



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 AM GMT

PDB ID : 2IIP  
Title : Human Nicotinamide N-methyltransferase  
Authors : Bernstein, G.; Min, J.; Wu, H.; Tempel, W.; Zeng, H.; Loppnau, P.; Avvakumov, G.V.; Wasney, G.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-09-28  
Resolution : 2.05 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

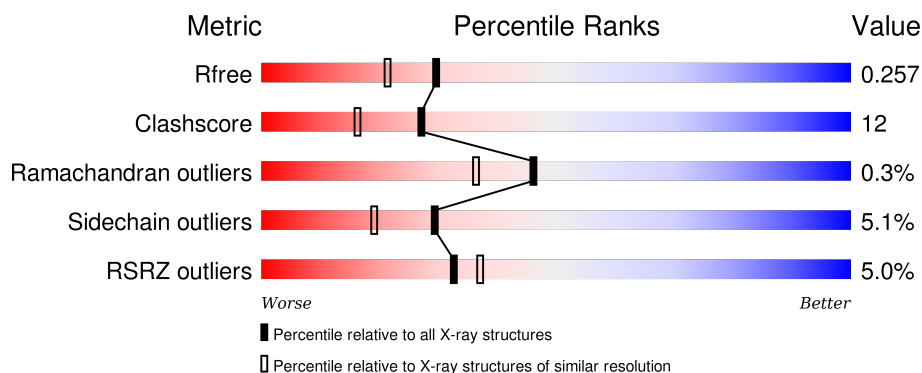
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	283	<div> <div>4%</div> <div>72% 19% • 6%</div> </div>
1	B	283	<div> <div>4%</div> <div>68% 24% • 7%</div> </div>
1	C	283	<div> <div>5%</div> <div>68% 19% • 11%</div> </div>
1	D	283	<div> <div>6%</div> <div>69% 19% • 11%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8481 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 Nicotinamide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			2069	1329	334	394	12			
1	B	264	Total	C	N	O	S	0	2	0
			2070	1329	335	394	12			
1	C	251	Total	C	N	O	S	0	1	0
			1979	1276	318	374	11			
1	D	251	Total	C	N	O	S	0	1	0
			1974	1272	317	374	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	SEE REMARK 999	UNP P40261
A	-17	GLY	-	CLONING ARTIFACT	UNP P40261
A	-16	SER	-	CLONING ARTIFACT	UNP P40261
A	-15	SER	-	CLONING ARTIFACT	UNP P40261
A	-14	HIS	-	EXPRESSION TAG	UNP P40261
A	-13	HIS	-	EXPRESSION TAG	UNP P40261
A	-12	HIS	-	EXPRESSION TAG	UNP P40261
A	-11	HIS	-	EXPRESSION TAG	UNP P40261
A	-10	HIS	-	EXPRESSION TAG	UNP P40261
A	-9	HIS	-	EXPRESSION TAG	UNP P40261
A	-8	SER	-	CLONING ARTIFACT	UNP P40261
A	-7	SER	-	CLONING ARTIFACT	UNP P40261
A	-6	GLY	-	CLONING ARTIFACT	UNP P40261
A	-5	LEU	-	CLONING ARTIFACT	UNP P40261
A	-4	VAL	-	CLONING ARTIFACT	UNP P40261
A	-3	PRO	-	CLONING ARTIFACT	UNP P40261
A	-2	ARG	-	CLONING ARTIFACT	UNP P40261
A	-1	GLY	-	CLONING ARTIFACT	UNP P40261
A	0	SER	-	CLONING ARTIFACT	UNP P40261
A	100	ALA	LYS	ENGINEERED	UNP P40261
A	101	ALA	GLU	ENGINEERED	UNP P40261

