



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:47 PM GMT

PDB ID : 1MT6
Title : Structure of histone H3 K4-specific methyltransferase SET7/9 with AdoHcy
Authors : Jacobs, S.A.; Harp, J.M.; Devarakonda, S.; Kim, Y.; Rastinejad, F.; Khorasanizadeh, S.
Deposited on : 2002-09-20
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

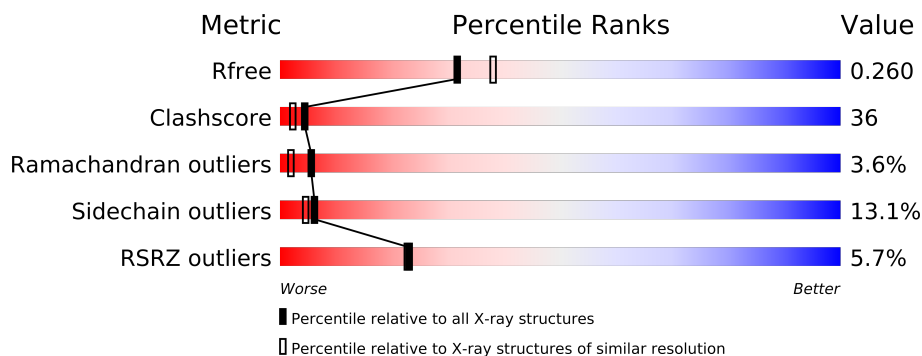
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

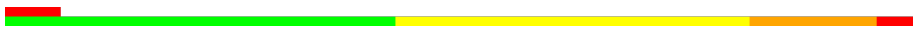
The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	280	

2 Entry composition i

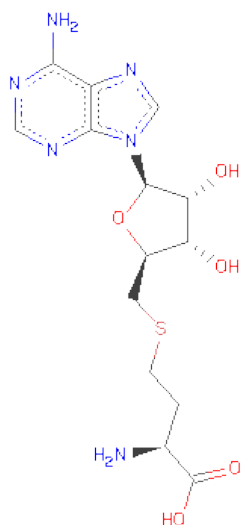
There are 3 unique types of molecules in this entry. The entry contains 2389 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SET9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2192	1382	356	443	11			

- 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		

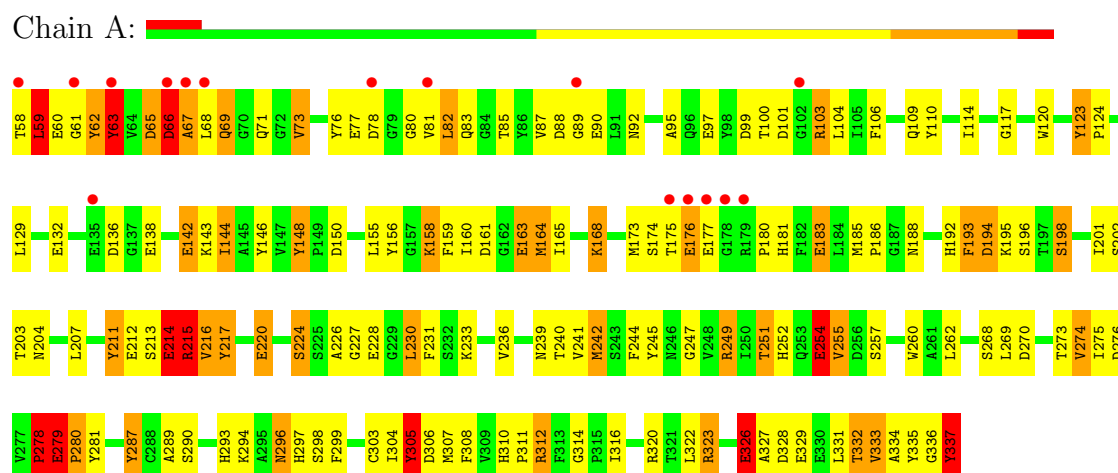
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		

