



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 10:40 AM GMT

PDB ID : 3MTG
Title : Crystal structure of human S-adenosyl homocysteine hydrolase-like 1 protein
Authors : Wisniewska, M.; Siponen, M.I.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Schutz, P.; Thorsell, A.G.; Tresaugues, L.; van der Berg, S.; Wahlberg, E.; Weigelt, J.; Welin, M.; Schuler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2010-04-30
Resolution : 2.64 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>

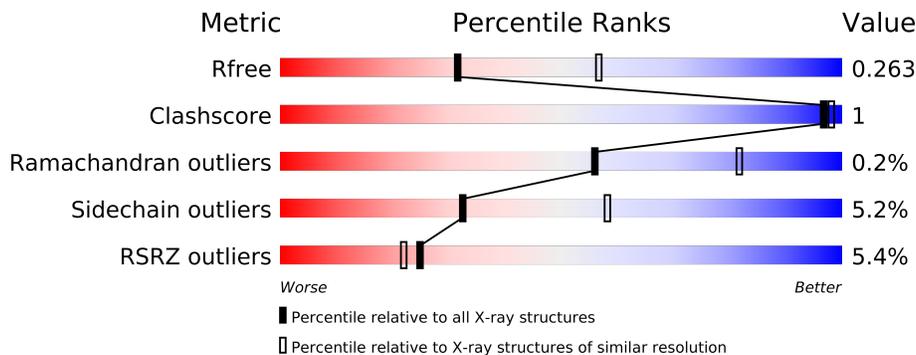
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.64 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	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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	444	
1	B	444	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6792 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.

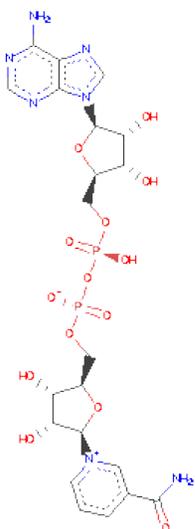
- Molecule 1 is a protein called Putative adenosylhomocysteinase2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	Total 3322	C 2095	N 576	O 624	S 27	0	0	0
1	B	423	Total 3268	C 2063	N 566	O 613	S 26	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	SER	-	EXPRESSION TAG	UNP O43865
A	88	MET	-	EXPRESSION TAG	UNP O43865
A	508	ALA	THR	ENGINEERED MUTATION	UNP O43865
B	87	SER	-	EXPRESSION TAG	UNP O43865
B	88	MET	-	EXPRESSION TAG	UNP O43865
B	508	ALA	THR	ENGINEERED MUTATION	UNP O43865

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

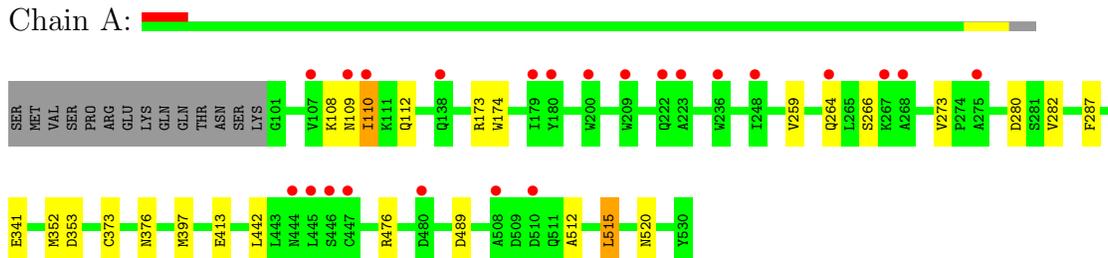
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	59	Total	O	0	0
			59	59		

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.

