



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:10 AM EDT

PDB ID : 2PB5 / pdb_00002pb5
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 : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

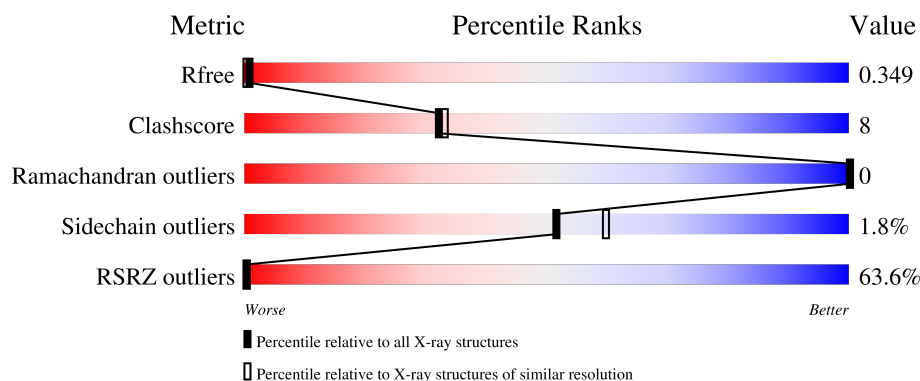
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	265	63% 86% 13% .
1	B	265	64% 78% 21% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4647 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.

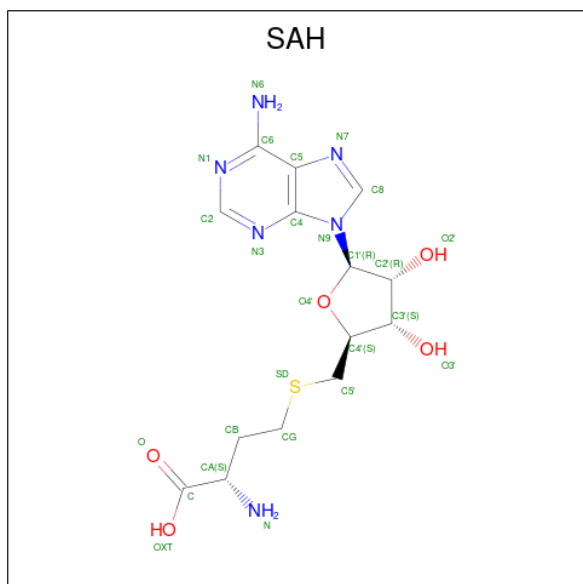
- Molecule 1 is a protein called diphthine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2086	1349	346	383	8			
1	B	265	Total	C	N	O	S	0	0	0
			2086	1349	346	383	8			

There are 2 discrepancies between the modelled and reference sequences:

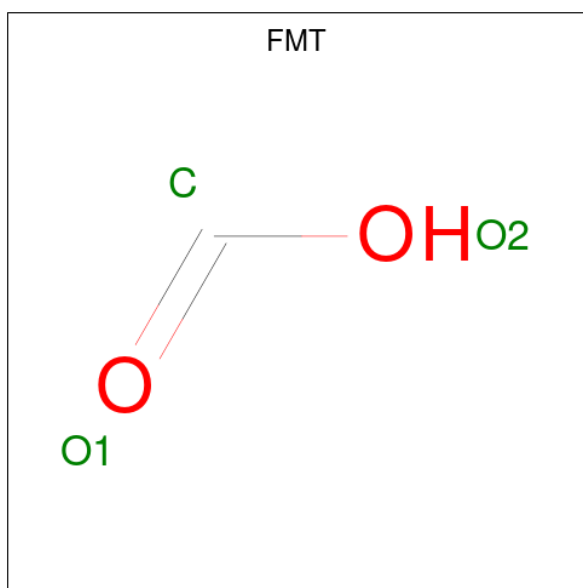
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	LEU	engineered mutation	UNP O58456
B	74	MET	LEU	engineered mutation	UNP O58456

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



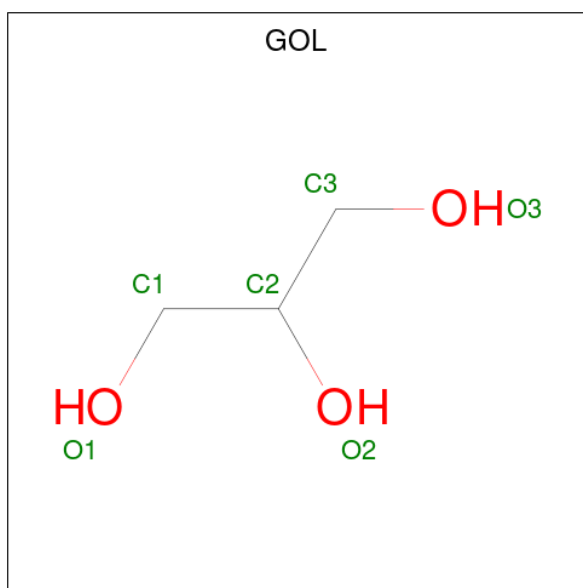
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

