



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 11:59 AM BST

PDB ID : 6OVG
Title : L-Methionine Depletion with an Engineered Human Enzyme Disrupts Prostate Cancer Metabolism
Authors : Yan, W.; Irani, S.; Zhang, J.
Deposited on : 2019-05-07
Resolution : 2.72 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

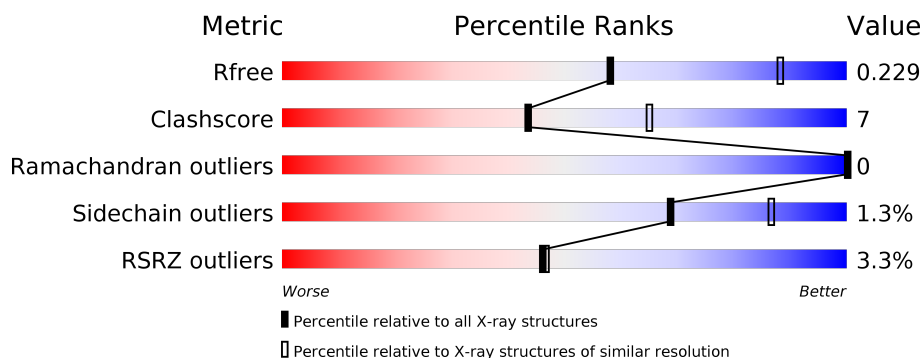
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 on 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 $\leq 5\%$. 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	415	<div> <div></div> <div>79% 13% 7%</div> </div>
1	B	415	<div> <div>4%</div> <div>81% 11% 7%</div> </div>
1	C	415	<div> <div></div> <div>80% 13% 7%</div> </div>
1	D	415	<div> <div>5%</div> <div>78% 14% 7%</div> </div>
1	E	415	<div> <div>5%</div> <div>78% 15% 7%</div> </div>
1	F	415	<div> <div>%</div> <div>78% 15% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	415	<div><div></div><div>3%</div><div>79%</div><div>14%</div><div>7%</div></div>
1	H	415	<div><div></div><div>6%</div><div>72%</div><div>20%</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24368 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-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	0	0
			2982	1902	508	551	1	20			
1	B	386	Total	C	N	O	P	S	0	0	0
			2993	1908	510	554	1	20			
1	C	387	Total	C	N	O	P	S	0	0	0
			3000	1913	511	555	1	20			
1	D	386	Total	C	N	O	P	S	0	0	0
			2989	1903	510	555	1	20			
1	E	388	Total	C	N	O	P	S	0	0	0
			3004	1915	512	556	1	20			
1	F	387	Total	C	N	O	P	S	0	0	0
			3000	1913	511	555	1	20			
1	G	388	Total	C	N	O	P	S	0	0	0
			3007	1918	512	556	1	20			
1	H	387	Total	C	N	O	P	S	0	0	0
			2997	1910	511	555	1	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P32929
A	-8	GLY	-	expression tag	UNP P32929
A	-7	GLY	-	expression tag	UNP P32929
A	-6	HIS	-	expression tag	UNP P32929
A	-5	HIS	-	expression tag	UNP P32929
A	-4	HIS	-	expression tag	UNP P32929
A	-3	HIS	-	expression tag	UNP P32929
A	-2	HIS	-	expression tag	UNP P32929
A	-1	HIS	-	expression tag	UNP P32929
A	0	GLY	-	expression tag	UNP P32929
A	1	GLY	-	expression tag	UNP P32929
A	59	ILE	GLU	conflict	UNP P32929
A	63	LEU	SER	conflict	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MET	LEU	conflict	UNP P32929
A	119	ALA	ARG	conflict	UNP P32929
A	268	ARG	LYS	conflict	UNP P32929
A	311	GLY	THR	conflict	UNP P32929
A	339	VAL	GLU	conflict	UNP P32929
A	353	SER	ILE	conflict	UNP P32929
B	-9	MET	-	initiating methionine	UNP P32929
B	-8	GLY	-	expression tag	UNP P32929
B	-7	GLY	-	expression tag	UNP P32929
B	-6	HIS	-	expression tag	UNP P32929
B	-5	HIS	-	expression tag	UNP P32929
B	-4	HIS	-	expression tag	UNP P32929
