



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 01:16 PM EDT

PDB ID : 1XCJ  
Title : Guanidinoacetate methyltransferase containing S-adenosylhomocysteine and  
guanidinoacetate  
Authors : Komoto, J.; Yamada, T.; Takata, Y.; Takusagawa, F.  
Deposited on : unknown  
Resolution : 2.00 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 : rb-20030345  
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) : rb-20030345

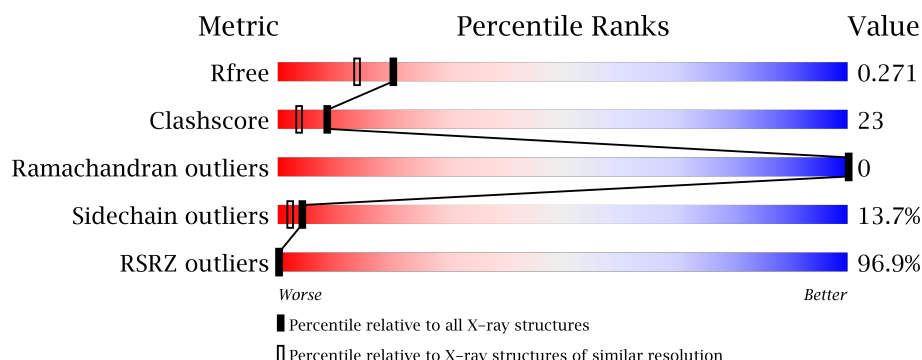
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	235	<div> <div>94%</div> <div>55% 36% 6%</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
3	NMG	A	237	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1910 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.

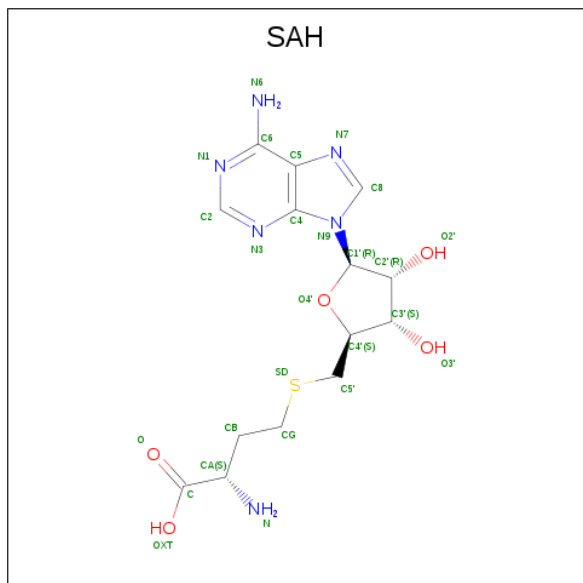
- Molecule 1 is a protein called Guanidinoacetate N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1816	1172	306	326	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

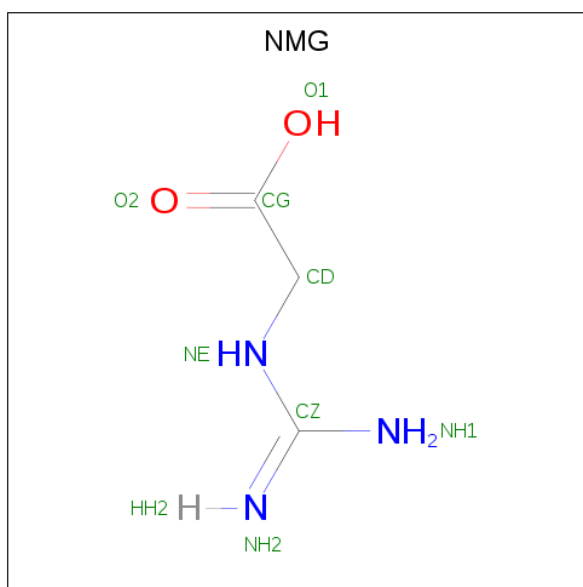
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	VAL	GLU	SEE REMARK 999	UNP P10868

