wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 08:47 AM EDT

PDB ID	:	1YDO
Title	:	Crystal Structure of the Bacillis subtilis HMG-CoA Lyase, Northeast Structural Genomics Target SR181.
Authors	:	Forouhar, F.; Hussain, M.; Edstrom, W.; Vorobiev, S.M.; Xiao, R.; Ciano, M.; Shih, L.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-12-24
Resolution	:	2.71 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

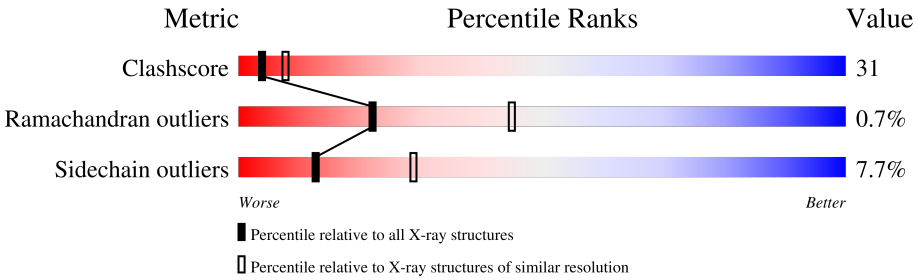
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.71 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))
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	47% 43% 6% ·
1	B	307	51% 39% 7% ·
1	C	307	52% 40% 5% ·
1	D	307	50% 41% 6% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9560 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 HMG-CoA Lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	Se	0	0	0
			2288	1448	392	438	3	7			
1	B	298	Total	C	N	O	S	Se	0	0	0
			2288	1448	392	438	3	7			
1	C	298	Total	C	N	O	S	Se	0	0	0
			2288	1448	392	438	3	7			
1	D	298	Total	C	N	O	S	Se	0	0	0
			2288	1448	392	438	3	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	102	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	219	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	225	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	258	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	262	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	284	MSE	MET	MODIFIED RESIDUE	UNP O34873
A	300	LEU	-	CLONING ARTIFACT	UNP O34873
A	301	GLU	-	CLONING ARTIFACT	UNP O34873
A	302	HIS	-	EXPRESSION TAG	UNP O34873
A	303	HIS	-	EXPRESSION TAG	UNP O34873
A	304	HIS	-	EXPRESSION TAG	UNP O34873
A	305	HIS	-	EXPRESSION TAG	UNP O34873
A	306	HIS	-	EXPRESSION TAG	UNP O34873
A	307	HIS	-	EXPRESSION TAG	UNP O34873
B	1	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	102	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	219	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	225	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	258	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	262	MSE	MET	MODIFIED RESIDUE	UNP O34873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	284	MSE	MET	MODIFIED RESIDUE	UNP O34873
B	300	LEU	-	CLONING ARTIFACT	UNP O34873
B	301	GLU	-	CLONING ARTIFACT	UNP O34873
B	302	HIS	-	EXPRESSION TAG	UNP O34873
B	303	HIS	-	EXPRESSION TAG	UNP O34873
B	304	HIS	-	EXPRESSION TAG	UNP O34873
B	305	HIS	-	EXPRESSION TAG	UNP O34873
B	306	HIS	-	EXPRESSION TAG	UNP O34873
B	307	HIS	-	EXPRESSION TAG	UNP O34873
C	1	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	102	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	219	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	225	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	258	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	262	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	284	MSE	MET	MODIFIED RESIDUE	UNP O34873
C	300	LEU	-	CLONING ARTIFACT	UNP O34873
C	301	GLU	-	CLONING ARTIFACT	UNP O34873
C	302	HIS	-	EXPRESSION TAG	UNP O34873
C	303	HIS	-	EXPRESSION TAG	UNP O34873
C	304	HIS	-	EXPRESSION TAG	UNP O34873
C	305	HIS	-	EXPRESSION TAG	UNP O34873
C	306	HIS	-	EXPRESSION TAG	UNP O34873
C	307	HIS	-	EXPRESSION TAG	UNP O34873
D	1	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	102	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	219	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	225	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	258	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	262	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	284	MSE	MET	MODIFIED RESIDUE	UNP O34873
D	300	LEU	-	CLONING ARTIFACT	UNP O34873
D	301	GLU	-	CLONING ARTIFACT	UNP O34873
D	302	HIS	-	EXPRESSION TAG	UNP O34873
D	303	HIS	-	EXPRESSION TAG	UNP O34873
D	304	HIS	-	EXPRESSION TAG	UNP O34873
D	305	HIS	-	EXPRESSION TAG	UNP O34873
D	306	HIS	-	EXPRESSION TAG	UNP O34873
D	307	HIS	-	EXPRESSION TAG	UNP O34873