B	-3	HIS	-	expression tag	UNP P32929
B	-2	HIS	-	expression tag	UNP P32929
B	-1	HIS	-	expression tag	UNP P32929
B	0	GLY	-	expression tag	UNP P32929
B	1	GLY	-	expression tag	UNP P32929
B	59	ILE	GLU	conflict	UNP P32929
B	63	LEU	SER	conflict	UNP P32929
B	91	MET	LEU	conflict	UNP P32929
B	119	ALA	ARG	conflict	UNP P32929
B	268	ARG	LYS	conflict	UNP P32929
B	311	GLY	THR	conflict	UNP P32929
B	339	VAL	GLU	conflict	UNP P32929
B	353	SER	ILE	conflict	UNP P32929
C	-9	MET	-	initiating methionine	UNP P32929
C	-8	GLY	-	expression tag	UNP P32929
C	-7	GLY	-	expression tag	UNP P32929
C	-6	HIS	-	expression tag	UNP P32929
C	-5	HIS	-	expression tag	UNP P32929
C	-4	HIS	-	expression tag	UNP P32929
C	-3	HIS	-	expression tag	UNP P32929
C	-2	HIS	-	expression tag	UNP P32929
C	-1	HIS	-	expression tag	UNP P32929
C	0	GLY	-	expression tag	UNP P32929
C	1	GLY	-	expression tag	UNP P32929
C	59	ILE	GLU	conflict	UNP P32929
C	63	LEU	SER	conflict	UNP P32929
C	91	MET	LEU	conflict	UNP P32929
C	119	ALA	ARG	conflict	UNP P32929
C	268	ARG	LYS	conflict	UNP P32929
C	311	GLY	THR	conflict	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
C	339	VAL	GLU	conflict	UNP P32929
C	353	SER	ILE	conflict	UNP P32929
D	-9	MET	-	initiating methionine	UNP P32929
D	-8	GLY	-	expression tag	UNP P32929
D	-7	GLY	-	expression tag	UNP P32929
D	-6	HIS	-	expression tag	UNP P32929
D	-5	HIS	-	expression tag	UNP P32929
D	-4	HIS	-	expression tag	UNP P32929
D	-3	HIS	-	expression tag	UNP P32929
D	-2	HIS	-	expression tag	UNP P32929
D	-1	HIS	-	expression tag	UNP P32929
D	0	GLY	-	expression tag	UNP P32929
D	1	GLY	-	expression tag	UNP P32929
D	59	ILE	GLU	conflict	UNP P32929
D	63	LEU	SER	conflict	UNP P32929
D	91	MET	LEU	conflict	UNP P32929
D	119	ALA	ARG	conflict	UNP P32929
D	268	ARG	LYS	conflict	UNP P32929
D	311	GLY	THR	conflict	UNP P32929
D	339	VAL	GLU	conflict	UNP P32929
D	353	SER	ILE	conflict	UNP P32929
E	-9	MET	-	initiating methionine	UNP P32929
E	-8	GLY	-	expression tag	UNP P32929
E	-7	GLY	-	expression tag	UNP P32929
E	-6	HIS	-	expression tag	UNP P32929
E	-5	HIS	-	expression tag	UNP P32929
E	-4	HIS	-	expression tag	UNP P32929
E	-3	HIS	-	expression tag	UNP P32929
E	-2	HIS	-	expression tag	UNP P32929
E	-1	HIS	-	expression tag	UNP P32929
E	0	GLY	-	expression tag	UNP P32929
E	1	GLY	-	expression tag	UNP P32929
E	59	ILE	GLU	conflict	UNP P32929
E	63	LEU	SER	conflict	UNP P32929
E	91	MET	LEU	conflict	UNP P32929
E	119	ALA	ARG	conflict	UNP P32929
E	268	ARG	LYS	conflict	UNP P32929
E	311	GLY	THR	conflict	UNP P32929
E	339	VAL	GLU	conflict	UNP P32929
E	353	SER	ILE	conflict	UNP P32929
F	-9	MET	-	initiating methionine	UNP P32929
F	-8	GLY	-	expression tag	UNP P32929

