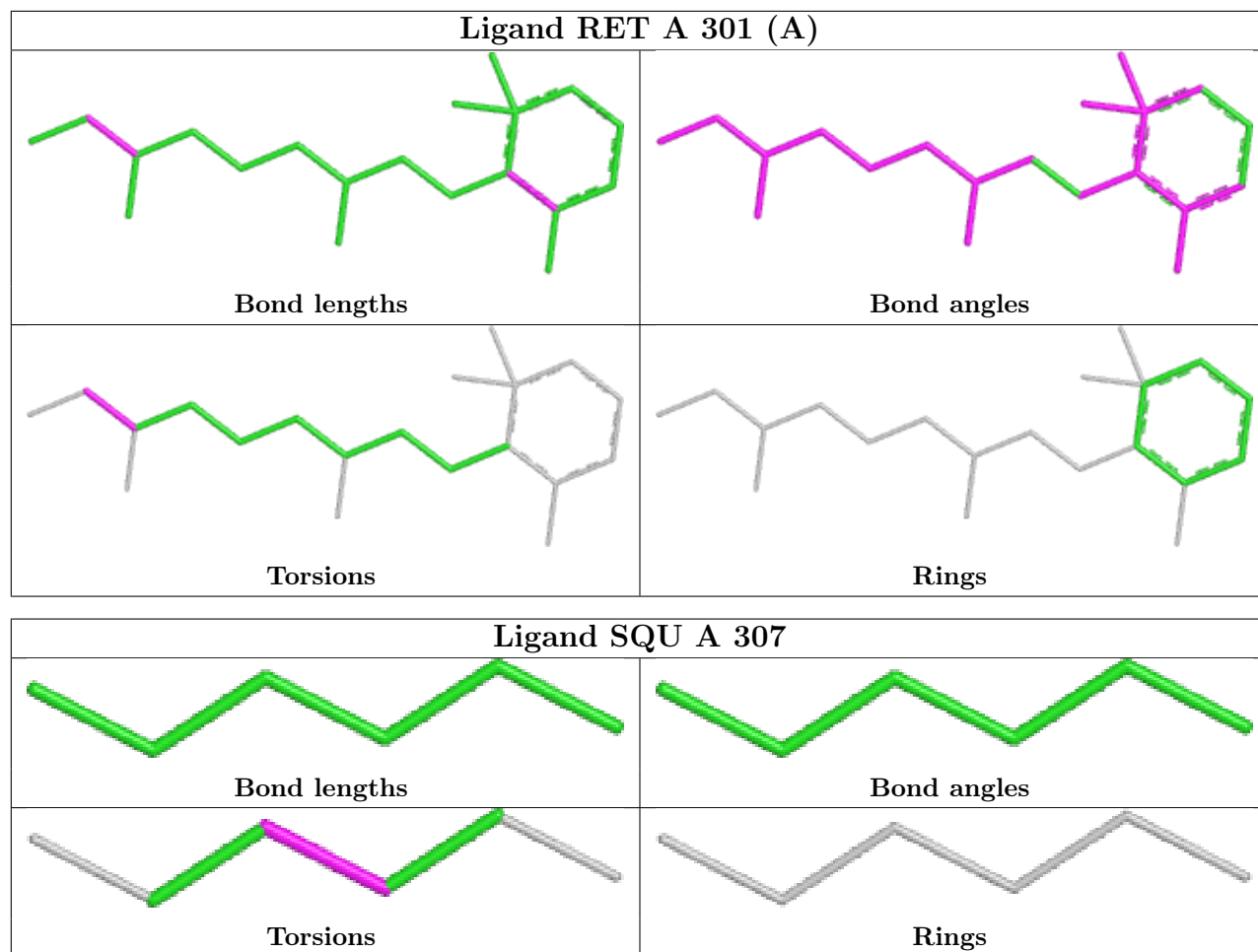


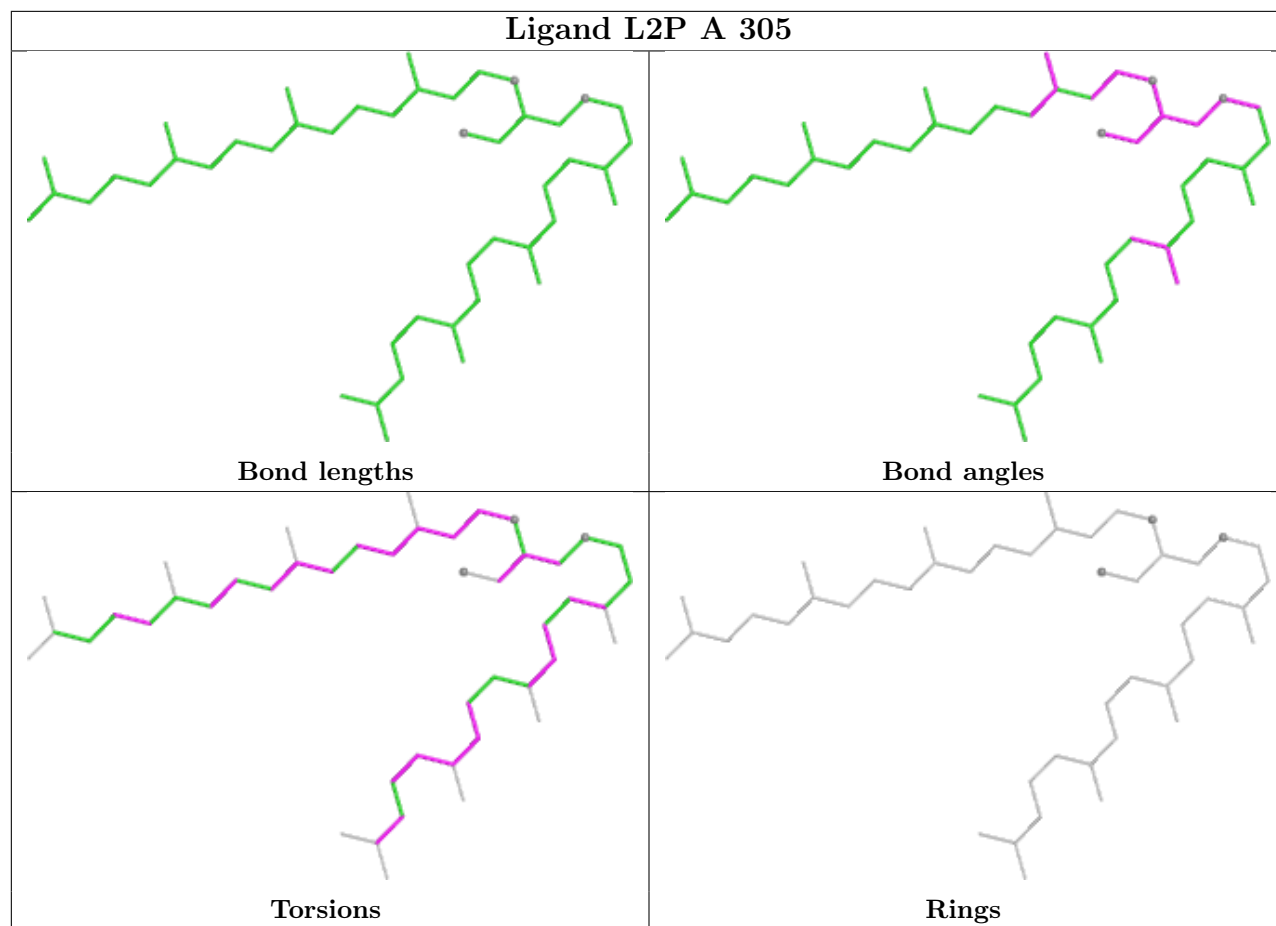












5.7 Other polymers [i](#)

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	230/230 (100%)	-0.80	2 (0%) 81 88	6, 10, 23, 58	230 (100%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157[A]	THR	2.6
1	A	161[A]	GLU	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	L2P	A	313	12/46	0.93	0.11	57,62,71,78	0
3	L2P	A	308	17/46	0.94	0.12	67,73,83,83	0
3	L2P	A	306	42/46	0.94	0.12	51,85,97,106	0
4	SQU	A	317	11/27	0.94	0.14	77,88,95,106	0
3	L2P	A	305	46/46	0.95	0.12	56,65,90,93	0

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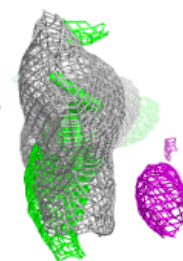
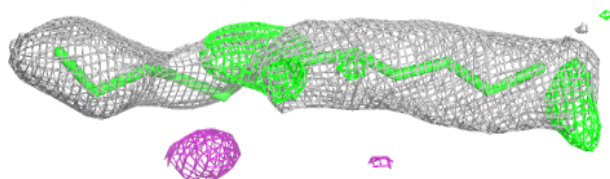
