



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:15 pm GMT

PDB ID : 2PB5  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

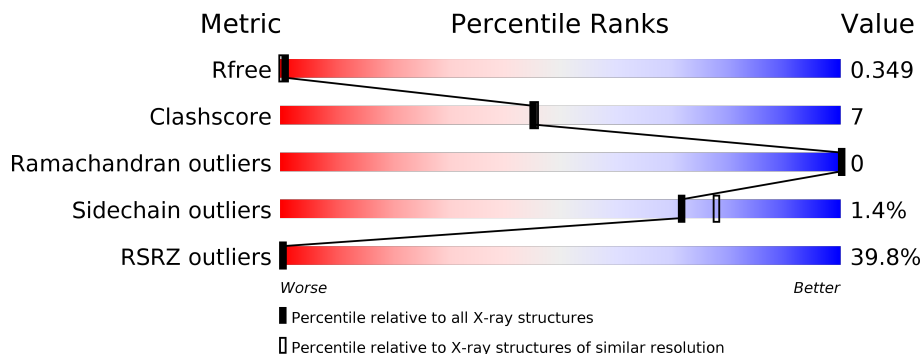
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>40%</div> <div>89%</div> <div>11%</div> </div>
1	B	265	<div> <div>39%</div> <div>82%</div> <div>17%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	A	701	-	-	-	X

## 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.

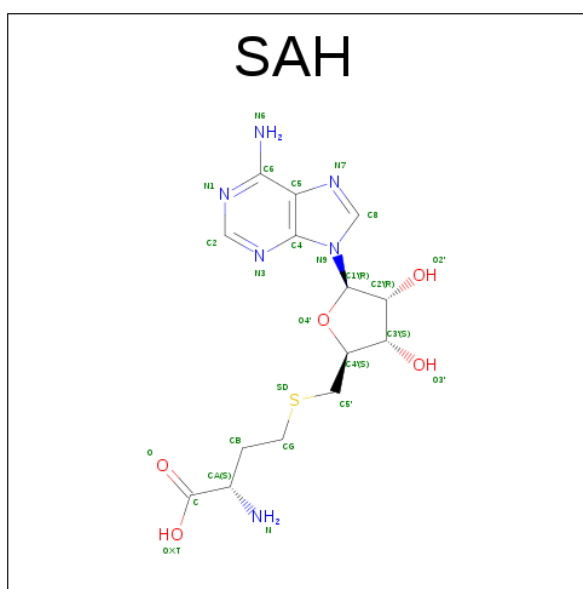
- Molecule 1 is a protein called diphthine synthase.

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	UNP O58456
B	74	MET	LEU	ENGINEERED	UNP O58456

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



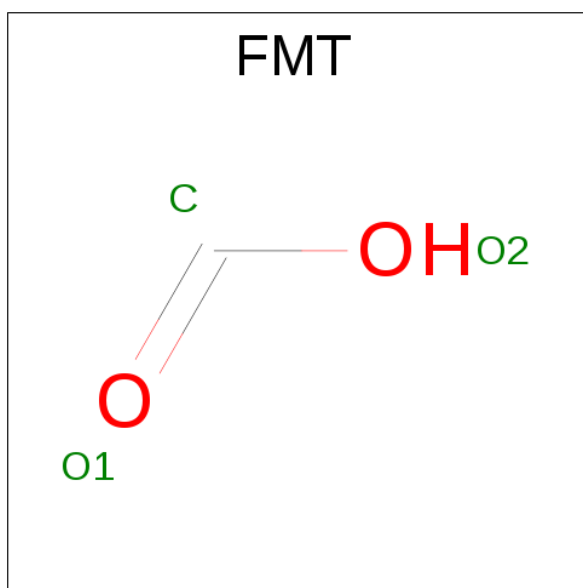
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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



