



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:08 AM UTC

PDB ID : 3AYN / pdb_00003ayn
Title : Crystal structure of squid isorhodopsin
Authors : Murakami, M.; Kouyama, T.
Deposited on : 2011-05-09
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

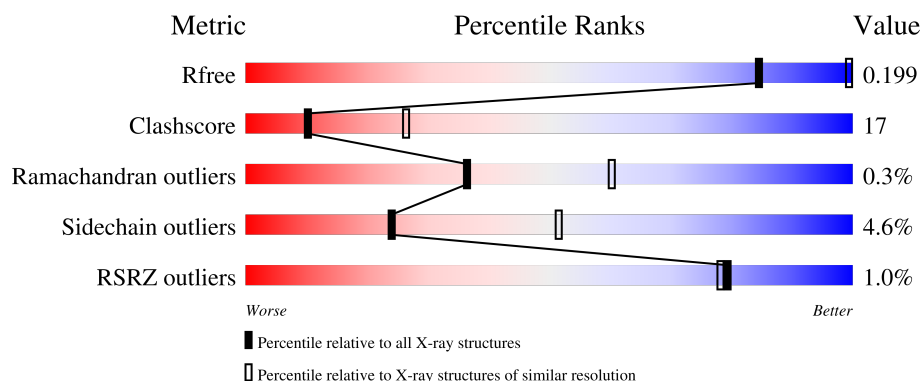
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	448	% 48% 28% • 22%
1	B	448	% 49% 25% • 23%

2 Entry composition [i](#)

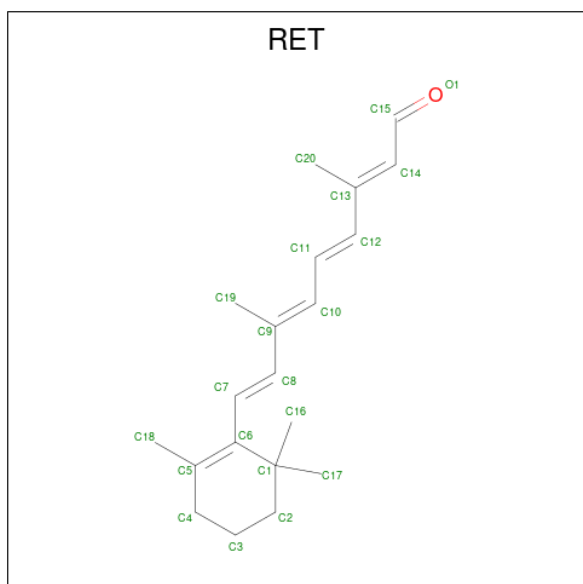
There are 7 unique types of molecules in this entry. The entry contains 5756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rhodopsin.

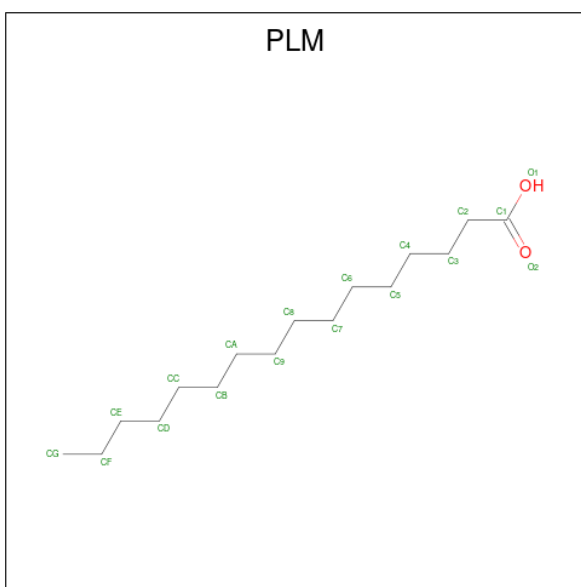
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2780	1838	443	473	26			
1	B	347	Total	C	N	O	S	0	0	0
			2762	1828	440	468	26			

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



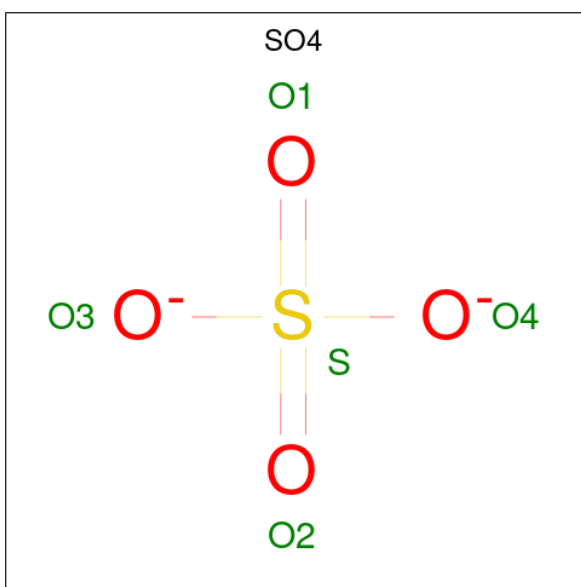
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



