W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:15 PM GMT

PDB ID : 4L0O
Title : Structure determination of cystathionine gamma-synthase from Helicobacter pylori
Authors : Tarique, K.F.; Rehman, S.A.A.; Gourinath, S.
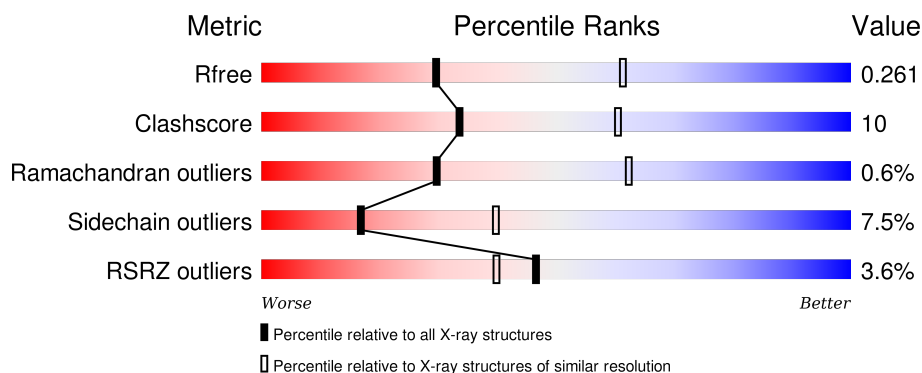Deposited on : 2013-05-31
Resolution : 2.76 Å(reported)

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 2.76 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		10
Ramachandran outliers		0.6%
Sidechain outliers		7.5%
RSRZ outliers		3.6%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	388	2% / 67% / 22% • 6%
1	C	388	2% / 76% / 16% • 6%
1	E	388	3% / 73% / 19% •• 6%
1	G	388	6% / 72% / 19% • 6%
1	H	388	% / 74% / 20% • •

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Mol	Chain	Length	Quality of chain
1	K	388	3% ■ 75% / 20% • •
1	M	388	6% ■ 71% / 19% • 6%
1	O	388	5% ■ 74% / 16% • 5%

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	PO4	K	401	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22365 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 Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	373	Total 2828	C 1801	N 480	O 537	S 10	0	0	0
1	A	363	Total 2756	C 1760	N 464	O 523	S 9	0	0	0
1	C	366	Total 2778	C 1771	N 468	O 530	S 9	0	0	0
1	E	364	Total 2728	C 1741	N 459	O 519	S 9	0	0	0
1	G	365	Total 2762	C 1760	N 464	O 529	S 9	0	0	0
1	K	378	Total 2865	C 1823	N 488	O 544	S 10	0	0	0
1	M	365	Total 2765	C 1763	N 465	O 528	S 9	0	0	0
1	O	367	Total 2773	C 1770	N 464	O 530	S 9	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	381	LEU	-	EXPRESSION TAG	UNP P56069
H	382	GLU	-	EXPRESSION TAG	UNP P56069
H	383	HIS	-	EXPRESSION TAG	UNP P56069
H	384	HIS	-	EXPRESSION TAG	UNP P56069
H	385	HIS	-	EXPRESSION TAG	UNP P56069
H	386	HIS	-	EXPRESSION TAG	UNP P56069
H	387	HIS	-	EXPRESSION TAG	UNP P56069
H	388	HIS	-	EXPRESSION TAG	UNP P56069
A	381	LEU	-	EXPRESSION TAG	UNP P56069
A	382	GLU	-	EXPRESSION TAG	UNP P56069
A	383	HIS	-	EXPRESSION TAG	UNP P56069
A	384	HIS	-	EXPRESSION TAG	UNP P56069
A	385	HIS	-	EXPRESSION TAG	UNP P56069