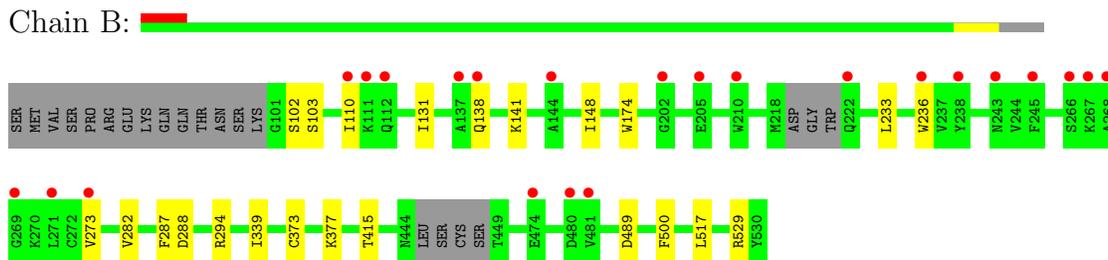
- Molecule 1: Putative adenosylhomocysteinase2

Chain A:



- Molecule 1: Putative adenosylhomocysteinase2

Chain B:



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.24Å 68.60Å 90.37Å 90.00° 115.27° 90.00°	Depositor
Resolution (Å)	33.59 – 2.64 32.73 – 2.64	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.59-2.64) 99.0 (32.73-2.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 2.65Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.203 , 0.249 0.209 , 0.263	Depositor DCC
R_{free} test set	628 reflections (2.12%)	DCC
Wilson B-factor (Å ²)	53.1	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 30251 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.51	0/3383	0.70	0/4592
1	B	0.48	0/3325	0.68	0/4509
All	All	0.50	0/6708	0.69	0/9101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3322	0	0	7	0
1	B	3268	0	0	3	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
3	A	55	0	0	0	0
3	B	59	0	0	0	0
All	All	6792	0	52	7	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 1.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ILE:O	1:A:110:ILE:CG2	2.30	0.75
1:A:109:ASN:ND2	1:A:112:GLN:OE1	2.22	0.72
1:A:352:MET:CE	1:B:500:PHE:CZ	2.97	0.48
1:A:512:ALA:O	1:A:515:LEU:O	2.34	0.45
1:A:353:ASP:OD1	1:B:294:ARG:NH2	2.51	0.44
1:A:280:ASP:O	1:B:529:ARG:NH2	2.51	0.43
1:A:397:MET:O	2:A:1:NAD:H2N	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

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	428/444 (96%)	406 (95%)	21 (5%)	1 (0%)	56	82
1	B	417/444 (94%)	389 (93%)	27 (6%)	1 (0%)	56	82
All	All	845/888 (95%)	795 (94%)	48 (6%)	2 (0%)	56	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	VAL
1	A	282	VAL

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	357/378 (94%)	339 (95%)	18 (5%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	351/378 (93%)	332 (95%)	19 (5%)	31	56
All	All	708/756 (94%)	671 (95%)	37 (5%)	32	58

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	110	ILE
1	A	173	ARG
1	A	174	TRP
1	A	259	VAL
1	A	264	GLN
1	A	266	SER
1	A	273	VAL
1	A	287	PHE
1	A	341	GLU
1	A	373	CYS
1	A	376	ASN
1	A	413	GLU
1	A	442	LEU
1	A	476	ARG
1	A	489	ASP
1	A	515	LEU
1	A	520	ASN
1	B	102	SER
1	B	103	SER
1	B	110	ILE
1	B	131	ILE
1	B	138	GLN
1	B	141	LYS
1	B	148	ILE
1	B	174	TRP
1	B	233	LEU
1	B	236	TRP
1	B	273	VAL
1	B	287	PHE
1	B	288	ASP
1	B	339	ILE
1	B	373	CYS
1	B	377	LYS
1	B	415	THR
1	B	489	ASP

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Mol	Chain	Res	Type
1	B	517	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	NAD	A	1	-	48,48,48	1.42	4 (8%)	73,73,73	1.90	10 (13%)
2	NAD	B	1	-	48,48,48	1.39	3 (6%)	73,73,73	1.78	8 (10%)