- 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
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0

- Molecule 3 is GUANIDINO ACETATE (three-letter code: NMG) (formula:  $C_3H_7N_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	3	3	2		

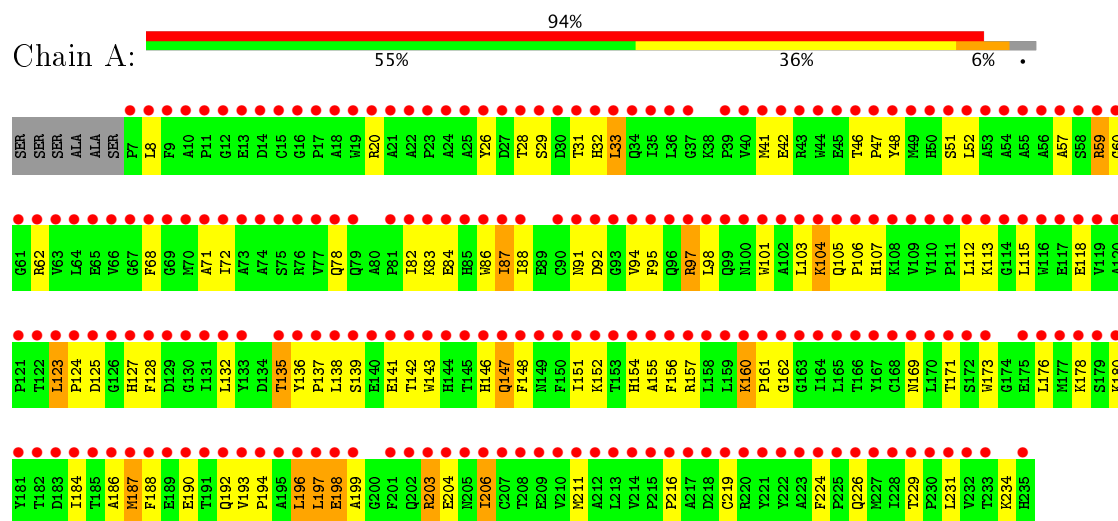
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		

### 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: Guanidinoacetate N-methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.19Å 41.40Å 42.32Å 104.25° 112.67° 104.45°	Depositor
Resolution (Å)	10.00 – 2.00 21.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 82.7 (21.97-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	22.65 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.224 , 0.279 0.220 , 0.271	Depositor DCC
$R_{free}$ test set	1310 reflections (10.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	436.54 , 5.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.45	EDS
Total number of atoms	1910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% 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: NMG, 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	0.38	0/1874	0.64	0/2555

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	1816	0	1770	83	0
2	A	26	0	19	0	0
3	A	8	0	5	2	0
4	A	60	0	0	4	0
All	All	1910	0	1794	83	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 23.