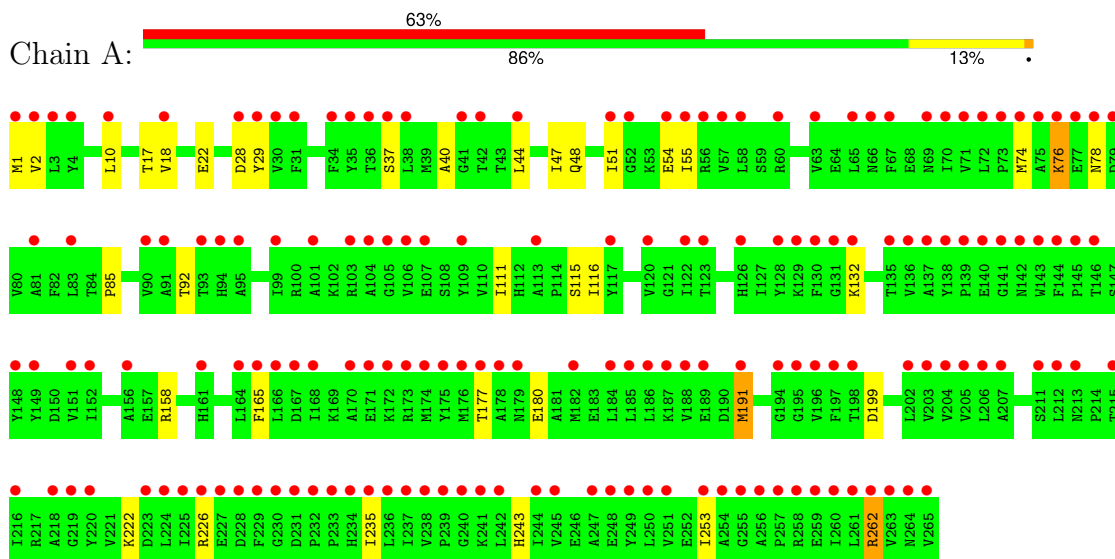
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	208	Total 208	O 208	0	0
5	B	232	Total 232	O 232	0	0

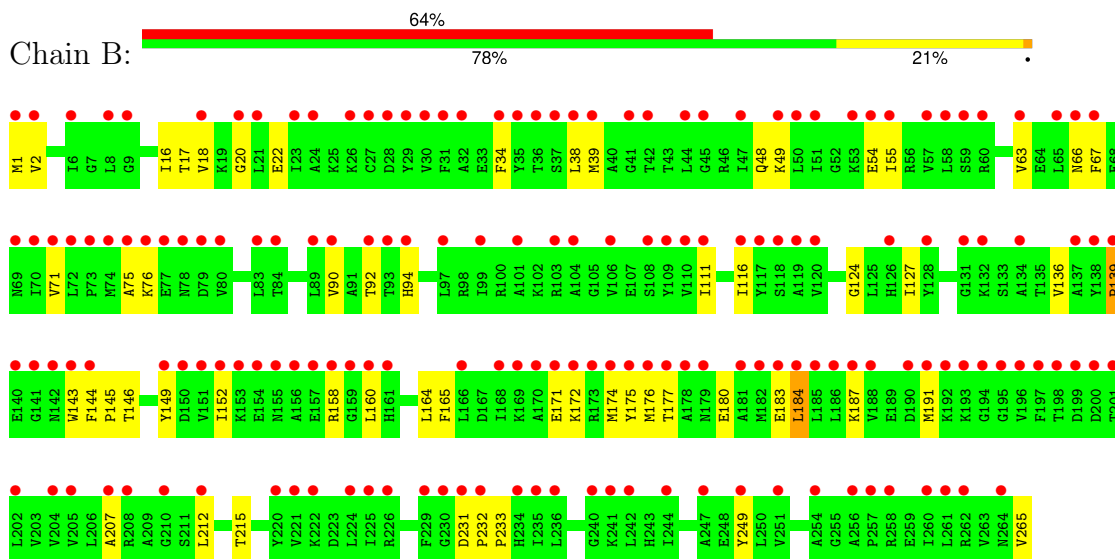
3 Residue-property plots

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: diphthine synthase



• Molecule 1: diphthine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 104.79Å 139.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.10 19.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.77-2.10) 99.8 (19.77-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.230 0.349 , 0.349	Depositor DCC
R_{free} test set	2286 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4647	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, SAH, FMT