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total I 1 1	0	0
2	B	1	Total I 1 1	0	0
2	C	1	Total I 1 1	0	0
2	D	1	Total I 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	119	Total O 119 119	0	0
3	C	90	Total O 90 90	0	0
3	D	93	Total O 93 93	0	0

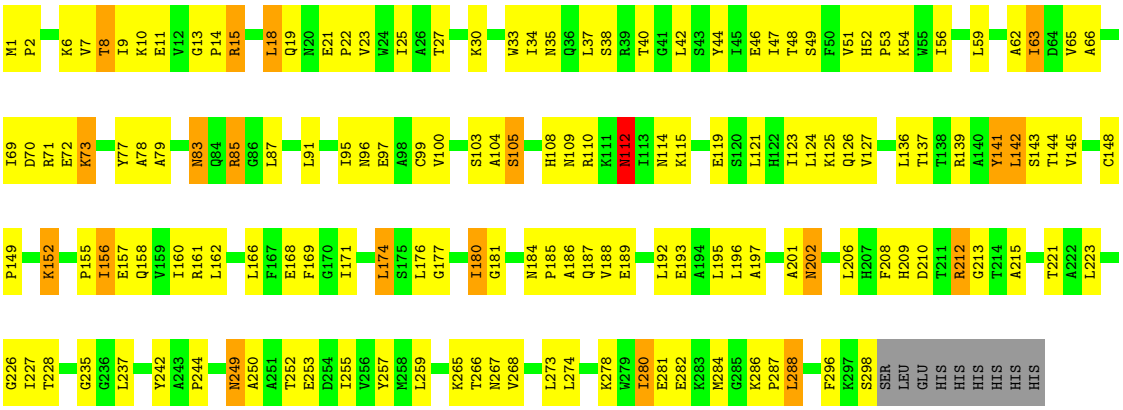
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

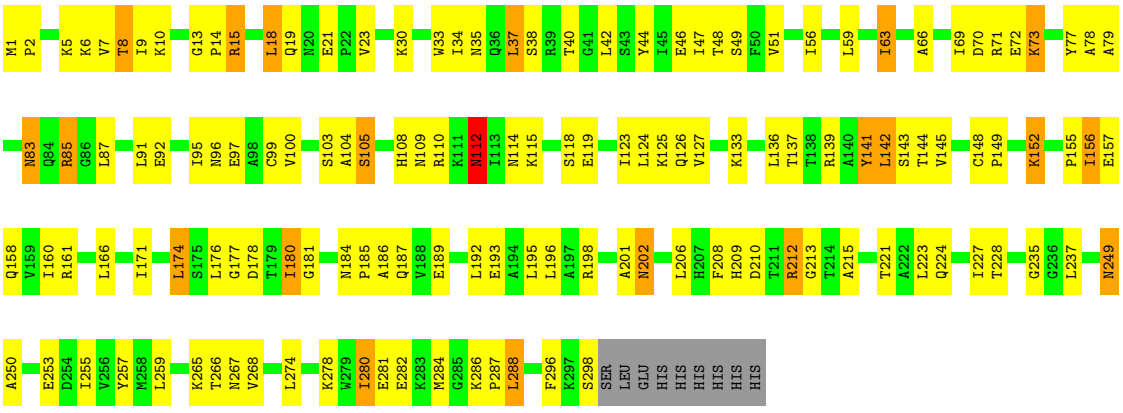
• Molecule 1: HMG-CoA Lyase

Chain A:



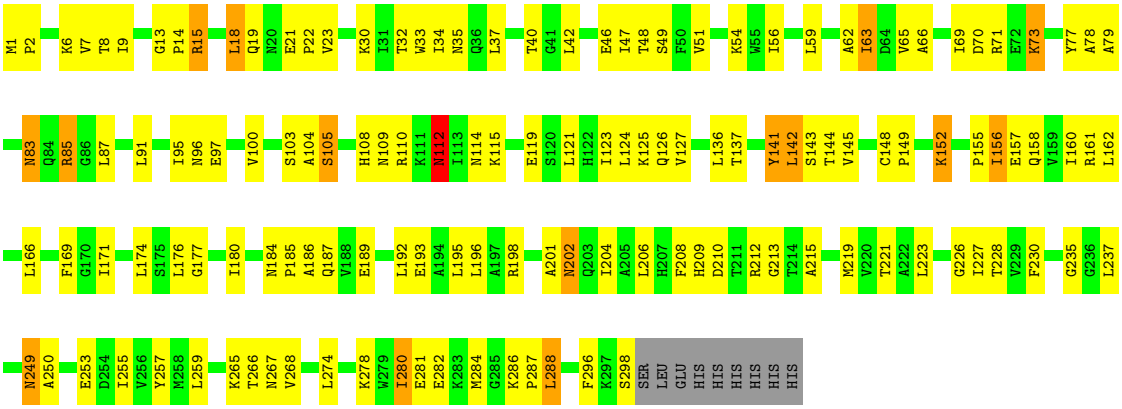
• Molecule 1: HMG-CoA Lyase

Chain B:



