



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 07:35 PM JST

PDB ID : 6A6E  
Title : Crystal structure of thermostable Cysteine desulfurase (FiSufS) from thermophilic *Fervidobacterium Islandicum* AW-1  
Authors : Dhanasingh, I.; Jin, H.S.; Lee, D.W.; Lee, S.H.  
Deposited on : 2018-06-27  
Resolution : 2.09 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

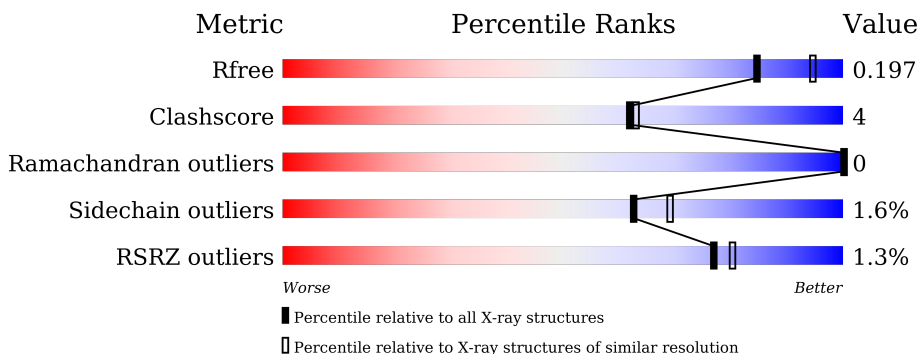
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

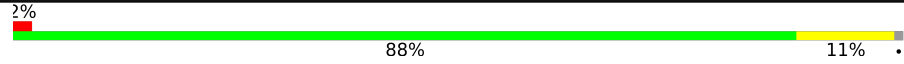
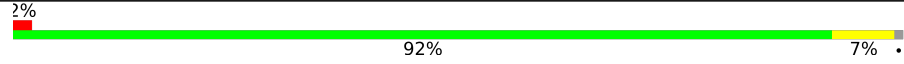
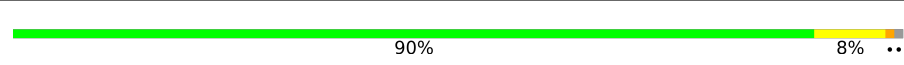
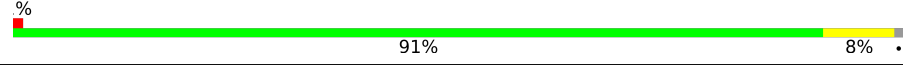
The reported resolution of this entry is 2.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	425	 2% 88% 11% .
1	B	425	 2% 92% 7% .
1	C	425	 90% 8% ..
1	D	425	 91% 8% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	A	503	-	X	-	-
4	CIT	C	505	-	X	-	-
4	CIT	D	506	-	-	-	X
5	PEG	A	508	-	-	-	X
5	PEG	A	511	-	-	-	X
5	PEG	A	512	-	-	-	X
5	PEG	B	504	-	-	-	X
5	PEG	C	507	-	-	-	X
5	PEG	C	508	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14912 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.

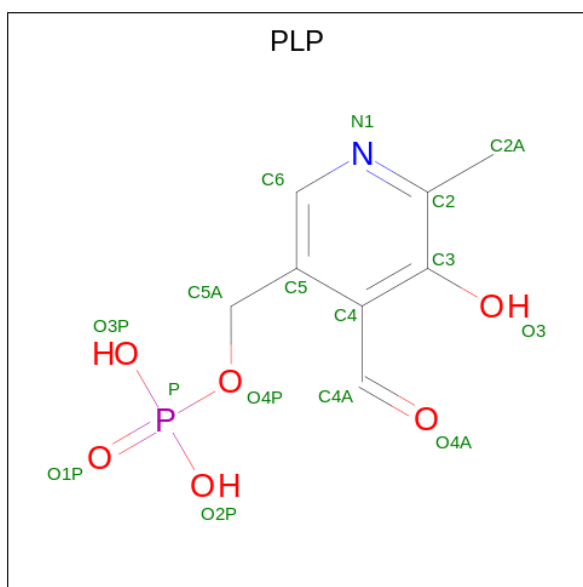
- Molecule 1 is a protein called Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	422	3346	2150	554	631	11	0	1	0
1	B	422	3340	2146	553	630	11	0	0	0
1	C	422	3340	2146	553	630	11	0	0	0
1	D	422	3346	2150	553	632	11	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