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	0.39	0/2127	0.91	5/2880 (0.2%)
1	B	0.41	0/2127	0.91	8/2880 (0.3%)
All	All	0.40	0/4254	0.91	13/5760 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ILE	N-CA-C	-6.76	102.68	110.05
1	A	243	HIS	N-CA-C	-5.91	101.77	110.52
1	B	66	ASN	N-CA-C	5.56	119.71	111.87
1	B	90	VAL	N-CA-C	-5.45	105.53	110.82
1	A	165	PHE	N-CA-C	-5.43	102.84	110.50
1	A	40	ALA	N-CA-C	5.40	119.13	112.54
1	B	139	PRO	N-CA-C	-5.30	103.23	111.13
1	A	92	THR	N-CA-C	-5.28	101.28	109.14
1	B	94	HIS	N-CA-C	5.25	117.08	111.36
1	B	92	THR	N-CA-C	5.15	119.86	111.37
1	B	71	VAL	N-CA-C	5.12	115.79	110.82
1	A	253	ILE	N-CA-C	5.07	116.17	111.81
1	B	54	GLU	N-CA-C	-5.06	103.37	110.50

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	2086	0	2139	32	0
1	B	2086	0	2139	40	0
2	A	26	0	19	2	0
3	A	3	0	1	0	0
4	B	6	0	7	3	0
5	A	208	0	0	3	0
5	B	232	0	0	1	0
All	All	4647	0	4305	68	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 8.

All (68) 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:B:144:PHE:CZ	1:B:191:MET:HE1	2.07	0.90
1:B:38:LEU:HD22	4:B:601:GOL:H11	1.59	0.82
1:B:144:PHE:CZ	1:B:191:MET:CE	2.66	0.79
1:A:191:MET:HA	1:A:191:MET:HE2	1.65	0.78
1:B:171:GLU:CD	1:B:171:GLU:H	1.93	0.77
1:B:38:LEU:HD12	1:B:175:TYR:OH	1.86	0.74
1:B:144:PHE:CE2	1:B:191:MET:HE1	2.23	0.74
1:A:76:LYS:HA	1:A:76:LYS:HE3	1.70	0.74
1:A:74:MET:HA	1:A:74:MET:HE2	1.71	0.72
1:B:1:MET:HA	1:B:75:ALA:O	1.90	0.72
1:A:1:MET:HG3	1:A:2:VAL:HG13	1.78	0.65
1:A:226:ARG:NH1	5:A:880:HOH:O	2.30	0.64
1:A:158:ARG:HD3	1:B:158:ARG:CZ	2.28	0.63
1:A:18:VAL:O	1:A:22:GLU:HG3	2.01	0.61
1:A:76:LYS:HA	1:A:76:LYS:CE	2.30	0.61
1:A:132:LYS:HD2	1:B:160:LEU:HD21	1.83	0.61
1:A:235:ILE:HG23	2:A:501:SAH:N3	2.17	0.60
1:B:38:LEU:CD2	4:B:601:GOL:H11	2.29	0.60
1:A:29:TYR:HE2	1:A:78:ASN:ND2	1.99	0.60
1:A:199:ASP:HB3	1:A:222:LYS:HB3	1.84	0.58
1:B:207:ALA:HB3	1:B:215:THR:HB	1.88	0.56
1:B:1:MET:HG3	1:B:76:LYS:HA	1.87	0.56
1:B:183:GLU:HG3	5:B:817:HOH:O	2.05	0.56
1:B:139:PRO:HD3	1:B:184:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:PRO:HB3	1:B:233:PRO:HA	1.87	0.55
1:A:28:ASP:HB2	1:A:78:ASN:HB3	1.88	0.55
1:A:17:THR:HA	1:B:17:THR:HA	1.90	0.54
1:A:262:ARG:N	1:A:262:ARG:HD3	2.22	0.53
1:B:18:VAL:O	1:B:22:GLU:HG3	2.09	0.53
1:B:48:GLN:HG2	1:B:55:ILE:HG13	1.91	0.53
1:B:116:ILE:HG21	1:B:165:PHE:HE1	1.73	0.53
1:B:144:PHE:CE1	1:B:191:MET:HE1	2.44	0.53
1:B:34:PHE:HB3	1:B:38:LEU:HD23	1.90	0.52
1:B:177:THR:OG1	1:B:180:GLU:HG3	2.09	0.52
1:A:226:ARG:HB2	5:A:765:HOH:O	2.07	0.52
1:A:74:MET:HE2	1:A:74:MET:CA	2.41	0.49
1:A:235:ILE:CG2	2:A:501:SAH:H1'	2.43	0.48
1:A:37:SER:HB3	1:A:85:PRO:HB2	1.93	0.48
1:A:111:ILE:HD11	1:B:212:LEU:HD21	1.96	0.47
1:B:1:MET:O	1:B:1:MET:HG2	2.15	0.47
1:B:144:PHE:CZ	1:B:191:MET:HE2	2.48	0.47
1:B:146:THR:O	1:B:149:TYR:HB3	2.14	0.47
1:B:172:LYS:O	1:B:174:MET:HG3	2.15	0.46
1:A:51:ILE:N	1:A:51:ILE:HD12	2.30	0.46
1:B:232:PRO:CB	1:B:233:PRO:HA	2.45	0.45
1:A:262:ARG:HG3	1:A:262:ARG:HH11	1.81	0.45
1:A:158:ARG:HD2	5:A:778:HOH:O	2.17	0.44
1:A:47:ILE:O	1:A:51:ILE:HD13	2.17	0.44
1:B:124:GLY:HA3	1:B:249:TYR:CD1	2.53	0.44
1:B:152:ILE:HD11	1:B:164:LEU:HD11	1.99	0.44
1:A:28:ASP:CB	1:A:78:ASN:HB3	2.48	0.43
1:B:136:VAL:HG12	1:B:176:MET:HE1	2.00	0.43
1:B:144:PHE:CE2	1:B:187:LYS:HE2	2.54	0.43
1:A:10:LEU:HD21	1:A:115:SER:C	2.43	0.43
1:A:116:ILE:HG12	1:A:235:ILE:HG21	2.01	0.43
1:B:171:GLU:CD	1:B:171:GLU:N	2.71	0.42
1:B:265:VAL:OXT	1:B:265:VAL:HG12	2.20	0.42
1:A:191:MET:HA	1:A:191:MET:CE	2.40	0.42
1:B:144:PHE:CE2	1:B:191:MET:CE	2.95	0.41
1:B:63:VAL:O	1:B:67:PHE:HB2	2.20	0.41
1:B:143:TRP:CD1	1:B:145:PRO:HD3	2.55	0.41
1:A:177:THR:OG1	1:A:180:GLU:HG3	2.20	0.41
1:A:1:MET:H2	1:A:78:ASN:C	2.28	0.41
1:B:20:GLY:HA2	1:B:111:ILE:HG21	2.03	0.41
1:B:39:MET:N	4:B:601:GOL:O1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASP:HA	1:B:232:PRO:HD3	1.95	0.40
1:A:48:GLN:HG2	1:A:55:ILE:HG13	2.03	0.40
1:A:44:LEU:HD11	1:A:55:ILE:HB	2.04	0.40

