



Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2022 – 02:18 PM EDT

PDB ID : 7ULM
Title : HMG-CoA reductase from Arabidopsis thaliana (HMG1) complexed with pitavastatin
Authors : Haywood, J.; Bond, C.S.
Deposited on : 2022-04-05
Resolution : 2.13 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

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 : 2.28.1
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) : 2.28.1

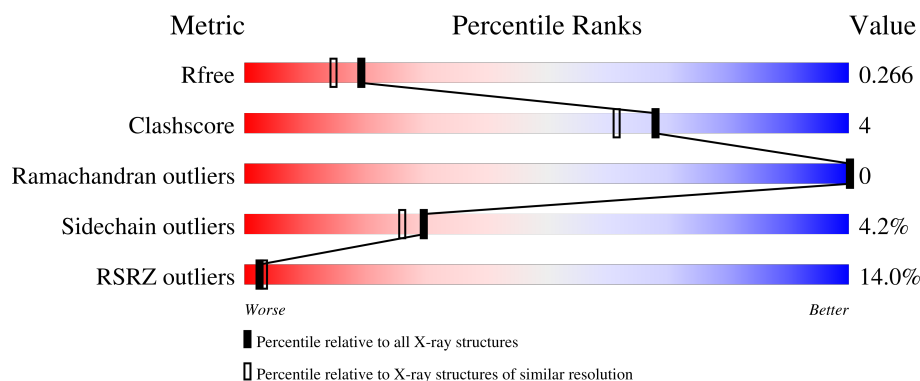
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 $\leq 5\%$. 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	AAA	592	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5130 atoms, of which 2548 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase 1.

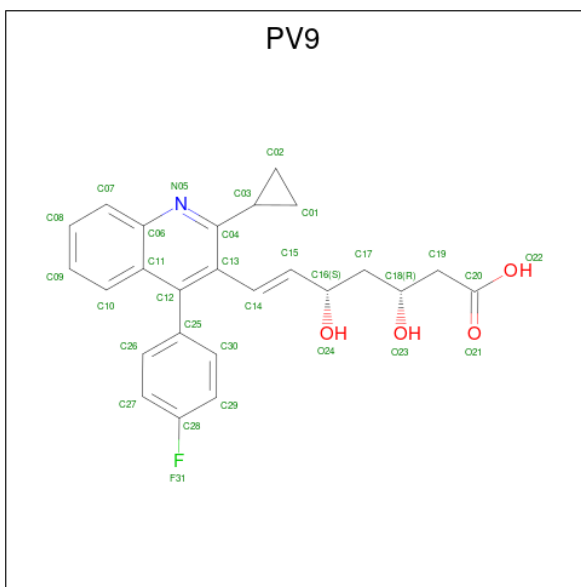
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	357	5043	1574	2517	440	489	23	80	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	AAA	1	14	3	8	3	0	0

- Molecule 3 is Pitavastatin (three-letter code: PV9) (formula: C₂₅H₂₄FNO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total	C	F	H	N	O	2	0
			54	25	1	23	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	19	Total	O	0	0
			19	19		

- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase 1



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.55Å 85.55Å 265.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.11 – 2.13 45.07 – 2.13	Depositor EDS
% Data completeness (in resolution range)	59.8 (45.11-2.13) 59.8 (45.07-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.264 0.228 , 0.266	Depositor DCC
R_{free} test set	905 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: GOL, PV9

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	AAA	0.79	0/2560	0.87	0/3461

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2526	2517	2477	19	0
2	AAA	6	8	8	0	0
3	AAA	31	23	0	0	0
4	AAA	19	0	0	1	0
All	All	2582	2548	2485	19	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 4.

