



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2018 – 04:57 PM EST

PDB ID : 5UTS
Title : Carbon Sulfoxide lyase, Egt2 in the Ergothioneine biosynthesis pathway
Authors : Irani, S.; Zhang, Y.
Deposited on : 2017-02-15
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

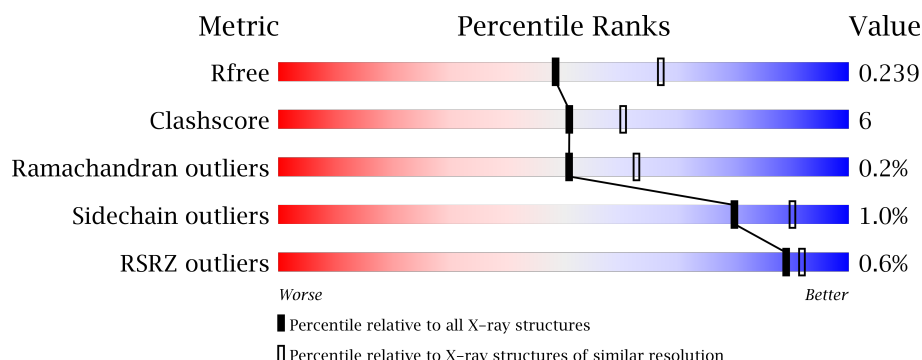
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	501	<div> <div>74%</div> <div>15%</div> <div>11%</div> </div>
1	B	501	<div> <div>71%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	C	501	<div> <div>%</div> <div>71%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	D	501	<div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	E	501	<div> <div>73%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	501	
1	G	501	
1	H	501	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	B	501	-	-	X	-
2	FMT	D	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28997 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 C-S Lyase Egt2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	G	445	Total	C	N	O	P	S	Se	0	0	0
			3536	2265	596	654	1	10	10			
1	C	436	Total	C	N	O	P	S	Se	0	0	0
			3475	2224	586	644	1	10	10			
1	H	436	Total	C	N	O	P	S	Se	0	0	0
			3476	2226	586	643	1	10	10			
1	D	438	Total	C	N	O	P	S	Se	0	0	0
			3491	2235	589	646	1	10	10			
1	E	436	Total	C	N	O	P	S	Se	0	0	0
			3475	2224	586	644	1	10	10			
1	F	439	Total	C	N	O	P	S	Se	0	0	0
			3500	2240	590	649	1	10	10			
1	B	436	Total	C	N	O	P	S	Se	0	0	0
			3476	2226	586	643	1	10	10			
1	A	447	Total	C	N	O	P	S	Se	0	0	0
			3555	2278	599	657	1	10	10			

