



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:21 AM BST

PDB ID : 6UH3
Title : Crystal structure of bacterial heliorhodopsin 48C12
Authors : Lu, Y.; Zhou, X.E.; Gao, X.; Xia, R.; Xu, Z.; Wang, N.; Leng, Y.; Melcher, K.; Xu, H.E.; He, Y.
Deposited on : 2019-09-26
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

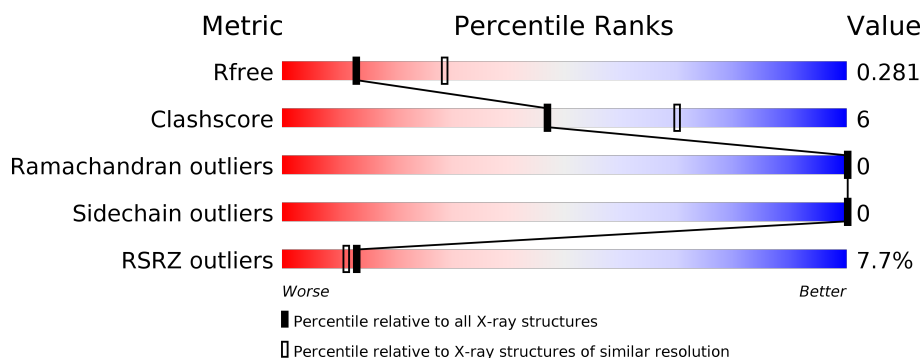
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	252	<div> <div>8%</div> <div>90%</div> <div>8%</div> </div>
1	B	252	<div> <div>7%</div> <div>89%</div> <div>8%</div> </div>

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
5	PEG	B	304	-	X	-	-
5	PEG	B	307	-	-	X	-

2 Entry composition [i](#)

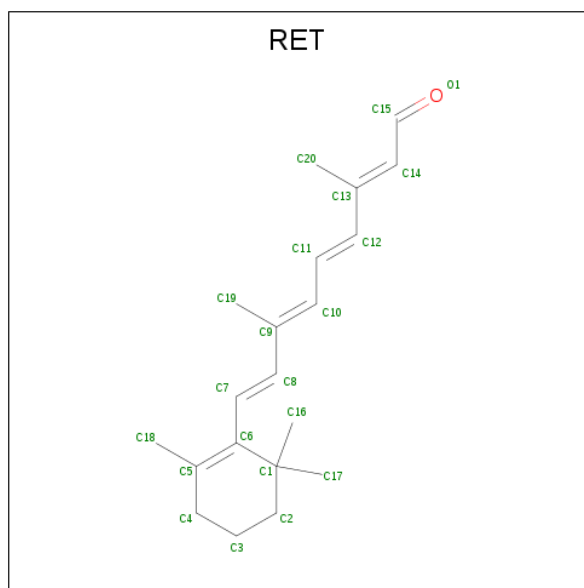
There are 6 unique types of molecules in this entry. The entry contains 4190 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heliorhodopsin.

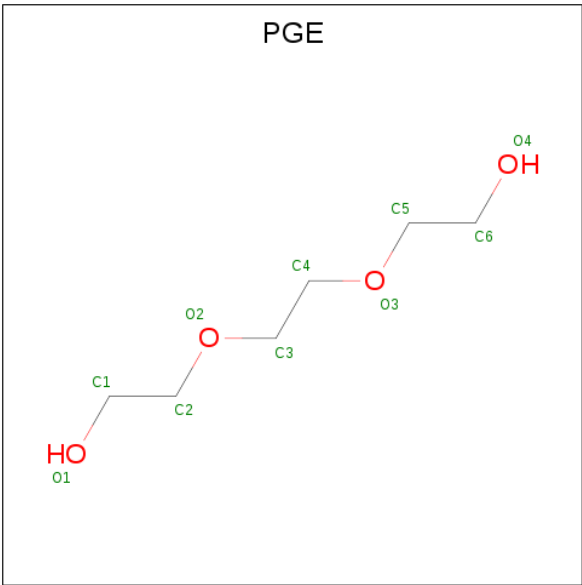
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1915	1286	300	323	6			
1	B	245	Total	C	N	O	S	0	0	0
			1907	1280	299	322	6			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



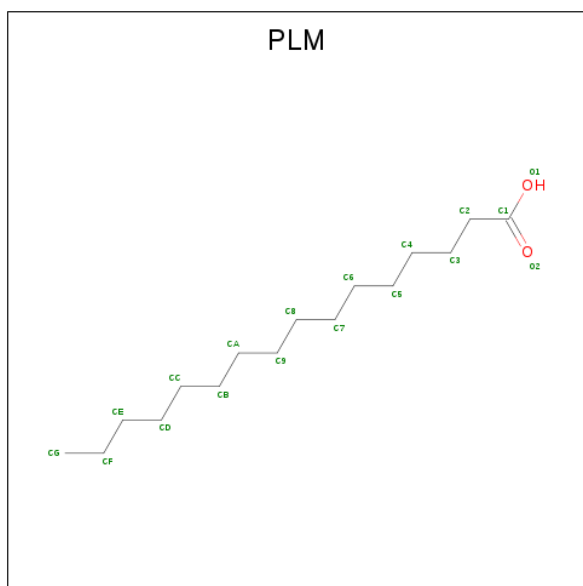
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

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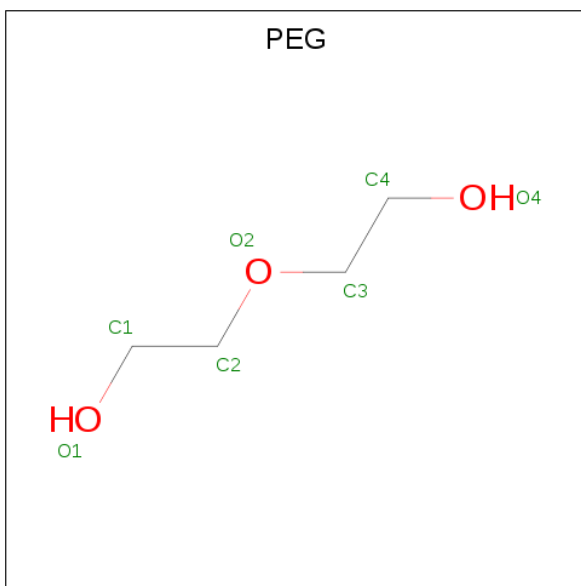
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	12	2		
4	A	1	Total	C	O	0	0
			18	16	2		
4	B	1	Total	C	O	0	0
			18	16	2		
4	B	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