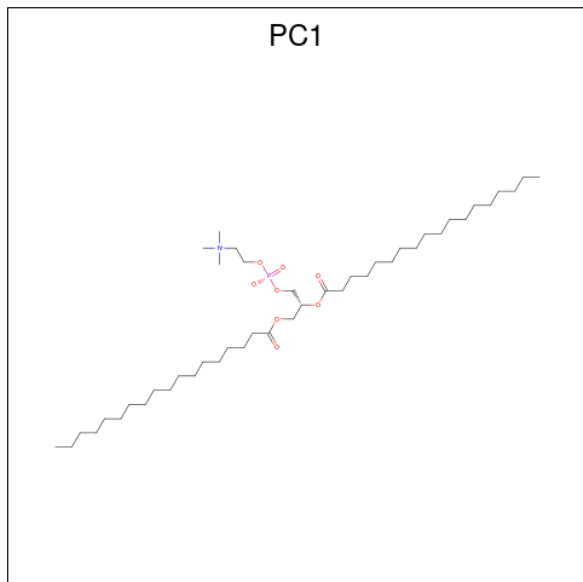
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



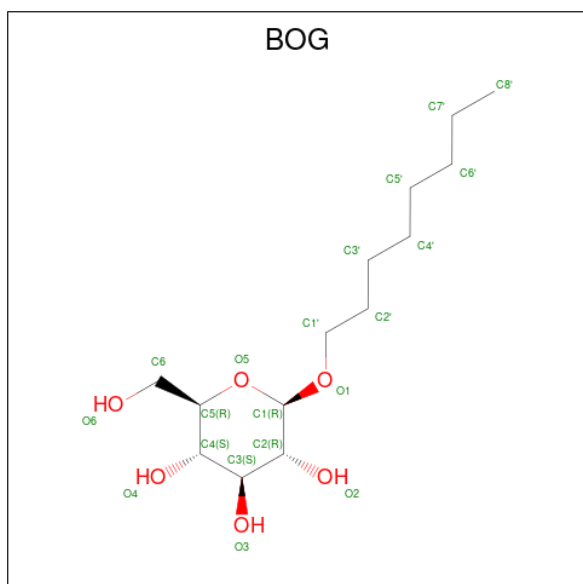
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	B	1	39	30	8	1	0	0

- Molecule 6 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	B	1	20	14	6		0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	29	Total 29	O 29	0	0
7	B	30	Total 30	O 30	0	0

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.

[illegible]

Chain B:

Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	Col 10	Col 11	Col 12	Col 13	Col 14	Col 15	Col 16
1	S318	H319	F322	R323	I326	F330	L334	T335	C336	C337	Q338	K342	F343	T344	E345	D346
2	M225	S228	N229	H230	E231	K232	E233	M234	A235	M236	M237	A238	K239	R240	L241	N242
3	I117	F118	G119	A120	M121	S122	I123	M124	A127	M128	I131	D132	R133	V136	I137	G138
4	MET	GLY	ARG	ASP	LEU	ARG	ASP	ASN	E9	T10	D31	Y35	I41	N52	V55	I56
5															V57	L58
6															F59	T60
7															R61	T62
8															K63	S64
9															L65	Q66
10															T67	
11															F72	I73
12															I74	N75
13															L76	
14															S79	
15															F83	S84
16															L85	V86
17															C203	N87
18															M204	G88
19															F205	
20															L206	K100
21															L207	W101
22															P212	I102
23															T216	F105
24															C219	K109
25															Y220	V110
26															P312	G112
27															L223	F113
28															V224	
29															V247	
30															I309	ALA
31															H310	GLN
32															N311	GLN
33															P312	GLN
34															ALA	ALA

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ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	122.54Å 122.54Å 158.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (15.00-2.70) 90.9 (15.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.180 , 0.200 0.182 , 0.199	Depositor DCC
R_{free} test set	1679 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5756	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PLM, BOG, RET, SO4, PC1

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	0.45	0/2865	0.91	5/3889 (0.1%)
1	B	0.47	1/2847 (0.0%)	0.94	7/3865 (0.2%)
All	All	0.46	1/5712 (0.0%)	0.92	12/7754 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	CYS	CA-C	5.89	1.59	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	244	LYS	N-CA-C	-7.53	104.59	114.31
1	B	119	GLY	N-CA-C	-7.08	103.92	112.49
1	B	245	GLU	N-CA-C	-6.33	105.41	113.01
1	A	229	ASN	N-CA-C	-6.18	104.54	111.28
1	A	66	GLN	N-CA-C	6.02	119.67	112.93