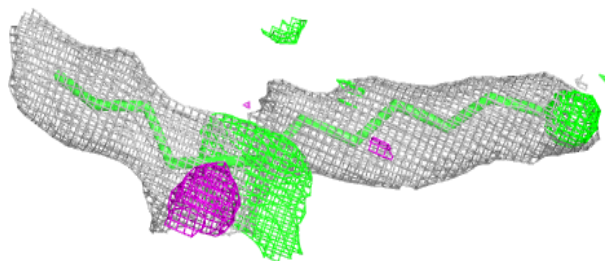
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SQU	A	318	8/27	0.95	0.09	46,52,58,61	0
3	L2P	A	310	26/46	0.96	0.10	54,66,81,82	0
3	L2P	A	311	10/46	0.96	0.10	55,63,67,67	0
3	L2P	A	312	10/46	0.96	0.08	48,62,67,70	0
3	L2P	A	304	46/46	0.96	0.10	59,71,84,86	0
3	L2P	A	302	46/46	0.96	0.11	50,65,75,76	0
3	L2P	A	309	10/46	0.96	0.08	40,45,53,58	0
3	L2P	A	315	8/46	0.97	0.08	47,62,74,75	0
3	L2P	A	316	18/46	0.97	0.07	49,55,59,69	0
4	SQU	A	307	6/27	0.97	0.07	49,57,59,59	0
3	L2P	A	303	40/46	0.97	0.08	28,53,79,84	0
3	L2P	A	314	10/46	0.97	0.07	48,58,62,64	0
4	SQU	A	319	8/27	0.97	0.07	44,56,68,69	0
2	RET	A	301[A]	20/21	0.99	0.03	14,15,17,17	20
2	RET	A	301[C]	20/21	0.99	0.03	11,15,18,19	20

