



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 7XJE / pdb_00007xje
Title : Crystal structure of bacteriorhodopsin in the K state refined against the extrapolated dataset
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

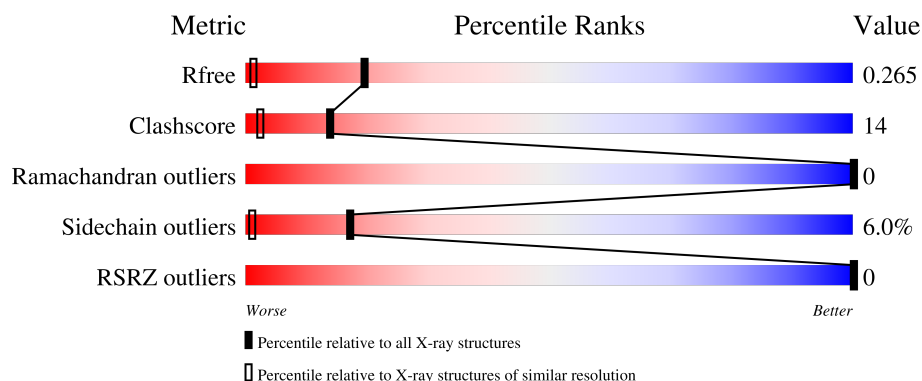
1 Overall quality at a glance

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	-	-	-

Continued on next page...

Continued from previous page...

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

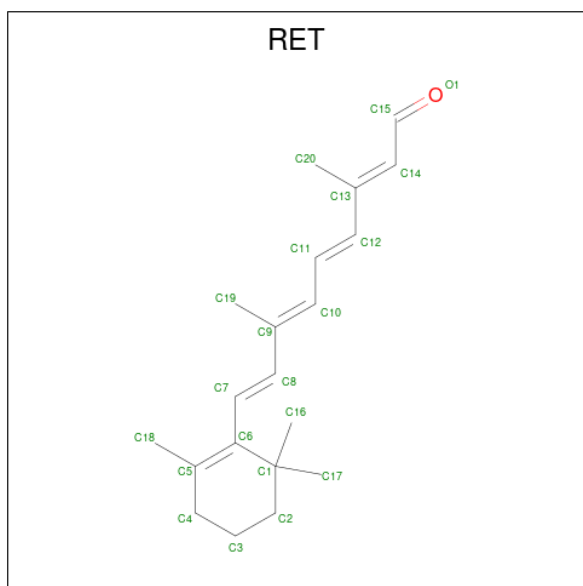
i

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.

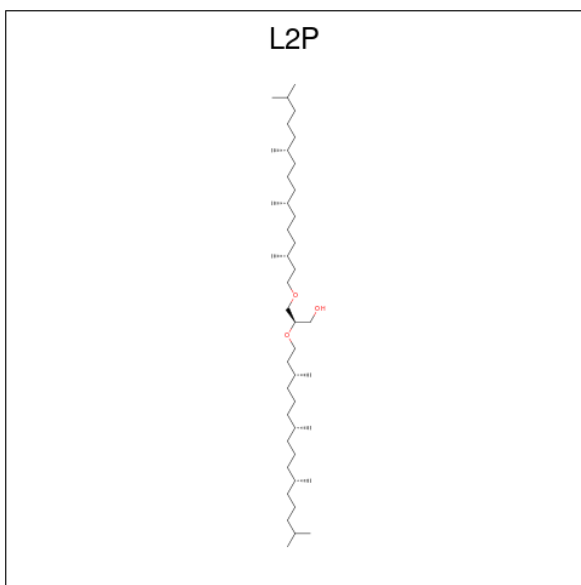
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	5	0
			1819	1215	277	317	10			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



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

- 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		0	0
			29	29			
3	A	1	Total	C	O	0	0
			29	26	3		
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			26	23	3		
3	A	1	Total	C		0	0
			5	5			
3	A	1	Total	C	O	0	0
			10	7	3		
3	A	1	Total	C	O	0	0
			18	17	1		
3	A	1	Total	C		0	0
			8	8			

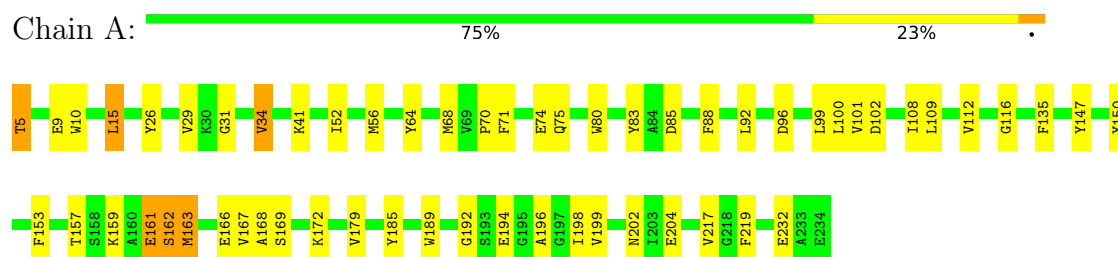
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	3
			26	26		

3 Residue-property plots

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

- Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.57 Å 60.57 Å 110.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.33 20.00 – 1.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.33) 99.6 (20.00-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.23 (at 1.33 Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.274 , 0.293 0.253 , 0.265	Depositor DCC
R_{free} test set	2436 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.237 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2085	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/1867	1.36	10/2548 (0.4%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	135	PHE	CA-CB-CG	-6.75	107.05	113.80
1	A	96	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	71	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	192	GLY	CA-C-O	-5.72	116.56	122.28
1	A	85	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	219	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	29	VAL	CA-C-O	-5.39	115.07	121.05
1	A	29	VAL	O-C-N	5.26	127.37	121.90
1	A	83	TYR	CA-CB-CG	-5.09	104.74	113.90
1	A	189	TRP	CA-CB-CG	5.08	123.25	113.60

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	1819	0	1858	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	27	2	0
3	A	220	0	343	39	0
4	A	26	0	0	1	0
All	All	2085	0	2228	62	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 14.

