



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 3LVY / pdb_00003lvY
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

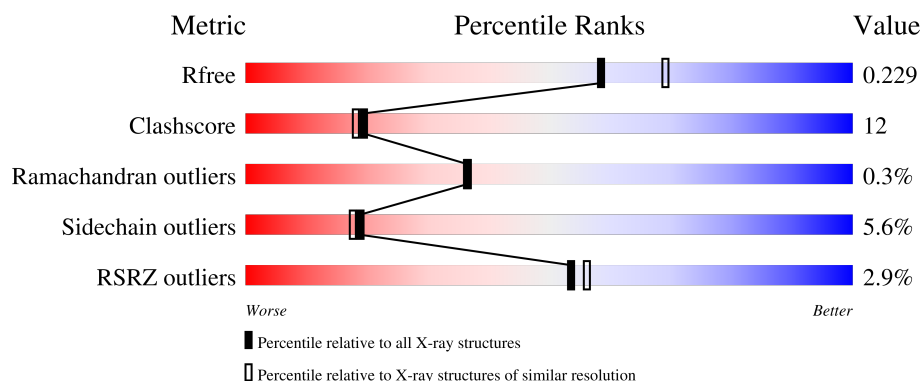
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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	207	76% 12% • 11%
1	B	207	71% 16% • 12%
1	C	207	69% 18% • 12%
1	D	207	70% 15% • 14%
1	E	207	7% 57% 24% • 16%

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Mol	Chain	Length	Quality of chain
1	F	207	

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	-

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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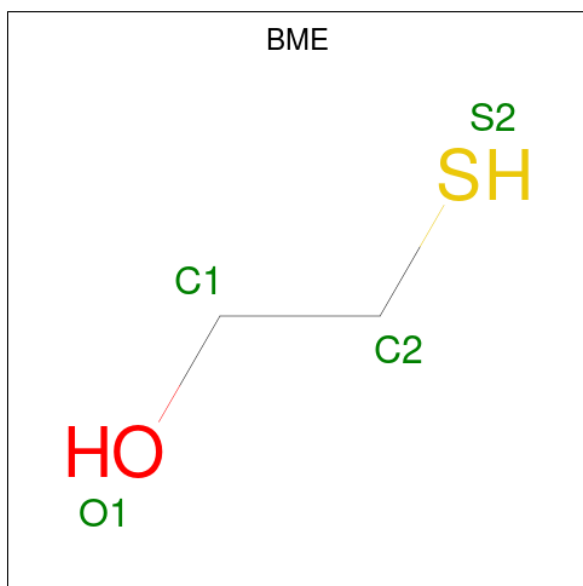
Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	HIS	-	expression tag	UNP Q8DUG8
E	-15	HIS	-	expression tag	UNP Q8DUG8
E	-14	HIS	-	expression tag	UNP Q8DUG8
E	-13	HIS	-	expression tag	UNP Q8DUG8
E	-12	HIS	-	expression tag	UNP Q8DUG8
E	-11	SER	-	expression tag	UNP Q8DUG8
E	-10	SER	-	expression tag	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 (CCD ID: BME) (formula: C_2H_6OS).

