



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 02:02 PM BST

PDB ID : 6XVY
Title : Human myelin protein P2 mutant R88Q
Authors : Ruskamo, S.; Lehtimaki, M.; Kursula, P.
Deposited on : 2020-01-22
Resolution : 1.80 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

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

i

X-RAY DIFFRACTION

A.

Ramachandran outliers

The numeric value for each fraction is indicated below the corresponding segment, with a dot

1

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9631 atoms, of which 4580 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.

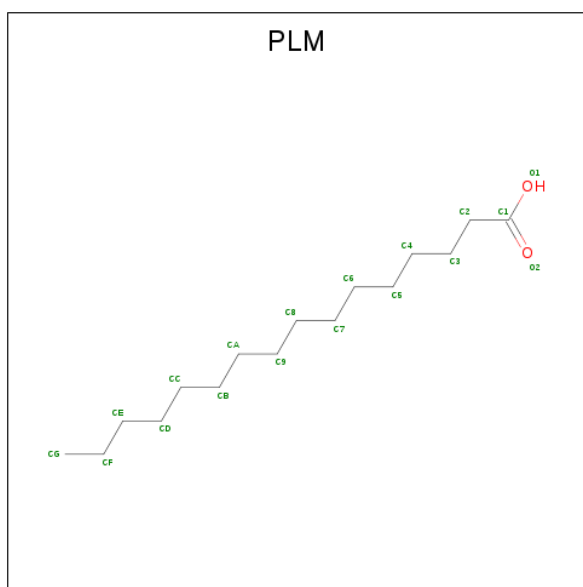
- Molecule 1 is a protein called Myelin P2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	133	Total	C	H	N	O	S	7	2	0
			2183	670	1121	185	200	7			
1	C	133	Total	C	H	N	O	S	7	0	0
			2147	659	1101	183	198	6			
1	D	133	Total	C	H	N	O	S	10	0	0
			2147	659	1101	183	198	6			
1	E	133	Total	C	H	N	O	S	6	4	0
			2190	671	1123	186	203	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P02689
B	88	GLN	ARG	engineered mutation	UNP P02689
C	-1	GLY	-	expression tag	UNP P02689
C	88	GLN	ARG	engineered mutation	UNP P02689
D	-1	GLY	-	expression tag	UNP P02689
D	88	GLN	ARG	engineered mutation	UNP P02689
E	-1	GLY	-	expression tag	UNP P02689
E	88	GLN	ARG	engineered mutation	UNP P02689

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			49	16	31	2		
2	C	1	Total	C	H	O	0	0
			49	16	31	2		
2	D	1	Total	C	H	O	0	0
			49	16	31	2		
2	E	1	Total	C	H	O	0	0
			49	16	31	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			18	6	5	7		
4	D	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 5 is water.

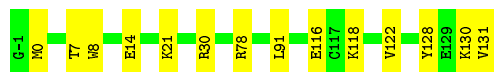
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	189	Total	O	0	0
			189	189		
5	C	173	Total	O	0	0
			173	173		
5	D	181	Total	O	0	1
			182	182		
5	E	184	Total	O	0	0
			184	184		

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: Myelin P2 protein

Chain B:  89% 11%



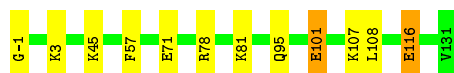
- Molecule 1: Myelin P2 protein

Chain C:  93% 7%




- Molecule 1: Myelin P2 protein

Chain D:  91% 8% •



- Molecule 1: Myelin P2 protein

Chain E:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.88Å 64.88Å 264.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 37.69 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.80) 99.5 (37.69-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.159 , 0.199 0.159 , 0.199	Depositor DCC
R_{free} test set	2670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9631	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, CL, CIT

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	B	0.47	0/1073	0.73	2/1433 (0.1%)
1	C	0.49	0/1057	0.73	0/1412
1	D	0.48	0/1057	0.73	1/1412 (0.1%)
1	E	0.49	0/1090	0.67	0/1456
All	All	0.48	0/4277	0.71	3/5713 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	78	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	78	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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	B	1062	1121	1119	9	0
1	C	1046	1101	1101	6	0
1	D	1046	1101	1101	8	0
1	E	1067	1123	1112	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	31	31	0	0
2	C	18	31	31	1	0
2	D	18	31	31	0	0
2	E	18	31	31	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	1	0
4	C	13	5	5	0	0
4	D	13	5	5	0	0
5	B	189	0	0	3	4
5	C	173	0	0	3	3
5	D	182	0	0	5	1
5	E	184	0	0	7	2
All	All	5051	4580	4567	37	5

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 4.

