



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:25 PM BST

PDB ID : 3AYM  
Title : Crystal structure of the batho intermediate of squid rhodopsin  
Authors : Murakami, M.; Kouyama, T.  
Deposited on : 2011-05-09  
Resolution : 2.80 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](mailto: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.

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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

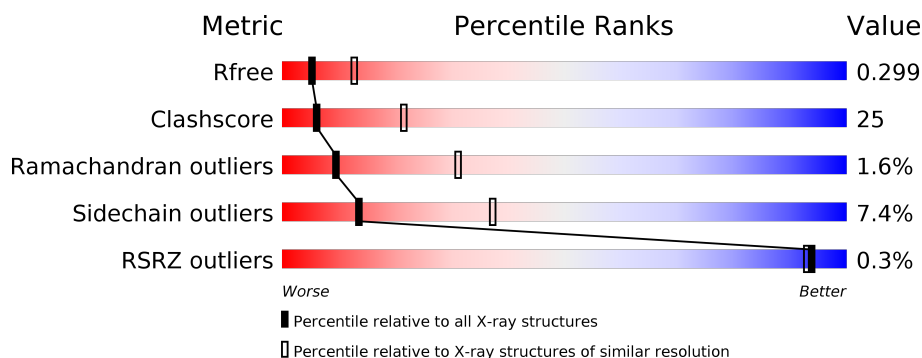
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

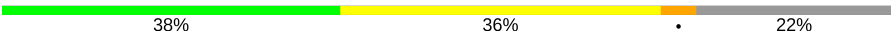
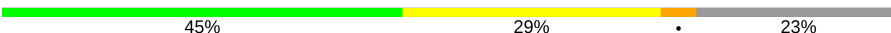
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	
1	B	448	

## 2 Entry composition [i](#)

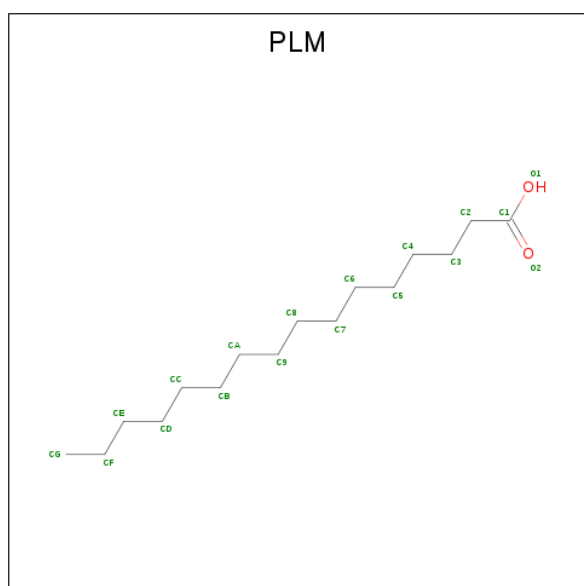
There are 7 unique types of molecules in this entry. The entry contains 5742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

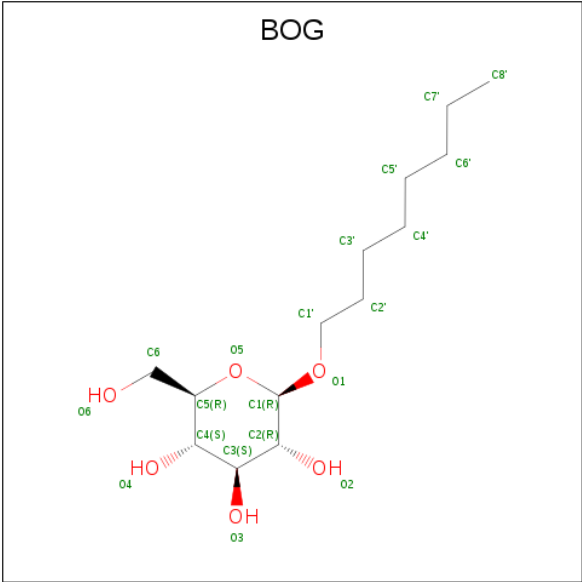
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2780	1838	443	473	26			
1	B	347	Total	C	N	O	S	0	0	0
			2762	1828	440	468	26			

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



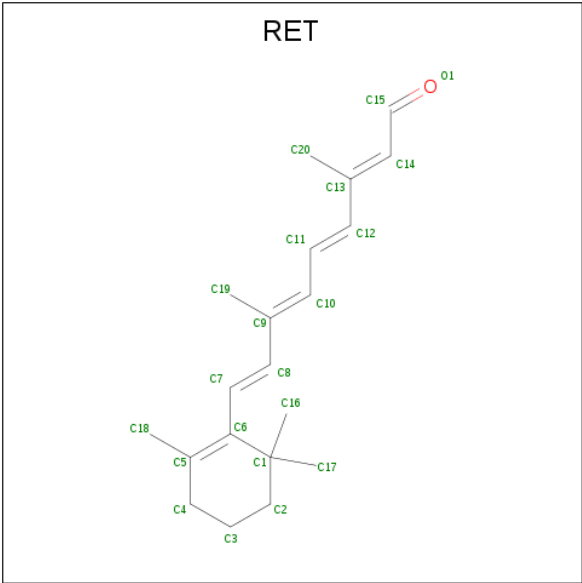
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