All (62) 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)
3:A:305:L2P:H13	3:A:305:L2P:H422	1.56	0.87
1:A:163:MET:HG2	1:A:168:ALA:HB2	1.57	0.84
1:A:217:VAL:HG11	3:A:310:L2P:H222	1.67	0.76
1:A:108:ILE:HG21	3:A:307:L2P:H2	1.67	0.75
3:A:304:L2P:H492	3:A:304:L2P:H201	1.69	0.74
1:A:31:GLY:O	1:A:34:VAL:HG13	1.91	0.70
1:A:80:TRP:HH2	3:A:302:L2P:H122	1.61	0.65
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.32	0.65
1:A:109:LEU:HD23	3:A:307:L2P:H121	1.78	0.64
1:A:102:ASP:O	1:A:159:LYS:HE2	1.98	0.63
1:A:92:LEU:HD11	3:A:302:L2P:H302	1.79	0.62
1:A:199:VAL:HG22	3:A:305:L2P:H151	1.82	0.61
3:A:304:L2P:H493	3:A:304:L2P:H522	1.84	0.59
1:A:52:ILE:HG12	3:A:302:L2P:H242	1.84	0.59
1:A:41:LYS:HD2	1:A:99:LEU:HD13	1.84	0.59
1:A:150:TYR:CZ	3:A:303:L2P:H192	2.38	0.58
3:A:303:L2P:C29	3:A:303:L2P:H511	2.35	0.57
3:A:303:L2P:H511	3:A:303:L2P:H291	1.86	0.57
1:A:92:LEU:HD11	3:A:302:L2P:C30	2.35	0.57
1:A:56:MET:HE3	3:A:302:L2P:H192	1.88	0.55
1:A:166:GLU:HG2	1:A:167:VAL:N	2.21	0.55
3:A:304:L2P:H492	3:A:304:L2P:C20	2.36	0.55
1:A:70:PRO:HA	1:A:74:GLU:O	2.08	0.54
1:A:52:ILE:CD1	3:A:302:L2P:H242	2.37	0.53
3:A:303:L2P:H201	3:A:303:L2P:H251	1.91	0.53
1:A:64:TYR:CE2	3:A:302:L2P:H112	2.44	0.53
1:A:101:VAL:O	1:A:159:LYS:HD2	2.10	0.52
1:A:5:THR:O	1:A:5:THR:OG1	2.27	0.52
1:A:9:GLU:HA	1:A:202[B]:ASN:HD22	1.74	0.52
1:A:56:MET:HE2	1:A:56:MET:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:HG22	3:A:305:L2P:H421	1.93	0.51
1:A:185:TYR:CE1	2:A:301:RET:H203	2.45	0.51
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.74	0.50
3:A:305:L2P:H422	3:A:305:L2P:C13	2.36	0.50
1:A:80:TRP:CH2	3:A:302:L2P:H122	2.45	0.49
1:A:112:VAL:HG21	3:A:307:L2P:C42	2.43	0.49
1:A:52:ILE:HD11	3:A:302:L2P:H301	1.94	0.48
1:A:52:ILE:CG1	3:A:302:L2P:H242	2.44	0.47
1:A:196:ALA:HB3	1:A:198:ILE:HD12	1.97	0.47
1:A:5:THR:HA	1:A:10:TRP:CD1	2.49	0.46
3:A:302:L2P:H572	3:A:302:L2P:H53	1.61	0.46
1:A:108:ILE:CG2	3:A:307:L2P:H2	2.43	0.46
1:A:161:GLU:HG3	1:A:162:SER:N	2.30	0.46
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.72	0.45
1:A:64:TYR:HE2	3:A:302:L2P:H112	1.80	0.45
1:A:68:MET:HE3	1:A:75:GLN:HB3	1.98	0.44
1:A:112:VAL:HG21	3:A:307:L2P:H421	1.99	0.44
1:A:52:ILE:HD11	3:A:302:L2P:H242	1.99	0.44
1:A:88:PHE:CD1	3:A:302:L2P:H271	2.53	0.43
1:A:56:MET:CE	3:A:302:L2P:H192	2.48	0.43
1:A:26:TYR:OH	3:A:310:L2P:H112	2.18	0.43
2:A:301:RET:H181	2:A:301:RET:H7	1.61	0.43
3:A:305:L2P:H161	3:A:305:L2P:H143	1.71	0.43
1:A:194[A]:GLU:OE1	1:A:204[A]:GLU:OE2	2.38	0.42
1:A:116:GLY:HA2	4:A:422:HOH:O	2.20	0.41
3:A:303:L2P:H412	3:A:303:L2P:O1	2.20	0.41
3:A:302:L2P:O1	3:A:302:L2P:H142	2.20	0.41
1:A:163:MET:HE3	1:A:163:MET:HB2	1.63	0.41
1:A:88:PHE:CD1	3:A:302:L2P:H251	2.56	0.40
3:A:304:L2P:H192	3:A:304:L2P:H151	2.04	0.40
1:A:101:VAL:O	1:A:102:ASP:HB3	2.21	0.40
1:A:147:TYR:HE1	3:A:303:L2P:H111	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/230 (101%)	228 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/184 (103%)	178 (94%)	11 (6%)	18	1

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	15	LEU
1	A	34	VAL
1	A	100	LEU
1	A	157	THR
1	A	161	GLU
1	A	162	SER
1	A	163	MET
1	A	169	SER
1	A	172	LYS
1	A	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	RET	A	301	1	20,20,21	2.13	3 (15%)	27,27,28	3.07	14 (51%)
3	L2P	A	311	-	7,7,45	0.31	0	6,6,53	0.20	0
3	L2P	A	306	-	8,8,45	0.43	0	7,7,53	1.00	1 (14%)
3	L2P	A	310	-	17,17,45	0.35	0	16,16,53	0.32	0
3	L2P	A	304	-	27,27,45	0.26	0	30,30,53	1.07	1 (3%)
3	L2P	A	303	-	39,39,45	0.65	0	41,41,53	1.68	7 (17%)
3	L2P	A	308	-	4,4,45	0.39	0	3,3,53	0.25	0
3	L2P	A	305	-	28,28,45	0.57	0	30,32,53	2.55	8 (26%)
3	L2P	A	309	-	9,9,45	0.65	0	9,9,53	2.76	1 (11%)
3	L2P	A	307	-	25,25,45	0.71	0	25,25,53	1.98	7 (28%)
3	L2P	A	302	-	45,45,45	0.47	0	51,53,53	2.14	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
2	RET	A	301	1	-	4/13/30/31	0/1/1/1
3	L2P	A	311	-	-	3/5/5/51	-
3	L2P	A	306	-	-	3/6/6/51	-
3	L2P	A	310	-	-	10/15/15/51	-
3	L2P	A	304	-	1/1/5/9	13/26/26/51	-
3	L2P	A	303	-	1/1/3/9	29/40/40/51	-
3	L2P	A	308	-	-	1/2/2/51	-
3	L2P	A	305	-	2/2/5/9	17/31/31/51	-
3	L2P	A	309	-	-	2/8/8/51	-
3	L2P	A	307	-	-	14/25/25/51	-
3	L2P	A	302	-	4/4/9/9	23/51/51/51	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C14-C13	7.94	1.39	1.33
2	A	301	RET	C5-C6	2.84	1.39	1.34
2	A	301	RET	C20-C13	-2.39	1.46	1.50

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C11-C10-C9	-8.95	114.72	127.28
3	A	309	L2P	O2-C2-C1	8.25	138.22	109.70
3	A	302	L2P	O2-C41-C42	7.99	125.55	108.77
3	A	305	L2P	O2-C41-C42	7.40	124.32	108.77
3	A	303	L2P	O2-C2-C3	6.28	125.35	108.64
3	A	302	L2P	C41-O2-C2	6.16	132.55	115.53
3	A	307	L2P	O1-C1-C2	5.47	121.97	109.42
3	A	305	L2P	C41-O2-C2	5.29	130.14	115.53
3	A	305	L2P	O2-C2-C3	4.88	121.63	108.64
3	A	305	L2P	O1-C1-C2	4.61	119.98	109.42
3	A	302	L2P	O3-C3-C2	4.51	123.38	111.77
3	A	302	L2P	O2-C2-C3	4.42	120.40	108.64
2	A	301	RET	C19-C9-C8	4.39	124.79	118.09
3	A	305	L2P	O2-C2-C1	4.28	122.71	109.06
2	A	301	RET	C2-C3-C4	4.23	120.57	111.28
2	A	301	RET	C7-C6-C5	-4.22	111.83	121.56
3	A	307	L2P	O2-C2-C3	4.10	119.56	108.64
3	A	303	L2P	O1-C1-C2	4.08	118.78	109.42
2	A	301	RET	C2-C1-C6	3.82	115.98	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	L2P	O1-C1-C2	3.78	118.09	109.42
2	A	301	RET	C8-C9-C10	-3.63	113.31	119.01
2	A	301	RET	C3-C4-C5	-3.48	107.85	114.06
3	A	303	L2P	C11-O1-C1	3.47	128.87	113.58
2	A	301	RET	C20-C13-C12	-3.47	112.78	118.09
2	A	301	RET	C17-C1-C2	-3.43	95.79	108.95
2	A	301	RET	C17-C1-C6	3.33	115.47	110.24
2	A	301	RET	C1-C6-C7	3.31	124.63	115.65
3	A	305	L2P	O3-C3-C2	3.28	120.21	111.77
3	A	307	L2P	O3-C3-C2	3.22	120.06	111.77
3	A	303	L2P	O2-C2-C1	3.21	119.29	109.06
3	A	307	L2P	C11-O1-C1	3.17	127.53	113.58
3	A	302	L2P	C11-O1-C1	3.15	127.44	113.58
3	A	302	L2P	O2-C2-C1	3.10	118.95	109.06
3	A	307	L2P	C41-O2-C2	3.03	123.90	115.53
3	A	307	L2P	O2-C2-C1	2.89	118.28	109.06
2	A	301	RET	C7-C8-C9	-2.63	122.34	126.23
3	A	305	L2P	C11-O1-C1	2.58	124.95	113.58
3	A	307	L2P	O2-C41-C42	2.53	117.94	109.37
3	A	303	L2P	O1-C11-C12	2.36	122.70	110.32
2	A	301	RET	C3-C2-C1	-2.30	106.30	114.43
2	A	301	RET	C18-C5-C6	-2.29	121.98	124.48
3	A	303	L2P	C41-O2-C2	2.27	121.80	115.53
3	A	302	L2P	C60-C58-C59	2.23	120.49	110.53
3	A	302	L2P	C44-C43-C42	2.20	119.11	111.27
3	A	302	L2P	C1-C2-C3	2.19	116.86	111.80
3	A	304	L2P	C19-C18-C20	2.12	118.85	111.27
3	A	306	L2P	O1-C11-C12	2.12	124.93	111.44
3	A	303	L2P	C56-C55-C53	2.10	125.00	114.37
3	A	305	L2P	O1-C11-C12	2.01	122.98	110.29

