

Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 01:07 AM EDT

PDB ID	:	2PB6
Title	:	Crystal structure of PH0725 from Pyrococcus horikoshii OT3
Authors	:	Yamamoto, H.; Taketa, M.; Ono, N.; Matsuura, Y.; Kunishima, N.; RIKEN
		Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-28
Resolution	:	2.20 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

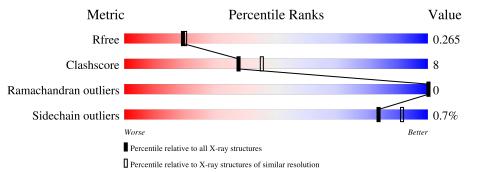
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	:::::::::::::::::::::::::::::::::::::::	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	4898 (2.20-2.20)		
Clashscore	141614	5594 (2.20-2.20)		
Ramachandran outliers	138981	5503 (2.20-2.20)		
Sidechain outliers	138945	5504 (2.20-2.20)		

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%

Mol	Chain	Length	Quality of chain	
1	А	265	86%	14%
1	В	265	80%	20%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4555 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.

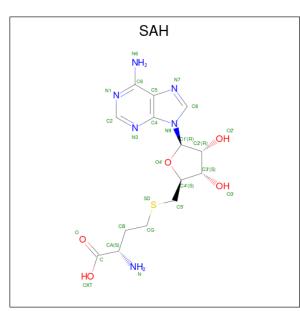
• Molecule 1 is a protein called Probable diphthine synthase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A 26	265	Total	С	Ν	0	S	1	0	0
		203	2080	1344	346	382	8	1		
1	р	265	Total	С	Ν	0	S	2	0	0
1	D	265	2080	1344	346	382	8	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	220	CYS	TYR	engineered mutation	UNP O58456
В	220	CYS	TYR	engineered mutation	UNP O58456

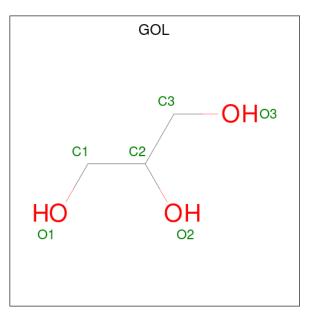
• Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	А	1	Total 26	C 14	N 6	O 5	S 1	0	0

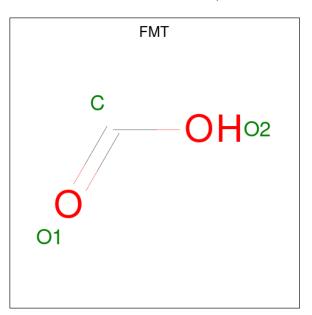


• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 3	C 1	O 2	0	0



• Molecule 5 is water.

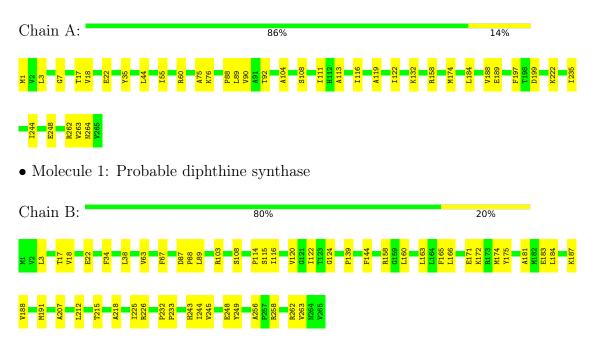
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	162	Total O 162 162	0	0
5	В	192	Total O 192 192	0	0



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. 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: Probable diphthine synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	104.79Å 104.79Å 139.74Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 - 2.20	Depositor
Resolution (A)	19.72 - 2.19	EDS
% Data completeness	99.9 (19.76-2.20)	Depositor
(in resolution range)	99.7(19.72-2.19)	EDS
R _{merge}	0.06	Depositor
R _{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$4.01 (at 2.19 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
D D.	0.203 , 0.221	Depositor
R, R_{free}	0.256 , 0.265	DCC
R_{free} test set	1996 reflections (4.95%)	wwPDB-VP
Wilson B-factor $(Å^2)$	38.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 39.8	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	0.93	EDS
Total number of atoms	4555	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: FMT, SAH, GOL

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		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/2120	0.60	0/2871	
1	В	0.36	0/2120	0.63	0/2871	
All	All	0.35	0/4240	0.62	0/5742	

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	А	2080	0	2137	24	0
1	В	2080	0	2137	47	1
2	А	26	0	19	2	0
3	В	12	0	14	3	0
4	В	3	0	1	0	0
5	А	162	0	0	0	0
5	В	192	0	0	0	1
All	All	4555	0	4308	65	1

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 8.



