wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:29 AM GMT

PDB ID	:	2H5L
Title	:	S-Adenosylhomocysteine hydrolase containing NAD and 3-deaza-D-eritadeni ne
Authors	:	Yamada, T.; Komoto, J.; Takusagawa, F.
Deposited on	:	2006-05-26
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

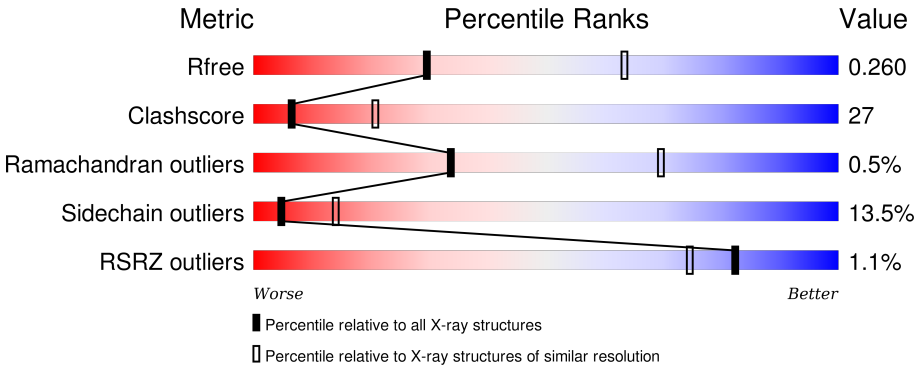
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	431	58% 35% 7%
1	B	431	% 55% 38% 7%
1	C	431	% 55% 38% 7%
1	D	431	4% 55% 38% 7%
1	E	431	% 55% 37% 7%

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Mol	Chain	Length	Quality of chain
1	F	431	56% 36% 7%
1	G	431	% 54% 39% 7%
1	H	431	54% 37% 9%

2 Entry composition (i)

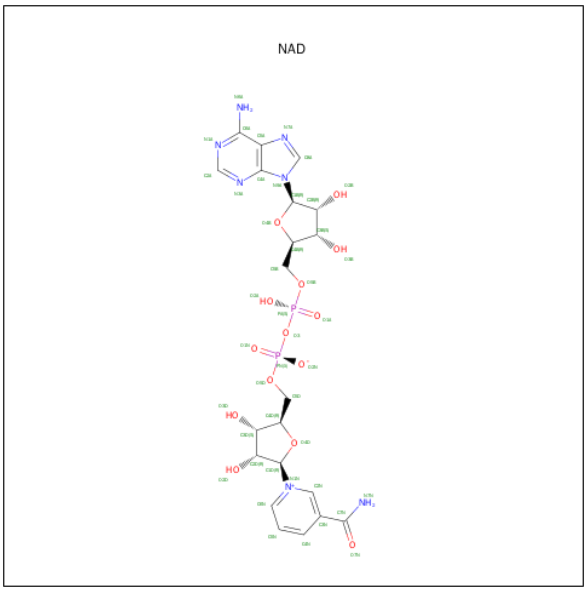
There are 4 unique types of molecules in this entry. The entry contains 27338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

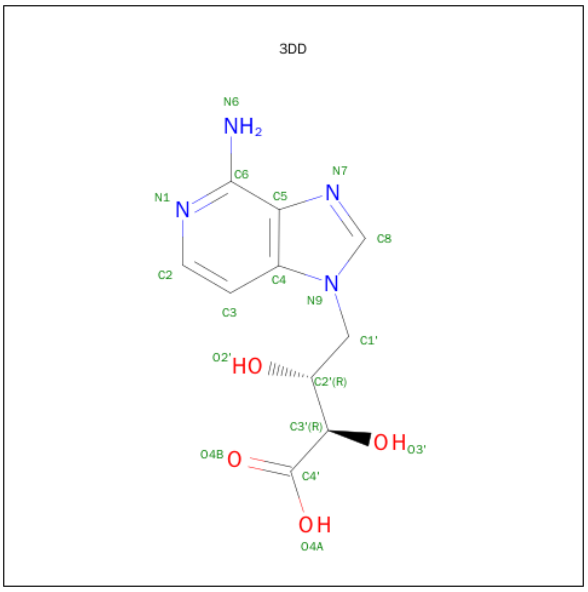
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	E	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	F	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	G	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	H	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (2R,3R)-4-(4-AMINO-1H-IMIDAZO[4,5-C]PYRIDIN-1-YL)-2,3-DIHYDROXYBUTANOIC ACID (three-letter code: 3DD) (formula: $C_{10}H_{12}N_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 18 10 4 4	0	0
3	B	1	Total C N O 18 10 4 4	0	0
3	C	1	Total C N O 18 10 4 4	0	0
3	D	1	Total C N O 18 10 4 4	0	0
3	E	1	Total C N O 18 10 4 4	0	0
3	F	1	Total C N O 18 10 4 4	0	0
3	G	1	Total C N O 18 10 4 4	0	0
3	H	1	Total C N O 18 10 4 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	30	Total O 30 30	0	0
4	C	28	Total O 28 28	0	0
4	D	34	Total O 34 34	0	0

