



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2025 – 10:21 pm BST

PDB ID : 9HEE / pdb_00009hee
Title : Crystal structure of methionine gamma-lyase from *Brevibacterium aurantiacum* having disordered N-terminus and devoid of PLP cofactor
Authors : Kopecny, D.; Ferchaud, N.; Briozzo, P.
Deposited on : 2024-11-13
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

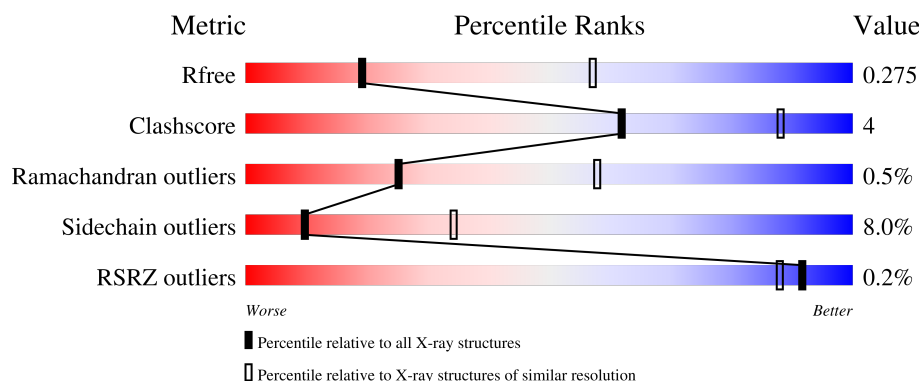
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	164625	1999 (3.28-3.20)
Clashscore	180529	2147 (3.28-3.20)
Ramachandran outliers	177936	2118 (3.28-3.20)
Sidechain outliers	177891	2117 (3.28-3.20)
RSRZ outliers	164620	2001 (3.28-3.20)

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 $\leq 5\%$. 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	413	 67% 9% 24%
1	B	413	 64% 11% 24%
1	C	413	 67% 8% 24%
1	D	413	 63% 11% 24%
1	E	413	 65% 10% 24%