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

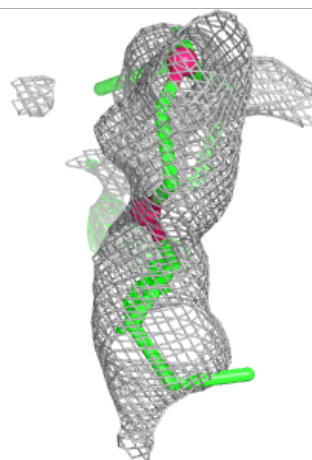
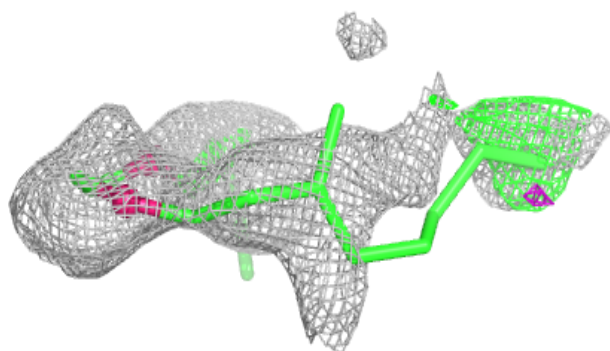
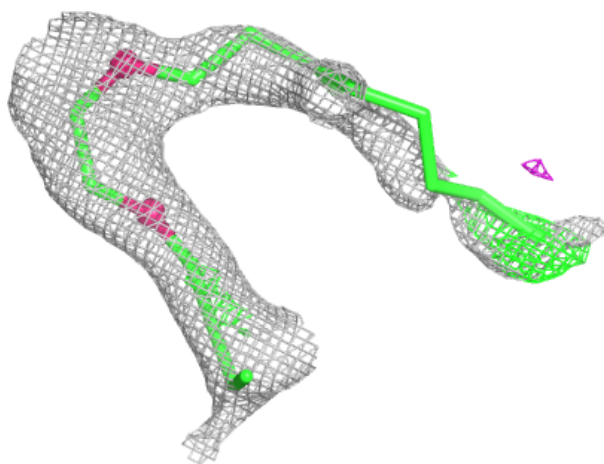
Electron density around L2P A 313:

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



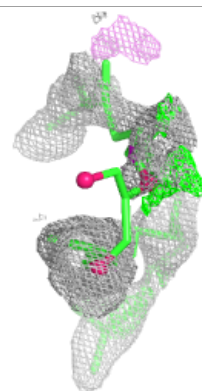
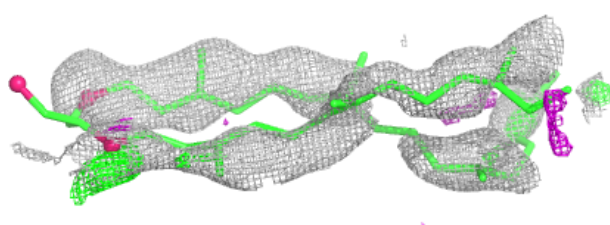
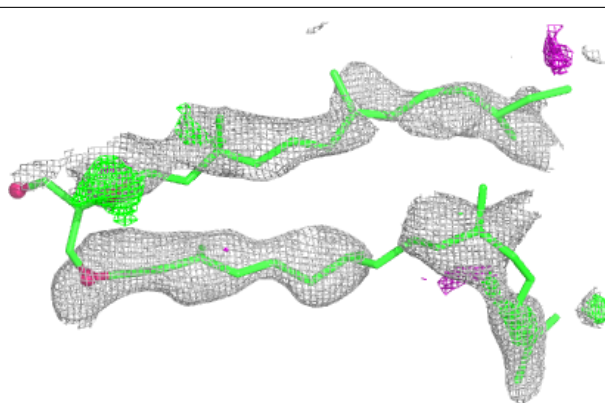
Electron density around L2P A 308:

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and green (positive)