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

- Molecule 4 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



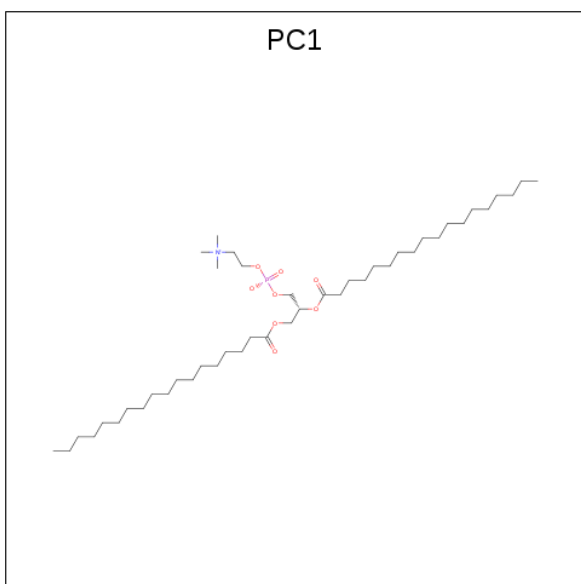
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			20	20		
4	B	1	Total	C	0	0
			20	20		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



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

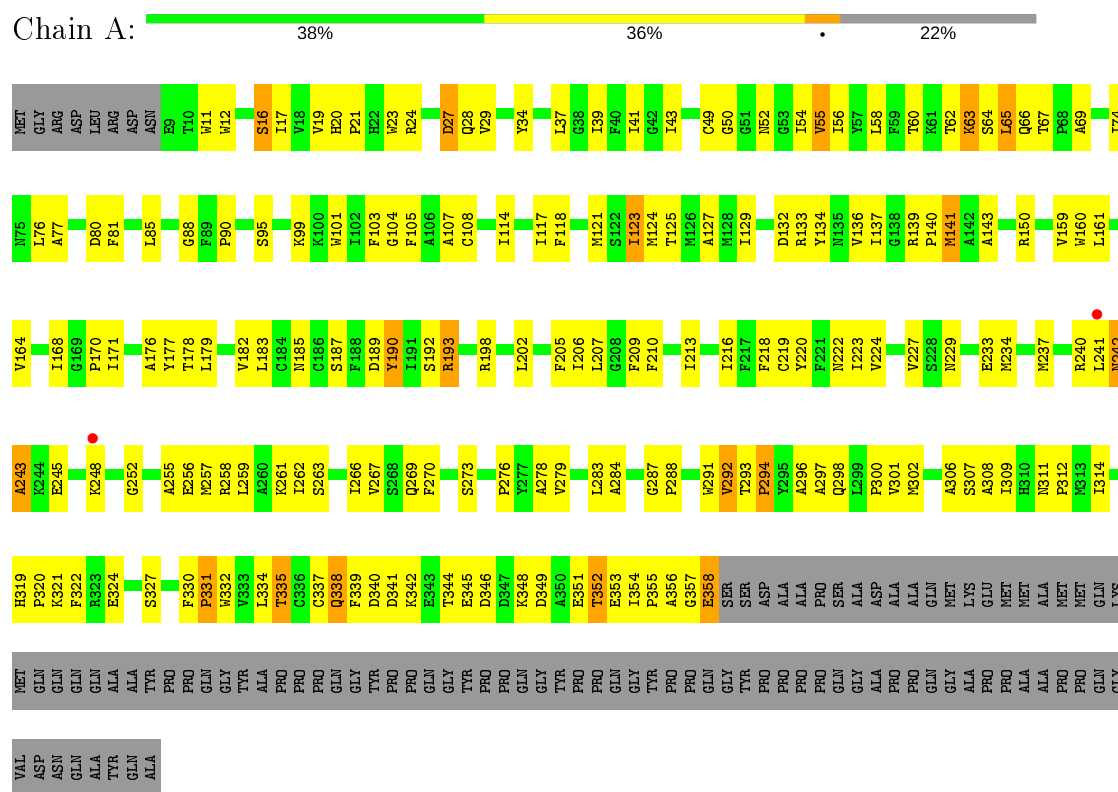
- Molecule 7 is water.

