



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 01:49 PM EST

PDB ID : 5TSU  
Title : Active conformation for Engineered human cystathionine gamma lyase (E59N, R119L, E339V) to depleting methionine  
Authors : Yan, W.; Zhang, Y.  
Deposited on : 2016-10-31  
Resolution : 2.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

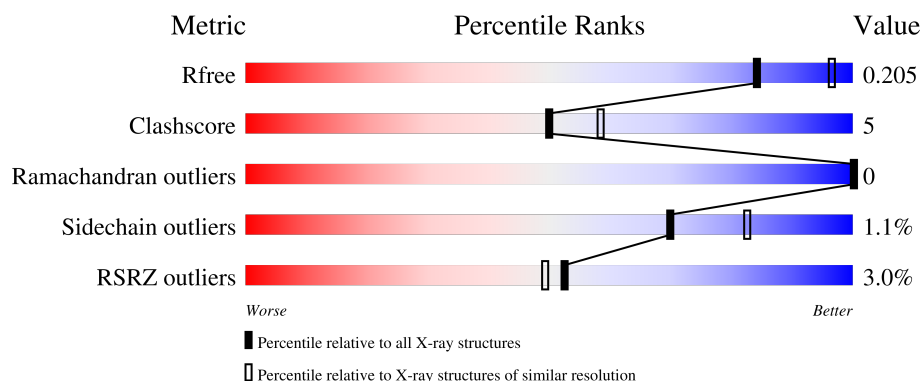
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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  $\geq 3$ , 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	422	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	B	422	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	D	422	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>9%</div> </div> </div>
1	F	422	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	G	422	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	422	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>81%</div><div>10%</div><div>9%</div></div></div>
2	C	422	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>81%</div><div>10%</div><div>9%</div></div></div>
2	E	422	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>11%</div><div>9%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24978 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
			2985	1905	507	553	1	19			
1	B	385	Total	C	N	O	P	S	0	0	0
			2992	1909	508	555	1	19			
1	D	384	Total	C	N	O	P	S	0	0	0
			2976	1898	505	553	1	19			
1	F	381	Total	C	N	O	P	S	0	0	0
			2961	1889	503	549	1	19			
1	G	386	Total	C	N	O	P	S	0	0	0
			2996	1913	508	555	1	19			
1	H	386	Total	C	N	O	P	S	0	0	0
			3001	1915	509	557	1	19			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP P32929
A	-15	GLY	-	expression tag	UNP P32929
A	-14	GLY	-	expression tag	UNP P32929
A	-13	HIS	-	expression tag	UNP P32929
A	-12	HIS	-	expression tag	UNP P32929
A	-11	HIS	-	expression tag	UNP P32929
A	-10	HIS	-	expression tag	UNP P32929
A	-9	HIS	-	expression tag	UNP P32929
A	-8	HIS	-	expression tag	UNP P32929
A	-7	GLY	-	expression tag	UNP P32929
A	-6	LEU	-	expression tag	UNP P32929
A	-5	GLU	-	expression tag	UNP P32929
A	-4	VAL	-	expression tag	UNP P32929
A	-3	LEU	-	expression tag	UNP P32929
A	-2	PHE	-	expression tag	UNP P32929
A	-1	GLN	-	expression tag	UNP P32929
A	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P32929
A	59	ASN	GLU	engineered mutation	UNP P32929
A	119	LEU	ARG	engineered mutation	UNP P32929
A	339	VAL	GLU	engineered mutation	UNP P32929
B	-16	MET	-	expression tag	UNP P32929
B	-15	GLY	-	expression tag	UNP P32929
B	-14	GLY	-	expression tag	UNP P32929
B	-13	HIS	-	expression tag	UNP P32929
B	-12	HIS	-	expression tag	UNP P32929
B	-11	HIS	-	expression tag	UNP P32929
B	-10	HIS	-	expression tag	UNP P32929
B	-9	HIS	-	expression tag	UNP P32929
B	-8	HIS	-	expression tag	UNP P32929
B	-7	GLY	-	expression tag	UNP P32929
B	-6	LEU	-	expression tag	UNP P32929
B	-5	GLU	-	expression tag	UNP P32929
B	-4	VAL	-	expression tag	UNP P32929
B	-3	LEU	-	expression tag	UNP P32929
B	-2	PHE	-	expression tag	UNP P32929
B	-1	GLN	-	expression tag	UNP P32929
B	0	GLY	-	expression tag	UNP P32929
B	1	PRO	-	expression tag	UNP P32929
B	59	ASN	GLU	engineered mutation	UNP P32929
B	119	LEU	ARG	engineered mutation	UNP P32929
B	339	VAL	GLU	engineered mutation	UNP P32929
D	-16	MET	-	expression tag	UNP P32929
D	-15	GLY	-	expression tag	UNP P32929
D	-14	GLY	-	expression tag	UNP P32929
D	-13	HIS	-	expression tag	UNP P32929
D	-12	HIS	-	expression tag	UNP P32929
D	-11	HIS	-	expression tag	UNP P32929
D	-10	HIS	-	expression tag	UNP P32929
D	-9	HIS	-	expression tag	UNP P32929
D	-8	HIS	-	expression tag	UNP P32929
D	-7	GLY	-	expression tag	UNP P32929
D	-6	LEU	-	expression tag	UNP P32929
D	-5	GLU	-	expression tag	UNP P32929
D	-4	VAL	-	expression tag	UNP P32929
D	-3	LEU	-	expression tag	UNP P32929
D	-2	PHE	-	expression tag	UNP P32929
D	-1	GLN	-	expression tag	UNP P32929
D	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	PRO	-	expression tag	UNP P32929
D	59	ASN	GLU	engineered mutation	UNP P32929
D	119	LEU	ARG	engineered mutation	UNP P32929
D	339	VAL	GLU	engineered mutation	UNP P32929
F	-16	MET	-	expression tag	UNP P32929
F	-15	GLY	-	expression tag	UNP P32929
F	-14	GLY	-	expression tag	UNP P32929
F	-13	HIS	-	expression tag	UNP P32929
F	-12	HIS	-	expression tag	UNP P32929
F	-11	HIS	-	expression tag	UNP P32929
F	-10	HIS	-	expression tag	UNP P32929
F	-9	HIS	-	expression tag	UNP P32929
F	-8	HIS	-	expression tag	UNP P32929
F	-7	GLY	-	expression tag	UNP P32929
F	-6	LEU	-	expression tag	UNP P32929
F	-5	GLU	-	expression tag	UNP P32929
F	-4	VAL	-	expression tag	UNP P32929
F	-3	LEU	-	expression tag	UNP P32929
F	-2	PHE	-	expression tag	UNP P32929
F	-1	GLN	-	expression tag	UNP P32929
F	0	GLY	-	expression tag	UNP P32929
F	1	PRO	-	expression tag	UNP P32929
F	59	ASN	GLU	engineered mutation	UNP P32929
F	119	LEU	ARG	engineered mutation	UNP P32929
F	339	VAL	GLU	engineered mutation	UNP P32929
G	-16	MET	-	expression tag	UNP P32929
G	-15	GLY	-	expression tag	UNP P32929
G	-14	GLY	-	expression tag	UNP P32929
G	-13	HIS	-	expression tag	UNP P32929
G	-12	HIS	-	expression tag	UNP P32929
G	-11	HIS	-	expression tag	UNP P32929
G	-10	HIS	-	expression tag	UNP P32929
G	-9	HIS	-	expression tag	UNP P32929
G	-8	HIS	-	expression tag	UNP P32929
G	-7	GLY	-	expression tag	UNP P32929
G	-6	LEU	-	expression tag	UNP P32929
G	-5	GLU	-	expression tag	UNP P32929
G	-4	VAL	-	expression tag	UNP P32929
G	-3	LEU	-	expression tag	UNP P32929
G	-2	PHE	-	expression tag	UNP P32929
G	-1	GLN	-	expression tag	UNP P32929
G	0	GLY	-	expression tag	UNP P32929

