



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2021 – 04:10 pm GMT

PDB ID : 7P8M  
Title : Crystal structure of L147A/I351A variant of S-adenosylmethionine synthetase from *Methanocaldococcus jannaschii* in complex with DMNB-SAM (4,5-dimethoxy-2-nitro benzene S-adenosyl-methionine)  
Authors : Herrmann, E.; Peters, A.; Cornelissen, N.V.; Rentmeister, A.; Kuemmel, D.  
Deposited on : 2021-07-23  
Resolution : 1.71 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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

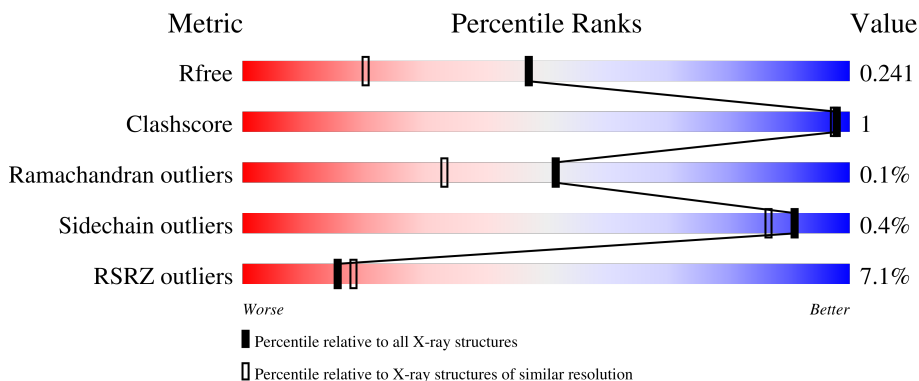
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	426	
1	C	426	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13292 atoms, of which 6417 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 S-adenosylmethionine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	404	6339	1986	3190	533	614	16	0	0	0
1	C	408	6408	2004	3227	540	620	17	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

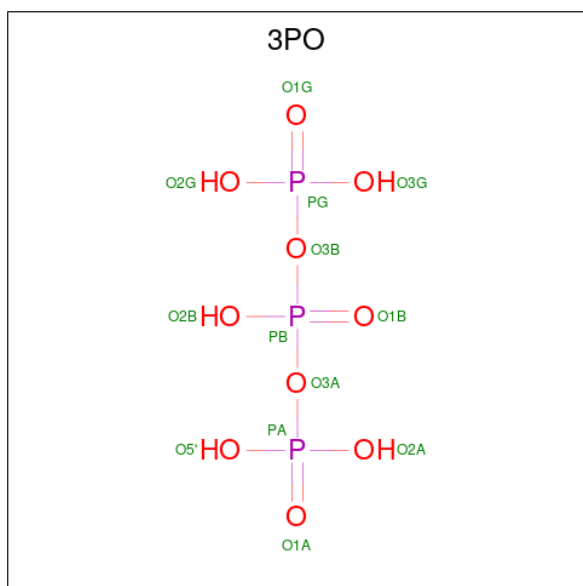
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q58605
A	-18	GLY	-	expression tag	UNP Q58605
A	-17	SER	-	expression tag	UNP Q58605
A	-16	SER	-	expression tag	UNP Q58605
A	-15	HIS	-	expression tag	UNP Q58605
A	-14	HIS	-	expression tag	UNP Q58605
A	-13	HIS	-	expression tag	UNP Q58605
A	-12	HIS	-	expression tag	UNP Q58605
A	-11	HIS	-	expression tag	UNP Q58605
A	-10	HIS	-	expression tag	UNP Q58605
A	-9	SER	-	expression tag	UNP Q58605
A	-8	SER	-	expression tag	UNP Q58605
A	-7	GLY	-	expression tag	UNP Q58605
A	-6	LEU	-	expression tag	UNP Q58605
A	-5	VAL	-	expression tag	UNP Q58605
A	-4	PRO	-	expression tag	UNP Q58605
A	-3	ARG	-	expression tag	UNP Q58605
A	-2	GLY	-	expression tag	UNP Q58605
A	-1	SER	-	expression tag	UNP Q58605
A	0	HIS	-	expression tag	UNP Q58605
A	147	ALA	LEU	engineered mutation	UNP Q58605
A	351	ALA	ILE	engineered mutation	UNP Q58605
C	-19	MET	-	initiating methionine	UNP Q58605
C	-18	GLY	-	expression tag	UNP Q58605
C	-17	SER	-	expression tag	UNP Q58605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q58605
C	-15	HIS	-	expression tag	UNP Q58605
C	-14	HIS	-	expression tag	UNP Q58605
C	-13	HIS	-	expression tag	UNP Q58605
C	-12	HIS	-	expression tag	UNP Q58605
C	-11	HIS	-	expression tag	UNP Q58605
C	-10	HIS	-	expression tag	UNP Q58605
C	-9	SER	-	expression tag	UNP Q58605
C	-8	SER	-	expression tag	UNP Q58605
C	-7	GLY	-	expression tag	UNP Q58605
C	-6	LEU	-	expression tag	UNP Q58605
C	-5	VAL	-	expression tag	UNP Q58605
C	-4	PRO	-	expression tag	UNP Q58605
C	-3	ARG	-	expression tag	UNP Q58605
C	-2	GLY	-	expression tag	UNP Q58605
C	-1	SER	-	expression tag	UNP Q58605
C	0	HIS	-	expression tag	UNP Q58605
C	147	ALA	LEU	engineered mutation	UNP Q58605
C	351	ALA	ILE	engineered mutation	UNP Q58605