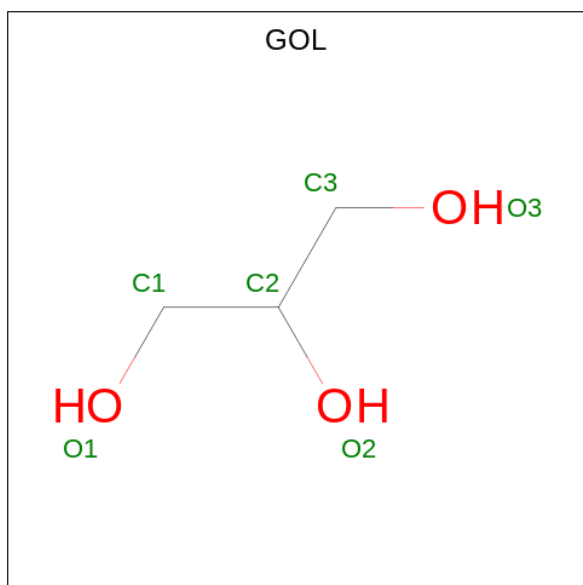
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP A0A1B0VPZ3
A	-2	SER	-	expression tag	UNP A0A1B0VPZ3
A	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
A	0	HIS	-	expression tag	UNP A0A1B0VPZ3
B	-3	SER	-	expression tag	UNP A0A1B0VPZ3
B	-2	SER	-	expression tag	UNP A0A1B0VPZ3
B	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
B	0	HIS	-	expression tag	UNP A0A1B0VPZ3
C	-3	SER	-	expression tag	UNP A0A1B0VPZ3
C	-2	SER	-	expression tag	UNP A0A1B0VPZ3
C	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
C	0	HIS	-	expression tag	UNP A0A1B0VPZ3
D	-3	SER	-	expression tag	UNP A0A1B0VPZ3
D	-2	SER	-	expression tag	UNP A0A1B0VPZ3
D	-1	GLY	-	expression tag	UNP A0A1B0VPZ3
D	0	HIS	-	expression tag	UNP A0A1B0VPZ3

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



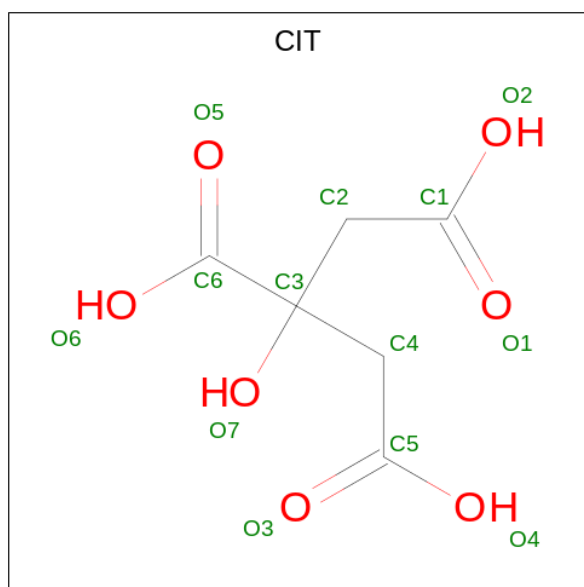
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