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	PRO	-	expression tag	UNP P32929
G	59	ASN	GLU	engineered mutation	UNP P32929
G	119	LEU	ARG	engineered mutation	UNP P32929
G	339	VAL	GLU	engineered mutation	UNP P32929
H	-16	MET	-	expression tag	UNP P32929
H	-15	GLY	-	expression tag	UNP P32929
H	-14	GLY	-	expression tag	UNP P32929
H	-13	HIS	-	expression tag	UNP P32929
H	-12	HIS	-	expression tag	UNP P32929
H	-11	HIS	-	expression tag	UNP P32929
H	-10	HIS	-	expression tag	UNP P32929
H	-9	HIS	-	expression tag	UNP P32929
H	-8	HIS	-	expression tag	UNP P32929
H	-7	GLY	-	expression tag	UNP P32929
H	-6	LEU	-	expression tag	UNP P32929
H	-5	GLU	-	expression tag	UNP P32929
H	-4	VAL	-	expression tag	UNP P32929
H	-3	LEU	-	expression tag	UNP P32929
H	-2	PHE	-	expression tag	UNP P32929
H	-1	GLN	-	expression tag	UNP P32929
H	0	GLY	-	expression tag	UNP P32929
H	1	PRO	-	expression tag	UNP P32929
H	59	ASN	GLU	engineered mutation	UNP P32929
H	119	LEU	ARG	engineered mutation	UNP P32929
H	339	VAL	GLU	engineered mutation	UNP P32929

- Molecule 2 is a protein called Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	386	Total	C	N	O	S	0	0	0
			2984	1906	508	551	19			
2	E	385	Total	C	N	O	S	0	0	0
			2978	1903	507	549	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P32929
C	-15	GLY	-	expression tag	UNP P32929
C	-14	GLY	-	expression tag	UNP P32929
C	-13	HIS	-	expression tag	UNP P32929
C	-12	HIS	-	expression tag	UNP P32929

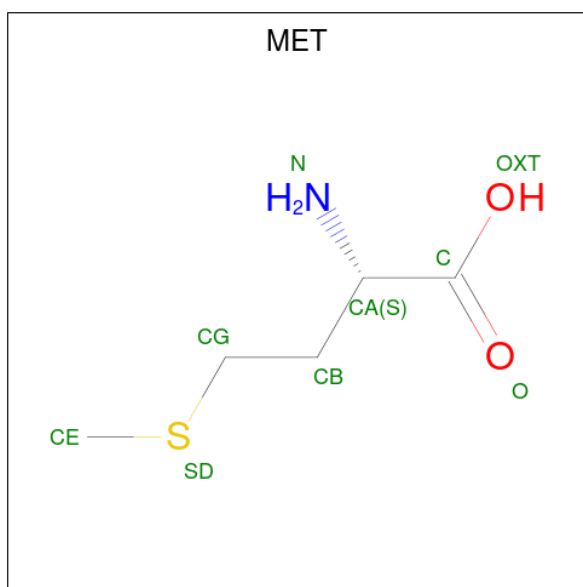
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP P32929
C	-10	HIS	-	expression tag	UNP P32929
C	-9	HIS	-	expression tag	UNP P32929
C	-8	HIS	-	expression tag	UNP P32929
C	-7	GLY	-	expression tag	UNP P32929
C	-6	LEU	-	expression tag	UNP P32929
C	-5	GLU	-	expression tag	UNP P32929
C	-4	VAL	-	expression tag	UNP P32929
C	-3	LEU	-	expression tag	UNP P32929
C	-2	PHE	-	expression tag	UNP P32929
C	-1	GLN	-	expression tag	UNP P32929
C	0	GLY	-	expression tag	UNP P32929
C	1	PRO	-	expression tag	UNP P32929
C	59	ASN	GLU	engineered mutation	UNP P32929
C	119	LEU	ARG	engineered mutation	UNP P32929
C	339	VAL	GLU	engineered mutation	UNP P32929
E	-16	MET	-	initiating methionine	UNP P32929
E	-15	GLY	-	expression tag	UNP P32929
E	-14	GLY	-	expression tag	UNP P32929
E	-13	HIS	-	expression tag	UNP P32929
E	-12	HIS	-	expression tag	UNP P32929
E	-11	HIS	-	expression tag	UNP P32929
E	-10	HIS	-	expression tag	UNP P32929
E	-9	HIS	-	expression tag	UNP P32929
E	-8	HIS	-	expression tag	UNP P32929
E	-7	GLY	-	expression tag	UNP P32929
E	-6	LEU	-	expression tag	UNP P32929
E	-5	GLU	-	expression tag	UNP P32929
E	-4	VAL	-	expression tag	UNP P32929
E	-3	LEU	-	expression tag	UNP P32929
E	-2	PHE	-	expression tag	UNP P32929
E	-1	GLN	-	expression tag	UNP P32929
E	0	GLY	-	expression tag	UNP P32929
E	1	PRO	-	expression tag	UNP P32929
E	59	ASN	GLU	engineered mutation	UNP P32929
E	119	LEU	ARG	engineered mutation	UNP P32929
E	339	VAL	GLU	engineered mutation	UNP P32929