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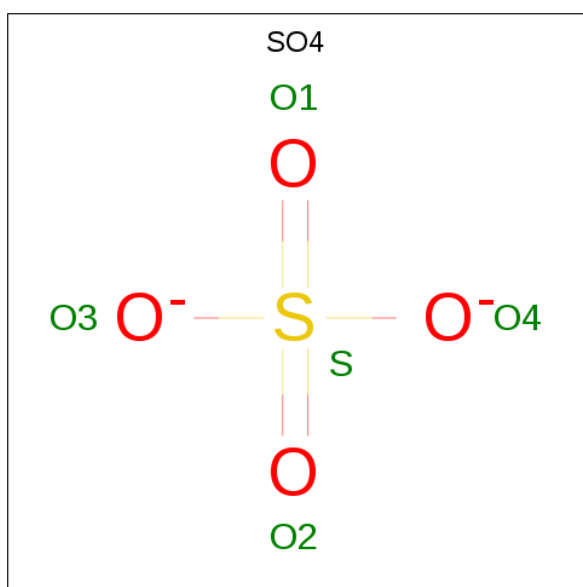
Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	GLY	-	expression tag	UNP P32929
F	-6	HIS	-	expression tag	UNP P32929
F	-5	HIS	-	expression tag	UNP P32929
F	-4	HIS	-	expression tag	UNP P32929
F	-3	HIS	-	expression tag	UNP P32929
F	-2	HIS	-	expression tag	UNP P32929
F	-1	HIS	-	expression tag	UNP P32929
F	0	GLY	-	expression tag	UNP P32929
F	1	GLY	-	expression tag	UNP P32929
F	59	ILE	GLU	conflict	UNP P32929
F	63	LEU	SER	conflict	UNP P32929
F	91	MET	LEU	conflict	UNP P32929
F	119	ALA	ARG	conflict	UNP P32929
F	268	ARG	LYS	conflict	UNP P32929
F	311	GLY	THR	conflict	UNP P32929
F	339	VAL	GLU	conflict	UNP P32929
F	353	SER	ILE	conflict	UNP P32929
G	-9	MET	-	initiating methionine	UNP P32929
G	-8	GLY	-	expression tag	UNP P32929
G	-7	GLY	-	expression tag	UNP P32929
G	-6	HIS	-	expression tag	UNP P32929
G	-5	HIS	-	expression tag	UNP P32929
G	-4	HIS	-	expression tag	UNP P32929
G	-3	HIS	-	expression tag	UNP P32929
G	-2	HIS	-	expression tag	UNP P32929
G	-1	HIS	-	expression tag	UNP P32929
G	0	GLY	-	expression tag	UNP P32929
G	1	GLY	-	expression tag	UNP P32929
G	59	ILE	GLU	conflict	UNP P32929
G	63	LEU	SER	conflict	UNP P32929
G	91	MET	LEU	conflict	UNP P32929
G	119	ALA	ARG	conflict	UNP P32929
G	268	ARG	LYS	conflict	UNP P32929
G	311	GLY	THR	conflict	UNP P32929
G	339	VAL	GLU	conflict	UNP P32929
G	353	SER	ILE	conflict	UNP P32929
H	-9	MET	-	initiating methionine	UNP P32929
H	-8	GLY	-	expression tag	UNP P32929
H	-7	GLY	-	expression tag	UNP P32929
H	-6	HIS	-	expression tag	UNP P32929
H	-5	HIS	-	expression tag	UNP P32929
H	-4	HIS	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	HIS	-	expression tag	UNP P32929
H	-2	HIS	-	expression tag	UNP P32929
H	-1	HIS	-	expression tag	UNP P32929
H	0	GLY	-	expression tag	UNP P32929
H	1	GLY	-	expression tag	UNP P32929
H	59	ILE	GLU	conflict	UNP P32929
H	63	LEU	SER	conflict	UNP P32929
H	91	MET	LEU	conflict	UNP P32929
H	119	ALA	ARG	conflict	UNP P32929
H	268	ARG	LYS	conflict	UNP P32929
H	311	GLY	THR	conflict	UNP P32929
H	339	VAL	GLU	conflict	UNP P32929
H	353	SER	ILE	conflict	UNP P32929