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

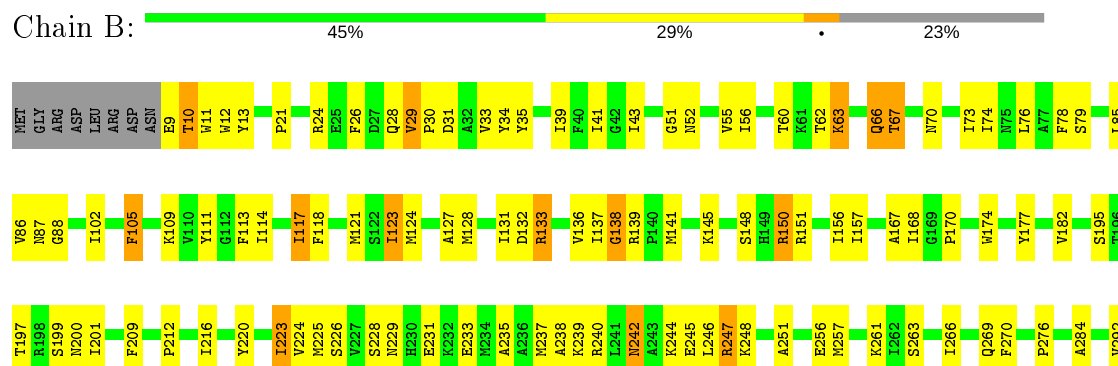
### 3 Residue-property plots

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: Rhodopsin



#### • Molecule 1: Rhodopsin



SER	GLN	T293
	GLY	P294
ALA	ALA	T295
	PRO	A296
PRO	PRO	A297
	GLN	Q298
GLY	GLY	L299
	ALA	P300
PRO	PRO	V301
	PRO	X302
MET	ALA	K305
	PRO	A306
MET	PRO	L309
	GLN	H310
GLN	GLY	N311
	VAL	P312
ASP	ASP	L316
	ASN	V317
ASN	GLN	S318
	GLN	H319
TYR	TYR	P320
	GLN	R321
ALA	ALA	F322
	ALA	R323
GLN	GLY	E324
	GLY	A325
TYR	TYR	T326
	ALA	S327
PRO	PRO	Q328
	GLN	T329
GLN	GLN	F330
	GLY	P331
TYR	TYR	T335
	PRO	C336
PRO	PRO	C337
	GLN	Q338
GLY	GLY	F339
	TYR	D340
PRO	PRO	D341
	GLN	K342
GLY	GLY	D349
	TYR	A350
PRO	PRO	P353
	GLN	T354
GLY	GLY	P355
	PRO	ALA
PRO	PRO	GLY
	GLY	GLY
GLN	GLN	GLU
	GLY	SER
TYR	TYR	ASP
	PRO	ALA
PRO	PRO	ALA
	PRO	PRO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.36Å 122.36Å 158.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 44.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	67.7 (15.00-2.80) 67.6 (44.02-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.56 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.295 , 0.345 0.298 , 0.299	Depositor DCC
$R_{free}$ test set	1088 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.088 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PLM, PC1, SO4, RET, BOG

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	0.73	0/2865	0.73	1/3889 (0.0%)
1	B	0.75	0/2847	0.74	0/3865
All	All	0.74	0/5712	0.73	1/7754 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CG-OD2	-9.35	109.88	118.30

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	2780	0	2766	161	0
1	B	2762	0	2752	119	0
2	A	17	0	31	0	0
3	A	20	0	28	2	0
3	B	20	0	28	4	0
4	A	20	0	27	1	0
4	B	20	0	27	2	0
5	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	39	0	49	2	0
7	A	29	0	0	7	0
7	B	30	0	0	2	0
All	All	5742	0	5708	280	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 25.

The worst 5 of 280 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:21:PRO:HA	1:A:24:ARG:HD3	1.30	1.11
1:B:67:THR:HG21	3:B:1005:BOG:H5	1.43	1.00
1:A:20:HIS:ND1	1:A:21:PRO:HD2	1.81	0.94
1:A:332:TRP:O	1:A:335:THR:HG23	1.67	0.93
1:B:150:ARG:HD2	1:B:150:ARG:H	1.32	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%)	308 (88%)	33 (10%)	7 (2%)	7	24
1	B	345/448 (77%)	317 (92%)	24 (7%)	4 (1%)	13	39
All	All	693/896 (77%)	625 (90%)	57 (8%)	11 (2%)	9	31

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	243	ALA
1	A	292	VAL
1	B	138	GLY
1	A	352	THR

### 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%)	275 (93%)	21 (7%)	14	39
1	B	295/369 (80%)	272 (92%)	23 (8%)	12	35
All	All	591/738 (80%)	547 (93%)	44 (7%)	13	37

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ASP
1	B	66	GLN
1	B	335	THR
1	A	358	GLU
1	B	29	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	328	GLN
1	B	222	ASN
1	A	269	GLN
1	B	70	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

7 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	RET	A	1000	1	20,20,21	1.82	2 (10%)	27,27,28	1.76	5 (18%)
2	PLM	A	1001	-	16,16,17	0.35	0	15,15,17	0.67	0
6	PC1	B	1004	-	38,38,53	1.90	3 (7%)	41,43,61	1.00	2 (4%)
3	BOG	B	1005	-	20,20,20	1.76	5 (25%)	25,25,25	2.69	10 (40%)
3	BOG	A	1005	-	20,20,20	1.73	4 (20%)	25,25,25	2.65	9 (36%)
5	SO4	B	449	-	4,4,4	0.33	0	6,6,6	0.25	0
4	RET	B	1000	1	20,20,21	1.97	5 (25%)	27,27,28	2.05	8 (29%)

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
4	RET	A	1000	1	-	1/13/30/31	0/1/1/1
2	PLM	A	1001	-	-	5/13/14/15	-
6	PC1	B	1004	-	-	16/42/42/57	-
3	BOG	B	1005	-	-	4/11/31/31	0/1/1/1
3	BOG	A	1005	-	-	8/11/31/31	0/1/1/1
4	RET	B	1000	1	-	5/13/30/31	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)
6	B	1004	PC1	O21-C21	8.43	1.58	1.34
4	A	1000	RET	C1-C6	6.25	1.62	1.53
4	B	1000	RET	C1-C6	5.26	1.61	1.53
6	B	1004	PC1	O31-C31	5.17	1.48	1.33
4	A	1000	RET	C2-C3	-3.96	1.42	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1005	BOG	C1'-O1-C1	-8.61	99.56	113.84
3	B	1005	BOG	C1'-O1-C1	-8.14	100.34	113.84
4	B	1000	RET	C8-C9-C10	-6.31	109.25	118.94
4	A	1000	RET	C8-C9-C10	-5.15	111.04	118.94
3	B	1005	BOG	C1-C2-C3	-4.45	100.73	110.00

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1004	PC1	C1-O11-P-O12
6	B	1004	PC1	C1-O11-P-O14
3	A	1005	BOG	O5-C5-C6-O6
3	A	1005	BOG	C4-C5-C6-O6
3	A	1005	BOG	O1-C1'-C2'-C3'

