wwPDB X-ray Structure Validation Summary Report (i)

Feb 26, 2018 – 12:52 PM EST

PDB ID	:	5V1X
Title	:	Carbon Sulfoxide lyase, Egt2 Y134F in complex with its substrate
Authors	:	Irani, S.; Zhang, Y.
Deposited on	:	2017-03-02
Resolution	:	2.56 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

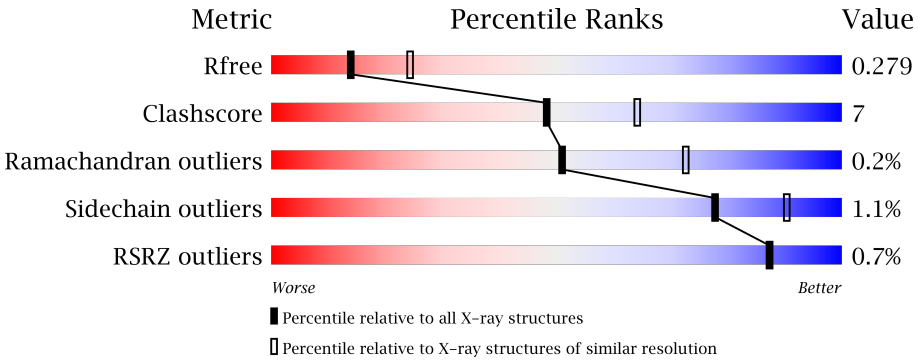
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	501	.% 77% 10% 12%
1	B	501	2% 71% 16% • 13%
1	C	501	.% 69% 18% 13%
1	D	501	73% 16% • 11%
1	E	501	72% 15% • 13%

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Mol	Chain	Length	Quality of chain
1	F	501	76% 10% 13%
1	G	501	72% 16% 12%
1	H	501	76% 11% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	8VV	A	501	-	-	-	X
3	8VV	C	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28336 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 Hercynylcysteine sulfoxide lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	438	Total	C	N	O	P	S	0	0	0
			3490	2234	589	646	1	20			
1	F	436	Total	C	N	O	P	S	0	0	0
			3475	2226	586	642	1	20			
1	D	447	Total	C	N	O	P	S	0	0	0
			3554	2278	599	656	1	20			
1	C	438	Total	C	N	O	P	S	0	0	0
			3490	2235	589	645	1	20			
1	A	439	Total	C	N	O	P	S	0	0	0
			3494	2237	590	646	1	20			
1	B	436	Total	C	N	O	P	S	0	0	0
			3475	2226	586	642	1	20			
1	G	441	Total	C	N	O	P	S	0	0	0
			3510	2245	592	652	1	20			
1	H	438	Total	C	N	O	P	S	0	0	0
			3490	2235	589	645	1	20			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	MET	-	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	134	PHE	TYR	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	MET	-	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	134	PHE	TYR	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	-6	MET	-	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	134	PHE	TYR	engineered mutation	UNP A7UX13
D	474	LEU	-	expression tag	UNP A7UX13
D	475	GLU	-	expression tag	UNP A7UX13
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
C	-6	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	PHE	-	expression tag	UNP A7UX13
C	134	PHE	TYR	engineered mutation	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
C	492	PHE	-	expression tag	UNP A7UX13
C	493	GLU	-	expression tag	UNP A7UX13
C	494	LYS	-	expression tag	UNP A7UX13
A	-6	MET	-	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	134	PHE	TYR	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	LEU	-	expression tag	UNP A7UX13
A	485	SER	-	expression tag	UNP A7UX13
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
B	-6	MET	-	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
B	1	PHE	-	expression tag	UNP A7UX13
B	134	PHE	TYR	engineered mutation	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
G	-6	MET	-	initiating methionine	UNP A7UX13

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Chain	Residue	Modelled	Actual	Comment	Reference
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	134	PHE	TYR	engineered mutation	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
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
H	-6	MET	-	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	134	PHE	TYR	engineered mutation	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