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		

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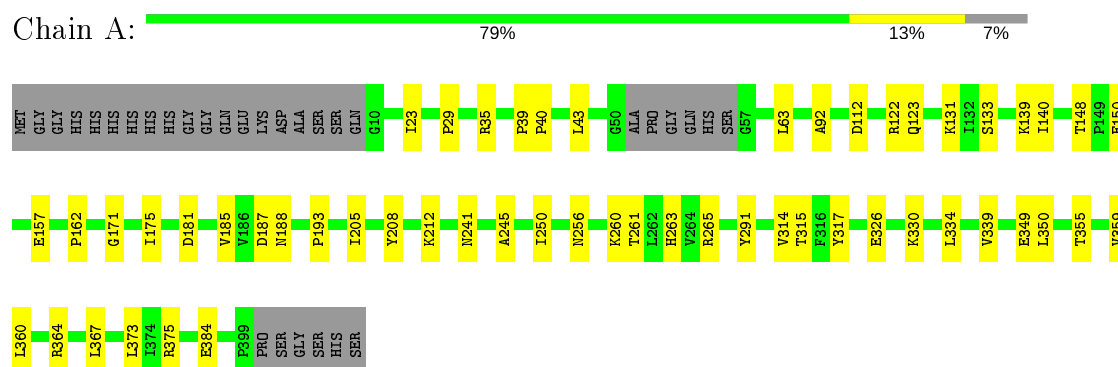
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	55	Total 55	O 55	0	0
3	C	66	Total 66	O 66	0	0
3	D	61	Total 61	O 61	0	0
3	E	44	Total 44	O 44	0	0
3	F	35	Total 35	O 35	0	0
3	G	39	Total 39	O 39	0	0
3	H	18	Total 18	O 18	0	0

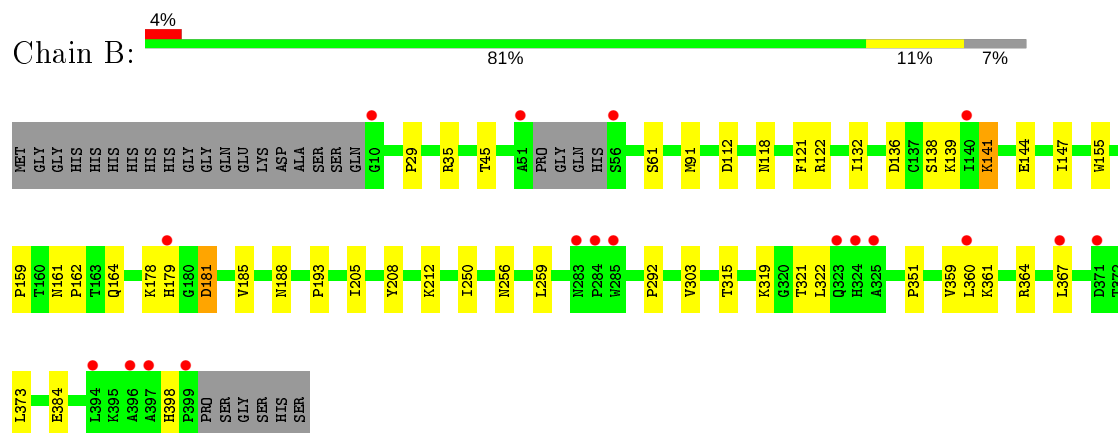
3 Residue-property plots [i](#)

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.