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Chain	Residue	Modelled	Actual	Comment	Reference
A	386	HIS	-	EXPRESSION TAG	UNP P56069
A	387	HIS	-	EXPRESSION TAG	UNP P56069
A	388	HIS	-	EXPRESSION TAG	UNP P56069
C	381	LEU	-	EXPRESSION TAG	UNP P56069
C	382	GLU	-	EXPRESSION TAG	UNP P56069
C	383	HIS	-	EXPRESSION TAG	UNP P56069
C	384	HIS	-	EXPRESSION TAG	UNP P56069
C	385	HIS	-	EXPRESSION TAG	UNP P56069
C	386	HIS	-	EXPRESSION TAG	UNP P56069
C	387	HIS	-	EXPRESSION TAG	UNP P56069
C	388	HIS	-	EXPRESSION TAG	UNP P56069
E	381	LEU	-	EXPRESSION TAG	UNP P56069
E	382	GLU	-	EXPRESSION TAG	UNP P56069
E	383	HIS	-	EXPRESSION TAG	UNP P56069
E	384	HIS	-	EXPRESSION TAG	UNP P56069
E	385	HIS	-	EXPRESSION TAG	UNP P56069
E	386	HIS	-	EXPRESSION TAG	UNP P56069
E	387	HIS	-	EXPRESSION TAG	UNP P56069
E	388	HIS	-	EXPRESSION TAG	UNP P56069
G	381	LEU	-	EXPRESSION TAG	UNP P56069
G	382	GLU	-	EXPRESSION TAG	UNP P56069
G	383	HIS	-	EXPRESSION TAG	UNP P56069
G	384	HIS	-	EXPRESSION TAG	UNP P56069
G	385	HIS	-	EXPRESSION TAG	UNP P56069
G	386	HIS	-	EXPRESSION TAG	UNP P56069
G	387	HIS	-	EXPRESSION TAG	UNP P56069
G	388	HIS	-	EXPRESSION TAG	UNP P56069
K	381	LEU	-	EXPRESSION TAG	UNP P56069
K	382	GLU	-	EXPRESSION TAG	UNP P56069
K	383	HIS	-	EXPRESSION TAG	UNP P56069
K	384	HIS	-	EXPRESSION TAG	UNP P56069
K	385	HIS	-	EXPRESSION TAG	UNP P56069
K	386	HIS	-	EXPRESSION TAG	UNP P56069
K	387	HIS	-	EXPRESSION TAG	UNP P56069
K	388	HIS	-	EXPRESSION TAG	UNP P56069
M	381	LEU	-	EXPRESSION TAG	UNP P56069
M	382	GLU	-	EXPRESSION TAG	UNP P56069
M	383	HIS	-	EXPRESSION TAG	UNP P56069
M	384	HIS	-	EXPRESSION TAG	UNP P56069
M	385	HIS	-	EXPRESSION TAG	UNP P56069
M	386	HIS	-	EXPRESSION TAG	UNP P56069
M	387	HIS	-	EXPRESSION TAG	UNP P56069

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Chain	Residue	Modelled	Actual	Comment	Reference
M	388	HIS	-	EXPRESSION TAG	UNP P56069
O	381	LEU	-	EXPRESSION TAG	UNP P56069
O	382	GLU	-	EXPRESSION TAG	UNP P56069
O	383	HIS	-	EXPRESSION TAG	UNP P56069
O	384	HIS	-	EXPRESSION TAG	UNP P56069
O	385	HIS	-	EXPRESSION TAG	UNP P56069
O	386	HIS	-	EXPRESSION TAG	UNP P56069
O	387	HIS	-	EXPRESSION TAG	UNP P56069
O	388	HIS	-	EXPRESSION TAG	UNP P56069