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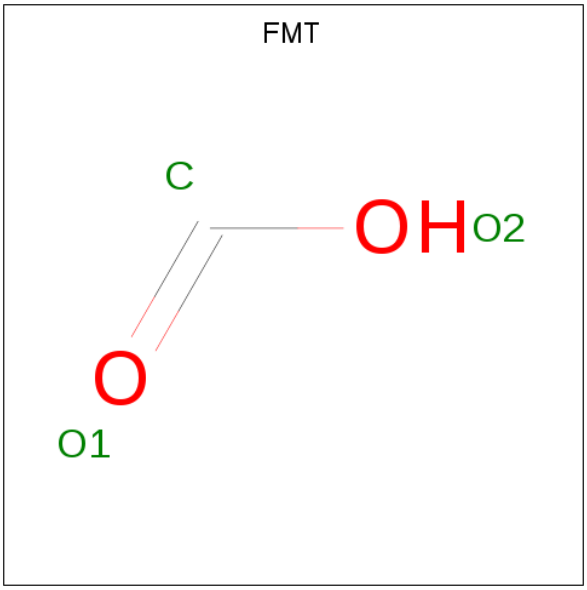
Chain	Residue	Modelled	Actual	Comment	Reference
H	478	LEU	-	expression tag	UNP A7UX13
H	479	GLN	-	expression tag	UNP A7UX13
H	480	GLY	-	expression tag	UNP A7UX13
H	481	ASP	-	expression tag	UNP A7UX13
H	482	HIS	-	expression tag	UNP A7UX13
H	483	GLY	-	expression tag	UNP A7UX13
H	484	LEU	-	expression tag	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

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			3	1	2		
2	D	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

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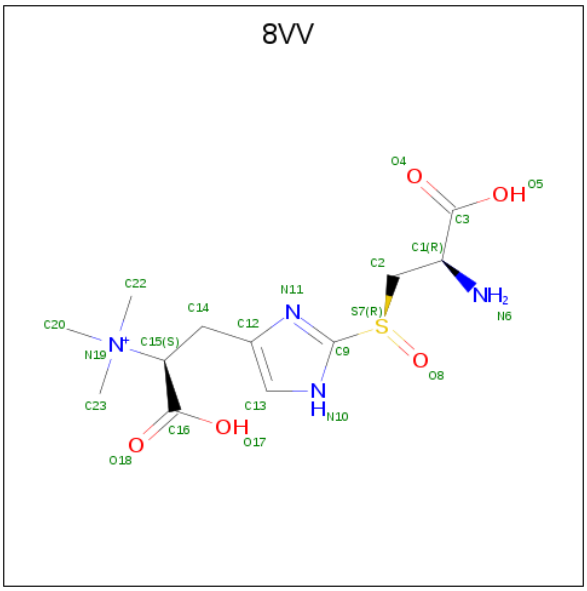
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 3 1 2	0	0
2	H	1	Total C O 3 1 2	0	0

- Molecule 3 is (2 {S})-3-[2-[(2 {R})-2-azanyl-3-oxidanyl-3-oxidanylidene-propyl]sulfinyl-1 {H}-imidazol-4-yl]-2-(trimethyl-$l^{4}-azanyl)propanoic acid (three-letter code: 8VV) (formula: $C_{12}H_{21}N_4O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O S 22 12 4 5 1	0	0
3	A	1	Total C N O S 22 12 4 5 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	49	Total O 49 49	0	0
4	F	42	Total O 42 42	0	0
4	D	33	Total O 33 33	0	0
4	C	33	Total O 33 33	0	0

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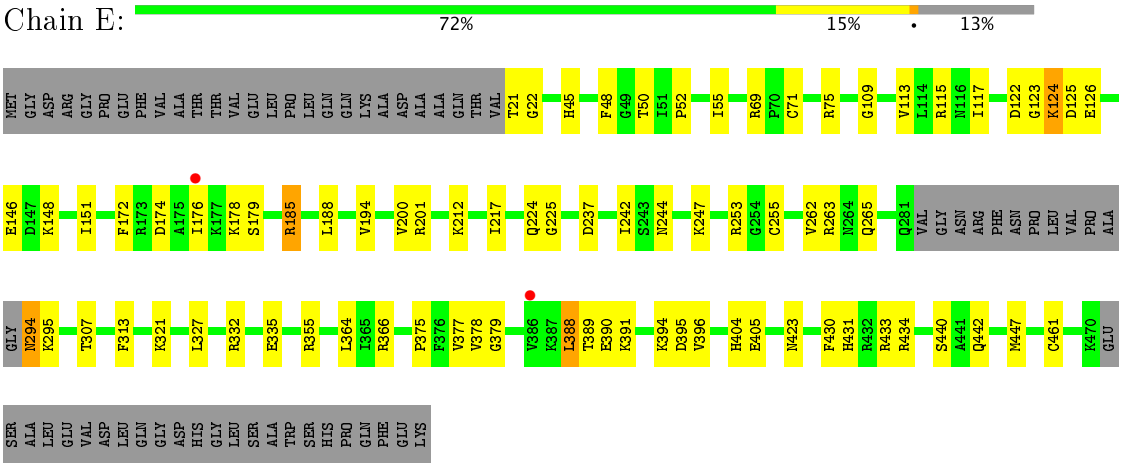
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0
4	B	31	Total O 31 31	0	0
4	G	39	Total O 39 39	0	0
4	H	38	Total O 38 38	0	0

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.

