



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 05:12 pm BST

PDB ID : 1FCZ  
Title : ISOTYPE SELECTIVITY OF THE HUMAN RETINOIC ACID NUCLEAR RECEPTOR HRAR: THE COMPLEX WITH THE PANAGONIST RETINOID BMS181156  
Authors : Klaholz, B.P.; Mitschler, A.; Moras, D.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2000-07-19  
Resolution : 1.38 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](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 : 2.11  
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) : 2.11

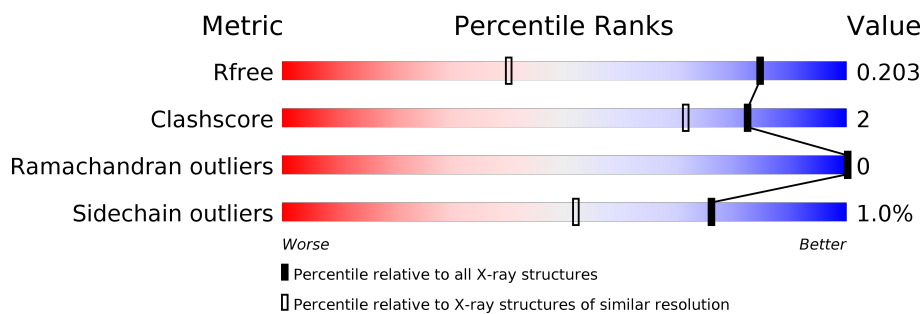
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.38 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)

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	235	

## 2 Entry composition [i](#)

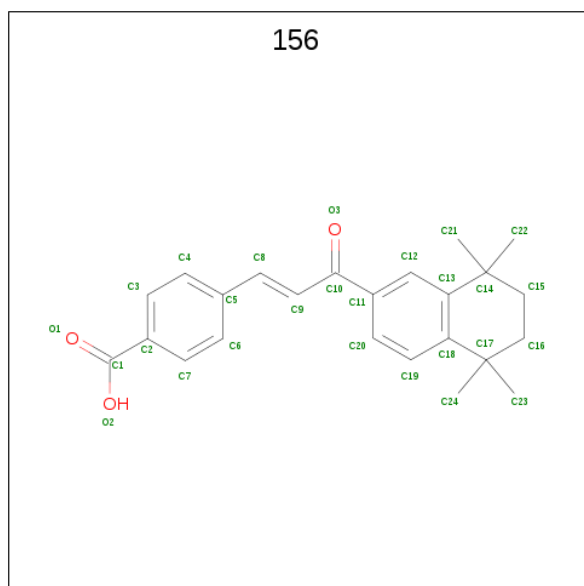
There are 4 unique types of molecules in this entry. The entry contains 2265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOIC ACID RECEPTOR GAMMA-1.

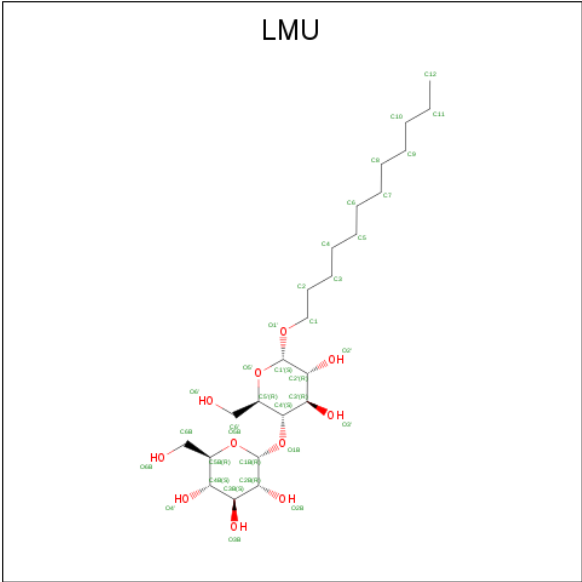
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	12	0
			1898	1208	317	352	21			

