wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 06:30 AM EDT

PDB ID	:	1LT7
Title	:	Oxidized Homo sapiens betaine-homocysteine S-methyltransferase in complex with four Sm(III) ions
Authors	:	Evans, J.C.; Huddler, D.P.; Jiracek, J.; Castro, C.; Millian, N.S.; Garrow, T.A.; Ludwig, M.L.
Deposited on	:	2002-05-20
Resolution	:	2.15 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
https://www.wwpdb.org/validation/2017/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:

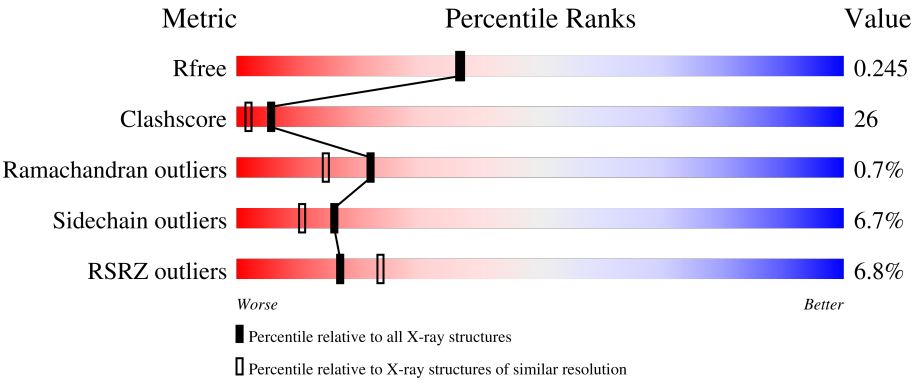
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	406	5% 48% 25% . 25%
1	B	406	5% 47% 26% . 22%

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	CIT	A	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5146 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 BETAINE-HOMOCYSTEINE METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2368	1511	414	434	9			
1	B	315	Total	C	N	O	S	0	0	0
			2450	1565	428	447	10			

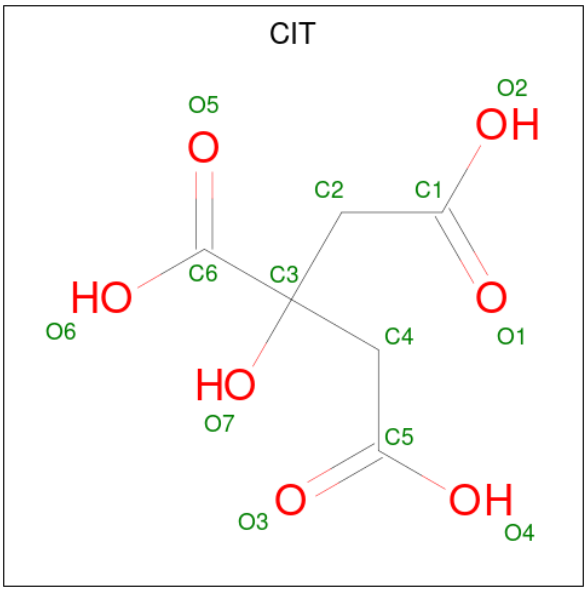
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	engineered mutation	UNP Q93088
A	104	ALA	CYS	engineered mutation	UNP Q93088
A	131	ALA	CYS	engineered mutation	UNP Q93088
A	186	ALA	CYS	engineered mutation	UNP Q93088
A	201	ALA	CYS	engineered mutation	UNP Q93088
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
A	256	ALA	CYS	engineered mutation	UNP Q93088
B	2	ALA	PRO	engineered mutation	UNP Q93088
B	104	ALA	CYS	engineered mutation	UNP Q93088
B	131	ALA	CYS	engineered mutation	UNP Q93088
B	186	ALA	CYS	engineered mutation	UNP Q93088
B	201	ALA	CYS	engineered mutation	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	256	ALA	CYS	engineered mutation	UNP Q93088

- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Sm	0	0
			2	2		
2	B	2	Total	Sm	0	0
			2	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