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	MSE	-	initiating methionine	UNP A7UX13
G	-5	GLY	-	expression tag	UNP A7UX13
G	-4	ASP	-	expression tag	UNP A7UX13
G	-3	ARG	-	expression tag	UNP A7UX13
G	-2	GLY	-	expression tag	UNP A7UX13
G	-1	PRO	-	expression tag	UNP A7UX13
G	0	GLU	-	expression tag	UNP A7UX13
G	1	PHE	-	expression tag	UNP A7UX13
G	474	LEU	-	expression tag	UNP A7UX13
G	475	GLU	-	expression tag	UNP A7UX13
G	476	VAL	-	expression tag	UNP A7UX13
G	477	ASP	-	expression tag	UNP A7UX13
G	478	LEU	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	479	GLN	-	expression tag	UNP A7UX13
G	480	GLY	-	expression tag	UNP A7UX13
G	481	ASP	-	expression tag	UNP A7UX13
G	482	HIS	-	expression tag	UNP A7UX13
G	483	GLY	-	expression tag	UNP A7UX13
G	484	LEU	-	expression tag	UNP A7UX13
G	485	SER	-	expression tag	UNP A7UX13
G	486	ALA	-	expression tag	UNP A7UX13
G	487	TRP	-	expression tag	UNP A7UX13
G	488	SER	-	expression tag	UNP A7UX13
G	489	HIS	-	expression tag	UNP A7UX13
G	490	PRO	-	expression tag	UNP A7UX13
G	491	GLN	-	expression tag	UNP A7UX13
G	492	PHE	-	expression tag	UNP A7UX13
G	493	GLU	-	expression tag	UNP A7UX13
G	494	LYS	-	expression tag	UNP A7UX13
C	-6	MSE	-	initiating methionine	UNP A7UX13
C	-5	GLY	-	expression tag	UNP A7UX13
C	-4	ASP	-	expression tag	UNP A7UX13
C	-3	ARG	-	expression tag	UNP A7UX13
C	-2	GLY	-	expression tag	UNP A7UX13
C	-1	PRO	-	expression tag	UNP A7UX13
C	0	GLU	-	expression tag	UNP A7UX13
C	1	PHE	-	expression tag	UNP A7UX13
C	474	LEU	-	expression tag	UNP A7UX13
C	475	GLU	-	expression tag	UNP A7UX13
C	476	VAL	-	expression tag	UNP A7UX13
C	477	ASP	-	expression tag	UNP A7UX13
C	478	LEU	-	expression tag	UNP A7UX13
C	479	GLN	-	expression tag	UNP A7UX13
C	480	GLY	-	expression tag	UNP A7UX13
C	481	ASP	-	expression tag	UNP A7UX13
C	482	HIS	-	expression tag	UNP A7UX13
C	483	GLY	-	expression tag	UNP A7UX13
C	484	LEU	-	expression tag	UNP A7UX13
C	485	SER	-	expression tag	UNP A7UX13
C	486	ALA	-	expression tag	UNP A7UX13
C	487	TRP	-	expression tag	UNP A7UX13
C	488	SER	-	expression tag	UNP A7UX13
C	489	HIS	-	expression tag	UNP A7UX13
C	490	PRO	-	expression tag	UNP A7UX13
C	491	GLN	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	492	PHE	-	expression tag	UNP A7UX13
C	493	GLU	-	expression tag	UNP A7UX13
C	494	LYS	-	expression tag	UNP A7UX13
H	-6	MSE	-	initiating methionine	UNP A7UX13
H	-5	GLY	-	expression tag	UNP A7UX13
H	-4	ASP	-	expression tag	UNP A7UX13
H	-3	ARG	-	expression tag	UNP A7UX13
H	-2	GLY	-	expression tag	UNP A7UX13
H	-1	PRO	-	expression tag	UNP A7UX13
H	0	GLU	-	expression tag	UNP A7UX13
H	1	PHE	-	expression tag	UNP A7UX13
H	474	LEU	-	expression tag	UNP A7UX13
H	475	GLU	-	expression tag	UNP A7UX13
H	476	VAL	-	expression tag	UNP A7UX13
H	477	ASP	-	expression tag	UNP A7UX13
H	478	LEU	-	expression tag	UNP A7UX13
H	479	GLN	-	expression tag	UNP A7UX13
H	480	GLY	-	expression tag	UNP A7UX13
H	481	ASP	-	expression tag	UNP A7UX13
H	482	HIS	-	expression tag	UNP A7UX13
H	483	GLY	-	expression tag	UNP A7UX13
H	484	LEU	-	expression tag	UNP A7UX13
H	485	SER	-	expression tag	UNP A7UX13
H	486	ALA	-	expression tag	UNP A7UX13
H	487	TRP	-	expression tag	UNP A7UX13
H	488	SER	-	expression tag	UNP A7UX13
H	489	HIS	-	expression tag	UNP A7UX13
H	490	PRO	-	expression tag	UNP A7UX13
H	491	GLN	-	expression tag	UNP A7UX13
H	492	PHE	-	expression tag	UNP A7UX13
H	493	GLU	-	expression tag	UNP A7UX13
H	494	LYS	-	expression tag	UNP A7UX13
D	-6	MSE	-	initiating methionine	UNP A7UX13
D	-5	GLY	-	expression tag	UNP A7UX13
D	-4	ASP	-	expression tag	UNP A7UX13
D	-3	ARG	-	expression tag	UNP A7UX13
D	-2	GLY	-	expression tag	UNP A7UX13
D	-1	PRO	-	expression tag	UNP A7UX13
D	0	GLU	-	expression tag	UNP A7UX13
D	1	PHE	-	expression tag	UNP A7UX13
D	474	LEU	-	expression tag	UNP A7UX13
D	475	GLU	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	476	VAL	-	expression tag	UNP A7UX13
D	477	ASP	-	expression tag	UNP A7UX13
D	478	LEU	-	expression tag	UNP A7UX13
D	479	GLN	-	expression tag	UNP A7UX13
D	480	GLY	-	expression tag	UNP A7UX13
D	481	ASP	-	expression tag	UNP A7UX13
D	482	HIS	-	expression tag	UNP A7UX13
D	483	GLY	-	expression tag	UNP A7UX13
D	484	LEU	-	expression tag	UNP A7UX13
D	485	SER	-	expression tag	UNP A7UX13
D	486	ALA	-	expression tag	UNP A7UX13
D	487	TRP	-	expression tag	UNP A7UX13
D	488	SER	-	expression tag	UNP A7UX13
D	489	HIS	-	expression tag	UNP A7UX13
D	490	PRO	-	expression tag	UNP A7UX13
D	491	GLN	-	expression tag	UNP A7UX13
D	492	PHE	-	expression tag	UNP A7UX13
D	493	GLU	-	expression tag	UNP A7UX13
D	494	LYS	-	expression tag	UNP A7UX13
E	-6	MSE	-	initiating methionine	UNP A7UX13
E	-5	GLY	-	expression tag	UNP A7UX13
E	-4	ASP	-	expression tag	UNP A7UX13
E	-3	ARG	-	expression tag	UNP A7UX13
E	-2	GLY	-	expression tag	UNP A7UX13
E	-1	PRO	-	expression tag	UNP A7UX13
E	0	GLU	-	expression tag	UNP A7UX13
E	1	PHE	-	expression tag	UNP A7UX13
E	474	LEU	-	expression tag	UNP A7UX13
E	475	GLU	-	expression tag	UNP A7UX13
E	476	VAL	-	expression tag	UNP A7UX13
E	477	ASP	-	expression tag	UNP A7UX13
E	478	LEU	-	expression tag	UNP A7UX13
E	479	GLN	-	expression tag	UNP A7UX13
E	480	GLY	-	expression tag	UNP A7UX13
E	481	ASP	-	expression tag	UNP A7UX13
E	482	HIS	-	expression tag	UNP A7UX13
E	483	GLY	-	expression tag	UNP A7UX13
E	484	LEU	-	expression tag	UNP A7UX13
E	485	SER	-	expression tag	UNP A7UX13
E	486	ALA	-	expression tag	UNP A7UX13
E	487	TRP	-	expression tag	UNP A7UX13
E	488	SER	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	489	HIS	-	expression tag	UNP A7UX13
E	490	PRO	-	expression tag	UNP A7UX13
E	491	GLN	-	expression tag	UNP A7UX13
E	492	PHE	-	expression tag	UNP A7UX13
E	493	GLU	-	expression tag	UNP A7UX13
E	494	LYS	-	expression tag	UNP A7UX13
F	-6	MSE	-	initiating methionine	UNP A7UX13
F	-5	GLY	-	expression tag	UNP A7UX13
F	-4	ASP	-	expression tag	UNP A7UX13
F	-3	ARG	-	expression tag	UNP A7UX13
F	-2	GLY	-	expression tag	UNP A7UX13
F	-1	PRO	-	expression tag	UNP A7UX13
F	0	GLU	-	expression tag	UNP A7UX13
F	1	PHE	-	expression tag	UNP A7UX13
F	474	LEU	-	expression tag	UNP A7UX13
F	475	GLU	-	expression tag	UNP A7UX13
F	476	VAL	-	expression tag	UNP A7UX13
F	477	ASP	-	expression tag	UNP A7UX13
F	478	LEU	-	expression tag	UNP A7UX13
F	479	GLN	-	expression tag	UNP A7UX13
F	480	GLY	-	expression tag	UNP A7UX13
F	481	ASP	-	expression tag	UNP A7UX13
F	482	HIS	-	expression tag	UNP A7UX13
F	483	GLY	-	expression tag	UNP A7UX13
F	484	LEU	-	expression tag	UNP A7UX13
F	485	SER	-	expression tag	UNP A7UX13
F	486	ALA	-	expression tag	UNP A7UX13
F	487	TRP	-	expression tag	UNP A7UX13
F	488	SER	-	expression tag	UNP A7UX13
F	489	HIS	-	expression tag	UNP A7UX13
F	490	PRO	-	expression tag	UNP A7UX13
F	491	GLN	-	expression tag	UNP A7UX13
F	492	PHE	-	expression tag	UNP A7UX13
F	493	GLU	-	expression tag	UNP A7UX13
F	494	LYS	-	expression tag	UNP A7UX13
B	-6	MSE	-	initiating methionine	UNP A7UX13
B	-5	GLY	-	expression tag	UNP A7UX13
B	-4	ASP	-	expression tag	UNP A7UX13
B	-3	ARG	-	expression tag	UNP A7UX13
B	-2	GLY	-	expression tag	UNP A7UX13
B	-1	PRO	-	expression tag	UNP A7UX13
B	0	GLU	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