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	NAD	A	1	-	-	0/30/62/62	0/3/5/5
2	NAD	B	1	-	-	0/30/62/62	0/3/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAD	O7N-C7N	7.26	1.41	1.24
2	A	1	NAD	O7N-C7N	7.17	1.41	1.24
2	A	1	NAD	C2A-N3A	3.43	1.39	1.32
2	B	1	NAD	C2A-N3A	3.41	1.38	1.32
2	A	1	NAD	C2A-N1A	2.77	1.39	1.33
2	B	1	NAD	C2A-N1A	2.75	1.39	1.33
2	A	1	NAD	C2N-N1N	2.13	1.38	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAD	N3A-C2A-N1A	-11.45	119.13	128.71
2	B	1	NAD	N3A-C2A-N1A	-10.61	119.84	128.71
2	A	1	NAD	O4D-C1D-N1N	5.34	113.42	107.95
2	B	1	NAD	N3A-C4A-N9A	4.17	132.95	125.43
2	A	1	NAD	N3A-C4A-N9A	4.10	132.84	125.43
2	B	1	NAD	O4D-C1D-N1N	3.86	111.90	107.95
2	B	1	NAD	C3N-C7N-N7N	3.07	121.26	117.77
2	A	1	NAD	C3N-C7N-N7N	3.01	121.19	117.77
2	A	1	NAD	C5A-C4A-N3A	-2.54	120.18	125.70
2	A	1	NAD	C2A-N3A-C4A	2.52	121.18	114.01
2	A	1	NAD	O4B-C1B-N9A	2.51	110.78	108.44
2	A	1	NAD	O7N-C7N-C3N	-2.43	116.83	119.58
2	B	1	NAD	C5A-C4A-N3A	-2.41	120.46	125.70
2	B	1	NAD	C2A-N3A-C4A	2.23	120.36	114.01
2	A	1	NAD	N7A-C8A-N9A	-2.19	108.15	114.36
2	B	1	NAD	N7A-C8A-N9A	-2.18	108.18	114.36
2	B	1	NAD	O7N-C7N-C3N	-2.14	117.17	119.58
2	A	1	NAD	PN-O3-PA	-2.00	124.36	132.95

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	430/444 (96%)	0.17	23 (5%) 25 22	30, 84, 127, 149	0
1	B	423/444 (95%)	0.20	23 (5%) 25 22	28, 81, 139, 170	0
All	All	853/888 (96%)	0.19	46 (5%) 25 22	28, 82, 134, 170	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	GLN	8.3
1	B	269	GLY	5.8
1	B	137	ALA	5.7
1	A	445	LEU	5.5
1	A	444	ASN	5.3
1	B	267	LYS	4.8
1	A	446	SER	4.7
1	B	474	GLU	4.6
1	B	111	LYS	4.4
1	B	245	PHE	4.0
1	B	202	GLY	3.9
1	A	447	CYS	3.9
1	B	480	ASP	3.7
1	B	273	VAL	3.6
1	A	275	ALA	3.3
1	A	267	LYS	3.3
1	B	271	LEU	3.3
1	B	481	VAL	3.2
1	B	268	ALA	3.0
1	A	200	TRP	3.0
1	A	138	GLN	3.0
1	A	109	ASN	3.0
1	B	243	ASN	2.9
1	B	236	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	180	TYR	2.8
1	A	236	TRP	2.7
1	B	210	TRP	2.7
1	B	138	GLN	2.6
1	B	144	ALA	2.5
1	A	480	ASP	2.5
1	B	266	SER	2.5
1	A	107	VAL	2.5
1	A	268	ALA	2.4
1	A	510	ASP	2.3
1	A	110	ILE	2.3
1	A	508	ALA	2.3
1	A	209	TRP	2.3
1	B	110	ILE	2.2
1	A	222	GLN	2.1
1	B	112	GLN	2.1
1	A	223	ALA	2.1
1	A	264	GLN	2.1
1	A	179	ILE	2.0
1	B	238	TYR	2.0
1	A	248	ILE	2.0
1	B	205	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	NAD	B	1	44/44	0.16	0.12	42,52,59,60	0
2	NAD	A	1	44/44	0.16	-0.18	47,55,65,67	0

6.5 Other polymers

There are no such residues in this entry.