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Mol	Chain	Length	Quality of chain
1	F	413	 66% 10% 24%
1	G	413	 67% 8% 24%
1	H	413	 64% 11% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18176 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	A	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	B	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	C	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	D	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	E	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	F	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	G	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			
1	H	314	Total	C	N	O	S	0	0	0
			2272	1426	404	431	11			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
A	-18	GLY	-	expression tag	UNP A0A2H1K3G9
A	-17	SER	-	expression tag	UNP A0A2H1K3G9
A	-16	SER	-	expression tag	UNP A0A2H1K3G9
A	-15	HIS	-	expression tag	UNP A0A2H1K3G9
A	-14	HIS	-	expression tag	UNP A0A2H1K3G9
A	-13	HIS	-	expression tag	UNP A0A2H1K3G9
A	-12	HIS	-	expression tag	UNP A0A2H1K3G9
A	-11	HIS	-	expression tag	UNP A0A2H1K3G9
A	-10	HIS	-	expression tag	UNP A0A2H1K3G9
A	-9	SER	-	expression tag	UNP A0A2H1K3G9
A	-8	SER	-	expression tag	UNP A0A2H1K3G9
A	-7	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A2H1K3G9
A	-5	VAL	-	expression tag	UNP A0A2H1K3G9
A	-4	PRO	-	expression tag	UNP A0A2H1K3G9
A	-3	ARG	-	expression tag	UNP A0A2H1K3G9
A	-2	GLY	-	expression tag	UNP A0A2H1K3G9
A	-1	SER	-	expression tag	UNP A0A2H1K3G9
A	0	HIS	-	expression tag	UNP A0A2H1K3G9
B	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
B	-18	GLY	-	expression tag	UNP A0A2H1K3G9
B	-17	SER	-	expression tag	UNP A0A2H1K3G9
B	-16	SER	-	expression tag	UNP A0A2H1K3G9
B	-15	HIS	-	expression tag	UNP A0A2H1K3G9
B	-14	HIS	-	expression tag	UNP A0A2H1K3G9
B	-13	HIS	-	expression tag	UNP A0A2H1K3G9
B	-12	HIS	-	expression tag	UNP A0A2H1K3G9
B	-11	HIS	-	expression tag	UNP A0A2H1K3G9
B	-10	HIS	-	expression tag	UNP A0A2H1K3G9
B	-9	SER	-	expression tag	UNP A0A2H1K3G9
B	-8	SER	-	expression tag	UNP A0A2H1K3G9
B	-7	GLY	-	expression tag	UNP A0A2H1K3G9
B	-6	LEU	-	expression tag	UNP A0A2H1K3G9
B	-5	VAL	-	expression tag	UNP A0A2H1K3G9
B	-4	PRO	-	expression tag	UNP A0A2H1K3G9
B	-3	ARG	-	expression tag	UNP A0A2H1K3G9
B	-2	GLY	-	expression tag	UNP A0A2H1K3G9
B	-1	SER	-	expression tag	UNP A0A2H1K3G9
B	0	HIS	-	expression tag	UNP A0A2H1K3G9
C	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
C	-18	GLY	-	expression tag	UNP A0A2H1K3G9
C	-17	SER	-	expression tag	UNP A0A2H1K3G9
C	-16	SER	-	expression tag	UNP A0A2H1K3G9
C	-15	HIS	-	expression tag	UNP A0A2H1K3G9
C	-14	HIS	-	expression tag	UNP A0A2H1K3G9
C	-13	HIS	-	expression tag	UNP A0A2H1K3G9
C	-12	HIS	-	expression tag	UNP A0A2H1K3G9
C	-11	HIS	-	expression tag	UNP A0A2H1K3G9
C	-10	HIS	-	expression tag	UNP A0A2H1K3G9
C	-9	SER	-	expression tag	UNP A0A2H1K3G9
C	-8	SER	-	expression tag	UNP A0A2H1K3G9
C	-7	GLY	-	expression tag	UNP A0A2H1K3G9
C	-6	LEU	-	expression tag	UNP A0A2H1K3G9
C	-5	VAL	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A2H1K3G9
C	-3	ARG	-	expression tag	UNP A0A2H1K3G9
C	-2	GLY	-	expression tag	UNP A0A2H1K3G9
C	-1	SER	-	expression tag	UNP A0A2H1K3G9
C	0	HIS	-	expression tag	UNP A0A2H1K3G9
D	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
D	-18	GLY	-	expression tag	UNP A0A2H1K3G9
D	-17	SER	-	expression tag	UNP A0A2H1K3G9
D	-16	SER	-	expression tag	UNP A0A2H1K3G9
D	-15	HIS	-	expression tag	UNP A0A2H1K3G9
D	-14	HIS	-	expression tag	UNP A0A2H1K3G9
D	-13	HIS	-	expression tag	UNP A0A2H1K3G9
D	-12	HIS	-	expression tag	UNP A0A2H1K3G9
D	-11	HIS	-	expression tag	UNP A0A2H1K3G9
D	-10	HIS	-	expression tag	UNP A0A2H1K3G9
D	-9	SER	-	expression tag	UNP A0A2H1K3G9
D	-8	SER	-	expression tag	UNP A0A2H1K3G9
D	-7	GLY	-	expression tag	UNP A0A2H1K3G9
D	-6	LEU	-	expression tag	UNP A0A2H1K3G9
D	-5	VAL	-	expression tag	UNP A0A2H1K3G9
D	-4	PRO	-	expression tag	UNP A0A2H1K3G9
D	-3	ARG	-	expression tag	UNP A0A2H1K3G9
D	-2	GLY	-	expression tag	UNP A0A2H1K3G9
D	-1	SER	-	expression tag	UNP A0A2H1K3G9
D	0	HIS	-	expression tag	UNP A0A2H1K3G9
E	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
E	-18	GLY	-	expression tag	UNP A0A2H1K3G9
E	-17	SER	-	expression tag	UNP A0A2H1K3G9
E	-16	SER	-	expression tag	UNP A0A2H1K3G9
E	-15	HIS	-	expression tag	UNP A0A2H1K3G9
E	-14	HIS	-	expression tag	UNP A0A2H1K3G9
E	-13	HIS	-	expression tag	UNP A0A2H1K3G9
E	-12	HIS	-	expression tag	UNP A0A2H1K3G9
E	-11	HIS	-	expression tag	UNP A0A2H1K3G9
E	-10	HIS	-	expression tag	UNP A0A2H1K3G9
E	-9	SER	-	expression tag	UNP A0A2H1K3G9
E	-8	SER	-	expression tag	UNP A0A2H1K3G9
E	-7	GLY	-	expression tag	UNP A0A2H1K3G9
E	-6	LEU	-	expression tag	UNP A0A2H1K3G9
E	-5	VAL	-	expression tag	UNP A0A2H1K3G9
E	-4	PRO	-	expression tag	UNP A0A2H1K3G9
E	-3	ARG	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A2H1K3G9
E	-1	SER	-	expression tag	UNP A0A2H1K3G9
E	0	HIS	-	expression tag	UNP A0A2H1K3G9
F	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
F	-18	GLY	-	expression tag	UNP A0A2H1K3G9
F	-17	SER	-	expression tag	UNP A0A2H1K3G9
F	-16	SER	-	expression tag	UNP A0A2H1K3G9
F	-15	HIS	-	expression tag	UNP A0A2H1K3G9
F	-14	HIS	-	expression tag	UNP A0A2H1K3G9
F	-13	HIS	-	expression tag	UNP A0A2H1K3G9
F	-12	HIS	-	expression tag	UNP A0A2H1K3G9
F	-11	HIS	-	expression tag	UNP A0A2H1K3G9
F	-10	HIS	-	expression tag	UNP A0A2H1K3G9
F	-9	SER	-	expression tag	UNP A0A2H1K3G9
F	-8	SER	-	expression tag	UNP A0A2H1K3G9
F	-7	GLY	-	expression tag	UNP A0A2H1K3G9
F	-6	LEU	-	expression tag	UNP A0A2H1K3G9
F	-5	VAL	-	expression tag	UNP A0A2H1K3G9
F	-4	PRO	-	expression tag	UNP A0A2H1K3G9
F	-3	ARG	-	expression tag	UNP A0A2H1K3G9
F	-2	GLY	-	expression tag	UNP A0A2H1K3G9
F	-1	SER	-	expression tag	UNP A0A2H1K3G9
F	0	HIS	-	expression tag	UNP A0A2H1K3G9
G	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
G	-18	GLY	-	expression tag	UNP A0A2H1K3G9
G	-17	SER	-	expression tag	UNP A0A2H1K3G9
G	-16	SER	-	expression tag	UNP A0A2H1K3G9
G	-15	HIS	-	expression tag	UNP A0A2H1K3G9
G	-14	HIS	-	expression tag	UNP A0A2H1K3G9
G	-13	HIS	-	expression tag	UNP A0A2H1K3G9
G	-12	HIS	-	expression tag	UNP A0A2H1K3G9
G	-11	HIS	-	expression tag	UNP A0A2H1K3G9
G	-10	HIS	-	expression tag	UNP A0A2H1K3G9
G	-9	SER	-	expression tag	UNP A0A2H1K3G9
G	-8	SER	-	expression tag	UNP A0A2H1K3G9
G	-7	GLY	-	expression tag	UNP A0A2H1K3G9
G	-6	LEU	-	expression tag	UNP A0A2H1K3G9
G	-5	VAL	-	expression tag	UNP A0A2H1K3G9
G	-4	PRO	-	expression tag	UNP A0A2H1K3G9
G	-3	ARG	-	expression tag	UNP A0A2H1K3G9
G	-2	GLY	-	expression tag	UNP A0A2H1K3G9
G	-1	SER	-	expression tag	UNP A0A2H1K3G9