- Molecule 2 is TRIPHOSPHATE (three-letter code: 3PO) (formula:  $H_5O_{10}P_3$ ).

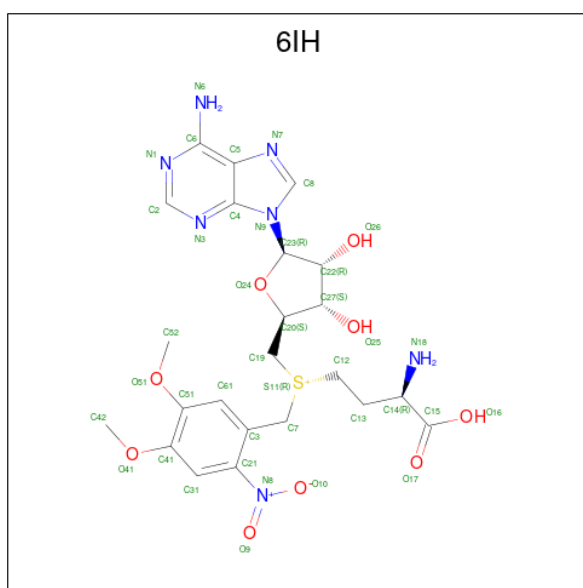


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			13	10	3		
2	C	1	Total	O	P	0	0
			13	10	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is 4,5-dimethoxy-2-nitro benzoyl-S-adenosyl-methionine (three-letter code: 6IH) (formula: C<sub>23</sub>H<sub>30</sub>N<sub>7</sub>O<sub>9</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O S 40 23 7 9 1	0	0

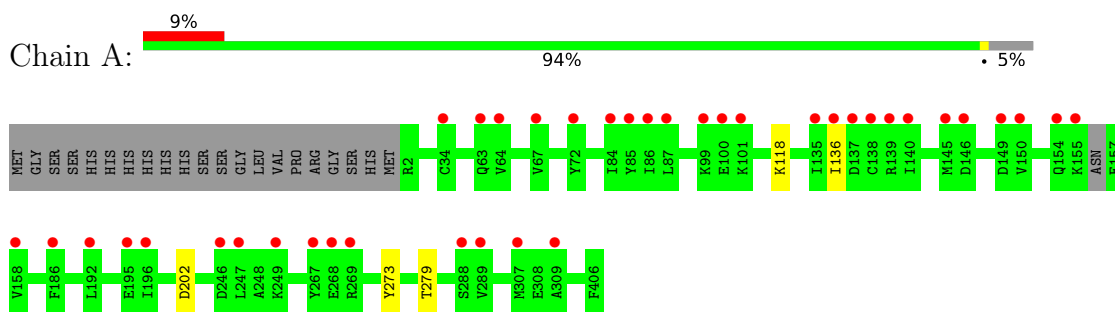
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	232	Total O 232 232	0	0
5	C	244	Total O 244 244	0	0