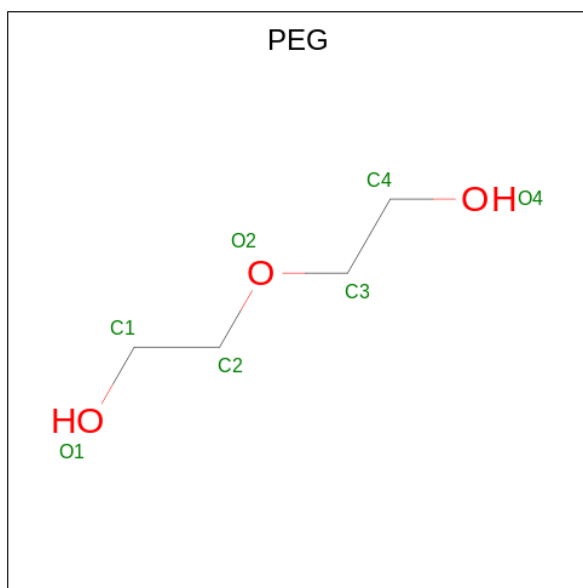
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

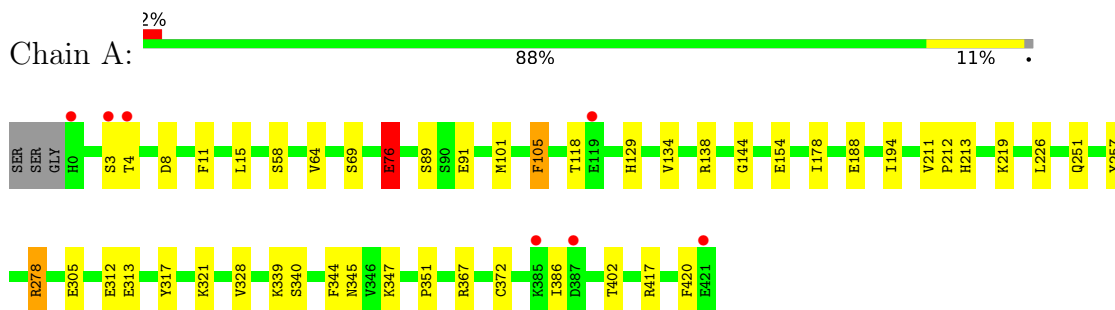
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	311	Total O 311 311	0	0
6	B	331	Total O 331 331	0	0
6	C	307	Total O 307 307	0	0
6	D	277	Total O 277 277	0	0



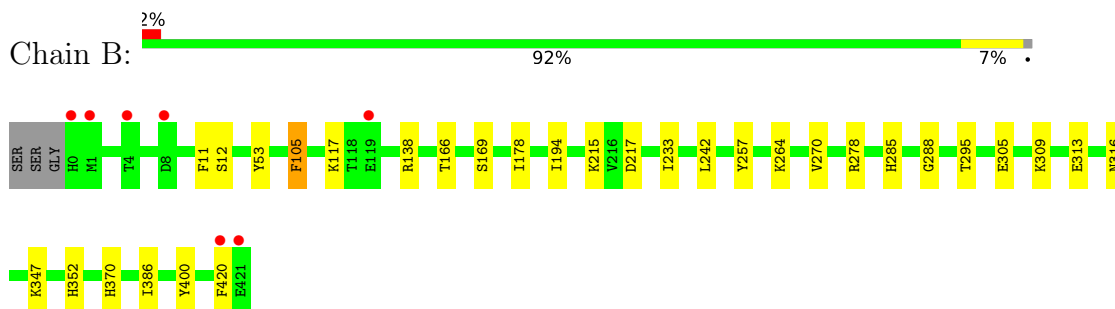
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