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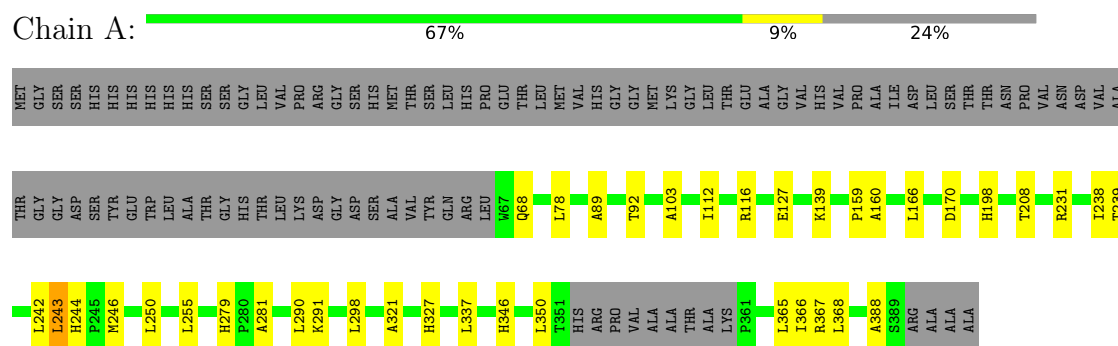
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A2H1K3G9
H	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
H	-18	GLY	-	expression tag	UNP A0A2H1K3G9
H	-17	SER	-	expression tag	UNP A0A2H1K3G9
H	-16	SER	-	expression tag	UNP A0A2H1K3G9
H	-15	HIS	-	expression tag	UNP A0A2H1K3G9
H	-14	HIS	-	expression tag	UNP A0A2H1K3G9
H	-13	HIS	-	expression tag	UNP A0A2H1K3G9
H	-12	HIS	-	expression tag	UNP A0A2H1K3G9
H	-11	HIS	-	expression tag	UNP A0A2H1K3G9
H	-10	HIS	-	expression tag	UNP A0A2H1K3G9
H	-9	SER	-	expression tag	UNP A0A2H1K3G9
H	-8	SER	-	expression tag	UNP A0A2H1K3G9
H	-7	GLY	-	expression tag	UNP A0A2H1K3G9
H	-6	LEU	-	expression tag	UNP A0A2H1K3G9
H	-5	VAL	-	expression tag	UNP A0A2H1K3G9
H	-4	PRO	-	expression tag	UNP A0A2H1K3G9
H	-3	ARG	-	expression tag	UNP A0A2H1K3G9
H	-2	GLY	-	expression tag	UNP A0A2H1K3G9
H	-1	SER	-	expression tag	UNP A0A2H1K3G9
H	0	HIS	-	expression tag	UNP A0A2H1K3G9

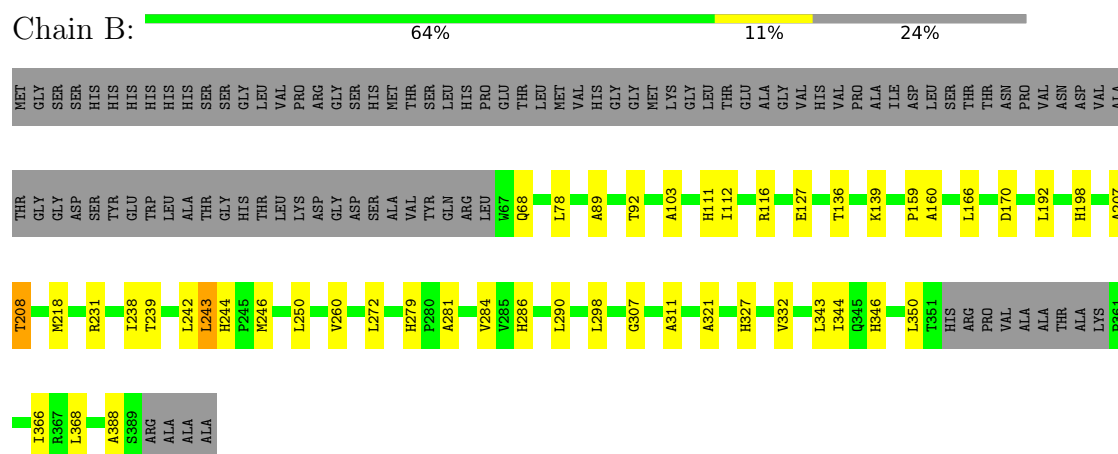
3 Residue-property plots

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.