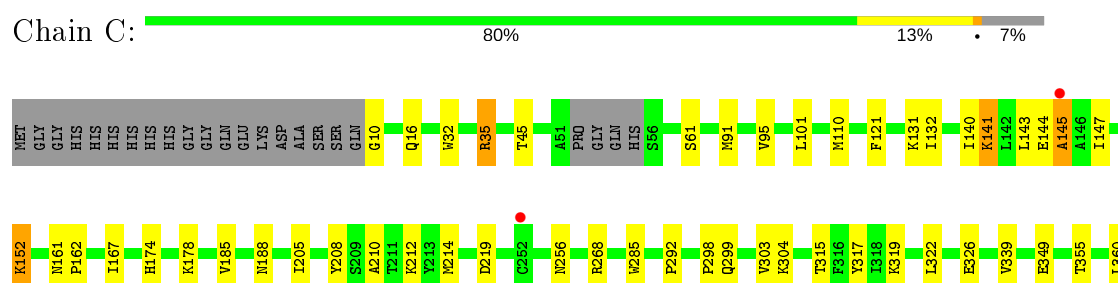
• Molecule 1: Cystathionine gamma-lyase



• Molecule 1: Cystathionine gamma-lyase

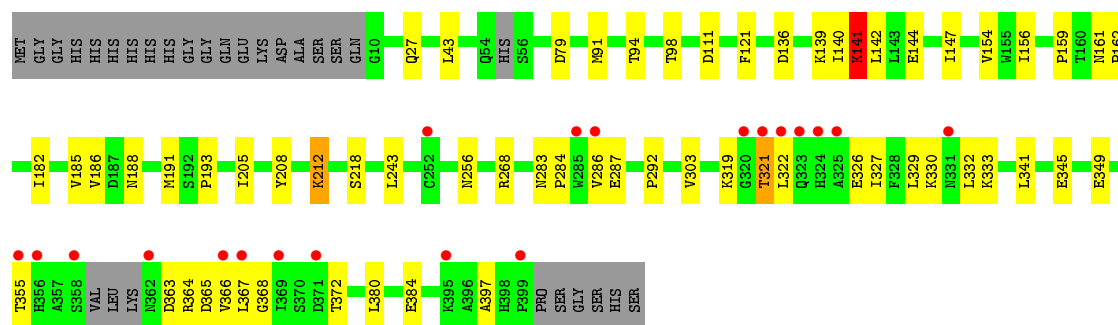
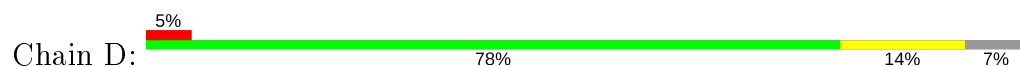


• Molecule 1: Cystathionine gamma-lyase

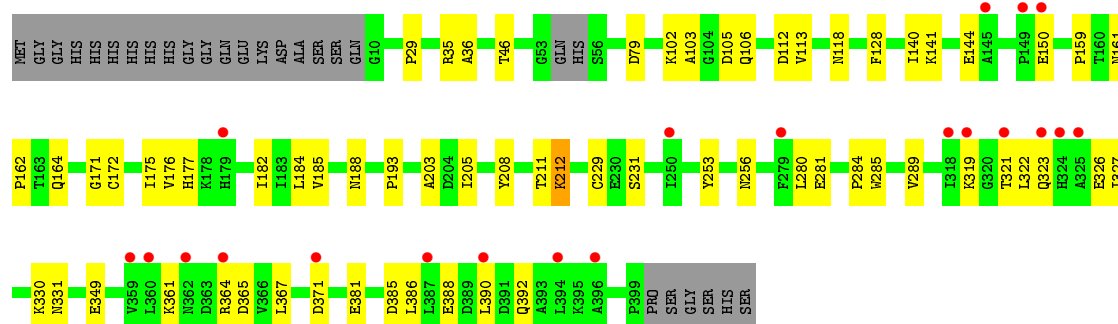
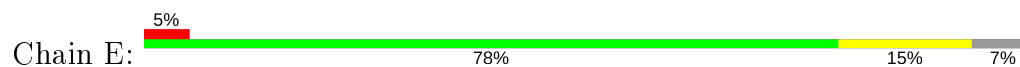




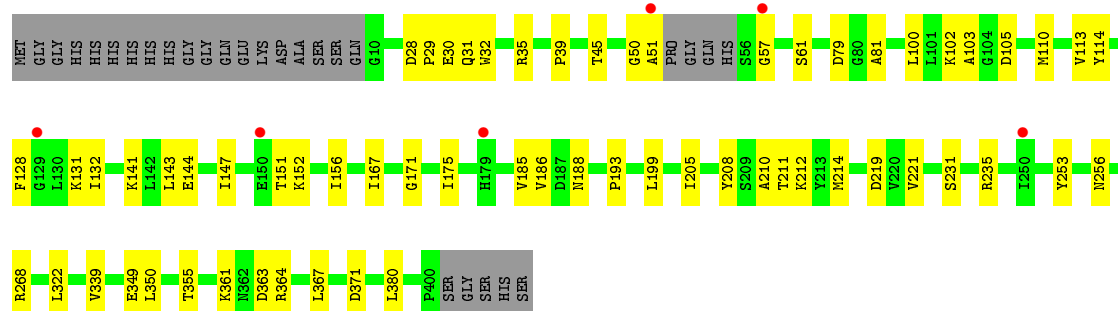
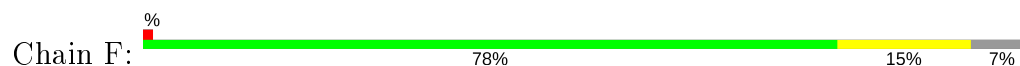
• Molecule 1: Cystathionine gamma-lyase