All (8) chirality outliers are listed below:

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

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	RET	C12-C13-C14-C15
2	A	301	RET	C20-C13-C14-C15
3	A	302	L2P	C41-C42-C43-C44
3	A	302	L2P	C51-C52-C53-C54
3	A	303	L2P	O2-C2-C3-O3
3	A	303	L2P	C16-C17-C18-C19
3	A	305	L2P	O2-C2-C3-O3
3	A	305	L2P	C11-C12-C13-C14
3	A	305	L2P	C44-C43-C45-C46
3	A	307	L2P	C1-C2-C3-O3
3	A	307	L2P	O2-C2-C3-O3
3	A	307	L2P	C42-C41-O2-C2
3	A	303	L2P	C11-C12-C13-C15
3	A	305	L2P	C2-C1-O1-C11
3	A	303	L2P	C12-C11-O1-C1
3	A	307	L2P	C45-C46-C47-C48
3	A	302	L2P	C53-C55-C56-C57
3	A	302	L2P	C16-C17-C18-C19
3	A	304	L2P	C16-C17-C18-C19
3	A	304	L2P	C24-C23-C25-C26
3	A	305	L2P	C14-C13-C15-C16
3	A	309	L2P	O1-C1-C2-C3
3	A	307	L2P	C50-C51-C52-C53
3	A	302	L2P	C42-C43-C45-C46
3	A	302	L2P	C25-C26-C27-C28
3	A	307	L2P	O1-C11-C12-C13
3	A	310	L2P	O1-C11-C12-C13
3	A	303	L2P	C21-C22-C23-C25
3	A	304	L2P	C23-C25-C26-C27
3	A	304	L2P	C45-C46-C47-C48
3	A	302	L2P	C46-C47-C48-C49
3	A	305	L2P	C42-C41-O2-C2
3	A	302	L2P	C56-C57-C58-C59
3	A	303	L2P	C26-C27-C28-C29
3	A	303	L2P	C25-C26-C27-C28
3	A	309	L2P	O2-C2-C3-O3
3	A	310	L2P	C17-C18-C20-C21
3	A	304	L2P	C26-C27-C28-C30
3	A	307	L2P	C43-C45-C46-C47
3	A	303	L2P	C46-C47-C48-C50
3	A	303	L2P	C13-C15-C16-C17
3	A	306	L2P	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	303	L2P	C52-C53-C55-C56
3	A	310	L2P	C12-C13-C15-C16
3	A	310	L2P	C20-C21-C22-C23
3	A	303	L2P	C23-C25-C26-C27
3	A	303	L2P	C43-C45-C46-C47
3	A	303	L2P	C51-C52-C53-C55
3	A	305	L2P	C45-C46-C47-C48
3	A	304	L2P	C20-C21-C22-C23
3	A	303	L2P	C53-C55-C56-C57
3	A	305	L2P	C12-C11-O1-C1
3	A	302	L2P	C19-C18-C20-C21
3	A	304	L2P	C21-C22-C23-C24
2	A	301	RET	C10-C11-C12-C13
3	A	311	L2P	C25-C26-C27-C28
3	A	303	L2P	C12-C13-C15-C16
3	A	310	L2P	C13-C15-C16-C17
3	A	303	L2P	O1-C1-C2-O2
3	A	303	L2P	C18-C20-C21-C22
3	A	303	L2P	O2-C41-C42-C43
3	A	310	L2P	C21-C22-C23-C25
3	A	302	L2P	C23-C25-C26-C27
3	A	307	L2P	C12-C13-C15-C16
3	A	302	L2P	C26-C27-C28-C29
3	A	310	L2P	C22-C23-C25-C26
3	A	307	L2P	C53-C55-C56-C57
3	A	302	L2P	C52-C53-C55-C56
3	A	305	L2P	C16-C17-C18-C20
3	A	305	L2P	C15-C16-C17-C18
3	A	302	L2P	C48-C50-C51-C52
3	A	303	L2P	C1-C2-O2-C41
3	A	307	L2P	O1-C1-C2-C3
3	A	302	L2P	O2-C41-C42-C43
3	A	305	L2P	O2-C41-C42-C43
3	A	310	L2P	C18-C20-C21-C22
3	A	303	L2P	C1-C2-C3-O3
3	A	304	L2P	C12-C13-C15-C16
3	A	302	L2P	O1-C1-C2-O2
3	A	305	L2P	C19-C18-C20-C21
3	A	311	L2P	C20-C21-C22-C23
3	A	303	L2P	O1-C11-C12-C13
3	A	304	L2P	C26-C27-C28-C29
3	A	303	L2P	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	303	L2P	C20-C21-C22-C23
3	A	307	L2P	C2-C1-O1-C11
3	A	302	L2P	O1-C1-C2-C3
3	A	307	L2P	C51-C52-C53-C55
3	A	307	L2P	C13-C15-C16-C17
3	A	305	L2P	C46-C47-C48-C49
3	A	302	L2P	C21-C22-C23-C24
3	A	305	L2P	C16-C17-C18-C19
3	A	303	L2P	C45-C46-C47-C48
3	A	308	L2P	C25-C26-C27-C28
3	A	311	L2P	C23-C25-C26-C27
3	A	305	L2P	O1-C1-C2-C3
3	A	305	L2P	C41-C42-C43-C45
3	A	303	L2P	C26-C27-C28-C30
3	A	306	L2P	C12-C13-C15-C16
3	A	303	L2P	C47-C48-C50-C51
3	A	310	L2P	C25-C26-C27-C28
3	A	305	L2P	O1-C1-C2-O2
3	A	303	L2P	C42-C43-C45-C46
3	A	307	L2P	C12-C11-O1-C1
3	A	303	L2P	C22-C23-C25-C26
3	A	306	L2P	O1-C11-C12-C13
3	A	302	L2P	C18-C20-C21-C22
3	A	302	L2P	C54-C53-C55-C56
2	A	301	RET	C11-C10-C9-C8
3	A	302	L2P	C17-C18-C20-C21
3	A	303	L2P	O1-C1-C2-C3
3	A	304	L2P	C15-C16-C17-C18
3	A	304	L2P	C21-C22-C23-C25
3	A	302	L2P	C44-C43-C45-C46
3	A	302	L2P	C51-C52-C53-C55
3	A	310	L2P	C16-C17-C18-C20
3	A	304	L2P	C19-C18-C20-C21
3	A	304	L2P	C51-C52-C53-C55
3	A	302	L2P	C42-C41-O2-C2

There are no ring outliers.