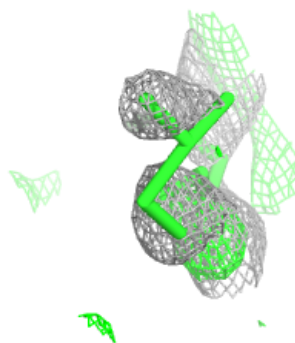
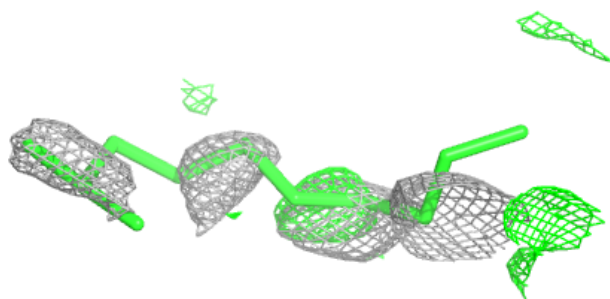
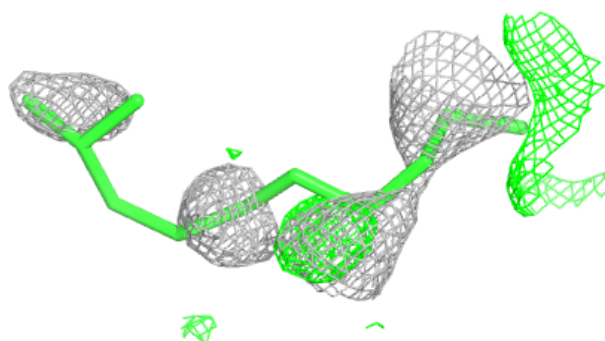


Electron density around L2P A 306:

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and green (positive)

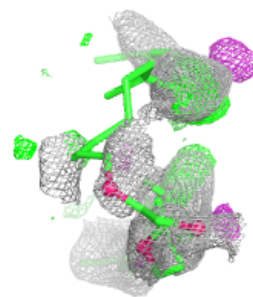
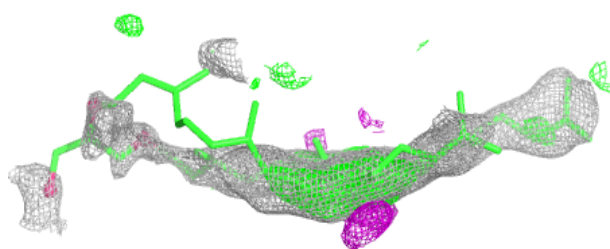
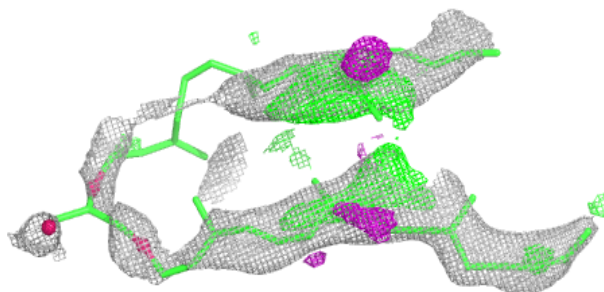
**Electron density around SQU A 317:**

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and green (positive)

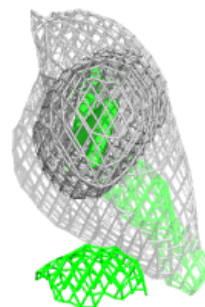
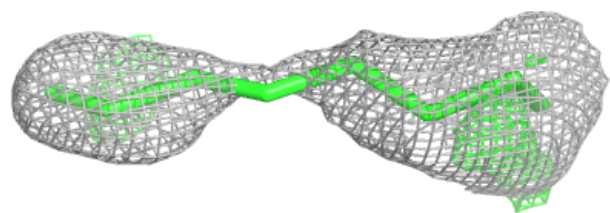
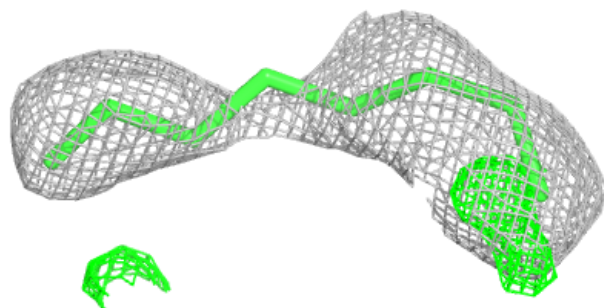


Electron density around L2P A 305:

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

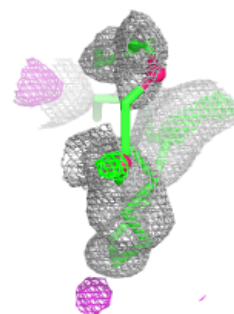
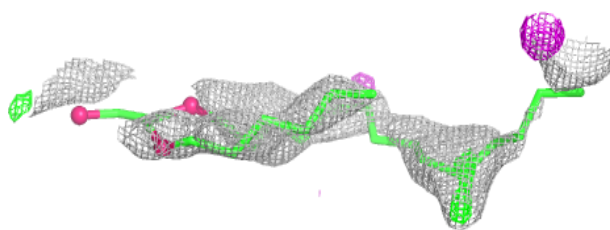
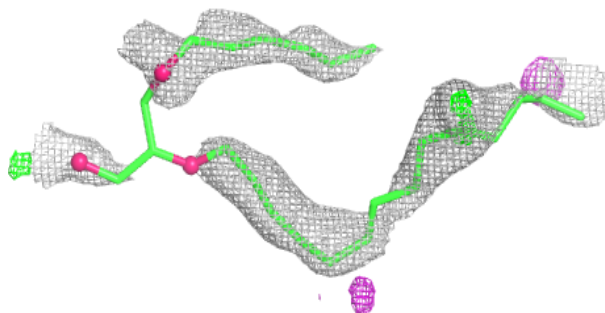
**Electron density around SQU A 318:**