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

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



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

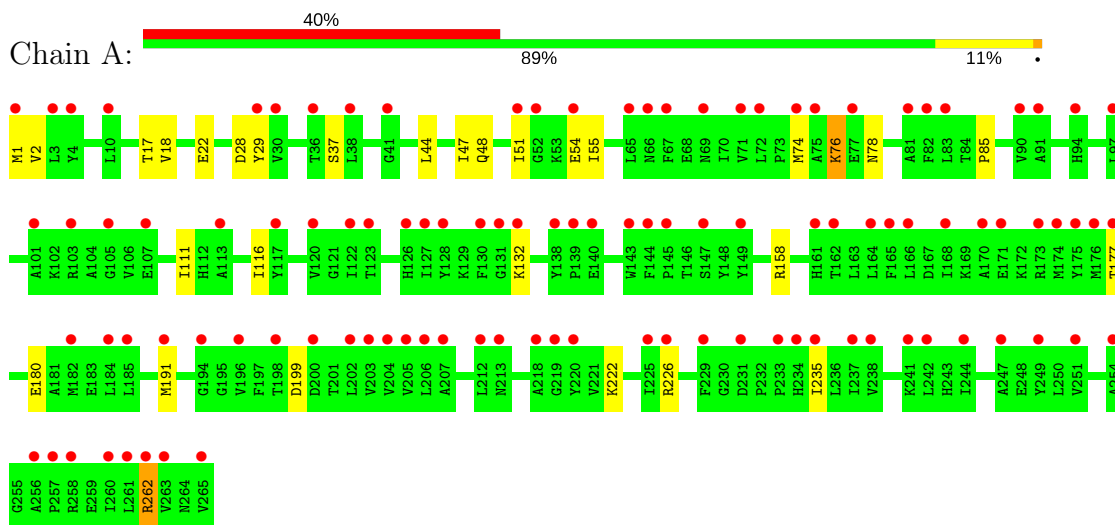
- Molecule 5 is water.

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

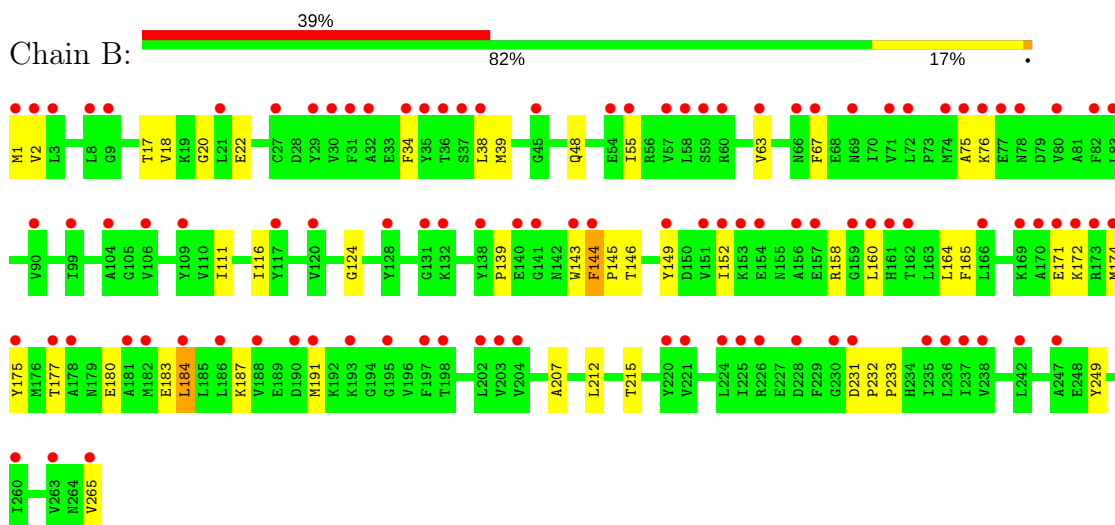
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	104.79Å 104.79Å 139.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.10 19.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.77-2.10) 100.0 (19.72-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.09Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.203 , 0.230 0.350 , 0.349	Depositor DCC
$R_{free}$ test set	2284 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, SAH

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	0.32	0/2127	0.61	0/2880
1	B	0.35	0/2127	0.61	0/2880
All	All	0.34	0/4254	0.61	0/5760

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

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	29	0
1	B	2086	0	2139	38	0
2	A	26	0	19	2	0
3	B	6	0	7	3	0
4	A	3	0	1	0	0
5	A	208	0	0	3	0
5	B	232	0	0	1	0
All	All	4647	0	4305	63	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 7.