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	2780	0	2766	103	0
1	B	2762	0	2752	92	0
2	A	20	0	27	0	0
2	B	20	0	27	1	0
3	A	34	0	62	0	0
3	B	17	0	31	0	0
4	B	5	0	0	0	0
5	B	39	0	49	1	0
6	B	20	0	28	3	0
7	A	29	0	0	3	0
7	B	30	0	0	2	0
All	All	5756	0	5742	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 195 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:354:ILE:H	1:B:354:ILE:HD13	1.29	0.98
1:B:150:ARG:HD2	1:B:150:ARG:H	1.29	0.96
1:B:79:SER:HB2	1:B:121:MET:HE2	1.47	0.95
1:A:284:ALA:HB2	1:A:292:VAL:HG21	1.47	0.94
1:A:21:PRO:HA	1:A:24:ARG:HD3	1.48	0.93

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	348/448 (78%)	316 (91%)	32 (9%)	0	100	100
1	B	345/448 (77%)	316 (92%)	27 (8%)	2 (1%)	21	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	693/896 (77%)	632 (91%)	59 (8%)	2 (0%)	36 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLN
1	B	223	ILE

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	296/369 (80%)	285 (96%)	11 (4%)	30 59
1	B	295/369 (80%)	279 (95%)	16 (5%)	20 45
All	All	591/738 (80%)	564 (95%)	27 (5%)	24 51

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	LEU
1	B	117	ILE
1	B	247	ARG
1	B	102	ILE
1	B	123	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	70	ASN
1	B	135	ASN
1	B	328	GLN
1	B	242	ASN
1	A	242	ASN

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 ⓘ

8 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	$\# Z > 2$
4	SO4	B	449	-	4,4,4	0.38	0	6,6,6	0.10	0
3	PLM	A	1001	-	15,16,17	0.27	0	14,15,17	0.65	0
2	RET	B	1000	1	20,20,21	1.93	4 (20%)	27,27,28	1.14	4 (14%)
3	PLM	A	1004	-	15,16,17	0.28	0	14,15,17	0.63	0
5	PC1	B	1004	-	38,38,53	1.62	3 (7%)	41,43,61	0.98	1 (2%)
6	BOG	B	1005	-	20,20,20	1.84	8 (40%)	25,25,25	2.82	11 (44%)
3	PLM	B	1001	-	15,16,17	0.31	0	14,15,17	0.62	0
2	RET	A	1000	1	20,20,21	2.10	4 (20%)	27,27,28	1.20	4 (14%)

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	PLM	A	1001	-	-	5/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	B	1000	1	-	2/13/30/31	0/1/1/1
3	PLM	A	1004	-	-	6/14/14/15	-
5	PC1	B	1004	-	-	13/42/42/57	-
6	BOG	B	1005	-	-	4/11/31/31	0/1/1/1
3	PLM	B	1001	-	-	8/14/14/15	-
2	RET	A	1000	1	-	2/13/30/31	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	PC1	O21-C21	7.27	1.54	1.34
2	A	1000	RET	C14-C13	6.42	1.38	1.33
2	B	1000	RET	C14-C13	5.98	1.37	1.33
2	A	1000	RET	C1-C6	5.01	1.60	1.53
2	B	1000	RET	C1-C6	4.14	1.59	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1005	BOG	C1'-O1-C1	-8.12	99.80	113.68
6	B	1005	BOG	O1-C1-C2	-4.90	100.83	108.27
6	B	1005	BOG	C1-C2-C3	-4.32	100.93	110.01
6	B	1005	BOG	O5-C5-C4	-4.28	101.98	109.70
6	B	1005	BOG	O3-C3-C2	-3.68	101.71	110.38

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	PLM	C1-C2-C3-C4
5	B	1004	PC1	C1-O11-P-O12
5	B	1004	PC1	C1-O11-P-O14
5	B	1004	PC1	C1-O11-P-O13
5	B	1004	PC1	C32-C31-O31-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