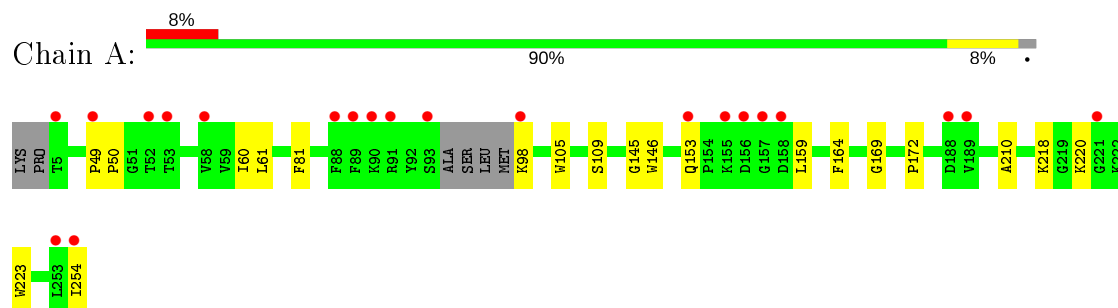
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total	O	0	0
			17	17		
6	B	19	Total	O	0	0
			19	19		

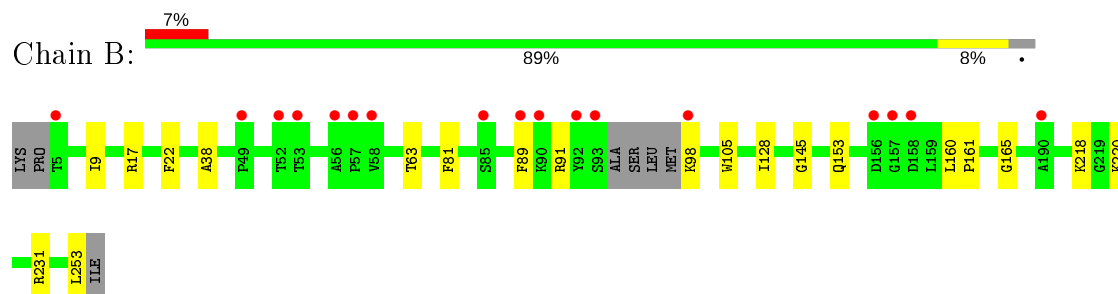
3 Residue-property plots [i](#)

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: Heliorhodopsin



• Molecule 1: Heliorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.45Å 102.14Å 56.77Å 90.00° 94.04° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.00-2.70) 76.1 (49.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.264 , 0.279 0.266 , 0.281	Depositor DCC
R_{free} test set	1032 reflections (7.17%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4190	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% 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: PEG, PLM, PGE, 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	0.38	0/1967	0.58	0/2678
1	B	0.38	0/1959	0.58	0/2667
All	All	0.38	0/3926	0.58	0/5345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1969	20	0
1	B	1907	0	1958	22	0
2	A	20	0	27	4	0
2	B	20	0	27	8	0
3	A	110	0	154	8	0
3	B	100	0	140	5	0
4	A	32	0	51	4	0
4	B	36	0	62	4	0
5	B	14	0	20	5	0
6	A	17	0	0	1	0
6	B	19	0	0	0	0
All	All	4190	0	4408	53	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 6.