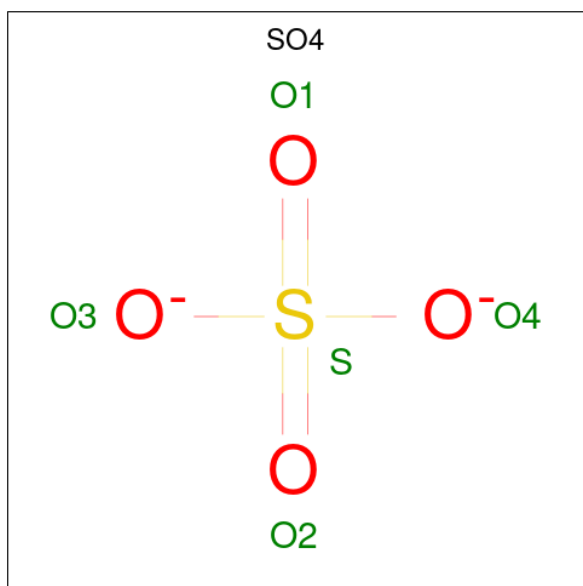
- Molecule 3 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).





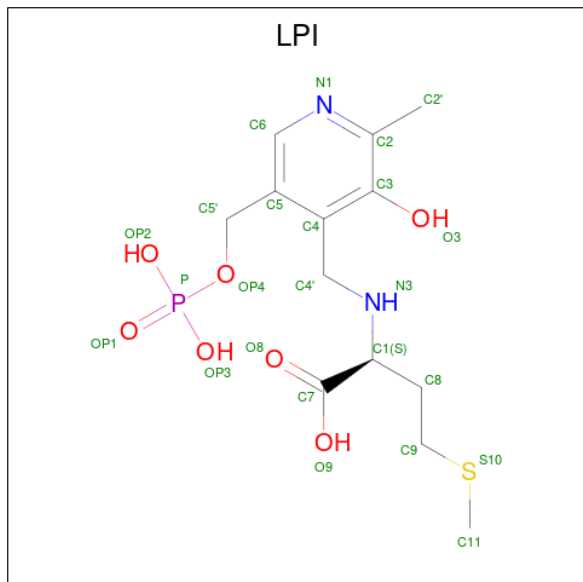
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



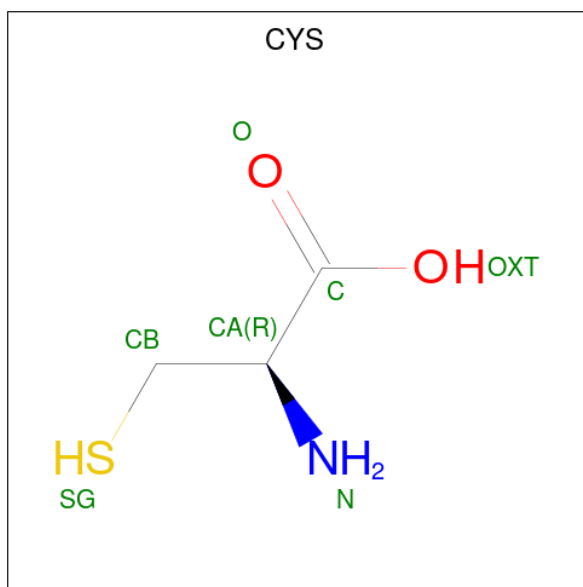
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is N-({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)-L-methionine (three-letter code: LPI) (formula:  $C_{13}H_{21}N_2O_7PS$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
5	E	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
6	G	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
6	H	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

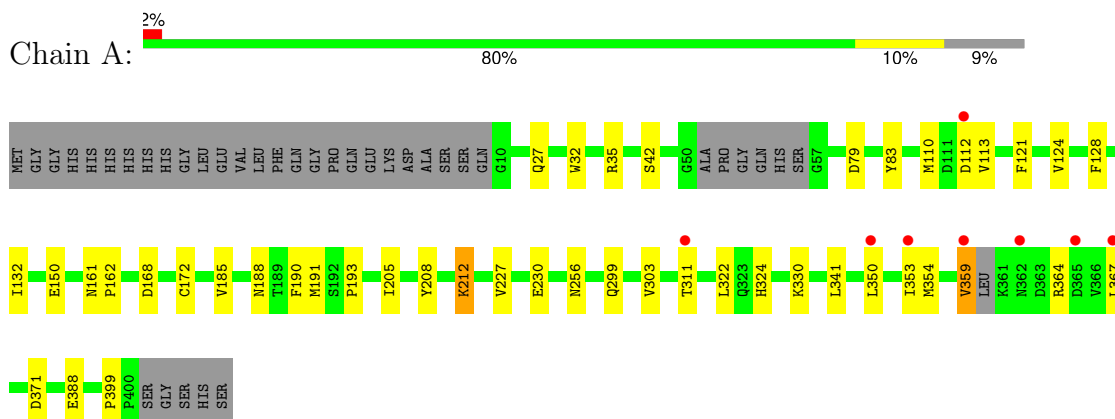
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		
7	B	139	Total	O	0	0
			139	139		
7	C	176	Total	O	0	0
			176	176		
7	D	157	Total	O	0	0
			157	157		
7	E	103	Total	O	0	0
			103	103		
7	F	63	Total	O	0	0
			63	63		
7	G	94	Total	O	0	0
			94	94		
7	H	103	Total	O	0	0
			103	103		

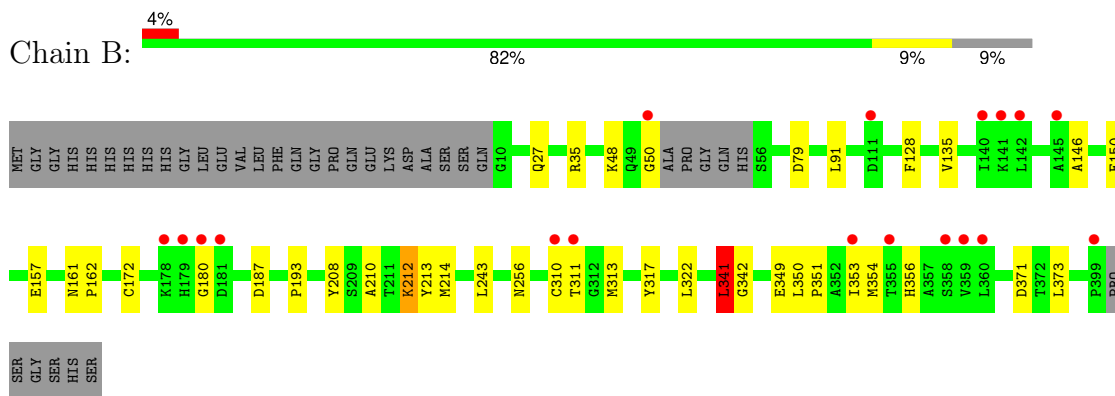
### 3 Residue-property plots [i](#)

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.

