



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:50 pm GMT

PDB ID : 3LVY  
Title : Crystal Structure of Carboxymuconolactone Decarboxylase Family Protein SMU.961 from Streptococcus mutans  
Authors : Kim, Y.; Xu, X.; Cui, H.; Chin, S.; Edwards, A.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-02-22  
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

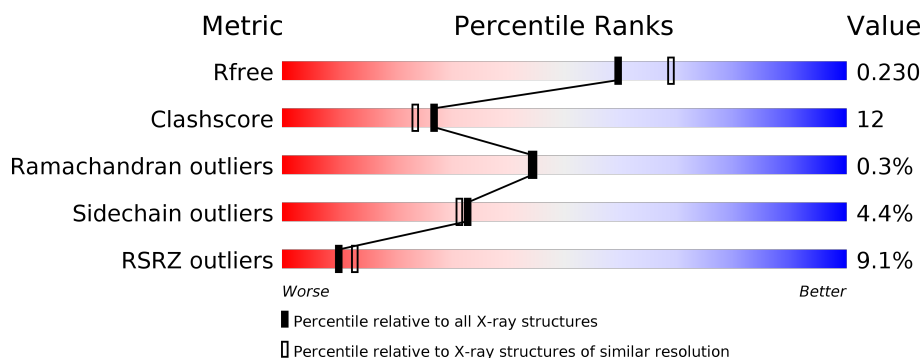
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	207	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	207	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	207	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	207	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>
1	E	207	<div> <div>20%</div> <div> <div></div> <div>58%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	F	207	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>•</div> <div>12%</div> </div> </div>

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	BME	A	191	-	-	X	X
2	BME	B	191	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8818 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 Carboxymuconolactone decarboxylase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	Se	0	3	0
			1427	895	245	280	4	3			
1	B	183	Total	C	N	O	S	Se	0	5	0
			1439	904	245	284	3	3			
1	C	183	Total	C	N	O	S	Se	0	2	0
			1415	890	242	277	3	3			
1	D	179	Total	C	N	O	S	Se	0	1	0
			1381	869	235	272	3	2			
1	E	174	Total	C	N	O	S	Se	5	1	0
			1331	835	229	262	3	2			
1	F	183	Total	C	N	O	S	Se	4	0	0
			1393	876	238	274	3	2			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
A	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
A	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
A	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
A	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8
A	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
A	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
A	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
A	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
A	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
A	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
A	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
A	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
A	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
A	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
A	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8
A	185	SER	-	EXPRESSION TAG	UNP Q8DUG8
B	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
B	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
B	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
B	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
B	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8
B	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
B	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
B	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
B	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
B	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
B	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8
B	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
B	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
B	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
B	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
B	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
B	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8
B	185	SER	-	EXPRESSION TAG	UNP Q8DUG8
C	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
C	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
C	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
C	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
C	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
C	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
C	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
C	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
C	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
C	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8
C	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
C	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
C	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
C	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
C	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
C	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8
C	185	SER	-	EXPRESSION TAG	UNP Q8DUG8
D	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
D	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
D	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
D	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
D	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8
D	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
D	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
D	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
D	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
D	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
D	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8
D	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
D	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
D	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
D	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
D	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
D	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8
D	185	SER	-	EXPRESSION TAG	UNP Q8DUG8
E	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
E	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
E	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
E	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
E	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8