7 monomers are involved in 41 short contacts:

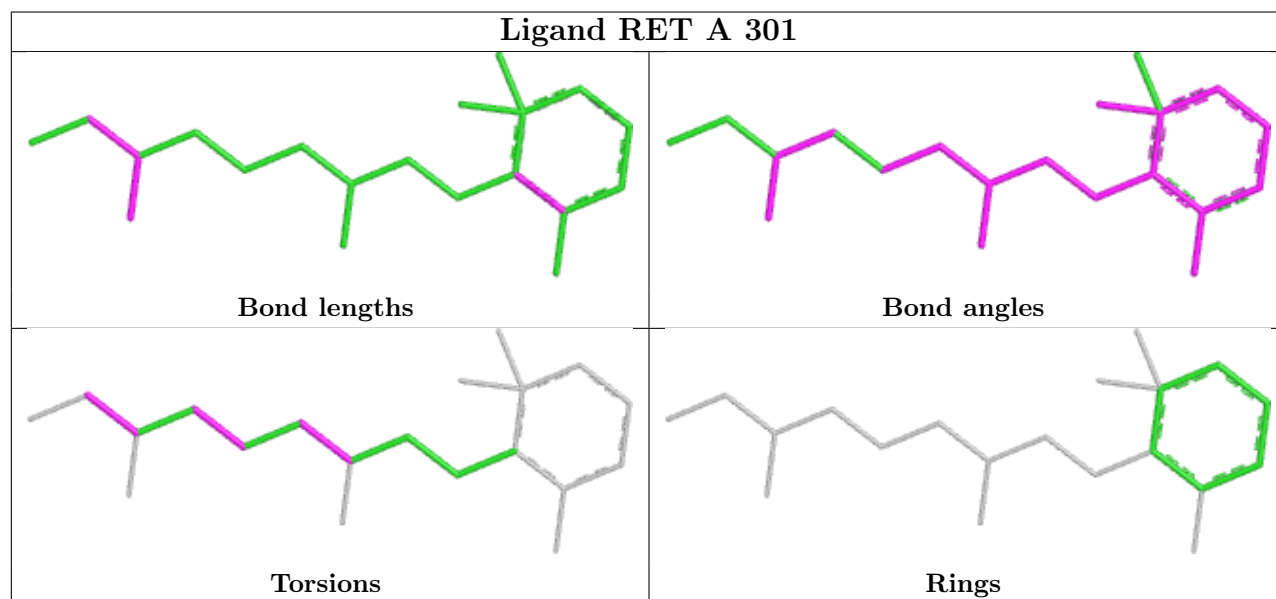
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	2	0
3	A	310	L2P	2	0

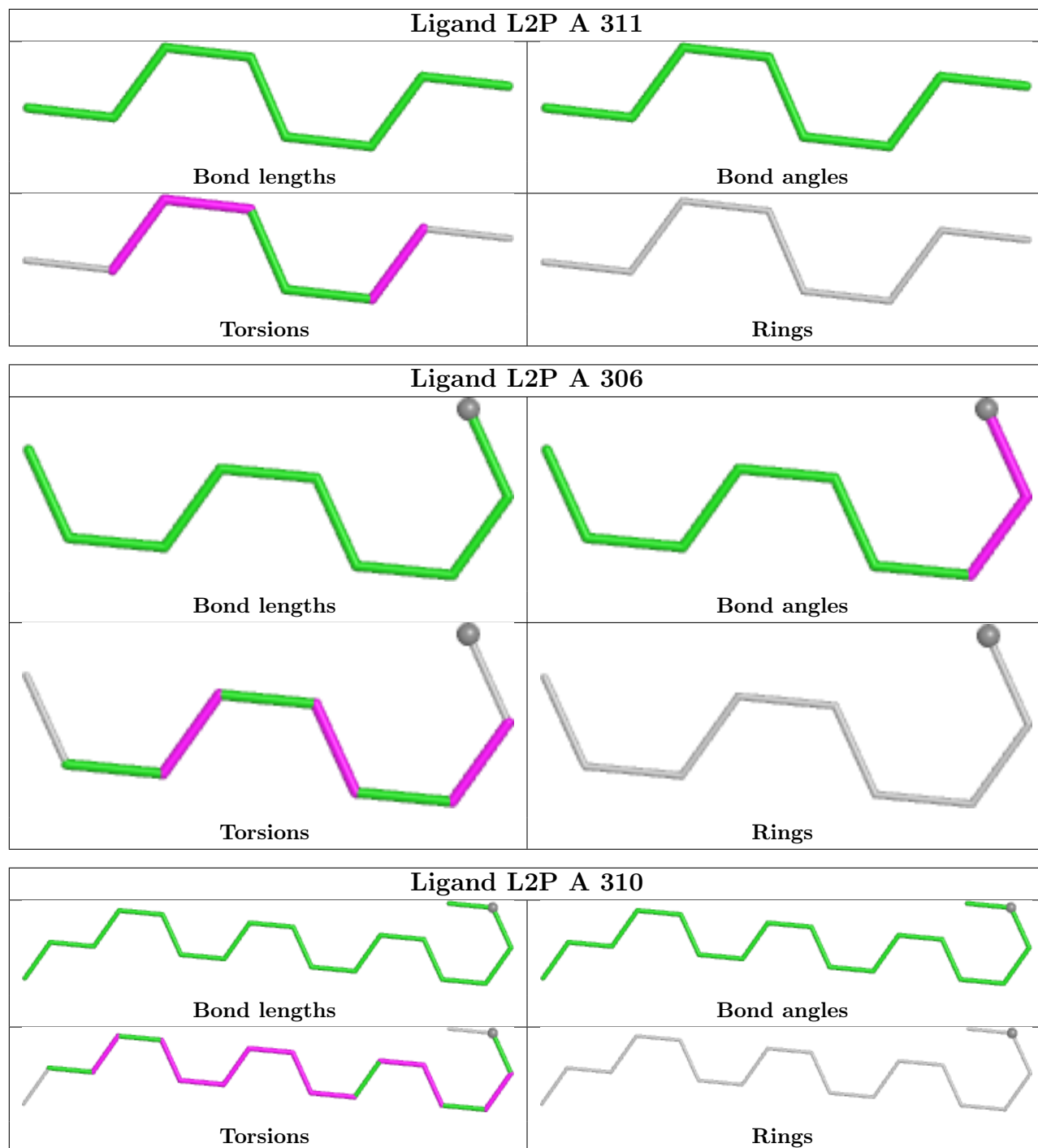
Continued on next page...

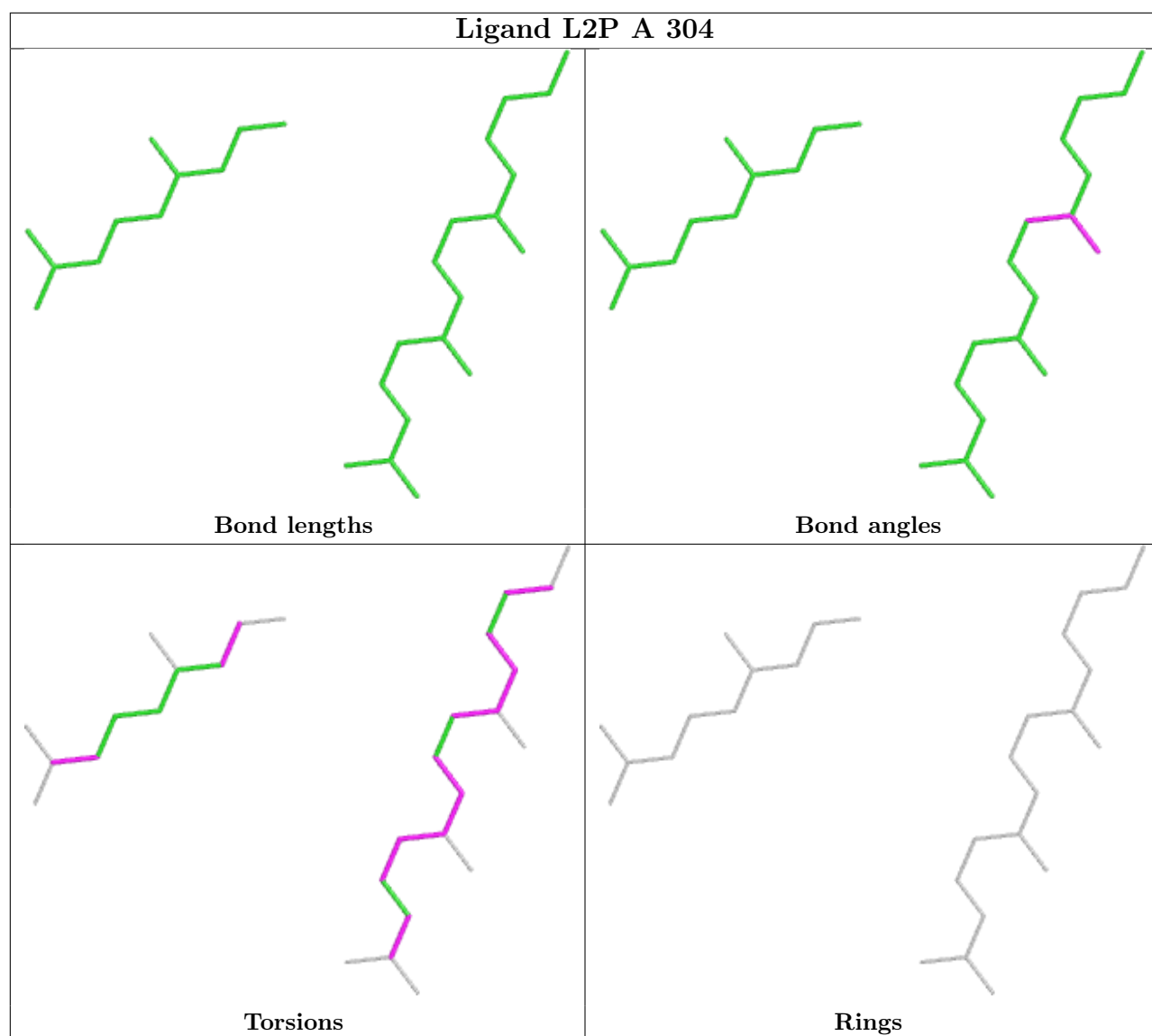
Continued from previous page...