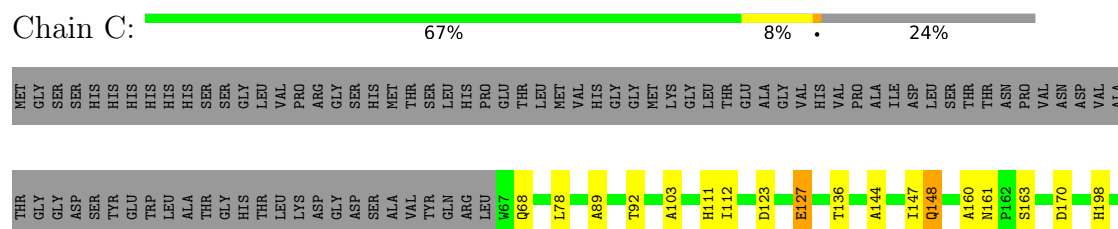
• Molecule 1: Cystathionine gamma-synthase



• Molecule 1: Cystathionine gamma-synthase



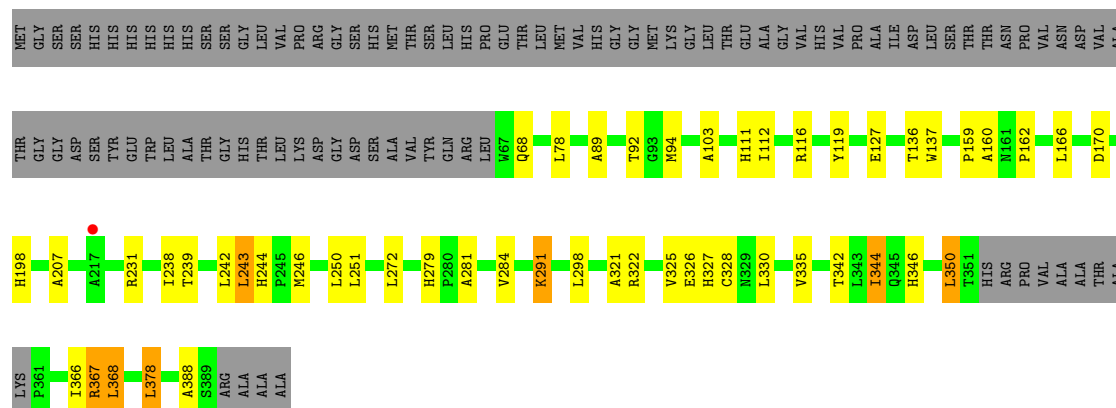
• Molecule 1: Cystathionine gamma-synthase





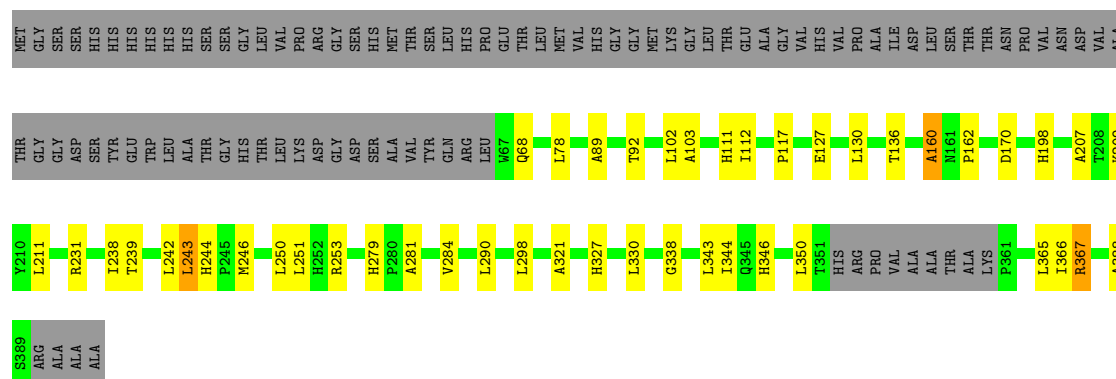
• Molecule 1: Cystathionine gamma-synthase

Chain D: 63% 11% 24%



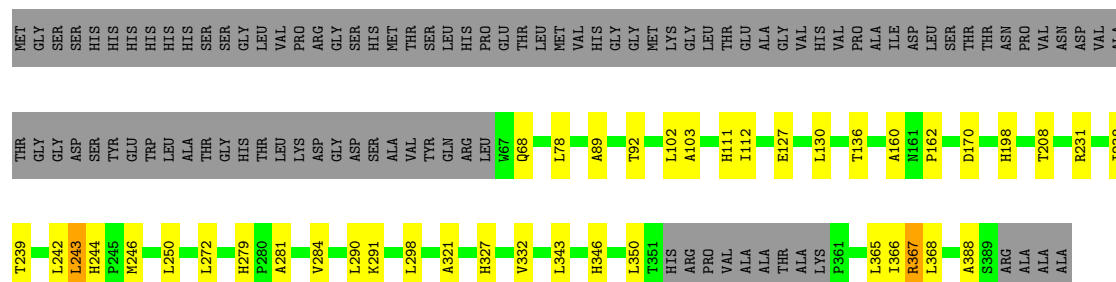
• Molecule 1: Cystathionine gamma-synthase

Chain E: 65% 10% 24%



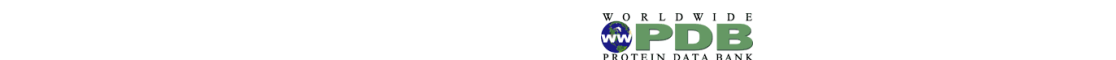
• Molecule 1: Cystathionine gamma-synthase