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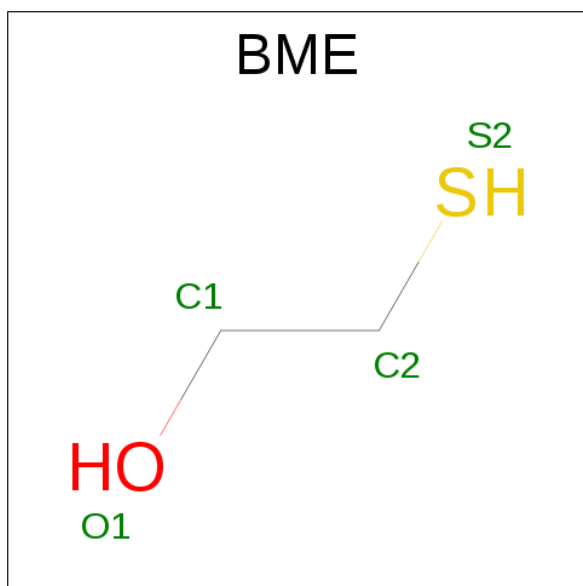
Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8
E	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
E	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
E	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
E	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
E	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
E	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8
E	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
E	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
E	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
E	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
E	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
E	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8
E	185	SER	-	EXPRESSION TAG	UNP Q8DUG8
F	-21	MSE	-	EXPRESSION TAG	UNP Q8DUG8
F	-20	GLY	-	EXPRESSION TAG	UNP Q8DUG8
F	-19	SER	-	EXPRESSION TAG	UNP Q8DUG8
F	-18	SER	-	EXPRESSION TAG	UNP Q8DUG8
F	-17	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-16	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-15	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-14	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-13	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-12	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	-11	SER	-	EXPRESSION TAG	UNP Q8DUG8
F	-10	SER	-	EXPRESSION TAG	UNP Q8DUG8
F	-9	GLY	-	EXPRESSION TAG	UNP Q8DUG8
F	-8	ARG	-	EXPRESSION TAG	UNP Q8DUG8
F	-7	GLU	-	EXPRESSION TAG	UNP Q8DUG8
F	-6	ASN	-	EXPRESSION TAG	UNP Q8DUG8
F	-5	LEU	-	EXPRESSION TAG	UNP Q8DUG8
F	-4	TYR	-	EXPRESSION TAG	UNP Q8DUG8
F	-3	PHE	-	EXPRESSION TAG	UNP Q8DUG8
F	-2	GLN	-	EXPRESSION TAG	UNP Q8DUG8
F	-1	GLY	-	EXPRESSION TAG	UNP Q8DUG8
F	0	HIS	-	EXPRESSION TAG	UNP Q8DUG8
F	184	GLY	-	EXPRESSION TAG	UNP Q8DUG8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	185	SER	-	EXPRESSION TAG	UNP Q8DUG8

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



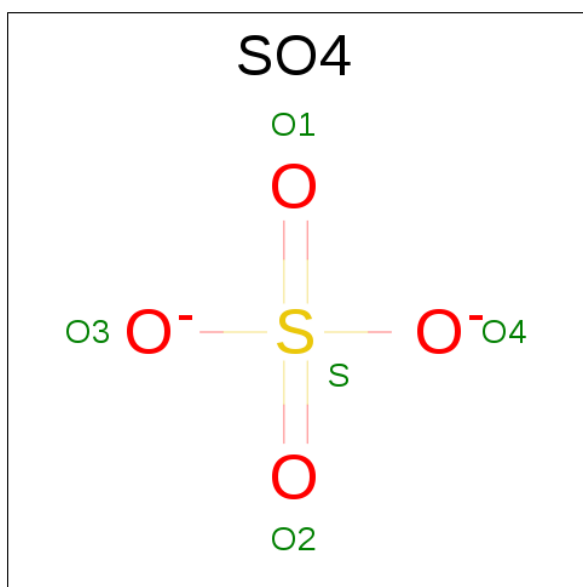
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code:  $SO_4$ ) (formula:  $O_4S$ ).