The worst 5 of 37 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)
3:E:202:CL:CL	5:E:318:HOH:O	2.04	1.09
1:E:129:GLU:OE2	5:E:301:HOH:O	1.98	0.80
1:E:116:GLU:OE1	5:E:302:HOH:O	2.01	0.77
1:E:56[B]:THR:HG23	5:E:318:HOH:O	1.92	0.69
1:C:120:LYS:NZ	5:C:302:HOH:O	2.26	0.69

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:349:HOH:O	5:C:314:HOH:O[5_555]	1.97	0.23
5:B:305:HOH:O	5:C:366:HOH:O[5_555]	2.02	0.18
5:B:349:HOH:O	5:C:435:HOH:O[5_555]	2.04	0.16
5:D:433:HOH:O	5:E:467:HOH:O[8_565]	2.07	0.13
5:B:427:HOH:O	5:E:459:HOH:O[4_554]	2.17	0.03

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	B	133/133 (100%)	133 (100%)	0	0	100	100
1	C	131/133 (98%)	131 (100%)	0	0	100	100
1	D	131/133 (98%)	131 (100%)	0	0	100	100
1	E	135/133 (102%)	135 (100%)	0	0	100	100
All	All	530/532 (100%)	530 (100%)	0	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	B	119/117 (102%)	118 (99%)	1 (1%)	81	78
1	C	117/117 (100%)	116 (99%)	1 (1%)	78	75
1	D	117/117 (100%)	115 (98%)	2 (2%)	60	51
1	E	121/117 (103%)	119 (98%)	2 (2%)	60	51
All	All	474/468 (101%)	468 (99%)	6 (1%)	69	62

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	101	GLU
1	E	131	VAL
1	D	116	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	130	LYS
1	E	44	LYS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	CIT	C	203	-	3,12,12	1.38	1 (33%)	3,17,17	1.55	1 (33%)
4	CIT	D	203	-	3,12,12	1.27	0	3,17,17	1.36	0
2	PLM	C	201	-	14,17,17	0.41	0	13,17,17	0.45	0
2	PLM	D	201	-	14,17,17	0.53	0	13,17,17	0.38	0
2	PLM	B	201	-	14,17,17	0.39	0	13,17,17	0.46	0
2	PLM	E	201	-	14,17,17	0.62	0	13,17,17	0.48	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
4	CIT	C	203	-	-	3/6/16/16	-
4	CIT	D	203	-	-	3/6/16/16	-
2	PLM	C	201	-	-	6/13/15/15	-
2	PLM	D	201	-	-	6/13/15/15	-
2	PLM	B	201	-	-	7/13/15/15	-
2	PLM	E	201	-	-	7/13/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	203	CIT	O7-C3	2.14	1.46	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	CIT	C3-C2-C1	-2.22	111.44	114.98

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	203	CIT	C1-C2-C3-C6
4	D	203	CIT	C1-C2-C3-O7
4	D	203	CIT	C1-C2-C3-C4
4	D	203	CIT	C1-C2-C3-C6
2	B	201	PLM	C8-C9-CA-CB