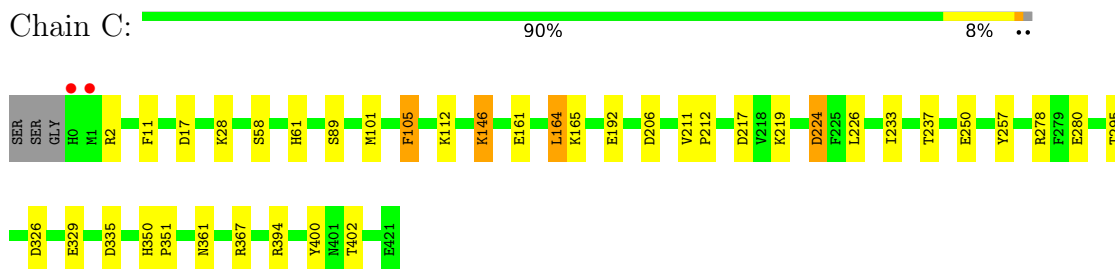
- Molecule 1: Cysteine desulfurase



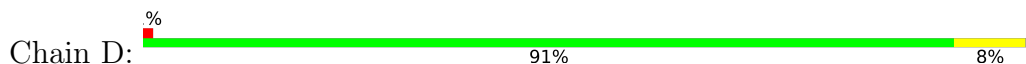
- Molecule 1: Cysteine desulfurase

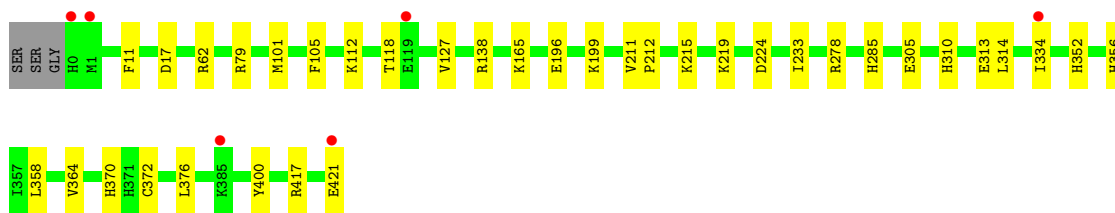


- Molecule 1: Cysteine desulfurase



- Molecule 1: Cysteine desulfurase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.30Å 218.72Å 89.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.75 – 2.09 26.76 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.75-2.09) 98.7 (26.76-2.09)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.90 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.142 , 0.187 0.155 , 0.197	Depositor DCC
$R_{free}$ test set	6103 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, PEG, CSS, GOL, PLP

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	0.90	2/3412 (0.1%)	0.88	2/4617 (0.0%)
1	B	0.95	1/3403 (0.0%)	0.91	2/4605 (0.0%)
1	C	0.94	1/3403 (0.0%)	0.92	8/4605 (0.2%)
1	D	0.92	0/3412	0.88	3/4617 (0.1%)
All	All	0.93	4/13630 (0.0%)	0.90	15/18444 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	GLU	CD-OE1	8.75	1.35	1.25
1	B	313	GLU	CD-OE2	8.52	1.35	1.25
1	C	280	GLU	CD-OE1	5.81	1.32	1.25
1	A	340	SER	CB-OG	-5.63	1.34	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	ASP	CB-CG-OD1	8.14	125.63	118.30
1	B	217	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	278	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	217	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	217	ASP	CB-CG-OD2	-6.53	112.43	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	PHE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3346	0	3353	38	0
1	B	3340	0	3345	23	0
1	C	3340	0	3345	28	0
1	D	3346	0	3351	26	0
2	A	15	0	6	1	0
2	B	15	0	6	0	0
2	C	15	0	6	1	0
2	D	15	0	6	0	0
3	A	24	0	32	0	0
3	B	6	0	8	3	0
3	C	18	0	24	1	0
3	D	12	0	16	0	0
4	A	26	0	10	5	0
4	B	13	0	5	2	0
4	C	39	0	15	2	0
4	D	39	0	15	2	0
5	A	35	0	50	6	0
5	B	21	0	30	0	0
5	C	21	0	30	0	0
6	A	311	0	0	17	0
6	B	331	0	0	14	0
6	C	307	0	0	12	0
6	D	277	0	0	13	0
All	All	14912	0	13653	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 120 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HG3	6:A:1481:HOH:O	1.40	1.21
1:D:101:MET:HG3	6:D:860:HOH:O	1.38	1.19
1:C:101:MET:HG3	6:C:894:HOH:O	1.41	1.18
1:A:129:HIS:HE2	4:A:503:CIT:H42	1.28	0.97
1:A:305:GLU:HB3	5:A:511:PEG:H42	1.48	0.92