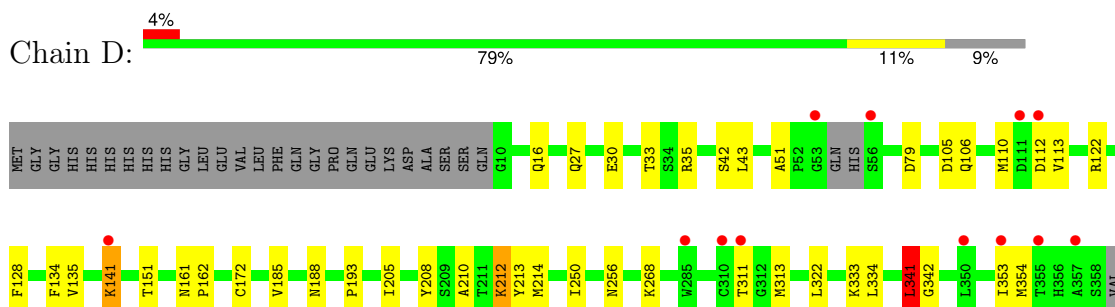
- Molecule 1: Cystathionine gamma-lyase



- Molecule 1: Cystathionine gamma-lyase

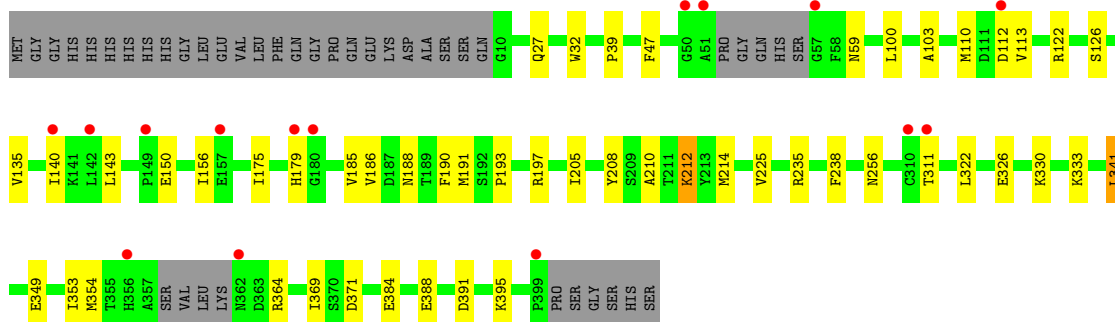
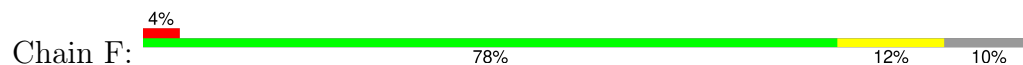


- Molecule 1: Cystathionine gamma-lyase

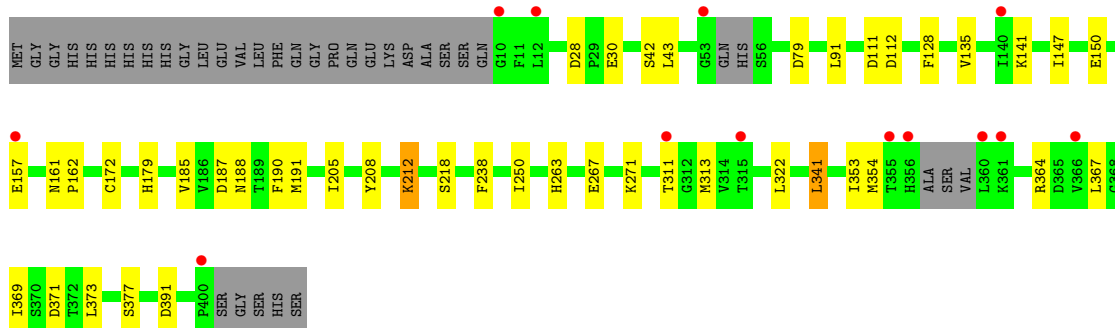
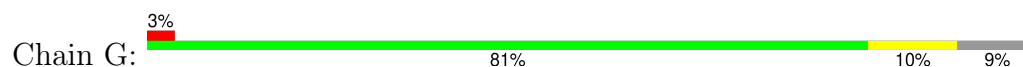




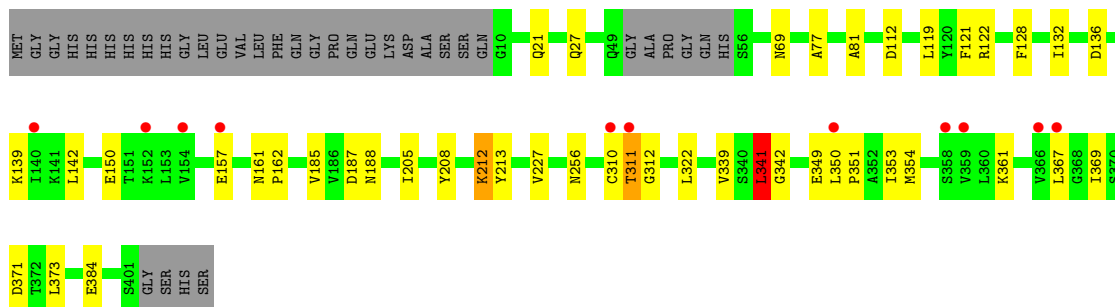
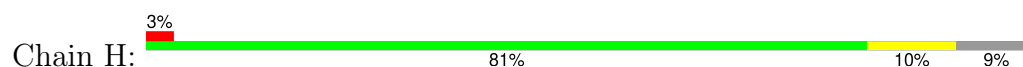
• Molecule 1: Cystathionine gamma-lyase