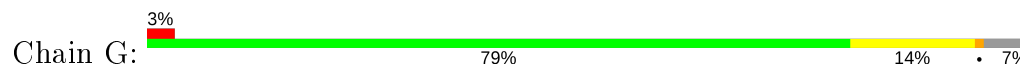
• Molecule 1: Cystathionine gamma-lyase

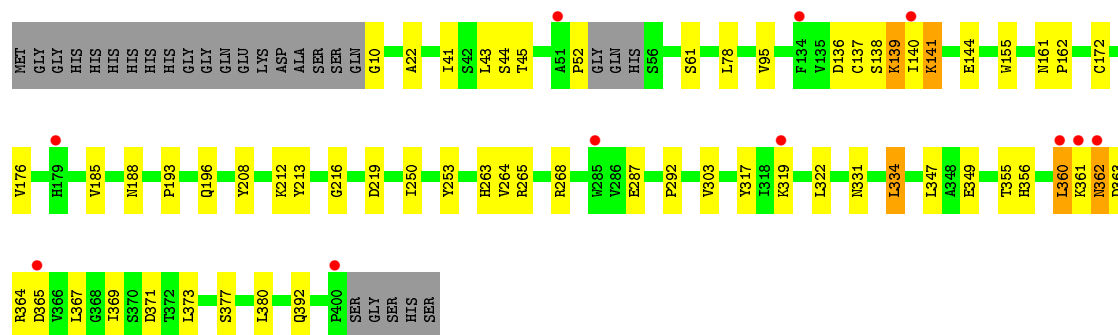


• Molecule 1: Cystathionine gamma-lyase

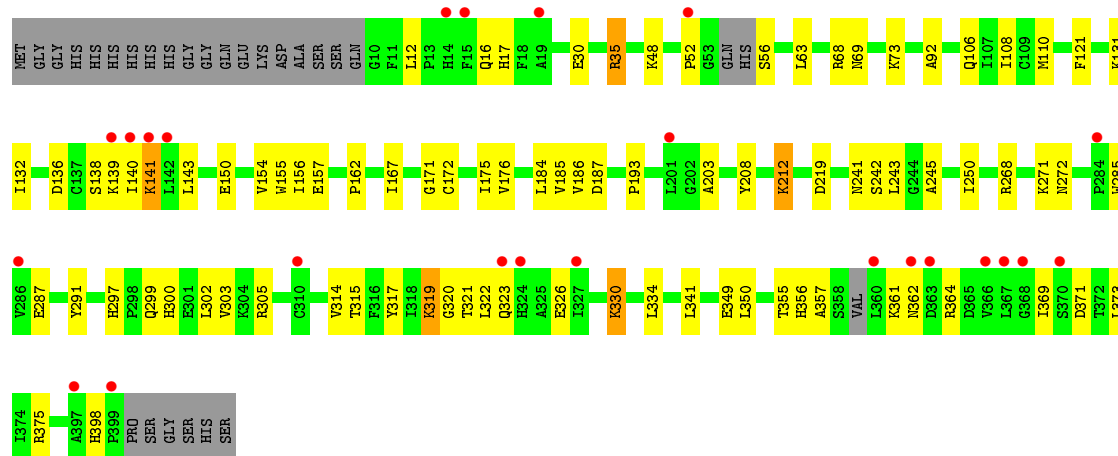
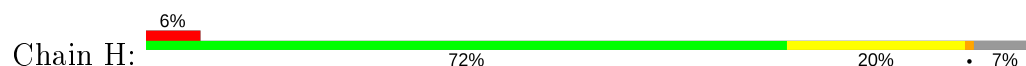