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	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	B	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
All	All	526/530 (99%)	516 (98%)	10 (2%)	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	A	222/222 (100%)	218 (98%)	4 (2%)	51	60
1	B	222/222 (100%)	218 (98%)	4 (2%)	51	60
All	All	444/444 (100%)	436 (98%)	8 (2%)	51	60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	76	LYS
1	A	191	MET
1	A	262	ARG
1	B	2	VAL
1	B	49	LYS
1	B	127	ILE
1	B	184	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	SAH	A	501	-	27,28,28	1.45	3 (11%)	36,40,40	1.49	7 (19%)
3	FMT	A	701	-	2,2,2	1.81	1 (50%)	1,1,1	0.62	0
4	GOL	B	601	-	5,5,5	0.93	0	5,5,5	0.25	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	A	501	-	-	0/15/31/31	0/3/3/3
4	GOL	B	601	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	O4'-C1'	4.17	1.51	1.42
2	A	501	SAH	C4-N9	2.85	1.43	1.37
3	A	701	FMT	O1-C	2.29	1.34	1.22
2	A	501	SAH	C2-N3	2.23	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAH	N3-C2-N1	-3.52	123.25	128.58
2	A	501	SAH	O4'-C1'-C2'	-3.02	100.15	106.62
2	A	501	SAH	C2-N1-C6	2.87	123.45	118.73
2	A	501	SAH	C1'-N9-C8	2.80	133.30	127.09
2	A	501	SAH	CB-CA-N	2.75	117.28	110.12
2	A	501	SAH	CB-CG-SD	-2.70	107.42	113.45
2	A	501	SAH	O4'-C1'-N9	2.19	112.30	108.09

There are no chirality outliers.