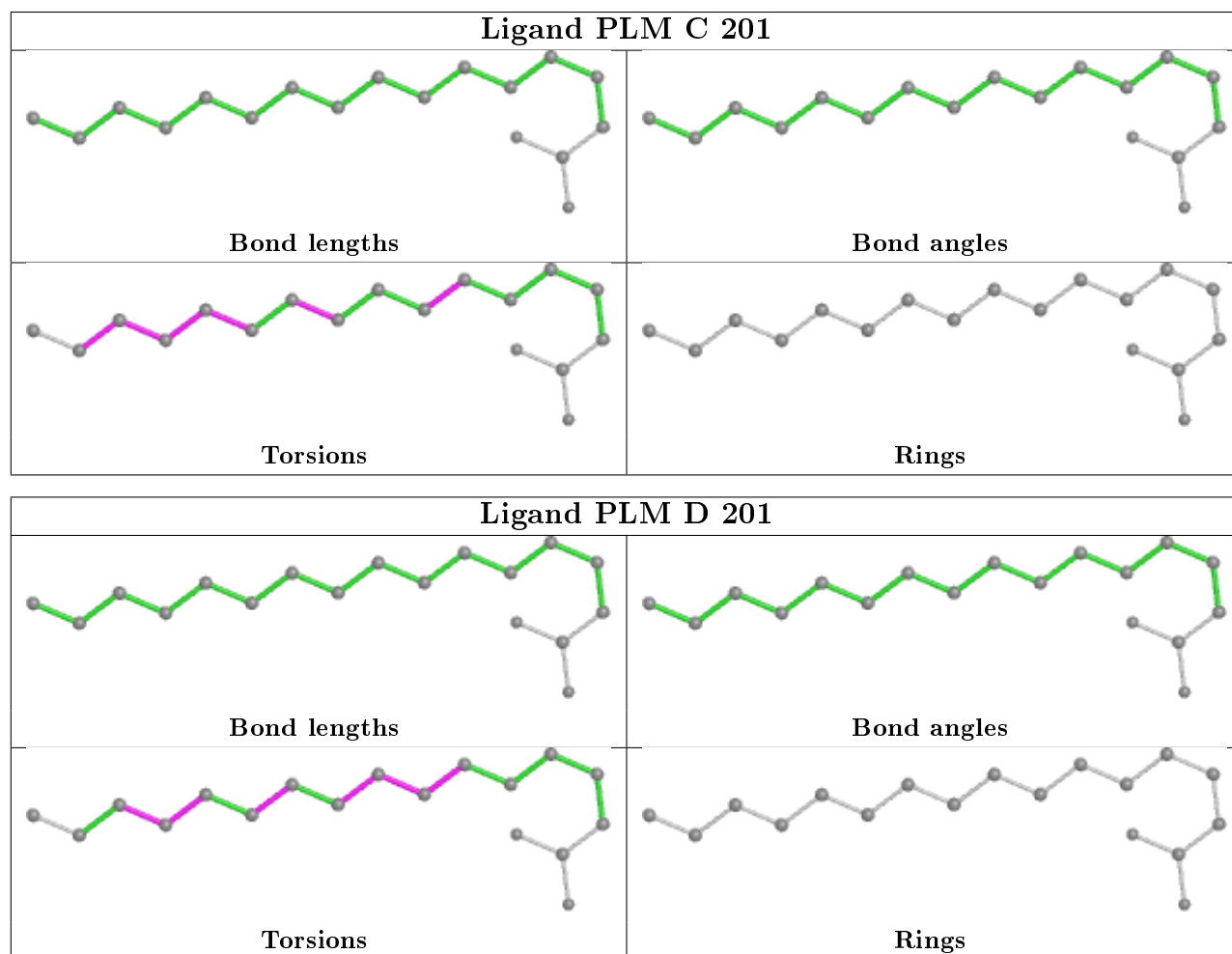
There are no ring outliers.