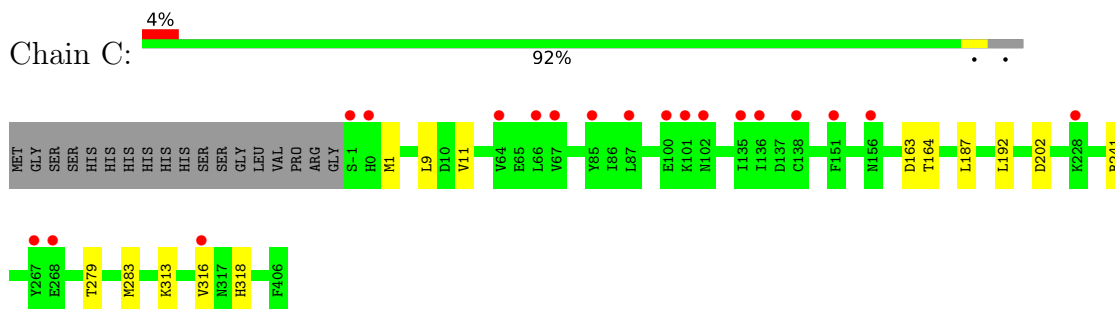
### 3 Residue-property plots [i](#)

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: S-adenosylmethionine synthase



- Molecule 1: S-adenosylmethionine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.49Å 76.49Å 280.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.85 – 1.71 48.19 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.85-1.71) 99.8 (48.19-1.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.71Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.191 , 0.239 0.199 , 0.241	Depositor DCC
$R_{free}$ test set	1103 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MG, 3PO, 6IH

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	0.27	0/3190	0.50	0/4299
1	C	0.28	0/3224	0.50	0/4346
All	All	0.28	0/6414	0.50	0/8645

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	A	3149	3190	3225	3	0
1	C	3181	3227	3256	6	0
2	A	13	0	0	0	0
2	C	13	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	C	40	0	0	0	0
5	A	232	0	0	0	0
5	C	244	0	0	1	0
All	All	6875	6417	6481	9	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 1.

All (9) 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:C:241:ARG:NH2	5:C:602:HOH:O	2.32	0.62
1:C:187:LEU:HA	1:C:192:LEU:HD22	1.85	0.58
1:A:118:LYS:HG2	1:A:136:ILE:HD12	1.98	0.46
1:A:202:ASP:HB2	1:A:279:THR:HA	1.98	0.46
1:C:313:LYS:HD3	1:C:318:HIS:CE1	2.51	0.45
1:A:118:LYS:CG	1:A:136:ILE:HD12	2.48	0.43
1:C:202:ASP:HB2	1:C:279:THR:HA	1.99	0.43
1:C:163:ASP:OD1	1:C:164:THR:N	2.51	0.43
1:C:9:LEU:HG	1:C:11:VAL:HG22	2.03	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	A	400/426 (94%)	395 (99%)	5 (1%)	0	100	100
1	C	406/426 (95%)	398 (98%)	7 (2%)	1 (0%)	47	30
All	All	806/852 (95%)	793 (98%)	12 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	283	MET

### 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	A	348/367 (95%)	347 (100%)	1 (0%)	92	89
1	C	352/367 (96%)	350 (99%)	2 (1%)	86	80
All	All	700/734 (95%)	697 (100%)	3 (0%)	91	86

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

Mol	Chain	Res	Type
1	A	273	TYR
1	C	1	MET
1	C	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