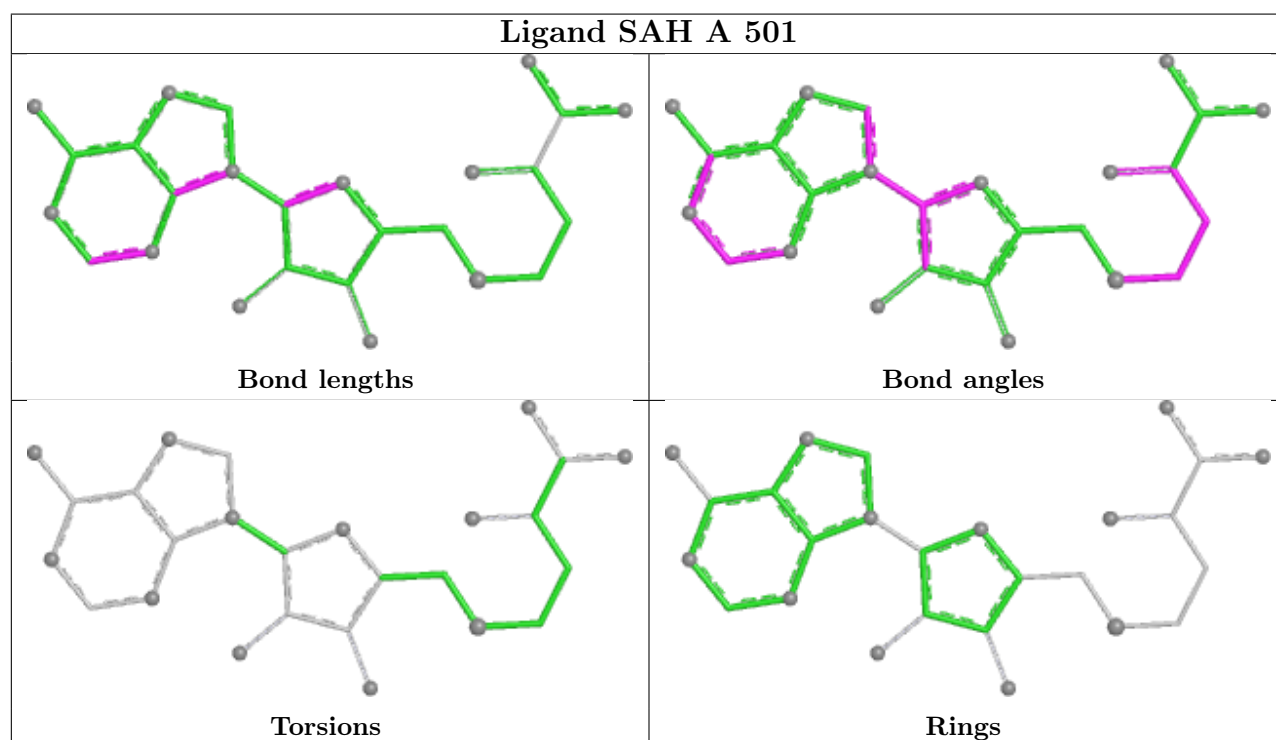
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SAH	2	0
4	B	601	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 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	A	265/265 (100%)	2.45	167 (63%) 0 0	21, 31, 54, 70	0
1	B	265/265 (100%)	2.44	170 (64%) 0 0	22, 30, 50, 62	0
All	All	530/530 (100%)	2.45	337 (63%) 0 0	21, 30, 52, 70	0