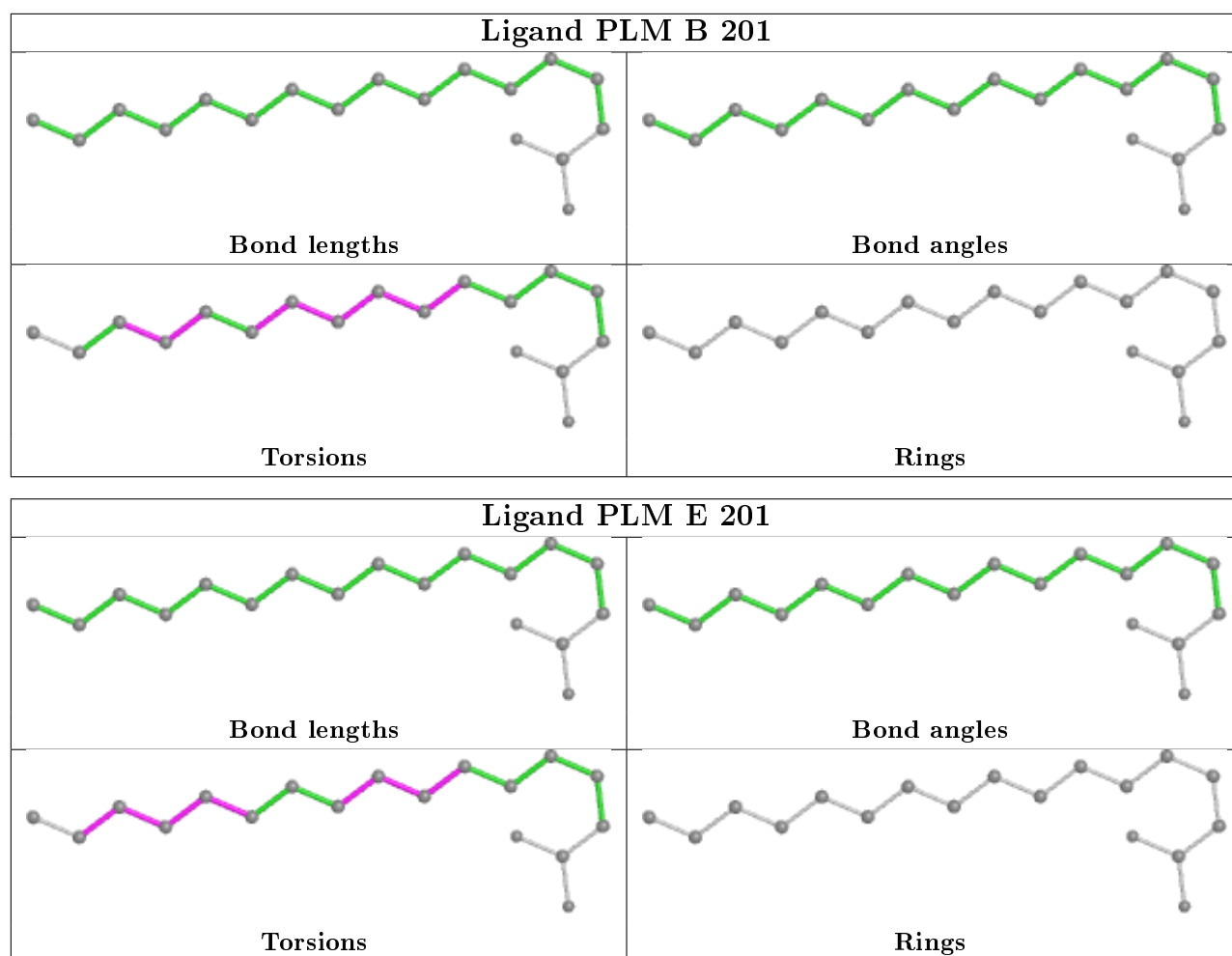
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	PLM	1	0
2	E	201	PLM	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 ⓘ

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	B	133/133 (100%)	-0.60	0 100 100	12, 18, 33, 46	3 (2%)
1	C	133/133 (100%)	-0.67	0 100 100	12, 18, 32, 41	2 (1%)
1	D	133/133 (100%)	-0.59	0 100 100	13, 20, 33, 54	3 (2%)
1	E	133/133 (100%)	-0.58	0 100 100	11, 18, 32, 38	1 (0%)
All	All	532/532 (100%)	-0.61	0 100 100	11, 19, 33, 54	9 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