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: SET9



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	70.35Å 76.04Å 166.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.20 28.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (28.64-2.20) 93.0 (28.64-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.263 0.223 , 0.260	Depositor DCC
R_{free} test set	2132 reflections (9.93%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.914	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21496 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2389	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.00	60/2246 (2.7%)	1.57	24/3051 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	GLU	C-O	13.29	1.48	1.23
1	A	220	GLU	CG-CD	10.87	1.68	1.51
1	A	193	PHE	CE1-CZ	9.91	1.56	1.37
1	A	337	TYR	CD2-CE2	9.35	1.53	1.39
1	A	215	ARG	CZ-NH1	9.34	1.45	1.33
1	A	156	TYR	CD2-CE2	9.28	1.53	1.39
1	A	216	VAL	CA-CB	8.59	1.72	1.54
1	A	305	TYR	CD1-CE1	8.17	1.51	1.39
1	A	148	TYR	CE2-CZ	-8.14	1.27	1.38
1	A	215	ARG	CZ-NH2	8.07	1.43	1.33
1	A	215	ARG	CB-CG	-8.07	1.30	1.52
1	A	120	TRP	CB-CG	-7.77	1.36	1.50
1	A	296	ASN	C-O	7.67	1.38	1.23
1	A	332	THR	C-O	7.58	1.37	1.23
1	A	298	SER	CB-OG	7.37	1.51	1.42
1	A	305	TYR	CD2-CE2	7.14	1.50	1.39
1	A	144	ILE	CA-CB	7.01	1.71	1.54
1	A	228	GLU	CG-CD	6.98	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	VAL	CA-CB	-6.97	1.40	1.54
1	A	214	GLU	CG-CD	6.87	1.62	1.51
1	A	287	TYR	CD1-CE1	6.85	1.49	1.39
1	A	326	GLU	CD-OE1	6.76	1.33	1.25
1	A	148	TYR	CD2-CE2	6.75	1.49	1.39
1	A	163	GLU	CD-OE1	6.75	1.33	1.25
1	A	254	GLU	CG-CD	6.72	1.62	1.51
1	A	333	VAL	CB-CG1	6.68	1.66	1.52
1	A	244	PHE	CD1-CE1	6.68	1.52	1.39
1	A	77	GLU	CG-CD	6.62	1.61	1.51
1	A	333	VAL	C-O	6.55	1.35	1.23
1	A	214	GLU	CD-OE2	6.50	1.32	1.25
1	A	123	TYR	CE2-CZ	6.35	1.46	1.38
1	A	312	ARG	CB-CG	6.30	1.69	1.52
1	A	308	PHE	CE1-CZ	6.25	1.49	1.37
1	A	230	LEU	CG-CD1	6.19	1.74	1.51
1	A	215	ARG	NE-CZ	6.07	1.41	1.33
1	A	164	MET	CG-SD	6.04	1.96	1.81
1	A	183	GLU	CG-CD	5.92	1.60	1.51
1	A	312	ARG	CZ-NH2	5.78	1.40	1.33