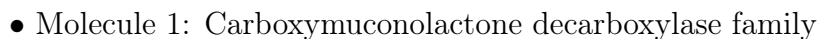
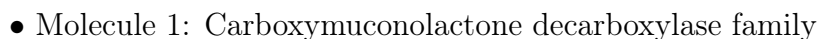
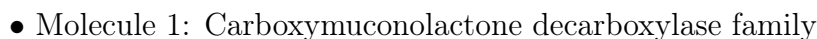
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	151	Total	O	0	0
			151	151		
5	B	162	Total	O	0	0
			162	162		
5	C	59	Total	O	0	0
			59	59		
5	D	34	Total	O	0	0
			34	34		
5	E	5	Total	O	0	0
			5	5		
5	F	6	Total	O	0	0
			6	6		

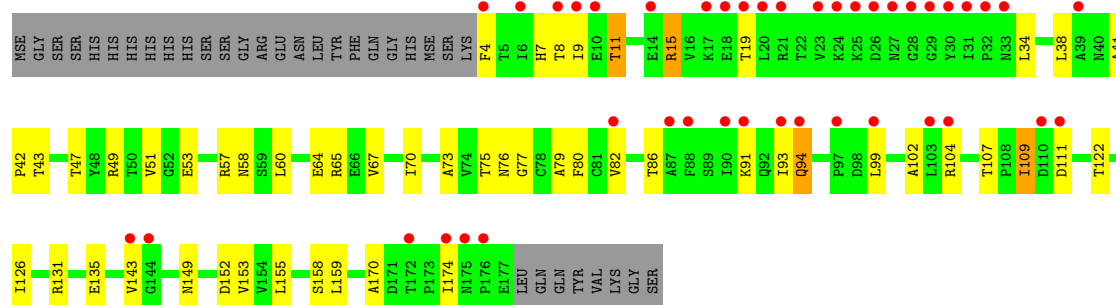


- Molecule 1: Carboxymuconolactone decarboxylase family

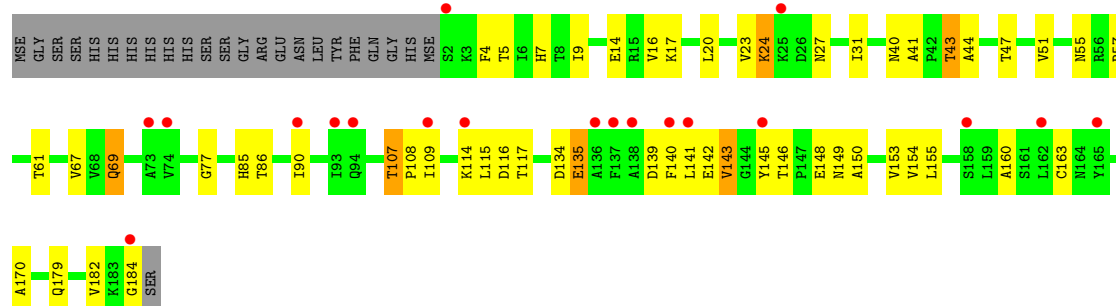




- Molecule 1: Carboxymuconolactone decarboxylase family



- Molecule 1: Carboxymuconolactone decarboxylase family



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.00Å 73.74Å 183.71Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	34.16 – 2.10 34.16 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.16-2.10) 99.1 (34.16-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, $R_{free}$	0.184 , 0.236 0.175 , 0.230	Depositor DCC
$R_{free}$ test set	3779 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: CL, SO4, BME

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	0.71	0/1447	0.74	0/1967
1	B	0.68	0/1459	0.72	0/1985
1	C	0.51	0/1435	0.60	0/1951
1	D	0.49	0/1400	0.58	0/1906
1	E	0.30	0/1350	0.54	0/1839
1	F	0.32	0/1413	0.53	0/1923
All	All	0.53	0/8504	0.62	0/11571

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	LYS	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	1427	0	1433	28	0
1	B	1439	0	1446	27	0
1	C	1415	0	1430	33	0
1	D	1381	0	1386	37	0
1	E	1331	0	1335	45	0
1	F	1393	0	1402	39	0
2	A	4	0	6	5	0
2	B	4	0	6	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	D	5	0	0	0	0
5	A	151	0	0	3	0
5	B	162	0	0	4	0
5	C	59	0	0	1	0
5	D	34	0	0	1	0
5	E	5	0	0	0	0
5	F	6	0	0	0	0
All	All	8818	0	8444	194	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 12.