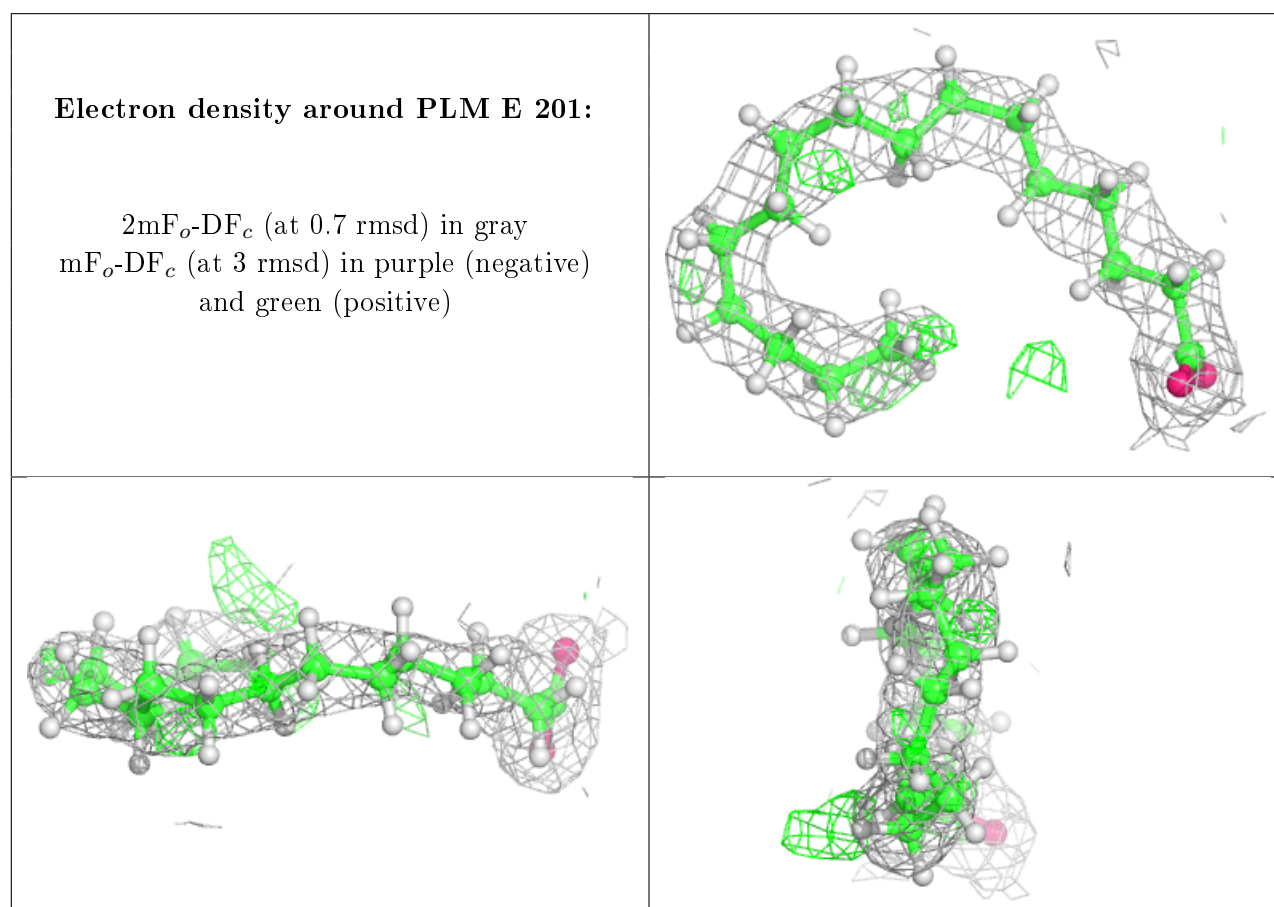
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	D	203	13/13	0.76	0.24	19,44,56,60	18
2	PLM	E	201	18/18	0.90	0.14	22,36,48,49	0
2	PLM	D	201	18/18	0.91	0.13	23,35,53,57	0
2	PLM	C	201	18/18	0.91	0.11	20,34,40,41	0

Continued on next page...

Continued from previous page...