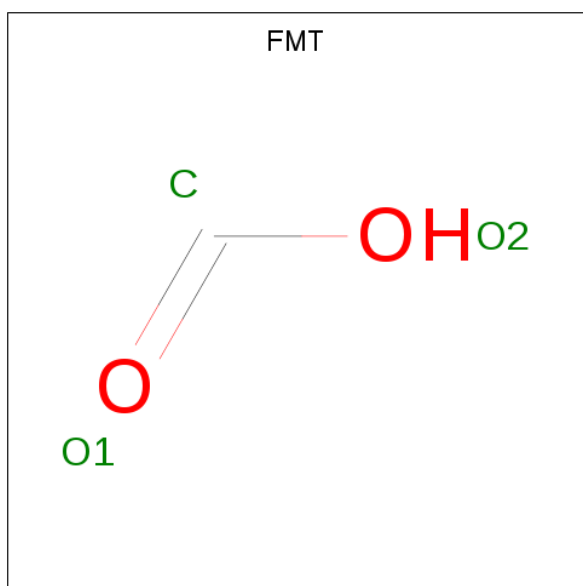
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PHE	-	expression tag	UNP A7UX13
B	474	LEU	-	expression tag	UNP A7UX13
B	475	GLU	-	expression tag	UNP A7UX13
B	476	VAL	-	expression tag	UNP A7UX13
B	477	ASP	-	expression tag	UNP A7UX13
B	478	LEU	-	expression tag	UNP A7UX13
B	479	GLN	-	expression tag	UNP A7UX13
B	480	GLY	-	expression tag	UNP A7UX13
B	481	ASP	-	expression tag	UNP A7UX13
B	482	HIS	-	expression tag	UNP A7UX13
B	483	GLY	-	expression tag	UNP A7UX13
B	484	LEU	-	expression tag	UNP A7UX13
B	485	SER	-	expression tag	UNP A7UX13
B	486	ALA	-	expression tag	UNP A7UX13
B	487	TRP	-	expression tag	UNP A7UX13
B	488	SER	-	expression tag	UNP A7UX13
B	489	HIS	-	expression tag	UNP A7UX13
B	490	PRO	-	expression tag	UNP A7UX13
B	491	GLN	-	expression tag	UNP A7UX13
B	492	PHE	-	expression tag	UNP A7UX13
B	493	GLU	-	expression tag	UNP A7UX13
B	494	LYS	-	expression tag	UNP A7UX13
A	-6	MSE	-	initiating methionine	UNP A7UX13
A	-5	GLY	-	expression tag	UNP A7UX13
A	-4	ASP	-	expression tag	UNP A7UX13
A	-3	ARG	-	expression tag	UNP A7UX13
A	-2	GLY	-	expression tag	UNP A7UX13
A	-1	PRO	-	expression tag	UNP A7UX13
A	0	GLU	-	expression tag	UNP A7UX13
A	1	PHE	-	expression tag	UNP A7UX13
A	474	LEU	-	expression tag	UNP A7UX13
A	475	GLU	-	expression tag	UNP A7UX13
A	476	VAL	-	expression tag	UNP A7UX13
A	477	ASP	-	expression tag	UNP A7UX13
A	478	LEU	-	expression tag	UNP A7UX13
A	479	GLN	-	expression tag	UNP A7UX13
A	480	GLY	-	expression tag	UNP A7UX13
A	481	ASP	-	expression tag	UNP A7UX13
A	482	HIS	-	expression tag	UNP A7UX13
A	483	GLY	-	expression tag	UNP A7UX13
A	484	LEU	-	expression tag	UNP A7UX13
A	485	SER	-	expression tag	UNP A7UX13