All (53) 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:22:PHE:HE1	4:B:314:PLM:HG3	1.22	1.02
1:B:128:ILE:HD11	3:B:308:PGE:H5	1.55	0.88
1:B:22:PHE:CE1	4:B:314:PLM:HG3	2.10	0.87
1:B:220:LYS:HD2	5:B:307:PEG:H32	1.60	0.82
1:A:159:LEU:HD13	3:A:302:PGE:O1	1.84	0.78
1:B:81:PHE:HB3	3:B:309:PGE:H12	1.72	0.72
1:A:223:TRP:HH2	4:A:313:PLM:H91	1.56	0.70
1:A:164:PHE:HE1	3:A:302:PGE:H62	1.62	0.65
1:A:60:ILE:HG22	1:A:61:LEU:HG	1.78	0.65
1:A:98:LYS:N	1:A:153:GLN:HE22	1.95	0.65
3:A:304:PGE:H12	3:A:306:PGE:O1	2.02	0.60
2:B:301:RET:H171	2:B:301:RET:H8	1.84	0.60
1:A:210:ALA:HB2	2:A:301:RET:H183	1.87	0.55
1:B:145:GLY:HA3	2:B:301:RET:H172	1.90	0.54
1:A:169:GLY:O	1:A:172:PRO:HD2	2.09	0.53
1:B:81:PHE:HB3	3:B:309:PGE:C1	2.39	0.52
1:B:165:GLY:HA3	2:B:301:RET:H31	1.90	0.52
1:B:98:LYS:N	1:B:153:GLN:HE22	2.07	0.52
2:A:301:RET:H171	2:A:301:RET:H8	1.92	0.51
1:A:81:PHE:HD2	3:A:310:PGE:O2	1.94	0.49
1:A:164:PHE:CE1	3:A:302:PGE:H62	2.47	0.49
1:A:109:SER:OG	3:A:308:PGE:H52	2.15	0.47
1:A:254:ILE:HG22	1:A:254:ILE:O	2.15	0.47
1:A:218:LYS:HB3	6:A:401:HOH:O	2.15	0.47
1:B:231:ARG:HD3	3:B:310:PGE:H12	1.96	0.47
1:B:17:ARG:HH11	4:B:314:PLM:H81	1.80	0.46
1:A:223:TRP:CH2	4:A:313:PLM:H91	2.45	0.46
3:A:308:PGE:H1	4:A:314:PLM:HG2	1.98	0.46
1:B:165:GLY:HA3	2:B:301:RET:C3	2.45	0.46
2:A:301:RET:H181	2:A:301:RET:H7	1.59	0.46
1:B:160:LEU:HB3	1:B:161:PRO:HD3	1.98	0.45
1:B:91:ARG:N	1:B:91:ARG:HD2	2.31	0.45
1:B:220:LYS:CD	5:B:307:PEG:H32	2.41	0.45
1:A:146:TRP:HD1	1:A:146:TRP:O	1.99	0.45
1:A:220:LYS:O	1:A:223:TRP:N	2.50	0.45
1:B:145:GLY:CA	2:B:301:RET:H21	2.47	0.45
1:B:105:TRP:HA	1:B:105:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LYS:HD2	5:B:307:PEG:C3	2.41	0.44
4:A:314:PLM:HB2	4:A:314:PLM:HF1	1.98	0.44
2:B:301:RET:H181	2:B:301:RET:H7	1.60	0.43
3:B:303:PGE:H4	5:B:307:PEG:H31	2.00	0.43
1:B:253:LEU:O	1:B:253:LEU:HG	2.17	0.43
1:A:81:PHE:CD2	3:A:310:PGE:O2	2.72	0.43
1:A:146:TRP:CD1	1:A:146:TRP:C	2.92	0.43
1:B:9:ILE:HG21	1:B:89:PHE:CD1	2.53	0.43
1:A:105:TRP:HA	1:A:105:TRP:CE3	2.55	0.42
2:B:301:RET:H171	2:B:301:RET:C8	2.50	0.42
2:B:301:RET:H11	2:B:301:RET:H191	1.92	0.42
1:B:218:LYS:HG2	5:B:307:PEG:O1	2.20	0.41
1:A:145:GLY:HA3	2:A:301:RET:H21	2.02	0.41
1:B:38:ALA:HA	1:B:63:THR:O	2.21	0.41
4:B:315:PLM:HF2	4:B:315:PLM:HC2	1.82	0.40
1:A:49:PRO:HA	1:A:50:PRO:HD3	1.95	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	242/252 (96%)	233 (96%)	9 (4%)	0	100	100
1	B	241/252 (96%)	233 (97%)	8 (3%)	0	100	100
All	All	483/504 (96%)	466 (96%)	17 (4%)	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	203/208 (98%)	203 (100%)	0	100	100
1	B	202/208 (97%)	202 (100%)	0	100	100
All	All	405/416 (97%)	405 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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](#)

29 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	PGE	A	307	-	9,9,9	0.51	0	8,8,8	0.37	0
4	PLM	A	314	-	14,17,17	0.24	0	13,17,17	0.60	0
4	PLM	B	314	-	14,17,17	0.23	0	13,17,17	0.41	0
4	PLM	A	313	-	10,13,17	0.22	0	9,13,17	0.53	0
5	PEG	B	307	-	6,6,6	0.59	0	5,5,5	1.80	2 (40%)
3	PGE	A	302	-	9,9,9	0.55	0	8,8,8	0.53	0
3	PGE	A	306	-	9,9,9	0.53	0	8,8,8	0.27	0
5	PEG	B	304	-	6,6,6	0.55	0	5,5,5	1.87	2 (40%)
3	PGE	A	309	-	9,9,9	0.51	0	8,8,8	0.26	0
3	PGE	A	310	-	9,9,9	0.51	0	8,8,8	0.36	0
3	PGE	A	308	-	9,9,9	0.50	0	8,8,8	0.29	0
3	PGE	B	313	-	9,9,9	0.54	0	8,8,8	0.38	0
3	PGE	A	312	-	9,9,9	0.51	0	8,8,8	0.45	0
3	PGE	B	311	-	9,9,9	0.54	0	8,8,8	0.32	0
3	PGE	B	306	-	9,9,9	0.51	0	8,8,8	0.37	0
3	PGE	B	308	-	9,9,9	0.53	0	8,8,8	0.51	0
3	PGE	B	310	-	9,9,9	0.50	0	8,8,8	0.29	0
4	PLM	B	315	-	14,17,17	0.19	0	13,17,17	0.77	0
3	PGE	A	311	-	9,9,9	0.48	0	8,8,8	0.23	0
3	PGE	B	312	-	9,9,9	0.52	0	8,8,8	0.20	0
3	PGE	B	305	-	9,9,9	0.52	0	8,8,8	0.27	0
3	PGE	A	304	-	9,9,9	0.51	0	8,8,8	0.47	0
3	PGE	A	303	-	9,9,9	0.49	0	8,8,8	0.29	0
2	RET	B	301	1	20,20,21	1.70	5 (25%)	27,27,28	1.81	8 (29%)
2	RET	A	301	1	20,20,21	1.68	5 (25%)	27,27,28	1.85	8 (29%)
3	PGE	B	309	-	9,9,9	0.50	0	8,8,8	0.37	0
3	PGE	A	305	-	9,9,9	0.53	0	8,8,8	0.32	0
3	PGE	B	302	-	9,9,9	0.51	0	8,8,8	0.26	0
3	PGE	B	303	-	9,9,9	0.50	0	8,8,8	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	307	-	-	1/7/7/7	-
4	PLM	A	314	-	-	4/13/15/15	-
4	PLM	B	314	-	-	9/13/15/15	-
4	PLM	A	313	-	-	0/9/11/15	-
5	PEG	B	307	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	302	-	-	2/7/7/7	-
3	PGE	A	306	-	-	3/7/7/7	-
5	PEG	B	304	-	-	4/4/4/4	-
3	PGE	A	309	-	-	3/7/7/7	-
3	PGE	A	310	-	-	4/7/7/7	-
3	PGE	A	308	-	-	2/7/7/7	-
3	PGE	B	313	-	-	4/7/7/7	-
3	PGE	A	312	-	-	4/7/7/7	-
3	PGE	B	311	-	-	5/7/7/7	-
3	PGE	B	306	-	-	1/7/7/7	-
3	PGE	B	308	-	-	3/7/7/7	-
3	PGE	B	310	-	-	2/7/7/7	-
4	PLM	B	315	-	-	4/13/15/15	-
3	PGE	A	311	-	-	5/7/7/7	-
3	PGE	B	312	-	-	4/7/7/7	-
3	PGE	B	305	-	-	3/7/7/7	-
3	PGE	A	304	-	-	2/7/7/7	-
3	PGE	A	303	-	-	2/7/7/7	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	PGE	B	309	-	-	3/7/7/7	-
3	PGE	A	305	-	-	0/7/7/7	-
3	PGE	B	302	-	-	1/7/7/7	-
3	PGE	B	303	-	-	4/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	RET	C11-C10	3.46	1.54	1.43
2	B	301	RET	C12-C13	3.41	1.53	1.45
2	A	301	RET	C8-C9	3.26	1.52	1.45
2	B	301	RET	C8-C9	3.16	1.52	1.45
2	A	301	RET	C11-C10	3.13	1.53	1.43
2	A	301	RET	C7-C6	2.59	1.54	1.45
2	A	301	RET	C12-C13	2.54	1.51	1.45
2	B	301	RET	C7-C6	2.46	1.53	1.45
2	A	301	RET	C10-C9	-2.45	1.32	1.35
2	B	301	RET	C10-C9	-2.39	1.32	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C18-C5-C6	-4.42	119.56	124.53
2	A	301	RET	C18-C5-C6	-3.90	120.15	124.53
2	A	301	RET	C11-C10-C9	-3.80	121.88	127.31
2	B	301	RET	C11-C10-C9	-3.32	122.57	127.31
2	B	301	RET	C7-C8-C9	-3.25	121.32	126.23
5	B	304	PEG	O2-C2-C1	3.01	123.30	110.07
2	A	301	RET	C7-C8-C9	-2.97	121.75	126.23
5	B	307	PEG	O2-C3-C4	2.89	122.76	110.07
5	B	307	PEG	O4-C4-C3	2.64	127.14	111.81
2	B	301	RET	C3-C4-C5	-2.60	109.44	114.08
2	A	301	RET	C3-C4-C5	-2.60	109.44	114.08
2	A	301	RET	C1-C6-C7	2.56	123.03	115.78
2	B	301	RET	C20-C13-C12	2.46	121.95	118.08
2	A	301	RET	C18-C5-C4	2.31	118.06	113.62
2	A	301	RET	C7-C6-C5	-2.26	115.99	121.46
2	B	301	RET	C1-C6-C7	2.24	122.12	115.78
5	B	304	PEG	C3-O2-C2	2.21	122.85	113.29
2	B	301	RET	C18-C5-C4	2.08	117.62	113.62
2	B	301	RET	C7-C6-C5	-2.07	116.46	121.46
2	A	301	RET	C2-C3-C4	-2.03	106.84	111.38