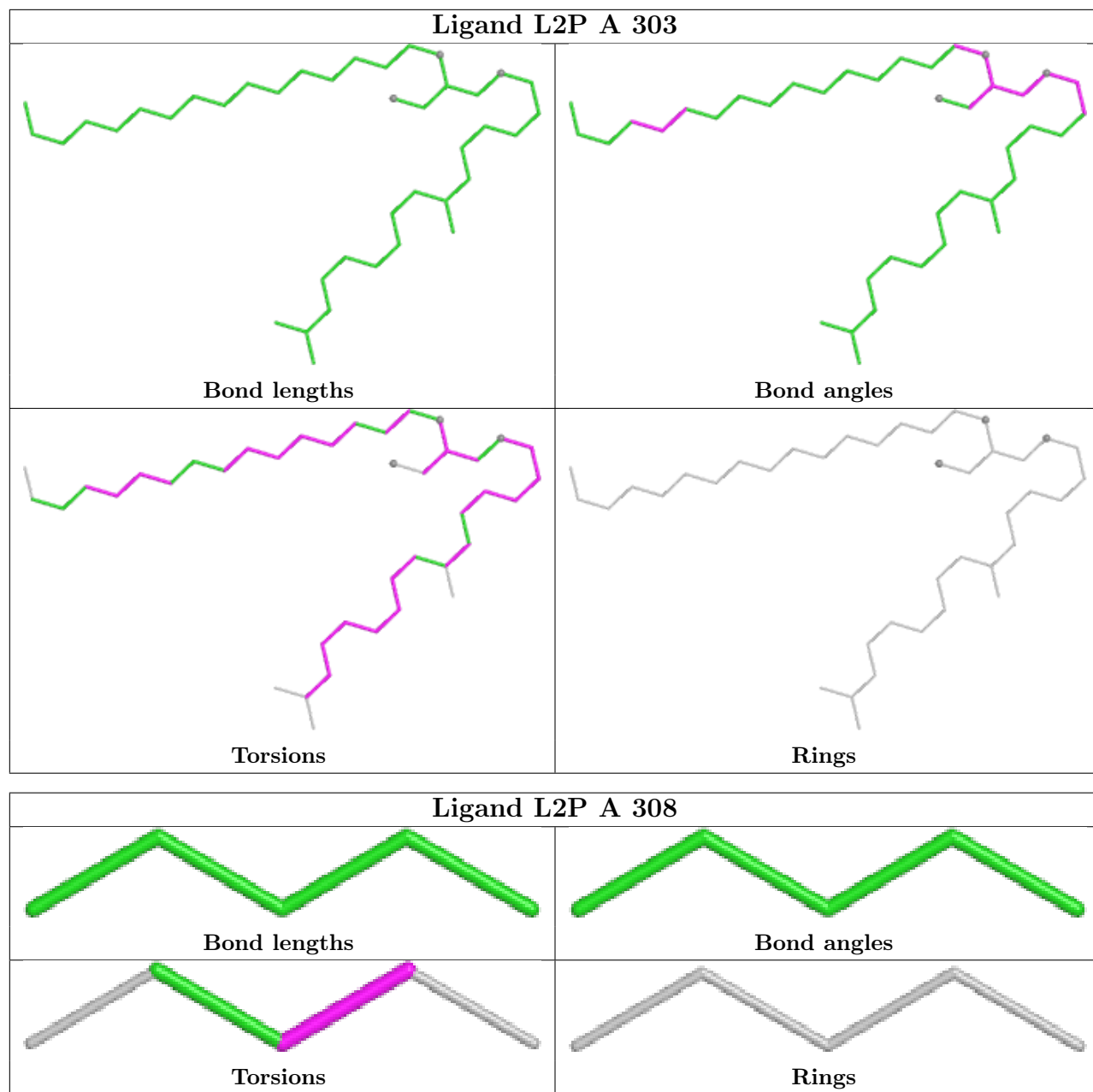
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	L2P	4	0
3	A	303	L2P	6	0
3	A	305	L2P	5	0
3	A	307	L2P	5	0
3	A	302	L2P	17	0