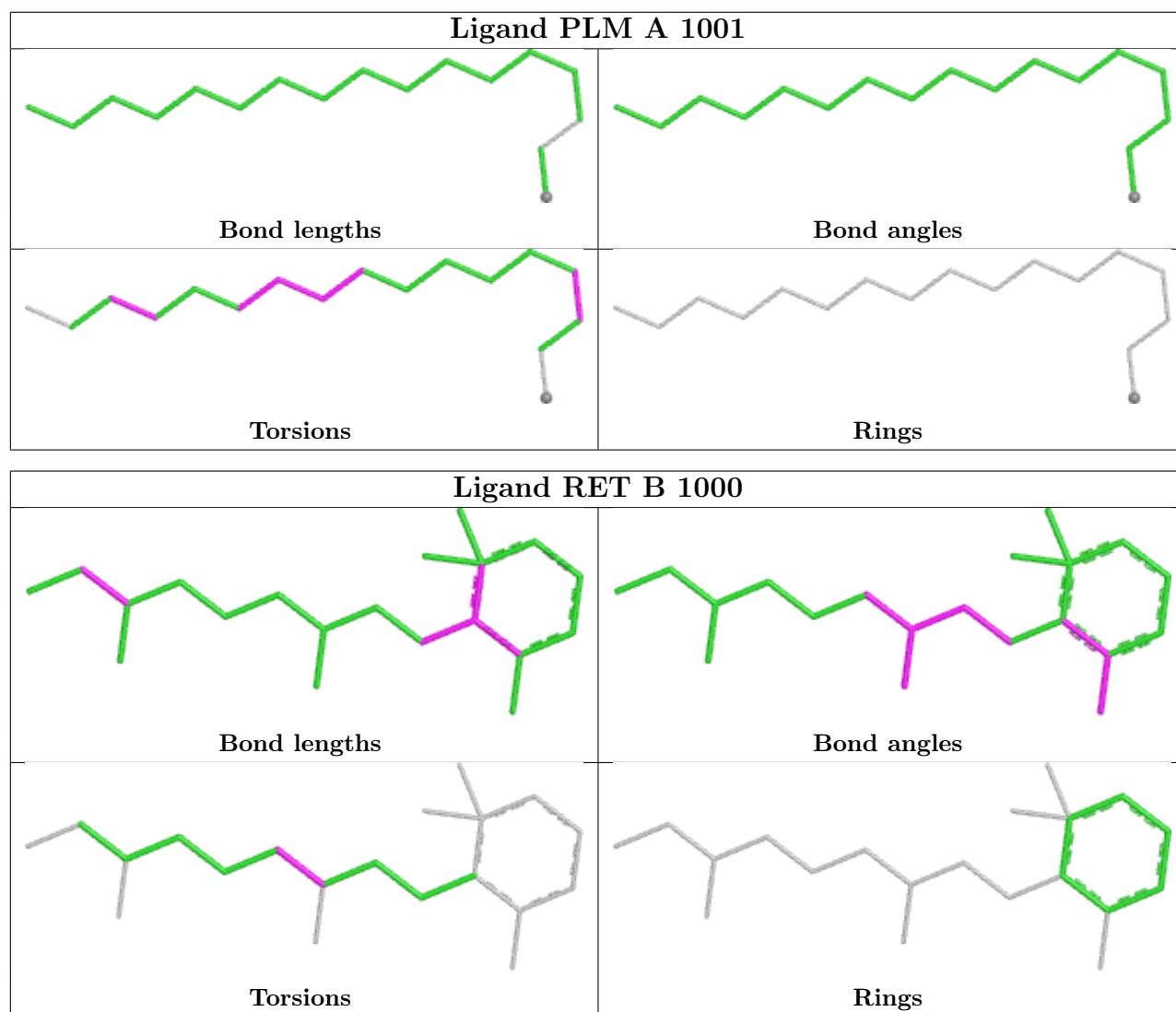
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	RET	1	0

