WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 29, 2024 – 03:09 PM EDT

PDB ID	:	8VOM
Title	:	Double alanine Apex domain mutant of bacteriophage P2 central spike protein, membrane-piercing module
Authors	:	Leiman, P.G.; Miller, J.M.
Deposited on	:	2024-01-15
Resolution	:	1.25 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.37.1
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)	:	2.37.1

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 1.25 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.
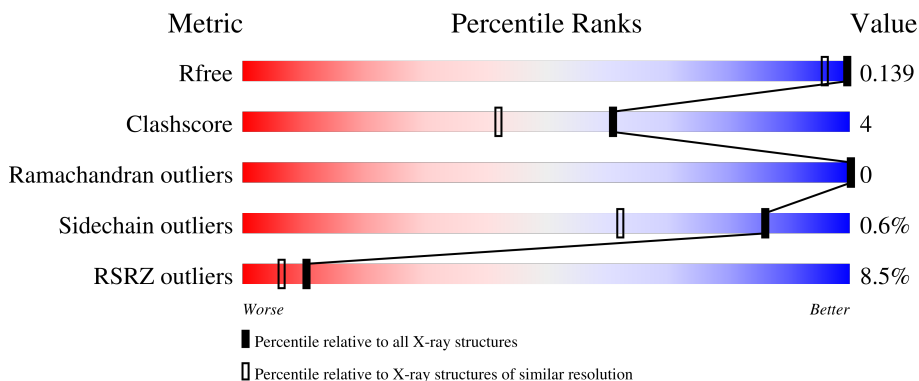
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 <=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	118	7% / 75% 8% · 17%
1	B	118	7% / 74% 8% · 17%
1	C	118	7% / 80% 6% 14%
1	D	118	7% / 81% 5% · 13%
1	E	118	8% / 75% 8% 17%

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Mol	Chain	Length	Quality of chain
1	F	118	8% 77% 8% 15%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10246 atoms, of which 4851 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 Spike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	98	Total	C	H	N	O	S	0	6	0
			1516	460	774	126	153	3			
1	B	98	Total	C	H	N	O	S	0	4	0
			1498	453	767	128	147	3			
1	C	101	Total	C	H	N	O	S	0	5	0
			1518	462	773	125	155	3			
1	D	103	Total	C	H	N	O	S	0	4	0
			1558	473	796	131	155	3			
1	E	98	Total	C	H	N	O	S	0	8	0
			1552	470	795	129	155	3			
1	F	100	Total	C	H	N	O	S	0	7	0
			1540	467	788	127	155	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	GLY	-	expression tag	UNP P31340
A	95	SER	-	expression tag	UNP P31340
A	96	GLY	-	expression tag	UNP P31340
A	97	SER	-	expression tag	UNP P31340
A	197	ALA	HIS	engineered mutation	UNP P31340
A	199	ALA	HIS	engineered mutation	UNP P31340
B	94	GLY	-	expression tag	UNP P31340
B	95	SER	-	expression tag	UNP P31340
B	96	GLY	-	expression tag	UNP P31340
B	97	SER	-	expression tag	UNP P31340
B	197	ALA	HIS	engineered mutation	UNP P31340
B	199	ALA	HIS	engineered mutation	UNP P31340
C	94	GLY	-	expression tag	UNP P31340
C	95	SER	-	expression tag	UNP P31340
C	96	GLY	-	expression tag	UNP P31340
C	97	SER	-	expression tag	UNP P31340
C	197	ALA	HIS	engineered mutation	UNP P31340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	199	ALA	HIS	engineered mutation	UNP P31340
D	94	GLY	-	expression tag	UNP P31340
D	95	SER	-	expression tag	UNP P31340
D	96	GLY	-	expression tag	UNP P31340
D	97	SER	-	expression tag	UNP P31340
D	197	ALA	HIS	engineered mutation	UNP P31340
D	199	ALA	HIS	engineered mutation	UNP P31340
E	94	GLY	-	expression tag	UNP P31340
E	95	SER	-	expression tag	UNP P31340
E	96	GLY	-	expression tag	UNP P31340
E	97	SER	-	expression tag	UNP P31340
E	197	ALA	HIS	engineered mutation	UNP P31340
E	199	ALA	HIS	engineered mutation	UNP P31340
F	94	GLY	-	expression tag	UNP P31340
F	95	SER	-	expression tag	UNP P31340
F	96	GLY	-	expression tag	UNP P31340
F	97	SER	-	expression tag	UNP P31340
F	197	ALA	HIS	engineered mutation	UNP P31340
F	199	ALA	HIS	engineered mutation	UNP P31340