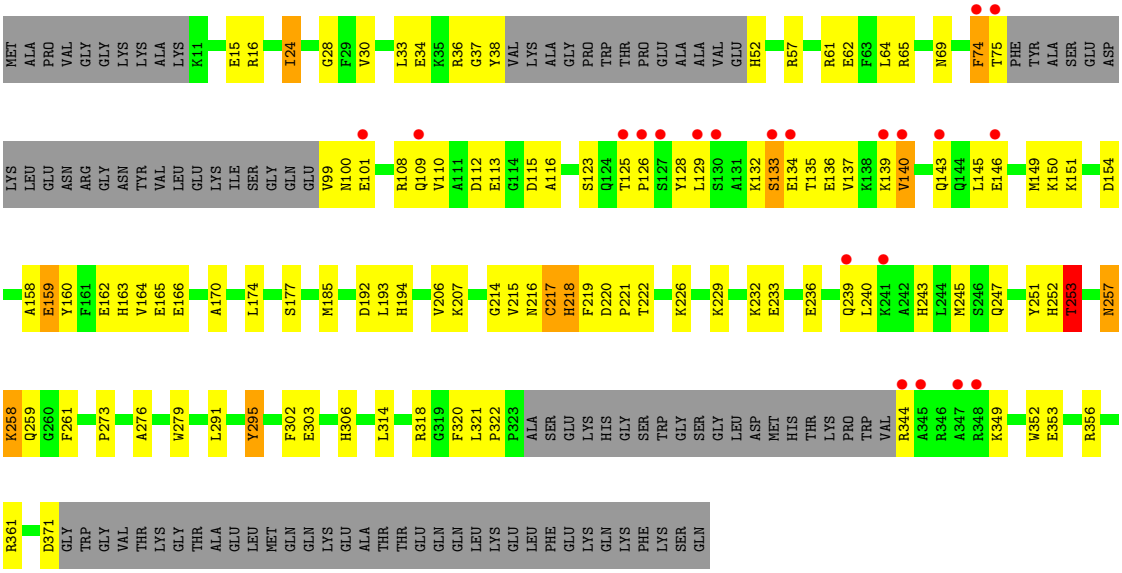
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	150	Total O 150 150	0	0
4	B	148	Total O 148 148	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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.

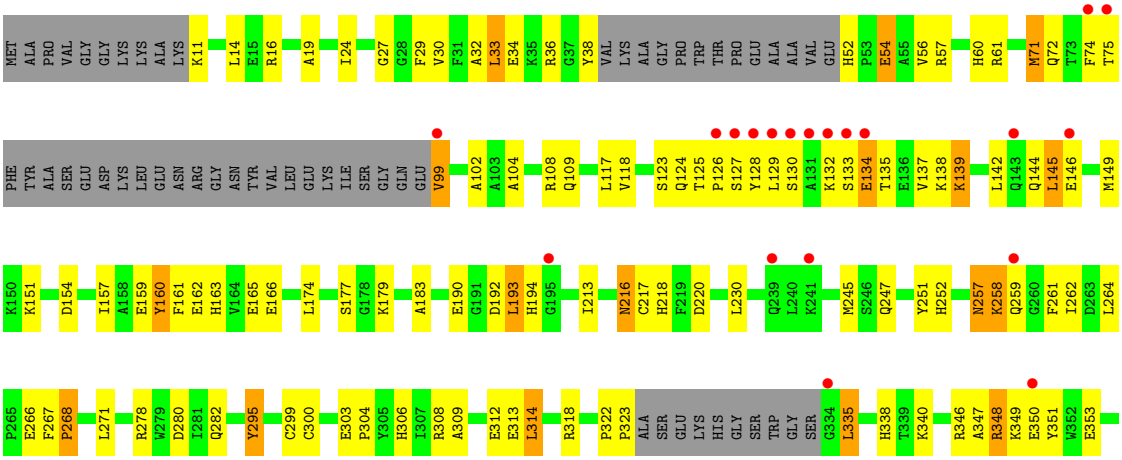
• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE

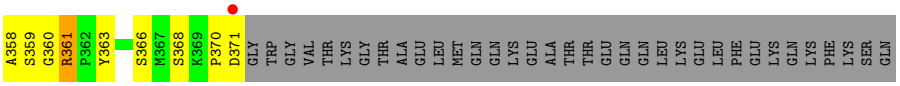
Chain A:



• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE

Chain B:




A358
S359
G360
R361
P362
Y363
S366
M367
S368
K369
P370
D371
GLY
TRP
GLY
VAL
THR
LYS
GLY
THR
ALA
GLU
LEU
MET
GLN
GLN
LYS
GLU
ALA
THR
THR
GLU
GLN
GLN
LEU
LYS
GLU
LEU
PHE
GLU
LYS
GLN
LYS
PHE
LYS
SER
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.99Å 90.08Å 89.08Å 90.00° 122.10° 90.00°	Depositor
Resolution (Å)	9.99 – 2.15 9.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.3 (9.99-2.15) 98.7 (9.99-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.15Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.249 0.203 , 0.245	Depositor DCC
R_{free} test set	7403 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.52 , 95.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SM, CIT

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	0.70	0/2421	0.80	3/3274 (0.1%)
1	B	0.66	1/2507 (0.0%)	0.77	3/3392 (0.1%)
All	All	0.68	1/4928 (0.0%)	0.78	6/6666 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	ALA	CA-CB	5.06	1.63	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	CYS	N-CA-C	6.01	127.24	111.00
1	B	217	CYS	N-CA-C	5.81	126.69	111.00
1	A	253	THR	N-CA-CB	-5.38	100.08	110.30
1	B	361	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	158	ALA	N-CA-C	-5.19	96.99	111.00

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	2368	0	2350	121	0
1	B	2450	0	2432	126	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	13	0	4	10	0
3	B	13	0	4	0	0
4	A	150	0	0	31	0
4	B	148	0	0	28	0
All	All	5146	0	4790	244	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 26.

The worst 5 of 244 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:A:356:ARG:NH2	3:A:601:CIT:H21	1.34	1.39
1:B:366:SER:HB3	4:B:673:HOH:O	1.33	1.28
1:B:368:SER:HB2	4:B:664:HOH:O	1.50	1.07
1:A:356:ARG:NH2	3:A:601:CIT:C2	2.19	1.05
1:A:215:VAL:HB	4:A:748:HOH:O	1.67	0.94

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	297/406 (73%)	282 (95%)	14 (5%)	1 (0%)	41 37
1	B	307/406 (76%)	295 (96%)	9 (3%)	3 (1%)	15 9
All	All	604/812 (74%)	577 (96%)	23 (4%)	4 (1%)	22 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	B	27	GLY
1	B	134	GLU
1	B	160	TYR

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	242/323 (75%)	230 (95%)	12 (5%)	24 21
1	B	251/323 (78%)	230 (92%)	21 (8%)	11 6
All	All	493/646 (76%)	460 (93%)	33 (7%)	16 11

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	TYR
1	B	304	PRO
1	B	348	ARG
1	B	14	LEU
1	A	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	257	ASN
1	B	306	HIS
1	B	354	ASN
1	B	338	HIS
1	A	259	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	CIT	B	602	-	3,12,12	2.31	1 (33%)	3,17,17	0.64	0
3	CIT	A	601	2	3,12,12	3.33	1 (33%)	3,17,17	1.84	1 (33%)

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	CIT	B	602	-	-	0/6/16/16	-
3	CIT	A	601	2	-	0/6/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	CIT	O7-C3	-5.66	1.34	1.43
3	B	602	CIT	O7-C3	-3.75	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	CIT	C3-C4-C5	2.75	119.39	114.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	CIT	10	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^{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	305/406 (75%)	0.14	21 (6%)	16	23	15, 35, 60, 76	0
1	B	315/406 (77%)	0.27	21 (6%)	17	24	15, 36, 55, 80	0
All	All	620/812 (76%)	0.20	42 (6%)	17	24	15, 36, 59, 80	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	SER	14.0
1	B	128	TYR	10.7
1	B	129	LEU	8.5
1	B	131	ALA	7.2
1	A	344	ARG	6.3

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	CIT	A	601	13/13	0.84	0.17	24,27,32,34	13
3	CIT	B	602	13/13	0.87	0.14	30,33,35,37	13
2	SM	A	503	1/1	0.90	0.06	53,53,53,53	1
2	SM	B	502	1/1	0.94	0.07	46,46,46,46	1
2	SM	B	504	1/1	0.94	0.12	49,49,49,49	1
2	SM	A	501	1/1	0.95	0.06	35,35,35,35	1

6.5 Other polymers (i)

There are no such residues in this entry.