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).
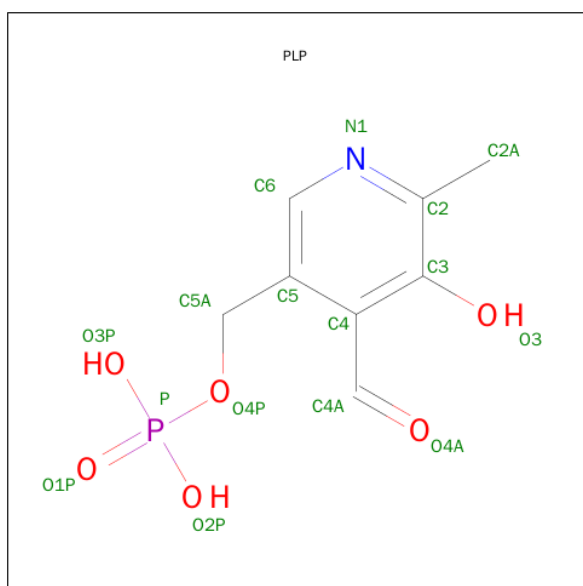
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	A	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	M	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	O	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
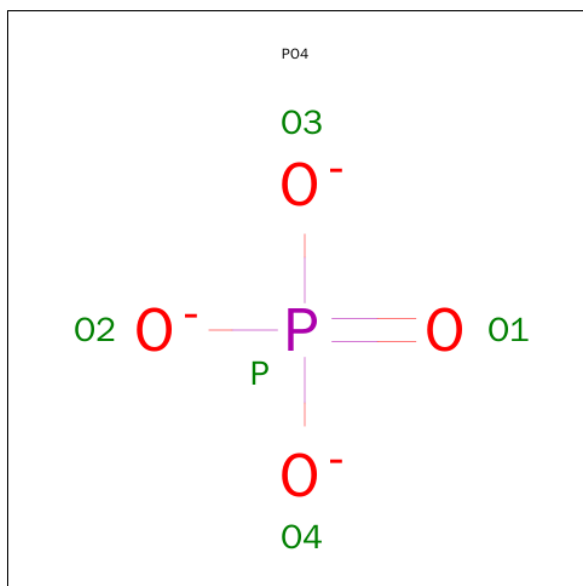
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	K	1	5	4	1	0	0

