



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 08:48 AM BST

PDB ID : 2J4Y  
Title : Crystal structure of a rhodopsin stabilizing mutant expressed in mammalian cells  
Authors : Standfuss, J.; Xie, G.; Edwards, P.C.; Burghammer, M.; Oprian, D.D.; Schertler, G.F.X.  
Deposited on : 2006-09-07  
Resolution : 3.40 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

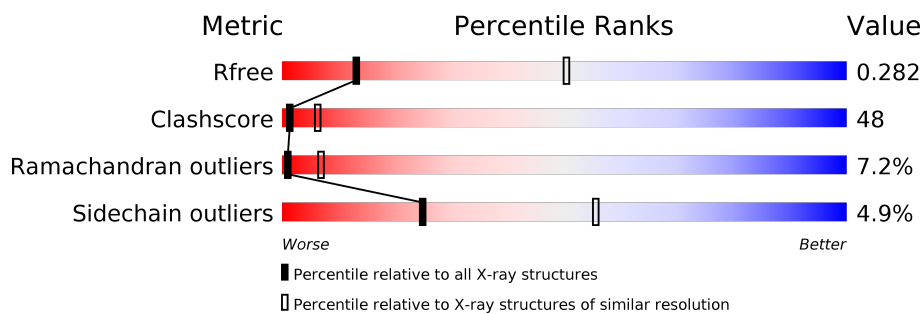
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5252 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.

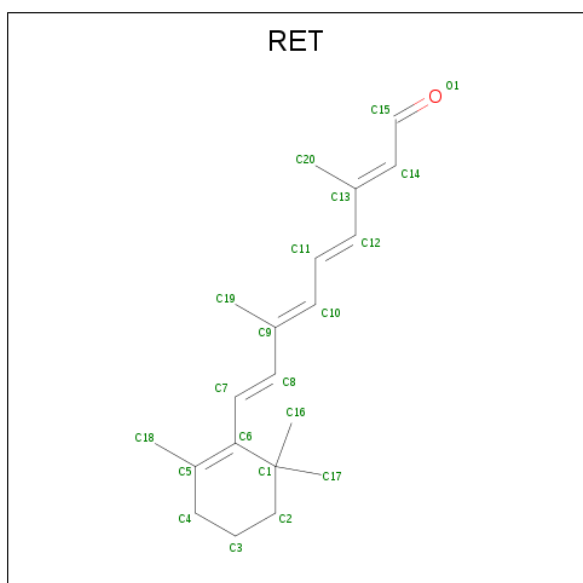
- Molecule 1 is a protein called RHODOPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	1
			2592	1725	400	439	28			
1	B	328	Total	C	N	O	S	0	0	1
			2592	1725	400	439	28			

There are 6 discrepancies between the modelled and reference sequences:

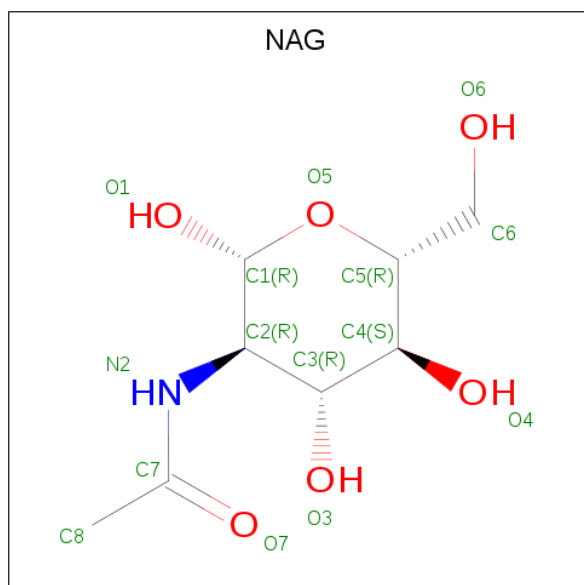
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P02699
A	2	CYS	ASN	engineered mutation	UNP P02699
A	282	CYS	ASP	engineered mutation	UNP P02699
B	0	ACE	-	acetylation	UNP P02699
B	2	CYS	ASN	engineered mutation	UNP P02699
B	282	CYS	ASP	engineered mutation	UNP P02699

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.30 Å   109.30 Å   77.70 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 3.40 44.70 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-3.40) 95.9 (44.70-3.40)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.40 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.290 , 0.330 0.259 , 0.282	Depositor DCC
$R_{free}$ test set	407 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 1.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.340 for -h,-k,l 0.256 for h,-h-k,-l 0.258 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: RET, NAG, ACE

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	0.62	0/2672	0.77	0/3641
1	B	0.62	0/2672	0.77	0/3641
All	All	0.62	0/5344	0.77	0/7282

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	TYR	Sidechain

### 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	2592	0	2567	274	0
1	B	2592	0	2567	268	0
2	A	20	0	27	0	0
2	B	20	0	27	1	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
All	All	5252	0	5214	507	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 48.