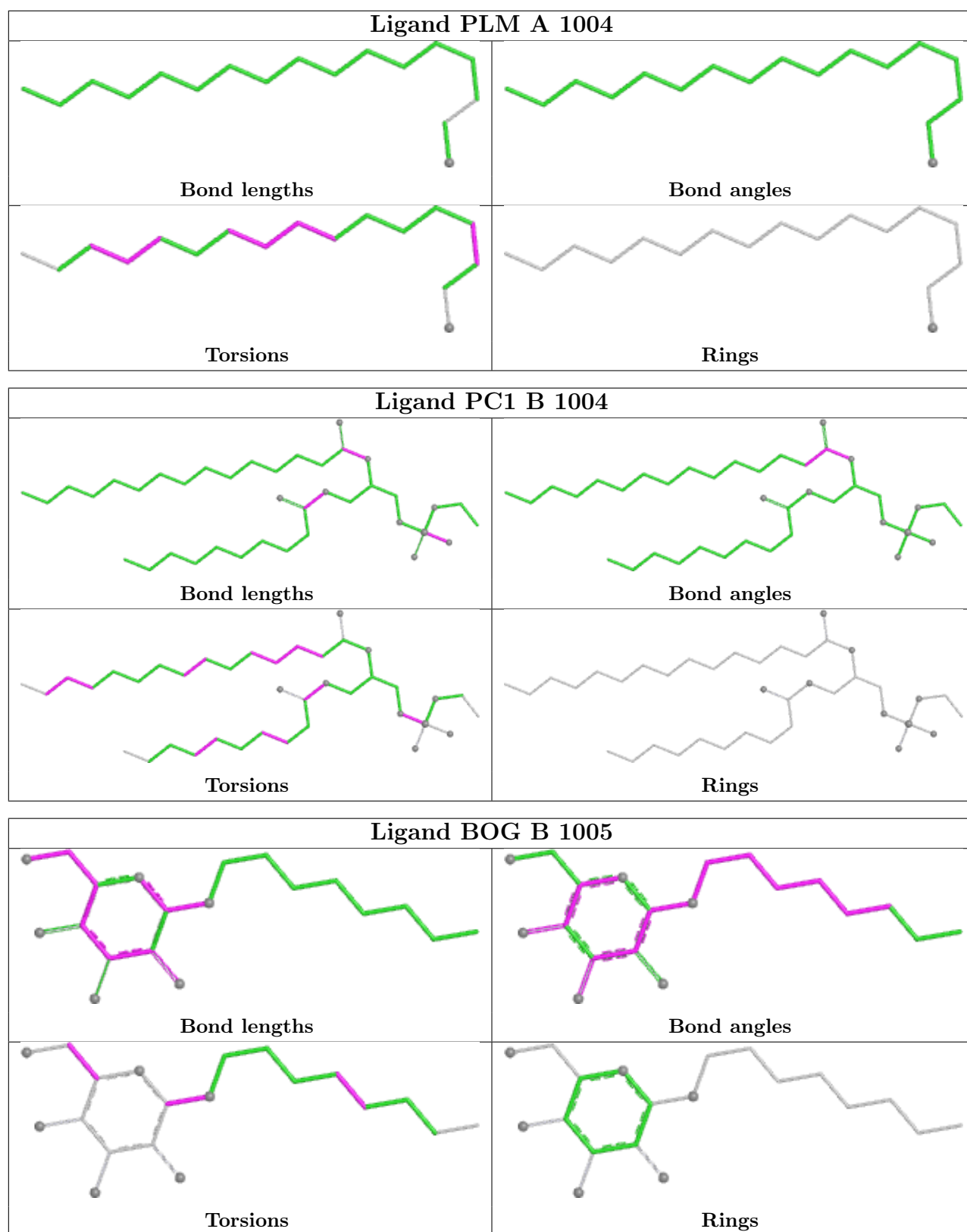
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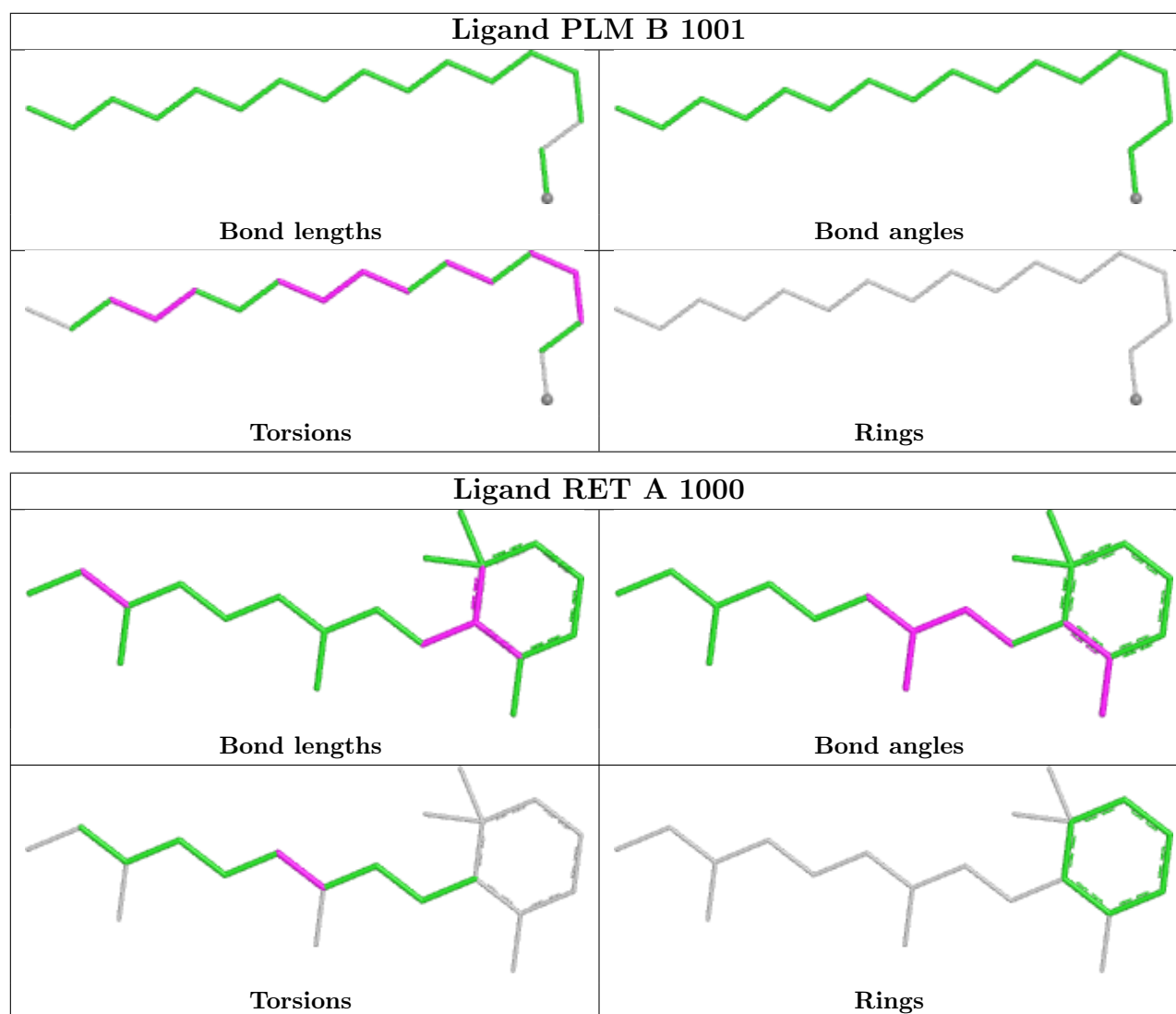
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	PC1	1	0
6	B	1005	BOG	3	0