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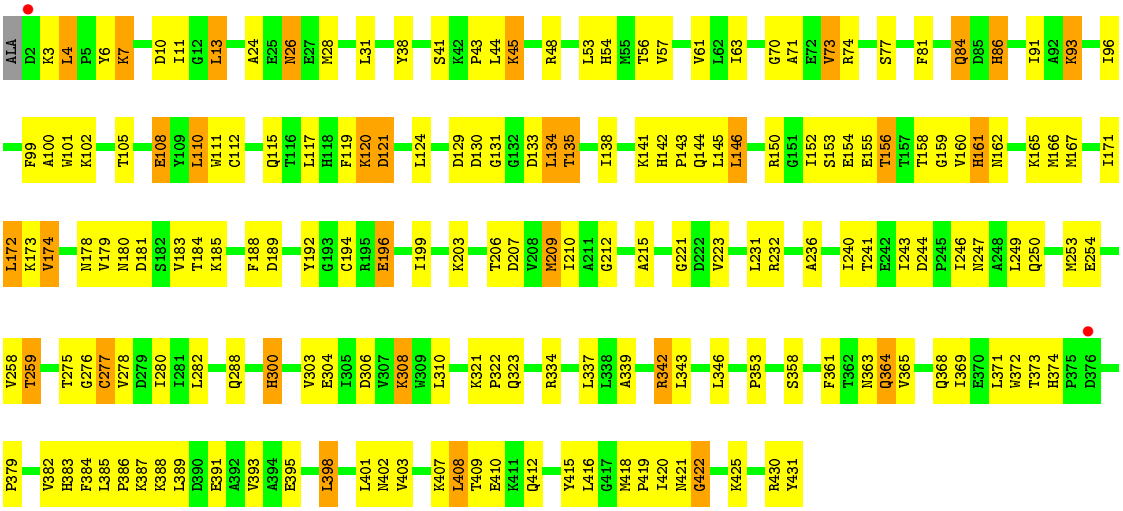
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	53	Total O 53 53	0	0
4	F	35	Total O 35 35	0	0
4	G	33	Total O 33 33	0	0
4	H	30	Total O 30 30	0	0

3 Residue-property plots (i)

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

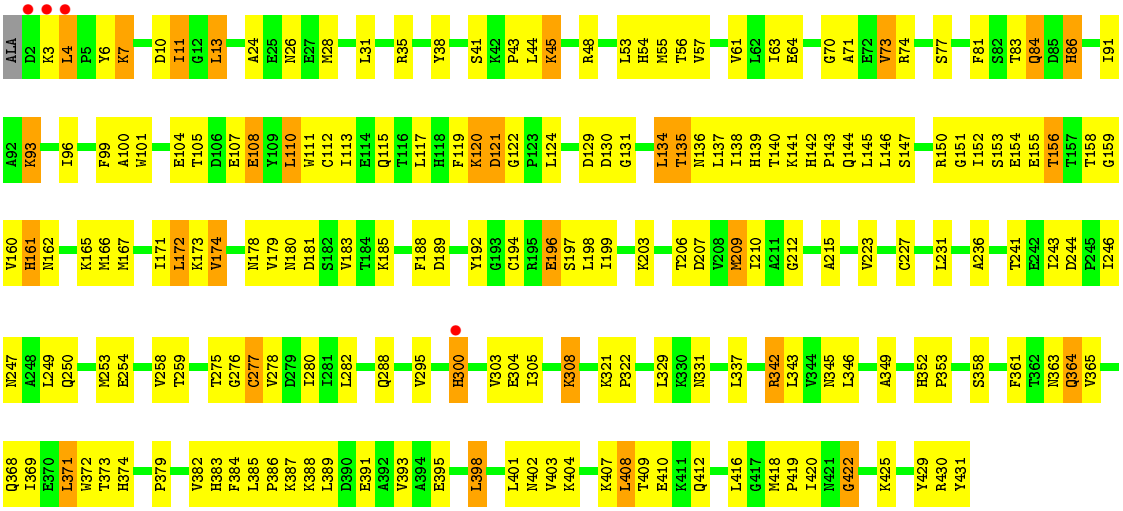
- Molecule 1: Adenosylhomocysteinase

Chain A:



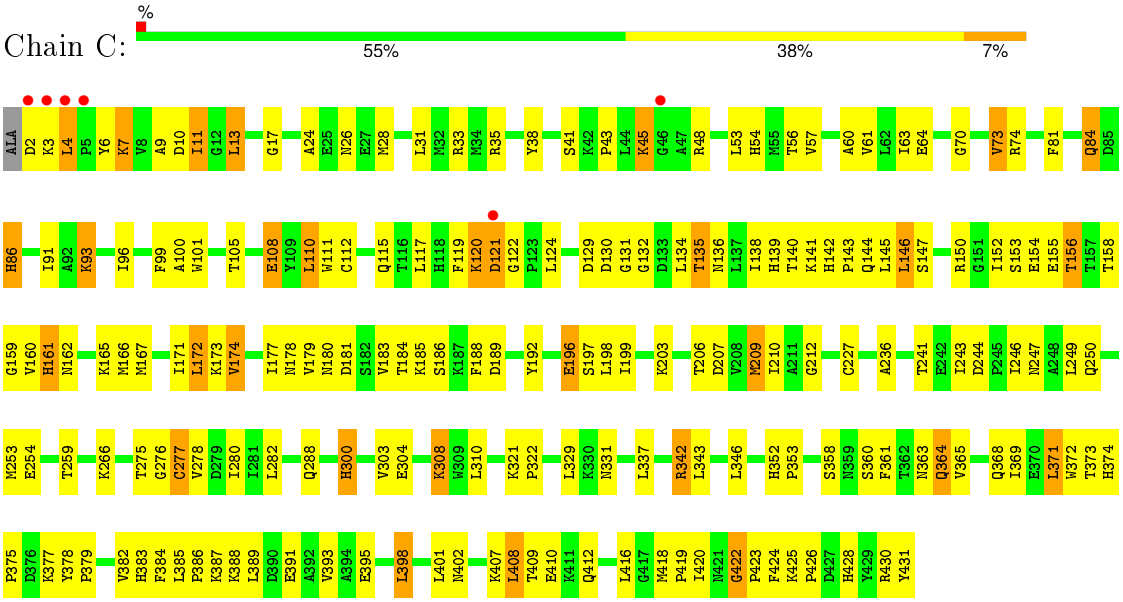
- Molecule 1: Adenosylhomocysteinase

Chain B:



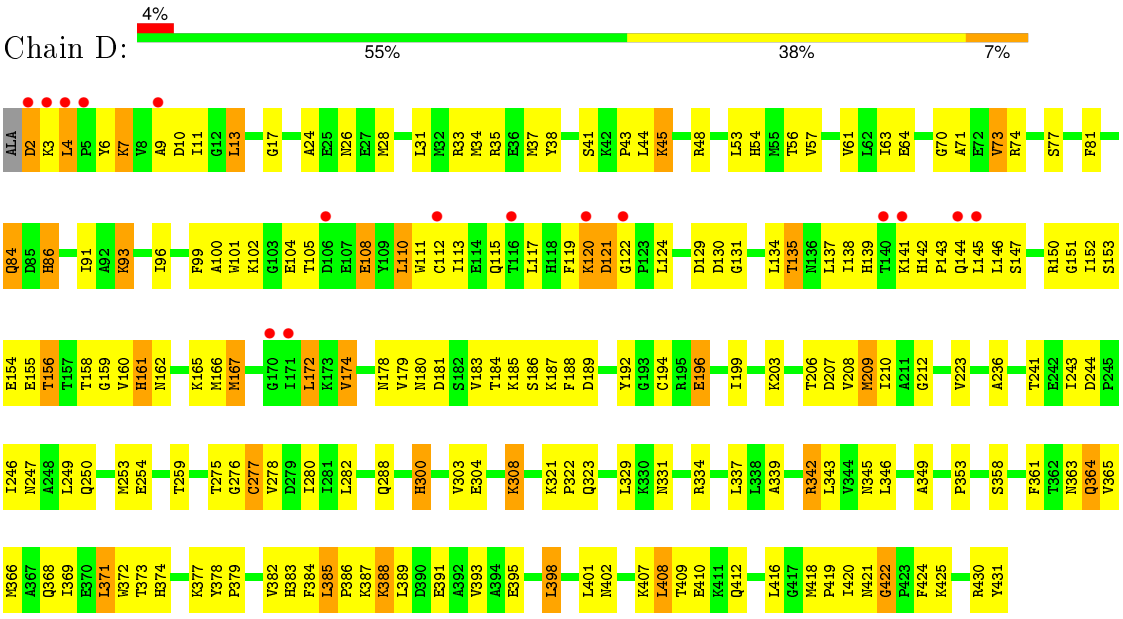
- Molecule 1: Adenosylhomocysteinase

Chain C:



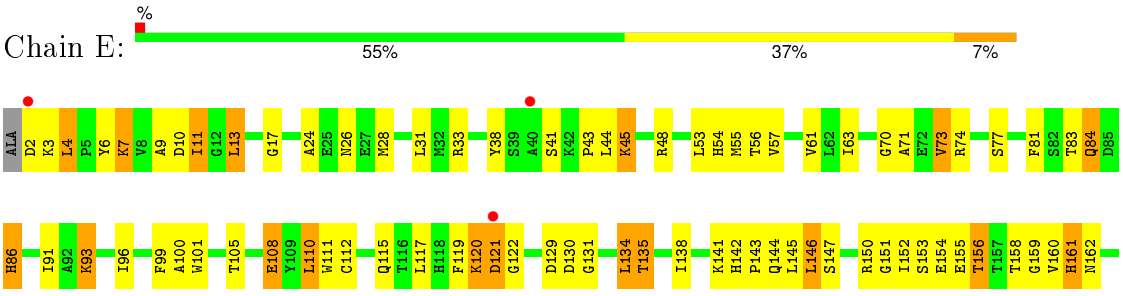
- Molecule 1: Adenosylhomocysteinase

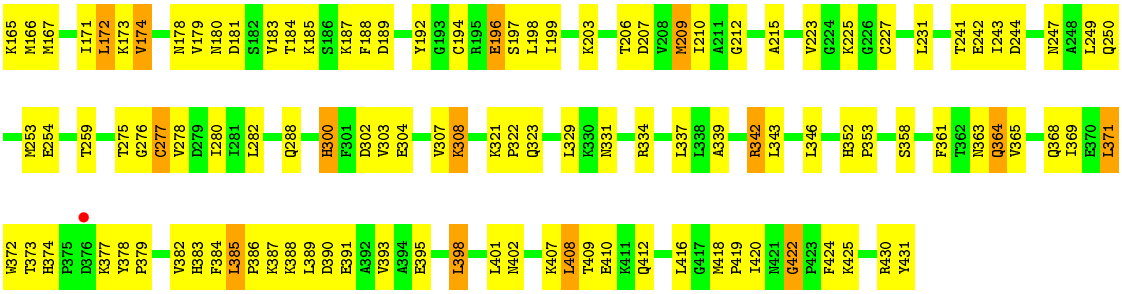
Chain D:



- Molecule 1: Adenosylhomocysteinase

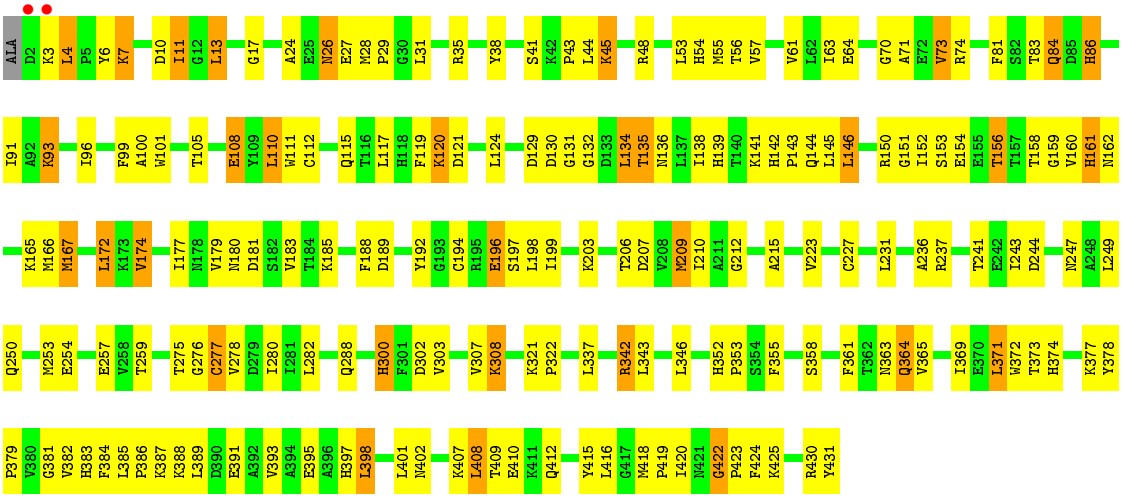
Chain E:





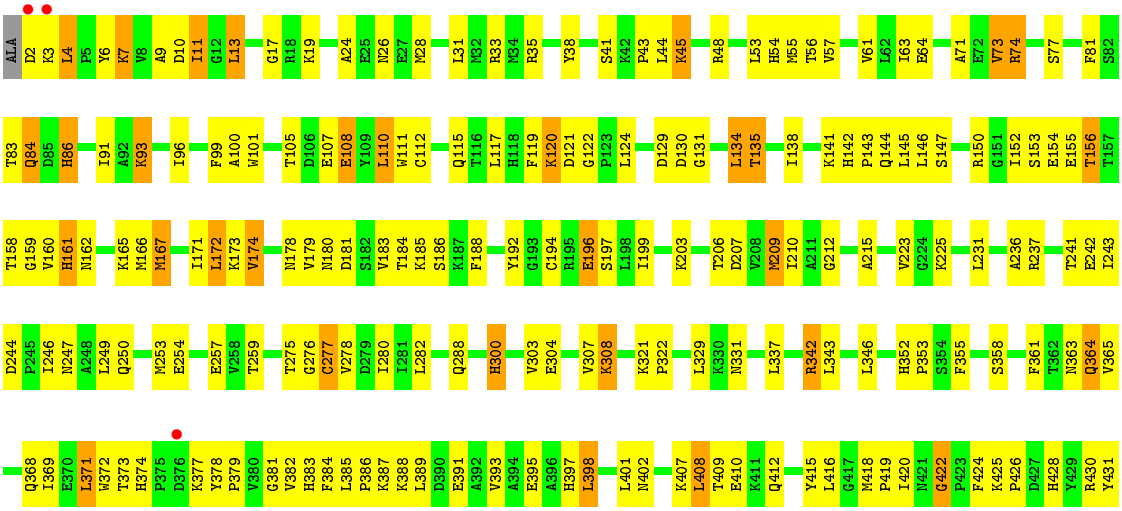
• Molecule 1: Adenosylhomocysteinase

Chain F:



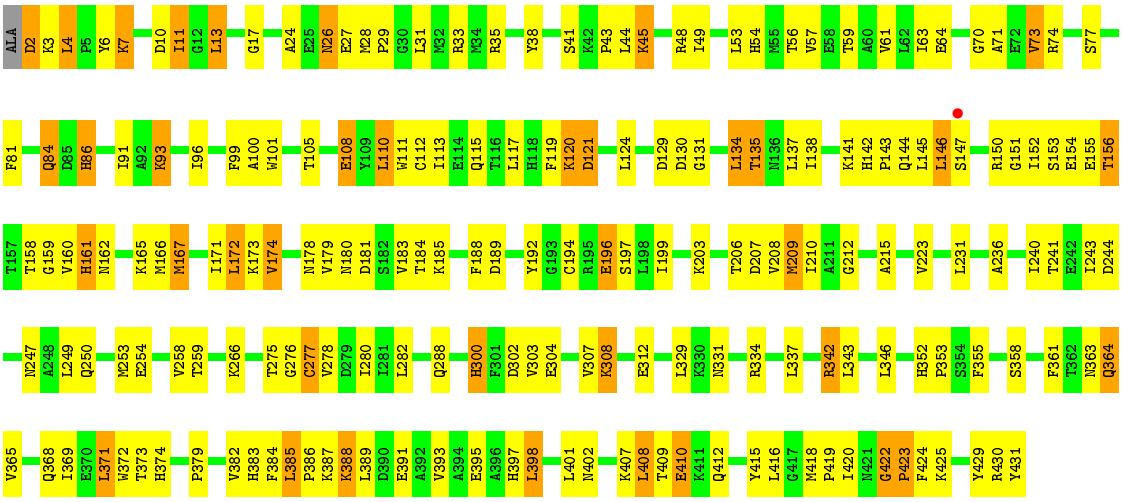
• Molecule 1: Adenosylhomocysteinase

Chain G:



• Molecule 1: Adenosylhomocysteinase

Chain H:


ALA D2 K3 L4 P5 Y6 K7 D10 I11 G12 L13 G17 A24 E25 N26 E27 M28 P29 G30 I31 N32 R33 N34 R35 Y38 S41 K42 P43 L44 K45 R48 I49 L53 H54 M55 T56 V57 E58 T59 A60 V61 L62 I63 E64 G70 A71 E72 V73 R74 S77
F81 Q84 D85 H86 I91 A92 K93 I96 F99 A100 W101 T105 E108 Y109 L110 W111 C112 I113 E114 Q115 T116 L117 H118 F119 K120 D121 L124 D129 D130 G131 L134 T135 N136 L137 I138 K141 H142 P143 Q144 L145 L146 S147 R150 G151 I152 S153 E154 E155 T156
T157 T158 G159 V160 H161 N162 K165 M166 M167 I171 L172 K173 V174 N178 V179 N180 D181 S182 V183 T184 K185 F188 D189 Y192 G193 C194 R195 E196 S197 L198 I199 K203 T206 D207 V208 M209 I210 A211 G212 A215 V223 L231 A236 I240 T241 E242 I243 D244
N247 A248 I249 Q250 M253 E254 V258 T259 K266 T275 G276 C277 V278 D279 I280 I281 L282 Q288 H300 F301 D302 V303 E304 V307 K308 E312 L329 K330 N331 R334 L337 R342 L343 L346 H352 P353 S354 F355 S358 F361 Y362 N363 Q364
V365 Q368 I369 E370 L371 W372 T373 H374 P379 V382 H383 F384 L385 P386 K387 K388 L389 D390 E391 A392 V393 A394 E395 A396 H397 L398 L401 N402 K407 L408 T409 E410 K411 Q412 Y415 L416 G417 M418 P419 I420 N421 G422 P423 F424 K425 Y429 R430 Y431

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.50Å 178.60Å 112.66Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 91.92 – 2.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 92.3 (91.92-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.77Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.248 , 0.283 0.229 , 0.260	Depositor DCC
R_{free} test set	7705 reflections (10.06%)	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 10.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 78969 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27338	wwPDB-VP
Average B, all atoms (Å^2)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DD, 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	0.39	0/3384	0.60	0/4579
1	B	0.39	0/3384	0.60	0/4579
1	C	0.39	0/3384	0.61	0/4579
1	D	0.40	0/3384	0.61	0/4579
1	E	0.38	0/3384	0.61	0/4579
1	F	0.39	0/3384	0.61	0/4579
1	G	0.38	0/3384	0.61	0/4579
1	H	0.38	0/3384	0.61	0/4579
All	All	0.39	0/27072	0.61	0/36632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3319	0	3341	193	0
1	B	3319	0	3341	205	0
1	C	3319	0	3341	198	0
1	D	3319	0	3341	207	0
1	E	3319	0	3341	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3319	0	3341	187	0
1	G	3319	0	3341	200	0
1	H	3319	0	3341	199	0
2	A	44	0	26	6	0
2	B	44	0	26	5	0
2	C	44	0	26	6	0
2	D	44	0	26	6	0
2	E	44	0	26	6	0
2	F	44	0	26	5	0
2	G	44	0	26	5	0
2	H	44	0	26	4	0
3	A	18	0	11	0	0
3	B	18	0	11	0	0
3	C	18	0	11	0	0
3	D	18	0	11	0	0
3	E	18	0	11	0	0
3	F	18	0	11	0	0
3	G	18	0	11	0	0
3	H	18	0	11	0	0
4	A	47	0	0	2	0
4	B	30	0	0	1	0
4	C	28	0	0	2	0
4	D	34	0	0	10	0
4	E	53	0	0	1	0
4	F	35	0	0	1	0
4	G	33	0	0	3	0
4	H	30	0	0	2	0
All	All	27338	0	27024	1480	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 27.