All (83) 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:A:154:HIS:CD2	1:A:157:ARG:HH12	1.75	1.05
1:A:57:ALA:HB1	1:A:82:ILE:HD11	1.42	0.99
1:A:78:GLN:HE22	1:A:107:HIS:H	1.15	0.93
1:A:154:HIS:HD2	1:A:157:ARG:HH12	1.18	0.87
1:A:31:THR:HG23	1:A:32:HIS:ND1	1.90	0.86
1:A:8:LEU:HD23	1:A:171:THR:HG23	1.58	0.85
1:A:78:GLN:HG3	1:A:105:GLN:HE21	1.43	0.84
1:A:147:GLN:HE22	1:A:169:ASN:HD22	1.32	0.77
1:A:147:GLN:H	1:A:147:GLN:HE21	1.34	0.73
1:A:60:GLY:HA2	1:A:82:ILE:HD13	1.71	0.72
1:A:152:LYS:HD3	1:A:198:GLU:HB3	1.71	0.71
1:A:188:PHE:HE1	1:A:206:ILE:HD11	1.55	0.70
1:A:68:PHE:HB2	1:A:87:ILE:HD11	1.75	0.69
1:A:68:PHE:CZ	1:A:71:ALA:HB2	2.29	0.68
1:A:78:GLN:NE2	1:A:107:HIS:H	1.92	0.66
1:A:152:LYS:HG2	1:A:199:ALA:HB2	1.81	0.62
1:A:97:ARG:HB3	1:A:97:ARG:HH11	1.63	0.62
1:A:60:GLY:HA2	1:A:82:ILE:CD1	2.30	0.61
1:A:135:THR:HG22	1:A:146:HIS:CE1	2.36	0.61
1:A:154:HIS:HD2	1:A:157:ARG:NH1	1.93	0.60
1:A:224:PHE:HE2	1:A:226:GLN:HE21	1.49	0.60
1:A:115:LEU:HB2	1:A:118:GLU:HG3	1.84	0.60
1:A:147:GLN:NE2	1:A:169:ASN:HD22	1.99	0.60
1:A:139:SER:OG	1:A:142:THR:HG22	2.01	0.59
1:A:46:THR:HB	1:A:47:PRO:HD3	1.84	0.59
1:A:78:GLN:HG3	1:A:105:GLN:NE2	2.17	0.59
1:A:82:ILE:HG22	1:A:83:LYS:N	2.17	0.59
1:A:135:THR:HG23	1:A:136:TYR:N	2.18	0.59
1:A:26:TYR:CE1	1:A:33:LEU:HG	2.38	0.58
1:A:160:LYS:NZ	1:A:161:PRO:O	2.37	0.58
1:A:62:ARG:HD3	1:A:84:GLU:OE1	2.04	0.57
1:A:206:ILE:O	1:A:206:ILE:HG23	2.05	0.57
1:A:147:GLN:HG2	1:A:148:PHE:N	2.21	0.56
1:A:32:HIS:CD2	1:A:42:GLU:HG2	2.42	0.54
1:A:78:GLN:HE21	1:A:106:PRO:HD2	1.72	0.54
1:A:203:ARG:O	1:A:206:ILE:HG22	2.07	0.54
1:A:197:LEU:HD11	1:A:203:ARG:HG2	1.88	0.54
1:A:188:PHE:CD2	1:A:192:GLN:HG3	2.43	0.53
1:A:78:GLN:HE22	1:A:107:HIS:N	1.96	0.52
1:A:91:ASN:HB3	1:A:94:VAL:HG23	1.92	0.52
1:A:203:ARG:NH2	1:A:206:ILE:O	2.43	0.52
1:A:188:PHE:CE1	1:A:206:ILE:HD11	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HD3	1:A:162:GLY:O	2.11	0.51
1:A:203:ARG:CZ	1:A:206:ILE:HG23	2.41	0.51