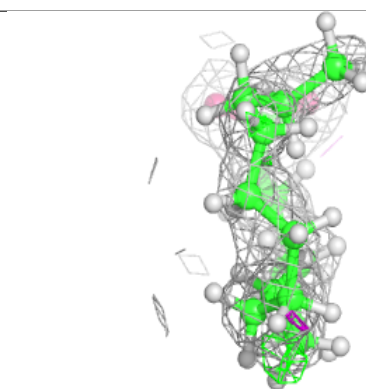
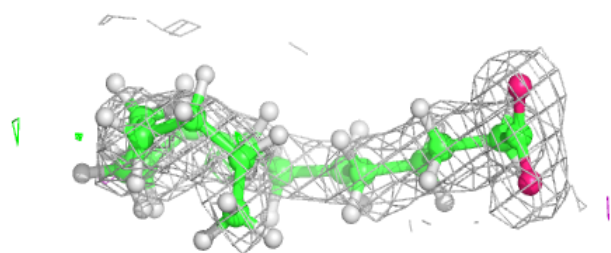
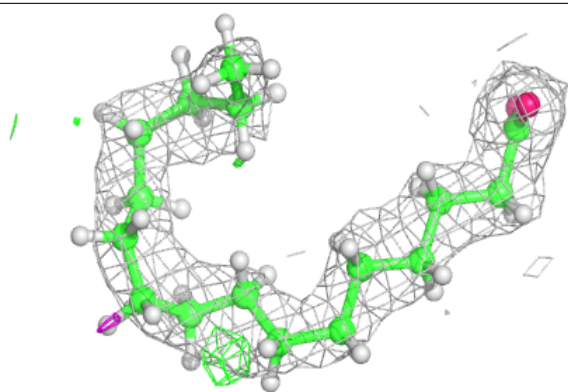
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLM	B	201	18/18	0.93	0.12	15,29,41,41	0
4	CIT	C	203	13/13	0.94	0.15	15,26,51,52	0
3	CL	B	202	1/1	0.96	0.05	36,36,36,36	0
3	CL	C	202	1/1	0.96	0.05	36,36,36,36	0
3	CL	D	202	1/1	0.96	0.06	44,44,44,44	0
3	CL	E	202	1/1	0.98	0.05	33,33,33,33	0

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.

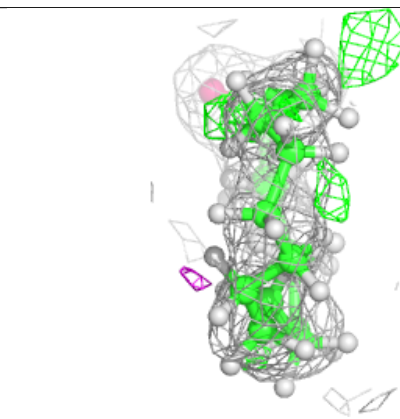
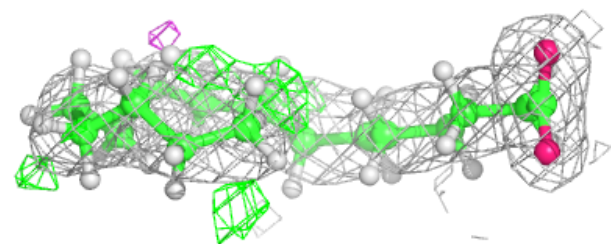
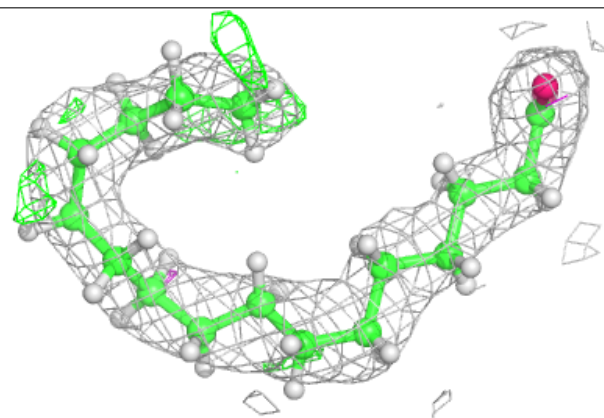


