



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:54 am GMT

PDB ID : 3OXG
Title : human lysine methyltransferase Smyd3 in complex with AdoHcy (Form III)
Authors : Xu, S.; Wu, J.; Sun, B.; Zhong, C.; Ding, J.
Deposited on : 2010-09-21
Resolution : 3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

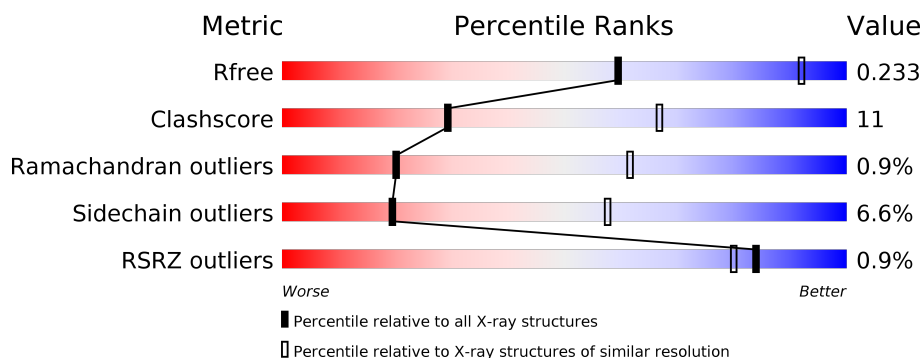
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1074 (3.50-3.34)
Clashscore	112137	1179 (3.50-3.34)
Ramachandran outliers	110173	1147 (3.50-3.34)
Sidechain outliers	110143	1148 (3.50-3.34)
RSRZ outliers	101464	1100 (3.50-3.34)

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. 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	464	<div> <div></div> <div>66%</div> <div>23%</div> <div>9%</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	SAH	A	432	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3426 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 SET and MYND domain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3397	2142	596	621	38	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP Q9H7B4
A	-34	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-33	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-32	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-31	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-30	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-29	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-28	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-27	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-26	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-25	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-24	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-23	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-22	LEU	-	EXPRESSION TAG	UNP Q9H7B4
A	-21	VAL	-	EXPRESSION TAG	UNP Q9H7B4
A	-20	PRO	-	EXPRESSION TAG	UNP Q9H7B4
A	-19	ARG	-	EXPRESSION TAG	UNP Q9H7B4
A	-18	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-17	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-16	HIS	-	EXPRESSION TAG	UNP Q9H7B4
A	-15	MET	-	EXPRESSION TAG	UNP Q9H7B4
A	-14	ALA	-	EXPRESSION TAG	UNP Q9H7B4
A	-13	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-12	MET	-	EXPRESSION TAG	UNP Q9H7B4
A	-11	THR	-	EXPRESSION TAG	UNP Q9H7B4
A	-10	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-9	GLY	-	EXPRESSION TAG	UNP Q9H7B4

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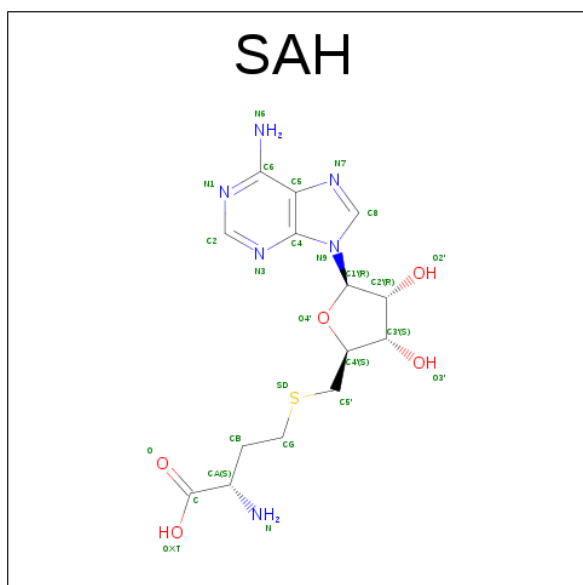
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLN	-	EXPRESSION TAG	UNP Q9H7B4
A	-7	GLN	-	EXPRESSION TAG	UNP Q9H7B4
A	-6	MET	-	EXPRESSION TAG	UNP Q9H7B4
A	-5	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-4	ARG	-	EXPRESSION TAG	UNP Q9H7B4
A	-3	GLY	-	EXPRESSION TAG	UNP Q9H7B4
A	-2	SER	-	EXPRESSION TAG	UNP Q9H7B4
A	-1	GLU	-	EXPRESSION TAG	UNP Q9H7B4
A	0	PHE	-	EXPRESSION TAG	UNP Q9H7B4
A	13	ASN	LYS	SEE REMARK 999	UNP Q9H7B4
A	140	ARG	LYS	SEE REMARK 999	UNP Q9H7B4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Zn 3 3	0	0