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	315	PLM	C1-C2-C3-C4
5	B	304	PEG	C1-C2-O2-C3
3	B	312	PGE	O2-C3-C4-O3
3	B	309	PGE	O2-C3-C4-O3
4	B	315	PLM	C8-C9-CA-CB
3	B	313	PGE	O2-C3-C4-O3
3	B	308	PGE	O2-C3-C4-O3
3	B	302	PGE	O2-C3-C4-O3
3	B	311	PGE	O2-C3-C4-O3
3	A	310	PGE	O2-C3-C4-O3
3	A	307	PGE	O2-C3-C4-O3
3	A	309	PGE	O2-C3-C4-O3
5	B	307	PEG	O1-C1-C2-O2
4	A	314	PLM	C6-C7-C8-C9
4	B	314	PLM	C2-C3-C4-C5
3	A	310	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	A	308	PGE	O1-C1-C2-O2
3	B	311	PGE	O1-C1-C2-O2
3	A	312	PGE	O3-C5-C6-O4
3	B	312	PGE	O3-C5-C6-O4
4	B	314	PLM	C6-C7-C8-C9
3	B	308	PGE	O1-C1-C2-O2
3	A	311	PGE	O1-C1-C2-O2
3	B	312	PGE	O1-C1-C2-O2
3	B	303	PGE	O3-C5-C6-O4
4	B	314	PLM	C4-C5-C6-C7
4	B	314	PLM	CC-CD-CE-CF
3	B	303	PGE	O2-C3-C4-O3
3	B	306	PGE	O2-C3-C4-O3
4	B	314	PLM	C5-C6-C7-C8
4	B	314	PLM	CB-CC-CD-CE
3	A	304	PGE	O2-C3-C4-O3
4	A	314	PLM	CC-CD-CE-CF
4	B	315	PLM	C2-C3-C4-C5
3	B	305	PGE	C4-C3-O2-C2
3	A	312	PGE	C6-C5-O3-C4
3	B	313	PGE	C4-C3-O2-C2
3	A	311	PGE	C3-C4-O3-C5
3	B	311	PGE	C6-C5-O3-C4
3	B	303	PGE	C6-C5-O3-C4
4	B	314	PLM	C1-C2-C3-C4
3	B	313	PGE	C1-C2-O2-C3
4	A	314	PLM	CB-CC-CD-CE
3	B	311	PGE	C1-C2-O2-C3
3	A	311	PGE	C6-C5-O3-C4
3	A	309	PGE	C1-C2-O2-C3
3	B	312	PGE	C3-C4-O3-C5
3	A	311	PGE	C1-C2-O2-C3
5	B	304	PEG	O2-C3-C4-O4
3	A	303	PGE	O3-C5-C6-O4
3	A	302	PGE	O2-C3-C4-O3
4	B	314	PLM	C7-C8-C9-CA
3	B	305	PGE	C3-C4-O3-C5
3	A	302	PGE	O3-C5-C6-O4
5	B	304	PEG	O1-C1-C2-O2
3	B	305	PGE	O3-C5-C6-O4
3	B	309	PGE	C1-C2-O2-C3
4	A	314	PLM	C8-C9-CA-CB