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	6.6
1	B	175	TYR	5.8
1	A	261	LEU	5.6
1	A	262	ARG	5.5
1	A	138	TYR	5.3
1	B	132	LYS	5.3
1	A	105	GLY	5.3
1	B	159	GLY	5.2
1	B	1	MET	5.2
1	A	263	VAL	5.1
1	A	229	PHE	5.0
1	A	143	TRP	4.9
1	B	170	ALA	4.9
1	A	128	TYR	4.9
1	B	131	GLY	4.9
1	B	172	LYS	4.9
1	B	74	MET	4.9
1	B	171	GLU	4.8
1	B	58	LEU	4.7
1	A	256	ALA	4.6
1	A	74	MET	4.5
1	A	90	VAL	4.5
1	B	225	ILE	4.5
1	A	257	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	191	MET	4.2
1	B	104	ALA	4.2
1	B	141	GLY	4.2
1	B	197	PHE	4.2
1	A	168	ILE	4.1
1	A	38	LEU	4.1
1	A	175	TYR	4.1
1	A	220	TYR	4.1
1	A	198	THR	4.1
1	A	225	ILE	4.1
1	B	160	LEU	4.0
1	B	128	TYR	4.0
1	A	51	ILE	4.0
1	A	218	ALA	4.0
1	A	219	GLY	4.0
1	A	176	MET	4.0
1	B	195	GLY	4.0
1	A	75	ALA	3.9
1	B	90	VAL	3.9
1	B	55	ILE	3.9
1	A	251	VAL	3.9
1	B	120	VAL	3.9
1	B	190	ASP	3.8
1	A	70	ILE	3.8
1	B	78	ASN	3.8
1	A	196	VAL	3.8
1	B	27	CYS	3.8
1	A	184	LEU	3.8
1	A	204	VAL	3.8
1	B	221	VAL	3.8
1	A	165	PHE	3.8
1	A	130	PHE	3.7
1	B	181	ALA	3.7
1	B	149	TYR	3.7
1	B	178	ALA	3.7
1	A	41	GLY	3.7
1	A	71	VAL	3.7
1	B	188	VAL	3.7
1	B	173	ARG	3.7
1	A	191	MET	3.6
1	A	260	ILE	3.6
1	B	2	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	51	ILE	3.6
1	A	166	LEU	3.6
1	A	247	ALA	3.6
1	B	69	ASN	3.6
1	A	106	VAL	3.5
1	A	203	VAL	3.5
1	B	31	PHE	3.5
1	A	72	LEU	3.5
1	B	151	VAL	3.5
1	B	142	ASN	3.5
1	B	144	PHE	3.5
1	B	156	ALA	3.5
1	A	202	LEU	3.5
1	A	101	ALA	3.5
1	B	32	ALA	3.5
1	B	193	LYS	3.5
1	A	232	PRO	3.4
1	A	67	PHE	3.4
1	A	195	GLY	3.4
1	A	77	GLU	3.4
1	A	173	ARG	3.4
1	B	260	ILE	3.4
1	B	240	GLY	3.4
1	A	226	ARG	3.4
1	A	1	MET	3.4
1	A	207	ALA	3.4
1	A	117	TYR	3.4
1	B	36	THR	3.4
1	B	138	TYR	3.4
1	B	177	THR	3.4
1	B	226	ARG	3.4
1	B	76	LYS	3.4
1	A	174	MET	3.3
1	A	132	LYS	3.3
1	A	164	LEU	3.3
1	B	57	VAL	3.3
1	B	106	VAL	3.3
1	A	144	PHE	3.3
1	A	182	MET	3.3
1	A	137	ALA	3.3
1	A	170	ALA	3.2
1	B	37	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	103	ARG	3.2
1	B	29	TYR	3.2
1	B	186	LEU	3.2
1	B	71	VAL	3.2
1	A	149	TYR	3.2
1	A	242	LEU	3.2
1	B	224	LEU	3.2
1	B	35	TYR	3.1
1	B	158	ARG	3.1
1	B	75	ALA	3.1
1	B	60	ARG	3.1
1	A	58	LEU	3.1
1	A	131	GLY	3.1
1	A	194	GLY	3.1
1	B	34	PHE	3.1
1	B	21	LEU	3.1
1	B	161	HIS	3.1
1	B	26	LYS	3.1
1	A	141	GLY	3.1
1	B	153	LYS	3.1
1	A	212	LEU	3.1
1	B	222	LYS	3.0
1	B	256	ALA	3.0
1	A	120	VAL	3.0
1	A	188	VAL	3.0
1	A	244	ILE	3.0
1	A	103	ARG	3.0
1	A	36	THR	3.0
1	A	73	PRO	3.0
1	A	145	PRO	3.0
1	A	76	LYS	3.0
1	A	185	LEU	3.0
1	B	41	GLY	3.0
1	A	177	THR	3.0
1	A	65	LEU	3.0
1	B	72	LEU	3.0
1	B	198	THR	3.0
1	A	233	PRO	3.0
1	A	54	GLU	2.9
1	A	235	ILE	2.9
1	A	231	ASP	2.9
1	B	154	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	38	LEU	2.9
1	B	110	VAL	2.9
1	B	111	ILE	2.9
1	B	157	GLU	2.9
1	A	211	SER	2.9
1	A	241	LYS	2.9
1	B	89	LEU	2.9
1	B	166	LEU	2.9
1	A	57	VAL	2.9
1	B	196	VAL	2.9
1	A	249	TYR	2.9
1	B	117	TYR	2.9
1	A	178	ALA	2.9
1	A	240	GLY	2.9
1	B	230	GLY	2.9
1	B	182	MET	2.8
1	A	136	VAL	2.8
1	A	206	LEU	2.8