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	486	ALA	-	expression tag	UNP A7UX13
A	487	TRP	-	expression tag	UNP A7UX13
A	488	SER	-	expression tag	UNP A7UX13
A	489	HIS	-	expression tag	UNP A7UX13
A	490	PRO	-	expression tag	UNP A7UX13
A	491	GLN	-	expression tag	UNP A7UX13
A	492	PHE	-	expression tag	UNP A7UX13
A	493	GLU	-	expression tag	UNP A7UX13
A	494	LYS	-	expression tag	UNP A7UX13

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 3 1 2	0	0
2	C	1	Total C O 3 1 2	0	0
2	H	1	Total C O 3 1 2	0	0
2	D	1	Total C O 3 1 2	0	0
2	E	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0
2	A	1	Total C O 3 1 2	0	0

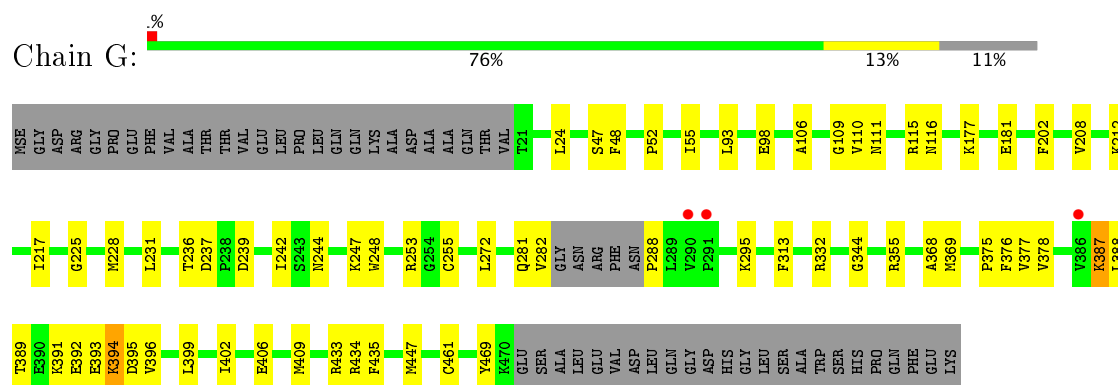
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	128	Total 128	O 128	0	0
3	C	120	Total 120	O 120	0	0
3	H	119	Total 119	O 119	0	0
3	D	143	Total 143	O 143	0	0
3	E	120	Total 120	O 120	0	0
3	F	116	Total 116	O 116	0	0
3	B	128	Total 128	O 128	0	0
3	A	118	Total 118	O 118	0	0