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).
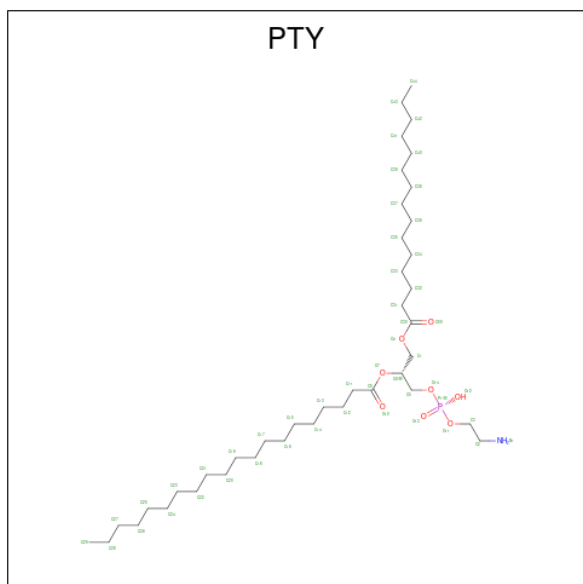
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	C	1	129	40	79	1	8	1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	E	1	129	40	79	1	8	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	125	Total	O	0	0
			125	125		
3	C	136	Total	O	0	0
			136	136		
3	D	146	Total	O	0	0
			146	146		
3	E	130	Total	O	0	0
			130	130		
3	F	135	Total	O	0	0
			135	135		

# 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.
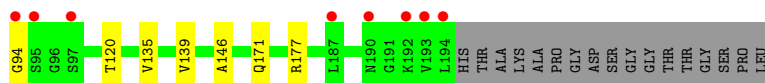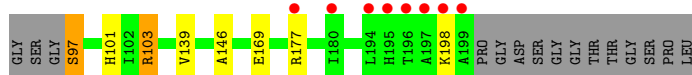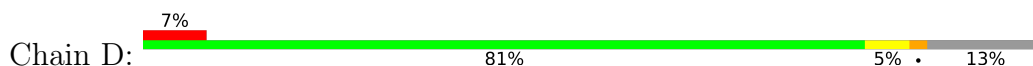
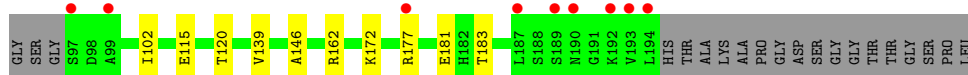- Molecule 1: Spike protein
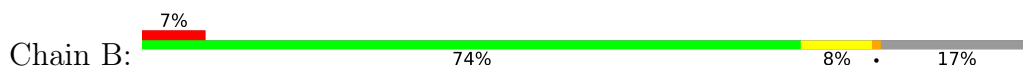
- Molecule 1: Spike protein
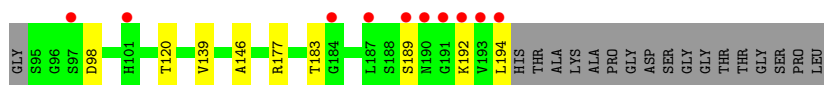

- Molecule 1: Spike protein

- Molecule 1: Spike protein

- Molecule 1: Spike protein

- Molecule 1: Spike protein

Chain F:
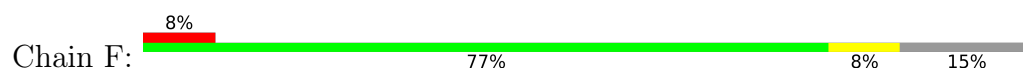
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.01Å 52.81Å 78.37Å 90.00° 108.68° 90.00°	Depositor
Resolution (Å)	44.06 – 1.25 44.06 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.06-1.25) 99.8 (44.06-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.84 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.119 , 0.139 0.118 , 0.139	Depositor DCC
R_{free} test set	3109 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 59.5	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10246	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4582e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: PTY