- Molecule 2 is 4-[3-OXO-3-(5,5,8,8-TETRAMETHYL-5,6,7,8-TETRAHYDRO-NAPHTHAL EN-2-YL)-PROPENYL]-BENZOIC ACID (three-letter code: 156) (formula: C<sub>24</sub>H<sub>26</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	24	3		

- Molecule 3 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		

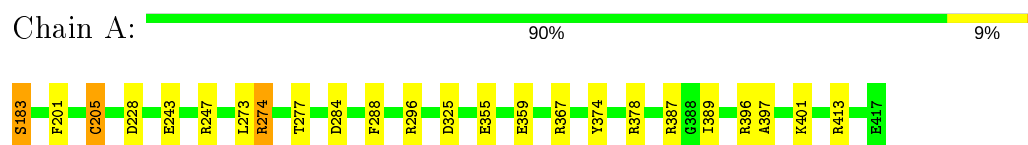
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	305	Total	O	0	0
			305	305		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: RETINOIC ACID RECEPTOR GAMMA-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.88Å 59.88Å 155.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.38 19.80 – 1.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (6.00-1.38) 99.9 (19.80-1.38)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 1.38Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, $R_{free}$	0.131 , 0.174 0.188 , 0.203	Depositor DCC
$R_{free}$ test set	2992 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.58% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMU, 156

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	0.64	0/1979	1.23	18/2668 (0.7%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	247	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	A	183	SER	N-CA-CB	9.87	125.31	110.50
1	A	413	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	A	325	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	288	PHE	CB-CG-CD2	-7.18	115.78	120.80
1	A	274	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	228	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	325	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	374	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	A	247	ARG	NH1-CZ-NH2	6.02	126.02	119.40
1	A	396	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	296	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	374	TYR	CB-CG-CD2	5.80	124.48	121.00
1	A	183	SER	CA-CB-OG	5.64	126.44	111.20
1	A	367	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	378	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	284	ASP	CB-CG-OD2	-5.13	113.68	118.30

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	1898	0	1952	10	0
2	A	27	0	25	0	0
3	A	35	0	46	0	0
4	A	305	0	0	6	0
All	All	2265	0	2023	10	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 2.

All (10) 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:401:LYS:HE3	4:A:672:HOH:O	1.85	0.75
1:A:397:ALA:O	1:A:401:LYS:HG3	1.93	0.68
1:A:243[B]:GLU:HG3	4:A:515:HOH:O	2.00	0.61
1:A:273:LEU:O	1:A:277:THR:HG23	2.01	0.60
1:A:387:ARG:HG3	4:A:661:HOH:O	2.13	0.47
1:A:205:CYS:HB3	4:A:765:HOH:O	2.13	0.47
1:A:355:GLU:O	1:A:359[B]:GLU:HG3	2.14	0.47
1:A:183:SER:N	4:A:773:HOH:O	2.49	0.45
1:A:401:LYS:NZ	4:A:655:HOH:O	2.50	0.41
1:A:201:PHE:CZ	1:A:274:ARG:HB3	2.56	0.41

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	245/235 (104%)	244 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/207 (106%)	216 (99%)	3 (1%)	67	39

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	CYS
1	A	389[A]	ILE
1	A	389[B]	ILE

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	156	A	450	-	27,29,29	1.14	2 (7%)	41,44,44	2.24	9 (21%)
3	LMU	A	451	-	36,36,36	0.69	1 (2%)	47,47,47	1.26	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	156	A	450	-	-	2/9/32/32	0/3/3/3
3	LMU	A	451	-	-	9/21/61/61	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	156	C7-C2	3.77	1.47	1.39
2	A	450	156	C2-C1	-2.75	1.44	1.47
3	A	451	LMU	O4'-C4B	-2.13	1.38	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	156	C3-C2-C1	8.33	131.56	120.37
2	A	450	156	C7-C2-C1	-5.49	113.00	120.37
2	A	450	156	C4-C3-C2	4.34	127.38	121.13
2	A	450	156	C11-C10-C9	4.27	124.03	119.23
3	A	451	LMU	C1-O1'-C1'	-4.12	107.02	113.84
2	A	450	156	C6-C7-C2	-3.63	115.91	121.13
3	A	451	LMU	C4B-C3B-C2B	-3.49	104.72	110.82
3	A	451	LMU	O4'-C4B-C5B	3.47	117.92	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	156	O3-C10-C9	-2.98	116.12	120.76
2	A	450	156	C8-C9-C10	2.86	126.31	121.64
3	A	451	LMU	O4'-C4B-C3B	-2.83	103.80	110.35
2	A	450	156	C7-C6-C5	2.82	124.92	121.25
2	A	450	156	C3-C4-C5	-2.54	117.94	121.25

There are no chirality outliers.