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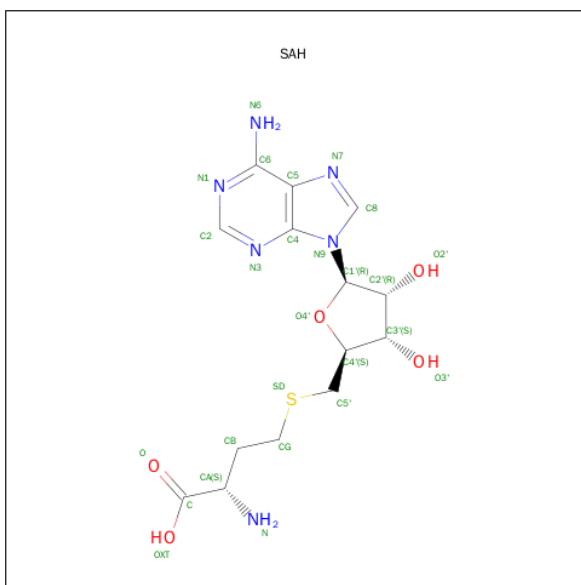
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	GLU	ENGINEERED	UNP P40261
B	-18	MET	-	SEE REMARK 999	UNP P40261
B	-17	GLY	-	CLONING ARTIFACT	UNP P40261
B	-16	SER	-	CLONING ARTIFACT	UNP P40261
B	-15	SER	-	CLONING ARTIFACT	UNP P40261
B	-14	HIS	-	EXPRESSION TAG	UNP P40261
B	-13	HIS	-	EXPRESSION TAG	UNP P40261
B	-12	HIS	-	EXPRESSION TAG	UNP P40261
B	-11	HIS	-	EXPRESSION TAG	UNP P40261
B	-10	HIS	-	EXPRESSION TAG	UNP P40261
B	-9	HIS	-	EXPRESSION TAG	UNP P40261
B	-8	SER	-	CLONING ARTIFACT	UNP P40261
B	-7	SER	-	CLONING ARTIFACT	UNP P40261
B	-6	GLY	-	CLONING ARTIFACT	UNP P40261
B	-5	LEU	-	CLONING ARTIFACT	UNP P40261
B	-4	VAL	-	CLONING ARTIFACT	UNP P40261
B	-3	PRO	-	CLONING ARTIFACT	UNP P40261
B	-2	ARG	-	CLONING ARTIFACT	UNP P40261
B	-1	GLY	-	CLONING ARTIFACT	UNP P40261
B	0	SER	-	CLONING ARTIFACT	UNP P40261
B	100	ALA	LYS	ENGINEERED	UNP P40261
B	101	ALA	GLU	ENGINEERED	UNP P40261
B	103	ALA	GLU	ENGINEERED	UNP P40261
C	-18	MET	-	SEE REMARK 999	UNP P40261
C	-17	GLY	-	CLONING ARTIFACT	UNP P40261
C	-16	SER	-	CLONING ARTIFACT	UNP P40261
C	-15	SER	-	CLONING ARTIFACT	UNP P40261
C	-14	HIS	-	EXPRESSION TAG	UNP P40261
C	-13	HIS	-	EXPRESSION TAG	UNP P40261
C	-12	HIS	-	EXPRESSION TAG	UNP P40261
C	-11	HIS	-	EXPRESSION TAG	UNP P40261
C	-10	HIS	-	EXPRESSION TAG	UNP P40261
C	-9	HIS	-	EXPRESSION TAG	UNP P40261
C	-8	SER	-	CLONING ARTIFACT	UNP P40261
C	-7	SER	-	CLONING ARTIFACT	UNP P40261
C	-6	GLY	-	CLONING ARTIFACT	UNP P40261
C	-5	LEU	-	CLONING ARTIFACT	UNP P40261
C	-4	VAL	-	CLONING ARTIFACT	UNP P40261
C	-3	PRO	-	CLONING ARTIFACT	UNP P40261
C	-2	ARG	-	CLONING ARTIFACT	UNP P40261
C	-1	GLY	-	CLONING ARTIFACT	UNP P40261
C	0	SER	-	CLONING ARTIFACT	UNP P40261

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ALA	LYS	ENGINEERED	UNP P40261
C	101	ALA	GLU	ENGINEERED	UNP P40261
C	103	ALA	GLU	ENGINEERED	UNP P40261
D	-18	MET	-	SEE REMARK 999	UNP P40261
D	-17	GLY	-	CLONING ARTIFACT	UNP P40261
D	-16	SER	-	CLONING ARTIFACT	UNP P40261
D	-15	SER	-	CLONING ARTIFACT	UNP P40261
D	-14	HIS	-	EXPRESSION TAG	UNP P40261
D	-13	HIS	-	EXPRESSION TAG	UNP P40261
D	-12	HIS	-	EXPRESSION TAG	UNP P40261
D	-11	HIS	-	EXPRESSION TAG	UNP P40261
D	-10	HIS	-	EXPRESSION TAG	UNP P40261
D	-9	HIS	-	EXPRESSION TAG	UNP P40261
D	-8	SER	-	CLONING ARTIFACT	UNP P40261
D	-7	SER	-	CLONING ARTIFACT	UNP P40261
D	-6	GLY	-	CLONING ARTIFACT	UNP P40261
D	-5	LEU	-	CLONING ARTIFACT	UNP P40261
D	-4	VAL	-	CLONING ARTIFACT	UNP P40261
D	-3	PRO	-	CLONING ARTIFACT	UNP P40261
D	-2	ARG	-	CLONING ARTIFACT	UNP P40261
D	-1	GLY	-	CLONING ARTIFACT	UNP P40261
D	0	SER	-	CLONING ARTIFACT	UNP P40261
D	100	ALA	LYS	ENGINEERED	UNP P40261
D	101	ALA	GLU	ENGINEERED	UNP P40261
D	103	ALA	GLU	ENGINEERED	UNP P40261