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	350/448 (78%)	-0.41	4 (1%) 78 76	28, 51, 114, 136	0
1	B	347/448 (77%)	-0.58	3 (0%) 81 80	27, 44, 96, 118	0
All	All	697/896 (77%)	-0.49	7 (1%) 79 78	27, 48, 105, 136	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	4.4
1	A	241	LEU	4.2
1	A	239	LYS	3.8
1	B	239	LYS	3.1
1	A	356	ALA	3.0

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

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

6.3 Carbohydrates [i](#)

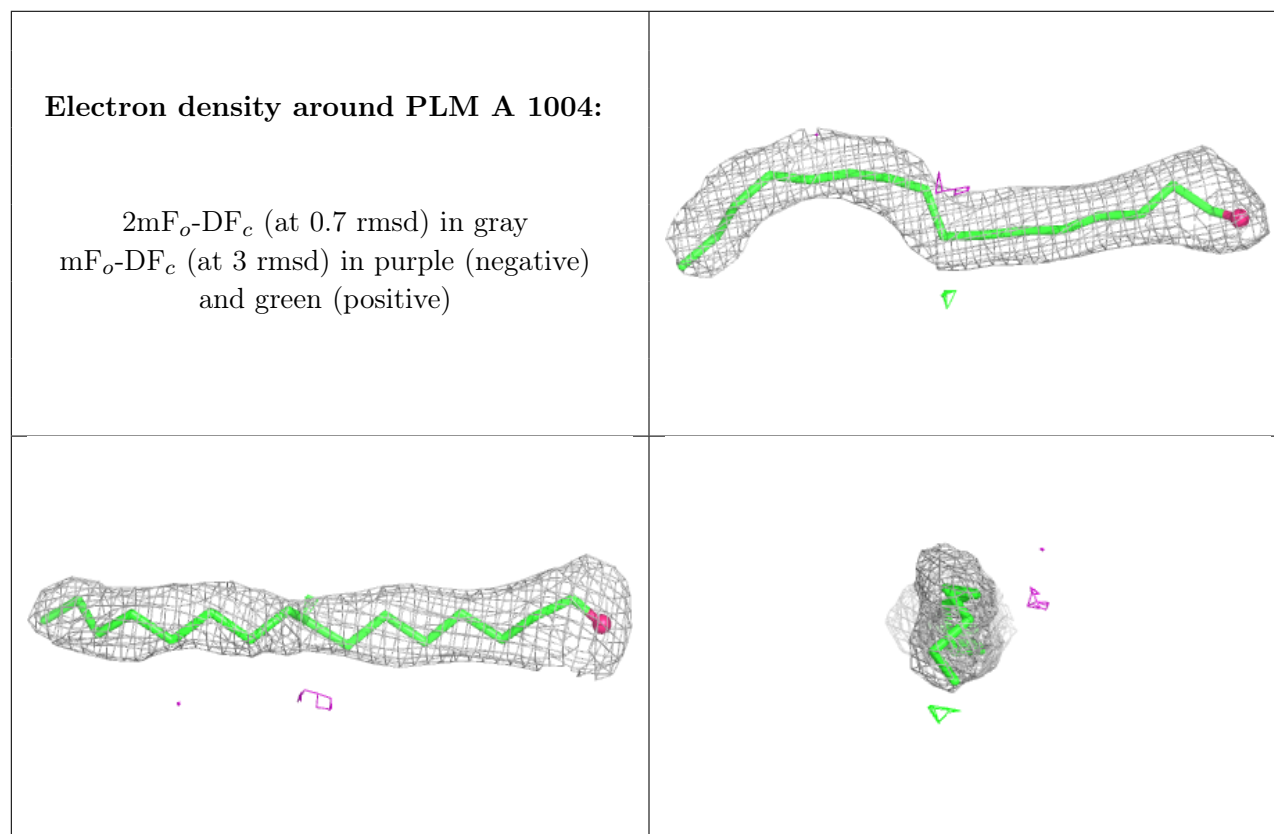
There are no oligosaccharides in this entry.