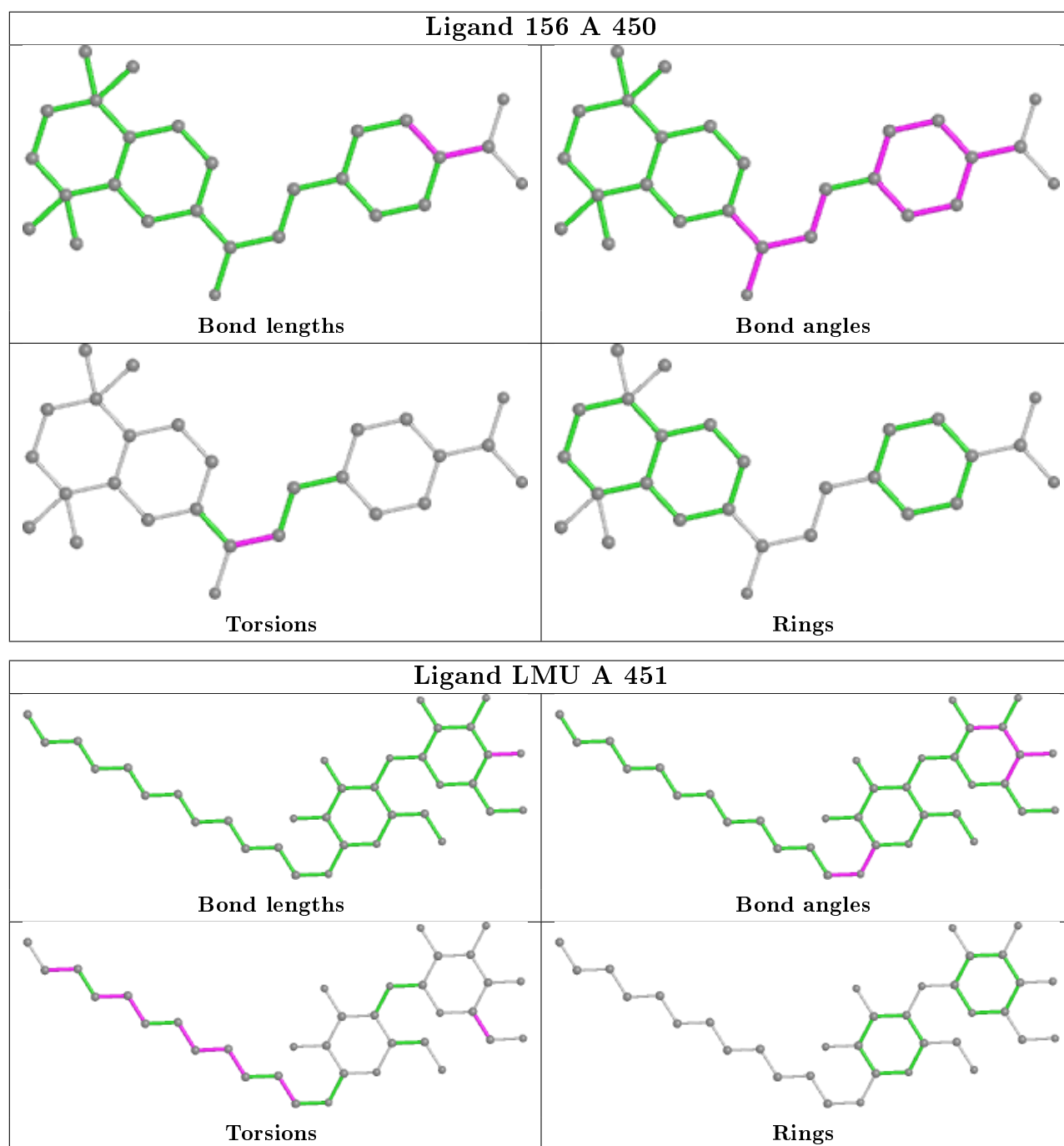
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	451	LMU	O5B-C5B-C6B-O6B
3	A	451	LMU	C4B-C5B-C6B-O6B
2	A	450	156	O3-C10-C9-C8
3	A	451	LMU	C7-C8-C9-C10
2	A	450	156	C11-C10-C9-C8
3	A	451	LMU	O1'-C1-C2-C3
3	A	451	LMU	C2-C3-C4-C5
3	A	451	LMU	C3-C4-C5-C6
3	A	451	LMU	C9-C10-C11-C12
3	A	451	LMU	C6-C7-C8-C9
3	A	451	LMU	C4-C5-C6-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