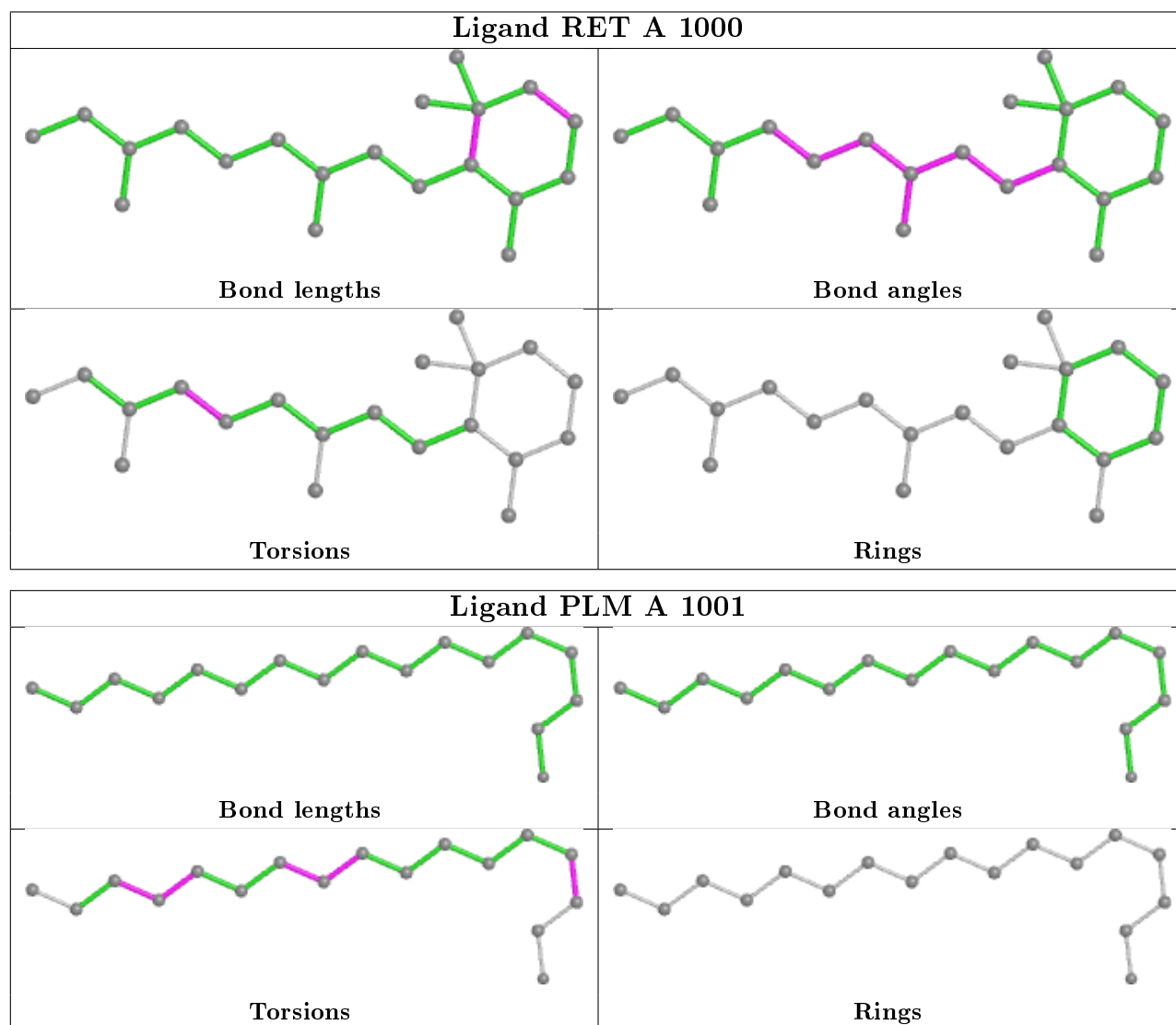
There are no ring outliers.