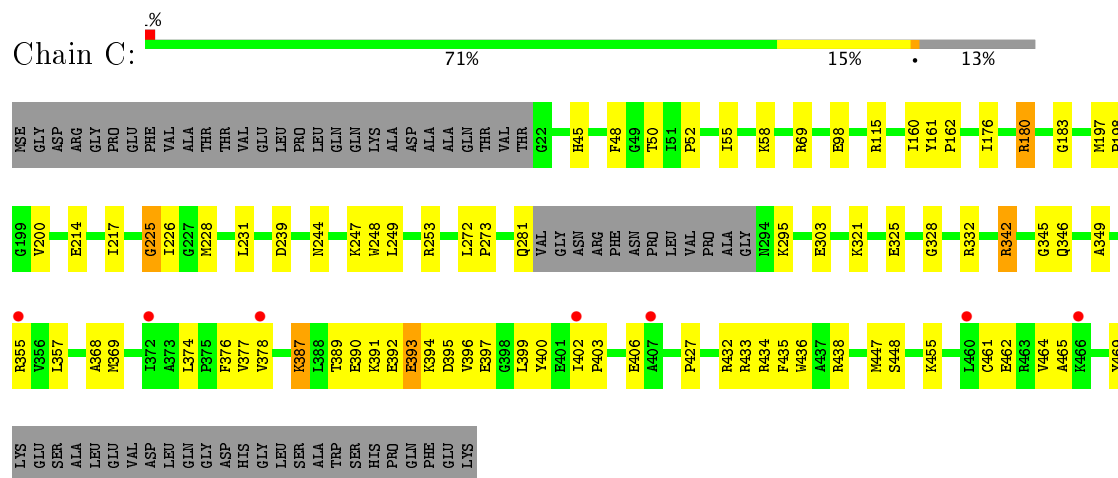
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