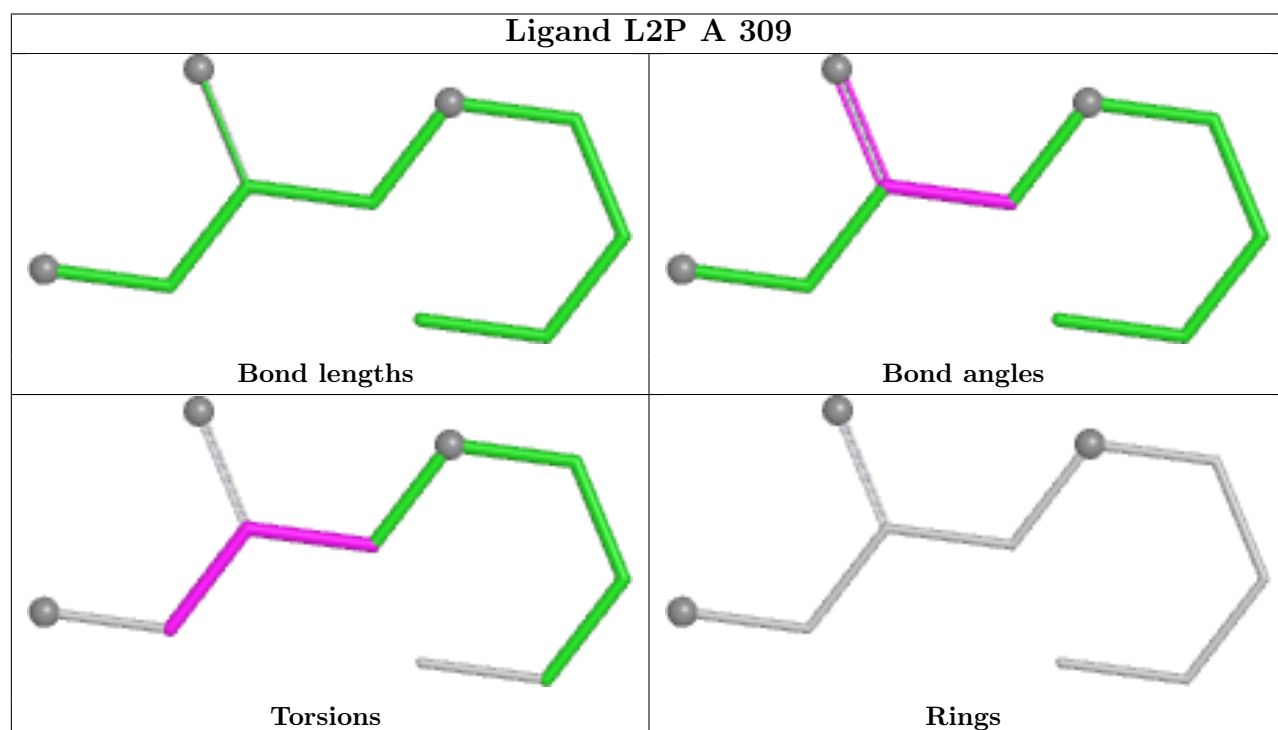
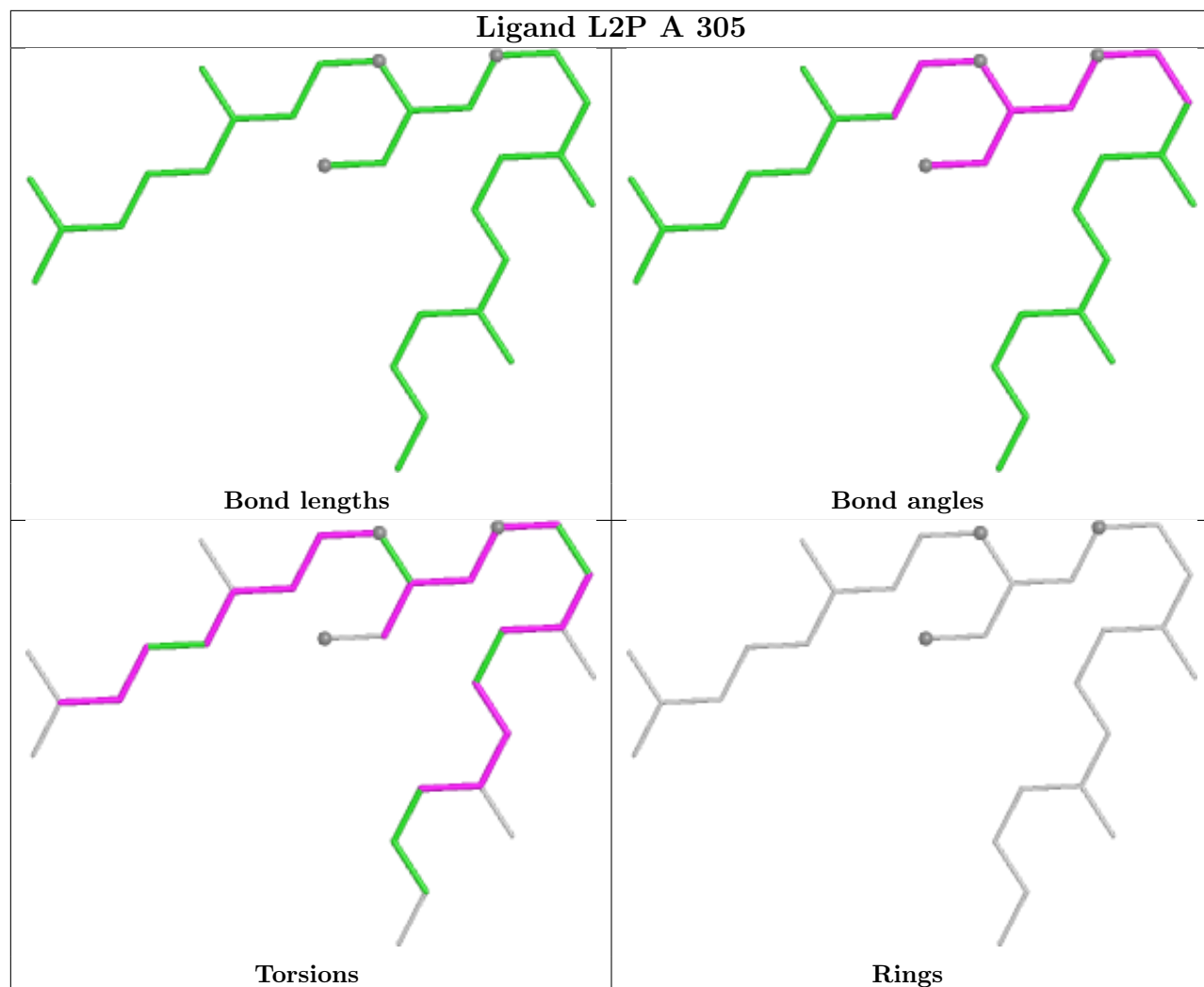
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