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

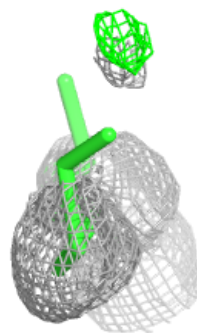
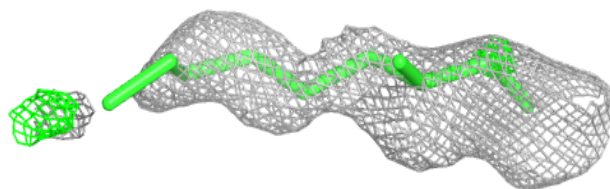
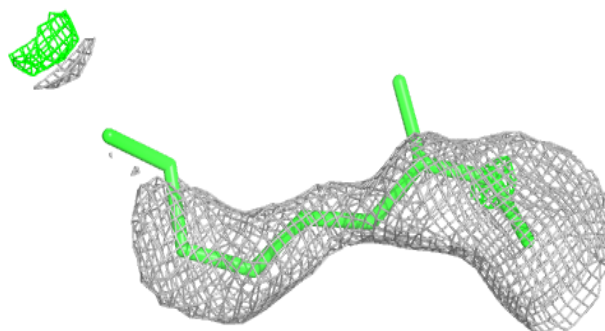


Electron density around L2P A 310:

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

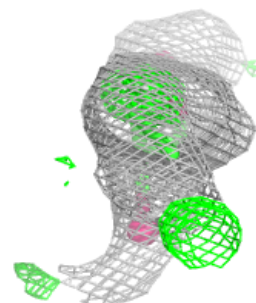
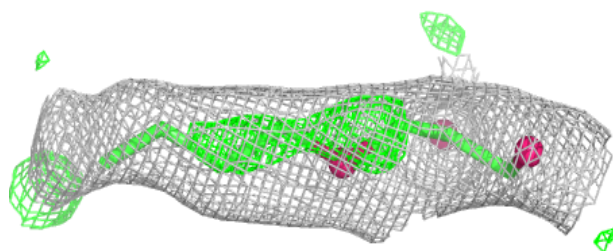
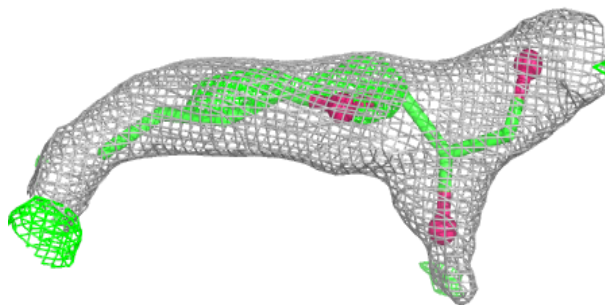
**Electron density around L2P A 311:**

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

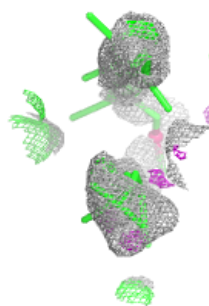
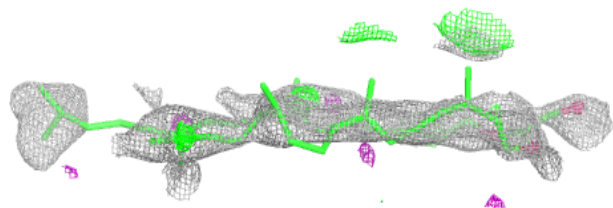
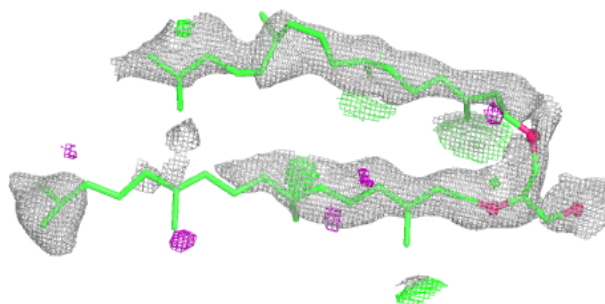


Electron density around L2P A 312:

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

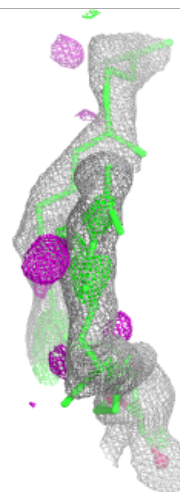
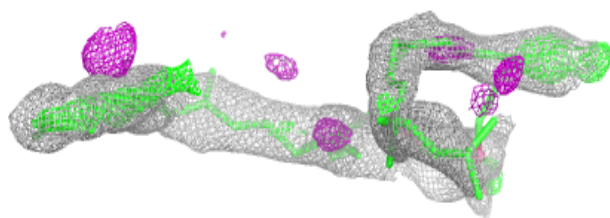
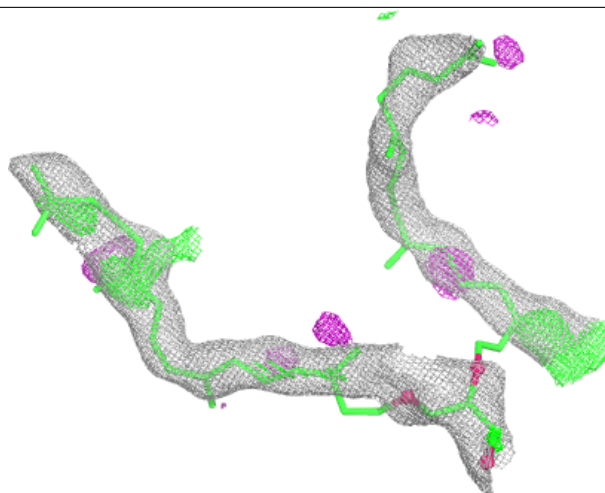
**Electron density around L2P A 304:**

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



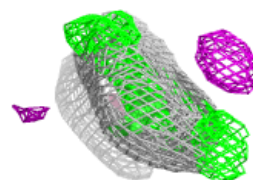
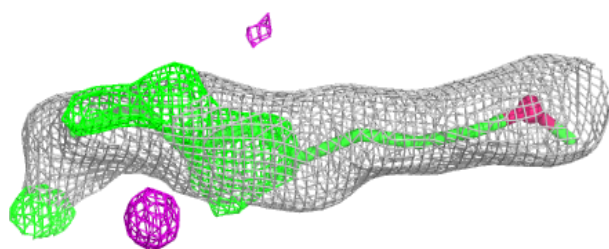
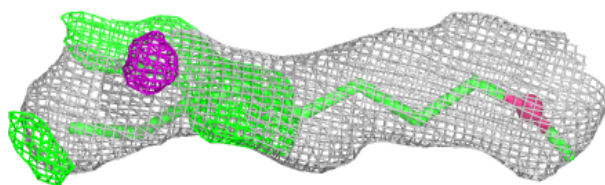
Electron density around L2P A 302:

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

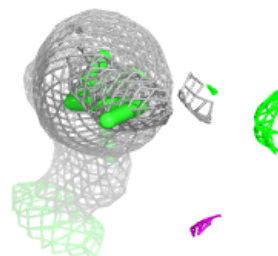
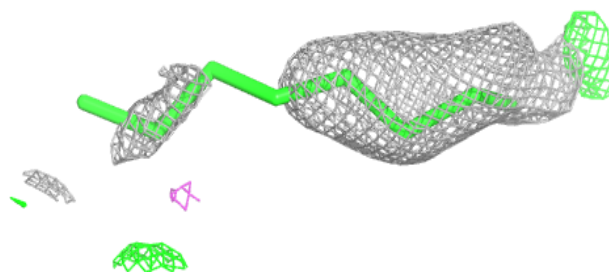
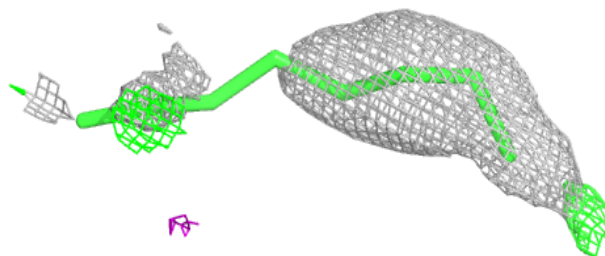


Electron density around L2P A 309:

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

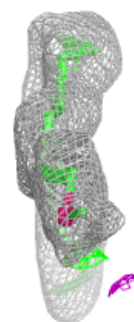
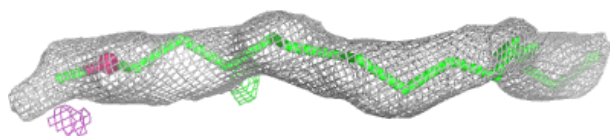
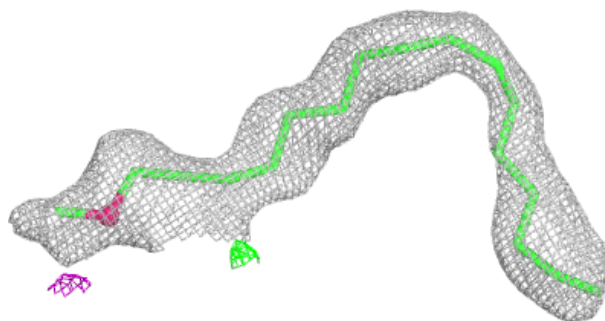
**Electron density around L2P A 315:**

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and green (positive)