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	420/425 (99%)	404 (96%)	16 (4%)	0	100	100
1	B	419/425 (99%)	405 (97%)	14 (3%)	0	100	100
1	C	419/425 (99%)	403 (96%)	16 (4%)	0	100	100
1	D	420/425 (99%)	405 (96%)	15 (4%)	0	100	100
All	All	1678/1700 (99%)	1617 (96%)	61 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/372 (100%)	365 (98%)	6 (2%)	62	69
1	B	370/372 (100%)	363 (98%)	7 (2%)	57	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	370/372 (100%)	364 (98%)	6 (2%)	62	69
1	D	371/372 (100%)	366 (99%)	5 (1%)	69	75
All	All	1482/1488 (100%)	1458 (98%)	24 (2%)	62	69

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	105	PHE
1	C	226	LEU
1	C	164	LEU
1	C	400	TYR
1	B	11	PHE

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

Mol	Chain	Res	Type
1	A	0	HIS
1	B	285	HIS
1	B	352	HIS
1	D	285	HIS
1	D	370	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	CSS	C	372	1	4,6,7	0.82	0	1,6,8	0.01	0
1	CSS	B	372	1	4,6,7	0.88	0	1,6,8	0.78	0
1	CSS	A	372	1	4,6,7	1.20	1 (25%)	1,6,8	0.29	0
1	CSS	D	372	1	4,6,7	1.08	0	1,6,8	0.60	0

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	CSS	C	372	1	-	0/1/5/7	-
1	CSS	B	372	1	-	0/1/5/7	-
1	CSS	A	372	1	-	0/1/5/7	-
1	CSS	D	372	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	CSS	CB-CA	2.02	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	372	CSS	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

34 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
5	PEG	A	509	-	6,6,6	0.69	0	5,5,5	0.52	0
5	PEG	A	504	-	6,6,6	0.75	0	5,5,5	0.87	0
4	CIT	D	504	-	12,12,12	1.18	0	17,17,17	1.66	4 (23%)
4	CIT	A	503	-	12,12,12	1.03	1 (8%)	17,17,17	2.90	9 (52%)
5	PEG	B	504	-	6,6,6	0.61	0	5,5,5	0.61	0
4	CIT	D	506	-	12,12,12	1.34	1 (8%)	17,17,17	2.26	5 (29%)
2	PLP	C	501	1	15,15,16	2.81	2 (13%)	20,22,23	2.15	5 (25%)
4	CIT	C	509	-	12,12,12	1.49	2 (16%)	17,17,17	2.51	10 (58%)
3	GOL	A	510	-	5,5,5	0.48	0	5,5,5	0.60	0
5	PEG	A	512	-	6,6,6	0.61	0	5,5,5	0.95	0
5	PEG	A	511	-	6,6,6	0.61	0	5,5,5	0.31	0
5	PEG	C	510	-	6,6,6	0.73	0	5,5,5	0.49	0
3	GOL	D	502	-	5,5,5	0.39	0	5,5,5	0.46	0
5	PEG	B	503	-	6,6,6	0.35	0	5,5,5	0.47	0
5	PEG	C	507	-	6,6,6	0.71	0	5,5,5	0.63	0
5	PEG	A	508	-	6,6,6	0.57	0	5,5,5	0.52	0
3	GOL	D	503	-	5,5,5	0.44	0	5,5,5	0.65	0
4	CIT	C	506	-	12,12,12	2.03	4 (33%)	17,17,17	2.17	6 (35%)
3	GOL	C	502	-	5,5,5	0.68	0	5,5,5	1.12	0
2	PLP	D	501	1	15,15,16	2.29	4 (26%)	20,22,23	1.76	5 (25%)
3	GOL	C	503	-	5,5,5	0.69	0	5,5,5	0.91	0
4	CIT	A	506	-	12,12,12	1.35	1 (8%)	17,17,17	1.74	7 (41%)
3	GOL	A	502	-	5,5,5	0.55	0	5,5,5	0.80	0
5	PEG	B	505	-	6,6,6	0.44	0	5,5,5	0.28	0
4	CIT	D	505	-	12,12,12	1.14	0	17,17,17	1.77	7 (41%)
2	PLP	B	501	1	15,15,16	3.43	4 (26%)	20,22,23	1.84	5 (25%)
3	GOL	A	505	-	5,5,5	0.22	0	5,5,5	0.50	0
5	PEG	C	508	-	6,6,6	0.46	0	5,5,5	0.30	0
2	PLP	A	501	1	15,15,16	2.59	4 (26%)	20,22,23	2.07	5 (25%)
4	CIT	C	505	-	12,12,12	1.94	3 (25%)	17,17,17	2.50	7 (41%)
3	GOL	C	504	-	5,5,5	0.73	0	5,5,5	0.58	0
4	CIT	B	502	-	12,12,12	1.82	2 (16%)	17,17,17	1.29	2 (11%)
3	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	506	-	5,5,5	0.27	0	5,5,5	0.76	0