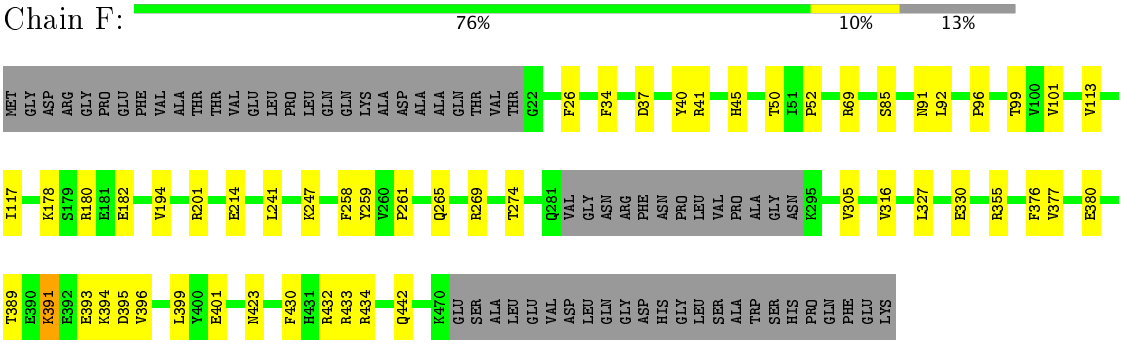
- Molecule 1: Hercynylcysteine sulfoxide lyase

Chain E:



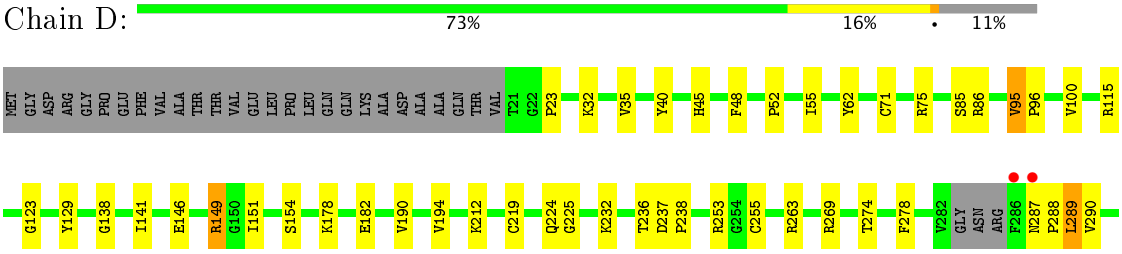
- Molecule 1: Hercynylcysteine sulfoxide lyase

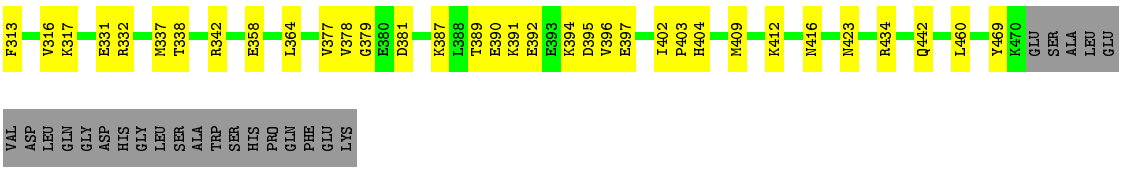
Chain F:



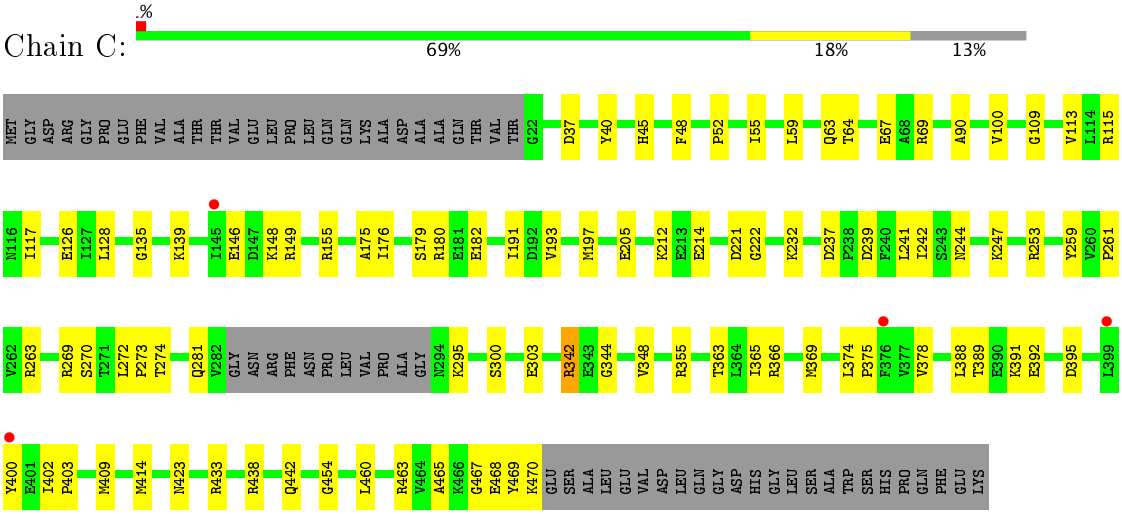
- Molecule 1: Hercynylcysteine sulfoxide lyase

Chain D:

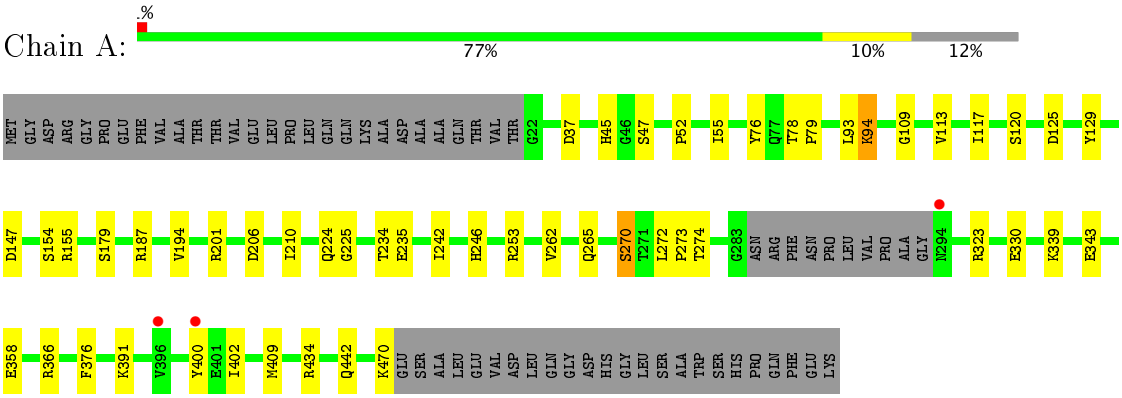




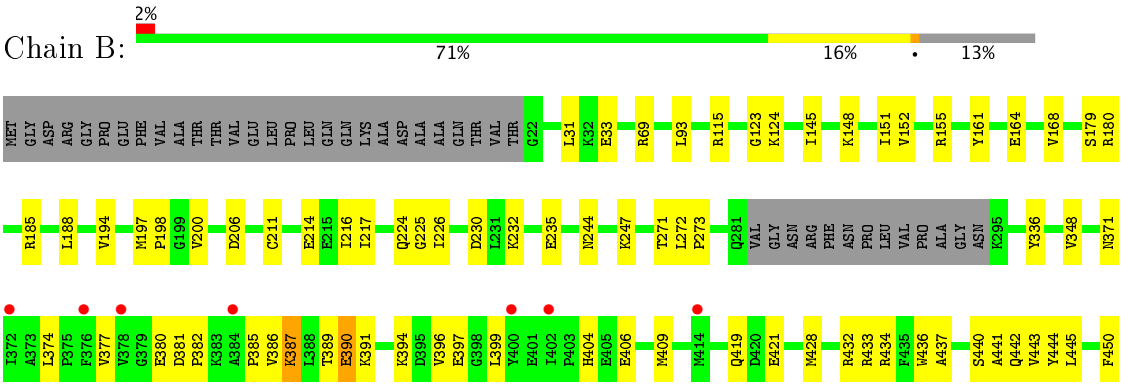
• Molecule 1: Hercynylcysteine sulfoxide lyase