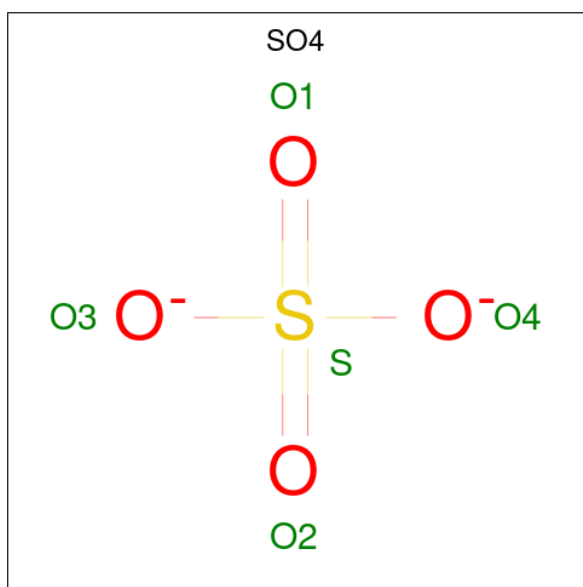


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

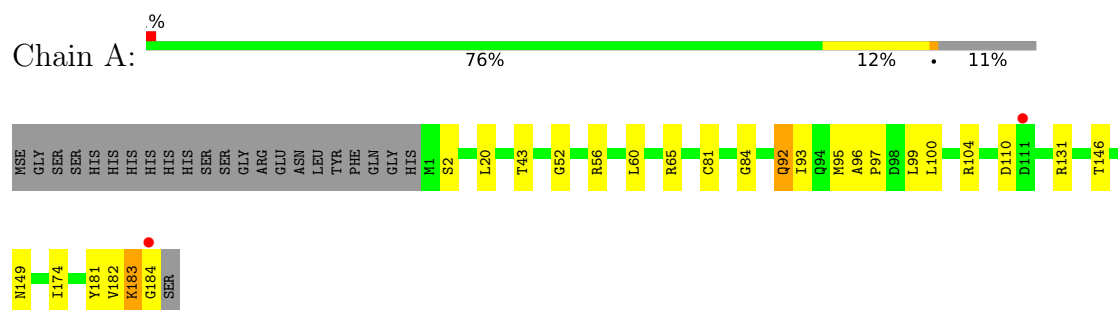
- Molecule 5 is water.

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		

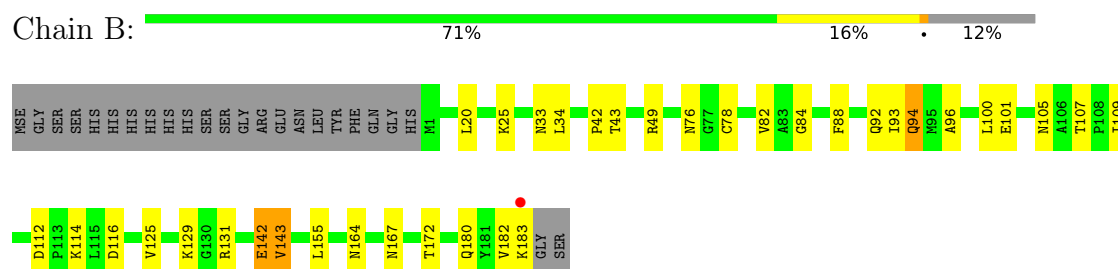
3 Residue-property plots [i](#)

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.

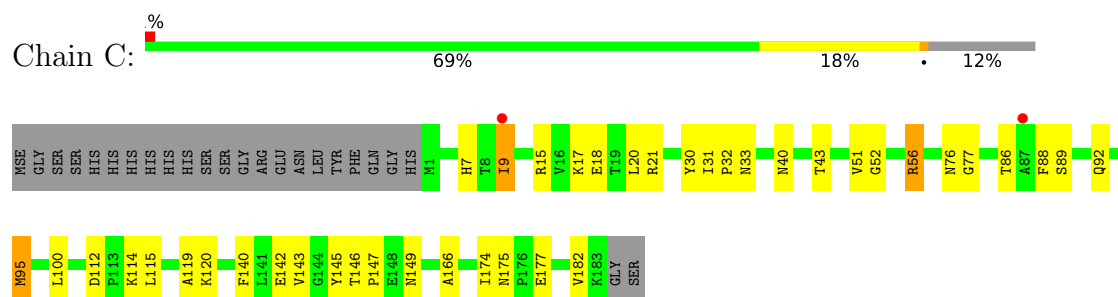
- Molecule 1: Carboxymuconolactone decarboxylase family



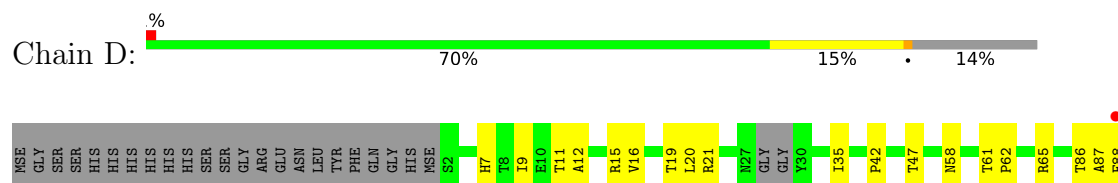
- Molecule 1: Carboxymuconolactone decarboxylase family