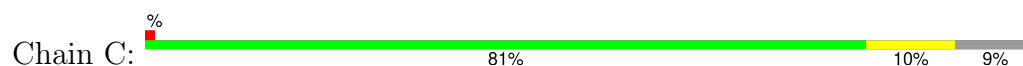
• Molecule 1: Cystathionine gamma-lyase

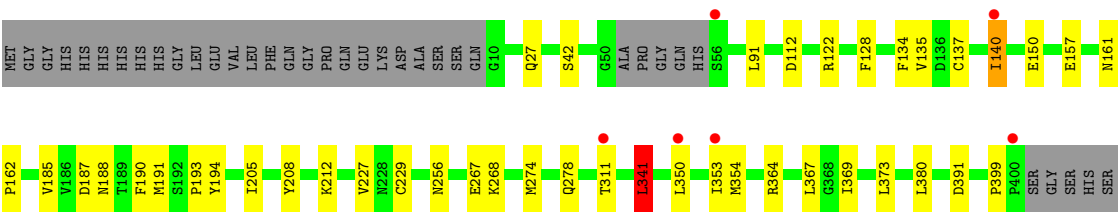


• Molecule 1: Cystathionine gamma-lyase

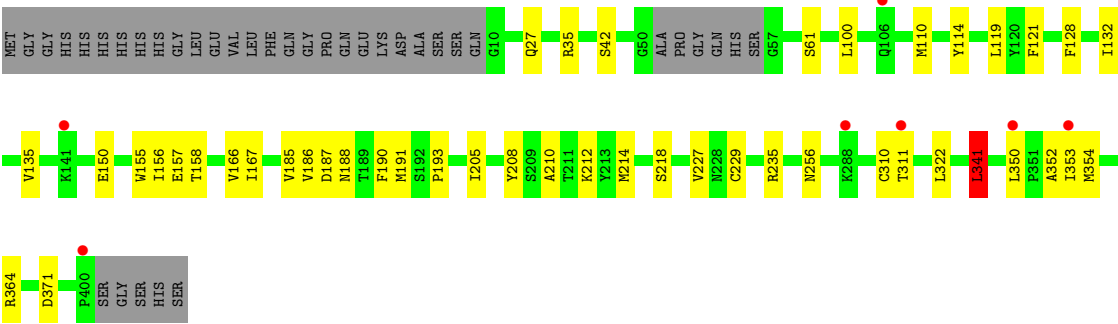
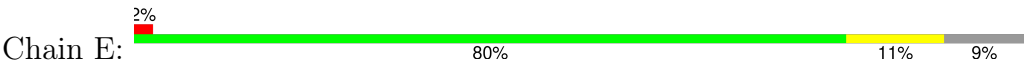


• Molecule 2: Cystathionine gamma-lyase





● Molecule 2: Cystathionine gamma-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.89Å 163.68Å 181.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.20 49.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.04-2.20) 95.7 (49.04-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.171 , 0.202 0.176 , 0.205	Depositor DCC
$R_{free}$ test set	8378 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	24978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, LLP, LPI

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	0.31	0/3026	0.50	1/4105 (0.0%)
1	B	0.28	0/3033	0.47	1/4115 (0.0%)
1	D	0.28	0/3017	0.47	1/4093 (0.0%)
1	F	0.26	0/3001	0.46	0/4071
1	G	0.27	0/3038	0.46	0/4122
1	H	0.28	0/3043	0.46	1/4130 (0.0%)
2	C	0.29	0/3051	0.50	1/4141 (0.0%)
2	E	0.27	0/3045	0.47	1/4133 (0.0%)
All	All	0.28	0/24254	0.47	6/32910 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	341	LEU	CA-CB-CG	6.03	129.18	115.30
1	A	359	VAL	N-CA-C	-5.86	95.18	111.00
2	E	341	LEU	CA-CB-CG	5.79	128.61	115.30
1	B	341	LEU	CA-CB-CG	5.17	127.18	115.30
1	H	341	LEU	CA-CB-CG	5.12	127.07	115.30

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	2985	0	2974	32	0
1	B	2992	0	2983	27	0
1	D	2976	0	2959	33	0
1	F	2961	0	2945	37	0
1	G	2996	0	2984	33	0
1	H	3001	0	2993	34	0
2	C	2984	0	2986	30	0
2	E	2978	0	2982	33	0
3	A	9	0	8	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	C	24	0	0	0	0
5	E	24	0	0	3	0
6	F	7	0	4	1	0
6	G	7	0	4	0	0
6	H	7	0	4	3	0
7	A	177	0	0	4	0
7	B	139	0	0	1	0
7	C	176	0	0	4	0
7	D	157	0	0	6	0
7	E	103	0	0	5	0
7	F	63	0	0	4	0
7	G	94	0	0	7	0
7	H	103	0	0	5	0
All	All	24978	0	23826	248	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 5.

The worst 5 of 248 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:G:157:GLU:HG2	1:G:187:ASP:HB3	1.35	1.03
1:H:157:GLU:HG2	1:H:187:ASP:HB3	1.45	0.98
1:G:391:ASP:OD1	7:G:601:HOH:O	1.88	0.90
1:H:212:LLP:H4'1	6:H:501:CYS:N	1.90	0.86
1:F:47:PHE:O	7:F:601:HOH:O	1.95	0.83

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	377/422 (89%)	365 (97%)	12 (3%)	0	100	100
1	B	380/422 (90%)	371 (98%)	9 (2%)	0	100	100
1	D	377/422 (89%)	367 (97%)	10 (3%)	0	100	100
1	F	374/422 (89%)	363 (97%)	11 (3%)	0	100	100
1	G	379/422 (90%)	371 (98%)	8 (2%)	0	100	100
1	H	381/422 (90%)	373 (98%)	8 (2%)	0	100	100
2	C	382/422 (90%)	372 (97%)	10 (3%)	0	100	100
2	E	381/422 (90%)	372 (98%)	9 (2%)	0	100	100
All	All	3031/3376 (90%)	2954 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	326/356 (92%)	324 (99%)	2 (1%)	84	91
1	B	327/356 (92%)	325 (99%)	2 (1%)	84	91
1	D	324/356 (91%)	318 (98%)	6 (2%)	52	67
1	F	322/356 (90%)	317 (98%)	5 (2%)	58	73
1	G	327/356 (92%)	324 (99%)	3 (1%)	75	86
1	H	329/356 (92%)	326 (99%)	3 (1%)	75	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	329/357 (92%)	325 (99%)	4 (1%)	67	80
2	E	328/357 (92%)	325 (99%)	3 (1%)	75	86
All	All	2612/2850 (92%)	2584 (99%)	28 (1%)	70	82