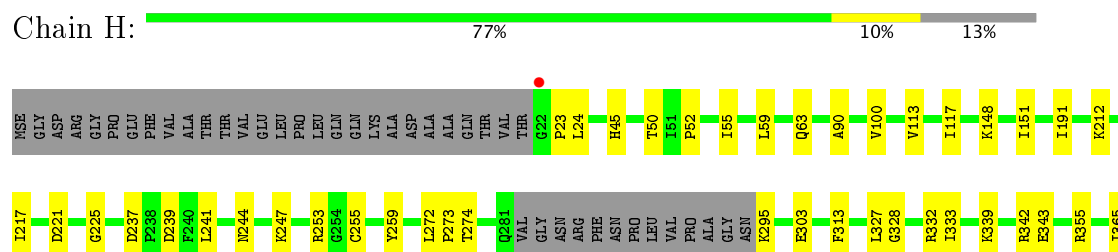
• Molecule 1: C-S Lyase Egt2

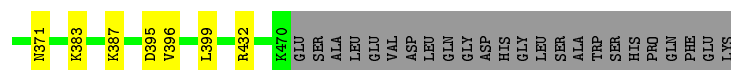


• Molecule 1: C-S Lyase Egt2



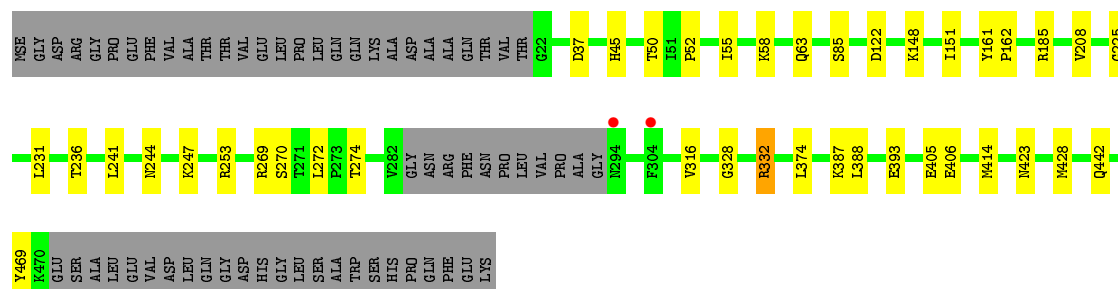
• Molecule 1: C-S Lyase Egt2





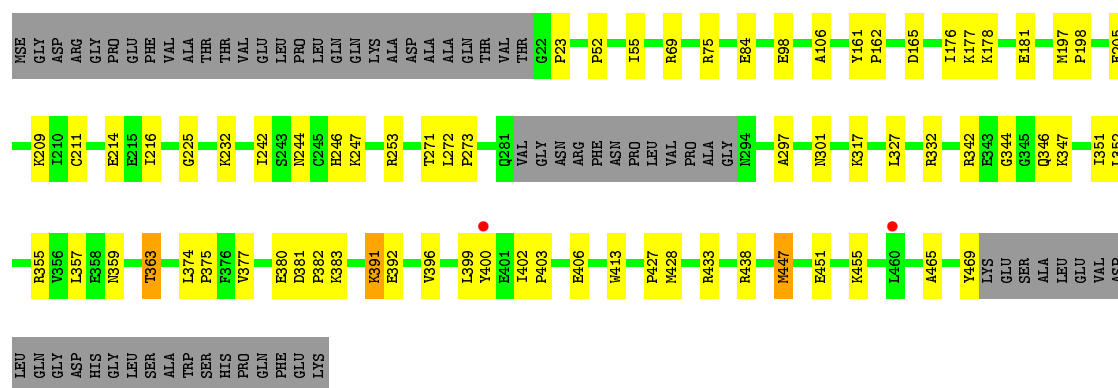
• Molecule 1: C-S Lyase Egt2

Chain D: 79% 8% 13%



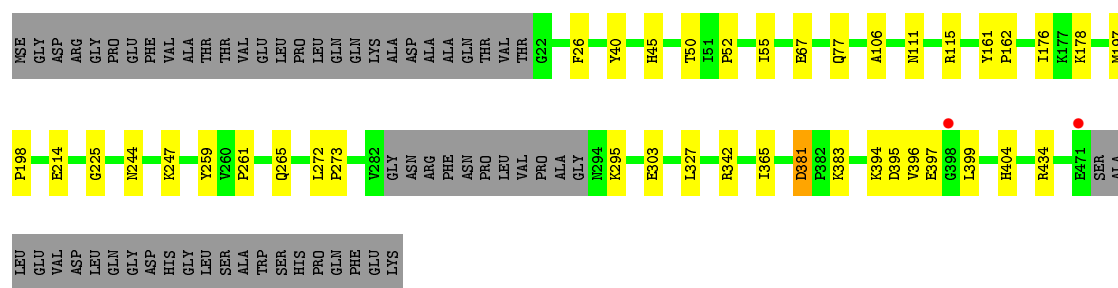
• Molecule 1: C-S Lyase Egt2

Chain E: 73% 14% 13%



• Molecule 1: C-S Lyase Egt2

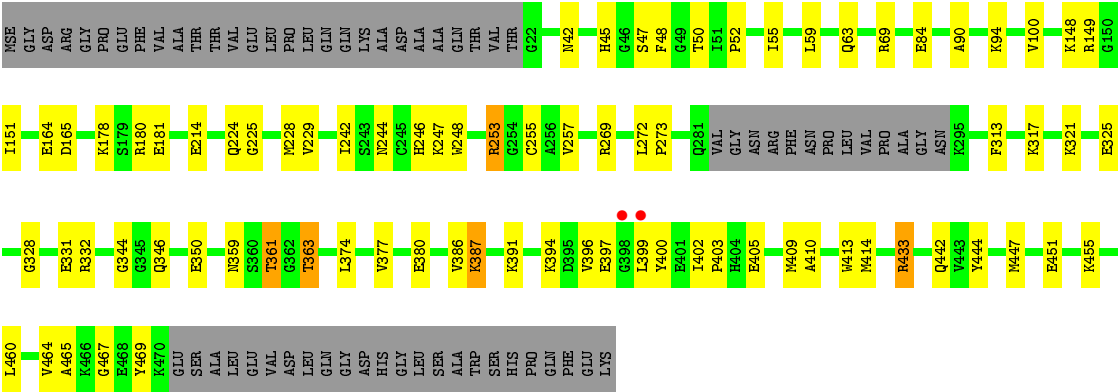
Chain F: 80% 8% 12%



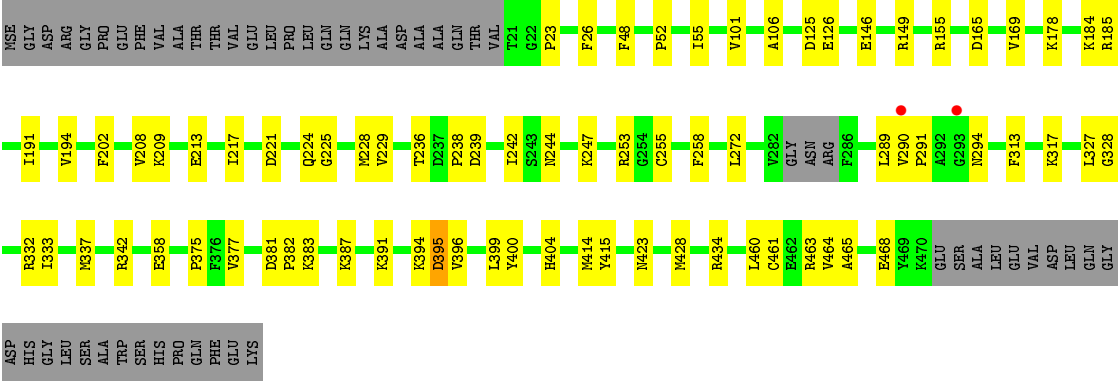
• Molecule 1: C-S Lyase Egt2

Chain B: 71% 15% 13%





● Molecule 1: C-S Lyase Egt2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.84Å 195.34Å 107.79Å 90.00° 91.32° 90.00°	Depositor
Resolution (Å)	49.35 – 2.30 49.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.9 (49.35-2.30) 81.8 (49.35-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.210 , 0.241 0.206 , 0.239	Depositor DCC
R_{free} test set	1855 reflections (1.20%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	1.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 17.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.002 for l,k,-h 0.148 for h,-k,-l 0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28997	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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](#)