- Molecule 1: Carboxymuconolactone decarboxylase family

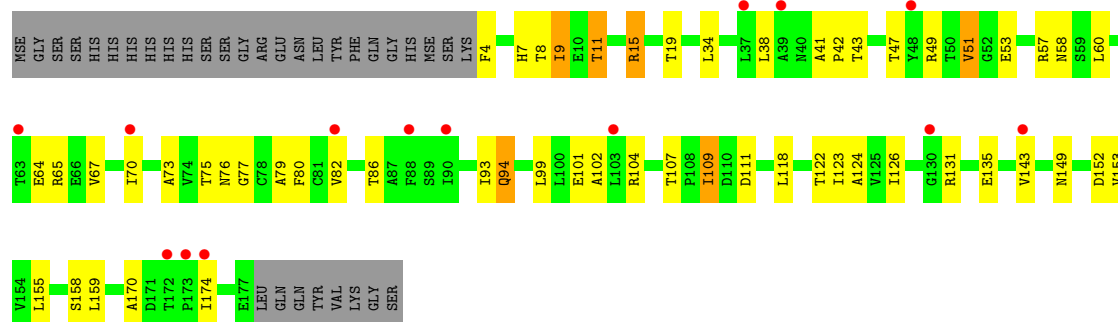


- Molecule 1: Carboxymuconolactone decarboxylase family

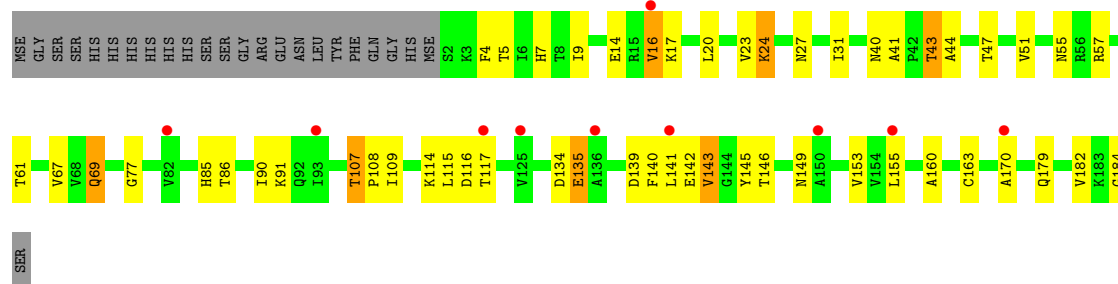




- Molecule 1: Carboxymuconolactone decarboxylase family



- 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, α , β , γ	98.00Å 73.74Å 183.71Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	34.16 – 2.10 34.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.16-2.10) 99.2 (34.16-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.184 , 0.236 0.178 , 0.229	Depositor DCC
R_{free} test set	3809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME, CL, SO4

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	0.89	0/1447	1.00	0/1967
1	B	0.88	1/1459 (0.1%)	0.98	5/1985 (0.3%)
1	C	0.65	1/1435 (0.1%)	0.88	0/1951
1	D	0.62	0/1400	0.87	0/1906
1	E	0.42	0/1350	0.88	0/1839
1	F	0.40	0/1413	0.85	0/1923
All	All	0.68	2/8504 (0.0%)	0.91	5/11571 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	125	VAL	CA-CB	6.09	1.61	1.54
1	C	166	ALA	CA-CB	5.90	1.62	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ASP	CA-C-N	5.78	125.90	119.32
1	B	112	ASP	C-N-CA	5.78	125.90	119.32
1	B	96	ALA	CA-C-N	5.28	124.91	119.05
1	B	96	ALA	C-N-CA	5.28	124.91	119.05
1	B	49	ARG	CA-CB-CG	-5.21	103.67	114.10

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 ⓘ

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	34	0
1	D	1381	0	1386	38	0
1	E	1331	0	1335	46	0
1	F	1393	0	1402	37	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	2	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	195	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.