All (19) 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:AAA:200:ALA:O	1:AAA:204:ARG:HG3	1.96	0.66
1:AAA:322:ASP:O	1:AAA:326:VAL:HG23	2.05	0.57
1:AAA:516:LEU:O	1:AAA:520:SER:HB2	2.07	0.55
1:AAA:323:THR:O	1:AAA:327:VAL:HG23	2.08	0.53
1:AAA:402:VAL:O	1:AAA:406:GLU:HB2	2.10	0.51
1:AAA:404:TRP:CZ3	1:AAA:453:GLY:HA2	2.46	0.50
1:AAA:291:LYS:HE3	4:AAA:708:HOH:O	2.14	0.48
1:AAA:487:MET:HB3	1:AAA:496:ILE:HD11	1.98	0.46
1:AAA:208:GLN:HG3	1:AAA:213:ARG:O	2.16	0.45
1:AAA:295:THR:HA	1:AAA:353:PHE:O	2.16	0.45
1:AAA:408:ARG:O	1:AAA:504:SER:HA	2.18	0.44
1:AAA:353:PHE:CD2	1:AAA:370:VAL:HG22	2.53	0.43
1:AAA:398:LYS:HB2	1:AAA:398:LYS:HE2	1.82	0.43
1:AAA:474:PRO:O	1:AAA:477:ASN:HB3	2.19	0.42
1:AAA:480:SER:HA	1:AAA:504:SER:O	2.19	0.42
1:AAA:402:VAL:O	1:AAA:406:GLU:CB	2.66	0.42
1:AAA:500:VAL:HG11	1:AAA:551:VAL:HG12	2.01	0.42
1:AAA:297:ALA:HA	1:AAA:351:VAL:O	2.20	0.42
1:AAA:421:GLU:H	1:AAA:421:GLU:HG3	1.58	0.41

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	AAA	352/592 (60%)	330 (94%)	22 (6%)	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	AAA	260/490 (53%)	248 (95%)	12 (5%)	27	22

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	267[A]	CYS
1	AAA	267[B]	CYS
1	AAA	301	ARG
1	AAA	319	GLU
1	AAA	394	CYS
1	AAA	398	LYS
1	AAA	421	GLU
1	AAA	458	HIS
1	AAA	477	ASN
1	AAA	479	GLU
1	AAA	520	SER
1	AAA	542	ARG

Sometimes 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 ⓘ

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	GOL	AAA	601	-	5,5,5	0.15	0	5,5,5	0.40	0
3	PV9	AAA	602	-	30,34,34	1.48	5 (16%)	38,48,48	2.89	10 (26%)

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	GOL	AAA	601	-	-	0/4/4/4	-
3	PV9	AAA	602	-	-	4/19/23/23	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	602	PV9	C12-C25	3.55	1.54	1.49
3	AAA	602	PV9	C13-C14	2.80	1.53	1.47
3	AAA	602	PV9	C16-C15	2.73	1.56	1.50
3	AAA	602	PV9	C11-C06	-2.32	1.38	1.42
3	AAA	602	PV9	C06-N05	-2.03	1.34	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	602	PV9	C02-C03-C04	14.96	138.07	119.37
3	AAA	602	PV9	C11-C06-N05	-4.01	118.56	122.81
3	AAA	602	PV9	C04-N05-C06	3.44	123.50	117.04
3	AAA	602	PV9	C16-C15-C14	-3.31	117.73	125.29
3	AAA	602	PV9	O23-C18-C19	-2.49	104.31	109.48
3	AAA	602	PV9	C13-C04-C03	-2.24	119.06	122.86
3	AAA	602	PV9	C26-C25-C12	-2.18	117.47	120.77
3	AAA	602	PV9	C30-C25-C26	2.17	121.92	117.59
3	AAA	602	PV9	C01-C03-C04	-2.08	116.77	119.37
3	AAA	602	PV9	C03-C04-N05	2.04	119.18	116.39

There are no chirality outliers.