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

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	1/3601 (0.0%)	0.43	0/4865
1	B	0.28	0/3519	0.45	1/4750 (0.0%)
1	C	0.37	3/3518 (0.1%)	0.49	2/4750 (0.0%)
1	D	0.27	0/3534	0.42	0/4771
1	E	0.32	0/3518	0.45	0/4750
1	F	0.29	1/3543 (0.0%)	0.43	1/4783 (0.0%)
1	G	0.26	1/3581 (0.0%)	0.43	0/4837
1	H	0.25	0/3519	0.41	0/4750
All	All	0.29	6/28333 (0.0%)	0.44	4/38256 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	393	GLU	CG-CD	-7.55	1.40	1.51
1	F	381	ASP	CB-CG	-7.00	1.37	1.51
1	A	202	PHE	C-N	6.03	1.45	1.34
1	C	180	ARG	CB-CG	-5.96	1.36	1.52
1	C	393	GLU	CB-CG	-5.77	1.41	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	C	393	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	F	381	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	C	180	ARG	CG-CD-NE	-5.36	100.55	111.80

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	3555	0	3540	45	0
1	B	3476	0	3461	67	0
1	C	3475	0	3454	73	0
1	D	3491	0	3476	27	0
1	E	3475	0	3454	54	0
1	F	3500	0	3482	30	0
1	G	3536	0	3526	53	0
1	H	3476	0	3461	29	0
2	A	3	0	1	0	0
2	B	3	0	1	2	0
2	C	3	0	1	0	0
2	D	3	0	1	0	0
2	E	3	0	1	0	0
2	G	3	0	1	1	0
2	H	3	0	1	0	0
3	A	118	0	0	0	0
3	B	128	0	0	2	0
3	C	120	0	0	1	0
3	D	143	0	0	2	0
3	E	120	0	0	2	0
3	F	116	0	0	1	0
3	G	128	0	0	4	0
3	H	119	0	0	2	0
All	All	28997	0	27861	362	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 6.

The worst 5 of 362 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:C:295:LYS:NZ	1:C:303:GLU:OE2	1.84	1.11
1:A:125:ASP:OD1	1:A:185:ARG:NH1	1.91	1.04
1:B:178:LYS:NZ	1:B:181:GLU:OE1	1.89	1.03
1:A:126:GLU:OE2	1:A:155:ARG:NH1	1.89	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ARG:NH1	1:F:67:GLU:OE2	1.92	1.01

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	442/501 (88%)	429 (97%)	12 (3%)	1 (0%)	51	63
1	B	431/501 (86%)	414 (96%)	16 (4%)	1 (0%)	51	63
1	C	431/501 (86%)	416 (96%)	14 (3%)	1 (0%)	51	63
1	D	433/501 (86%)	418 (96%)	14 (3%)	1 (0%)	51	63
1	E	431/501 (86%)	417 (97%)	13 (3%)	1 (0%)	51	63
1	F	434/501 (87%)	419 (96%)	14 (3%)	1 (0%)	51	63
1	G	440/501 (88%)	424 (96%)	15 (3%)	1 (0%)	51	63
1	H	431/501 (86%)	414 (96%)	16 (4%)	1 (0%)	51	63
All	All	3473/4008 (87%)	3351 (96%)	114 (3%)	8 (0%)	51	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	GLY
1	A	225	GLY
1	C	225	GLY
1	F	225	GLY
1	E	225	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	385/417 (92%)	381 (99%)	4 (1%)	80	90
1	B	376/417 (90%)	370 (98%)	6 (2%)	68	82
1	C	376/417 (90%)	370 (98%)	6 (2%)	68	82
1	D	378/417 (91%)	375 (99%)	3 (1%)	85	93
1	E	376/417 (90%)	370 (98%)	6 (2%)	68	82
1	F	379/417 (91%)	379 (100%)	0	100	100
1	G	383/417 (92%)	380 (99%)	3 (1%)	85	93
1	H	376/417 (90%)	375 (100%)	1 (0%)	94	97
All	All	3029/3336 (91%)	3000 (99%)	29 (1%)	80	90

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	178	LYS
1	E	391	LYS
1	A	294	ASN
1	E	342	ARG
1	E	447	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	111	ASN
1	F	265	GLN
1	F	404	HIS
1	A	63	GLN
1	A	416	ASN

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	A	247	1	24,24,25	2.71	6 (25%)	28,32,34	1.37	5 (17%)
1	LLP	B	247	1	24,24,25	2.72	6 (25%)	28,32,34	1.32	3 (10%)
1	LLP	C	247	1	24,24,25	2.71	6 (25%)	28,32,34	1.41	5 (17%)
1	LLP	D	247	1	24,24,25	2.71	6 (25%)	28,32,34	1.36	5 (17%)
1	LLP	E	247	1	24,24,25	2.70	6 (25%)	28,32,34	1.33	3 (10%)
1	LLP	F	247	1	24,24,25	2.74	6 (25%)	28,32,34	1.31	3 (10%)
1	LLP	G	247	1	24,24,25	2.70	6 (25%)	28,32,34	1.37	4 (14%)
1	LLP	H	247	1	24,24,25	2.70	6 (25%)	28,32,34	1.39	4 (14%)