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	135	VAL
1	H	341	LEU
1	F	59	ASN
1	G	341	LEU
2	E	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	106	GLN
2	E	256	ASN
1	H	256	ASN
1	G	179	HIS
1	G	398	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	2.55	5 (21%)	25,32,34	1.18	3 (12%)
1	LLP	A	212	1	23,24,25	2.49	6 (26%)	25,32,34	1.34	2 (8%)
1	LLP	B	212	1	23,24,25	2.61	5 (21%)	25,32,34	1.28	3 (12%)
1	LLP	H	212	1	23,24,25	2.58	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	G	212	1	23,24,25	2.52	6 (26%)	25,32,34	1.19	3 (12%)
1	LLP	D	212	1	23,24,25	2.47	6 (26%)	25,32,34	1.25	3 (12%)

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	A	212	1	-	7/16/17/19	0/1/1/1
1	LLP	B	212	1	-	10/16/17/19	0/1/1/1
1	LLP	H	212	1	-	7/16/17/19	0/1/1/1
1	LLP	G	212	1	-	7/16/17/19	0/1/1/1
1	LLP	D	212	1	-	5/16/17/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	LLP	C4-C4'	7.96	1.63	1.46
1	A	212	LLP	C4-C4'	7.58	1.62	1.46
1	F	212	LLP	C4-C4'	7.56	1.62	1.46
1	H	212	LLP	C4-C4'	7.53	1.62	1.46
1	G	212	LLP	C4-C4'	7.33	1.62	1.46

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LLP	C4-C4'-NZ	-3.47	108.01	124.04
1	D	212	LLP	C4-C4'-NZ	-3.43	108.20	124.04
1	B	212	LLP	C4-C4'-NZ	-3.15	109.50	124.04
1	H	212	LLP	C4-C4'-NZ	-3.08	109.83	124.04
1	F	212	LLP	C4-C4'-NZ	-3.04	110.02	124.04

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	212	LLP	3	0
1	A	212	LLP	2	0
1	B	212	LLP	2	0
1	H	212	LLP	4	0
1	G	212	LLP	2	0
1	D	212	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
6	CYS	F	501	-	5,6,6	1.07	1 (20%)	3,7,7	1.64	1 (33%)
4	SO4	A	502	-	4,4,4	0.24	0	6,6,6	0.09	0
6	CYS	G	501	-	5,6,6	1.09	1 (20%)	3,7,7	1.71	1 (33%)
3	MET	A	501	-	7,8,8	0.91	1 (14%)	5,9,9	1.28	1 (20%)
4	SO4	B	501	-	4,4,4	0.16	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	LPI	E	501	-	24,24,24	0.84	0	29,33,33	1.23	4 (13%)
5	LPI	C	501	2	24,24,24	0.84	0	29,33,33	1.56	3 (10%)
4	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.09	0
6	CYS	H	501	-	5,6,6	1.17	1 (20%)	3,7,7	1.90	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYS	F	501	-	-	0/6/6/6	-
6	CYS	G	501	-	-	0/6/6/6	-
3	MET	A	501	-	-	1/8/8/8	-
5	LPI	E	501	-	-	11/19/19/19	0/1/1/1
5	LPI	C	501	2	-	6/19/19/19	0/1/1/1
6	CYS	H	501	-	-	2/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	501	CYS	OXT-C	-2.43	1.22	1.30
3	A	501	MET	OXT-C	-2.35	1.23	1.30
6	G	501	CYS	OXT-C	-2.32	1.23	1.30
6	F	501	CYS	OXT-C	-2.27	1.23	1.30

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	LPI	C4'-C4-C5	5.44	125.67	119.75
6	H	501	CYS	OXT-C-O	-3.22	116.77	124.08
5	E	501	LPI	C6-C5-C4	2.94	120.29	118.06
6	G	501	CYS	OXT-C-O	-2.93	117.42	124.08
6	F	501	CYS	OXT-C-O	-2.84	117.63	124.08

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	LPI	C7-C1-C8-C9

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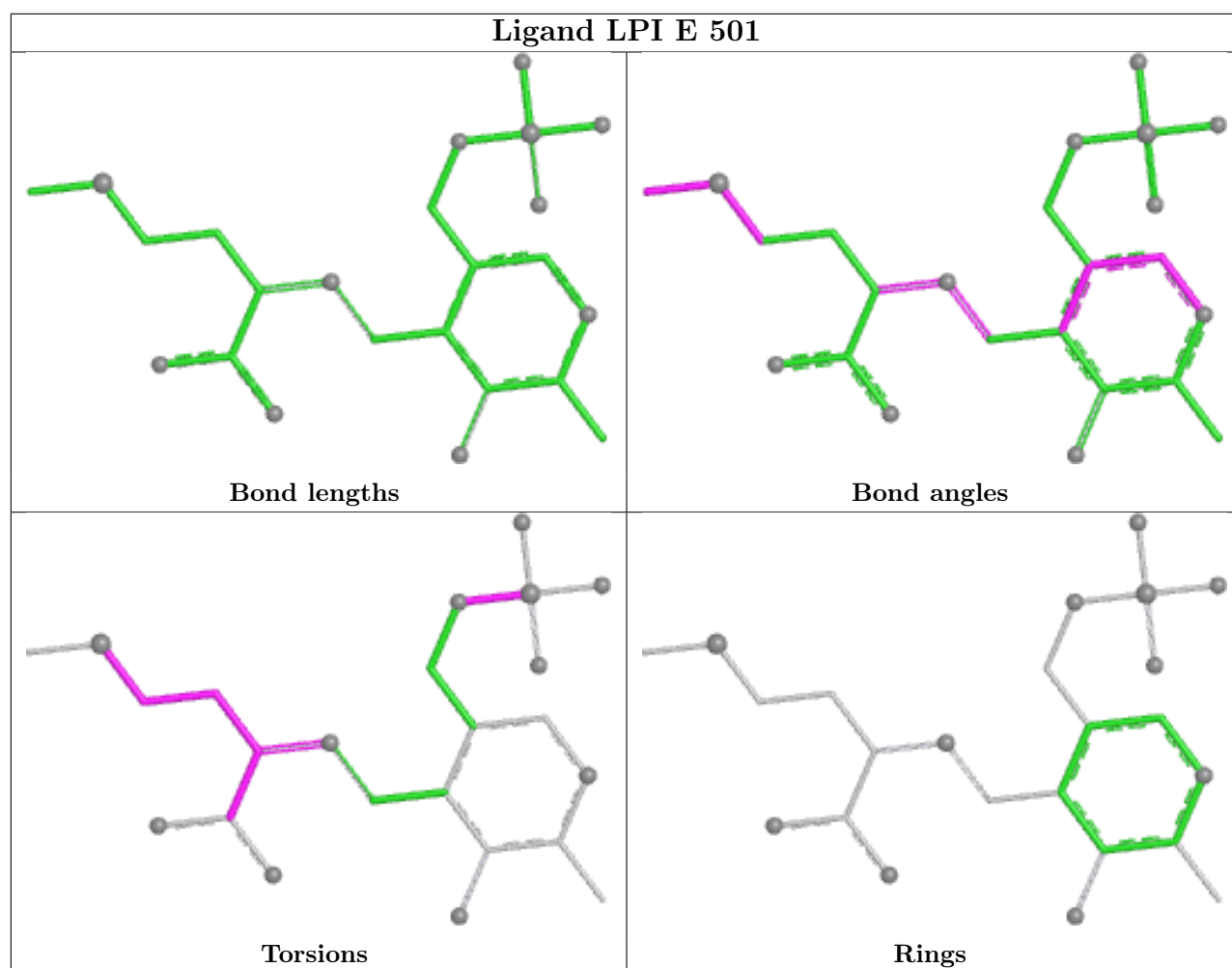
Mol	Chain	Res	Type	Atoms
5	C	501	LPI	N3-C1-C8-C9
5	C	501	LPI	C7-C1-N3-C4'
5	E	501	LPI	C5'-OP4-P-OP1
5	E	501	LPI	C5'-OP4-P-OP3