Chain F: 66% 10% 24%



• Molecule 1: Cystathionine gamma-synthase

Chain G: 67% 8% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.85Å 165.85Å 209.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.76 – 3.24 32.76 – 3.24	Depositor EDS
% Data completeness (in resolution range)	65.8 (32.76-3.24) 65.6 (32.76-3.24)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.247 , 0.284 0.243 , 0.275	Depositor DCC
R_{free} test set	1518 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	121.5	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 107.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18176	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.63	0/2313	1.02	0/3155
1	B	0.62	0/2313	1.02	0/3155
1	C	0.66	0/2313	1.03	5/3155 (0.2%)
1	D	0.63	0/2313	1.04	0/3155
1	E	0.56	0/2313	1.00	0/3155
1	F	0.58	0/2313	0.99	0/3155
1	G	0.56	0/2313	1.01	0/3155
1	H	0.59	0/2313	1.00	2/3155 (0.1%)
All	All	0.60	0/18504	1.01	7/25240 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	SER	CA-C-N	6.53	131.40	122.19
1	C	163	SER	C-N-CA	6.53	131.40	122.19
1	H	206	SER	CA-C-N	5.82	132.66	121.54
1	H	206	SER	C-N-CA	5.82	132.66	121.54
1	C	161	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	206	SER	CA-C-N	5.06	128.78	120.63
1	C	206	SER	C-N-CA	5.06	128.78	120.63

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	2272	0	2272	19	0
1	B	2272	0	2272	25	0
1	C	2272	0	2272	15	0
1	D	2272	0	2272	25	0
1	E	2272	0	2272	21	0
1	F	2272	0	2272	18	0
1	G	2272	0	2272	18	0
1	H	2272	0	2272	22	0
All	All	18176	0	18176	145	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 4.