All (195) 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:89:SER:HB3	1:C:95:MSE:HE2	1.23	1.10
1:C:95:MSE:HE1	1:C:100:LEU:HD13	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:76:ASN:HD22	1:B:164:ASN:HD22	1.08	0.94
1:C:95:MSE:CE	1:C:100:LEU:HD13	2.00	0.92
1:D:114:LYS:HG3	1:D:143:VAL:HG13	1.50	0.92
1:A:84:GLY:HA3	2:A:191:BME:H12	1.51	0.90
1:E:7:HIS:HD2	1:E:11:THR:HB	1.40	0.86
1:E:7:HIS:CD2	1:E:11:THR:HB	2.11	0.85
1:F:179:GLN:O	1:F:182:VAL:HG12	1.77	0.85
1:A:184:GLY:CA	1:D:134:ASP:H	1.85	0.83
1:B:180[B]:GLN:HE21	1:B:180[B]:GLN:H	1.20	0.82
1:E:4:PHE:HD1	1:E:170:ALA:HB2	1.45	0.81
1:D:7:HIS:HD2	1:D:11:THR:OG1	1.63	0.81
1:C:95:MSE:HE1	1:C:100:LEU:CD1	2.09	0.80
1:E:53:GLU:OE2	1:E:57[B]:ARG:HD2	1.83	0.79
1:A:100:LEU:O	1:A:104:ARG:HG3	1.84	0.78
1:F:146:THR:H	1:F:149:ASN:HD22	1.32	0.77
1:C:89:SER:CB	1:C:95:MSE:HE2	2.11	0.77
1:A:104:ARG:NH2	1:A:181:TYR:O	2.18	0.77
1:E:122:THR:O	1:E:126:ILE:HG13	1.86	0.76
1:B:105:ASN:HB2	1:B:107:THR:HG23	1.69	0.75
1:E:93:ILE:O	1:E:94:GLN:HG2	1.87	0.74
1:D:95:MSE:SE	1:D:100:LEU:HD23	2.38	0.74
1:C:52:GLY:O	1:C:56:ARG:HD3	1.88	0.73
1:F:140:PHE:HD2	1:F:141:LEU:HD12	1.53	0.73
1:E:4:PHE:CD1	1:E:170:ALA:HB2	2.24	0.72
1:E:149:ASN:O	1:E:153:VAL:HG23	1.90	0.71
1:C:9:ILE:HD11	1:C:21:ARG:NH2	2.05	0.70
1:B:76:ASN:HD22	1:B:164:ASN:ND2	1.88	0.69
1:D:88:PHE:CZ	1:D:92[A]:GLN:HG2	2.27	0.69
1:F:146:THR:H	1:F:149:ASN:ND2	1.90	0.69
1:E:152:ASP:O	1:E:155:LEU:HB3	1.93	0.69
1:F:69:GLN:HG3	1:F:85:HIS:CE1	2.29	0.68
1:F:149:ASN:O	1:F:153:VAL:HG23	1.93	0.68
2:A:191:BME:H11	5:A:289:HOH:O	1.94	0.67
1:B:180[B]:GLN:H	1:B:180[B]:GLN:NE2	1.92	0.67
1:F:9:ILE:O	1:F:17:LYS:HE2	1.95	0.67
1:C:95:MSE:HE3	1:C:100:LEU:HB2	1.77	0.67
1:B:84:GLY:HA3	2:B:191:BME:H22	1.76	0.67
1:E:86:THR:HG21	1:E:104:ARG:NH1	2.10	0.66
1:D:146:THR:H	1:D:149:ASN:HD22	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HG2	1:A:184:GLY:H	1.62	0.64
1:B:25:LYS:HD3	5:B:318:HOH:O	1.98	0.64
1:E:34:LEU:HB2	1:E:80:PHE:CE2	2.33	0.64
1:E:79:ALA:O	1:E:82:VAL:HG12	1.97	0.64
1:C:9:ILE:HG22	5:C:383:HOH:O	1.98	0.63
1:E:8:THR:HG22	1:E:9:ILE:H	1.62	0.62
1:D:88:PHE:CE2	1:D:92[A]:GLN:HG2	2.36	0.61