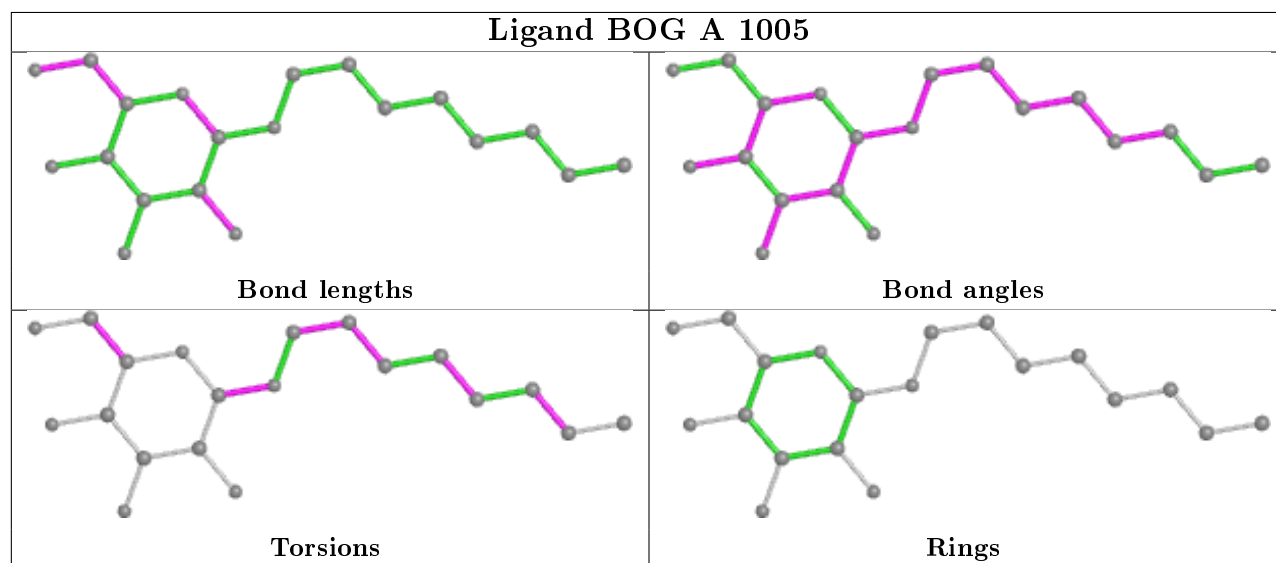
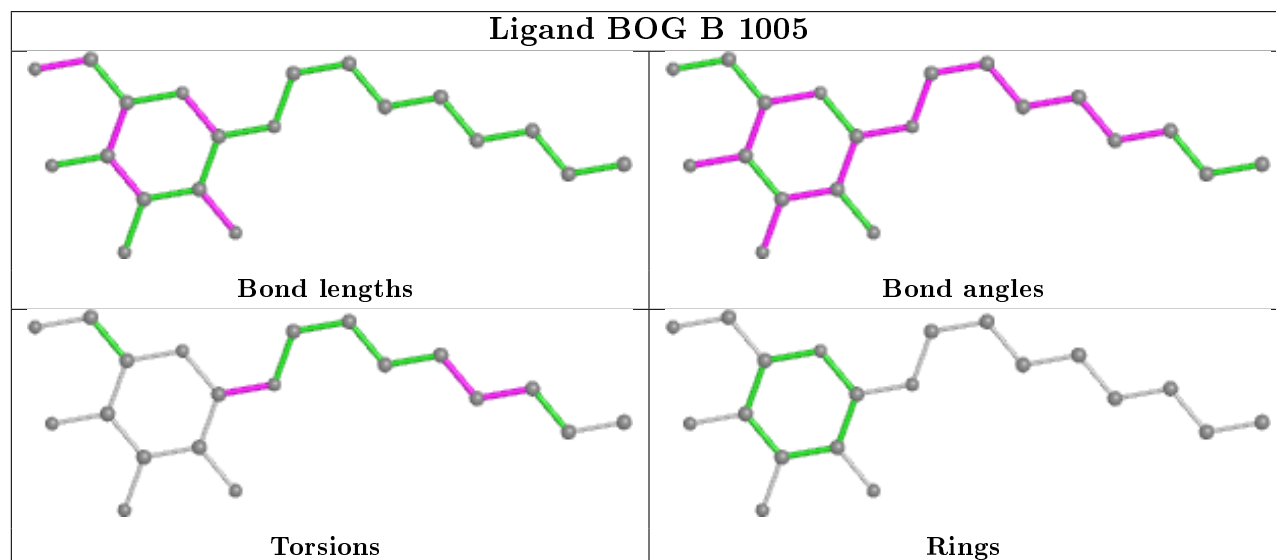
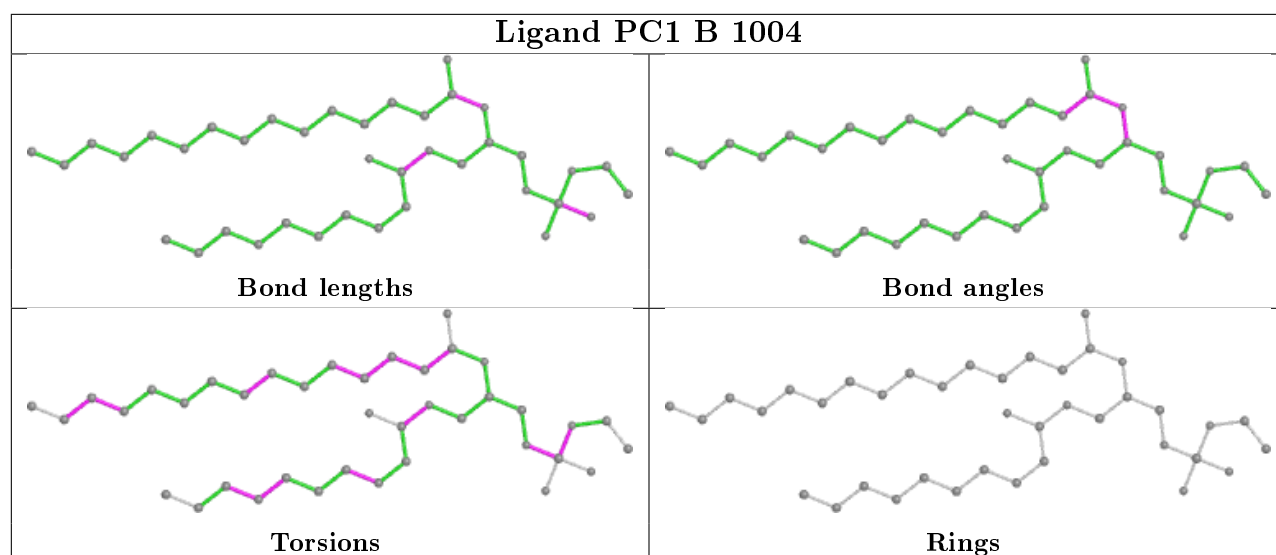
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	RET	1	0
6	B	1004	PC1	2	0
3	B	1005	BOG	4	0
3	A	1005	BOG	2	0
4	B	1000	RET	2	0