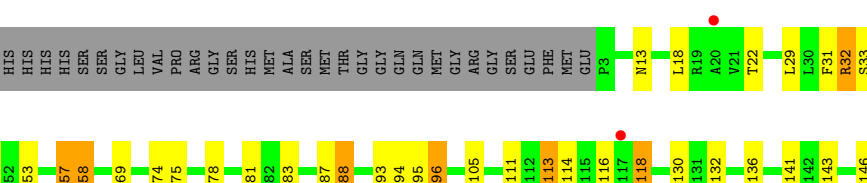
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 



Index	Residue	Category	Secondary Color
1	Met	Grey	Grey
2	Gly	Grey	Grey
3	Ser	Grey	Grey
4	Ser	Grey	Grey
5	His	Grey	Grey
6	His	Grey	Grey
7	His	Grey	Grey
8	His	Grey	Grey
9	His	Grey	Grey
10	Ser	Grey	Grey
11	Ser	Grey	Grey
12	Gly	Grey	Grey
13	Leu	Grey	Grey
14	Val	Grey	Grey
15	Pro	Grey	Grey
16	Arg	Grey	Grey
17	Gly	Grey	Grey
18	Ser	Grey	Grey
19	His	Grey	Grey
20	Met	Grey	Grey
21	Ala	Grey	Grey
22	Ser	Grey	Grey
23	Met	Grey	Grey
24	Thr	Grey	Grey
25	Gly	Grey	Grey
26	Gln	Grey	Grey
27	Gln	Grey	Grey
28	Met	Grey	Grey
29	Gly	Grey	Grey
30	Arg	Grey	Grey
31	Gly	Grey	Grey
32	Ser	Grey	Grey
33	Glu	Grey	Grey
34	Phe	Grey	Grey
35	Met	Grey	Grey
36	Glu	Grey	Grey
37	P3	Green	Green
38	N13	Yellow	Yellow
39	L18	Yellow	Yellow
40	R19	Red	Red
41	A20	Yellow	Yellow
42	V21	Yellow	Yellow
43	T22	Yellow	Yellow
44	L29	Yellow	Yellow
45	L30	Green	Green
46	F31	Green	Green
47	R32	Red	Red
48	S33	Green	Green
49	D34	Yellow	Yellow
50	P35	Green	Green
51	L36	Yellow	Yellow
52	A37	Green	Green
53	T39	Yellow	Yellow
54	V40	Yellow	Yellow
55	G46	Yellow	Yellow
56	C49	Yellow	Yellow
57	D50	Red	Red
58	R51	Green	Green
59	C52	Green	Green
60	L53	Green	Green
61	E57	Red	Red
62	K58	Red	Red
63	K69	Yellow	Yellow
64	K74	Yellow	Yellow
65	C75	Yellow	Yellow
66	K78	Yellow	Yellow
67	P81	Yellow	Yellow
68	D82	Green	Green
69	H83	Green	Green
70	C87	Yellow	Yellow
71	K88	Red	Red
72	C93	Yellow	Yellow
73	K94	Yellow	Yellow
74	P95	Yellow	Yellow
75	R96	Red	Red
76	L105	Yellow	Yellow
77	K111	Yellow	Yellow
78	L112	Green	Green
79	M113	Yellow	Yellow
80	D114	Yellow	Yellow
81	G115	Green	Green
82	A116	Yellow	Yellow
83	P117	Red	Red
84	S118	Red	Red
85	E130	Yellow	Yellow
86	L131	Yellow	Yellow
87	N132	Yellow	Yellow
88	L136	Yellow	Yellow
89	K141	Yellow	Yellow
90	E142	Green	Green
91	G143	Green	Green
92	Q146	Yellow	Yellow
93	F151	Yellow	Yellow
94	F154	Yellow	Yellow
95	M155	Red	Red
96	F157	Yellow	Yellow
97	N316	Green	Green
98	W302	Red	Red
99	E303	Yellow	Yellow
100	P310	Yellow	Yellow
101	L320	Red	Red
102	P321	Yellow	Yellow
103	D322	Yellow	Yellow
104	L325	Yellow	Yellow
105	Y326	Yellow	Yellow
106	Q327	Yellow	Yellow
107	L328	Yellow	Yellow
108	K329	Green	Green
109	V330	Yellow	Yellow
110	L331	Yellow	Yellow
111	D336	Yellow	Yellow
112	L339	Yellow	Yellow
113	L344	Yellow	Yellow
114	L348	Yellow	Yellow
115	E356	Yellow	Yellow
116	P357	Yellow	Yellow
117	F361	Yellow	Yellow
118	F362	Green	Green
119	P363	Yellow	Yellow
120	R369	Yellow	Yellow
121	V373	Yellow	Yellow
122	M374	Yellow	Yellow
123	K378	Yellow	Yellow
124	H382	Yellow	Yellow
125	Q383	Yellow	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	103.44Å 103.44Å 112.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.41 47.55 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.41) 99.6 (47.55-3.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.249 0.217 , 0.233	Depositor DCC
R_{free} test set	448 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.062 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3426	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.43	0/3461	0.54	0/4658