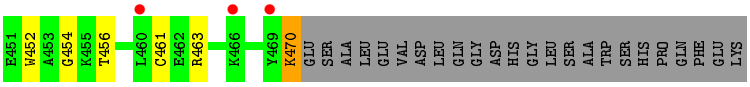


• Molecule 1: Hercynylcysteine sulfoxide lyase



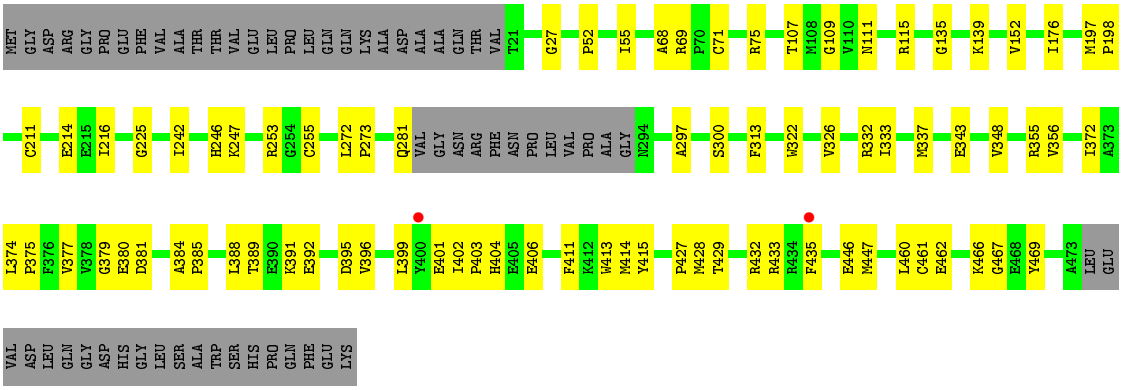
• Molecule 1: Hercynylcysteine sulfoxide lyase





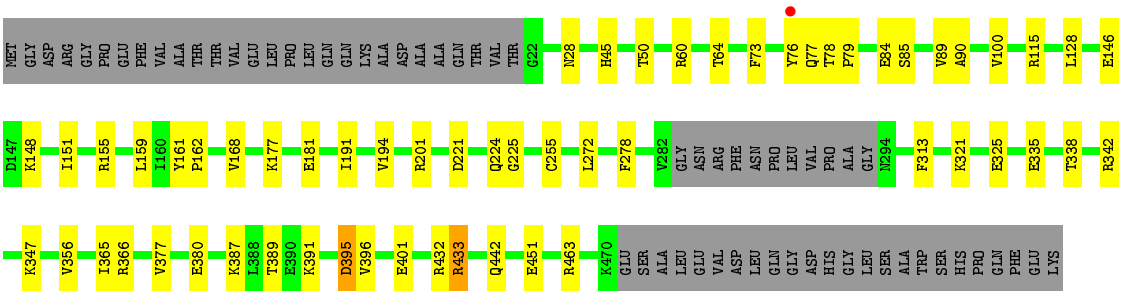
• Molecule 1: Hercynylcysteine sulfoxide lyase

Chain G:



• Molecule 1: Hercynylcysteine sulfoxide lyase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.90Å 195.07Å 107.60Å 90.00° 91.34° 90.00°	Depositor
Resolution (Å)	48.81 – 2.56 48.81 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.81-2.56) 98.1 (48.81-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.223 , 0.279 0.220 , 0.279	Depositor DCC
R_{free} test set	1974 reflections (1.46%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 29.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.119 for h,-k,-l 0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	28336	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FMT, LLP, 8VV