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

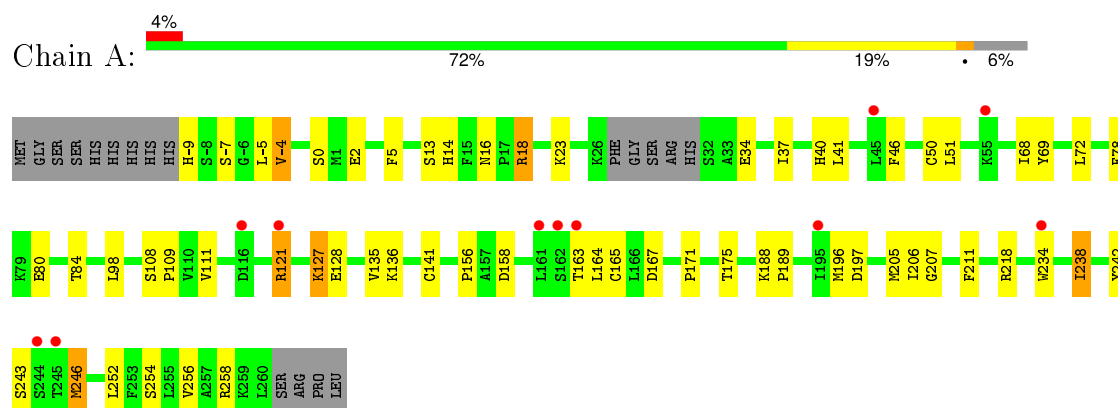
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	75	Total O 75 75	0	0
3	C	64	Total O 64 64	0	0
3	D	64	Total O 64 64	0	0

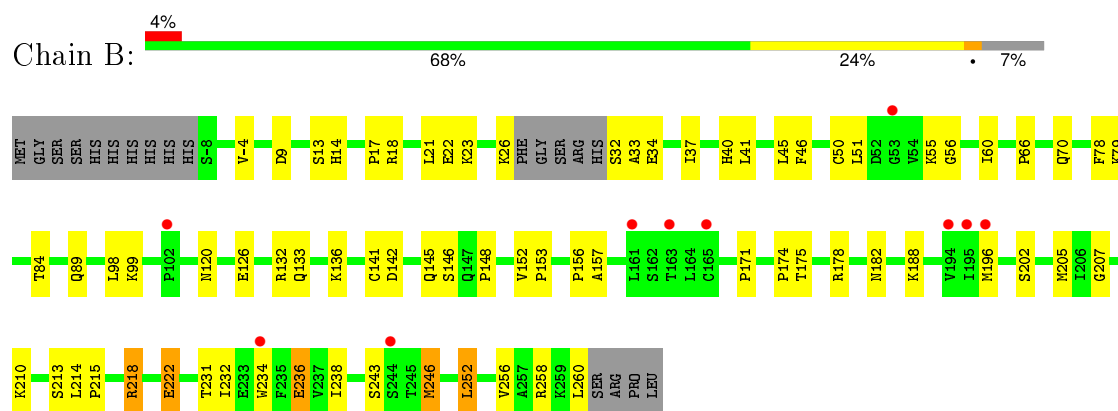
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

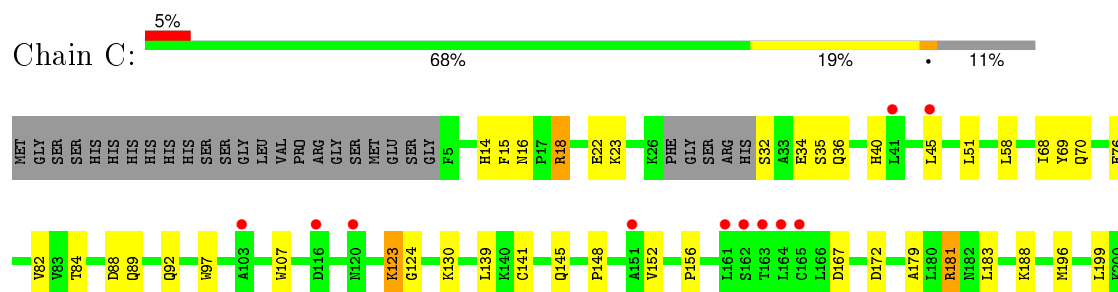
#### • Molecule 1: Nicotinamide N-methyltransferase



#### • Molecule 1: Nicotinamide N-methyltransferase

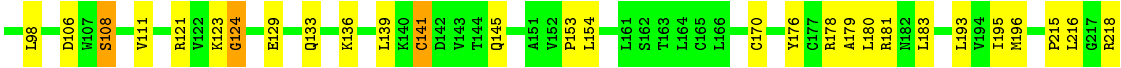
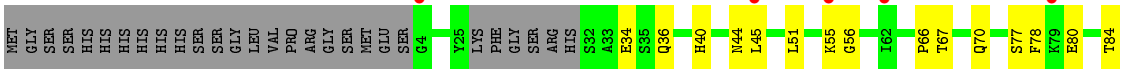


#### • Molecule 1: Nicotinamide N-methyltransferase





● Molecule 1: Nicotinamide N-methyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.02Å 62.01Å 107.07Å 82.35° 81.89° 68.30°	Depositor
Resolution (Å)	29.50 – 2.05 29.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.50-2.05) 95.2 (29.50-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.217 , 0.265 0.216 , 0.257	Depositor DCC
$R_{free}$ test set	2208 reflections (3.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66479 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.89	0/2114	0.88	2/2864 (0.1%)
1	B	0.88	0/2114	0.85	0/2863
1	C	0.81	0/2022	0.89	5/2740 (0.2%)
1	D	0.84	1/2017 (0.0%)	0.82	0/2734
All	All	0.86	1/8267 (0.0%)	0.86	7/11201 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	CYS	CB-SG	-7.06	1.70	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	LEU	CB-CG-CD2	-7.34	98.52	111.00
1	C	181	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	C	172	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	216	LEU	CB-CA-C	-5.60	99.56	110.20
1	A	167	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	167	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	218	ARG	NE-CZ-NH1	5.10	122.85	120.30

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	2069	0	2070	57	0
1	B	2070	0	2075	56	0
1	C	1979	0	1987	50	0
1	D	1974	0	1977	41	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	82	0	0	0	0
3	B	75	0	0	3	0
3	C	64	0	0	1	0
3	D	64	0	0	3	0
All	All	8481	0	8185	197	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 12.