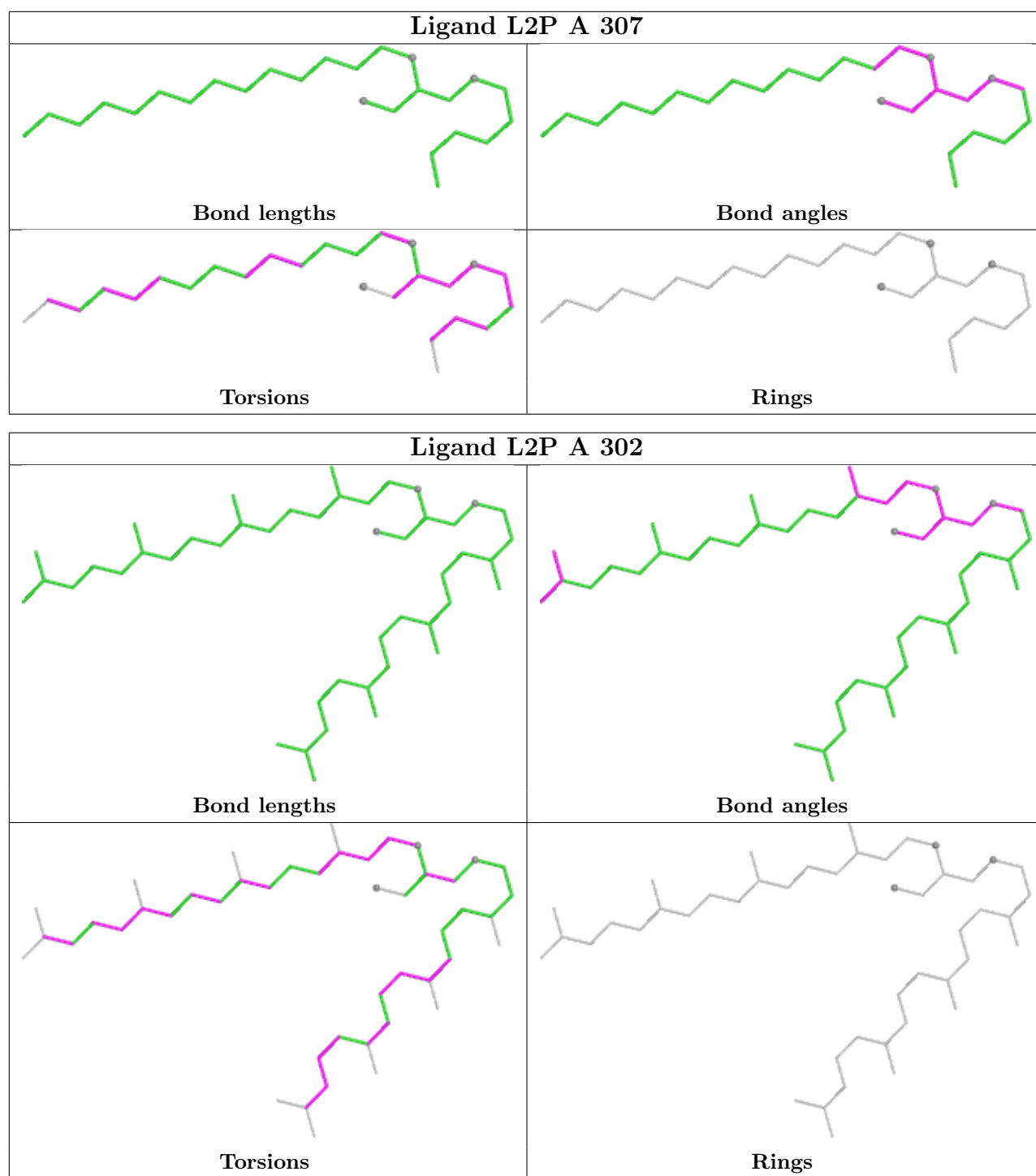












5.7 Other polymers [i](#)

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%)	-1.05	0 100 100	9, 23, 54, 89	5 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	L2P	A	308	5/46	0.97	0.08	61,68,82,94	0
3	L2P	A	304	29/46	0.98	0.07	38,59,79,86	0
3	L2P	A	305	29/46	0.98	0.07	52,85,128,147	0
3	L2P	A	307	26/46	0.98	0.07	41,77,98,122	0
3	L2P	A	303	40/46	0.98	0.06	34,58,88,101	0
3	L2P	A	309	10/46	0.98	0.05	35,59,75,78	0
3	L2P	A	310	18/46	0.98	0.05	41,58,98,117	0
2	RET	A	301	20/21	0.99	0.03	12,15,22,22	0
3	L2P	A	306	9/46	0.99	0.05	34,44,68,74	0

Continued on next page...

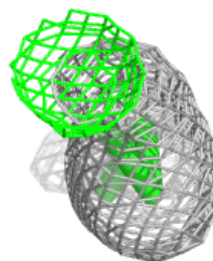
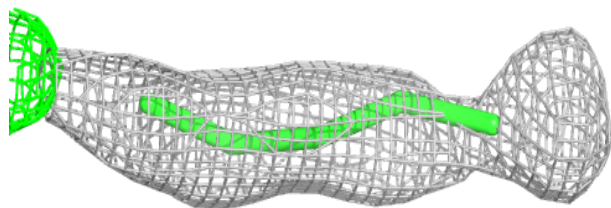
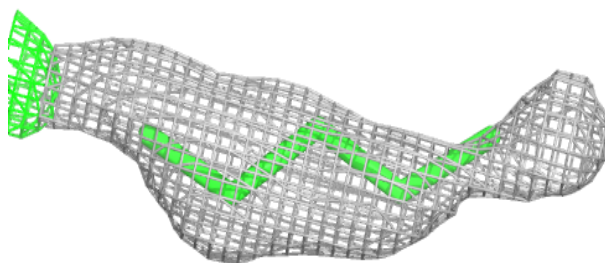
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	L2P	A	302	46/46	0.99	0.07	40,62,96,130	0
3	L2P	A	311	8/46	0.99	0.05	35,58,88,92	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.

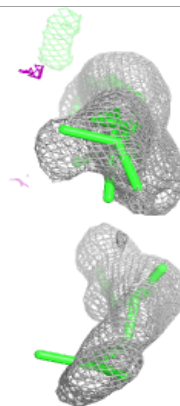
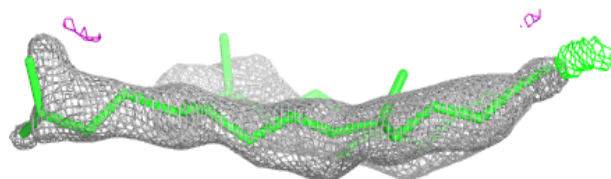
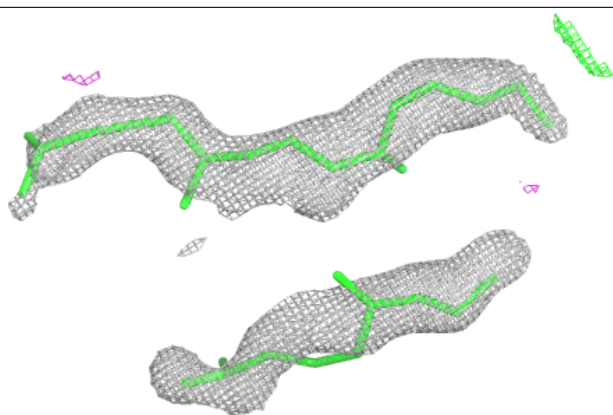
Electron density around L2P A 308:

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

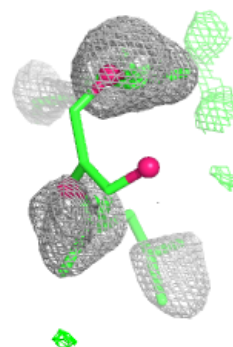
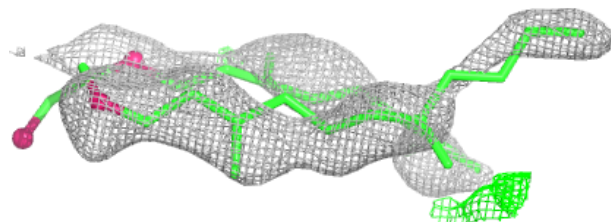
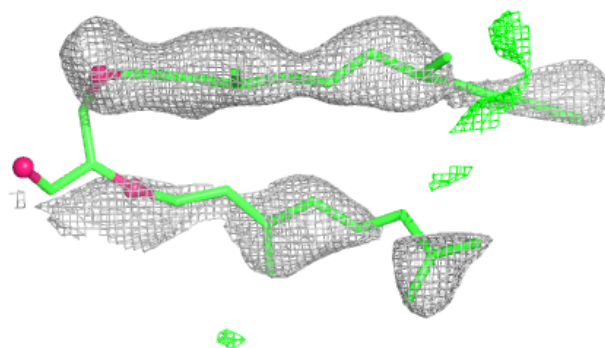


Electron density around L2P A 304:

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

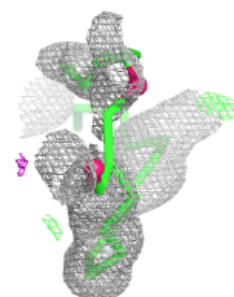
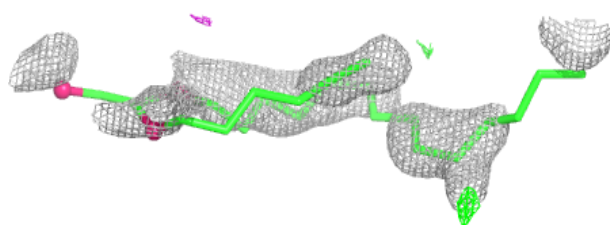
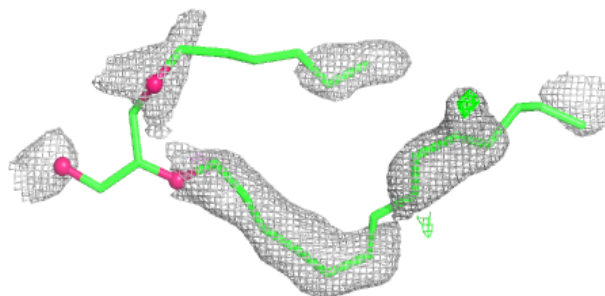
**Electron density around L2P A 305:**

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

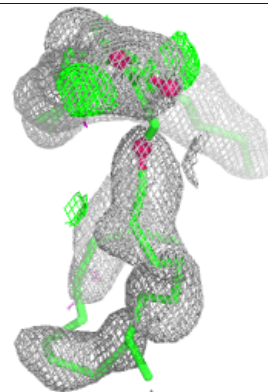
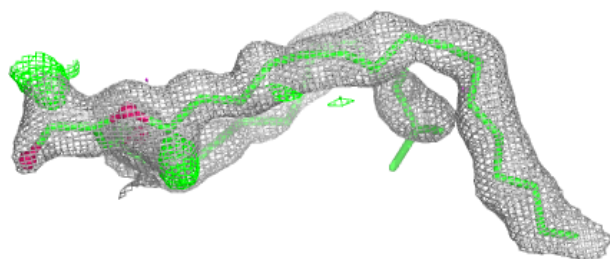
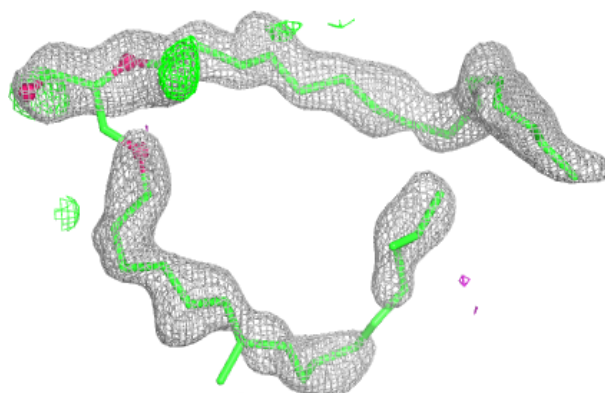