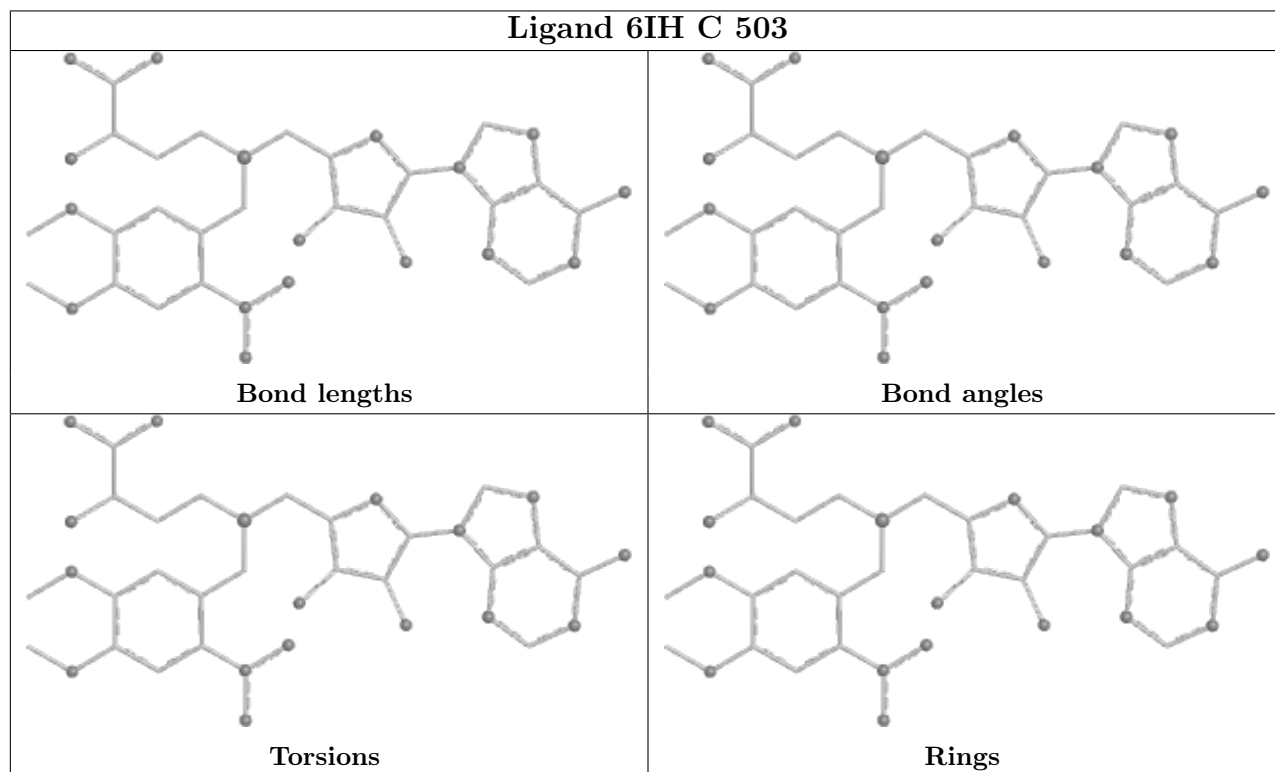
There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/426 (94%)	0.45	39 (9%) <b>7</b> <b>8</b>	21, 33, 63, 114	0
1	C	408/426 (95%)	0.27	19 (4%) <b>31</b> <b>35</b>	20, 30, 53, 91	0
All	All	812/852 (95%)	0.36	58 (7%) <b>16</b> <b>18</b>	20, 31, 59, 114	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	MET	4.4
1	A	146	ASP	4.2
1	C	151	PHE	4.0
1	A	34	CYS	4.0
1	A	85	TYR	3.6
1	C	100	GLU	3.6
1	A	268	GLU	3.5
1	A	135	ILE	3.4
1	A	139	ARG	3.4
1	C	268	GLU	3.4
1	C	85	TYR	3.4
1	A	64	VAL	3.4
1	C	87	LEU	3.3
1	A	136	ILE	3.1
1	C	-1	SER	3.2
1	A	87	LEU	3.1
1	A	289	VAL	3.1
1	A	155	LYS	3.0
1	A	138	CYS	2.9
1	A	249	LYS	2.9
1	A	247	LEU	2.9
1	C	138	CYS	2.6
1	A	246	ASP	2.6
1	A	309	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	64	VAL	2.6
1	C	156	ASN	2.6
1	A	137	ASP	2.5
1	A	67	VAL	2.5
1	A	100	GLU	2.5
1	A	196	ILE	2.5
1	C	66	LEU	2.5
1	C	102	ASN	2.4
1	A	84	ILE	2.4
1	A	192	LEU	2.3
1	C	136	ILE	2.3
1	A	99	LYS	2.3
1	A	186	PHE	2.3
1	C	0	HIS	2.3
1	A	288	SER	2.3
1	A	154	GLN	2.3
1	C	101	LYS	2.3
1	A	269	ARG	2.3
1	A	72	TYR	2.2
1	A	267	TYR	2.2
1	C	316	VAL	2.2
1	A	86	ILE	2.2
1	A	150	VAL	2.2
1	C	267	TYR	2.1
1	C	67	VAL	2.1
1	A	140	ILE	2.1
1	A	149	ASP	2.1
1	A	63	GLN	2.1
1	A	158	VAL	2.1
1	A	195	GLU	2.1
1	C	135	ILE	2.1
1	C	228	LYS	2.0
1	A	307	MET	2.0
1	A	101	LYS	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](#)