All (197) 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:123:LYS:HE2	1:C:124:GLY:H	1.10	1.15
1:B:234[B]:TRP:HE1	1:B:256:VAL:HG23	0.98	1.08
1:B:234[B]:TRP:NE1	1:B:256:VAL:HG23	1.71	1.05
1:B:234[B]:TRP:CZ3	1:B:236:GLU:HG2	1.94	1.02
1:B:234[B]:TRP:HE1	1:B:256:VAL:CG2	1.76	0.99
1:A:234[B]:TRP:HE1	1:A:256:VAL:HG23	1.29	0.93
1:D:45:LEU:HD21	1:D:196:MET:CE	2.00	0.92
1:A:23:LYS:HE3	1:A:246:MET:CE	2.03	0.88
1:A:234[B]:TRP:NE1	1:A:256:VAL:HG23	1.92	0.84
1:B:-4:VAL:HG21	3:B:4015:HOH:O	1.78	0.83
1:B:231:THR:HB	1:B:260:LEU:HD21	1.64	0.78
1:A:23:LYS:HE3	1:A:246:MET:HE2	1.66	0.78
1:D:45:LEU:HD21	1:D:196:MET:HE3	1.65	0.76
1:C:23:LYS:HE3	1:C:246:MET:HE2	1.68	0.76
1:C:123:LYS:HE2	1:C:124:GLY:N	1.95	0.75
1:D:45:LEU:CD2	1:D:196:MET:HE1	2.16	0.74
1:B:33:ALA:O	1:B:37:ILE:HG13	1.87	0.74
1:B:174:PRO:O	1:B:178[B]:ARG:HG3	1.89	0.72
1:C:238:ILE:HD12	1:C:240:GLN:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:HD21	1:C:196:MET:HE1	1.73	0.70
1:C:23:LYS:CE	1:C:246:MET:HE2	2.22	0.69
1:C:123:LYS:CE	1:C:124:GLY:H	1.99	0.69
1:C:34:GLU:OE2	1:C:246:MET:HG3	1.91	0.69
1:A:-9:HIS:HB3	1:B:136:LYS:O	1.94	0.68
1:D:45:LEU:HD21	1:D:196:MET:HE1	1.75	0.68
1:D:40:HIS:CE1	1:D:238:ILE:HG21	2.30	0.67
1:C:88:ASP:OD1	1:C:92:GLN:NE2	2.28	0.67
1:C:234[B]:TRP:HD1	1:C:256:VAL:HB	1.61	0.66
1:C:199:LEU:HD11	1:C:237:VAL:HG22	1.78	0.65
1:B:234[B]:TRP:NE1	1:B:256:VAL:CG2	2.47	0.65
1:B:234[B]:TRP:HD1	1:B:256:VAL:HB	1.61	0.65
1:B:41:LEU:HD22	1:B:196:MET:HE3	1.79	0.65
1:D:45:LEU:CD2	1:D:196:MET:CE	2.71	0.64
1:A:40:HIS:NE2	1:A:238:ILE:HD12	2.13	0.64
1:B:13:SER:HB3	1:B:14:HIS:ND1	2.13	0.63
1:B:126:GLU:HA	1:D:145:GLN:HE22	1.63	0.63
1:A:80:GLU:HG2	1:A:136:LYS:HE3	1.79	0.63
1:B:32:SER:N	3:B:4005:HOH:O	2.32	0.62
1:D:84:THR:HB	1:D:141:CYS:HB2	1.79	0.62
1:A:206:ILE:HD12	1:A:211:PHE:CE2	2.35	0.62
1:C:23:LYS:NZ	1:C:246:MET:CE	2.62	0.62
1:D:36:GLN:HG3	3:D:4050:HOH:O	2.01	0.61
1:B:23:LYS:HE2	1:B:205:MET:O	2.00	0.61
1:A:84:THR:HB	1:A:141:CYS:HB2	1.82	0.60
1:A:16:ASN:OD1	1:A:18:ARG:HD3	2.02	0.60
1:B:171:PRO:HD2	1:B:175:THR:HG21	1.83	0.60
1:A:23:LYS:CE	1:A:246:MET:HE2	2.31	0.60
1:B:37:ILE:HD13	1:B:252:LEU:HD11	1.84	0.60
1:D:40:HIS:CD2	1:D:238:ILE:HD13	2.37	0.60
1:B:84:THR:HB	1:B:141:CYS:HB2	1.82	0.60
1:D:66:PRO:HD2	1:D:67:THR:HG23	1.83	0.60
1:C:15:PHE:O	1:C:89:GLN:NE2	2.33	0.60
1:C:45:LEU:HD21	1:C:196:MET:CE	2.33	0.59
1:C:23:LYS:NZ	1:C:246:MET:HE1	2.17	0.59
1:C:23:LYS:HE3	1:C:246:MET:CE	2.34	0.58
1:D:240:GLN:O	1:D:251:GLY:HA2	2.02	0.58
1:C:156:PRO:HB2	1:C:188:LYS:HG2	1.84	0.58
1:B:218:ARG:NH1	3:B:4073:HOH:O	2.35	0.58
1:B:218:ARG:NH2	1:B:222:GLU:OE2	2.36	0.58
1:C:45:LEU:HD13	1:C:70:GLN:HA	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:CG1	1:D:124:GLY:HA2	2.35	0.57
1:B:41:LEU:HD22	1:B:196:MET:CE	2.34	0.57
1:B:243:SER:HB2	1:B:246:MET:HG2	1.87	0.57
1:A:34:GLU:OE2	1:A:246:MET:HG3	2.04	0.56
1:A:238:ILE:HD11	1:A:252:LEU:HB2	1.88	0.56
1:B:234[B]:TRP:HZ3	1:B:236:GLU:HG2	1.62	0.55
1:A:163:THR:HG22	1:A:196:MET:HE2	1.88	0.55