All (145) 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:242:LEU:HD12	1:B:92:THR:HG21	1.72	0.71
1:C:242:LEU:HD12	1:D:92:THR:HG21	1.74	0.68
1:E:242:LEU:HD12	1:F:92:THR:HG21	1.77	0.67
1:B:116:ARG:NH2	1:B:139:LYS:NZ	2.42	0.67
1:F:244:HIS:HD2	1:F:246:MET:HB3	1.62	0.65
1:A:244:HIS:HD2	1:A:246:MET:HB3	1.63	0.64
1:G:244:HIS:HD2	1:G:246:MET:HB3	1.62	0.63
1:A:92:THR:HG21	1:B:242:LEU:HD12	1.80	0.63
1:B:136:THR:HG21	1:H:80:GLY:HA2	1.81	0.63
1:H:244:HIS:HD2	1:H:246:MET:HB3	1.64	0.62
1:C:244:HIS:HD2	1:C:246:MET:HB3	1.62	0.62
1:D:244:HIS:HD2	1:D:246:MET:HB3	1.64	0.62
1:C:244:HIS:CD2	1:C:246:MET:HB3	2.35	0.62
1:B:244:HIS:HD2	1:B:246:MET:HB3	1.64	0.61
1:D:327:HIS:CD2	1:D:388:ALA:HB3	2.35	0.61
1:A:244:HIS:CD2	1:A:246:MET:HB3	2.36	0.61
1:D:244:HIS:CD2	1:D:246:MET:HB3	2.36	0.61
1:F:244:HIS:CD2	1:F:246:MET:HB3	2.36	0.61
1:E:244:HIS:HD2	1:E:246:MET:HB3	1.65	0.60
1:B:244:HIS:CD2	1:B:246:MET:HB3	2.37	0.60
1:G:244:HIS:CD2	1:G:246:MET:HB3	2.36	0.60
1:H:286:HIS:HB2	1:H:311:ALA:HB3	1.84	0.60
1:C:111:HIS:NE2	1:C:136:THR:HG23	2.17	0.60
1:B:111:HIS:NE2	1:B:136:THR:HG23	2.17	0.59
1:E:92:THR:HG21	1:F:242:LEU:HD12	1.84	0.59
1:E:244:HIS:CD2	1:E:246:MET:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:HIS:CD2	1:H:246:MET:HB3	2.38	0.59
1:F:246:MET:HE1	1:G:246:MET:HE1	1.85	0.58
1:G:92:THR:HG21	1:H:242:LEU:HD12	1.85	0.58
1:B:246:MET:HE1	1:C:246:MET:HE1	1.86	0.57
1:D:111:HIS:NE2	1:D:136:THR:HG23	2.19	0.56
1:E:111:HIS:NE2	1:E:136:THR:HG23	2.20	0.56
1:G:286:HIS:HB2	1:G:311:ALA:HB3	1.88	0.56
1:H:111:HIS:NE2	1:H:136:THR:HG23	2.20	0.56
1:C:92:THR:HG21	1:D:242:LEU:HD12	1.88	0.55
1:G:111:HIS:NE2	1:G:136:THR:HG23	2.21	0.55
1:F:111:HIS:NE2	1:F:136:THR:HG23	2.21	0.55
1:A:116:ARG:HH21	1:A:139:LYS:NZ	2.06	0.54
1:D:335:VAL:HG22	1:D:350:LEU:HD11	1.89	0.53
1:H:279:HIS:HD2	1:H:281:ALA:HB3	1.73	0.53
1:E:246:MET:HE1	1:H:246:MET:HE1	1.91	0.53
1:G:117:PRO:HB2	1:G:160:ALA:HB1	1.89	0.53
1:B:159:PRO:HB3	1:B:166:LEU:HD23	1.91	0.52
1:D:162:PRO:HB3	1:D:367:ARG:HE	1.75	0.52
1:F:162:PRO:HB3	1:F:367:ARG:HE	1.74	0.52
1:B:286:HIS:HB2	1:B:311:ALA:HB3	1.91	0.51
1:E:327:HIS:CD2	1:E:388:ALA:HB3	2.45	0.51
1:C:89:ALA:HB1	1:C:243:LEU:HD12	1.91	0.51
1:E:89:ALA:HB1	1:E:243:LEU:HD12	1.93	0.51
1:G:89:ALA:HB1	1:G:243:LEU:HD12	1.92	0.51
1:G:162:PRO:HB3	1:G:367:ARG:HE	1.76	0.51
1:B:260:VAL:HG11	1:C:372:LEU:HD22	1.92	0.51
1:D:89:ALA:HB1	1:D:243:LEU:HD12	1.92	0.51
1:B:89:ALA:HB1	1:B:243:LEU:HD12	1.93	0.50
1:C:144:ALA:HA	1:C:147:ILE:HD12	1.93	0.50
1:C:123:ASP:O	1:C:127:GLU:HB2	2.11	0.50
1:A:116:ARG:NH2	1:A:139:LYS:HZ2	2.09	0.50
1:E:162:PRO:HB3	1:E:367:ARG:HE	1.77	0.50
1:G:103:ALA:HB1	1:G:231:ARG:HG2	1.93	0.50
1:A:327:HIS:CD2	1:A:388:ALA:HB3	2.47	0.50
1:B:192:LEU:HD13	1:B:307:GLY:HA2	1.94	0.49
1:B:321:ALA:CB	1:B:346:HIS:CE1	2.95	0.49
1:D:344:ILE:HG23	1:D:368:LEU:HD12	1.94	0.49
1:H:89:ALA:HB1	1:H:243:LEU:HD12	1.93	0.49
1:H:103:ALA:HB1	1:H:231:ARG:HG2	1.94	0.49
1:A:89:ALA:HB1	1:A:243:LEU:HD12	1.93	0.49
1:A:321:ALA:CB	1:A:346:HIS:CE1	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HB1	1:B:231:ARG:HG2	1.95	0.49
1:D:327:HIS:CD2	1:D:388:ALA:CB	2.96	0.49
1:F:89:ALA:HB1	1:F:243:LEU:HD12	1.93	0.49
1:B:116:ARG:NH2	1:B:139:LYS:HZ3	2.10	0.49
1:C:103:ALA:HB1	1:C:231:ARG:HG2	1.95	0.49
1:H:162:PRO:HB3	1:H:367:ARG:HE	1.76	0.49
1:A:321:ALA:HB1	1:A:346:HIS:CE1	2.48	0.48
1:E:321:ALA:CB	1:E:346:HIS:CE1	2.96	0.48
1:D:170:ASP:OD2	1:D:198:HIS:HD2	1.96	0.48
1:G:327:HIS:CD2	1:G:388:ALA:HB3	2.48	0.48
1:E:103:ALA:HB1	1:E:231:ARG:HG2	1.95	0.48
1:B:321:ALA:HB1	1:B:346:HIS:CE1	2.48	0.48