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.
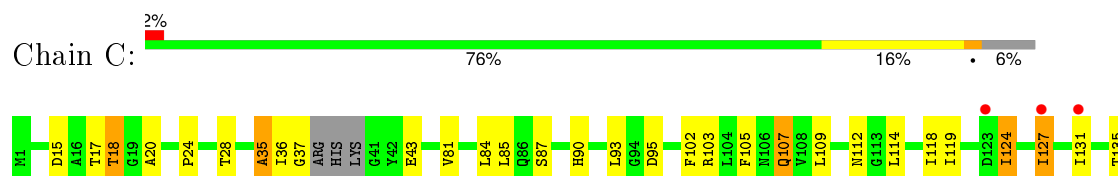
- Molecule 1: Cystathionine gamma-synthase
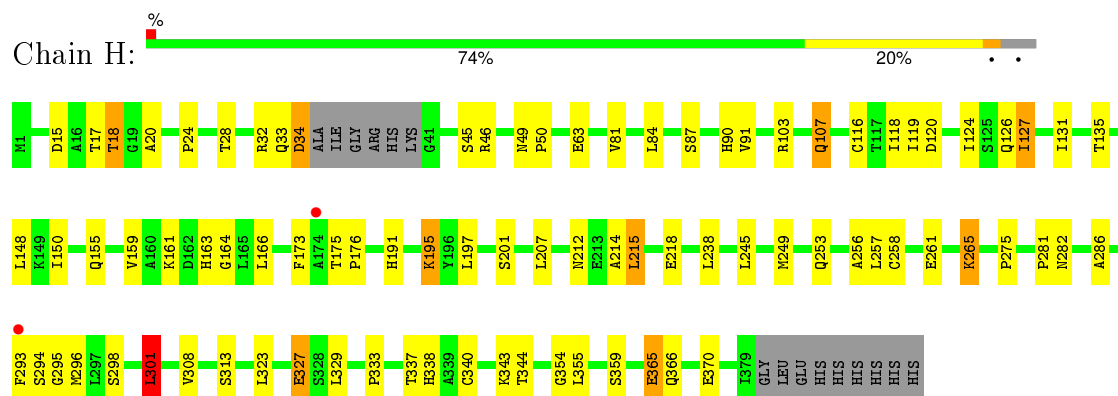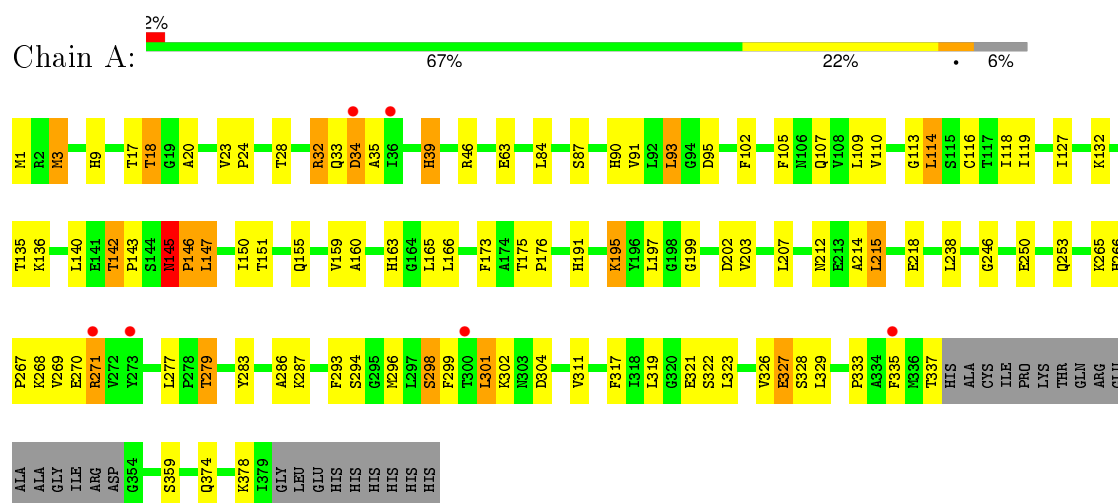
- Molecule 1: Cystathionine gamma-synthase

- Molecule 1: Cystathionine gamma-synthase

- Molecule 1: Cystathionine gamma-synthase

Chain E:

- Molecule 1: Cystathionine gamma-synthase

Chain G:

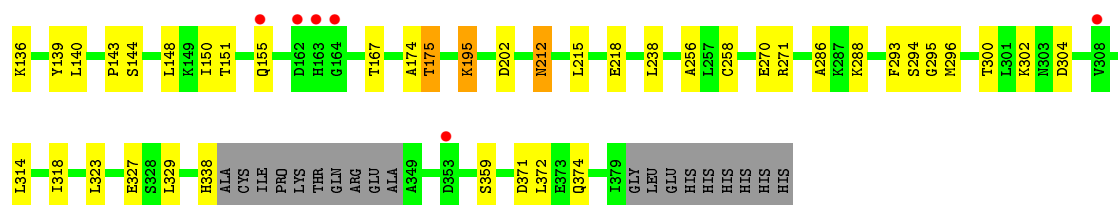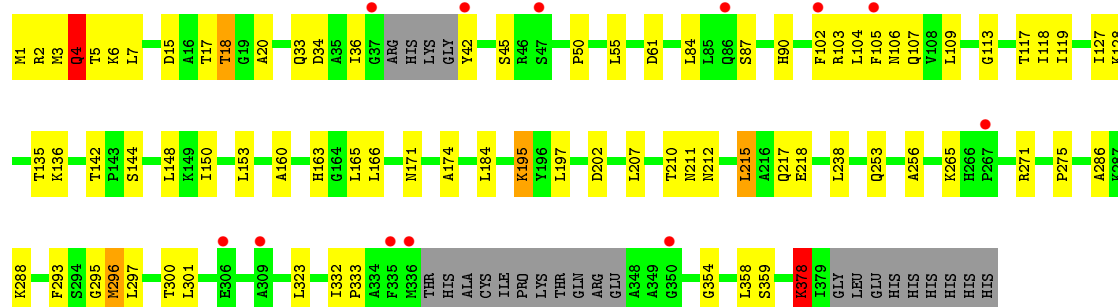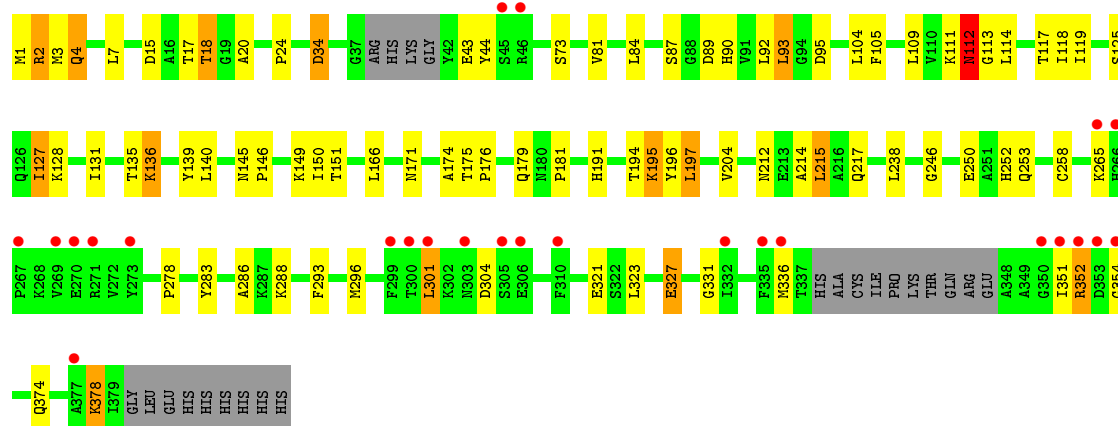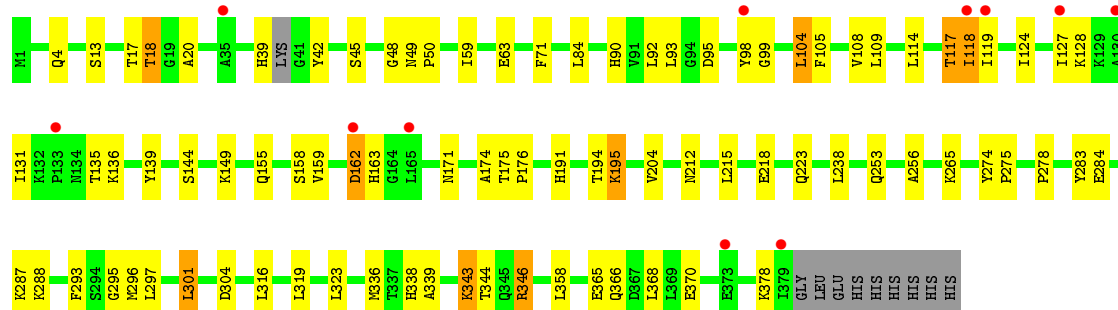