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 [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	3397	0	3408	70	0
2	A	3	0	0	0	0
3	A	26	0	19	11	0
All	All	3426	0	3427	74	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 11.

All (74) 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)
3:A:432:SAH:HA	3:A:432:SAH:H5'2	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB2	3:A:432:SAH:H5'1	1.38	1.01
1:A:130:GLU:HG2	3:A:432:SAH:H3'	1.53	0.90
1:A:130:GLU:CB	3:A:432:SAH:H5'1	2.02	0.89
1:A:208:CYS:HB2	1:A:263:CYS:SG	2.13	0.89
1:A:46:GLY:HA2	1:A:69:LYS:HD2	1.59	0.84
3:A:432:SAH:C5'	3:A:432:SAH:HA	2.07	0.84
1:A:130:GLU:HB2	3:A:432:SAH:C5'	2.14	0.78
1:A:320:LEU:HD23	1:A:321:PRO:HD2	1.69	0.73
1:A:263:CYS:SG	1:A:265:ARG:HB2	2.28	0.73
1:A:93:CYS:HB3	1:A:96:ARG:O	1.88	0.73
1:A:130:GLU:CG	3:A:432:SAH:H5'1	2.23	0.69
1:A:113:MET:SD	1:A:164:GLN:O	2.50	0.68
1:A:369:ARG:O	1:A:373:VAL:HG23	1.97	0.64
1:A:36:LEU:HD12	1:A:111:LYS:HG2	1.80	0.64
1:A:32:ARG:HG3	1:A:220:HIS:CE1	2.33	0.63
1:A:18:LEU:HG	1:A:203:LEU:HB3	1.81	0.62
1:A:130:GLU:HG2	3:A:432:SAH:C3'	2.26	0.62
1:A:166:PRO:O	1:A:169:PHE:HB3	2.00	0.61
1:A:361:PHE:O	1:A:363:PRO:HD3	2.01	0.59
1:A:264:PHE:C	1:A:264:PHE:CD1	2.76	0.59
1:A:38:TYR:OH	1:A:51:ARG:HA	2.02	0.59
3:A:432:SAH:H5'2	3:A:432:SAH:CA	2.19	0.57
1:A:143:GLY:O	1:A:146:GLN:HB2	2.05	0.56
1:A:344:LEU:HD12	1:A:382:HIS:CE1	2.41	0.55
1:A:166:PRO:O	1:A:169:PHE:CB	2.56	0.54
1:A:395:LEU:O	1:A:399:ILE:HG13	2.08	0.54
1:A:32:ARG:HG3	1:A:220:HIS:HE1	1.72	0.53
1:A:105:LEU:HD23	1:A:151:PHE:CE1	2.44	0.52
3:A:432:SAH:C	3:A:432:SAH:SD	2.98	0.52
1:A:388:GLN:O	1:A:391:LYS:HB3	2.10	0.51
1:A:264:PHE:C	1:A:264:PHE:HD1	2.13	0.51
1:A:29:LEU:HD22	1:A:407:GLU:HG2	1.93	0.51
1:A:136:LEU:HB2	1:A:141:LYS:HE3	1.93	0.51
1:A:328:LEU:HA	1:A:331:LEU:HD12	1.93	0.50
1:A:130:GLU:OE2	1:A:132:ASN:N	2.38	0.50
1:A:49:CYS:O	1:A:53:LEU:HD23	2.12	0.50
1:A:83:HIS:CD2	1:A:87:CYS:HB2	2.46	0.50
1:A:31:PHE:HE2	1:A:33:SER:HB2	1.77	0.48
1:A:49:CYS:C	1:A:51:ARG:H	2.16	0.48
1:A:396:ALA:HA	1:A:399:ILE:HD12	1.96	0.48
1:A:322:ASP:HA	1:A:327:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:HA	1:A:339:ILE:HD12	1.96	0.46
1:A:279:ASP:OD2	1:A:282:VAL:HG23	2.16	0.45
1:A:283:TRP:HB3	1:A:320:LEU:HD11	1.97	0.45
1:A:215:VAL:HG23	1:A:222:LEU:HB2	1.99	0.45
1:A:326:TYR:O	1:A:330:VAL:HG23	2.17	0.45
1:A:275:MET:HG2	1:A:361:PHE:CE1	2.53	0.44
1:A:400:MET:HA	1:A:403:THR:OG1	2.16	0.44
1:A:13:ASN:OD1	1:A:13:ASN:N	2.51	0.43
1:A:154:PHE:CD2	1:A:155:MET:HG2	2.53	0.43
1:A:386:PHE:N	1:A:387:PRO:HD2	2.33	0.43
1:A:116:ALA:O	1:A:118:SER:N	2.52	0.43
1:A:78:LYS:O	1:A:81:PRO:HD2	2.18	0.43
1:A:274:ASP:HA	1:A:277:THR:HG23	2.00	0.43
1:A:348:LEU:HD22	1:A:383:GLN:HG3	2.00	0.43
1:A:94:LYS:HA	1:A:95:PRO:HA	1.77	0.42
1:A:253:LEU:HD22	1:A:259:PHE:CZ	2.55	0.42
1:A:83:HIS:NE2	1:A:87:CYS:HB2	2.35	0.42
1:A:206:HIS:CG	1:A:207:SER:N	2.88	0.42
1:A:287:GLN:HA	1:A:290:LEU:HD12	2.02	0.41
1:A:356:GLU:HB3	1:A:357:PRO:HD3	2.01	0.41
1:A:57:GLU:O	1:A:58:LYS:C	2.59	0.41
1:A:88:LYS:HA	1:A:88:LYS:HD3	1.76	0.41
1:A:18:LEU:HD12	1:A:204:LEU:HG	2.03	0.41
1:A:205:ASN:OD1	3:A:432:SAH:O	2.38	0.41
1:A:374:MET:O	1:A:378:LYS:HB2	2.20	0.41
1:A:111:LYS:O	1:A:114:ASP:OD1	2.39	0.41
1:A:206:HIS:CE1	1:A:239:TYR:H	2.39	0.41
1:A:404:HIS:HB3	1:A:408:HIS:HB3	2.02	0.41
1:A:302:TRP:O	1:A:303:GLU:C	2.60	0.40
1:A:325:ILE:HG13	1:A:326:TYR:N	2.37	0.40
1:A:280:GLU:HA	1:A:283:TRP:CE2	2.56	0.40
1:A:51:ARG:O	1:A:53:LEU:HG	2.21	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	422/464 (91%)	370 (88%)	48 (11%)	4 (1%)	20 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	TRP
1	A	50	ASP
1	A	57	GLU
1	A	58	LYS