1:D:321:ALA:CB	1:D:346:HIS:CE1	2.97	0.48
1:F:321:ALA:CB	1:F:346:HIS:CE1	2.97	0.48
1:H:321:ALA:CB	1:H:346:HIS:CE1	2.96	0.48
1:H:327:HIS:CD2	1:H:388:ALA:HB3	2.49	0.48
1:D:279:HIS:HD2	1:D:281:ALA:HB3	1.79	0.48
1:G:321:ALA:CB	1:G:346:HIS:CE1	2.96	0.48
1:B:327:HIS:CD2	1:B:388:ALA:HB3	2.49	0.48
1:A:103:ALA:HB1	1:A:231:ARG:HG2	1.95	0.48
1:A:116:ARG:HH21	1:A:139:LYS:HZ2	1.61	0.48
1:H:321:ALA:HB1	1:H:346:HIS:CE1	2.49	0.47
1:G:321:ALA:HB1	1:G:346:HIS:CE1	2.49	0.47
1:E:321:ALA:HB1	1:E:346:HIS:CE1	2.50	0.47
1:F:103:ALA:HB1	1:F:231:ARG:HG2	1.96	0.47
1:G:333:HIS:NE2	1:G:345:GLN:HA	2.28	0.47
1:F:327:HIS:CD2	1:F:388:ALA:HB3	2.49	0.47
1:F:170:ASP:OD2	1:F:198:HIS:HD2	1.98	0.47
1:F:321:ALA:HB1	1:F:346:HIS:CE1	2.50	0.47
1:A:170:ASP:OD2	1:A:198:HIS:HD2	1.98	0.47
1:H:207:ALA:HB1	1:H:251:LEU:HD22	1.97	0.47
1:C:111:HIS:NE2	1:C:136:THR:CG2	2.78	0.46
1:E:207:ALA:HA	1:E:211:LEU:HB2	1.98	0.46
1:D:325:VAL:HG22	1:D:344:ILE:HD13	1.97	0.46
1:E:170:ASP:OD2	1:E:198:HIS:HD2	1.99	0.46
1:B:170:ASP:OD2	1:B:198:HIS:HD2	1.98	0.46
1:D:103:ALA:HB1	1:D:231:ARG:HG2	1.97	0.46
1:E:117:PRO:HD2	1:E:160:ALA:HB1	1.98	0.46
1:G:242:LEU:HD12	1:H:92:THR:HG21	1.98	0.46
1:H:170:ASP:OD2	1:H:198:HIS:HD2	1.98	0.46
1:C:279:HIS:HD2	1:C:281:ALA:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:HIS:NE2	1:D:136:THR:CG2	2.79	0.46
1:E:279:HIS:HD2	1:E:281:ALA:HB3	1.81	0.46
1:G:279:HIS:HD2	1:G:281:ALA:HB3	1.82	0.45
1:G:170:ASP:OD2	1:G:198:HIS:HD2	1.98	0.45
1:B:111:HIS:NE2	1:B:136:THR:CG2	2.78	0.45
1:A:246:MET:HE1	1:D:246:MET:HE1	1.99	0.45
1:E:102:LEU:HD22	1:F:130:LEU:HG	1.98	0.45
1:E:111:HIS:NE2	1:E:136:THR:CG2	2.80	0.45
1:G:111:HIS:NE2	1:G:136:THR:CG2	2.80	0.45
1:B:279:HIS:HD2	1:B:281:ALA:HB3	1.82	0.45
1:C:170:ASP:OD2	1:C:198:HIS:HD2	1.99	0.44
1:F:279:HIS:HD2	1:F:281:ALA:HB3	1.81	0.44
1:H:111:HIS:NE2	1:H:136:THR:CG2	2.80	0.44
1:D:321:ALA:HB3	1:D:346:HIS:CE1	2.51	0.44
1:F:111:HIS:NE2	1:F:136:THR:CG2	2.81	0.44
1:A:279:HIS:HD2	1:A:281:ALA:HB3	1.81	0.44
1:D:342:THR:HG21	1:D:378:LEU:HD21	2.00	0.44
1:F:332:VAL:HG23	1:F:343:LEU:HD23	2.00	0.44
1:A:159:PRO:HB3	1:A:166:LEU:HD23	2.00	0.44
1:A:116:ARG:NH2	1:A:139:LYS:NZ	2.65	0.44
1:D:207:ALA:HB1	1:D:251:LEU:HD22	2.00	0.43
1:E:207:ALA:HB1	1:E:251:LEU:HD22	2.00	0.43
1:E:130:LEU:HG	1:F:102:LEU:HD22	2.01	0.43
1:B:208:THR:HG23	1:B:218:MET:HA	2.02	0.42
1:A:337:LEU:HD23	1:A:337:LEU:N	2.35	0.42
1:E:253:ARG:HG2	1:H:214:HIS:CD2	2.55	0.42
1:B:332:VAL:HG23	1:B:343:LEU:HD23	2.02	0.41
1:H:209:LYS:O	1:H:210:TYR:HB2	2.20	0.41
1:B:321:ALA:HB3	1:B:346:HIS:CE1	2.56	0.41
1:C:148:GLN:NE2	1:C:148:GLN:HA	2.36	0.41
1:D:159:PRO:HB3	1:D:166:LEU:HD23	2.03	0.41
1:D:116:ARG:HD3	1:D:137:TRP:CZ3	2.55	0.41
1:D:321:ALA:HB1	1:D:346:HIS:CE1	2.56	0.41
1:A:321:ALA:HB3	1:A:346:HIS:CE1	2.55	0.41
1:H:291:LYS:HE3	1:H:291:LYS:HB3	1.96	0.41
1:D:94:MET:HE3	1:D:119:TYR:HE2	1.87	0.40
1:B:139:LYS:HE3	1:H:72:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	310/413 (75%)	292 (94%)	17 (6%)	1 (0%)	37	67
1	B	310/413 (75%)	295 (95%)	13 (4%)	2 (1%)	22	54
1	C	310/413 (75%)	298 (96%)	11 (4%)	1 (0%)	37	67
1	D	310/413 (75%)	297 (96%)	11 (4%)	2 (1%)	22	54
1	E	310/413 (75%)	298 (96%)	10 (3%)	2 (1%)	22	54
1	F	310/413 (75%)	296 (96%)	13 (4%)	1 (0%)	37	67
1	G	310/413 (75%)	295 (95%)	13 (4%)	2 (1%)	22	54
1	H	310/413 (75%)	296 (96%)	13 (4%)	1 (0%)	37	67
All	All	2480/3304 (75%)	2367 (95%)	101 (4%)	12 (0%)	25	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ALA
1	B	160	ALA
1	C	160	ALA
1	D	160	ALA
1	F	160	ALA
1	D	291	LYS
1	E	160	ALA
1	G	160	ALA
1	H	160	ALA
1	B	207	ALA
1	G	289	GLY
1	E	338	GLY