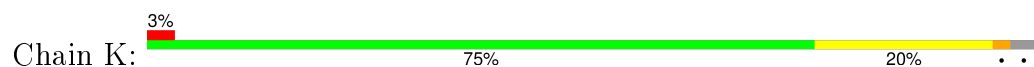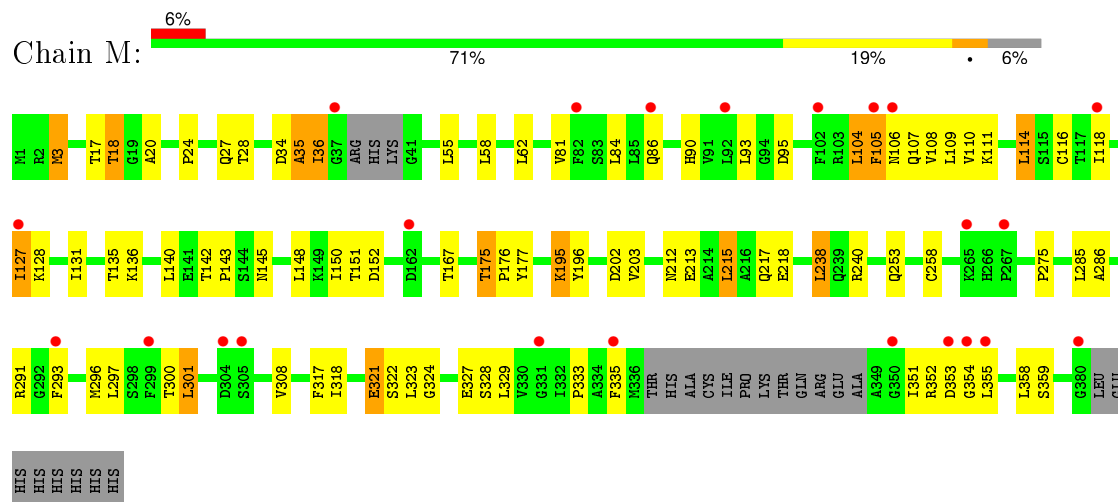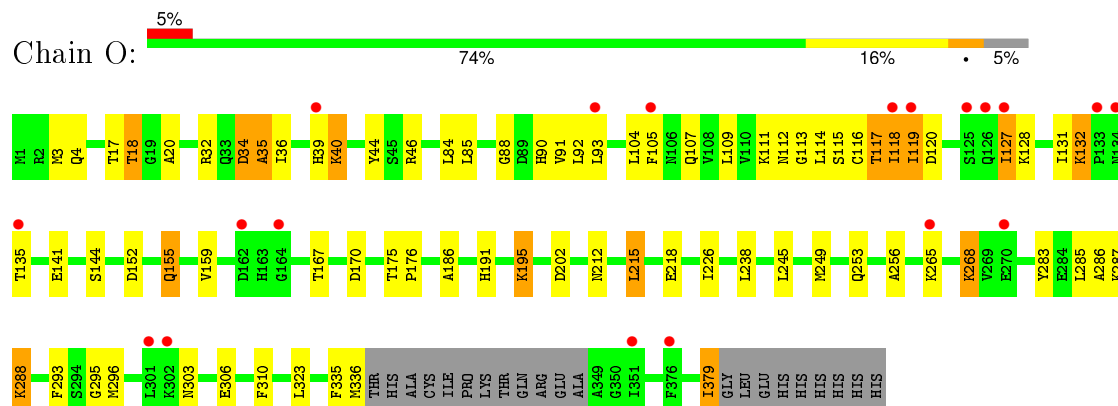- Molecule 1: Cystathionine gamma-synthase