The worst 5 of 194 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:184:GLY:HA2	1:D:134:ASP:N	1.63	1.14
1:C:95:MSE:HE1	1:C:100:LEU:HD13	1.33	1.10
1:C:89:SER:HB3	1:C:95:MSE:HE2	1.23	1.10
1:A:184:GLY:HA2	1:D:134:ASP:H	0.90	1.06
1:C:9:ILE:HD11	1:C:21:ARG:CZ	1.94	0.97

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	185/207 (89%)	184 (100%)	1 (0%)	0	100	100
1	B	186/207 (90%)	182 (98%)	4 (2%)	0	100	100
1	C	183/207 (88%)	181 (99%)	2 (1%)	0	100	100
1	D	176/207 (85%)	175 (99%)	1 (1%)	0	100	100
1	E	173/207 (84%)	158 (91%)	13 (8%)	2 (1%)	15	9
1	F	181/207 (87%)	165 (91%)	15 (8%)	1 (1%)	28	24
All	All	1084/1242 (87%)	1045 (96%)	36 (3%)	3 (0%)	44	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	135	GLU
1	E	76	ASN
1	E	42	PRO

### 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	156/169 (92%)	153 (98%)	3 (2%)	62	68
1	B	158/169 (94%)	152 (96%)	6 (4%)	38	38
1	C	155/169 (92%)	149 (96%)	6 (4%)	37	37
1	D	152/169 (90%)	149 (98%)	3 (2%)	60	66
1	E	145/169 (86%)	135 (93%)	10 (7%)	18	14
1	F	152/169 (90%)	140 (92%)	12 (8%)	14	10
All	All	918/1014 (90%)	878 (96%)	40 (4%)	33	31

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	11	THR
1	E	94	GLN
1	F	134	ASP
1	E	38	LEU
1	E	109	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	7	HIS
1	D	105	ASN
1	F	149	ASN
1	D	69	GLN
1	D	149	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	BME	A	191	-	3,3,3	0.38	0	2,2,2	0.32	0
2	BME	B	191	-	3,3,3	0.62	0	2,2,2	0.91	0
4	SO4	D	191	-	4,4,4	0.13	0	6,6,6	0.07	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
2	BME	A	191	-	-	0/1/1/1	0/0/0/0
2	BME	B	191	-	-	0/1/1/1	0/0/0/0
4	SO4	D	191	-	-	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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	191	BME	5	0
2	B	191	BME	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	181/207 (87%)	0.13	10 (5%) 26 32	28, 40, 59, 80	0
1	B	180/207 (86%)	-0.02	2 (1%) 80 84	28, 39, 64, 97	0
1	C	180/207 (86%)	0.30	8 (4%) 35 41	39, 62, 93, 112	0
1	D	177/207 (85%)	0.49	16 (9%) 10 13	38, 65, 107, 127	0
1	E	172/207 (83%)	1.21	42 (24%) 1 1	54, 87, 118, 129	167 (97%)
1	F	181/207 (87%)	0.62	19 (10%) 7 9	61, 79, 102, 112	168 (92%)
All	All	1071/1242 (86%)	0.45	97 (9%) 10 13	28, 64, 105, 129	335 (31%)

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	90	ILE	9.1
1	E	30	TYR	6.9
1	E	174	ILE	5.4
1	F	93	ILE	5.3
1	F	137	PHE	5.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no 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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BME	A	191	4/4	0.61	0.33	5.26	64,67,74,126	0
2	BME	B	191	4/4	0.79	0.25	4.35	44,49,52,140	0
3	CL	A	192	1/1	0.99	0.07	-	55,55,55,55	0
4	SO4	D	191	5/5	0.93	0.12	-	107,108,110,111	4
3	CL	B	192	1/1	0.99	0.05	-	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.