1:A:23:LYS:CD	1:A:207:GLY:H	2.20	0.55
1:B:234[B]:TRP:CD1	1:B:256:VAL:HB	2.42	0.55
1:C:14:HIS:HD2	1:C:209:GLN:OE1	1.89	0.55
1:A:23:LYS:NZ	1:A:207:GLY:H	2.04	0.55
1:A:23:LYS:CE	1:A:246:MET:CE	2.83	0.55
1:A:23:LYS:HE3	1:A:246:MET:HE1	1.88	0.55
1:A:234[B]:TRP:HD1	1:A:256:VAL:HB	1.70	0.55
1:C:58:LEU:HD11	1:C:82:VAL:HG23	1.89	0.55
1:A:156:PRO:HB2	1:A:188:LYS:HG3	1.89	0.54
1:A:23:LYS:HZ3	1:A:207:GLY:N	2.04	0.54
1:A:46:PHE:O	1:A:50:CYS:HB2	2.07	0.54
1:B:56:GLY:O	1:B:78:PHE:HA	2.06	0.54
1:D:106:ASP:OD1	1:D:108:SER:HB2	2.07	0.54
1:B:234[B]:TRP:CH2	1:B:236:GLU:HG2	2.40	0.54
1:A:163:THR:HG22	1:A:196:MET:CE	2.38	0.54
1:A:163:THR:CG2	1:A:196:MET:CE	2.87	0.53
1:C:243:SER:HB2	1:C:246:MET:HG2	1.91	0.53
1:C:45:LEU:CD2	1:C:196:MET:HE1	2.38	0.53
1:A:98:LEU:HD11	1:A:135:VAL:HB	1.90	0.53
1:A:69:TYR:HA	1:A:72:LEU:HD12	1.90	0.53
1:C:234[B]:TRP:CD1	1:C:256:VAL:HB	2.43	0.53
1:C:221:VAL:O	1:C:225:VAL:HG23	2.09	0.52
1:D:153:PRO:O	1:D:154:LEU:HD23	2.10	0.52
1:D:123:LYS:O	1:D:124:GLY:C	2.47	0.52
1:B:148:PRO:HG3	1:B:182:ASN:HB3	1.92	0.51
1:B:142:ASP:HA	2:B:4002:SAH:N1	2.26	0.50
1:D:236:GLU:HG2	1:D:237:VAL:N	2.26	0.50
1:B:205:MET:SD	1:B:210:LYS:HG3	2.51	0.50
1:D:235:PHE:CE1	1:D:255:LEU:HD23	2.46	0.50
1:A:196:MET:HG2	1:A:254:SER:HB2	1.93	0.50
1:A:163:THR:CG2	1:A:196:MET:HE2	2.42	0.50
1:D:129:GLU:O	1:D:133:GLN:HG2	2.12	0.50
1:C:23:LYS:CE	1:C:246:MET:CE	2.91	0.49
1:B:234[B]:TRP:CZ3	1:B:236:GLU:CG	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LYS:NZ	1:C:246:MET:HE2	2.25	0.49
1:A:234[B]:TRP:CD1	1:A:256:VAL:HB	2.49	0.48
1:A:121:ARG:HA	1:A:121:ARG:HH11	1.78	0.48
1:A:111:VAL:HG13	1:A:127:LYS:HG2	1.95	0.48
1:B:40:HIS:CD2	1:B:238:ILE:HD13	2.49	0.48
1:D:55:LYS:HG2	1:D:77:SER:HB3	1.96	0.48
1:D:45:LEU:HD23	1:D:196:MET:HE1	1.94	0.47
1:C:14:HIS:CD2	1:C:209:GLN:OE1	2.66	0.47
1:C:40:HIS:CE1	1:C:238:ILE:HG21	2.50	0.47
1:D:225:VAL:HG21	1:D:255:LEU:HD21	1.96	0.47
1:A:-4:VAL:HG13	1:A:0:SER:OG	2.14	0.47
1:C:23:LYS:HZ1	1:C:246:MET:CE	2.28	0.47
1:C:32:SER:HB3	1:C:35:SER:CB	2.44	0.47
1:A:5:PHE:CD2	1:A:171:PRO:HA	2.49	0.47
1:A:23:LYS:HZ3	1:A:207:GLY:H	1.62	0.46
1:B:234[B]:TRP:CD1	1:B:256:VAL:CG2	2.98	0.46
1:C:243:SER:HB2	1:C:246:MET:CG	2.45	0.46
1:C:23:LYS:HZ2	1:C:246:MET:HE1	1.80	0.46
1:D:238:ILE:HD12	1:D:240:GLN:HB3	1.97	0.46
1:C:139:LEU:HD22	1:C:152:VAL:HG21	1.98	0.46
1:D:80:GLU:HG2	1:D:136:LYS:HE2	1.97	0.46
1:B:156:PRO:HB2	1:B:188:LYS:HG2	1.97	0.46
1:C:234[B]:TRP:CZ3	1:C:236:GLU:HB3	2.51	0.46
1:A:68:ILE:C	1:A:68:ILE:HD12	2.36	0.46
1:B:214:LEU:HA	1:B:215:PRO:HD3	1.77	0.46
1:C:76:GLU:OE2	1:C:130:LYS:HD3	2.15	0.46
1:A:234[B]:TRP:CD1	1:A:256:VAL:HG23	2.51	0.45
1:C:216:LEU:N	1:C:216:LEU:HD23	2.24	0.45
1:A:40:HIS:CE1	1:A:238:ILE:HD12	2.52	0.45
1:B:133:GLN:O	1:B:136:LYS:HE2	2.16	0.44
1:A:23:LYS:HE2	1:A:205:MET:O	2.16	0.44
1:C:234[B]:TRP:HE1	1:C:256:VAL:HG23	1.83	0.44
1:A:171:PRO:HD2	1:A:175:THR:HG21	1.99	0.44
1:A:23:LYS:NZ	1:A:207:GLY:N	2.65	0.44
1:B:234[B]:TRP:CD1	1:B:256:VAL:CB	3.01	0.44