All (63) 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:38:LEU:HD22	3:B:601:GOL:H11	1.59	0.82
1:B:144:PHE:CZ	1:B:191:MET:CE	2.66	0.79
1:B:38:LEU:HD12	1:B:175:TYR:OH	1.86	0.74
1:A:76:LYS:HA	1:A:76:LYS:HE3	1.70	0.74
1:B:171:GLU:H	1:B:171:GLU:CD	1.93	0.72
1:B:1:MET:HA	1:B:75:ALA:O	1.90	0.72
1:B:144:PHE:CZ	1:B:191:MET:HE2	2.26	0.71
1:B:144:PHE:CZ	1:B:191:MET:HE1	2.27	0.68
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	3: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
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:116:ILE:HG21	1:B:165:PHE:HE1	1.73	0.53
1:B:48:GLN:HG2	1:B:55:ILE:HG13	1.91	0.53
1:B:177:THR:OG1	1:B:180:GLU:HG3	2.09	0.52
1:B:34:PHE:HB3	1:B:38:LEU:HD23	1.90	0.52
1:A:191:MET:HA	1:A:191:MET:CE	2.40	0.52
1:A:226:ARG:HB2	5:A:765:HOH:O	2.07	0.52
1:B:144:PHE:CE2	1:B:191:MET:CE	2.95	0.50
1:B:144:PHE:CE1	1:B:191:MET:HE1	2.47	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:HG2	1:B:1:MET:O	2.15	0.47
1:B:146:THR:O	1:B:149:TYR:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:174:MET:HG3	2.15	0.46
1:A:51:ILE:HD12	1:A:51:ILE:N	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:B:144:PHE:CE2	1:B:191:MET:HE1	2.51	0.44
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:A:74:MET:HA	1:A:74:MET:HE2	2.01	0.43
1:B:144:PHE:CE2	1:B:187:LYS:HE2	2.54	0.43
1:A:116:ILE:HG12	1:A:235:ILE:HG21	2.01	0.43
1:B:265:VAL:HG12	1:B:265:VAL:OXT	2.20	0.42
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:74:MET:CE	1:A:74:MET:HA	2.51	0.41
1:B:20:GLY:HA2	1:B:111:ILE:HG21	2.03	0.41
1:B:39:MET:N	3:B:601:GOL:O1	2.54	0.41
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	526/530 (99%)	516 (98%)	10 (2%)	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	222/222 (100%)	219 (99%)	3 (1%)	71	78
1	B	222/222 (100%)	219 (99%)	3 (1%)	71	78
All	All	444/444 (100%)	438 (99%)	6 (1%)	71	78

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	76	LYS
1	A	262	ARG
1	B	2	VAL
1	B	144	PHE
1	B	184	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	69	ASN
1	A	78	ASN
1	A	142	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	-	20,28,28	2.19	5 (25%)	20,40,40	2.05	5 (25%)
4	FMT	A	701	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	B	601	-	5,5,5	0.90	0	5,5,5	0.21	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	-	-	0/7/31/31	0/3/3/3
4	FMT	A	701	-	-	0/0/0/0	0/0/0/0
3	GOL	B	601	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	C8-N7	-2.33	1.30	1.34
2	A	501	SAH	C5'-SD	-2.33	1.75	1.81
2	A	501	SAH	C2'-C1'	2.26	1.57	1.53
2	A	501	SAH	C2-N3	3.44	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	O4'-C1'	7.50	1.51	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAH	N3-C2-N1	-6.44	123.25	128.86
2	A	501	SAH	CB-CG-SD	-3.19	107.42	113.57
2	A	501	SAH	C1'-N9-C4	-2.12	122.97	126.64
2	A	501	SAH	CG-CB-CA	2.02	118.77	112.97
2	A	501	SAH	C2-N1-C6	2.67	123.45	118.77