1:A:52:LEU:HD23	1:A:229:THR:HG23	1.91	0.51
1:A:204:GLU:HB2	4:A:1005:HOH:O	2.11	0.50
1:A:57:ALA:CB	1:A:82:ILE:HD11	2.29	0.50
1:A:216:PRO:HG2	1:A:219:CYS:HB2	1.94	0.49
1:A:135:THR:CG2	1:A:146:HIS:CE1	2.95	0.49
1:A:104:LYS:HG3	1:A:105:GLN:OE1	2.15	0.47
1:A:125:ASP:OD1	1:A:157:ARG:HD2	2.14	0.47
1:A:137:PRO:HD3	4:A:1009:HOH:O	2.15	0.47
1:A:143:TRP:NE1	1:A:171:THR:HG22	2.31	0.46
1:A:62:ARG:HD2	1:A:86:TRP:CE2	2.51	0.46
1:A:156:PHE:CZ	1:A:234:LYS:HE2	2.51	0.46
1:A:46:THR:HA	1:A:72:ILE:HG21	1.99	0.44
1:A:142:THR:HG21	4:A:1003:HOH:O	2.17	0.44
1:A:97:ARG:CB	1:A:97:ARG:HH11	2.29	0.44
1:A:203:ARG:HA	1:A:206:ILE:HG22	1.99	0.44
1:A:41:MET:SD	3:A:237:NMG:NH1	2.91	0.44
1:A:101:TRP:CH2	1:A:105:GLN:HG3	2.53	0.44
1:A:123:LEU:HA	1:A:124:PRO:HD3	1.83	0.44
1:A:193:VAL:N	1:A:194:PRO:CD	2.81	0.43
1:A:92:ASP:OD1	1:A:113:LYS:CE	2.66	0.43
1:A:186:ALA:O	1:A:190:GLU:HG3	2.18	0.43
1:A:82:ILE:CG2	1:A:83:LYS:N	2.81	0.43
1:A:135:THR:HG22	1:A:146:HIS:HE1	1.80	0.43
1:A:78:GLN:CG	1:A:105:GLN:HE21	2.23	0.43
1:A:187:MET:HG3	1:A:188:PHE:N	2.33	0.43
1:A:173:TRP:CD1	1:A:173:TRP:N	2.87	0.42
1:A:88:ILE:HA	1:A:112:LEU:O	2.19	0.42
1:A:196:LEU:HD23	1:A:206:ILE:HG13	2.01	0.42
1:A:151:ILE:HA	1:A:155:ALA:HB3	2.00	0.42
1:A:62:ARG:HG2	1:A:128:PHE:CD1	2.54	0.42
1:A:211:MET:HG2	4:A:1018:HOH:O	2.20	0.42
1:A:48:TYR:O	1:A:51:SER:HB3	2.20	0.41
1:A:154:HIS:CD2	1:A:157:ARG:NH1	2.60	0.41
1:A:95:PHE:CD2	1:A:98:LEU:HD23	2.56	0.41
1:A:78:GLN:NE2	1:A:106:PRO:HD2	2.33	0.41
1:A:184:ILE:O	1:A:187:MET:HG3	2.22	0.40
1:A:193:VAL:HG12	1:A:197:LEU:HD22	2.04	0.40
1:A:135:THR:O	3:A:237:NMG:HD2	2.21	0.40
1:A:124:PRO:O	1:A:127:HIS:HB2	2.21	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	227/235 (97%)	217 (96%)	10 (4%)	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	190/194 (98%)	164 (86%)	26 (14%)	4	2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	28	THR
1	A	29	SER
1	A	33	LEU
1	A	59	ARG
1	A	87	ILE
1	A	97	ARG
1	A	103	LEU
1	A	104	LYS
1	A	123	LEU