Electron density around L2P A 307:

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

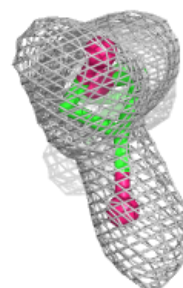
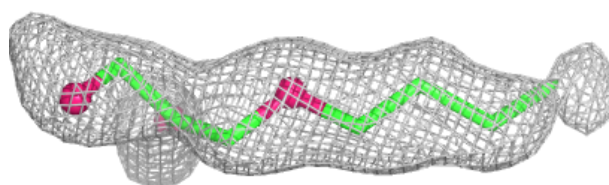
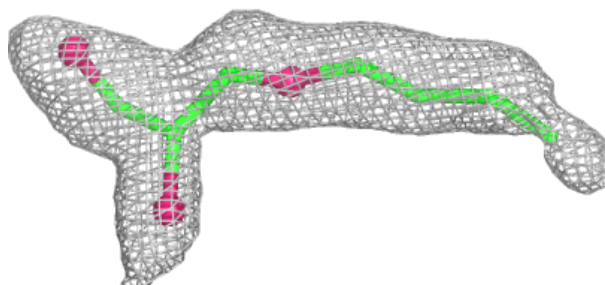
**Electron density around L2P A 303:**

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

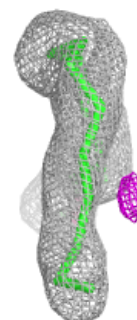
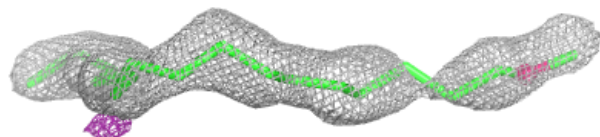
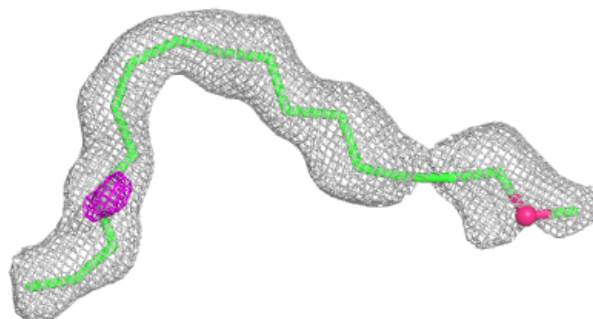


Electron density around L2P A 309:

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

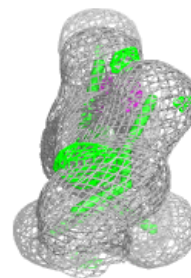
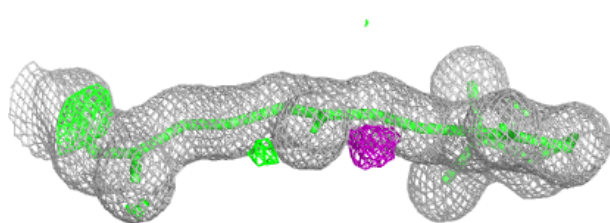
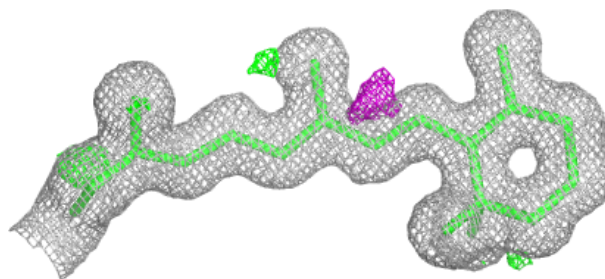
**Electron density around L2P A 310:**

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

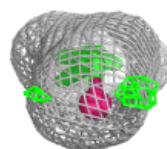
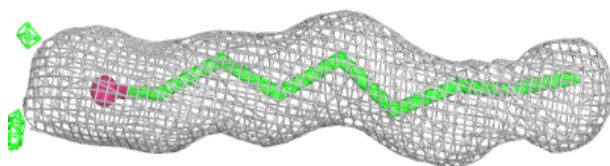
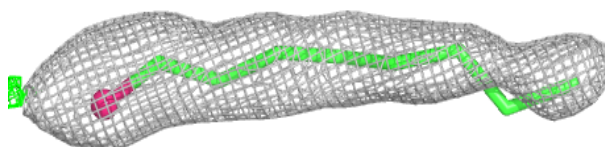


Electron density around RET A 301:

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

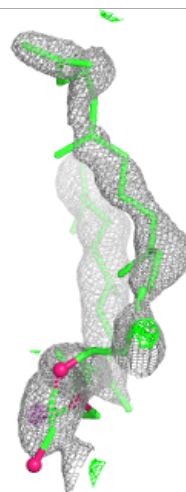
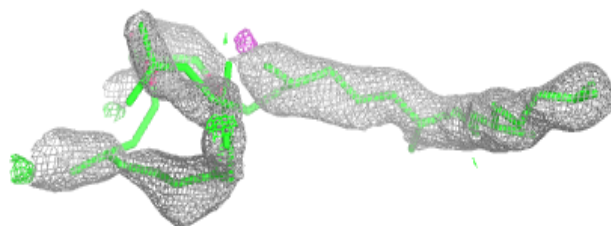
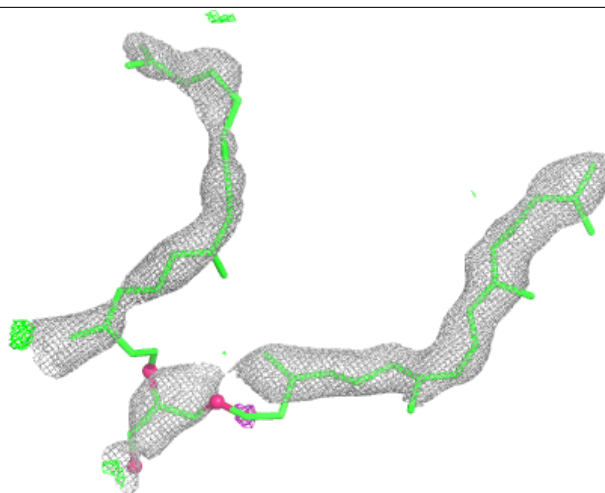
**Electron density around L2P A 306:**

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



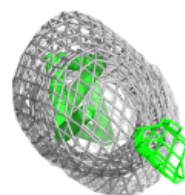
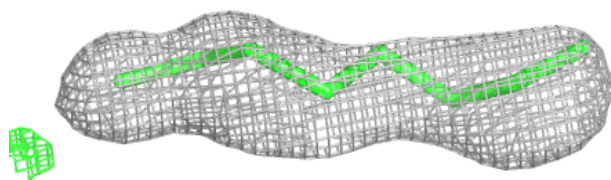
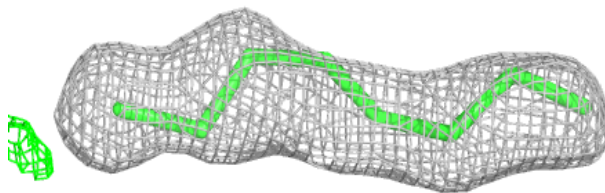
Electron density around L2P A 302:

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



Electron density around L2P A 311:

$2mF_o-DF_c$ (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.