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Mol	Chain	Res	Type	Atoms
3	B	311	PGE	O3-C5-C6-O4
3	A	306	PGE	O2-C3-C4-O3
3	A	310	PGE	C6-C5-O3-C4
5	B	307	PEG	O2-C3-C4-O4
3	A	311	PGE	O2-C3-C4-O3
3	A	306	PGE	O1-C1-C2-O2
3	B	310	PGE	C6-C5-O3-C4
3	A	309	PGE	C4-C3-O2-C2
3	A	303	PGE	O2-C3-C4-O3
3	A	310	PGE	C4-C3-O2-C2
3	B	308	PGE	C6-C5-O3-C4
3	B	310	PGE	O2-C3-C4-O3
5	B	304	PEG	C4-C3-O2-C2
3	A	306	PGE	C3-C4-O3-C5
3	A	308	PGE	C1-C2-O2-C3
4	B	315	PLM	CA-CB-CC-CD
3	B	313	PGE	O1-C1-C2-O2
3	B	309	PGE	O3-C5-C6-O4
3	B	303	PGE	O1-C1-C2-O2
4	B	314	PLM	CD-CE-CF-CG
3	A	312	PGE	O2-C3-C4-O3
3	A	304	PGE	O1-C1-C2-O2
3	A	312	PGE	C3-C4-O3-C5

There are no ring outliers.

16 monomers are involved in 36 short contacts:

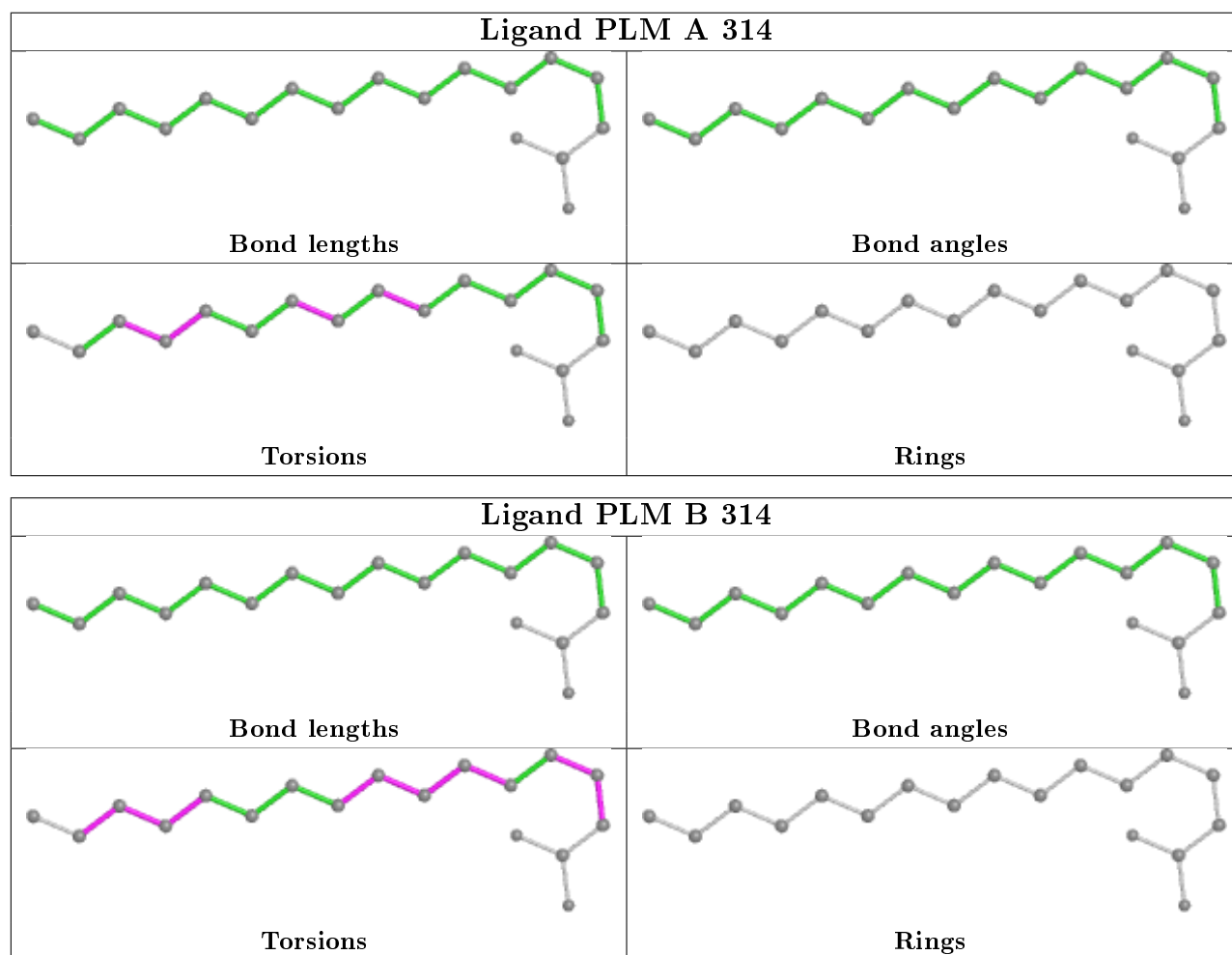
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	314	PLM	2	0
4	B	314	PLM	3	0
4	A	313	PLM	2	0
5	B	307	PEG	5	0
3	A	302	PGE	3	0
3	A	306	PGE	1	0
3	A	310	PGE	2	0
3	A	308	PGE	2	0
3	B	308	PGE	1	0
3	B	310	PGE	1	0
4	B	315	PLM	1	0
3	A	304	PGE	1	0
2	B	301	RET	8	0
2	A	301	RET	4	0