1	B	143	TRP	2.8
1	A	123	THR	2.8
1	A	238	VAL	2.8
1	A	161	HIS	2.8
1	B	140	GLU	2.8
1	A	10	LEU	2.8
1	B	8	LEU	2.8
1	A	139	PRO	2.8
1	A	205	VAL	2.8
1	B	152	ILE	2.8
1	B	169	LYS	2.8
1	B	262	ARG	2.8
1	A	234	HIS	2.8
1	A	254	ALA	2.8
1	B	184	LEU	2.8
1	A	30	VAL	2.8
1	B	66	ASN	2.7
1	B	179	ASN	2.7
1	B	264	ASN	2.7
1	B	9	GLY	2.7
1	B	109	TYR	2.7
1	B	235	ILE	2.7
1	B	28	ASP	2.7
1	A	146	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	2.7
1	B	50	LEU	2.7
1	B	108	SER	2.7
1	B	258	ARG	2.7
1	B	254	ALA	2.6
1	B	242	LEU	2.6
1	B	261	LEU	2.6
1	B	80	VAL	2.6
1	A	78	ASN	2.6
1	A	113	ALA	2.6
1	A	179	ASN	2.6
1	B	134	ALA	2.6
1	B	247	ALA	2.6
1	A	3	LEU	2.6
1	B	229	PHE	2.6
1	A	29	TYR	2.6
1	A	99	ILE	2.6
1	A	122	ILE	2.6
1	B	23	ILE	2.6
1	B	20	GLY	2.6
1	B	42	THR	2.6
1	B	83	LEU	2.6
1	B	139	PRO	2.6
1	A	55	ILE	2.6
1	A	63	VAL	2.6
1	A	107	GLU	2.6
1	A	94	HIS	2.6
1	A	172	LYS	2.6
1	A	186	LEU	2.6
1	B	77	GLU	2.5
1	A	245	VAL	2.5
1	A	264	ASN	2.5
1	B	150	ASP	2.5
1	A	156	ALA	2.5
1	B	185	LEU	2.5
1	B	30	VAL	2.5
1	A	35	TYR	2.5
1	A	167	ASP	2.5
1	B	232	PRO	2.5
1	B	97	LEU	2.5
1	A	253	ILE	2.5
1	B	63	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	37	SER	2.5
1	A	95	ALA	2.5
1	A	104	ALA	2.5
1	B	257	PRO	2.5
1	B	241	LYS	2.5
1	A	60	ARG	2.5
1	A	258	ARG	2.5
1	B	174	MET	2.4
1	B	44	LEU	2.4
1	B	53	LYS	2.4
1	A	255	GLY	2.4
1	B	67	PHE	2.4
1	A	213	ASN	2.4
1	A	152	ILE	2.4
1	B	70	ILE	2.4
1	B	99	ILE	2.4
1	B	204	VAL	2.4
1	B	249	TYR	2.4
1	B	24	ALA	2.4
1	B	137	ALA	2.4
1	A	230	GLY	2.4
1	A	18	VAL	2.4
1	A	93	THR	2.4
1	A	129	LYS	2.4
1	B	220	TYR	2.4
1	A	250	LEU	2.4
1	B	39	MET	2.4
1	B	208	ARG	2.4
1	B	118	SER	2.4
1	A	148	TYR	2.3
1	A	91	ALA	2.3
1	A	52	GLY	2.3
1	B	192	LYS	2.3
1	A	237	ILE	2.3
1	A	248	GLU	2.3
1	B	54	GLU	2.3
1	A	109	TYR	2.3
1	B	45	GLY	2.3
1	B	116	ILE	2.3
1	B	244	ILE	2.3
1	B	18	VAL	2.3
1	B	79	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	126	HIS	2.3
1	B	183	GLU	2.3
1	A	151	VAL	2.3
1	B	155	ASN	2.3
1	A	56	ARG	2.3
1	B	210	GLY	2.3
1	A	140	GLU	2.2
1	A	227	GLU	2.2
1	A	187	LYS	2.2
1	A	79	ASP	2.2
1	B	176	MET	2.2
1	A	236	LEU	2.2
1	B	65	LEU	2.2
1	B	6	ILE	2.2
1	B	93	THR	2.2
1	B	201	THR	2.2
1	A	2	VAL	2.2
1	B	205	VAL	2.2
1	A	28	ASP	2.2
1	B	202	LEU	2.2
1	B	236	LEU	2.2
1	A	142	ASN	2.2
1	A	42	THR	2.2
1	A	239	PRO	2.2
1	B	84	THR	2.2
1	B	168	ILE	2.2
1	B	231	ASP	2.2
1	B	126	HIS	2.2
1	A	66	ASN	2.2
1	A	215	THR	2.2
1	A	223	ASP	2.2
1	A	171	GLU	2.1
1	B	251	VAL	2.1
1	B	94	HIS	2.1
1	B	234	HIS	2.1
1	B	101	ALA	2.1
1	B	207	ALA	2.1
1	B	212	LEU	2.1
1	B	200	ASP	2.1
1	B	92	THR	2.1
1	A	31	PHE	2.1
1	A	34	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	59	SER	2.1
1	A	69	ASN	2.1
1	A	228	ASP	2.1
1	B	47	ILE	2.1
1	B	49	LYS	2.1
1	B	187	LYS	2.1
1	B	119	ALA	2.1
1	A	44	LEU	2.1
1	A	4	TYR	2.1
1	A	216	ILE	2.1
1	A	81	ALA	2.1
1	A	259	GLU	2.0
1	A	83	LEU	2.0
1	A	135	THR	2.0
1	B	73	PRO	2.0
1	A	189	GLU	2.0
1	A	197	PHE	2.0
1	B	199	ASP	2.0
1	B	194	GLY	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](#)