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:38:LEU:CD2	3:B:402:GOL:H11	2.08	0.83
1:B:38:LEU:HD22	3:B:402:GOL:H11	1.65	0.78
1:B:144:PHE:CE1	1:B:191:MET:HE1	2.22	0.74
1:B:244:ILE:O	1:B:248:GLU:HG3	1.88	0.73
1:A:132:LYS:HD2	1:B:160:LEU:HD21	1.71	0.73
1:A:235:ILE:HG23	2:A:301:SAH:N3	2.03	0.72
1:B:171:GLU:CD	1:B:171:GLU:H	1.94	0.67
1:B:38:LEU:HD12	1:B:175:TYR:OH	1.96	0.65
1:B:144:PHE:CE1	1:B:191:MET:CE	2.81	0.64
1:A:263:VAL:HG12	1:A:264:ASN:O	1.97	0.63
1:B:38:LEU:HD23	3:B:402:GOL:H11	1.80	0.62
1:B:18:VAL:O	1:B:22:GLU:HG3	2.00	0.62
1:B:207:ALA:HB3	1:B:215:THR:HB	1.82	0.59
1:B:38:LEU:CD1	1:B:175:TYR:OH	2.51	0.58
1:B:139:PRO:HD3	1:B:184:LEU:HD11	1.87	0.57
1:A:1:MET:HA	1:A:75:ALA:O	2.05	0.56
1:A:17:THR:HA	1:B:17:THR:HA	1.88	0.55
1:B:144:PHE:CD1	1:B:191:MET:HE1	2.42	0.55
1:B:38:LEU:HB2	1:B:175:TYR:OH	2.07	0.54
1:B:232:PRO:HB3	1:B:233:PRO:HA	1.90	0.54
1:A:18:VAL:O	1:A:22:GLU:HG3	2.08	0.53
1:A:199:ASP:HB3	1:A:222:LYS:HB3	1.90	0.53
1:A:158:ARG:HD3	1:B:158:ARG:CZ	2.38	0.53
1:B:166:LEU:HD22	1:B:181:ALA:HB2	1.93	0.51
1:B:226:ARG:NH1	1:B:226:ARG:HB2	2.25	0.51
1:A:1:MET:HG2	1:A:1:MET:O	2.12	0.50
1:B:225:ILE:HG23	1:B:226:ARG:HG3	1.94	0.50
1:B:184:LEU:O	1:B:188:VAL:HG23	2.12	0.50
1:A:116:ILE:HG12	1:A:235:ILE:HG21	1.94	0.48
1:B:87:ASP:OD1	1:B:88:PRO:HD2	2.13	0.48
1:A:184:LEU:O	1:A:188:VAL:HG23	2.14	0.47
1:B:244:ILE:HG23	1:B:245:VAL:N	2.30	0.47
1:A:235:ILE:CG2	2:A:301:SAH:H1'	2.45	0.47
1:B:226:ARG:HB2	1:B:226:ARG:HH11	1.80	0.46
1:B:172:LYS:O	1:B:174:MET:HG3	2.15	0.46
1:A:44:LEU:HD11	1:A:55:ILE:HB	1.98	0.46
1:B:63:VAL:O	1:B:67:PHE:HB2	2.16	0.45
1:B:144:PHE:CZ	1:B:187:LYS:HE3	2.51	0.45
1:B:116:ILE:HG21	1:B:165:PHE:HE2	1.81	0.45
1:A:35:TYR:CE2	1:A:60:ARG:HA	2.53	0.45

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Continued on next page...



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:89:LEU:HD12	1:B:122:ILE:HA	2.00	0.44
1:B:103:ARG:HH11	1:B:103:ARG:HG3	1.83	0.44
1:A:3:LEU:O	1:A:108:SER:HA	2.19	0.43
1:B:3:LEU:O	1:B:108:SER:HA	2.19	0.43
1:B:243:HIS:CD2	1:B:244:ILE:HG22	2.54	0.43
1:B:124:GLY:HA3	1:B:249:TYR:CD1	2.53	0.43
1:B:144:PHE:HZ	1:B:187:LYS:HE3	1.83	0.43
1:A:76:LYS:HE2	1:A:104:ALA:O	2.19	0.42
1:B:88:PRO:O	1:B:89:LEU:HB2	2.19	0.42
1:A:119:ALA:O	1:A:122:ILE:HG22	2.18	0.42
1:B:218:ALA:HB3	1:B:256:ALA:HB2	2.02	0.42
1:B:116:ILE:HG21	1:B:165:PHE:CE2	2.55	0.42
1:B:262:ARG:HG3	1:B:263:VAL:N	2.35	0.42
1:B:87:ASP:HB2	1:B:115:SER:HB2	2.01	0.42
1:A:111:ILE:HD11	1:B:212:LEU:HD21	2.02	0.42
1:A:90:VAL:O	1:A:92:THR:HG23	2.19	0.41
1:A:244:ILE:O	1:A:248:GLU:HG3	2.21	0.41
1:B:116:ILE:O	1:B:120:VAL:HG13	2.20	0.41
1:A:7:GLY:CA	1:A:88:PRO:HD3	2.50	0.41
1:B:183:GLU:HG2	1:B:225:ILE:HD11	2.03	0.41
1:B:244:ILE:CG2	1:B:245:VAL:N	2.84	0.41
1:A:113:ALA:CA	1:B:114:PRO:HG3	2.50	0.41
1:A:189:GLU:HG2	1:A:197:PHE:O	2.21	0.40
1:B:34:PHE:HB3	1:B:38:LEU:HD23	2.02	0.40
1:B:120:VAL:HG11	1:B:163:LEU:HD13	2.03	0.40

Continued from previous page...