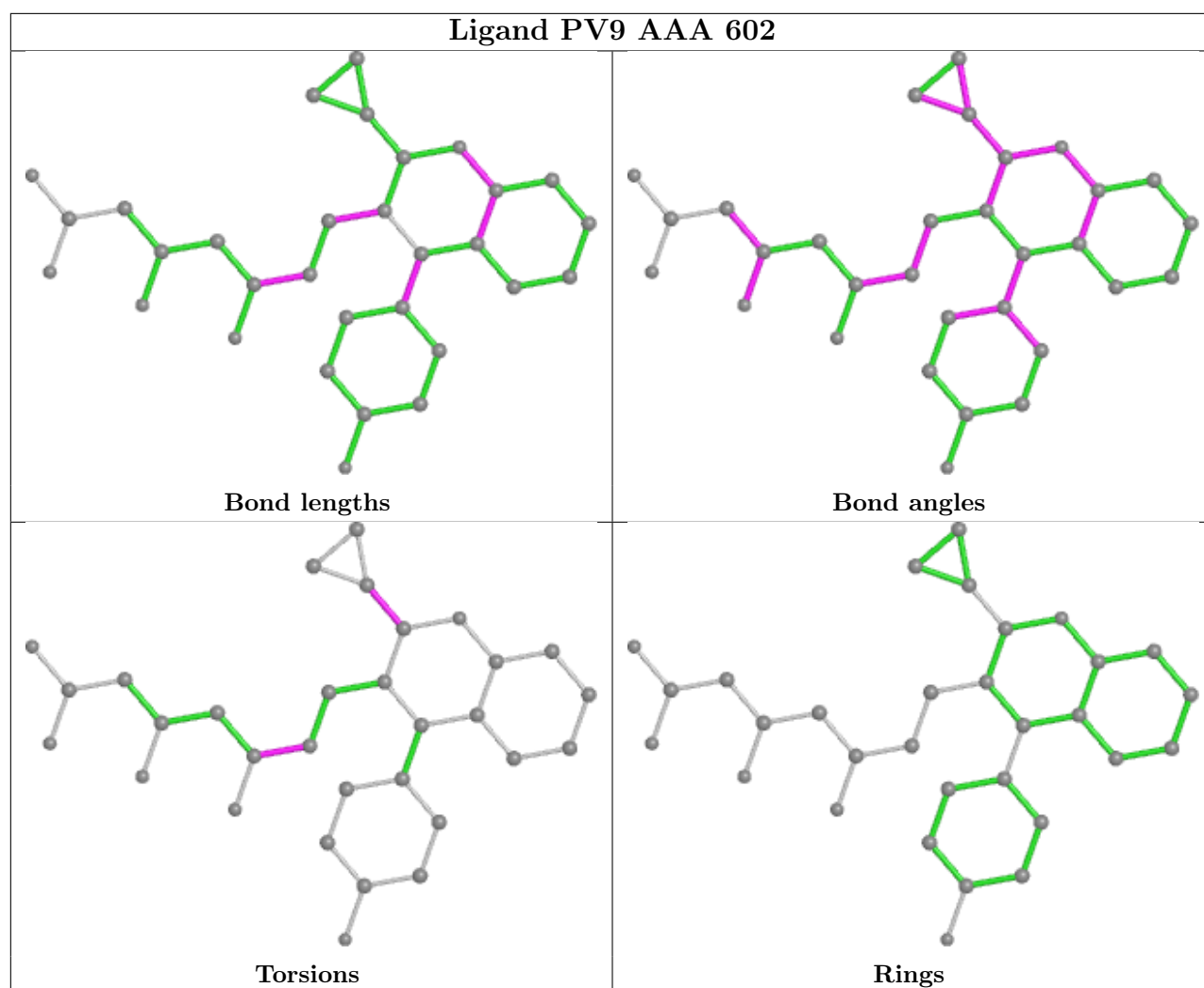
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	602	PV9	C02-C03-C04-C13
3	AAA	602	PV9	C02-C03-C04-N05
3	AAA	602	PV9	C01-C03-C04-C13
3	AAA	602	PV9	C14-C15-C16-O24

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 ⓘ

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	AAA	357/592 (60%)	0.59	50 (14%) 2 3	9, 26, 66, 82	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	199	ALA	5.0
1	AAA	331	SER	4.8
1	AAA	207	LEU	4.5
1	AAA	224	ASP	4.5
1	AAA	225	TYR	4.4
1	AAA	223	PHE	4.2
1	AAA	215	ILE	4.2
1	AAA	221	ASP	4.1
1	AAA	222	GLY	4.1
1	AAA	206	ALA	4.1
1	AAA	201	SER	4.0
1	AAA	209	ARG	4.0
1	AAA	202	ILE	4.0
1	AAA	400	ALA	3.9
1	AAA	205	GLU	3.7
1	AAA	401	ALA	3.7
1	AAA	220	LEU	3.7
1	AAA	203	ARG	3.6
1	AAA	219	PRO	3.6
1	AAA	447	ALA	3.5
1	AAA	213	ARG	3.4
1	AAA	452	LEU	3.3
1	AAA	453	GLY	3.2
1	AAA	478	VAL	3.2
1	AAA	204	ARG	3.2
1	AAA	216	GLU	3.1
1	AAA	404	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	334	PHE	3.0
1	AAA	451	SER	2.9
1	AAA	198	ARG	2.9
1	AAA	399	PRO	2.8
1	AAA	214	SER	2.8
1	AAA	455	PHE	2.7
1	AAA	239	TYR	2.7
1	AAA	533	THR	2.7
1	AAA	208	GLN	2.6
1	AAA	200	ALA	2.5
1	AAA	326	VAL	2.5
1	AAA	375	GLU	2.5
1	AAA	405	ILE	2.5
1	AAA	448	VAL	2.4
1	AAA	445	GLY	2.2
1	AAA	454	GLY	2.2
1	AAA	217	GLY	2.2
1	AAA	446	SER	2.2
1	AAA	449	ALA	2.1
1	AAA	379	ASP	2.1
1	AAA	483	CYS	2.1
1	AAA	320	ASN	2.1
1	AAA	402	VAL	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](#)