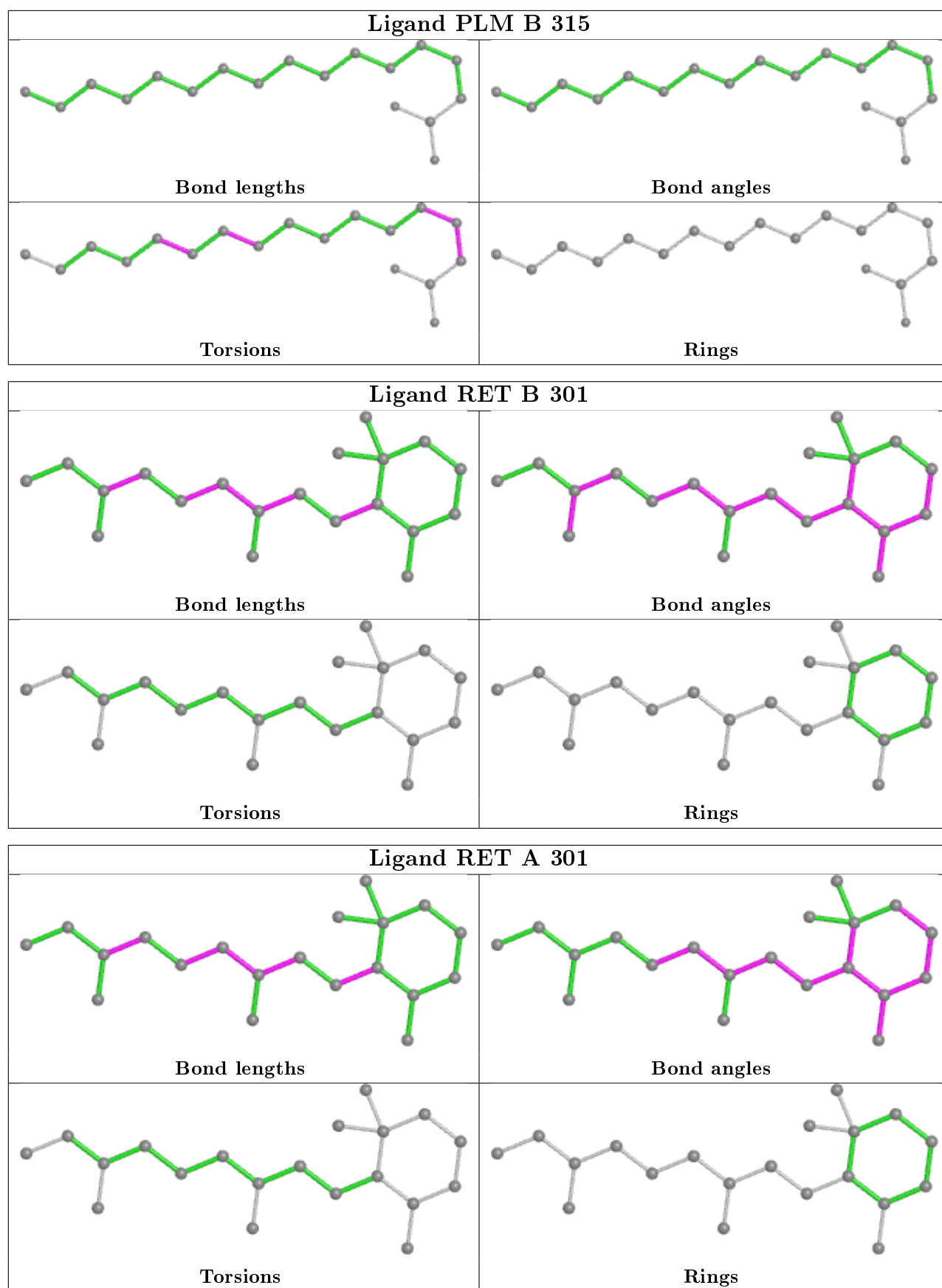
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	309	PGE	2	0
3	B	303	PGE	1	0

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





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	246/252 (97%)	0.22	21 (8%) 10 9	14, 29, 79, 155	0
1	B	245/252 (97%)	0.03	17 (6%) 16 15	14, 28, 73, 131	0
All	All	491/504 (97%)	0.12	38 (7%) 13 11	14, 29, 77, 155	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	24.4
1	B	92	TYR	10.2
1	A	91	ARG	7.9
1	A	88	PHE	6.8
1	A	90	LYS	6.6
1	A	89	PHE	5.5
1	B	52	THR	5.0
1	B	158	ASP	4.9
1	A	254	ILE	4.5
1	A	5	THR	4.4
1	B	5	THR	4.3
1	A	157	GLY	4.3
1	A	156	ASP	4.1
1	A	158	ASP	4.0
1	B	85	SER	3.9
1	A	155	LYS	3.9
1	B	58	VAL	3.8
1	B	89	PHE	3.7
1	A	98	LYS	3.7
1	A	253	LEU	3.5
1	A	52	THR	3.3
1	B	56	ALA	3.3
1	B	157	GLY	3.2
1	B	49	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	90	LYS	3.1
1	A	189	VAL	3.1
1	B	57	PRO	3.1
1	A	58	VAL	2.9
1	A	221	GLY	2.9
1	B	53	THR	2.9
1	A	153	GLN	2.9
1	A	53	THR	2.8
1	A	188	ASP	2.7
1	B	98	LYS	2.6
1	B	156	ASP	2.6
1	A	49	PRO	2.5
1	B	190	ALA	2.2
1	B	93	SER	2.1

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(\AA^2)	Q<0.9
3	PGE	B	308	10/10	0.60	0.38	41,47,53,57	0
3	PGE	B	313	10/10	0.66	0.32	55,59,65,67	0
5	PEG	B	307	7/7	0.68	0.29	56,57,62,67	0
3	PGE	A	302	10/10	0.69	0.40	43,52,60,63	0
3	PGE	A	312	10/10	0.70	0.20	56,70,74,81	0
3	PGE	B	303	10/10	0.70	0.22	51,57,59,62	0
3	PGE	A	306	10/10	0.72	0.29	49,54,60,62	0
5	PEG	B	304	7/7	0.74	0.19	53,72,76,76	0
4	PLM	A	313	14/18	0.75	0.36	28,40,59,61	0