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	A	247	1	-	0/15/17/19	0/1/1/1
1	LLP	B	247	1	-	0/15/17/19	0/1/1/1
1	LLP	C	247	1	-	0/15/17/19	0/1/1/1
1	LLP	D	247	1	-	0/15/17/19	0/1/1/1
1	LLP	E	247	1	-	0/15/17/19	0/1/1/1
1	LLP	F	247	1	-	0/15/17/19	0/1/1/1
1	LLP	G	247	1	-	0/15/17/19	0/1/1/1
1	LLP	H	247	1	-	0/15/17/19	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	247	LLP	C4-C5	-4.47	1.36	1.42
1	D	247	LLP	C4-C5	-4.40	1.36	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	LLP	C4-C5	-4.35	1.36	1.42
1	A	247	LLP	C4-C5	-4.31	1.36	1.42
1	E	247	LLP	C4-C5	-4.30	1.36	1.42

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	LLP	C4-C4'-NZ	-4.21	104.19	124.66
1	C	247	LLP	C4-C4'-NZ	-4.16	104.46	124.66
1	G	247	LLP	C4-C4'-NZ	-4.15	104.52	124.66
1	D	247	LLP	C4-C4'-NZ	-4.10	104.76	124.66
1	H	247	LLP	C4-C4'-NZ	-4.00	105.22	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	247	LLP	1	0
1	B	247	LLP	3	0
1	C	247	LLP	2	0
1	D	247	LLP	2	0
1	E	247	LLP	1	0
1	F	247	LLP	2	0
1	G	247	LLP	2	0
1	H	247	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	FMT	A	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	B	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	D	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	G	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	H	501	-	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMT	A	501	-	-	0/0/0/0	0/0/0/0
2	FMT	B	501	-	-	0/0/0/0	0/0/0/0
2	FMT	C	501	-	-	0/0/0/0	0/0/0/0
2	FMT	D	501	-	-	0/0/0/0	0/0/0/0
2	FMT	E	501	-	-	0/0/0/0	0/0/0/0
2	FMT	G	501	-	-	0/0/0/0	0/0/0/0
2	FMT	H	501	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FMT	2	0
2	G	501	FMT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	436/501 (87%)	-0.19	2 (0%) 90 93	21, 32, 51, 67	0
1	B	425/501 (84%)	-0.23	2 (0%) 90 93	22, 30, 45, 59	0
1	C	425/501 (84%)	-0.07	7 (1%) 72 77	17, 31, 64, 73	0
1	D	427/501 (85%)	-0.25	2 (0%) 90 93	20, 28, 43, 54	0
1	E	425/501 (84%)	-0.15	2 (0%) 90 93	21, 30, 61, 67	0
1	F	428/501 (85%)	-0.30	2 (0%) 90 93	20, 28, 43, 63	0
1	G	434/501 (86%)	-0.19	3 (0%) 87 90	20, 31, 49, 73	0
1	H	425/501 (84%)	-0.28	1 (0%) 94 96	22, 29, 44, 56	0
All	All	3425/4008 (85%)	-0.21	21 (0%) 89 92	17, 30, 50, 73	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	291	PRO	4.6
1	G	290	VAL	3.7
1	E	460	LEU	3.5
1	C	402	ILE	3.5
1	B	398	GLY	3.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	LLP	B	247	24/25	0.98	0.10	-	23,26,27,30	0
1	LLP	D	247	24/25	0.97	0.11	-	19,23,25,28	0
1	LLP	E	247	24/25	0.98	0.13	-	24,28,30,33	0
1	LLP	G	247	24/25	0.98	0.12	-	21,27,30,30	0
1	LLP	H	247	24/25	0.98	0.12	-	20,25,28,29	0
1	LLP	A	247	24/25	0.98	0.10	-	24,27,30,31	0
1	LLP	C	247	24/25	0.98	0.11	-	24,28,31,32	0
1	LLP	F	247	24/25	0.98	0.12	-	15,24,26,26	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FMT	D	501	3/3	0.95	0.15	3.75	27,27,30,37	0
2	FMT	E	501	3/3	0.98	0.17	1.27	33,33,35,35	0
2	FMT	G	501	3/3	0.93	0.12	0.19	30,30,31,34	0
2	FMT	C	501	3/3	0.99	0.12	0.07	33,33,33,35	0
2	FMT	H	501	3/3	0.94	0.12	-0.46	31,31,31,32	0
2	FMT	B	501	3/3	0.96	0.08	-2.26	27,27,30,33	0
2	FMT	A	501	3/3	0.98	0.10	-4.20	29,29,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.