• Molecule 1: Cystathionine gamma-lyase





● Molecule 1: Cystathionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	113.56 Å 164.33 Å 181.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.72 49.34 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.34-2.72) 99.1 (49.34-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.73 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.181 , 0.229 0.181 , 0.229	Depositor DCC
R_{free} test set	4561 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24368	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: LLP, SO4

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	0.29	0/3023	0.46	0/4100
1	B	0.28	0/3034	0.49	1/4115 (0.0%)
1	C	0.28	0/3042	0.47	0/4127
1	D	0.29	0/3030	0.49	0/4109
1	E	0.28	0/3046	0.46	0/4132
1	F	0.27	0/3042	0.46	0/4127
1	G	0.27	0/3050	0.47	0/4139
1	H	0.27	0/3038	0.46	0/4119
All	All	0.28	0/24305	0.47	1/32968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
1	D	0	2
1	G	0	4
1	H	0	1
All	All	0	11

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ASP	CB-CG-OD1	9.34	126.70	118.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	LYS	Peptide
1	C	140	ILE	Peptide
1	C	141	LYS	Peptide
1	C	145	ALA	Peptide
1	D	141	LYS	Peptide

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	2982	0	2972	30	0
1	B	2993	0	2982	30	0
1	C	3000	0	2989	35	0
1	D	2989	0	2966	52	0
1	E	3004	0	2992	51	0
1	F	3000	0	2989	38	0
1	G	3007	0	2997	40	0
1	H	2997	0	2982	60	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	68	0	0	0	0
3	B	55	0	0	0	0
3	C	66	0	0	2	0
3	D	61	0	0	2	0
3	E	44	0	0	1	0
3	F	35	0	0	1	0
3	G	39	0	0	1	0
3	H	18	0	0	1	0
All	All	24368	0	23869	320	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 7.

The worst 5 of 320 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:D:141:LYS:NZ	1:D:144:GLU:HB2	1.49	1.24
1:E:284:PRO:O	1:E:319:LYS:NZ	1.66	1.23
1:E:171:GLY:O	1:E:175:ILE:HD12	1.47	1.12
1:F:141:LYS:HE2	1:F:144:GLU:OE2	1.48	1.10
1:D:141:LYS:HZ2	1:D:144:GLU:HB2	1.28	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	379/415 (91%)	367 (97%)	12 (3%)	0	100	100
1	B	381/415 (92%)	371 (97%)	10 (3%)	0	100	100
1	C	382/415 (92%)	370 (97%)	12 (3%)	0	100	100
1	D	379/415 (91%)	363 (96%)	16 (4%)	0	100	100
1	E	383/415 (92%)	369 (96%)	14 (4%)	0	100	100
1	F	382/415 (92%)	371 (97%)	11 (3%)	0	100	100
1	G	383/415 (92%)	369 (96%)	14 (4%)	0	100	100
1	H	380/415 (92%)	365 (96%)	15 (4%)	0	100	100
All	All	3049/3320 (92%)	2945 (97%)	104 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	324/347 (93%)	319 (98%)	5 (2%)	65	85
1	B	325/347 (94%)	321 (99%)	4 (1%)	71	88
1	C	326/347 (94%)	320 (98%)	6 (2%)	59	82
1	D	324/347 (93%)	320 (99%)	4 (1%)	71	88
1	E	326/347 (94%)	321 (98%)	5 (2%)	65	85
1	F	326/347 (94%)	325 (100%)	1 (0%)	92	97
1	G	327/347 (94%)	326 (100%)	1 (0%)	92	97
1	H	325/347 (94%)	317 (98%)	8 (2%)	47	75
All	All	2603/2776 (94%)	2569 (99%)	34 (1%)	69	86

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	91	MET
1	E	106	GLN
1	H	319	LYS
1	D	333	LYS
1	B	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	256	ASN
1	E	256	ASN
1	H	106	GLN
1	D	118	ASN
1	H	179	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	LLP	F	212	1	23,24,25	2.70	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	D	212	1	23,24,25	2.70	5 (21%)	25,32,34	1.40	4 (16%)
1	LLP	B	212	1	23,24,25	2.70	6 (26%)	25,32,34	1.31	4 (16%)
1	LLP	C	212	1	23,24,25	2.73	6 (26%)	25,32,34	1.43	5 (20%)
1	LLP	H	212	1	23,24,25	2.71	7 (30%)	25,32,34	1.26	4 (16%)
1	LLP	E	212	1	23,24,25	2.70	8 (34%)	25,32,34	1.52	6 (24%)
1	LLP	A	212	1	23,24,25	2.70	6 (26%)	25,32,34	1.39	3 (12%)
1	LLP	G	212	1	23,24,25	2.73	6 (26%)	25,32,34	1.40	4 (16%)