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	0.37	0/767	0.73	0/1041
1	B	0.41	0/750	0.69	0/1020
1	C	0.43	0/767	0.70	0/1044
1	D	0.40	0/782	0.70	0/1063
1	E	0.37	0/788	0.69	0/1070
1	F	0.42	0/780	0.73	0/1062
All	All	0.40	0/4634	0.71	0/6300

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	2
1	B	0	4
1	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177[A]	ARG	Sidechain
1	A	177[B]	ARG	Sidechain
1	B	162[A]	ARG	Sidechain
1	B	162[B]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	177[A]	ARG	Sidechain

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	742	774	772	7	1
1	B	731	767	765	8	1
1	C	745	773	771	6	1
1	D	762	796	793	8	0
1	E	757	795	793	10	0
1	F	752	788	786	10	0
2	C	50	79	79	6	0
2	E	50	79	79	1	0
3	A	134	0	0	1	4
3	B	125	0	0	3	4
3	C	136	0	0	2	2
3	D	146	0	0	4	2
3	E	130	0	0	5	3
3	F	135	0	0	3	3
All	All	5395	4851	4838	42	13

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 42 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:E:115:GLU:OE2	3:E:401:HOH:O	2.06	0.74
1:B:99:ALA:HB1	3:B:357:HOH:O	1.86	0.73
1:E:172:LYS:NZ	3:E:403:HOH:O	2.22	0.72
1:E:102:ILE:HG23	1:F:98:ASP:HB3	1.81	0.63
1:D:103:ARG:NH2	3:D:303:HOH:O	2.35	0.59

The worst 5 of 13 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)
3:B:346:HOH:O	3:B:410:HOH:O[2_645]	1.88	0.32
3:A:424:HOH:O	3:A:426:HOH:O[2_655]	1.89	0.31
3:A:366:HOH:O	3:B:396:HOH:O[2_645]	1.96	0.24
3:B:423:HOH:O	3:C:425:HOH:O[2_645]	2.01	0.19
3:B:410:HOH:O	3:B:423:HOH:O[2_655]	2.03	0.17

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	102/118 (86%)	97 (95%)	5 (5%)	0	100	100
1	B	100/118 (85%)	97 (97%)	3 (3%)	0	100	100
1	C	104/118 (88%)	100 (96%)	4 (4%)	0	100	100
1	D	105/118 (89%)	99 (94%)	6 (6%)	0	100	100
1	E	104/118 (88%)	99 (95%)	5 (5%)	0	100	100
1	F	105/118 (89%)	101 (96%)	4 (4%)	0	100	100
All	All	620/708 (88%)	593 (96%)	27 (4%)	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	87/93 (94%)	86 (99%)	1 (1%)	73	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	85/93 (91%)	85 (100%)	0	100	100
1	C	87/93 (94%)	87 (100%)	0	100	100
1	D	88/93 (95%)	86 (98%)	2 (2%)	50	12
1	E	89/93 (96%)	89 (100%)	0	100	100
1	F	89/93 (96%)	89 (100%)	0	100	100
All	All	525/558 (94%)	522 (99%)	3 (1%)	86	62

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

Mol	Chain	Res	Type
1	A	98	ASP
1	D	97	SER
1	D	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	B	101	HIS
1	B	171	GLN
1	C	171	GLN
1	D	171	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 ⓘ

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	PTY	E	301	-	49,49,49	0.49	0	52,54,54	0.42	0
2	PTY	C	301	-	49,49,49	0.49	0	52,54,54	0.41	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
2	PTY	E	301	-	-	9/53/53/53	-
2	PTY	C	301	-	-	14/53/53/53	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	PTY	C5-O14-P1-O13
2	E	301	PTY	C3-O11-P1-O13
2	E	301	PTY	C3-O11-P1-O14
2	E	301	PTY	C5-O14-P1-O11
2	E	301	PTY	C5-O14-P1-O12

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PTY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	PTY	6	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 then 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.