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
5	PEG	A	509	-	-	2/4/4/4	-
5	PEG	A	504	-	-	3/4/4/4	-
4	CIT	D	504	-	-	7/16/16/16	-
4	CIT	A	503	-	-	13/16/16/16	-
5	PEG	B	504	-	-	2/4/4/4	-
4	CIT	D	506	-	-	9/16/16/16	-
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
4	CIT	C	509	-	-	5/16/16/16	-
3	GOL	A	510	-	-	0/4/4/4	-
5	PEG	A	512	-	-	2/4/4/4	-
5	PEG	A	511	-	-	3/4/4/4	-
5	PEG	C	510	-	-	3/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-
5	PEG	B	503	-	-	2/4/4/4	-
5	PEG	C	507	-	-	2/4/4/4	-
5	PEG	A	508	-	-	1/4/4/4	-
3	GOL	D	503	-	-	2/4/4/4	-
4	CIT	C	506	-	-	3/16/16/16	-
3	GOL	C	502	-	-	4/4/4/4	-
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
3	GOL	C	503	-	-	2/4/4/4	-
4	CIT	A	506	-	-	2/16/16/16	-
3	GOL	A	502	-	-	1/4/4/4	-
5	PEG	B	505	-	-	2/4/4/4	-
4	CIT	D	505	-	-	8/16/16/16	-
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
3	GOL	A	505	-	-	2/4/4/4	-
5	PEG	C	508	-	-	3/4/4/4	-
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	C	505	-	-	9/16/16/16	-
3	GOL	C	504	-	-	2/4/4/4	-
4	CIT	B	502	-	-	6/16/16/16	-
3	GOL	A	507	-	-	2/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C3-C2	9.82	1.50	1.40
2	B	501	PLP	C5-C4	8.69	1.50	1.40
2	B	501	PLP	C3-C2	8.46	1.49	1.40
2	D	501	PLP	C3-C2	6.56	1.47	1.40
2	A	501	PLP	C5-C4	5.97	1.47	1.40

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PLP	O4P-C5A-C5	5.77	120.35	109.35
4	A	503	CIT	O5-C6-C3	-5.35	114.67	122.25
2	A	501	PLP	O4P-C5A-C5	5.24	119.34	109.35
4	D	506	CIT	O7-C3-C6	5.24	116.22	108.86
4	C	505	CIT	O5-C6-C3	-5.08	115.05	122.25

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	GOL	O1-C1-C2-C3
3	A	507	GOL	C1-C2-C3-O3
3	C	502	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	C	504	GOL	C1-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	PEG	1	0
5	A	504	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	CIT	1	0
4	A	503	CIT	5	0
2	C	501	PLP	1	0
4	C	509	CIT	1	0
5	A	511	PEG	3	0
4	C	506	CIT	1	0
4	D	505	CIT	1	0
2	A	501	PLP	1	0
3	C	504	GOL	1	0
4	B	502	CIT	2	0
3	B	506	GOL	3	0