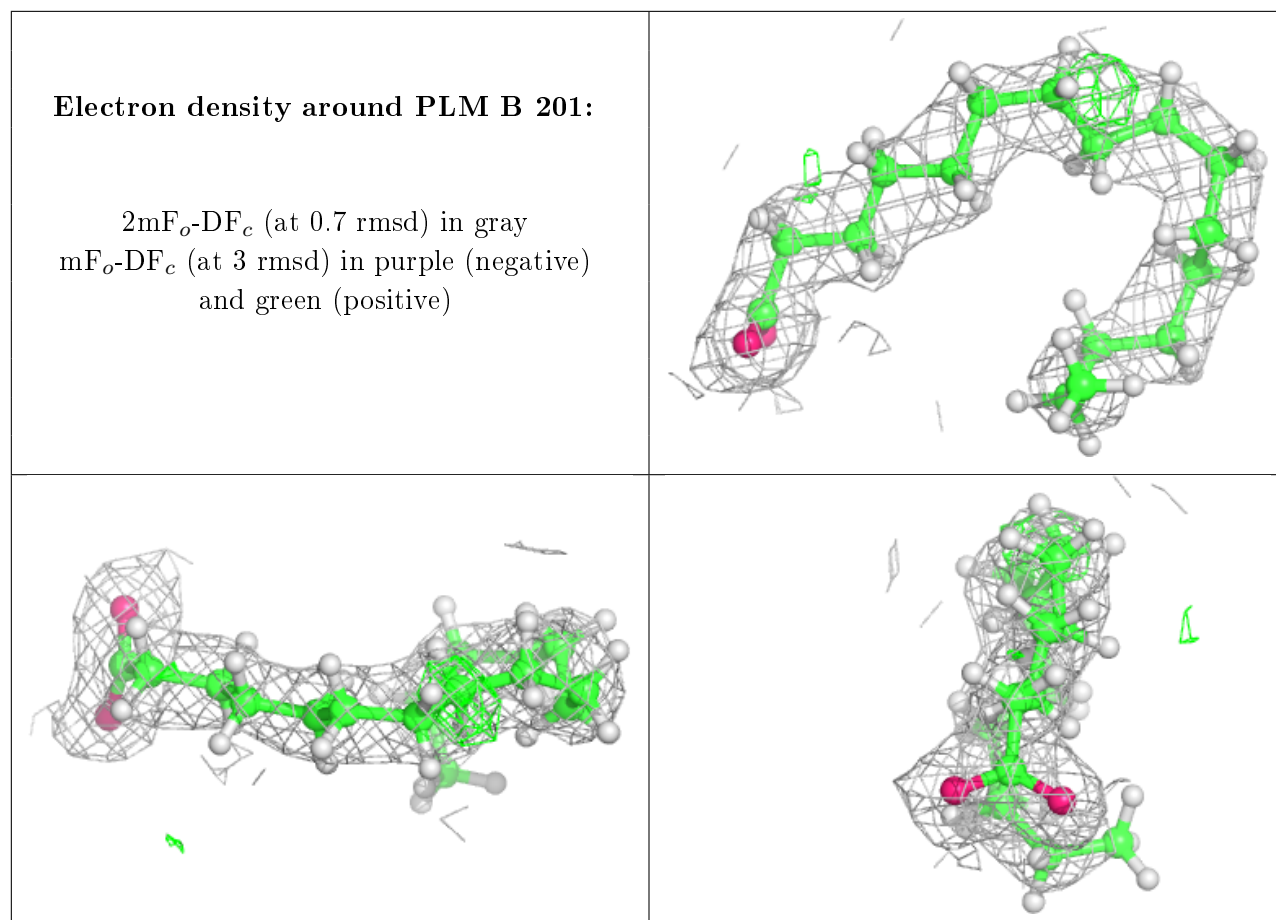
Electron density around PLM D 201:

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

**Electron density around PLM C 201:**

$2mF_o-DF_c$ (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.