Chain K:

• Molecule 1: Cystathionine gamma-synthase

Chain M:

• Molecule 1: Cystathionine gamma-synthase

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	115.81Å　174.89Å　324.75Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　2.76 48.28　–　2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.76) 99.8 (48.28-2.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.53 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234　,　0.278 0.221　,　0.261	Depositor DCC
R_{free} test set	4233 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 84795 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22365	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PLP

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	0.65	7/2808 (0.2%)	0.59	0/3804
1	C	0.57	1/2829 (0.0%)	0.57	0/3832
1	E	0.58	2/2777 (0.1%)	0.56	0/3764
1	G	0.64	4/2812 (0.1%)	0.59	0/3811
1	H	0.52	1/2881 (0.0%)	0.57	2/3904 (0.1%)
1	K	0.68	3/2919 (0.1%)	0.58	1/3954 (0.0%)
1	M	0.52	0/2815	0.55	0/3812
1	O	0.74	8/2825 (0.3%)	0.58	0/3829
All	All	0.62	26/22666 (0.1%)	0.57	3/30710 (0.0%)

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	39	HIS	C-O	11.43	1.45	1.23
1	E	378	LYS	CE-NZ	11.16	1.76	1.49
1	H	34	ASP	C-O	9.21	1.40	1.23
1	O	132	LYS	CE-NZ	9.14	1.72	1.49
1	K	338	HIS	CG-CD2	8.72	1.50	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	346	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	H	34	ASP	CA-C-O	-5.32	108.93	120.10
1	H	301	LEU	CA-CB-CG	5.14	127.13	115.30

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	2756	0	2762	72	0
1	C	2778	0	2775	44	0
1	E	2728	0	2708	53	0
1	G	2762	0	2748	59	0
1	H	2828	0	2824	52	0
1	K	2865	0	2858	55	0
1	M	2765	0	2764	64	0
1	O	2773	0	2762	76	0
2	A	15	0	5	4	0
2	C	15	0	5	3	0
2	E	15	0	4	1	0
2	G	15	0	6	2	0
2	H	15	0	5	3	0
2	M	15	0	5	3	0
2	O	15	0	5	0	0
3	K	5	0	0	0	0
All	All	22365	0	22236	454	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 10.

The worst 5 of 454 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:O:132:LYS:CE	1:O:132:LYS:NZ	1.71	1.53
1:O:268:LYS:CE	1:O:268:LYS:NZ	1.70	1.51
1:E:378:LYS:CE	1:E:378:LYS:NZ	1.77	1.48
1:O:118:ILE:O	1:O:119:ILE:HG23	1.49	1.10
1:M:35:ALA:HB1	1:M:36:ILE:HA	1.16	1.10

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	359/388 (92%)	339 (94%)	17 (5%)	3 (1%)	24	55
1	C	360/388 (93%)	341 (95%)	15 (4%)	4 (1%)	17	46
1	E	358/388 (92%)	337 (94%)	20 (6%)	1 (0%)	46	77
1	G	359/388 (92%)	343 (96%)	15 (4%)	1 (0%)	46	77
1	H	369/388 (95%)	350 (95%)	18 (5%)	1 (0%)	46	77
1	K	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	34	67
1	M	359/388 (92%)	343 (96%)	14 (4%)	2 (1%)	30	62
1	O	363/388 (94%)	339 (93%)	22 (6%)	2 (1%)	30	62
All	All	2901/3104 (94%)	2747 (95%)	138 (5%)	16 (1%)	30	62

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	35	ALA
1	C	35	ALA
1	K	99	GLY
1	M	353	ASP
1	A	294	SER

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	293/316 (93%)	266 (91%)	27 (9%)	11	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	295/316 (93%)	276 (94%)	19 (6%)	22	49
1	E	284/316 (90%)	265 (93%)	19 (7%)	20	46
1	G	292/316 (92%)	268 (92%)	24 (8%)	14	35
1	H	299/316 (95%)	275 (92%)	24 (8%)	15	37
1	K	302/316 (96%)	281 (93%)	21 (7%)	19	44
1	M	293/316 (93%)	268 (92%)	25 (8%)	13	34
1	O	293/316 (93%)	275 (94%)	18 (6%)	23	52
All	All	2351/2528 (93%)	2174 (92%)	177 (8%)	17	40

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	LYS
1	G	112	ASN
1	O	34	ASP
1	E	195	LYS
1	G	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	90	HIS
1	G	90	HIS
1	O	112	ASN
1	E	163	HIS
1	E	212	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)