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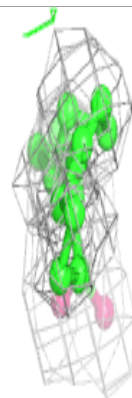
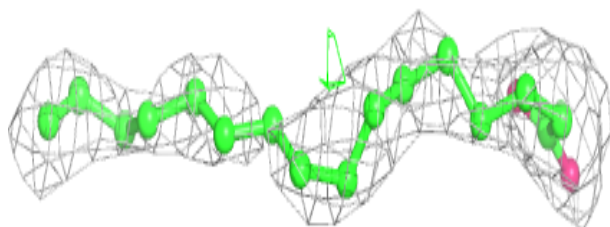
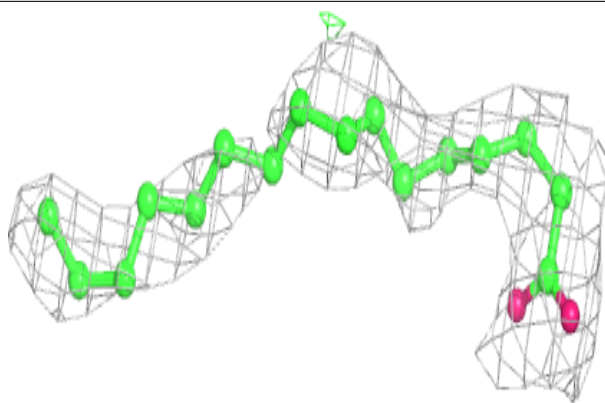
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PGE	A	309	10/10	0.75	0.20	52,57,64,68	0
3	PGE	A	304	10/10	0.77	0.36	51,58,65,68	0
3	PGE	B	312	10/10	0.77	0.21	58,60,67,69	0
3	PGE	A	311	10/10	0.78	0.34	52,55,65,67	0
3	PGE	B	302	10/10	0.78	0.24	44,48,52,53	0
3	PGE	B	311	10/10	0.78	0.27	30,36,44,47	0
4	PLM	B	314	18/18	0.79	0.25	37,48,59,63	0
3	PGE	A	307	10/10	0.79	0.34	40,42,57,66	0
4	PLM	A	314	18/18	0.80	0.38	30,43,61,65	0
3	PGE	A	305	10/10	0.81	0.35	43,48,50,54	0
3	PGE	B	309	10/10	0.82	0.34	32,34,39,43	0
4	PLM	B	315	18/18	0.83	0.24	28,37,52,52	0
3	PGE	A	308	10/10	0.85	0.27	31,35,50,53	0
3	PGE	A	310	10/10	0.86	0.32	32,39,44,47	0
3	PGE	B	310	10/10	0.86	0.15	37,49,53,56	0
3	PGE	B	306	10/10	0.86	0.25	23,33,49,51	0
3	PGE	A	303	10/10	0.86	0.22	49,52,58,60	0
3	PGE	B	305	10/10	0.89	0.13	36,42,48,50	0
2	RET	B	301	20/21	0.91	0.19	18,21,25,25	0
2	RET	A	301	20/21	0.91	0.19	18,22,25,26	0

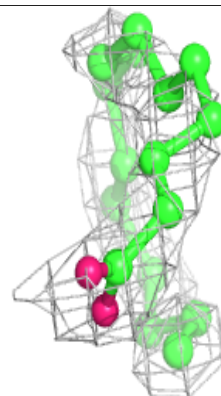
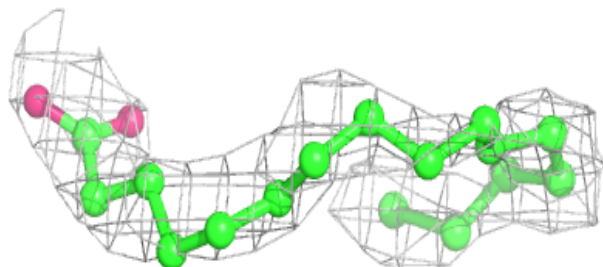
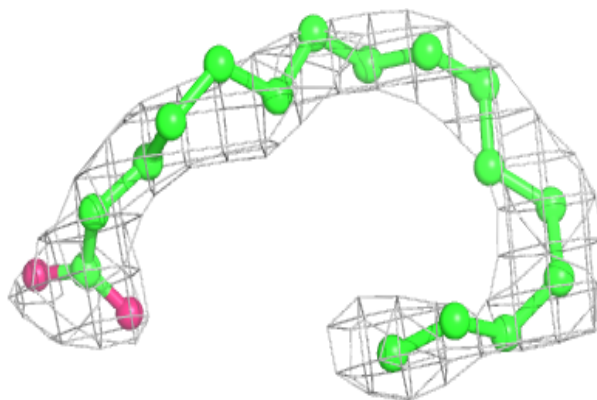
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM B 314:

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

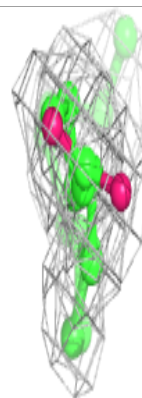
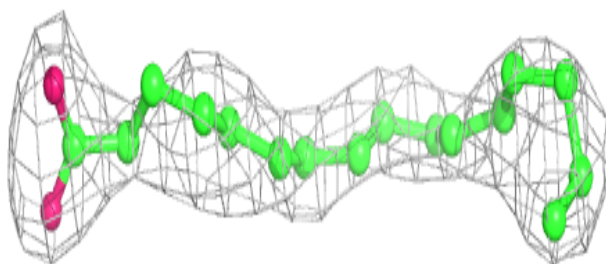
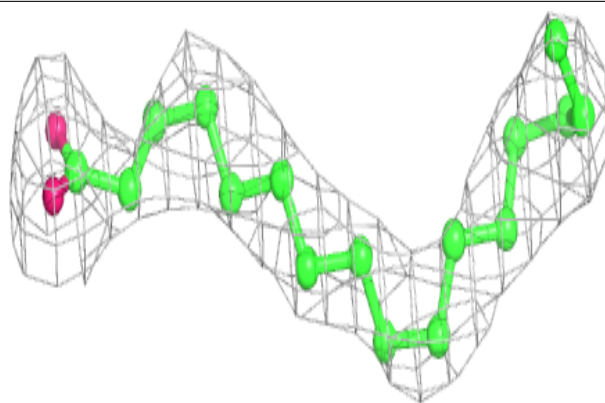
**Electron density around PLM A 314:**