5.3.2 Protein sidechains

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	229/306 (75%)	211 (92%)	18 (8%)	10	35
1	B	229/306 (75%)	212 (93%)	17 (7%)	11	37
1	C	229/306 (75%)	212 (93%)	17 (7%)	11	37
1	D	229/306 (75%)	207 (90%)	22 (10%)	7	26
1	E	229/306 (75%)	210 (92%)	19 (8%)	9	33
1	F	229/306 (75%)	210 (92%)	19 (8%)	9	33
1	G	229/306 (75%)	214 (93%)	15 (7%)	14	42
1	H	229/306 (75%)	210 (92%)	19 (8%)	9	33
All	All	1832/2448 (75%)	1686 (92%)	146 (8%)	10	34

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	78	LEU
1	A	112	ILE
1	A	127	GLU
1	A	208	THR
1	A	238	ILE
1	A	239	THR
1	A	243	LEU
1	A	250	LEU
1	A	255	LEU
1	A	290	LEU
1	A	291	LYS
1	A	298	LEU
1	A	350	LEU
1	A	365	LEU
1	A	366	ILE
1	A	367	ARG
1	A	368	LEU
1	B	68	GLN
1	B	78	LEU
1	B	112	ILE
1	B	127	GLU
1	B	208	THR

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Mol	Chain	Res	Type
1	B	238	ILE
1	B	239	THR
1	B	243	LEU
1	B	250	LEU
1	B	272	LEU
1	B	284	VAL
1	B	290	LEU
1	B	298	LEU
1	B	344	ILE
1	B	350	LEU
1	B	366	ILE
1	B	368	LEU
1	C	68	GLN
1	C	78	LEU
1	C	112	ILE
1	C	127	GLU
1	C	148	GLN
1	C	208	THR
1	C	238	ILE
1	C	239	THR
1	C	243	LEU
1	C	250	LEU
1	C	272	LEU
1	C	284	VAL
1	C	291	LYS
1	C	298	LEU
1	C	344	ILE
1	C	350	LEU
1	C	367	ARG
1	D	68	GLN
1	D	78	LEU
1	D	112	ILE
1	D	127	GLU
1	D	238	ILE
1	D	239	THR
1	D	243	LEU
1	D	250	LEU
1	D	272	LEU
1	D	284	VAL
1	D	291	LYS
1	D	298	LEU
1	D	322	ARG

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Mol	Chain	Res	Type
1	D	326	GLU
1	D	328	CYS
1	D	330	LEU
1	D	344	ILE
1	D	350	LEU
1	D	366	ILE
1	D	367	ARG
1	D	368	LEU
1	D	378	LEU
1	E	68	GLN
1	E	78	LEU
1	E	112	ILE
1	E	127	GLU
1	E	209	LYS
1	E	238	ILE
1	E	239	THR
1	E	243	LEU
1	E	250	LEU
1	E	284	VAL
1	E	290	LEU
1	E	298	LEU
1	E	330	LEU
1	E	343	LEU
1	E	344	ILE
1	E	350	LEU
1	E	365	LEU
1	E	366	ILE
1	E	367	ARG
1	F	68	GLN
1	F	78	LEU
1	F	112	ILE
1	F	127	GLU
1	F	208	THR
1	F	238	ILE
1	F	239	THR
1	F	243	LEU
1	F	250	LEU
1	F	272	LEU
1	F	284	VAL
1	F	290	LEU
1	F	291	LYS
1	F	298	LEU

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Mol	Chain	Res	Type
1	F	350	LEU
1	F	365	LEU
1	F	366	ILE
1	F	367	ARG
1	F	368	LEU
1	G	68	GLN
1	G	78	LEU
1	G	112	ILE
1	G	127	GLU
1	G	238	ILE
1	G	239	THR
1	G	243	LEU
1	G	250	LEU
1	G	298	LEU
1	G	345	GLN
1	G	350	LEU
1	G	365	LEU
1	G	366	ILE
1	G	367	ARG
1	G	368	LEU
1	H	68	GLN
1	H	78	LEU
1	H	112	ILE
1	H	127	GLU
1	H	238	ILE
1	H	239	THR
1	H	243	LEU
1	H	250	LEU
1	H	255	LEU
1	H	272	LEU
1	H	284	VAL
1	H	285	VAL
1	H	293	GLN
1	H	298	LEU
1	H	350	LEU
1	H	365	LEU
1	H	366	ILE
1	H	367	ARG
1	H	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	198	HIS
1	A	244	HIS
1	A	279	HIS
1	B	68	GLN
1	B	83	HIS
1	B	198	HIS
1	B	244	HIS
1	B	279	HIS
1	B	345	GLN
1	C	68	GLN
1	C	198	HIS
1	C	244	HIS
1	C	279	HIS
1	C	286	HIS
1	D	68	GLN
1	D	198	HIS
1	D	244	HIS
1	D	279	HIS
1	D	345	GLN
1	D	346	HIS
1	E	68	GLN
1	E	198	HIS
1	E	244	HIS
1	E	279	HIS
1	F	68	GLN
1	F	83	HIS
1	F	198	HIS
1	F	244	HIS
1	F	279	HIS
1	G	68	GLN
1	G	198	HIS
1	G	244	HIS
1	G	279	HIS
1	H	68	GLN
1	H	83	HIS
1	H	198	HIS
1	H	244	HIS
1	H	279	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	314/413 (76%)	-0.44	0 100 100	80, 129, 232, 262	0
1	B	314/413 (76%)	-0.36	0 100 100	89, 119, 220, 249	0
1	C	314/413 (76%)	-0.38	0 100 100	70, 110, 224, 258	0
1	D	314/413 (76%)	-0.48	1 (0%) 90 84	79, 131, 188, 207	0
1	E	314/413 (76%)	-0.41	0 100 100	131, 196, 239, 250	0
1	F	314/413 (76%)	-0.39	0 100 100	133, 205, 241, 258	0
1	G	314/413 (76%)	-0.42	1 (0%) 90 84	139, 206, 240, 247	0
1	H	314/413 (76%)	-0.30	2 (0%) 85 76	108, 177, 236, 251	0
All	All	2512/3304 (76%)	-0.40	4 (0%) 92 88	70, 168, 237, 262	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	155	ILE	2.4
1	G	97	MET	2.4
1	H	169	LEU	2.2
1	D	217	ALA	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.