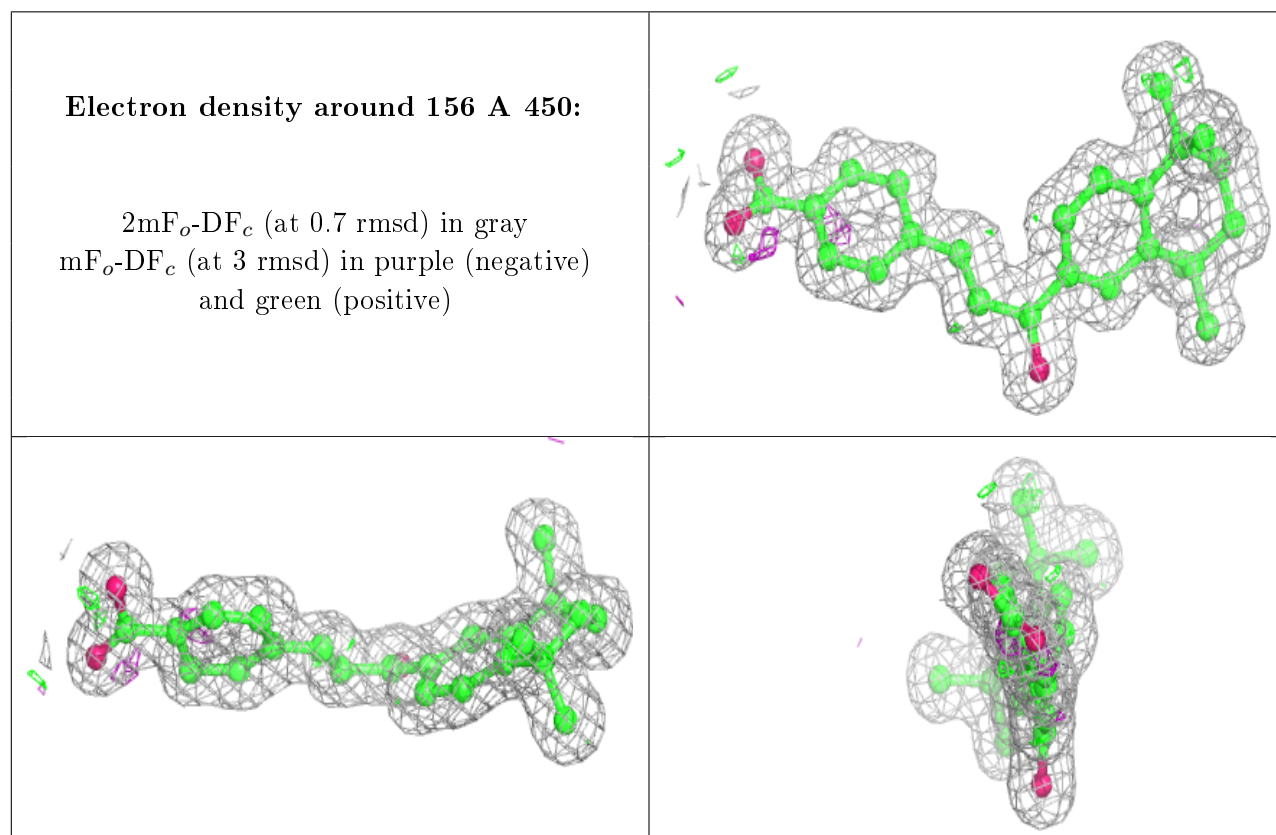
### 6.3 Carbohydrates ⓘ

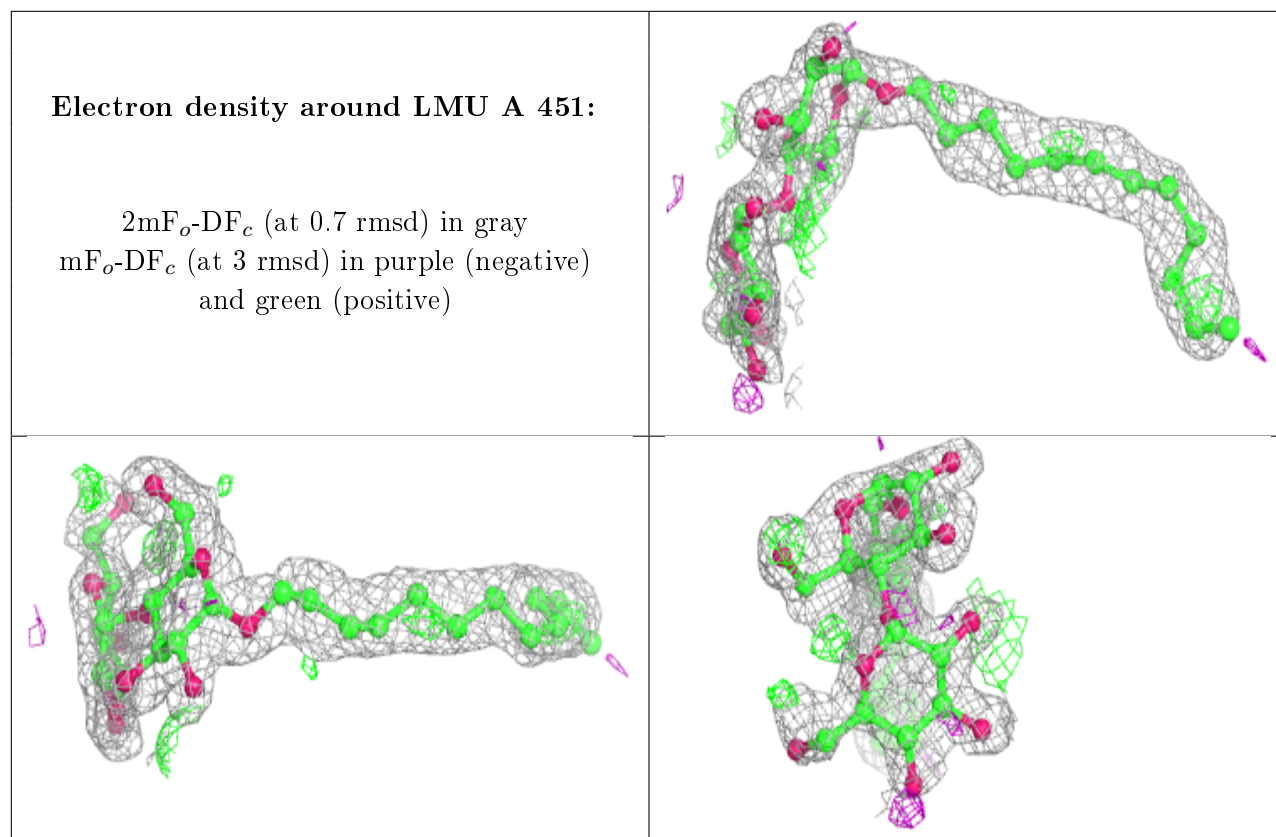
Unable to reproduce the depositors R factor - this section is therefore empty.

### 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.