The worst 5 of 1480 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:G:105:THR:H	1:G:108:GLU:HG3	1.18	1.08
1:F:275:THR:HG22	1:F:277:CYS:H	1.18	1.08
1:B:275:THR:HG22	1:B:277:CYS:H	1.16	1.08
1:E:275:THR:HG22	1:E:277:CYS:H	1.13	1.07
1:C:275:THR:HG22	1:C:277:CYS:H	1.17	1.07

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	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	34	69
1	B	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	34	69
1	C	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	34	69
1	D	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	34	69
1	E	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	34	69
1	F	428/431 (99%)	410 (96%)	16 (4%)	2 (0%)	34	69
1	G	428/431 (99%)	410 (96%)	16 (4%)	2 (0%)	34	69
1	H	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	34	69
All	All	3424/3448 (99%)	3271 (96%)	137 (4%)	16 (0%)	34	69

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	GLY
1	B	422	GLY
1	C	422	GLY
1	D	422	GLY
1	E	422	GLY

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	353/353 (100%)	307 (87%)	46 (13%)	5	15
1	B	353/353 (100%)	309 (88%)	44 (12%)	6	17
1	C	353/353 (100%)	305 (86%)	48 (14%)	5	14
1	D	353/353 (100%)	306 (87%)	47 (13%)	5	14
1	E	353/353 (100%)	303 (86%)	50 (14%)	4	12
1	F	353/353 (100%)	307 (87%)	46 (13%)	5	15
1	G	353/353 (100%)	305 (86%)	48 (14%)	5	14
1	H	353/353 (100%)	302 (86%)	51 (14%)	4	12
All	All	2824/2824 (100%)	2444 (86%)	380 (14%)	5	14

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	308	LYS
1	E	196	GLU
1	H	156	THR
1	D	371	LEU
1	E	41	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	364	GLN
1	E	250	GLN
1	H	247	ASN
1	D	368	GLN
1	E	26	ASN

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)

16 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	432	-	38,48,48	2.18	7 (18%)	47,73,73	1.67	8 (17%)
3	3DD	A	433	-	14,19,19	2.16	5 (35%)	10,27,27	1.46	3 (30%)
2	NAD	B	432	-	38,48,48	2.00	7 (18%)	47,73,73	1.73	9 (19%)
3	3DD	B	433	-	14,19,19	2.06	4 (28%)	10,27,27	1.52	3 (30%)
2	NAD	C	432	-	38,48,48	2.16	7 (18%)	47,73,73	1.75	9 (19%)
3	3DD	C	433	-	14,19,19	2.08	4 (28%)	10,27,27	1.62	3 (30%)
2	NAD	D	432	-	38,48,48	2.14	7 (18%)	47,73,73	1.78	9 (19%)
3	3DD	D	433	-	14,19,19	1.95	5 (35%)	10,27,27	1.43	2 (20%)
2	NAD	E	432	-	38,48,48	2.11	8 (21%)	47,73,73	1.69	9 (19%)
3	3DD	E	433	-	14,19,19	2.20	3 (21%)	10,27,27	1.49	3 (30%)
2	NAD	F	432	-	38,48,48	2.04	8 (21%)	47,73,73	1.74	9 (19%)
3	3DD	F	433	-	14,19,19	2.16	6 (42%)	10,27,27	1.57	3 (30%)
2	NAD	G	432	-	38,48,48	2.05	8 (21%)	47,73,73	1.73	9 (19%)
3	3DD	G	433	-	14,19,19	2.18	4 (28%)	10,27,27	1.47	3 (30%)
2	NAD	H	432	-	38,48,48	2.17	6 (15%)	47,73,73	1.84	9 (19%)
3	3DD	H	433	-	14,19,19	2.26	7 (50%)	10,27,27	1.47	3 (30%)