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	379/410 (92%)	354 (93%)	25 (7%)	19 57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	32	ARG
1	A	34	ASP
1	A	39	THR
1	A	40	VAL
1	A	50	ASP
1	A	74	LYS
1	A	75	CYS
1	A	88	LYS
1	A	96	ARG
1	A	113	MET
1	A	118	SER
1	A	155	MET

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Mol	Chain	Res	Type
1	A	191	GLN
1	A	217	ASN
1	A	228	ASP
1	A	263	CYS
1	A	264	PHE
1	A	272	ASP
1	A	289	SER
1	A	319	ARG
1	A	320	LEU
1	A	401	ARG
1	A	422	ASP
1	A	426	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	132	ASN
1	A	217	ASN
1	A	304	GLN
1	A	382	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	SAH	A	432	-	20,28,28	1.29	3 (15%)	20,40,40	2.00	5 (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
3	SAH	A	432	-	-	0/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	432	SAH	O4'-C1'	2.36	1.44	1.41
3	A	432	SAH	C2-N3	2.50	1.36	1.32
3	A	432	SAH	C5-C4	3.13	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	432	SAH	N3-C2-N1	-5.57	124.01	128.86
3	A	432	SAH	C4'-O4'-C1'	-4.54	104.94	109.77
3	A	432	SAH	C4-C5-N7	-2.38	107.11	109.41
3	A	432	SAH	C1'-N9-C4	-2.07	123.05	126.64
3	A	432	SAH	N6-C6-N1	2.23	123.19	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	432	SAH	11	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	424/464 (91%)	0.16	4 (0%) 84 80	70, 97, 128, 135	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	2.7
1	A	316	ASN	2.4
1	A	234	GLU	2.3
1	A	117	PRO	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SAH	A	432	26/26	0.84	0.26	0.54	49,56,57,57	26

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	429	1/1	1.00	0.13	-1.38	57,57,57,57	0
2	ZN	A	430	1/1	0.99	0.15	-1.68	56,56,56,56	0
2	ZN	A	431	1/1	0.99	0.10	-1.89	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.