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Mol	Chain	Res	Type
1	A	132	LEU
1	A	135	THR
1	A	138	LEU
1	A	141	GLU
1	A	147	GLN
1	A	160	LYS
1	A	176	LEU
1	A	178	LYS
1	A	180	LYS
1	A	187	MET
1	A	196	LEU
1	A	197	LEU
1	A	198	GLU
1	A	203	ARG
1	A	206	ILE
1	A	231	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	78	GLN
1	A	107	HIS
1	A	147	GLN
1	A	154	HIS
1	A	226	GLN

### 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 carbohydrates 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	SAH	A	236	-	20,28,28	0.98	1 (5%)	20,40,40	1.28	1 (5%)
3	NMG	A	237	-	4,7,7	0.76	0	4,8,8	1.36	1 (25%)

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	236	-	-	0/7/31/31	0/3/3/3
3	NMG	A	237	-	-	0/3/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	236	SAH	C8-N7	-2.09	1.30	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	237	NMG	CD-NE-CZ	2.71	125.04	122.43
2	A	236	SAH	O2'-C2'-C3'	3.67	123.58	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	237	NMG	2	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	229/235 (97%)	5.24	222 (96%) 0 0	9, 16, 26, 32	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	CYS	11.1
1	A	206	ILE	11.0
1	A	66	VAL	10.8
1	A	197	LEU	10.4
1	A	88	ILE	10.2
1	A	151	ILE	10.2
1	A	36	LEU	9.9
1	A	162	GLY	9.9
1	A	214	VAL	9.6
1	A	19	TRP	9.3
1	A	149	ASN	9.1
1	A	97	ARG	8.9
1	A	112	LEU	8.9
1	A	138	LEU	8.8
1	A	82	ILE	8.7
1	A	122	THR	8.6
1	A	143	TRP	8.5
1	A	208	THR	8.4
1	A	230	PRO	8.2
1	A	61	GLY	8.2
1	A	87	ILE	8.2
1	A	164	ILE	8.1
1	A	103	LEU	8.1
1	A	21	ALA	7.8
1	A	110	VAL	7.7
1	A	35	ILE	7.7
1	A	68	PHE	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	18	ALA	7.5
1	A	28	THR	7.5
1	A	173	TRP	7.4
1	A	73	ALA	7.4
1	A	102	ALA	7.4
1	A	131	ILE	7.3
1	A	135	THR	7.3
1	A	187	MET	7.3
1	A	54	ALA	7.2
1	A	72	ILE	7.1
1	A	168	CYS	7.0
1	A	10	ALA	7.0
1	A	142	THR	7.0
1	A	166	THR	6.9
1	A	55	ALA	6.9
1	A	115	LEU	6.9
1	A	210	VAL	6.8
1	A	201	PHE	6.8
1	A	106	PRO	6.8
1	A	215	PRO	6.7
1	A	193	VAL	6.6
1	A	95	PHE	6.6
1	A	120	ALA	6.5
1	A	125	ASP	6.5
1	A	233	THR	6.5
1	A	15	CYS	6.5
1	A	7	PRO	6.4
1	A	161	PRO	6.4
1	A	159	LEU	6.4
1	A	196	LEU	6.4
1	A	232	VAL	6.3
1	A	41	MET	6.3
1	A	23	PRO	6.3
1	A	49	MET	6.3
1	A	176	LEU	6.3
1	A	212	ALA	6.2
1	A	222	TYR	6.2
1	A	165	LEU	6.1
1	A	218	ASP	6.1
1	A	133	TYR	6.1
1	A	121	PRO	6.1
1	A	63	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	60	GLY	6.0
1	A	224	PHE	6.0
1	A	32	HIS	5.9
1	A	64	LEU	5.9
1	A	191	THR	5.9
1	A	188	PHE	5.9
1	A	44	TRP	5.8
1	A	150	PHE	5.8
1	A	171	THR	5.7
1	A	198	GLU	5.6
1	A	90	CYS	5.6
1	A	9	PHE	5.6
1	A	109	VAL	5.6
1	A	128	PHE	5.6