Ligand PTY E 301

Bond lengths — Bond angles — Torsions — Rings

Ligand PTY C 301

Bond lengths — Bond angles — Torsions — Rings
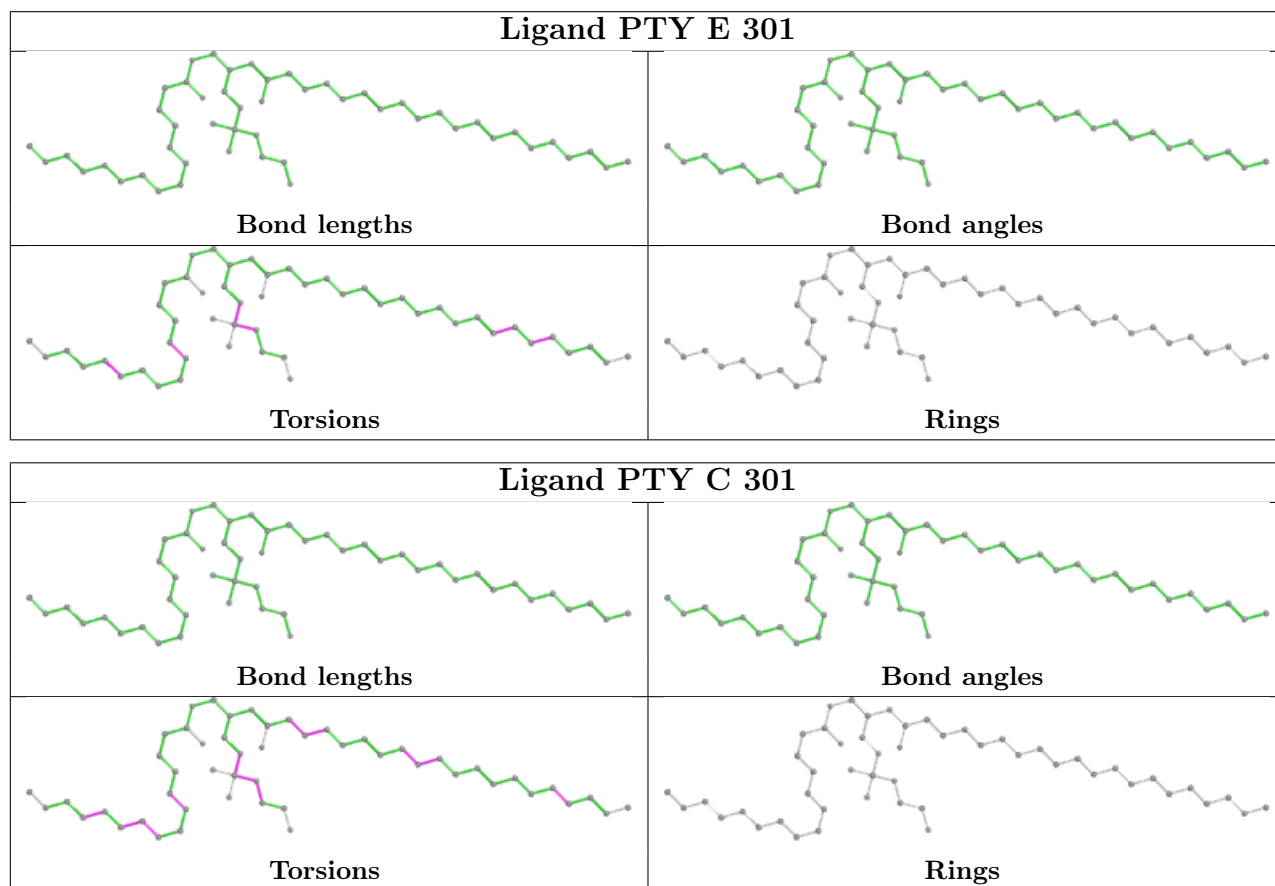
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	98/118 (83%)	0.06	8 (8%)	11	7	9, 14, 49, 65	0
1	B	98/118 (83%)	0.12	8 (8%)	11	7	10, 14, 47, 65	0
1	C	101/118 (85%)	0.15	8 (7%)	12	8	9, 15, 47, 70	0
1	D	103/118 (87%)	0.13	8 (7%)	13	8	9, 15, 36, 67	0
1	E	98/118 (83%)	0.15	9 (9%)	9	4	10, 14, 52, 70	0
1	F	100/118 (84%)	0.23	10 (10%)	7	3	9, 14, 67, 83	0
All	All	598/708 (84%)	0.14	51 (8%)	10	6	9, 14, 55, 83	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	8.7
1	F	192	LYS	6.0
1	C	194	LEU	6.0
1	E	192	LYS	5.9
1	F	191	GLY	5.9