## 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	421/425 (99%)	-0.17	7 (1%) 70 74	12, 24, 47, 85	0
1	B	421/425 (99%)	-0.34	7 (1%) 70 74	12, 21, 40, 82	0
1	C	421/425 (99%)	-0.28	2 (0%) 91 92	15, 23, 41, 82	0
1	D	421/425 (99%)	-0.16	6 (1%) 75 78	14, 27, 48, 76	0
All	All	1684/1700 (99%)	-0.24	22 (1%) 77 80	12, 23, 44, 85	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	HIS	5.4
1	C	0	HIS	4.8
1	D	0	HIS	4.5
1	A	0	HIS	4.0
1	A	4	THR	3.7

### 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	CSS	A	372	7/8	0.97	0.07	21,22,33,36	0
1	CSS	B	372	7/8	0.97	0.08	15,19,26,29	0
1	CSS	C	372	7/8	0.98	0.06	17,20,27,28	0
1	CSS	D	372	7/8	0.98	0.06	22,26,29,34	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(Å <sup>2</sup> )	Q<0.9
5	PEG	C	508	7/7	0.46	0.53	86,87,96,96	0
5	PEG	B	504	7/7	0.63	0.57	49,76,86,88	0
5	PEG	A	504	7/7	0.69	0.30	55,68,71,77	0
3	GOL	C	504	6/6	0.70	0.33	60,64,67,69	0
5	PEG	C	507	7/7	0.70	0.46	65,70,82,87	0
5	PEG	A	512	7/7	0.70	0.57	47,62,77,77	0
5	PEG	A	508	7/7	0.74	0.41	68,71,75,77	0
5	PEG	A	509	7/7	0.74	0.29	61,67,73,74	0
4	CIT	D	506	13/13	0.76	0.44	44,65,83,92	0
5	PEG	A	511	7/7	0.76	0.47	58,71,82,83	0
4	CIT	C	506	13/13	0.77	0.22	36,54,61,62	0
5	PEG	C	510	7/7	0.77	0.17	48,57,63,64	0
3	GOL	C	503	6/6	0.78	0.24	60,60,63,66	0
5	PEG	B	505	7/7	0.79	0.34	75,77,89,91	0
4	CIT	C	509	13/13	0.81	0.32	34,60,74,75	0
5	PEG	B	503	7/7	0.83	0.20	55,57,62,68	0
4	CIT	C	505	13/13	0.84	0.22	35,50,73,82	0
3	GOL	A	507	6/6	0.85	0.25	65,68,69,77	0
3	GOL	A	505	6/6	0.86	0.26	64,65,69,69	0
3	GOL	D	502	6/6	0.87	0.26	56,68,70,71	0
4	CIT	D	504	13/13	0.88	0.29	38,65,82,89	0
3	GOL	D	503	6/6	0.89	0.23	27,49,52,59	0
4	CIT	A	506	13/13	0.89	0.33	40,53,79,86	0
3	GOL	A	510	6/6	0.89	0.20	49,57,60,61	0
4	CIT	B	502	13/13	0.90	0.16	29,50,54,54	0
4	CIT	D	505	13/13	0.90	0.15	35,59,72,75	0
4	CIT	A	503	13/13	0.91	0.15	27,49,66,69	0
3	GOL	A	502	6/6	0.91	0.19	26,49,56,56	0
3	GOL	B	506	6/6	0.92	0.25	36,52,54,58	0
3	GOL	C	502	6/6	0.93	0.19	29,50,50,55	0
2	PLP	C	501	15/16	0.97	0.10	17,20,23,24	0
2	PLP	A	501	15/16	0.98	0.08	17,19,22,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLP	D	501	15/16	0.98	0.09	19,22,26,30	0
2	PLP	B	501	15/16	0.99	0.09	15,17,21,22	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.