1	A	99	GLN	5.5
1	A	228	ILE	5.5
1	A	71	ALA	5.5
1	A	178	LYS	5.4
1	A	101	TRP	5.4
1	A	136	TYR	5.4
1	A	57	ALA	5.4
1	A	79	GLN	5.4
1	A	94	VAL	5.4
1	A	170	LEU	5.3
1	A	205	ASN	5.3
1	A	145	THR	5.3
1	A	46	THR	5.3
1	A	184	ILE	5.2
1	A	40	VAL	5.2
1	A	48	TYR	5.2
1	A	186	ALA	5.2
1	A	147	GLN	5.2
1	A	185	THR	5.2
1	A	132	LEU	5.2
1	A	25	ALA	5.1
1	A	204	GLU	5.1
1	A	213	LEU	5.1
1	A	172	SER	5.1
1	A	156	PHE	5.1
1	A	225	PRO	5.1
1	A	52	LEU	5.1
1	A	34	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	75	SER	5.0
1	A	217	ALA	5.0
1	A	167	TYR	5.0
1	A	137	PRO	5.0
1	A	104	LYS	4.9
1	A	180	LYS	4.9
1	A	70	MET	4.9
1	A	59	ARG	4.8
1	A	216	PRO	4.8
1	A	231	LEU	4.8
1	A	223	ALA	4.8
1	A	86	TRP	4.8
1	A	146	HIS	4.7
1	A	179	SER	4.7
1	A	229	THR	4.7
1	A	93	GLY	4.7
1	A	123	LEU	4.7
1	A	158	LEU	4.7
1	A	124	PRO	4.7
1	A	26	TYR	4.6
1	A	31	THR	4.6
1	A	183	ASP	4.6
1	A	78	GLN	4.6
1	A	50	HIS	4.6
1	A	30	ASP	4.6
1	A	153	THR	4.6
1	A	181	TYR	4.6
1	A	148	PHE	4.5
1	A	118	GLU	4.5
1	A	203	ARG	4.5
1	A	119	VAL	4.5
1	A	160	LYS	4.5
1	A	81	PRO	4.5
1	A	177	MET	4.4
1	A	47	PRO	4.4
1	A	182	THR	4.4
1	A	116	TRP	4.4
1	A	74	ALA	4.3
1	A	92	ASP	4.3
1	A	17	PRO	4.3
1	A	33	LEU	4.3
1	A	77	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLN	4.2
1	A	157	ARG	4.2
1	A	111	PRO	4.1
1	A	141	GLU	4.1
1	A	107	HIS	4.1
1	A	163	GLY	4.1
1	A	24	ALA	4.1
1	A	192	GLN	4.0
1	A	29	SER	4.0
1	A	113	LYS	4.0
1	A	144	HIS	4.0
1	A	100	ASN	3.9
1	A	83	LYS	3.9
1	A	127	HIS	3.9
1	A	84	GLU	3.9
1	A	11	PRO	3.9
1	A	51	SER	3.9
1	A	39	PRO	3.8
1	A	98	LEU	3.8
1	A	221	TYR	3.8
1	A	69	GLY	3.7
1	A	14	ASP	3.7
1	A	202	GLN	3.7
1	A	199	ALA	3.7
1	A	227	MET	3.7
1	A	20	ARG	3.7
1	A	67	GLY	3.7
1	A	65	GLU	3.7
1	A	45	GLU	3.7
1	A	8	LEU	3.6
1	A	169	ASN	3.6
1	A	155	ALA	3.6
1	A	114	GLY	3.6
1	A	108	LYS	3.6
1	A	56	ALA	3.5
1	A	85	HIS	3.5
1	A	140	GLU	3.5
1	A	37	GLY	3.5
1	A	152	LYS	3.5
1	A	220	ARG	3.5
1	A	190	GLU	3.5
1	A	58	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	PRO	3.4
1	A	130	GLY	3.4
1	A	235	HIS	3.4
1	A	42	GLU	3.4
1	A	13	GLU	3.3
1	A	76	ARG	3.3
1	A	105	GLN	3.3
1	A	53	ALA	3.2
1	A	154	HIS	3.2
1	A	226	GLN	3.2
1	A	27	ASP	3.1
1	A	175	GLU	3.1
1	A	16	GLY	3.0
1	A	117	GLU	2.9
1	A	43	ARG	2.8
1	A	189	GLU	2.8
1	A	139	SER	2.8
1	A	129	ASP	2.8
1	A	195	ALA	2.8
1	A	22	ALA	2.7
1	A	12	GLY	2.7
1	A	62	ARG	2.6
1	A	209	GLU	2.6
1	A	219	CYS	2.5
1	A	126	GLY	2.4
1	A	91	ASN	2.3
1	A	211	MET	2.2

## 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( $\text{\AA}^2$ )	Q<0.9
3	NMG	A	237	8/8	0.79	0.46	0.97	3,3,3,3	0
2	SAH	A	236	26/26	0.60	0.40	-0.24	9,11,15,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.