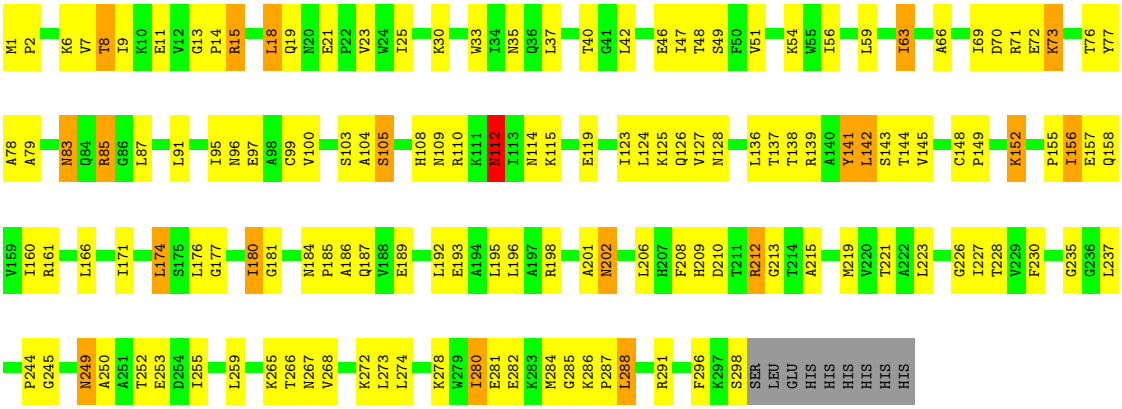
• Molecule 1: HMG-CoA Lyase

Chain C:



• Molecule 1: HMG-CoA Lyase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.69Å 104.67Å 97.44Å 90.00° 107.43° 90.00°	Depositor
Resolution (Å)	28.94 – 2.71	Depositor
% Data completeness (in resolution range)	81.7 (28.94-2.71)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9560	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0/2325	0.54	0/3144
1	B	0.45	0/2325	0.55	0/3144
1	C	0.43	0/2325	0.56	0/3144
1	D	0.44	0/2325	0.55	0/3144
All	All	0.44	0/9300	0.55	0/12576

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	2288	0	2308	151	0
1	B	2288	0	2308	147	0
1	C	2288	0	2308	138	0
1	D	2288	0	2308	144	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
3	A	102	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	119	0	0	14	0
3	C	90	0	0	7	0
3	D	93	0	0	11	0
All	All	9560	0	9232	565	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 31.

The worst 5 of 565 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:63:ILE:H	1:A:63:ILE:HD13	1.20	1.06
1:D:76:THR:HG22	3:D:509:HOH:O	1.59	1.01
1:B:63:ILE:HD13	1:B:63:ILE:H	1.25	1.00
1:D:63:ILE:HD13	1:D:63:ILE:H	1.25	0.99
1:D:100:VAL:HB	1:D:124:LEU:HD22	1.45	0.98

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	296/307 (96%)	269 (91%)	25 (8%)	2 (1%)	22	45
1	B	296/307 (96%)	267 (90%)	27 (9%)	2 (1%)	22	45
1	C	296/307 (96%)	268 (90%)	26 (9%)	2 (1%)	22	45
1	D	296/307 (96%)	268 (90%)	26 (9%)	2 (1%)	22	45
All	All	1184/1228 (96%)	1072 (90%)	104 (9%)	8 (1%)	22	45

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	152	LYS
1	B	112	ASN
1	B	152	LYS
1	C	112	ASN

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	247/249 (99%)	228 (92%)	19 (8%)	13	29
1	B	247/249 (99%)	227 (92%)	20 (8%)	11	26
1	C	247/249 (99%)	229 (93%)	18 (7%)	14	31
1	D	247/249 (99%)	228 (92%)	19 (8%)	13	29
All	All	988/996 (99%)	912 (92%)	76 (8%)	13	29

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	THR
1	D	202	ASN
1	D	18	LEU
1	D	112	ASN
1	D	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	19	GLN
1	C	158	GLN
1	D	158	GLN
1	C	35	ASN
1	C	96	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.