The worst 5 of 507 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:90:GLY:O	1:A:94:THR:HG23	1.52	1.08
1:A:228:PHE:CE2	1:A:233:ALA:HB2	1.91	1.05
1:B:228:PHE:CE2	1:B:233:ALA:HB2	1.93	1.03
1:A:143:MET:HG2	1:A:144:SER:H	1.22	1.03
1:B:90:GLY:O	1:B:94:THR:HG23	1.58	1.01

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	326/349 (93%)	241 (74%)	61 (19%)	24 (7%)	1	7
1	B	326/349 (93%)	240 (74%)	63 (19%)	23 (7%)	1	7
All	All	652/698 (93%)	481 (74%)	124 (19%)	47 (7%)	1	7

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	176	SER
1	A	177	ARG
1	A	195	HIS
1	A	230	VAL

### 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	278/296 (94%)	265 (95%)	13 (5%)	26	57
1	B	278/296 (94%)	264 (95%)	14 (5%)	24	54
All	All	556/592 (94%)	529 (95%)	27 (5%)	25	55

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

Mol	Chain	Res	Type
1	A	266	LEU
1	B	95	LEU
1	B	255	ILE
1	B	39	MET
1	A	110	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	312	GLN
1	B	73	ASN
1	B	312	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	NAG	B	1327	1	14,14,15	2.48	5 (35%)	17,19,21	1.54	4 (23%)
2	RET	A	1296	1	20,20,21	1.42	2 (10%)	27,27,28	1.69	5 (18%)
2	RET	B	1296	1	20,20,21	1.35	2 (10%)	27,27,28	1.72	7 (25%)
3	NAG	A	1327	1	14,14,15	2.41	5 (35%)	17,19,21	1.51	3 (17%)

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	NAG	B	1327	1	-	4/6/23/26	0/1/1/1
2	RET	A	1296	1	-	1/13/30/31	0/1/1/1
2	RET	B	1296	1	-	1/13/30/31	0/1/1/1
3	NAG	A	1327	1	-	4/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1327	NAG	C1-C2	6.28	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1327	NAG	C1-C2	5.25	1.60	1.52
3	B	1327	NAG	O5-C1	4.26	1.50	1.43
3	A	1327	NAG	C3-C2	4.23	1.61	1.52
3	A	1327	NAG	O5-C1	3.71	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1296	RET	C20-C13-C12	4.06	124.48	118.08
2	A	1296	RET	C8-C9-C10	-3.77	113.16	118.94
3	B	1327	NAG	O5-C5-C6	3.70	113.00	107.20
2	B	1296	RET	C8-C9-C10	-3.56	113.48	118.94
2	B	1296	RET	C20-C13-C12	3.55	123.68	118.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1327	NAG	O5-C5-C6-O6
3	B	1327	NAG	C4-C5-C6-O6
3	A	1327	NAG	C4-C5-C6-O6
3	A	1327	NAG	C1-C2-N2-C7
3	B	1327	NAG	C1-C2-N2-C7