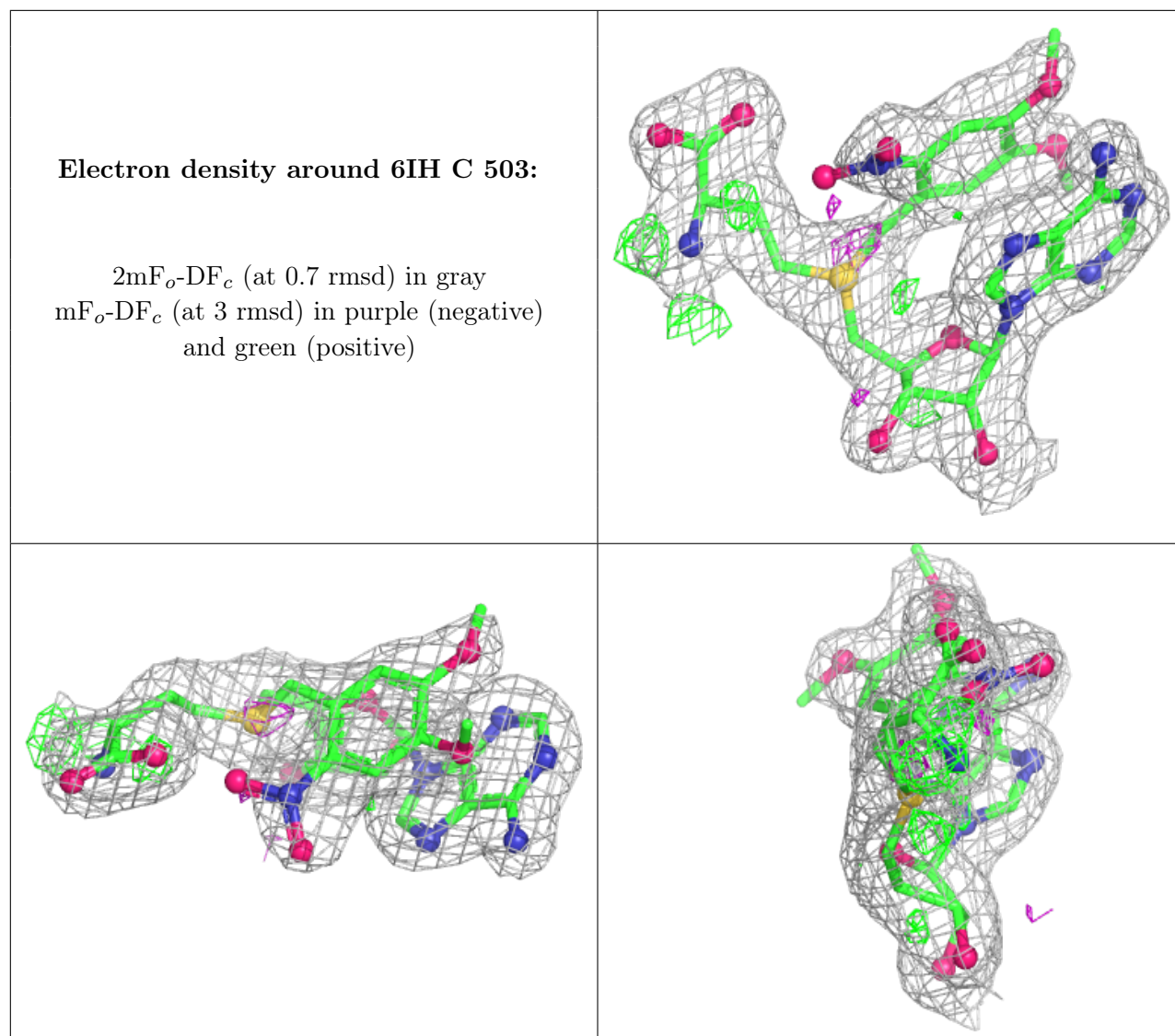
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	A	503	1/1	0.87	0.28	53,53,53,53	0
4	6IH	C	503	40/40	0.90	0.14	25,35,59,61	0
2	3PO	C	501	13/13	0.95	0.13	22,28,36,37	0
2	3PO	A	501	13/13	0.98	0.09	26,30,34,35	0
3	MG	A	502	1/1	0.98	0.10	28,28,28,28	0
3	MG	C	502	1/1	0.99	0.13	27,27,27,27	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.