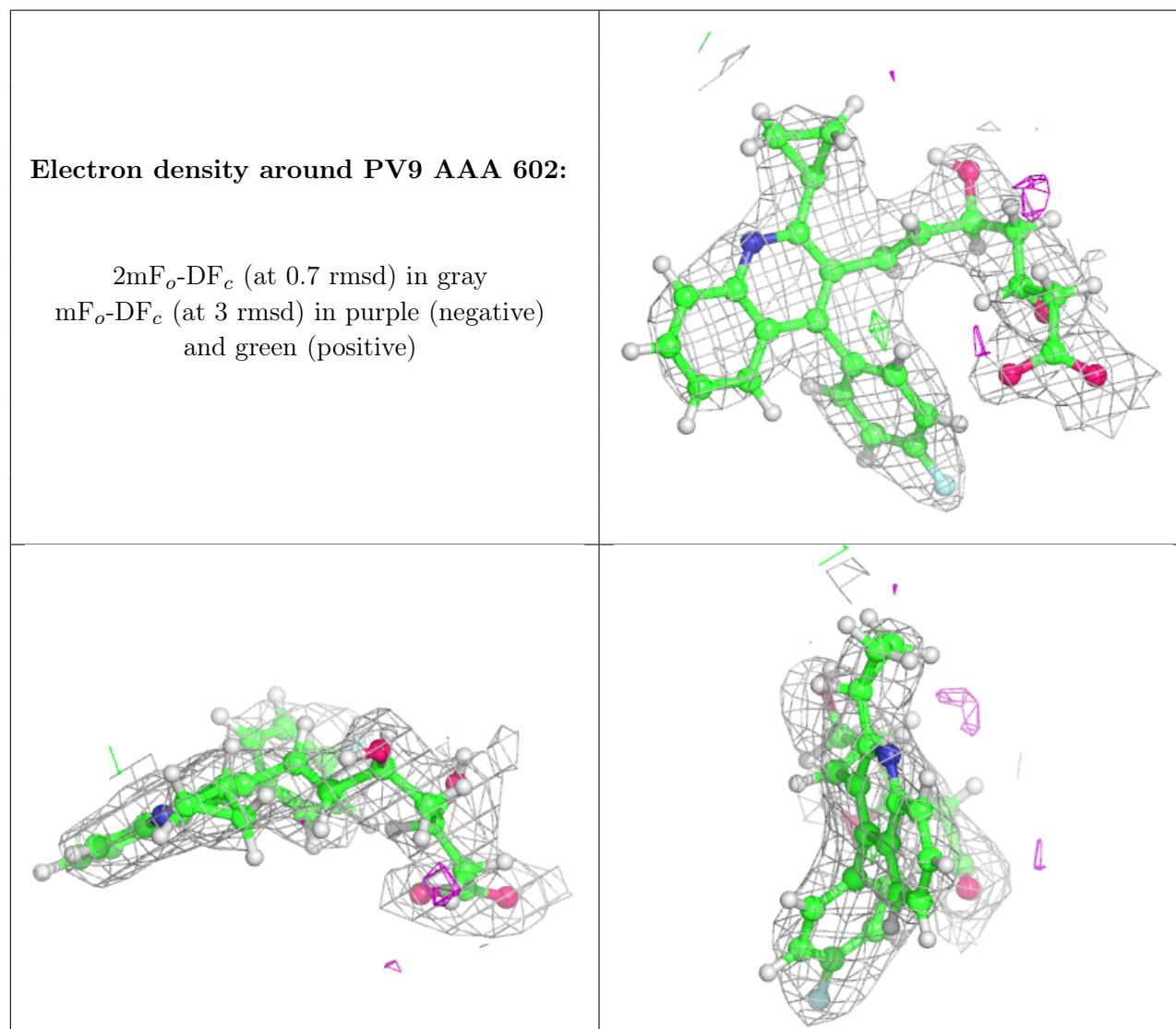
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	AAA	601	6/6	0.82	0.19	44,48,52,52	0
3	PV9	AAA	602	31/31	0.87	0.15	41,43,46,48	2

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](#)

There are no such residues in this entry.