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

There are no non-standard protein/DNA/RNA residues in this entry.
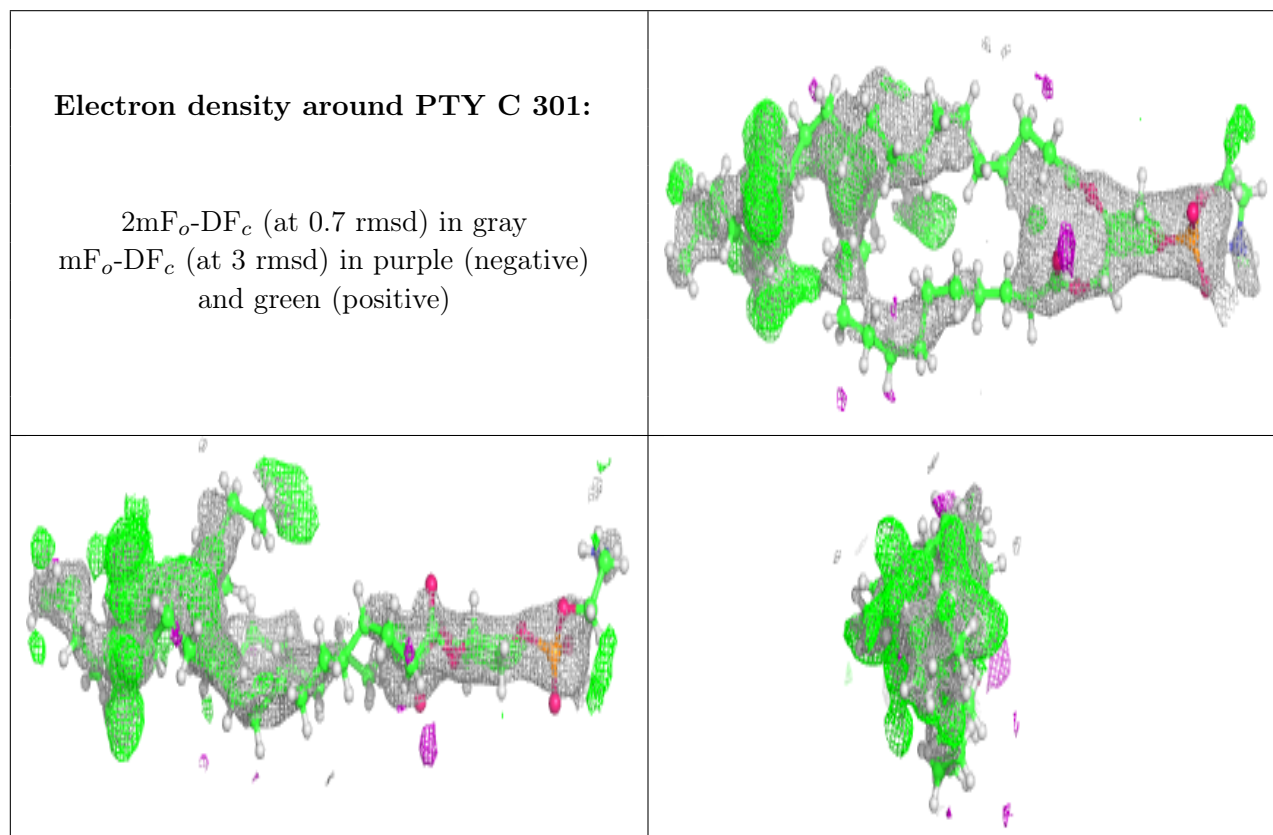
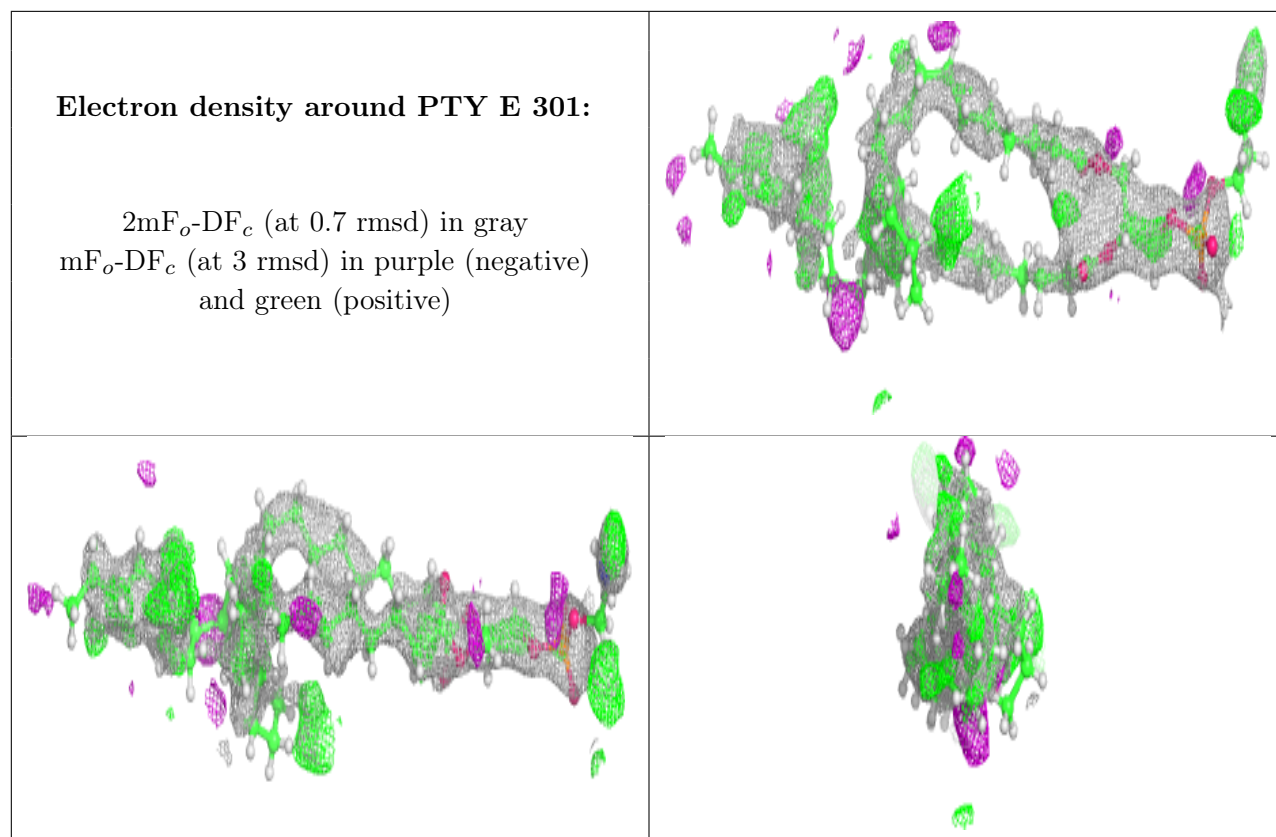## 6.3 Carbohydrates ⓘ

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
2	PTY	C	301	50/50	0.70	0.25	40,75,93,101	0
2	PTY	E	301	50/50	0.73	0.23	51,66,74,74	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 PTY C 301:

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

Electron density around PTY E 301:

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

6.5 Other polymers (i)

There are no such residues in this entry.