1	A	138	GLU	CG-CD	5.76	1.60	1.51
1	A	337	TYR	CA-C	5.57	1.67	1.52
1	A	194	ASP	CB-CG	5.51	1.63	1.51
1	A	211	TYR	CD2-CE2	-5.51	1.31	1.39
1	A	245	TYR	CD2-CE2	5.46	1.47	1.39
1	A	241	VAL	CA-CB	5.43	1.66	1.54
1	A	334	ALA	C-O	-5.36	1.13	1.23
1	A	287	TYR	CD2-CE2	5.34	1.47	1.39
1	A	148	TYR	CD1-CE1	5.30	1.47	1.39
1	A	196	SER	CB-OG	5.30	1.49	1.42
1	A	337	TYR	CD1-CE1	5.26	1.47	1.39
1	A	281	TYR	CE1-CZ	5.25	1.45	1.38
1	A	279	GLU	C-N	-5.24	1.24	1.34
1	A	164	MET	CB-CG	5.20	1.68	1.51
1	A	217	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	281	TYR	CG-CD1	5.17	1.45	1.39
1	A	97	GLU	CB-CG	-5.16	1.42	1.52
1	A	168	LYS	CD-CE	5.13	1.64	1.51
1	A	337	TYR	CB-CG	5.10	1.59	1.51
1	A	110	TYR	CB-CG	-5.04	1.44	1.51
1	A	142	GLU	CD-OE2	-5.02	1.20	1.25
1	A	220	GLU	CD-OE1	5.01	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ARG	NE-CZ-NH1	-11.11	114.74	120.30
1	A	279	GLU	CA-C-O	-8.81	101.61	120.10
1	A	194	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	323	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	A	59	LEU	CA-CB-CG	8.32	134.44	115.30
1	A	306	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	185	MET	CG-SD-CE	-7.68	87.92	100.20
1	A	242	MET	CG-SD-CE	-7.41	88.34	100.20
1	A	224	SER	C-N-CA	-6.70	104.95	121.70
1	A	312	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	164	MET	CG-SD-CE	-6.52	89.77	100.20
1	A	224	SER	CA-C-N	6.17	130.78	117.20
1	A	136	ASP	CB-CA-C	-5.93	98.54	110.40
1	A	202	SER	CB-CA-C	-5.82	99.05	110.10
1	A	323	ARG	CB-CG-CD	-5.74	96.69	111.60
1	A	66	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	278	PRO	CA-C-N	-5.63	104.81	117.20
1	A	194	ASP	OD1-CG-OD2	-5.54	112.78	123.30
1	A	144	ILE	CB-CA-C	-5.43	100.75	111.60
1	A	65	ASP	N-CA-C	5.38	125.54	111.00
1	A	279	GLU	CB-CA-C	5.31	121.02	110.40
1	A	242	MET	CB-CA-C	-5.24	99.91	110.40
1	A	323	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	A	337	TYR	CB-CG-CD2	5.13	124.08	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	TYR	Sidechain
1	A	215	ARG	Mainchain
1	A	278	PRO	Mainchain
1	A	279	GLU	Mainchain
1	A	305	TYR	Sidechain
1	A	337	TYR	Sidechain