1:A:111:VAL:HG21	1:A:128:GLU:HG2	1.99	0.44
1:B:45:LEU:HD13	1:B:70:GLN:HA	1.99	0.44
1:B:234[B]:TRP:CD1	1:B:256:VAL:HG23	2.46	0.44
1:B:40:HIS:CE1	1:B:238:ILE:HG21	2.52	0.44
1:D:246:MET:HE2	3:D:4055:HOH:O	2.17	0.44
1:B:132:ARG:HD3	1:D:178:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HB3	1:A:14:HIS:ND1	2.33	0.44
1:C:97:TRP:CD1	1:C:107:TRP:HD1	2.36	0.43
1:C:179:ALA:O	1:C:183:LEU:HG	2.18	0.43
1:A:-4:VAL:HG21	3:D:4008:HOH:O	2.17	0.43
1:B:40:HIS:CG	1:B:238:ILE:HD13	2.53	0.43
1:D:56:GLY:O	1:D:78:PHE:HA	2.18	0.43
1:D:111:VAL:HG12	1:D:124:GLY:HA2	2.01	0.43
1:A:13:SER:CB	1:A:14:HIS:ND1	2.81	0.43
1:A:2:GLU:HG3	1:D:215:PRO:O	2.19	0.43
1:D:170:CYS:SG	1:D:176:TYR:HA	2.58	0.43
1:D:179:ALA:O	1:D:183:LEU:HG	2.19	0.43
1:A:18:ARG:NH1	1:B:145:GLN:HE21	2.16	0.43
1:A:111:VAL:HG11	1:A:128:GLU:HG2	2.00	0.43
1:B:46:PHE:O	1:B:50:CYS:HB2	2.18	0.43
1:C:16:ASN:OD1	1:C:18:ARG:HD3	2.19	0.42
1:A:23:LYS:CE	1:A:207:GLY:H	2.31	0.42
1:D:193:LEU:HD21	1:D:195:ILE:HD11	2.00	0.42
1:D:234[B]:TRP:CD1	1:D:256:VAL:HG23	2.54	0.42
1:A:108:SER:HB2	1:A:109:PRO:HD3	2.01	0.42
1:D:45:LEU:HD13	1:D:70:GLN:HA	2.00	0.42
1:A:37:ILE:O	1:A:41:LEU:HG	2.20	0.42
1:A:234[B]:TRP:CZ2	1:A:254:SER:OG	2.69	0.42
1:B:17:PRO:O	1:B:21:LEU:HG	2.19	0.42
1:B:152:VAL:HA	1:B:153:PRO:HD3	1.78	0.42
1:B:99:LYS:O	1:D:181:ARG:NH1	2.45	0.42
1:C:84:THR:HA	1:C:139:LEU:O	2.19	0.42
1:C:145:GLN:NE2	3:C:4049:HOH:O	2.52	0.42
1:C:23:LYS:HD2	1:C:207:GLY:H	1.85	0.42
1:D:40:HIS:CE1	1:D:44:ASN:ND2	2.88	0.42
1:C:201:SER:HB2	1:C:249:ASN:HB3	2.02	0.42
1:A:164:LEU:HD23	1:A:197:ASP:HA	2.02	0.42
1:A:78:PHE:HE1	1:A:158:ASP:HB2	1.85	0.41
1:D:84:THR:HA	1:D:139:LEU:O	2.19	0.41
1:C:32:SER:O	1:C:36:GLN:HG2	2.20	0.41
1:A:37:ILE:HD12	1:A:242:TYR:CD1	2.55	0.41
1:B:218:ARG:HH21	1:B:222:GLU:HG3	1.84	0.41
1:B:218:ARG:HH21	1:B:222:GLU:CD	2.23	0.41
1:A:163:THR:HG21	1:A:196:MET:CE	2.50	0.41
1:D:40:HIS:HE1	1:D:236:GLU:OE2	2.02	0.41
1:B:23:LYS:CE	1:B:207:GLY:H	2.33	0.41
1:D:40:HIS:CE1	1:D:44:ASN:HD21	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:HIS:CE1	1:A:238:ILE:HG21	2.56	0.41
1:D:34:GLU:OE2	1:D:246:MET:HG3	2.21	0.41
1:B:21:LEU:HD21	1:B:66:PRO:HG2	2.03	0.41
1:C:68:ILE:HD12	1:C:68:ILE:C	2.40	0.41
1:B:222:GLU:HG2	1:B:232:ILE:HD13	2.03	0.41
1:B:202:SER:HA	1:B:213:SER:O	2.21	0.41
1:A:-5:LEU:HG	1:B:99:LYS:HD2	2.02	0.40
1:B:34:GLU:CD	1:B:34:GLU:H	2.24	0.40
1:C:32:SER:HB3	1:C:35:SER:HB3	2.02	0.40
1:B:60:ILE:HD12	1:B:157:ALA:HB2	2.02	0.40
1:C:141:CYS:HA	1:C:148:PRO:O	2.21	0.40
1:C:40:HIS:HE1	1:C:236:GLU:OE2	2.04	0.40
1:D:180:LEU:HD13	1:D:225:VAL:HA	2.04	0.40
1:C:69:TYR:HB3	1:C:107:TRP:CZ3	2.57	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	262/283 (93%)	253 (97%)	8 (3%)	1 (0%)	39	28
1	B	262/283 (93%)	255 (97%)	6 (2%)	1 (0%)	39	28
1	C	248/283 (88%)	239 (96%)	9 (4%)	0	100	100
1	D	248/283 (88%)	240 (97%)	7 (3%)	1 (0%)	39	28
All	All	1020/1132 (90%)	987 (97%)	30 (3%)	3 (0%)	46	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	GLY