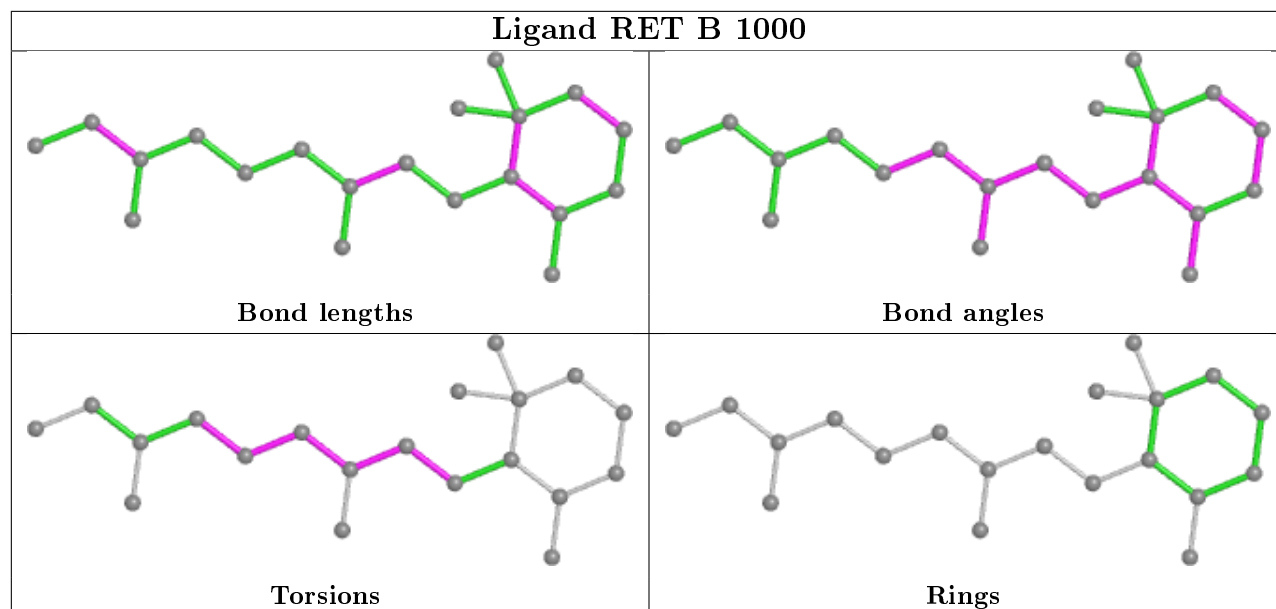
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	350/448 (78%)	-0.21	2 (0%) 89 86	28, 54, 115, 135	0
1	B	347/448 (77%)	-0.20	0 100 100	29, 49, 95, 124	0
All	All	697/896 (77%)	-0.20	2 (0%) 94 93	28, 52, 108, 135	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	LYS	2.2
1	A	241	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

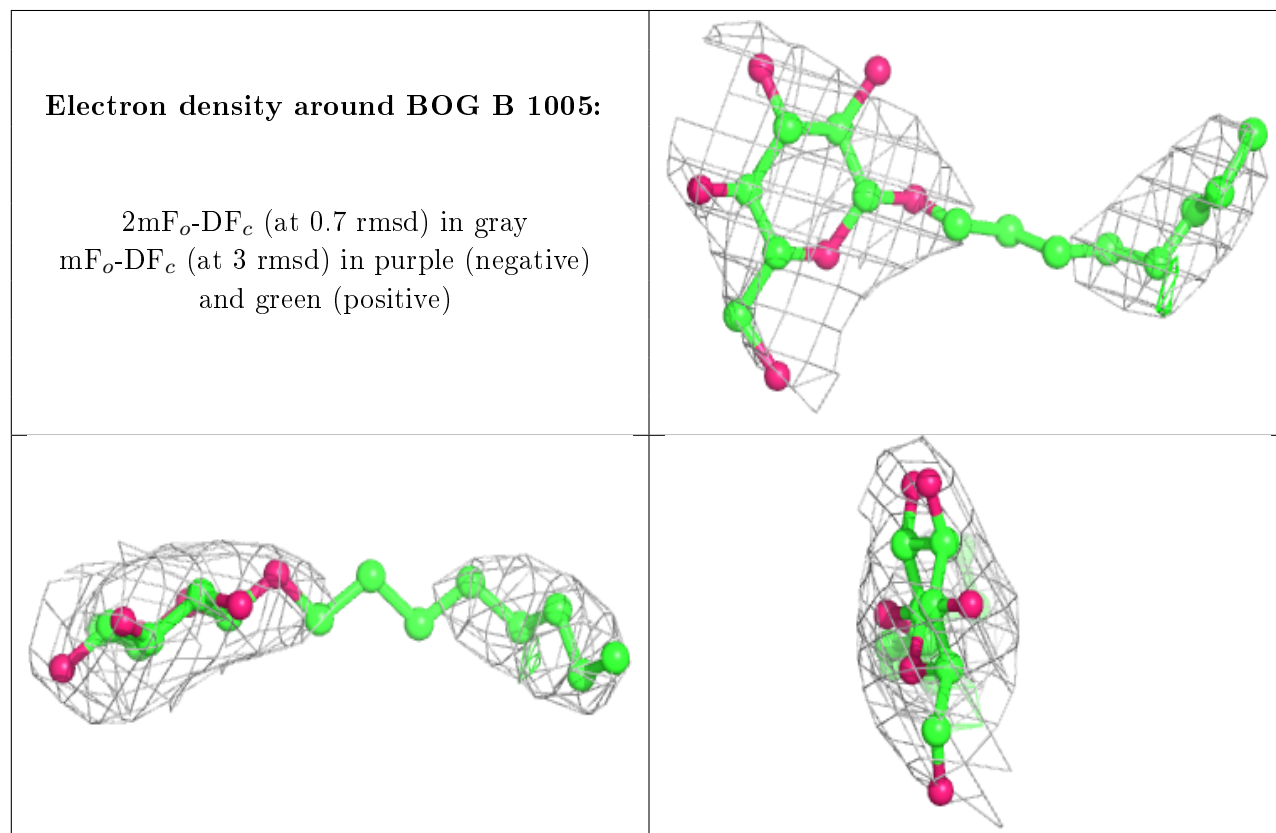
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BOG	B	1005	20/20	0.87	0.37	70,109,111,112	0
6	PC1	B	1004	39/54	0.90	0.31	44,65,119,120	0
2	PLM	A	1001	17/18	0.91	0.39	45,66,73,74	0