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2053	153	0
2	A	26	0	18	3	0
3	A	171	0	0	24	0
All	All	2389	0	2071	153	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:LEU:CG	1:A:230:LEU:CD1	1.74	1.60
1:A:326:GLU:HG3	3:A:477:HOH:O	1.54	1.03
1:A:188:ASN:HA	3:A:501:HOH:O	1.63	0.98
1:A:62:TYR:O	1:A:63:TYR:HB3	1.64	0.95
1:A:297:HIS:HD2	1:A:335:TYR:H	1.01	0.94
1:A:310:HIS:HD2	1:A:312:ARG:H	1.08	0.93
1:A:239:ASN:ND2	1:A:320:ARG:HD3	1.83	0.93
1:A:335:TYR:OH	2:A:1:SAH:H5'2	1.69	0.93
1:A:216:VAL:HB	3:A:505:HOH:O	1.70	0.89
1:A:297:HIS:CD2	1:A:335:TYR:H	1.91	0.89
1:A:326:GLU:HA	1:A:326:GLU:OE2	1.72	0.88
1:A:251:THR:HG23	1:A:254:GLU:HB2	1.54	0.88
1:A:307:MET:CE	3:A:440:HOH:O	2.21	0.87
1:A:336:GLY:C	1:A:337:TYR:CD1	2.47	0.87
1:A:251:THR:CG2	1:A:254:GLU:HB2	2.05	0.87
1:A:61:GLY:C	1:A:62:TYR:HD1	1.79	0.86
1:A:337:TYR:HB3	3:A:465:HOH:O	1.74	0.85
1:A:155:LEU:CB	1:A:164:MET:HE1	2.07	0.85
1:A:279:GLU:HB3	1:A:280:PRO:HD3	1.60	0.83
1:A:242:MET:HB3	3:A:505:HOH:O	1.79	0.82
1:A:310:HIS:CD2	1:A:311:PRO:HD2	2.14	0.82
1:A:269:LEU:HD22	1:A:275:ILE:HD11	1.63	0.81
1:A:239:ASN:HB2	3:A:428:HOH:O	1.81	0.80
1:A:61:GLY:C	1:A:62:TYR:CD1	2.54	0.79
1:A:279:GLU:CB	1:A:280:PRO:HD3	2.12	0.79
1:A:155:LEU:HB2	1:A:164:MET:CE	2.12	0.79
1:A:230:LEU:CB	1:A:230:LEU:CD1	2.59	0.79
1:A:239:ASN:HD22	1:A:320:ARG:HD3	1.48	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:VAL:HG21	1:A:242:MET:HE3	1.63	0.78
1:A:155:LEU:HB3	1:A:164:MET:HE1	1.67	0.76
1:A:252:HIS:HE1	1:A:270:ASP:O	1.68	0.76
1:A:155:LEU:HB2	1:A:164:MET:HE1	1.69	0.75
1:A:326:GLU:OE2	1:A:326:GLU:CA	2.36	0.74
1:A:142:GLU:OE1	1:A:158:LYS:NZ	2.21	0.74
1:A:310:HIS:CD2	1:A:312:ARG:H	1.99	0.73
1:A:63:TYR:C	1:A:63:TYR:CD2	2.62	0.73
1:A:296:ASN:HD21	2:A:1:SAH:HN1	1.33	0.73
1:A:216:VAL:CB	3:A:505:HOH:O	2.34	0.73
1:A:69:GLN:HG2	1:A:88:ASP:H	1.54	0.72
1:A:58:THR:O	1:A:59:LEU:HD22	1.89	0.71
1:A:279:GLU:CB	1:A:280:PRO:CD	2.69	0.71
1:A:62:TYR:O	1:A:63:TYR:CB	2.39	0.71
1:A:62:TYR:N	1:A:62:TYR:CD1	2.55	0.70
1:A:216:VAL:CG2	3:A:505:HOH:O	2.37	0.70
1:A:69:GLN:CG	1:A:88:ASP:H	2.04	0.70
1:A:159:PHE:CE1	1:A:164:MET:HB2	2.26	0.69
1:A:63:TYR:C	1:A:63:TYR:HD2	1.96	0.69
1:A:251:THR:HG23	1:A:254:GLU:H	1.57	0.69
1:A:230:LEU:CD2	1:A:230:LEU:CD1	2.69	0.68
1:A:236:VAL:HG11	1:A:242:MET:HE1	1.75	0.68