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	432	-	-	0/22/62/62	0/5/5/5
3	3DD	A	433	-	-	0/6/12/12	0/2/2/2
2	NAD	B	432	-	-	0/22/62/62	0/5/5/5
3	3DD	B	433	-	-	0/6/12/12	0/2/2/2
2	NAD	C	432	-	-	0/22/62/62	0/5/5/5
3	3DD	C	433	-	-	0/6/12/12	0/2/2/2
2	NAD	D	432	-	-	0/22/62/62	0/5/5/5
3	3DD	D	433	-	-	0/6/12/12	0/2/2/2
2	NAD	E	432	-	-	0/22/62/62	0/5/5/5
3	3DD	E	433	-	-	0/6/12/12	0/2/2/2
2	NAD	F	432	-	-	0/22/62/62	0/5/5/5
3	3DD	F	433	-	-	0/6/12/12	0/2/2/2
2	NAD	G	432	-	-	0/22/62/62	0/5/5/5
3	3DD	G	433	-	-	0/6/12/12	0/2/2/2
2	NAD	H	432	-	-	0/22/62/62	0/5/5/5
3	3DD	H	433	-	-	0/6/12/12	0/2/2/2

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	432	NAD	O4B-C1B	-4.86	1.35	1.41
2	A	432	NAD	O4B-C1B	-4.66	1.35	1.41
2	H	432	NAD	O4B-C1B	-4.55	1.35	1.41
2	G	432	NAD	O4B-C1B	-4.48	1.35	1.41
2	C	432	NAD	O4B-C1B	-4.28	1.35	1.41

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	432	NAD	O7N-C7N-C3N	-6.57	112.42	119.59
2	F	432	NAD	O7N-C7N-C3N	-6.30	112.71	119.59
2	D	432	NAD	O7N-C7N-C3N	-6.09	112.93	119.59
2	G	432	NAD	O7N-C7N-C3N	-6.08	112.95	119.59
2	B	432	NAD	O7N-C7N-C3N	-6.00	113.03	119.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	432	NAD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	432	NAD	5	0
2	C	432	NAD	6	0
2	D	432	NAD	6	0
2	E	432	NAD	6	0
2	F	432	NAD	5	0
2	G	432	NAD	5	0
2	H	432	NAD	4	0

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, 95^{th} 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	430/431 (99%)	-0.67	2 (0%)	91 88	2, 4, 15, 39	0
1	B	430/431 (99%)	-0.56	4 (0%)	85 79	2, 5, 18, 44	0
1	C	430/431 (99%)	-0.43	6 (1%)	78 69	2, 5, 18, 44	0
1	D	430/431 (99%)	-0.24	16 (3%)	45 33	2, 5, 21, 43	0
1	E	430/431 (99%)	-0.63	4 (0%)	85 79	2, 4, 16, 39	0
1	F	430/431 (99%)	-0.66	2 (0%)	91 88	2, 4, 14, 43	0
1	G	430/431 (99%)	-0.56	3 (0%)	89 84	2, 5, 17, 44	0
1	H	430/431 (99%)	-0.63	1 (0%)	95 94	2, 4, 15, 40	0
All	All	3440/3448 (99%)	-0.55	38 (1%)	82 74	2, 4, 17, 44	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ASP	8.4
1	F	2	ASP	7.5
1	G	2	ASP	7.0
1	B	2	ASP	6.6
1	D	2	ASP	4.5

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^{th} 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	3DD	F	433	18/18	0.91	0.16	0.83	2,2,8,9	0
3	3DD	H	433	18/18	0.90	0.16	0.70	2,3,6,9	0
3	3DD	E	433	18/18	0.92	0.15	0.45	2,2,5,10	0
3	3DD	D	433	18/18	0.92	0.15	0.32	2,2,6,14	0
3	3DD	G	433	18/18	0.92	0.14	0.22	2,4,8,11	0
3	3DD	A	433	18/18	0.92	0.14	-0.01	2,3,8,10	0
3	3DD	B	433	18/18	0.91	0.14	-0.04	2,2,8,14	0
2	NAD	H	432	44/44	0.94	0.14	-0.12	2,2,5,10	0
3	3DD	C	433	18/18	0.91	0.14	-0.22	2,5,9,12	0
2	NAD	A	432	44/44	0.95	0.12	-0.41	2,2,6,6	0
2	NAD	C	432	44/44	0.96	0.11	-0.57	2,2,6,8	0
2	NAD	F	432	44/44	0.96	0.11	-0.69	2,2,5,8	0
2	NAD	D	432	44/44	0.96	0.11	-0.70	2,3,6,8	0
2	NAD	B	432	44/44	0.96	0.11	-0.71	2,2,6,10	0
2	NAD	E	432	44/44	0.96	0.11	-0.80	2,2,5,7	0
2	NAD	G	432	44/44	0.96	0.10	-0.91	2,2,6,12	0

6.5 Other polymers (i)

There are no such residues in this entry.