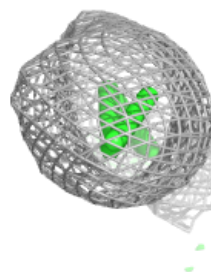
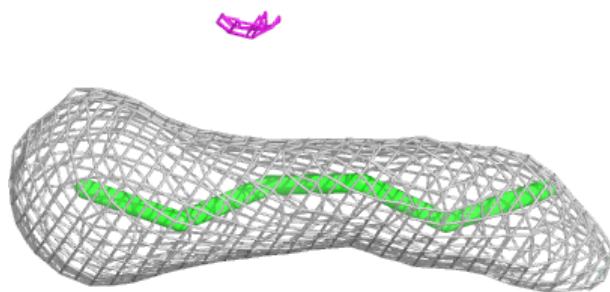
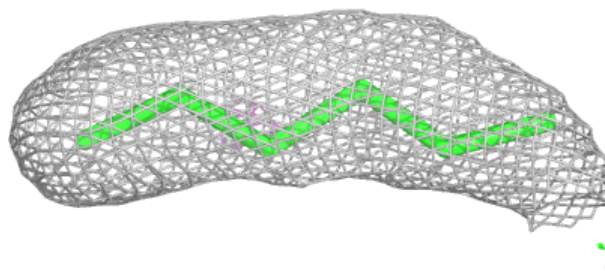


Electron density around L2P A 316:

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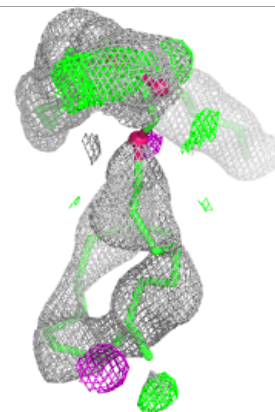
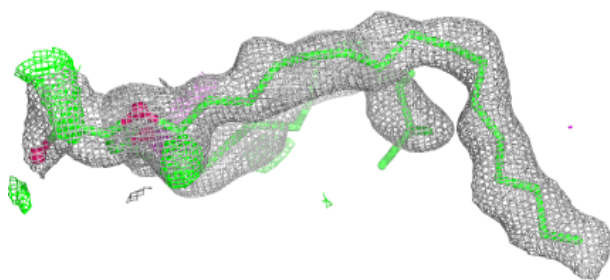
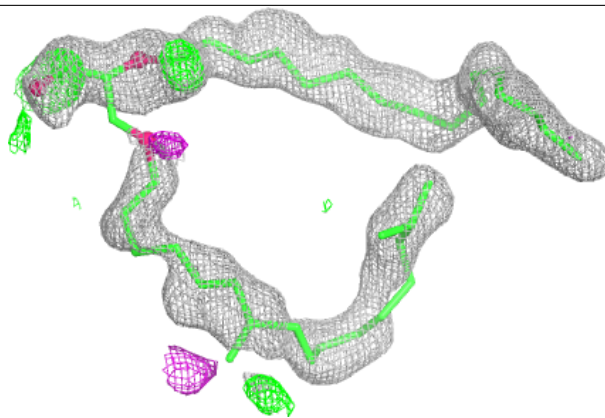
**Electron density around SQU A 307:**

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and green (positive)

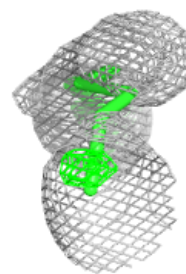
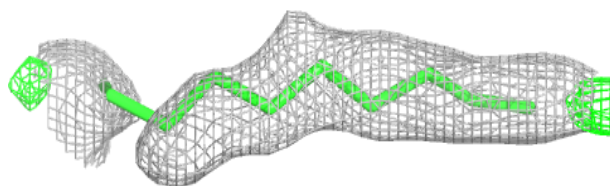
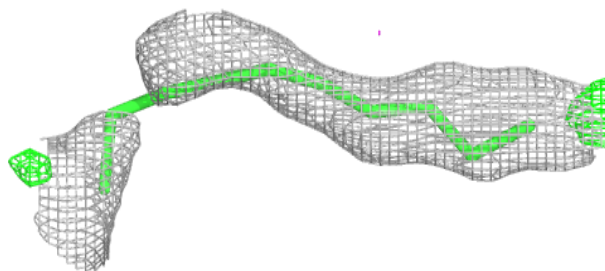


Electron density around L2P A 303:

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and green (positive)

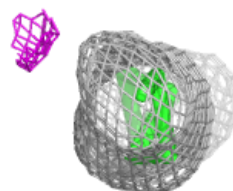
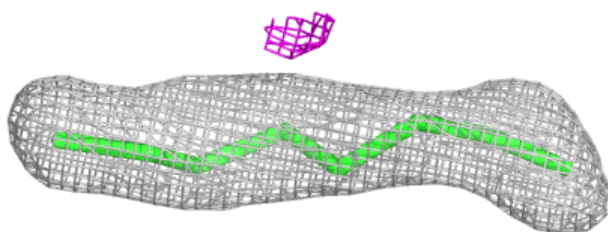
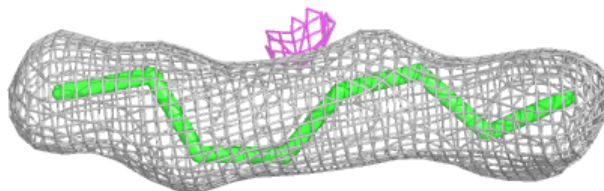
**Electron density around L2P A 314:**