1:A:297:HIS:HD2	1:A:335:TYR:N	1.83	0.68
1:A:251:THR:HG23	1:A:254:GLU:CB	2.24	0.67
1:A:336:GLY:C	1:A:337:TYR:HD1	1.95	0.66
1:A:336:GLY:O	1:A:337:TYR:HD1	1.80	0.65
1:A:165:ILE:HD13	1:A:165:ILE:N	2.10	0.65
1:A:175:THR:O	1:A:176:GLU:C	2.36	0.64
1:A:58:THR:HG22	1:A:59:LEU:N	2.13	0.63
1:A:249:ARG:HH21	1:A:249:ARG:HG2	1.62	0.63
1:A:198:SER:HA	1:A:249:ARG:O	1.99	0.62
1:A:144:ILE:HB	1:A:159:PHE:CD2	2.34	0.62
1:A:81:VAL:HG12	1:A:82:LEU:H	1.65	0.61
1:A:155:LEU:HB2	1:A:164:MET:HE3	1.82	0.61
1:A:236:VAL:HG21	1:A:242:MET:CE	2.31	0.61
1:A:337:TYR:CD2	3:A:503:HOH:O	2.51	0.60
1:A:143:LYS:HE3	3:A:474:HOH:O	2.01	0.60
1:A:71:GLN:OE1	1:A:85:THR:HG22	2.02	0.59
1:A:61:GLY:O	1:A:62:TYR:HD1	1.84	0.59
1:A:159:PHE:CZ	1:A:164:MET:HE2	2.37	0.59
1:A:87:VAL:O	1:A:88:ASP:HB2	2.02	0.58
1:A:117:GLY:O	1:A:132:GLU:HA	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:TYR:CE1	1:A:289:ALA:HB3	2.39	0.58
1:A:123:TYR:OH	1:A:129:LEU:HD22	2.03	0.57
1:A:327:ALA:O	1:A:328:ASP:HB2	2.04	0.57
1:A:305:TYR:CZ	1:A:333:VAL:HG21	2.39	0.57
1:A:146:TYR:CD2	1:A:311:PRO:HG3	2.40	0.57
1:A:310:HIS:CG	1:A:311:PRO:HD2	2.39	0.57
1:A:304:ILE:HB	1:A:322:LEU:HD21	1.85	0.56
1:A:63:TYR:HD2	1:A:63:TYR:O	1.88	0.56
1:A:337:TYR:N	1:A:337:TYR:CD1	2.72	0.56
1:A:217:TYR:HD2	1:A:233:LYS:HG3	1.71	0.56
1:A:255:VAL:HG11	1:A:274:VAL:HG11	1.88	0.56
1:A:226:ALA:O	1:A:227:GLY:C	2.39	0.56
1:A:99:ASP:C	1:A:101:ASP:N	2.59	0.56
1:A:99:ASP:C	1:A:101:ASP:H	2.10	0.55
1:A:213:SER:HB2	3:A:364:HOH:O	2.07	0.55
1:A:254:GLU:OE2	1:A:254:GLU:O	2.25	0.54
1:A:251:THR:HG23	1:A:254:GLU:N	2.23	0.54
1:A:160:ILE:HD12	1:A:165:ILE:HG13	1.90	0.54
1:A:99:ASP:N	1:A:103:ARG:O	2.40	0.54
1:A:106:PHE:C	1:A:106:PHE:CD1	2.82	0.53
1:A:168:LYS:HG2	3:A:421:HOH:O	2.09	0.53
1:A:69:GLN:HB3	1:A:89:GLY:H	1.75	0.52
1:A:99:ASP:O	1:A:101:ASP:N	2.43	0.52
1:A:279:GLU:HB2	1:A:280:PRO:CD	2.40	0.51
1:A:278:PRO:C	1:A:279:GLU:O	2.49	0.51
1:A:303:CYS:N	1:A:332:THR:O	2.42	0.51
1:A:68:LEU:HB2	1:A:69:GLN:NE2	2.25	0.51
1:A:81:VAL:HG12	1:A:82:LEU:N	2.25	0.51
1:A:150:ASP:OD1	1:A:150:ASP:C	2.47	0.50
1:A:201:ILE:HD11	1:A:247:GLY:HA2	1.93	0.50
1:A:76:TYR:HD1	1:A:80:GLY:O	1.95	0.49
1:A:66:ASP:OD2	1:A:67:ALA:N	2.46	0.49
1:A:173:MET:HE2	1:A:183:GLU:OE2	2.13	0.49
1:A:337:TYR:CE2	3:A:503:HOH:O	2.65	0.48