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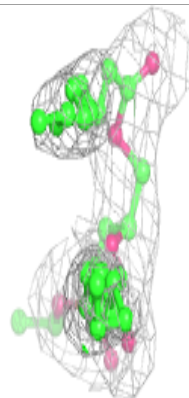
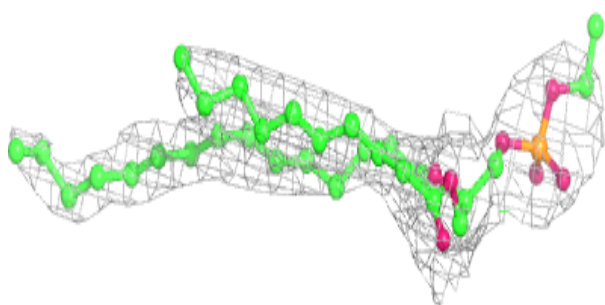
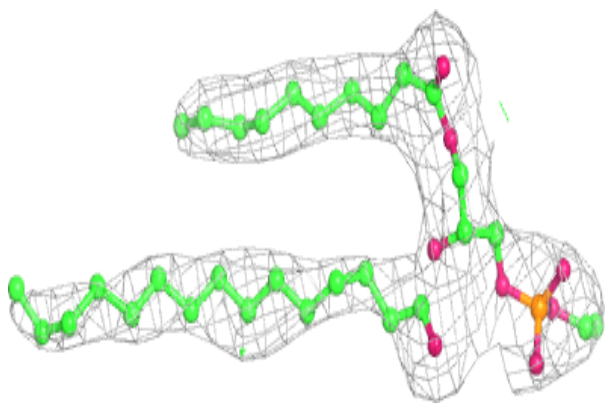
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BOG	A	1005	20/20	0.91	0.24	50,92,97,100	0
5	SO4	B	449	5/5	0.96	0.16	85,86,87,88	0
4	RET	A	1000	20/21	0.98	0.23	30,45,51,53	0
4	RET	B	1000	20/21	0.98	0.22	20,24,31,37	0

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.

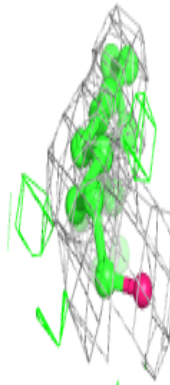
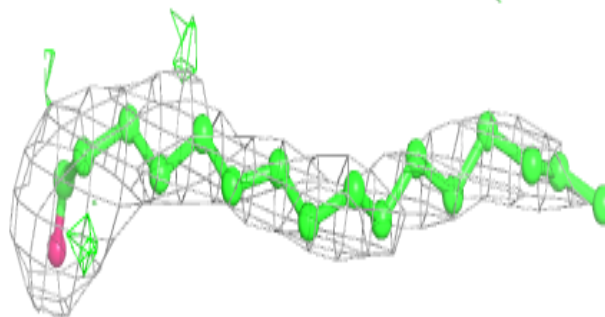
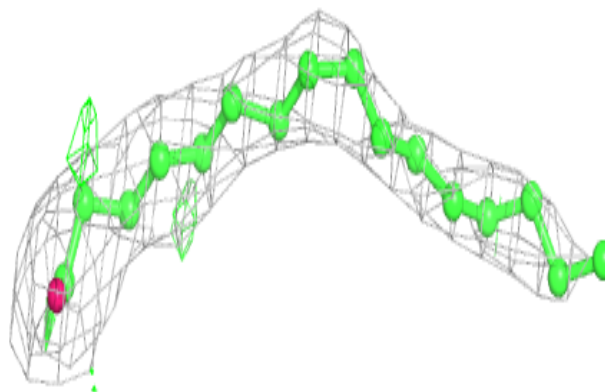


**Electron density around PC1 B 1004:**

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

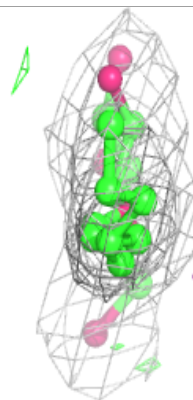
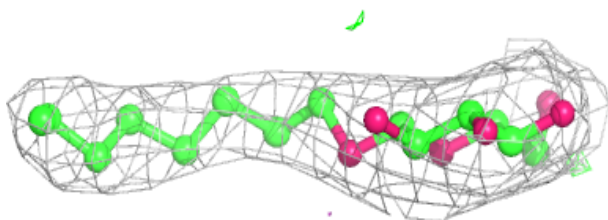
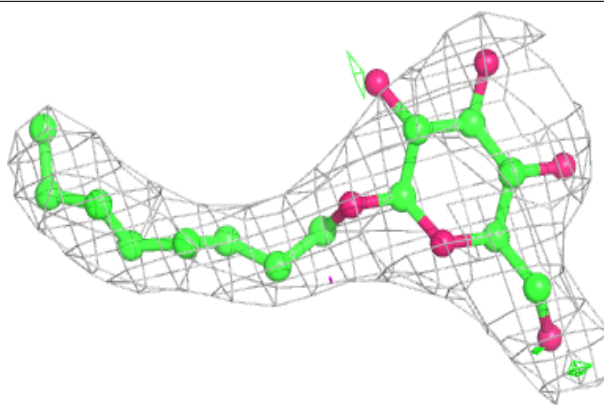
**Electron density around PLM A 1001:**