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and green (positive)

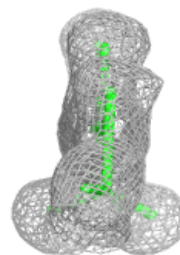
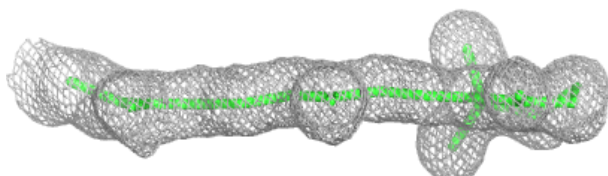
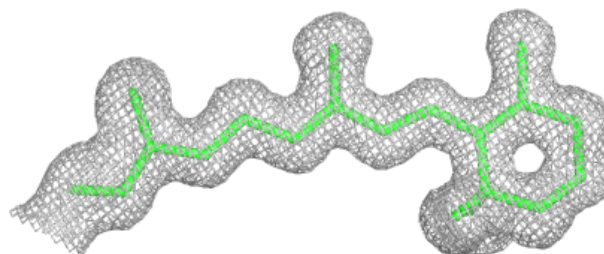


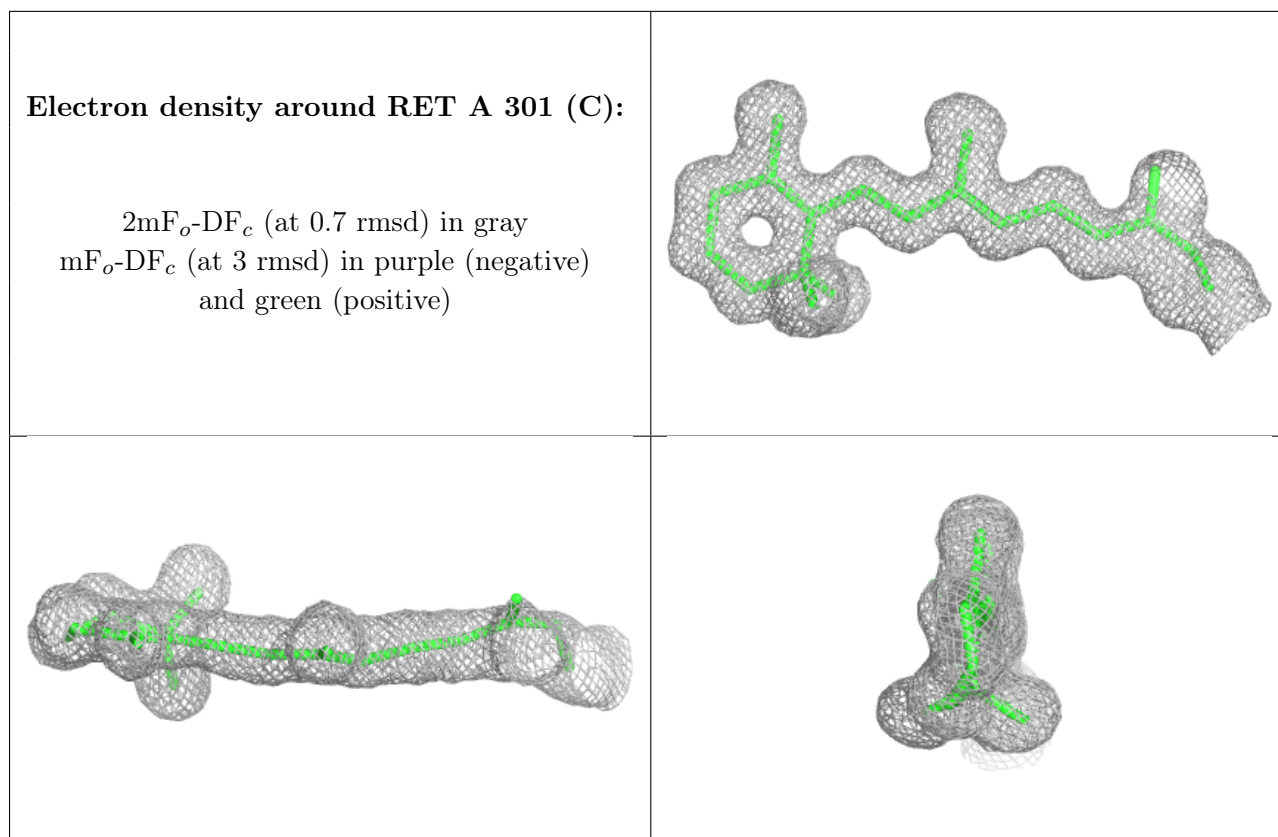
Electron density around SQU A 319:

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

**Electron density around RET A 301 (A):**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.