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
1	LLP	F	212	1	-	8/16/17/19	0/1/1/1
1	LLP	D	212	1	-	8/16/17/19	0/1/1/1
1	LLP	B	212	1	-	7/16/17/19	0/1/1/1
1	LLP	C	212	1	-	9/16/17/19	0/1/1/1
1	LLP	H	212	1	-	9/16/17/19	0/1/1/1
1	LLP	E	212	1	-	8/16/17/19	0/1/1/1
1	LLP	A	212	1	-	8/16/17/19	0/1/1/1
1	LLP	G	212	1	-	8/16/17/19	0/1/1/1

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	212	LLP	C4-C4'	8.50	1.62	1.46
1	C	212	LLP	C4-C4'	8.49	1.62	1.46
1	B	212	LLP	C4-C4'	8.48	1.62	1.46
1	F	212	LLP	C4-C4'	8.46	1.62	1.46
1	G	212	LLP	C4-C4'	8.40	1.62	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LLP	C4-C4'-NZ	-4.19	105.08	124.31
1	C	212	LLP	C4-C4'-NZ	-3.72	107.22	124.31
1	G	212	LLP	C4-C4'-NZ	-3.72	107.24	124.31
1	B	212	LLP	C4-C4'-NZ	-3.67	107.46	124.31
1	D	212	LLP	C4-C4'-NZ	-3.66	107.51	124.31

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	212	LLP	C5'-OP4-P-OP1
1	F	212	LLP	C5'-OP4-P-OP2
1	F	212	LLP	C5'-OP4-P-OP3
1	F	212	LLP	O-C-CA-CB
1	D	212	LLP	C4-C4'-NZ-CE

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	212	LLP	1	0
1	H	212	LLP	1	0
1	E	212	LLP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	C	501	-	4,4,4	0.16	0	6,6,6	0.12	0

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 [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, 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	383/415 (92%)	-0.34	0 100 100	17, 28, 56, 77	0
1	B	385/415 (92%)	-0.02	18 (4%) 31 30	17, 35, 71, 98	0
1	C	386/415 (93%)	-0.26	2 (0%) 91 92	17, 29, 58, 76	0
1	D	385/415 (92%)	0.10	20 (5%) 27 26	17, 37, 78, 106	0
1	E	387/415 (93%)	0.17	21 (5%) 25 25	22, 47, 87, 105	0
1	F	386/415 (93%)	-0.10	6 (1%) 72 74	24, 40, 75, 94	0
1	G	387/415 (93%)	0.08	11 (2%) 53 54	25, 46, 85, 112	0
1	H	386/415 (93%)	0.38	24 (6%) 20 20	27, 52, 90, 118	0
All	All	3085/3320 (92%)	0.00	102 (3%) 46 47	17, 39, 78, 118	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	57	GLY	5.9
1	G	362	ASN	4.6
1	E	359	VAL	4.6
1	H	366	VAL	4.4
1	H	367	LEU	4.1

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

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, 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	B-factors(Å ²)	Q<0.9
1	LLP	H	212	24/25	0.95	0.19	33,52,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	E	212	24/25	0.95	0.19	30,41,53,56	0
1	LLP	G	212	24/25	0.95	0.17	30,44,56,62	0
1	LLP	F	212	24/25	0.96	0.16	25,37,52,52	0
1	LLP	B	212	24/25	0.96	0.19	19,36,46,50	0
1	LLP	C	212	24/25	0.96	0.20	21,31,45,46	0
1	LLP	A	212	24/25	0.97	0.18	19,32,42,52	0
1	LLP	D	212	24/25	0.97	0.20	19,37,49,63	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
2	SO4	A	501	5/5	0.86	0.27	79,82,85,90	0
2	SO4	C	501	5/5	0.89	0.29	83,86,89,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.