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.

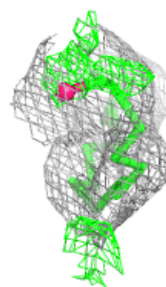
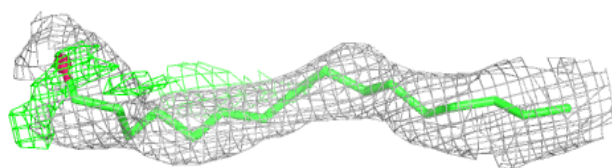
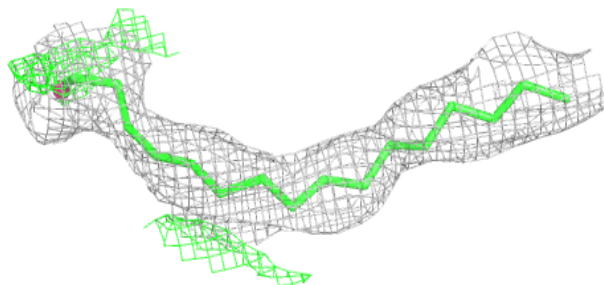
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PLM	A	1004	17/18	0.88	0.12	67,72,76,76	0
3	PLM	B	1001	17/18	0.89	0.12	45,65,68,69	0
5	PC1	B	1004	39/54	0.89	0.12	41,66,112,113	0
6	BOG	B	1005	20/20	0.89	0.11	71,104,106,106	0
3	PLM	A	1001	17/18	0.90	0.10	49,58,64,65	0
4	SO4	B	449	5/5	0.90	0.08	110,110,111,111	0
2	RET	A	1000	20/21	0.93	0.09	43,51,57,57	0
2	RET	B	1000	20/21	0.97	0.06	30,38,43,44	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.

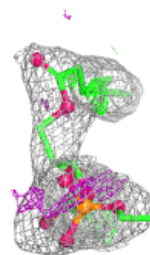
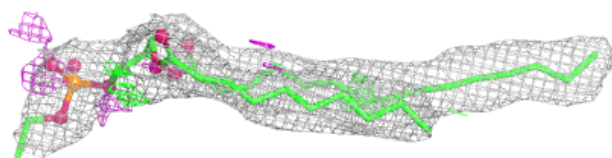
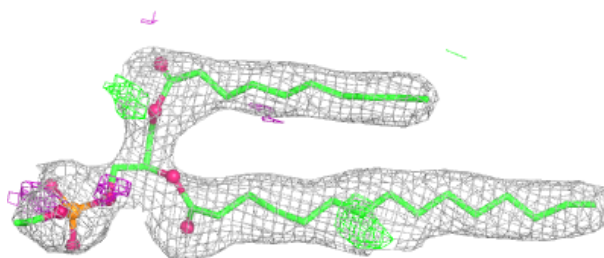


Electron density around PLM B 1001:

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

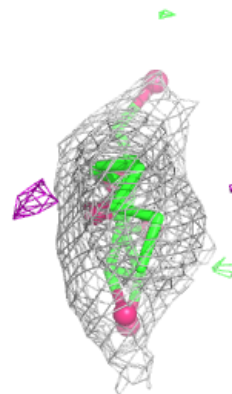
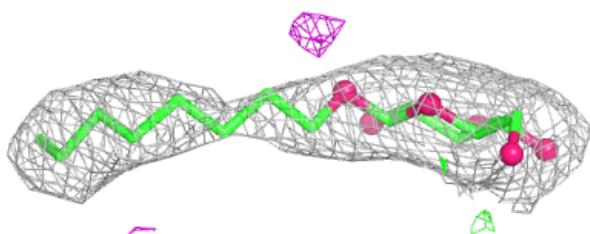
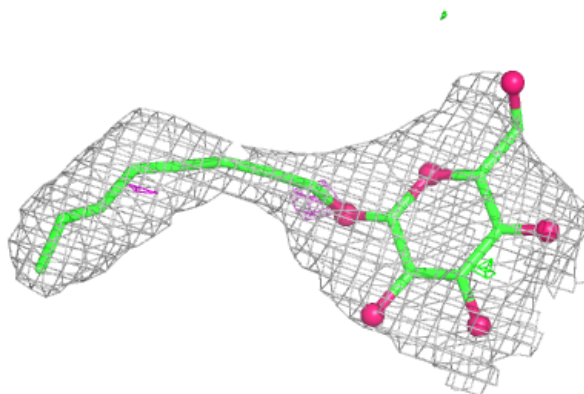
**Electron density around PC1 B 1004:**