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	0.27	0/3547	0.44	0/4804
1	B	0.29	0/3528	0.45	0/4778
1	C	0.30	1/3543 (0.0%)	0.46	0/4799
1	D	0.30	1/3610 (0.0%)	0.46	1/4893 (0.0%)
1	E	0.30	0/3543	0.45	1/4799 (0.0%)
1	F	0.26	0/3528	0.42	0/4778
1	G	0.27	0/3563	0.44	0/4826
1	H	0.26	0/3543	0.43	1/4799 (0.0%)
All	All	0.28	2/28405 (0.0%)	0.44	3/38476 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	ARG	CB-CG	-5.72	1.37	1.52
1	D	288	PRO	CG-CD	5.63	1.69	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	185	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	D	288	PRO	N-CD-CG	-7.61	91.78	103.20
1	H	433	ARG	NE-CZ-NH1	-6.58	117.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3494	0	3479	36	0
1	B	3475	0	3458	59	0
1	C	3490	0	3476	67	0
1	D	3554	0	3540	61	0
1	E	3490	0	3473	67	0
1	F	3475	0	3460	34	0
1	G	3510	0	3489	52	0
1	H	3490	0	3476	37	0
2	B	3	0	1	0	0
2	D	3	0	1	0	0
2	F	3	0	1	0	0
2	G	3	0	1	0	0
2	H	3	0	1	0	0
3	A	22	0	0	1	0
3	C	22	0	0	1	0
4	A	34	0	0	0	0
4	B	31	0	0	3	0
4	C	33	0	0	1	0
4	D	33	0	0	2	0
4	E	49	0	0	2	0
4	F	42	0	0	2	0
4	G	39	0	0	0	0
4	H	38	0	0	1	0
All	All	28336	0	27856	388	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 388 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:E:124:LYS:HE2	1:E:185:ARG:NH1	1.31	1.44
1:E:124:LYS:CE	1:E:185:ARG:HH11	1.28	1.44
1:E:124:LYS:HD3	1:E:185:ARG:HB3	1.40	1.03
1:F:52:PRO:O	4:F:601:HOH:O	1.77	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:LYS:NZ	1:E:125:ASP:OD2	1.93	0.99

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	434/501 (87%)	414 (95%)	19 (4%)	1 (0%)	51	72
1	B	431/501 (86%)	404 (94%)	26 (6%)	1 (0%)	51	72
1	C	433/501 (86%)	413 (95%)	20 (5%)	0	100	100
1	D	442/501 (88%)	423 (96%)	18 (4%)	1 (0%)	51	72
1	E	433/501 (86%)	416 (96%)	16 (4%)	1 (0%)	51	72
1	F	431/501 (86%)	410 (95%)	21 (5%)	0	100	100
1	G	436/501 (87%)	417 (96%)	18 (4%)	1 (0%)	51	72
1	H	433/501 (86%)	414 (96%)	18 (4%)	1 (0%)	51	72
All	All	3473/4008 (87%)	3311 (95%)	156 (4%)	6 (0%)	51	72

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	225	GLY
1	E	225	GLY
1	G	225	GLY
1	A	225	GLY
1	B	225	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	378/428 (88%)	375 (99%)	3 (1%)	85 93
1	B	376/428 (88%)	371 (99%)	5 (1%)	73 88
1	C	378/428 (88%)	372 (98%)	6 (2%)	68 85
1	D	385/428 (90%)	380 (99%)	5 (1%)	73 88
1	E	378/428 (88%)	373 (99%)	5 (1%)	73 88
1	F	376/428 (88%)	371 (99%)	5 (1%)	73 88
1	G	380/428 (89%)	378 (100%)	2 (0%)	91 96
1	H	378/428 (88%)	377 (100%)	1 (0%)	94 98
All	All	3029/3424 (88%)	2997 (99%)	32 (1%)	78 90

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	460	LEU
1	C	270	SER
1	G	152	VAL
1	C	149	ARG
1	C	281	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	56	GLN
1	D	28	ASN
1	D	419	GLN
1	C	63	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.70	7 (29%)	28,32,34	1.29	3 (10%)
1	LLP	B	247	1	24,24,25	2.70	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	C	247	1	24,24,25	2.71	7 (29%)	28,32,34	1.22	4 (14%)
1	LLP	D	247	1	24,24,25	2.68	7 (29%)	28,32,34	1.27	4 (14%)
1	LLP	E	247	1	24,24,25	2.68	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	F	247	1	24,24,25	2.72	6 (25%)	28,32,34	1.22	4 (14%)
1	LLP	G	247	1	24,24,25	2.69	7 (29%)	28,32,34	1.32	3 (10%)
1	LLP	H	247	1	24,24,25	2.69	7 (29%)	28,32,34	1.23	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 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	247	LLP	C4-C5	-3.97	1.36	1.42
1	H	247	LLP	C4-C5	-3.86	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	LLP	C4-C5	-3.84	1.37	1.42
1	D	247	LLP	C4-C5	-3.77	1.37	1.42
1	C	247	LLP	C4-C5	-3.67	1.37	1.42