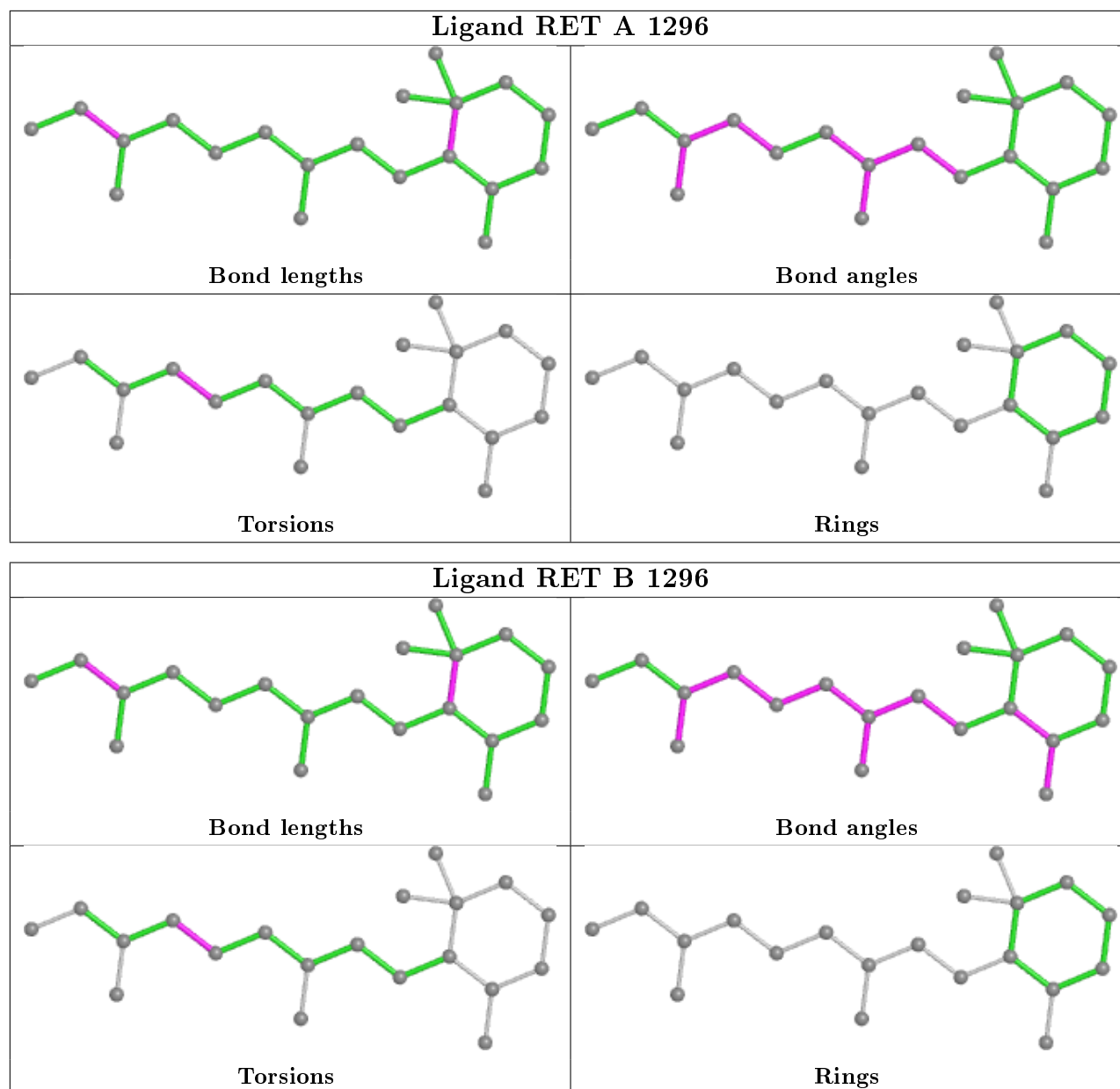
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1327	NAG	1	0
2	B	1296	RET	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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