1:A:158:LYS:HB3	1:A:165:ILE:HB	1.94	0.48
1:A:307:MET:HE2	3:A:440:HOH:O	1.98	0.48
1:A:212:GLU:OE1	1:A:290:SER:HA	2.14	0.48
1:A:249:ARG:HG2	1:A:249:ARG:NH2	2.28	0.48
1:A:323:ARG:NH1	1:A:329:GLU:OE2	2.37	0.47
1:A:336:GLY:O	1:A:337:TYR:CD1	2.62	0.47
1:A:87:VAL:HB	1:A:92:ASN:HD22	1.79	0.46
1:A:123:TYR:HB3	1:A:124:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:PHE:CD2	1:A:231:PHE:N	2.82	0.46
1:A:297:HIS:HA	1:A:333:VAL:O	2.15	0.46
1:A:217:TYR:CD2	1:A:233:LYS:HG3	2.49	0.46
1:A:204:ASN:O	1:A:312:ARG:NH2	2.48	0.45
1:A:103:ARG:HD2	3:A:487:HOH:O	2.16	0.45
1:A:254:GLU:OE2	1:A:254:GLU:HA	2.16	0.45
1:A:165:ILE:O	1:A:192:HIS:HD2	1.99	0.45
1:A:76:TYR:C	1:A:78:ASP:N	2.70	0.45
1:A:260:TRP:C	1:A:262:LEU:H	2.19	0.45
1:A:194:ASP:OD1	1:A:203:THR:HB	2.16	0.45
1:A:68:LEU:HA	3:A:360:HOH:O	2.16	0.44
1:A:240:THR:HB	1:A:242:MET:CE	2.48	0.44
1:A:294:LYS:HD3	1:A:294:LYS:HA	1.80	0.44
1:A:230:LEU:HD12	1:A:230:LEU:HA	2.00	0.43
1:A:337:TYR:CB	3:A:465:HOH:O	2.50	0.43
1:A:173:MET:O	1:A:174:SER:HB3	2.18	0.43
1:A:254:GLU:OE2	1:A:254:GLU:CA	2.66	0.43
1:A:181:HIS:CD2	3:A:436:HOH:O	2.71	0.43
1:A:61:GLY:HA3	3:A:453:HOH:O	2.18	0.43
1:A:76:TYR:C	1:A:78:ASP:H	2.21	0.43
1:A:90:GLU:HG2	3:A:424:HOH:O	2.20	0.42
1:A:173:MET:O	1:A:174:SER:CB	2.66	0.42
1:A:83:GLN:O	1:A:95:ALA:HA	2.19	0.42
1:A:297:HIS:HE1	1:A:299:PHE:CE2	2.37	0.42
1:A:310:HIS:HD2	1:A:312:ARG:N	1.92	0.42
1:A:290:SER:O	1:A:293:HIS:HE1	2.03	0.42
1:A:73:VAL:CG2	1:A:73:VAL:O	2.66	0.42
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.69	0.42
1:A:192:HIS:O	1:A:193:PHE:C	2.56	0.42
1:A:304:ILE:HG12	3:A:356:HOH:O	2.19	0.42
1:A:68:LEU:CA	3:A:360:HOH:O	2.67	0.41
1:A:307:MET:HE2	1:A:307:MET:HB3	1.77	0.41
1:A:214:GLU:HB2	3:A:444:HOH:O	2.20	0.41
1:A:66:ASP:CG	1:A:67:ALA:H	2.24	0.41
1:A:314:GLY:O	1:A:316:ILE:HG12	2.20	0.41
1:A:58:THR:CG2	1:A:59:LEU:N	2.83	0.41
1:A:247:GLY:HA3	1:A:276:ASP:O	2.20	0.41
1:A:220:GLU:CD	1:A:220:GLU:H	2.24	0.40
1:A:260:TRP:C	1:A:262:LEU:N	2.75	0.40
1:A:296:ASN:ND2	2:A:1:SAH:HG2	2.37	0.40
1:A:211:TYR:CE2	1:A:215:ARG:HD3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	278/280 (99%)	240 (86%)	28 (10%)	10 (4%)	5 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	66	ASP
1	A	67	ALA
1	A	224	SER
1	A	279	GLU
1	A	176	GLU
1	A	177	GLU
1	A	180	PRO
1	A	278	PRO
1	A	100	THR