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

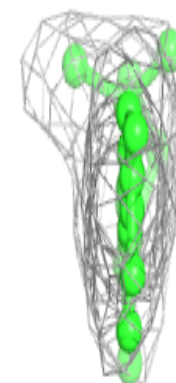
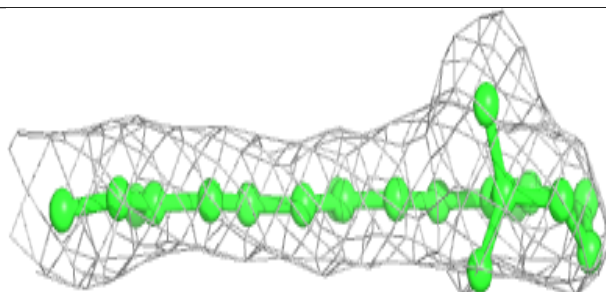
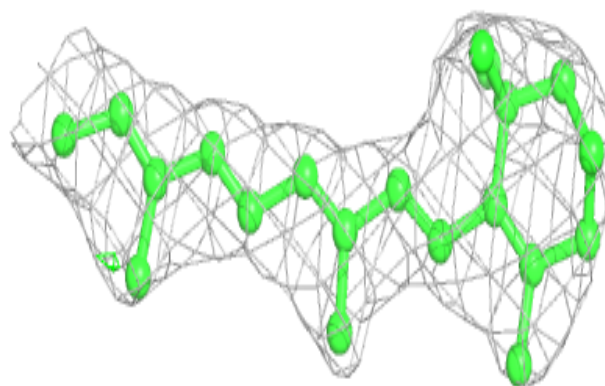


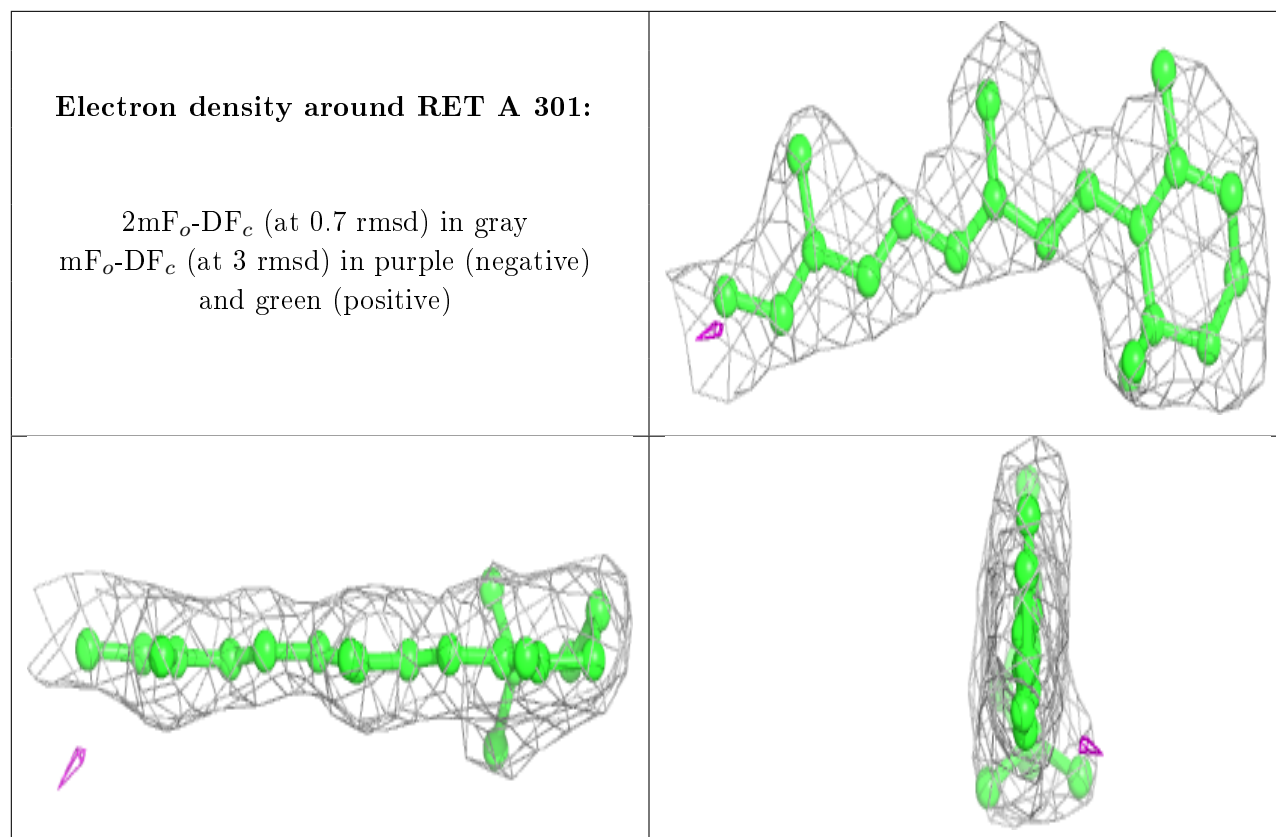
Electron density around PLM B 315:

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

**Electron density around RET B 301:**

$2mF_o-DF_c$ (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.