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
3	B	601	GOL	3	0

## 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	265/265 (100%)	1.91	107 (40%) <b>0</b> <b>0</b>	21, 31, 54, 70	0
1	B	265/265 (100%)	1.85	104 (39%) <b>0</b> <b>0</b>	22, 30, 50, 62	0
All	All	530/530 (100%)	1.88	211 (39%) <b>0</b> <b>0</b>	21, 30, 52, 70	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	6.6
1	B	74	MET	5.5
1	A	170	ALA	5.2
1	A	138	TYR	5.2
1	B	171	GLU	5.2
1	A	105	GLY	5.2
1	A	262	ARG	5.0
1	B	175	TYR	4.7
1	A	128	TYR	4.7
1	A	77	GLU	4.6
1	B	1	MET	4.6
1	A	143	TRP	4.5
1	B	226	ARG	4.5
1	A	90	VAL	4.4
1	B	172	LYS	4.4
1	A	1	MET	4.3
1	A	173	ARG	4.3
1	B	77	GLU	4.2
1	A	229	PHE	4.1
1	B	193	LYS	4.1
1	B	58	LEU	4.0
1	A	74	MET	4.0
1	A	140	GLU	3.9
1	B	170	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	225	ILE	3.8
1	A	191	MET	3.8
1	A	226	ARG	3.8
1	A	203	VAL	3.8
1	B	197	PHE	3.7
1	A	3	LEU	3.7
1	A	41	GLY	3.6
1	B	60	ARG	3.6
1	A	164	LEU	3.6
1	B	31	PHE	3.6
1	A	204	VAL	3.5
1	A	65	LEU	3.5
1	B	190	ASP	3.4
1	B	131	GLY	3.4
1	A	175	TYR	3.4
1	B	132	LYS	3.4
1	A	168	ILE	3.4
1	B	174	MET	3.3
1	A	256	ALA	3.3
1	A	225	ILE	3.3
1	A	117	TYR	3.2
1	B	149	TYR	3.2
1	B	83	LEU	3.2
1	A	71	VAL	3.2
1	B	67	PHE	3.2
1	A	238	VAL	3.2
1	A	263	VAL	3.2
1	A	38	LEU	3.2
1	A	101	ALA	3.2
1	B	260	ILE	3.2
1	A	171	GLU	3.2
1	A	130	PHE	3.2
1	B	75	ALA	3.2
1	B	195	GLY	3.2
1	A	219	GLY	3.1
1	A	198	THR	3.1
1	B	55	ILE	3.1
1	A	241	LYS	3.1
1	A	202	LEU	3.1
1	B	80	VAL	3.1
1	B	237	ILE	3.1
1	B	181	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	10	LEU	3.0
1	A	212	LEU	3.0
1	A	81	ALA	3.0
1	B	221	VAL	3.0
1	B	27	CYS	3.0
1	B	177	THR	3.0
1	A	176	MET	3.0
1	B	182	MET	3.0
1	B	160	LEU	3.0
1	B	78	ASN	3.0
1	B	90	VAL	2.9
1	A	261	LEU	2.9
1	B	21	LEU	2.9
1	B	228	ASP	2.9
1	A	29	TYR	2.9
1	B	178	ALA	2.9
1	B	82	PHE	2.9
1	A	166	LEU	2.9
1	A	165	PHE	2.9
1	A	257	PRO	2.9
1	B	34	PHE	2.9
1	B	120	VAL	2.9
1	A	220	TYR	2.8
1	B	37	SER	2.8
1	A	145	PRO	2.8
1	B	29	TYR	2.8
1	A	185	LEU	2.8
1	A	196	VAL	2.8
1	B	30	VAL	2.8
1	B	157	GLU	2.8
1	B	235	ILE	2.8
1	A	218	ALA	2.7
1	A	244	ILE	2.7
1	A	237	ILE	2.7
1	B	152	ILE	2.7
1	B	159	GLY	2.7