There are no ring outliers.

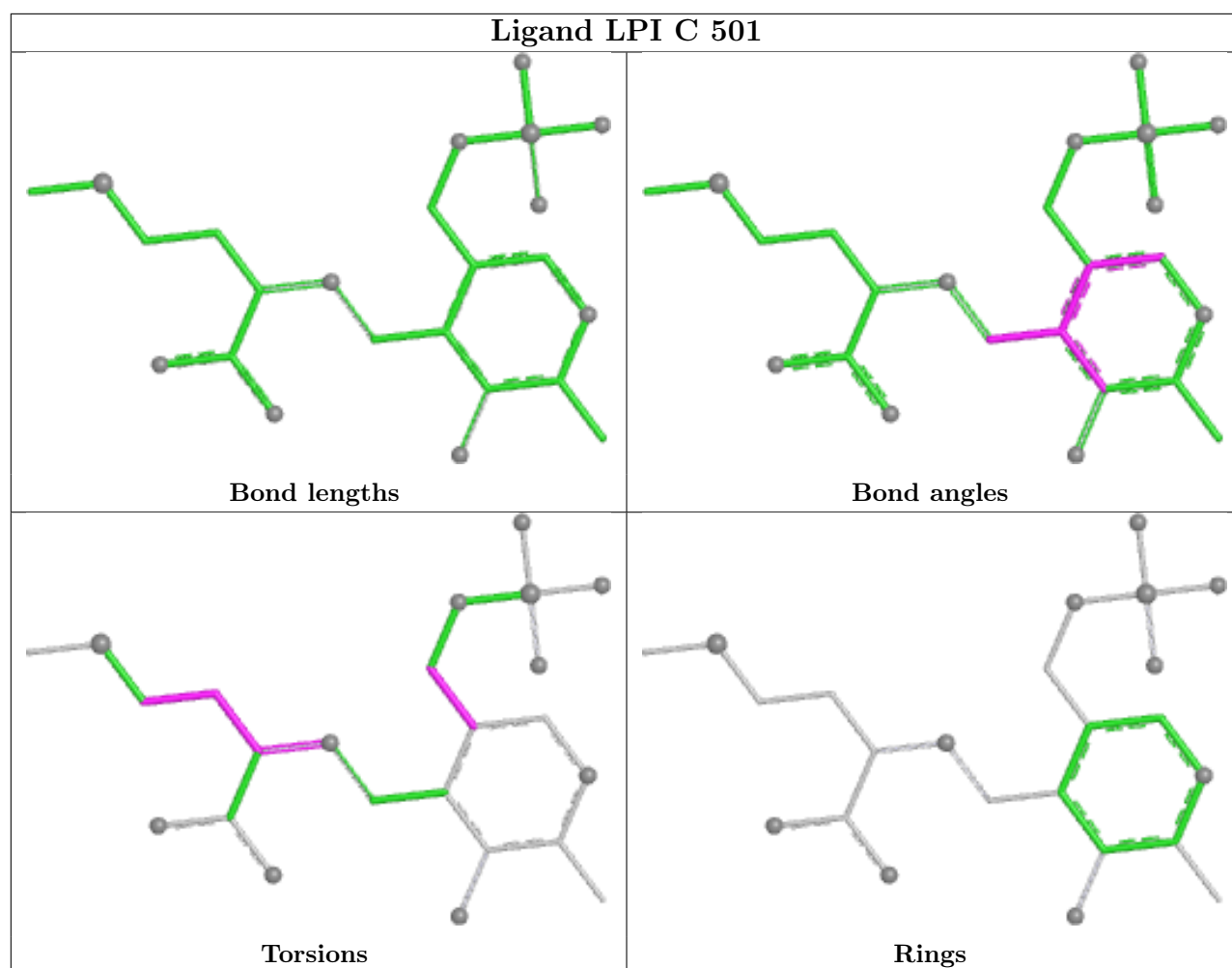
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	501	CYS	1	0
3	A	501	MET	2	0
5	E	501	LPI	3	0
6	H	501	CYS	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	383/422 (90%)	-0.32	8 (2%) 63 59	23, 35, 67, 102	0
1	B	384/422 (90%)	0.00	18 (4%) 37 34	25, 46, 84, 114	0
1	D	383/422 (90%)	-0.12	15 (3%) 44 40	23, 43, 85, 114	0
1	F	380/422 (90%)	0.45	15 (3%) 44 40	41, 66, 108, 140	0
1	G	385/422 (91%)	0.28	13 (3%) 48 45	32, 60, 97, 122	0
1	H	385/422 (91%)	-0.01	11 (2%) 54 51	29, 50, 91, 109	0
2	C	386/422 (91%)	-0.36	6 (1%) 70 67	23, 36, 64, 88	0
2	E	385/422 (91%)	0.03	7 (1%) 67 64	30, 53, 86, 102	0
All	All	3071/3376 (90%)	-0.01	93 (3%) 52 49	23, 48, 91, 140	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	311	THR	5.5
1	A	311	THR	5.5
1	B	311	THR	5.3
1	F	310	CYS	5.0
1	G	311	THR	4.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	G	212	24/25	0.93	0.11	43,51,61,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	F	212	24/25	0.94	0.11	46,56,62,63	0
1	LLP	H	212	24/25	0.94	0.10	34,43,50,54	0
1	LLP	B	212	24/25	0.95	0.10	35,42,51,63	0
1	LLP	D	212	24/25	0.96	0.08	31,39,48,52	0
1	LLP	A	212	24/25	0.96	0.07	22,30,34,37	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