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

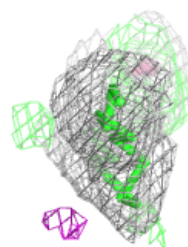
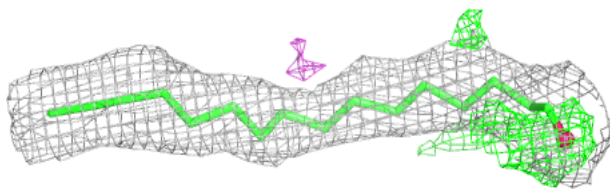
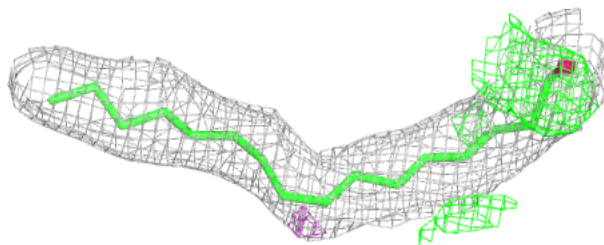


Electron density around BOG B 1005:

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

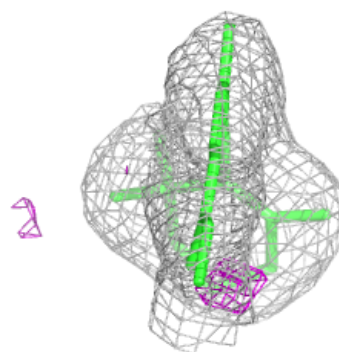
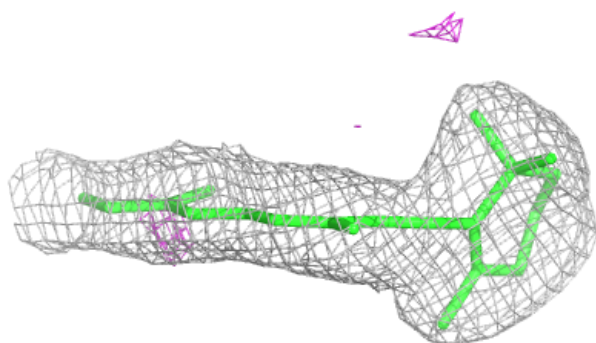
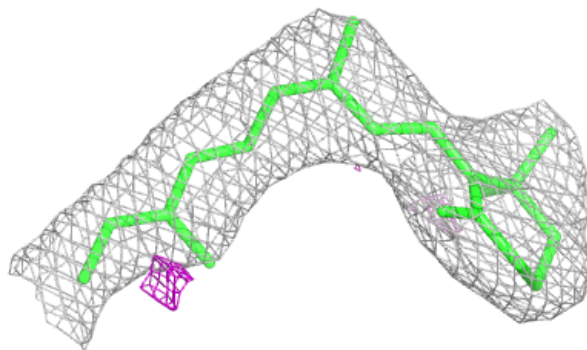
**Electron density around PLM A 1001:**

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

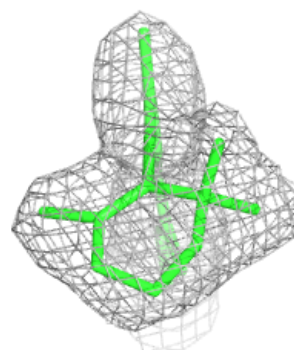
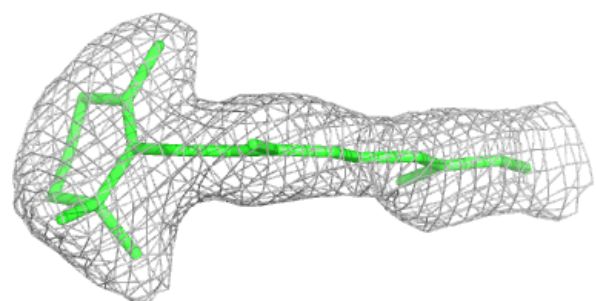
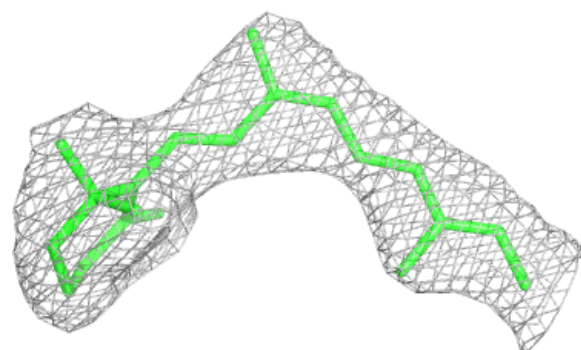


Electron density around RET A 1000:

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

**Electron density around RET B 1000:**

$2mF_o-DF_c$ (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.