All (1) 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)
1:B:248:GLU:OE2	5:B:681:HOH:O[3_655]	1.99	0.21

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	263/265~(99%)	258~(98%)	5(2%)	0	100	100
1	В	263/265~(99%)	256~(97%)	7 (3%)	0	100	100
All	All	526/530~(99%)	514 (98%)	12 (2%)	0	100	100

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

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	А	222/222 (100%)	220~(99%)	2(1%)	78 88		
1	В	222/222 (100%)	221 (100%)	1 (0%)	88 94		
All	All	444/444 (100%)	441 (99%)	3 (1%)	84 91		

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

Mol	Chain	Res	Type
1	А	174	MET
1	А	262	ARG
1	В	258	ARG

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

Mol	Chain	Res	Type
1	А	66	ASN
1	А	69	ASN
1	А	142	ASN
1	В	48	GLN
1	В	142	ASN



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)

4 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).

Mal	Mol Type Chain H		Res	Link	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	А	301	-	24,28,28	2.02	4 (16%)	25,40,40	1.82	8 (32%)
4	FMT	В	501	-	2,2,2	1.89	1 (50%)	1,1,1	0.62	0
3	GOL	В	401	-	$5,\!5,\!5$	0.88	0	$5,\!5,\!5$	0.22	0
3	GOL	В	402	-	$5,\!5,\!5$	0.93	0	$5,\!5,\!5$	0.24	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	SAH	А	301	-	-	0/11/31/31	0/3/3/3
3	GOL	В	401	-	-	0/4/4/4	-
3	GOL	В	402	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	А	301	SAH	O4'-C1'	7.49	1.51	1.41
2	А	301	SAH	C2-N3	3.63	1.37	1.32
2	А	301	SAH	C8-N7	-2.48	1.30	1.34
4	В	501	FMT	01-C	2.38	1.34	1.22
2	А	301	SAH	C2'-C1'	2.32	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	301	SAH	O4'-C1'-C2'	-4.44	100.44	106.93
2	А	301	SAH	N3-C2-N1	-3.42	123.33	128.68
2	А	301	SAH	C2-N1-C6	2.68	123.35	118.75
2	А	301	SAH	CB-CG-SD	-2.66	107.34	113.31
2	А	301	SAH	C5-C6-N6	2.48	124.12	120.35
2	А	301	SAH	CB-CA-N	2.48	116.66	110.17
2	А	301	SAH	C5-C6-N1	-2.45	114.79	120.35
2	А	301	SAH	C1'-N9-C4	-2.29	122.62	126.64

There are no chirality outliers.

There are no torsion outliers.

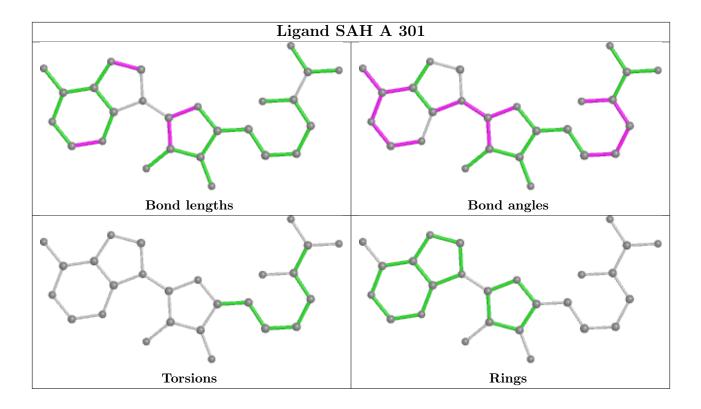
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	301	SAH	2	0
3	В	402	GOL	3	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.





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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

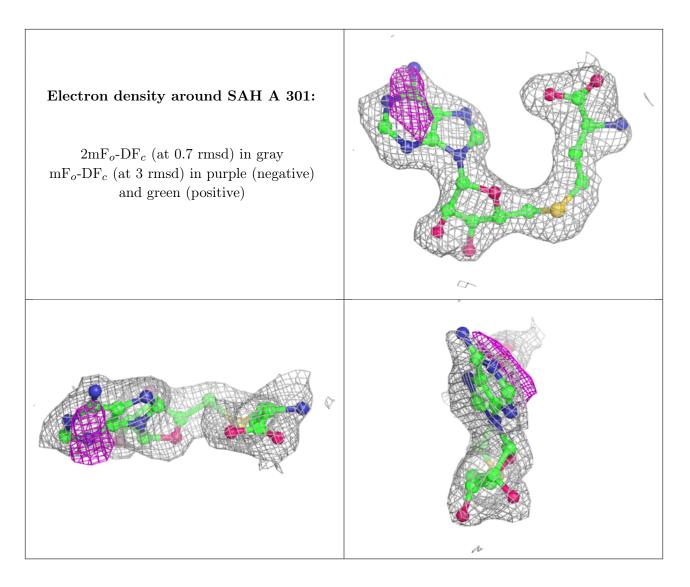
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

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.