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Mol	Chain	Res	Type
1	B	120	ASN
1	A	189	PRO

### 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	229/245 (94%)	218 (95%)	11 (5%)	31	22
1	B	229/245 (94%)	213 (93%)	16 (7%)	19	10
1	C	219/245 (89%)	209 (95%)	10 (5%)	33	24
1	D	218/245 (89%)	210 (96%)	8 (4%)	41	32
All	All	895/980 (91%)	850 (95%)	45 (5%)	29	20

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	SER
1	A	-4	VAL
1	A	18	ARG
1	A	51	LEU
1	A	121	ARG
1	A	127	LYS
1	A	165	CYS
1	A	238	ILE
1	A	243	SER
1	A	246	MET
1	A	258	ARG
1	B	9	ASP
1	B	18	ARG
1	B	22	GLU
1	B	26	LYS
1	B	51	LEU
1	B	55	LYS
1	B	79	LYS
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	98	LEU
1	B	146	SER
1	B	218	ARG
1	B	222	GLU
1	B	236	GLU
1	B	246	MET
1	B	252	LEU
1	B	258	ARG
1	C	18	ARG
1	C	22	GLU
1	C	51	LEU
1	C	123	LYS
1	C	181	ARG
1	C	209	GLN
1	C	216	LEU
1	C	237	VAL
1	C	254	SER
1	C	258	ARG
1	D	51	LEU
1	D	98	LEU
1	D	108	SER
1	D	121	ARG
1	D	216	LEU
1	D	218	ARG
1	D	254	SER
1	D	258	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	40	HIS
1	B	145	GLN
1	B	209	GLN
1	C	14	HIS
1	C	40	HIS
1	C	92	GLN
1	C	145	GLN
1	D	40	HIS
1	D	92	GLN
1	D	133	GLN
1	D	145	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 ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SAH	A	4001	-	20,28,28	1.29	3 (15%)	19,40,40	2.95	7 (36%)
2	SAH	B	4002	-	20,28,28	1.20	2 (10%)	19,40,40	2.89	5 (26%)
2	SAH	C	4003	-	20,28,28	1.42	3 (15%)	19,40,40	3.41	4 (21%)
2	SAH	D	4004	-	20,28,28	1.25	2 (10%)	19,40,40	3.34	4 (21%)