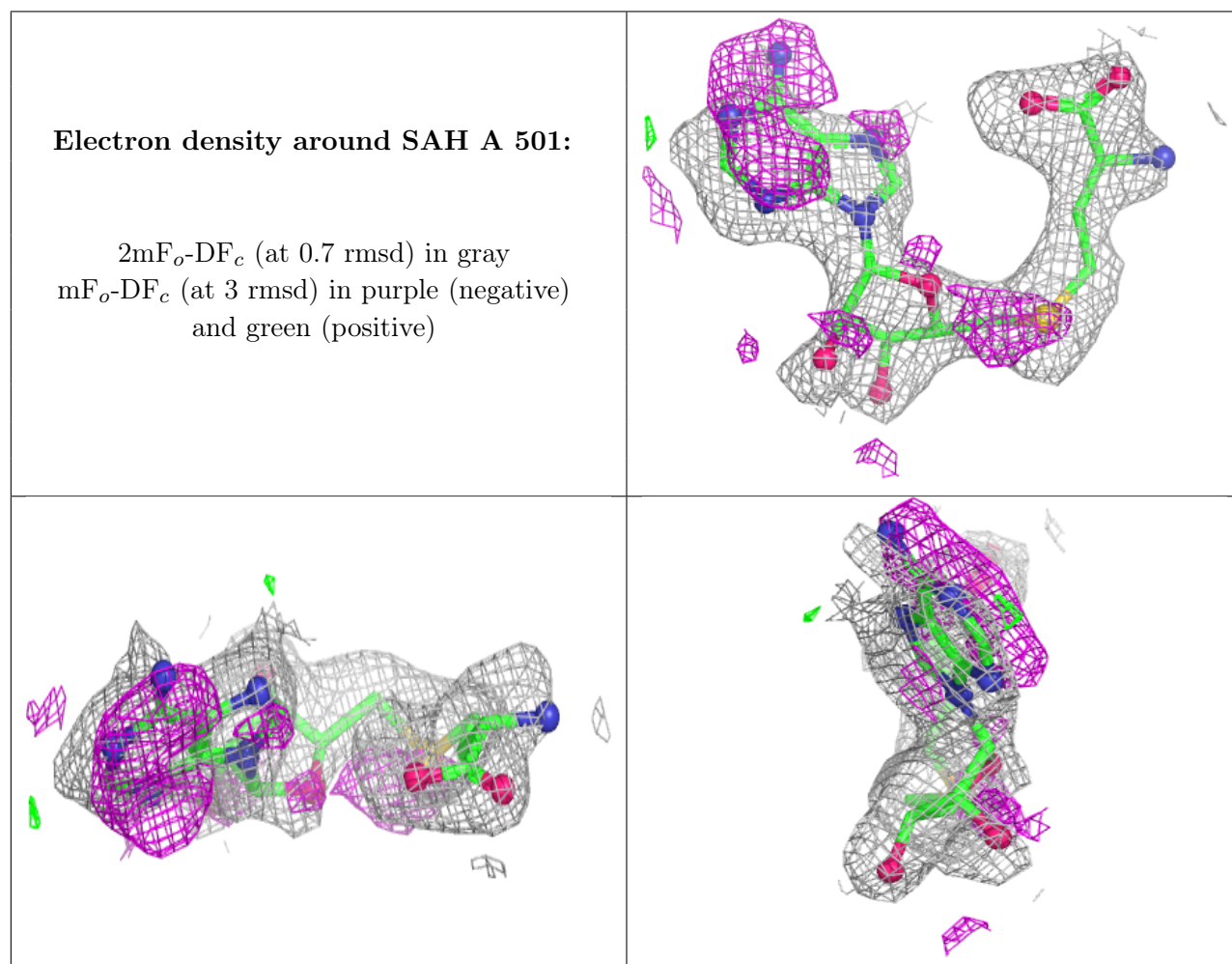
There are no oligosaccharides in this entry.

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	601	6/6	0.53	0.24	60,62,62,64	0
3	FMT	A	701	3/3	0.60	0.32	62,62,62,62	0
2	SAH	A	501	26/26	0.68	0.17	22,25,34,34	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 ⓘ

There are no such residues in this entry.