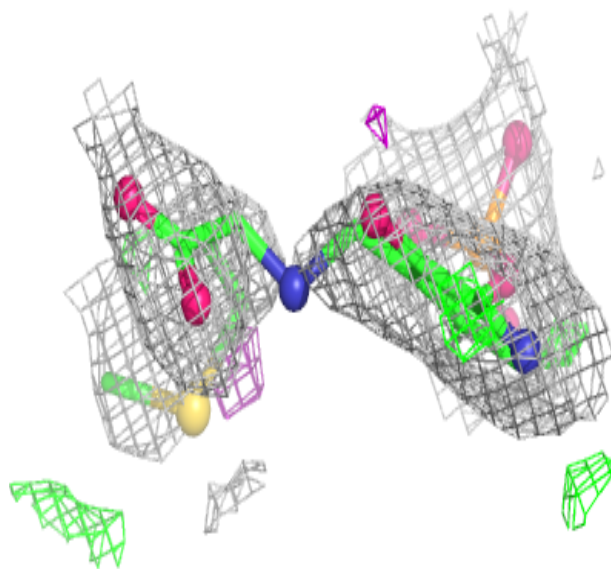
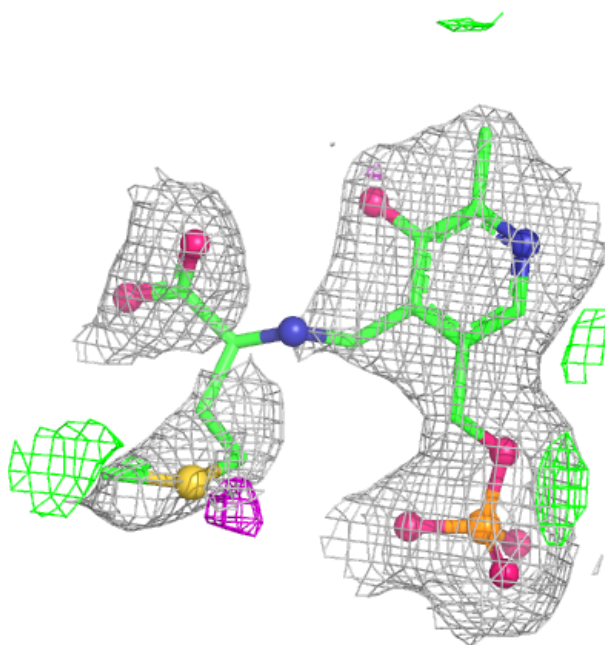
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	501	5/5	0.59	0.28	34,37,43,52	5
4	SO4	A	502	5/5	0.78	0.15	109,110,110,112	0
6	CYS	G	501	7/7	0.79	0.18	64,71,88,89	0
3	MET	A	501	9/9	0.86	0.21	41,64,85,87	0
6	CYS	F	501	7/7	0.89	0.17	72,72,83,87	0
6	CYS	H	501	7/7	0.89	0.14	48,53,72,81	0
5	LPI	E	501	24/24	0.91	0.11	39,49,53,58	3
4	SO4	D	501	5/5	0.91	0.09	62,64,73,73	0
5	LPI	C	501	24/24	0.92	0.12	23,35,64,80	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

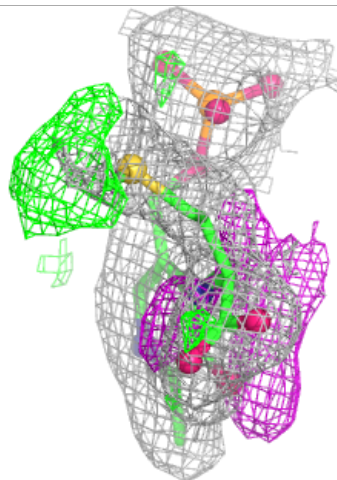
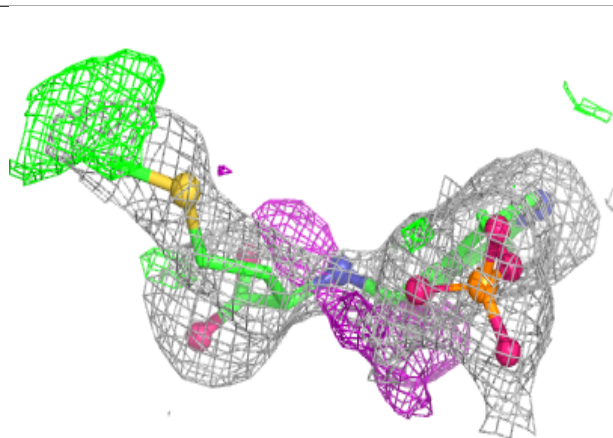
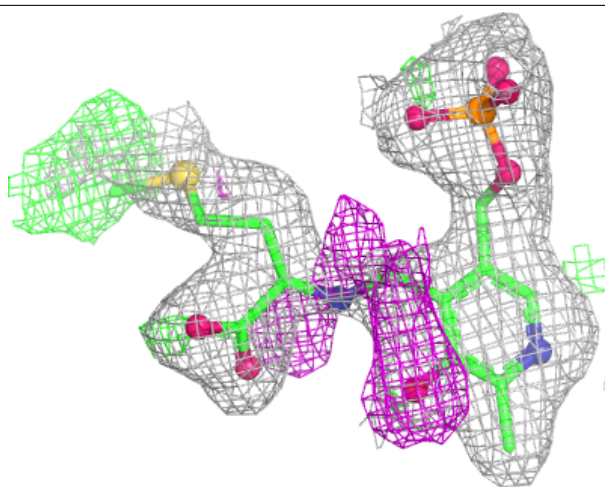
**Electron density around LPI E 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around LPI C 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.