8 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	PLP	A	401	-	15,15,16	3.53	3 (20%)	17,21,23	1.91	2 (11%)
2	PLP	C	401	-	15,15,16	3.61	3 (20%)	17,21,23	1.55	2 (11%)
2	PLP	E	401	-	15,15,16	3.63	3 (20%)	17,21,23	1.62	3 (17%)
2	PLP	G	401	1	15,15,16	3.11	7 (46%)	21,22,23	2.16	9 (42%)
2	PLP	H	401	-	15,15,16	3.80	3 (20%)	17,21,23	1.46	2 (11%)
3	PO4	K	401	-	4,4,4	2.12	4 (100%)	6,6,6	0.36	0
2	PLP	M	401	-	15,15,16	3.42	3 (20%)	17,21,23	2.01	4 (23%)
2	PLP	O	401	-	15,15,16	3.64	3 (20%)	17,21,23	1.57	2 (11%)

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	PLP	A	401	-	-	0/8/8/8	0/1/1/1
2	PLP	C	401	-	-	0/8/8/8	0/1/1/1
2	PLP	E	401	-	-	0/8/8/8	0/1/1/1
2	PLP	G	401	1	-	0/6/6/8	0/1/1/1
2	PLP	H	401	-	-	0/8/8/8	0/1/1/1
3	PO4	K	401	-	-	0/0/0/0	0/0/0/0
2	PLP	M	401	-	-	0/8/8/8	0/1/1/1
2	PLP	O	401	-	-	0/8/8/8	0/1/1/1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PLP	C3-C2	-6.60	1.36	1.40
2	G	401	PLP	O3-C3	-6.49	1.21	1.37
2	G	401	PLP	P-O2P	-3.89	1.40	1.54
2	G	401	PLP	P-O3P	-3.80	1.41	1.54
2	G	401	PLP	P-O4P	-2.87	1.50	1.60

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	PLP	O4A-C4A-C4	-5.17	114.67	125.11
2	A	401	PLP	O4A-C4A-C4	-4.73	115.56	125.11
2	G	401	PLP	O2P-P-O4P	-3.49	96.52	106.56
2	E	401	PLP	O4A-C4A-C4	-3.18	118.68	125.11
2	O	401	PLP	O4A-C4A-C4	-2.89	119.28	125.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	4	0
2	C	401	PLP	3	0
2	E	401	PLP	1	0
2	G	401	PLP	2	0
2	H	401	PLP	3	0
2	M	401	PLP	3	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	363/388 (93%)	0.15	6 (1%)	73	68	25, 43, 65, 81	0
1	C	366/388 (94%)	0.11	9 (2%)	61	54	23, 39, 62, 74	0
1	E	364/388 (93%)	0.29	12 (3%)	50	43	26, 42, 71, 88	0
1	G	365/388 (94%)	0.26	25 (6%)	20	15	22, 40, 68, 87	0
1	H	373/388 (96%)	0.06	2 (0%)	91	90	27, 39, 58, 79	0
1	K	378/388 (97%)	0.32	11 (2%)	55	48	27, 47, 71, 95	0
1	M	365/388 (94%)	0.37	23 (6%)	23	17	25, 47, 70, 96	0
1	O	367/388 (94%)	0.40	19 (5%)	31	24	28, 49, 75, 88	0
All	All	2941/3104 (94%)	0.25	107 (3%)	46	40	22, 43, 70, 96	0

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	164	GLY	5.7
1	O	133	PRO	4.7
1	G	335	PHE	4.7
1	O	119	ILE	4.5
1	A	273	TYR	4.3

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
2	PLP	O	401	15/16	0.93	0.22	1.35	47,54,57,57	0
2	PLP	M	401	15/16	0.94	0.19	0.55	41,42,43,43	0
2	PLP	E	401	15/16	0.92	0.20	0.49	49,51,52,52	0
2	PLP	C	401	15/16	0.96	0.18	0.47	34,39,43,44	0
2	PLP	H	401	15/16	0.92	0.19	-0.02	45,54,56,65	0
2	PLP	A	401	15/16	0.95	0.16	-0.53	38,42,43,44	0
3	PO4	K	401	5/5	0.97	0.10	-1.14	30,30,30,30	0
2	PLP	G	401	15/16	0.94	0.13	-2.23	30,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.