1	B	128	TYR	2.7
1	B	203	VAL	2.7
1	A	67	PHE	2.7
1	A	231	ASP	2.7
1	B	71	VAL	2.7
1	A	51	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	144	PHE	2.7
1	B	198	THR	2.7
1	A	54	GLU	2.6
1	B	106	VAL	2.6
1	B	204	VAL	2.6
1	B	35	TYR	2.6
1	A	206	LEU	2.6
1	B	224	LEU	2.6
1	B	173	ARG	2.6
1	A	182	MET	2.6
1	B	138	TYR	2.6
1	A	139	PRO	2.6
1	B	38	LEU	2.6
1	B	144	PHE	2.5
1	B	36	THR	2.5
1	B	45	GLY	2.5
1	B	151	VAL	2.5
1	B	188	VAL	2.5
1	A	162	THR	2.5
1	A	174	MET	2.5
1	A	107	GLU	2.5
1	A	103	ARG	2.5
1	A	258	ARG	2.5
1	B	72	LEU	2.5
1	B	184	LEU	2.5
1	B	57	VAL	2.5
1	A	83	LEU	2.5
1	A	205	VAL	2.5
1	A	4	TYR	2.5
1	A	260	ILE	2.5
1	A	82	PHE	2.4
1	A	123	THR	2.4
1	A	97	LEU	2.4
1	B	236	LEU	2.4
1	A	120	VAL	2.4
1	A	249	TYR	2.4
1	A	254	ALA	2.4
1	A	207	ALA	2.4
1	A	52	GLY	2.4
1	B	153	LYS	2.4
1	B	32	ALA	2.4
1	B	9	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	2.4
1	A	184	LEU	2.3
1	A	242	LEU	2.3
1	A	30	VAL	2.3
1	A	233	PRO	2.3
1	A	72	LEU	2.3
1	A	69	ASN	2.3
1	A	36	THR	2.3
1	B	140	GLU	2.3
1	B	76	LYS	2.3
1	B	2	VAL	2.3
1	A	66	ASN	2.3
1	A	213	ASN	2.3
1	B	3	LEU	2.2
1	A	200	ASP	2.2
1	A	75	ALA	2.2
1	B	247	ALA	2.2
1	A	149	TYR	2.2
1	A	194	GLY	2.2
1	B	109	TYR	2.2
1	B	238	VAL	2.2
1	B	143	TRP	2.2
1	A	235	ILE	2.2
1	B	166	LEU	2.2
1	B	186	LEU	2.2
1	B	202	LEU	2.2
1	A	251	VAL	2.2
1	A	161	HIS	2.2
1	B	63	VAL	2.2
1	B	66	ASN	2.2
1	A	131	GLY	2.2
1	B	162	THR	2.2
1	B	242	LEU	2.1
1	B	230	GLY	2.1
1	A	177	THR	2.1
1	B	104	ALA	2.1
1	A	132	LYS	2.1
1	B	69	ASN	2.1
1	B	99	ILE	2.1
1	B	54	GLU	2.1
1	B	59	SER	2.1
1	B	117	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	94	HIS	2.1
1	A	122	ILE	2.1
1	B	161	HIS	2.1
1	B	8	LEU	2.1
1	B	231	ASP	2.1
1	B	263	VAL	2.1
1	A	247	ALA	2.1
1	B	156	ALA	2.1
1	A	126	HIS	2.1
1	B	169	LYS	2.1
1	B	191	MET	2.0
1	A	113	ALA	2.0
1	B	154	GLU	2.0
1	B	220	TYR	2.0
1	A	127	ILE	2.0
1	B	265	VAL	2.0
1	A	147	SER	2.0
1	A	234	HIS	2.0
1	A	91	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FMT	A	701	3/3	0.71	0.34	10.85	62,62,62,62	0
2	SAH	A	501	26/26	0.74	0.31	1.63	22,25,34,34	0
3	GOL	B	601	6/6	0.67	0.28	0.81	60,62,62,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.