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	236/236 (100%)	205 (87%)	31 (13%)	6 4

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	60	GLU
1	A	62	TYR
1	A	63	TYR

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	69	GLN
1	A	73	VAL
1	A	82	LEU
1	A	103	ARG
1	A	104	LEU
1	A	109	GLN
1	A	114	ILE
1	A	158	LYS
1	A	161	ASP
1	A	163	GLU
1	A	186	PRO
1	A	195	LYS
1	A	198	SER
1	A	207	LEU
1	A	214	GLU
1	A	249	ARG
1	A	251	THR
1	A	254	GLU
1	A	255	VAL
1	A	257	SER
1	A	268	SER
1	A	273	THR
1	A	278	PRO
1	A	280	PRO
1	A	326	GLU
1	A	337	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	109	GLN
1	A	192	HIS
1	A	239	ASN
1	A	252	HIS
1	A	296	ASN
1	A	297	HIS
1	A	310	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

1 ligand is 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	1	-	28,28,28	2.43	11 (39%)	40,40,40	4.74	18 (45%)

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	1	-	-	0/15/31/31	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SAH	C8-N9	5.83	1.45	1.36
2	A	1	SAH	O4'-C1'	4.22	1.47	1.41
2	A	1	SAH	C2-N1	4.07	1.41	1.33
2	A	1	SAH	C5'-SD	-3.92	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SAH	C6-N6	3.74	1.47	1.35
2	A	1	SAH	CG-SD	3.32	1.94	1.81
2	A	1	SAH	C8-N7	-3.21	1.28	1.34
2	A	1	SAH	C2'-C3'	2.84	1.61	1.53
2	A	1	SAH	C2'-C1'	-2.73	1.49	1.53
2	A	1	SAH	CB-CA	-2.34	1.47	1.54
2	A	1	SAH	CA-N	2.12	1.60	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SAH	O4'-C1'-N9	-21.70	88.26	108.44
2	A	1	SAH	C2'-C1'-N9	-8.07	92.55	113.27
2	A	1	SAH	N3-C2-N1	-6.85	122.98	128.71
2	A	1	SAH	C8-N9-C4	-6.34	102.06	106.90
2	A	1	SAH	CG-CB-CA	6.08	123.40	113.22
2	A	1	SAH	CB-CA-N	5.63	123.91	110.14
2	A	1	SAH	CB-CG-SD	-5.63	102.72	113.57
2	A	1	SAH	C5'-C4'-C3'	5.36	128.87	114.98
2	A	1	SAH	O2'-C2'-C1'	-5.11	95.77	111.23
2	A	1	SAH	C4'-O4'-C1'	-4.88	104.44	109.75
2	A	1	SAH	C4-C5-N7	4.13	113.06	109.52
2	A	1	SAH	O4'-C4'-C3'	3.84	112.96	105.17
2	A	1	SAH	C2-N1-C6	3.75	125.55	118.77
2	A	1	SAH	O2'-C2'-C3'	-2.82	102.67	111.83
2	A	1	SAH	C8-N9-C1'	2.66	131.62	126.38
2	A	1	SAH	O4'-C1'-C2'	2.64	110.81	106.77
2	A	1	SAH	C5-C6-N6	2.49	126.34	120.72
2	A	1	SAH	C5-C6-N1	-2.14	112.10	119.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	280/280 (100%)	-0.03	16 (5%)	23 23	23, 45, 93, 102	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	4.6
1	A	102	GLY	4.4
1	A	177	GLU	4.2
1	A	61	GLY	4.0
1	A	66	ASP	3.5
1	A	178	GLY	3.5
1	A	67	ALA	3.1
1	A	63	TYR	2.9
1	A	81	VAL	2.8
1	A	58	THR	2.8
1	A	176	GLU	2.7
1	A	175	THR	2.4
1	A	135	GLU	2.3
1	A	179	ARG	2.3
1	A	78	ASP	2.2
1	A	89	GLY	2.1

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

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SAH	A	1	26/26	0.12	0.09	26,42,49,51	0

6.5 Other polymers

There are no such residues in this entry.