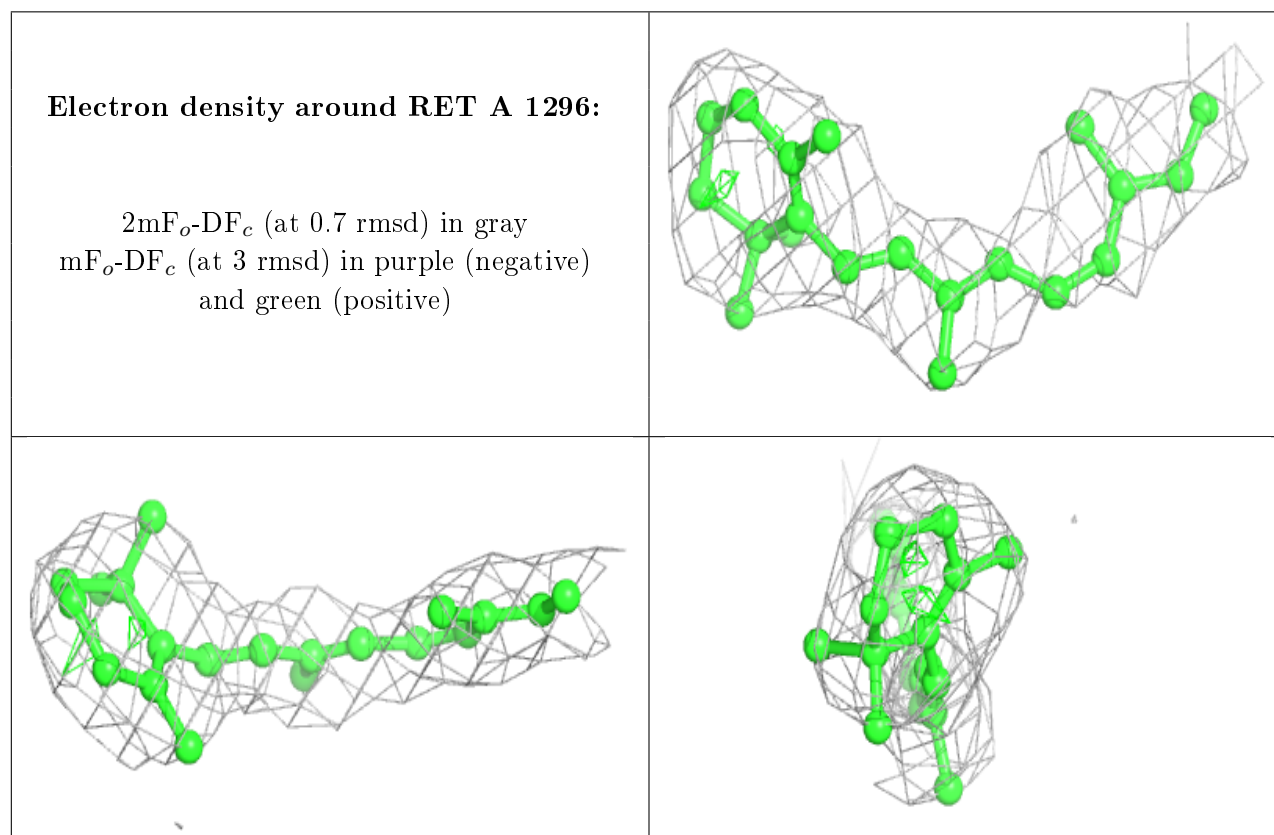
### 6.3 Carbohydrates ⓘ

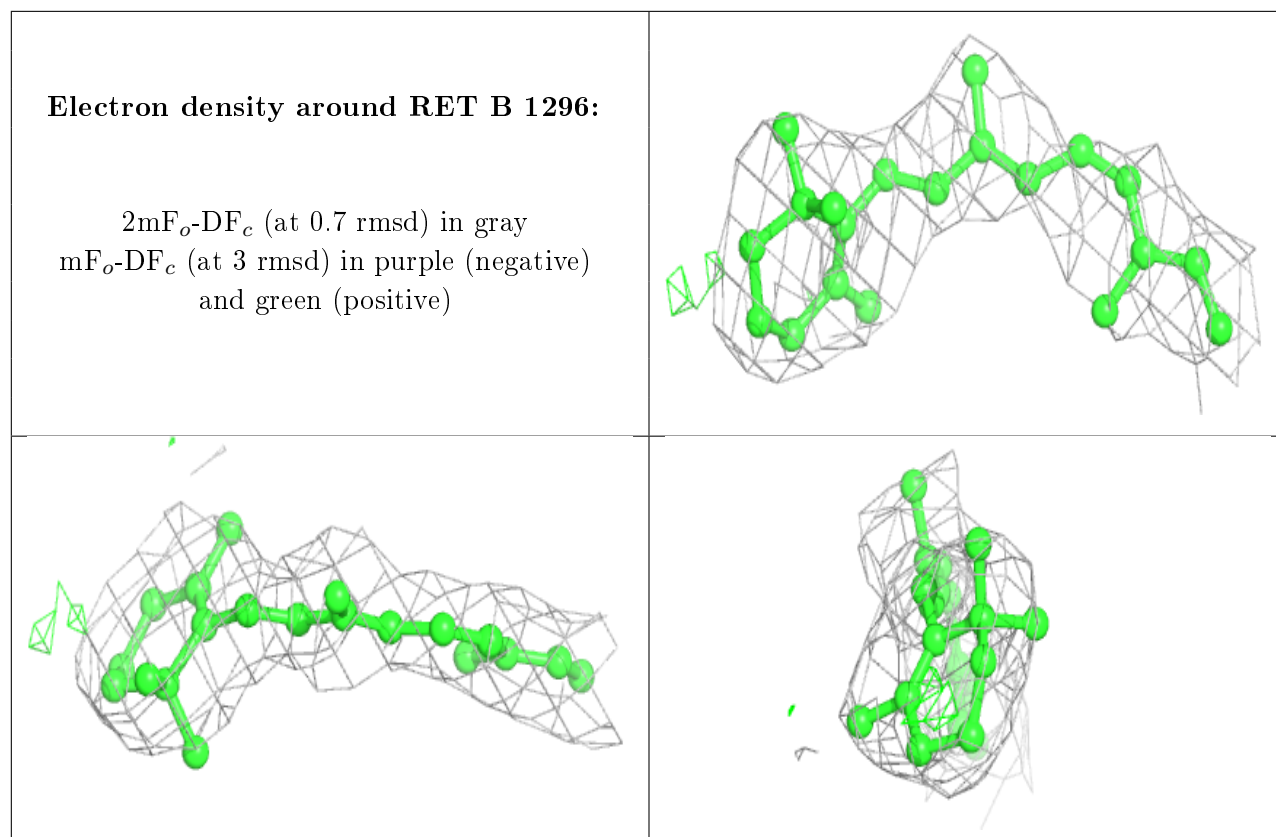
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.