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	LLP	C4-C4'-NZ	-3.81	106.15	124.66
1	B	247	LLP	C4-C4'-NZ	-3.56	107.38	124.66
1	E	247	LLP	C4-C4'-NZ	-3.52	107.55	124.66
1	G	247	LLP	C4-C4'-NZ	-3.48	107.76	124.66
1	H	247	LLP	C4-C4'-NZ	-3.46	107.88	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	247	LLP	1	0
1	C	247	LLP	1	0
1	E	247	LLP	1	0
1	F	247	LLP	1	0
1	G	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	$\#\|Z\|>2$
3	8VV	A	501	-	11,22,22	2.85	2 (18%)	9,32,32	1.25	2 (22%)
2	FMT	B	501	-	0,2,2	0.00	-	0,1,1	0.00	-
3	8VV	C	501	-	11,22,22	2.44	2 (18%)	9,32,32	1.69	1 (11%)
2	FMT	D	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	F	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
3	8VV	A	501	-	-	0/14/26/26	0/1/1/1
2	FMT	B	501	-	-	0/0/0/0	0/0/0/0
3	8VV	C	501	-	-	0/14/26/26	0/1/1/1
2	FMT	D	501	-	-	0/0/0/0	0/0/0/0
2	FMT	F	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	8VV	C2-S7	-8.50	1.71	1.81
3	C	501	8VV	C2-S7	-7.26	1.72	1.81
3	A	501	8VV	C15-N19	-3.03	1.48	1.54
3	C	501	8VV	C15-N19	-2.50	1.49	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	8VV	C14-C15-N19	-2.46	110.19	112.54
3	A	501	8VV	O8-S7-C2	2.69	108.83	105.55
3	C	501	8VV	O8-S7-C2	4.75	111.34	105.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	8VV	1	0
3	C	501	8VV	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, 95^{th} 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	438/501 (87%)	-0.05	3 (0%) 87 87	35, 47, 63, 88	0
1	B	435/501 (86%)	0.17	10 (2%) 61 58	31, 50, 91, 102	0
1	C	437/501 (87%)	-0.03	4 (0%) 84 84	35, 49, 67, 83	0
1	D	446/501 (89%)	0.05	2 (0%) 92 92	35, 52, 73, 87	0
1	E	437/501 (87%)	0.02	2 (0%) 90 91	33, 50, 69, 87	0
1	F	435/501 (86%)	-0.04	0 100 100	36, 48, 64, 85	0
1	G	440/501 (87%)	0.03	2 (0%) 90 91	35, 48, 78, 95	0
1	H	437/501 (87%)	-0.10	1 (0%) 94 95	35, 47, 63, 79	0
All	All	3505/4008 (87%)	0.01	24 (0%) 87 87	31, 49, 72, 102	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	PHE	5.7
1	B	402	ILE	5.4
1	B	469	TYR	4.5
1	C	145	ILE	3.6
1	B	372	ILE	3.5

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LLP	E	247	24/25	0.96	0.15	-	39,45,50,53	0
1	LLP	C	247	24/25	0.97	0.15	-	40,44,49,52	0
1	LLP	H	247	24/25	0.97	0.15	-	35,41,47,51	0
1	LLP	B	247	24/25	0.97	0.16	-	39,45,49,49	0
1	LLP	F	247	24/25	0.97	0.16	-	37,45,49,50	0
1	LLP	D	247	24/25	0.98	0.15	-	40,47,51,55	0
1	LLP	G	247	24/25	0.97	0.16	-	41,47,50,52	0
1	LLP	A	247	24/25	0.97	0.15	-	33,41,48,50	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	8VV	C	501	22/22	0.85	0.34	5.87	52,69,72,74	4
3	8VV	A	501	22/22	0.85	0.27	5.16	43,61,69,73	5
2	FMT	D	501	3/3	0.88	0.18	1.21	49,49,50,51	0
2	FMT	H	501	3/3	0.98	0.15	0.64	42,42,43,51	0
2	FMT	B	501	3/3	0.97	0.11	-1.25	45,45,45,47	0
2	FMT	F	501	3/3	0.94	0.12	-1.60	44,44,45,52	0
2	FMT	G	501	3/3	0.94	0.16	-	44,44,46,49	0

6.5 Other polymers (i)

There are no such residues in this entry.