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

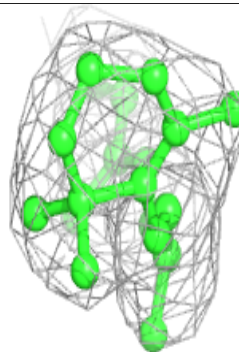
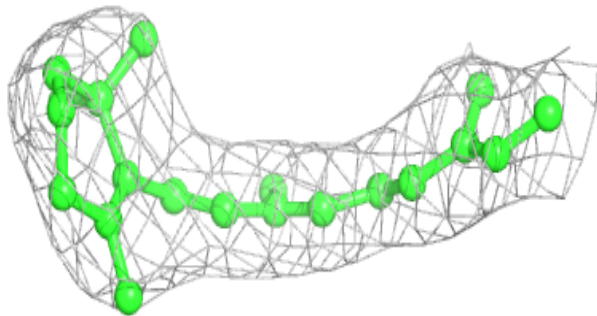
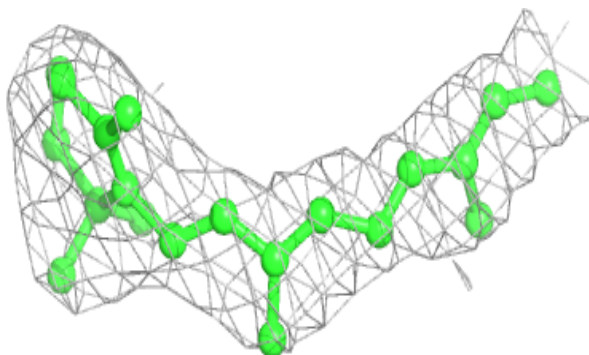


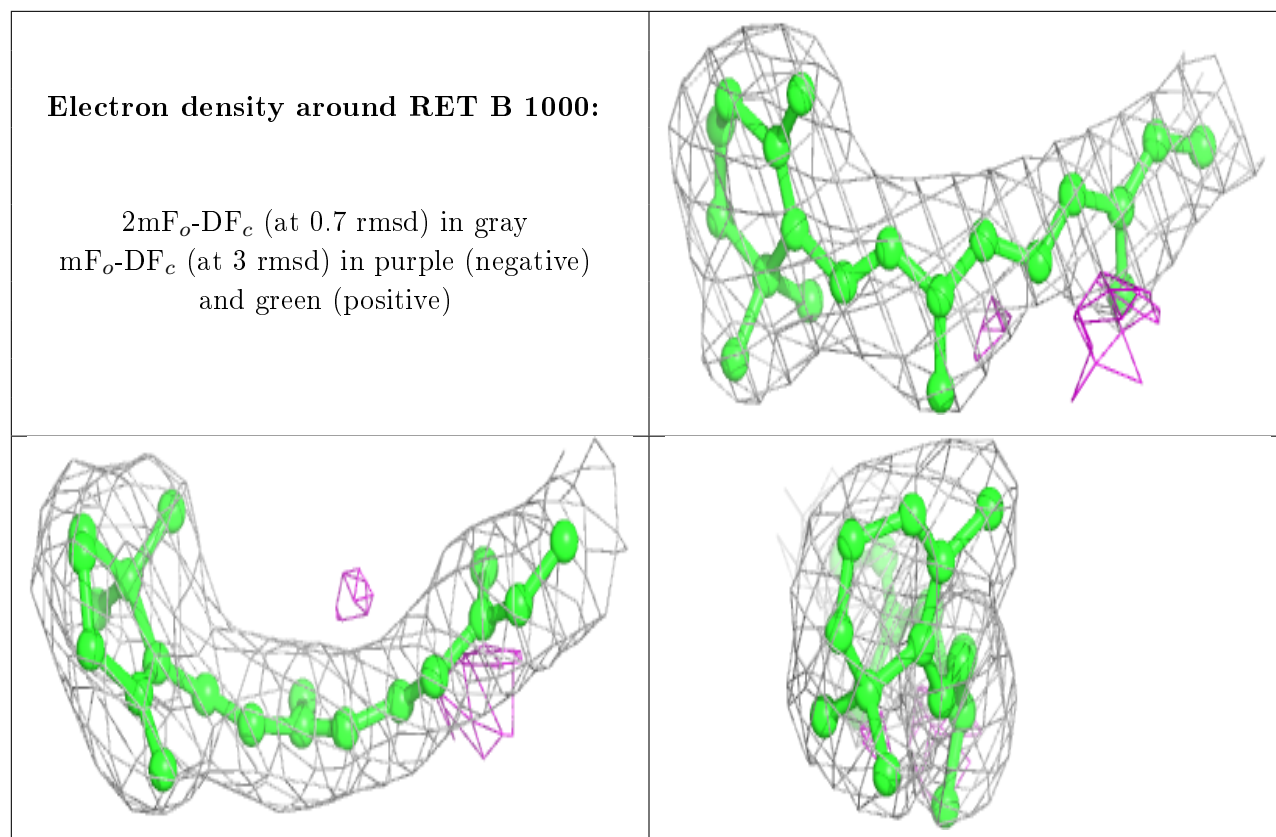
**Electron density around BOG A 1005:**

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

**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.