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	4001	-	-	0/7/31/31	0/3/3/3
2	SAH	B	4002	-	-	0/7/31/31	0/3/3/3
2	SAH	C	4003	-	-	0/7/31/31	0/3/3/3
2	SAH	D	4004	-	-	0/7/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	SAH	O4'-C4'	-2.87	1.38	1.45
2	C	4003	SAH	O4'-C4'	-2.09	1.40	1.45
2	B	4002	SAH	C2-N1	2.43	1.38	1.33
2	A	4001	SAH	C2-N1	2.70	1.39	1.33
2	D	4004	SAH	C2-N1	2.70	1.39	1.33
2	B	4002	SAH	C2-N3	3.03	1.37	1.32
2	A	4001	SAH	C2-N3	3.16	1.37	1.32
2	C	4003	SAH	C2-N1	3.18	1.39	1.33
2	D	4004	SAH	C2-N3	3.70	1.38	1.32
2	C	4003	SAH	C2-N3	4.47	1.40	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4003	SAH	N3-C2-N1	-13.47	118.58	128.89
2	D	4004	SAH	N3-C2-N1	-13.02	118.93	128.89
2	B	4002	SAH	N3-C2-N1	-10.97	120.49	128.89
2	A	4001	SAH	N3-C2-N1	-10.97	120.50	128.89
2	D	4004	SAH	C4'-O4'-C1'	-3.06	106.36	109.72
2	B	4002	SAH	C4'-O4'-C1'	-2.93	106.50	109.72
2	D	4004	SAH	C1'-N9-C4	-2.89	122.58	126.94
2	C	4003	SAH	C5'-SD-CG	-2.81	93.97	102.41
2	C	4003	SAH	C4-C5-N7	-2.61	107.08	109.48
2	A	4001	SAH	O3'-C3'-C4'	-2.36	103.97	111.05
2	B	4002	SAH	O4'-C4'-C5'	-2.35	102.44	108.85
2	A	4001	SAH	C5'-SD-CG	-2.35	95.36	102.41
2	C	4003	SAH	C1'-N9-C4	-2.22	123.59	126.94
2	A	4001	SAH	C1'-N9-C4	-2.16	123.68	126.94
2	D	4004	SAH	C5'-SD-CG	-2.16	95.92	102.41
2	A	4001	SAH	O4'-C4'-C5'	-2.09	103.17	108.85
2	B	4002	SAH	C4-C5-N7	-2.05	107.59	109.48
2	A	4001	SAH	O4'-C1'-N9	2.53	113.39	108.10
2	B	4002	SAH	CB-CG-SD	2.63	118.64	113.57
2	A	4001	SAH	C2'-C1'-N9	2.64	118.32	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4002	SAH	1	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	265/283 (93%)	0.13	11 (4%) 40 46	18, 26, 36, 52	0
1	B	264/283 (93%)	0.14	10 (3%) 44 50	19, 27, 36, 45	0
1	C	251/283 (88%)	0.30	14 (5%) 28 32	20, 29, 42, 54	0
1	D	251/283 (88%)	0.39	17 (6%) 20 23	19, 31, 43, 51	0
All	All	1031/1132 (91%)	0.24	52 (5%) 32 37	18, 28, 41, 54	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	GLY	4.4
1	D	161	LEU	4.1
1	B	195	ILE	3.7
1	C	120	ASN	3.6
1	A	234[A]	TRP	3.6
1	C	234[A]	TRP	3.5
1	D	234[A]	TRP	3.5
1	D	164	LEU	3.4
1	D	195	ILE	3.4
1	D	162	SER	3.3
1	D	165	CYS	3.0
1	A	195	ILE	3.0
1	B	234[A]	TRP	2.9
1	C	151	ALA	2.9
1	C	161	LEU	2.8
1	D	163	THR	2.8
1	D	45	LEU	2.7
1	B	161	LEU	2.7
1	A	116	ASP	2.6
1	D	143	VAL	2.6
1	A	55	LYS	2.6

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	A	244	SER	2.6
1	A	163	THR	2.6
1	D	79	LYS	2.6
1	C	164	LEU	2.6
1	D	166	LEU	2.6
1	D	62	ILE	2.6
1	C	209	GLN	2.6
1	C	162	SER	2.5
1	B	163	THR	2.5
1	C	163	THR	2.5
1	B	196	MET	2.5
1	A	161	LEU	2.4
1	C	116	ASP	2.4
1	C	165	CYS	2.4
1	C	208	GLU	2.4
1	D	121	ARG	2.4
1	D	151	ALA	2.4
1	B	244	SER	2.3
1	B	53	GLY	2.3
1	A	245	THR	2.3
1	B	165	CYS	2.2
1	C	45	LEU	2.2
1	C	103	ALA	2.2
1	D	55	LYS	2.1
1	C	41	LEU	2.1
1	B	102	PRO	2.1
1	B	194	VAL	2.1
1	D	124	GLY	2.0
1	A	121	ARG	2.0
1	A	45	LEU	2.0
1	A	162	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

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
2	SAH	C	4003	26/26	0.96	0.16	0.25	22,26,27,28	0
2	SAH	B	4002	26/26	0.96	0.14	0.17	13,21,22,24	0
2	SAH	D	4004	26/26	0.95	0.15	-0.19	18,25,27,28	0
2	SAH	A	4001	26/26	0.97	0.12	-0.30	12,19,23,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.