1:E:75:THR:C	1:E:77:GLY:H	2.08	0.61
1:B:114:LYS:HG3	1:B:143:VAL:HG13	1.81	0.61
1:B:84:GLY:HA3	2:B:191:BME:C2	2.31	0.60
1:E:64:GLU:O	1:E:67:VAL:HB	2.02	0.60
1:C:33:ASN:H	1:C:175:ASN:HD21	1.49	0.59
1:F:107:THR:HG23	1:F:108:PRO:HD2	1.85	0.59
1:A:81[A]:CYS:SG	2:A:191:BME:H22	2.43	0.59
1:E:86:THR:HG21	1:E:104:ARG:HH11	1.65	0.59
1:D:7:HIS:CD2	1:D:11:THR:OG1	2.52	0.58
1:C:51:VAL:HG22	1:D:47:THR:HG23	1.85	0.58
1:F:140:PHE:CE2	1:F:145:TYR:HB3	2.38	0.58
1:F:4:PHE:CD2	1:F:170:ALA:HB2	2.39	0.57
1:D:131:ARG:HD2	5:D:188:HOH:O	2.05	0.57
1:A:184:GLY:CA	1:D:134:ASP:HB2	2.34	0.57
1:C:146:THR:H	1:C:149:ASN:ND2	2.02	0.56
1:A:146:THR:H	1:A:149:ASN:HD22	1.52	0.56
1:E:8:THR:HG22	1:E:9:ILE:N	2.20	0.56
1:C:88:PHE:CD1	1:C:92:GLN:HG3	2.41	0.55
1:A:52:GLY:O	1:A:56[B]:ARG:HG3	2.05	0.55
1:B:182:VAL:O	1:B:183:LYS:HB3	2.06	0.55
1:C:9:ILE:HD11	1:C:21:ARG:NE	2.19	0.55
1:A:183:LYS:CG	1:A:184:GLY:H	2.19	0.55
1:B:93:ILE:C	1:B:94:GLN:HG2	2.31	0.55
1:F:23:VAL:HG13	1:F:27:ASN:HD22	1.71	0.55
1:C:88:PHE:CE1	1:C:92:GLN:HG3	2.42	0.54
1:D:15:ARG:HD2	1:D:42:PRO:HG2	1.87	0.54
1:D:87:ALA:O	1:D:91:LYS:HG2	2.07	0.54
1:B:34[B]:LEU:HD22	1:B:34[B]:LEU:O	2.06	0.54
1:E:131:ARG:NH2	1:F:77:GLY:O	2.41	0.54
1:D:20:LEU:HD21	1:D:35:ILE:HG22	1.91	0.53
1:B:180[B]:GLN:HE21	1:B:180[B]:GLN:N	2.00	0.53
1:D:146:THR:H	1:D:149:ASN:ND2	2.07	0.52
1:C:146:THR:H	1:C:149:ASN:HD22	1.57	0.52
1:F:139:ASP:O	1:F:142:GLU:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLY:HA2	1:D:134:ASP:CA	2.39	0.52
1:E:51:VAL:HG22	1:F:47:THR:HG23	1.92	0.52
1:E:51:VAL:CG1	1:E:159:LEU:HD13	2.40	0.52
1:E:174:ILE:H	1:E:174:ILE:HD12	1.75	0.52
1:E:60:LEU:O	1:E:65:ARG:NH1	2.44	0.51
1:A:92:GLN:NE2	1:A:92:GLN:HA	2.26	0.51
1:F:182:VAL:HG22	1:F:184:GLY:H	1.76	0.51
1:A:184:GLY:HA2	1:D:134:ASP:CB	2.40	0.50
1:F:14:GLU:C	1:F:16:VAL:H	2.19	0.50
1:E:174:ILE:HD12	1:E:174:ILE:N	2.26	0.50
1:B:180[B]:GLN:OE1	5:B:387:HOH:O	2.20	0.50
1:D:114:LYS:HG3	1:D:143:VAL:CG1	2.32	0.49
1:F:69:GLN:HG3	1:F:85:HIS:HE1	1.77	0.49
1:E:99:LEU:CD1	1:E:109:ILE:HG21	2.42	0.49
1:D:16:VAL:HG12	1:D:20:LEU:HG	1.94	0.49
1:D:146:THR:N	1:D:149:ASN:HD22	2.10	0.48
1:E:99:LEU:HD13	1:E:109:ILE:HG21	1.94	0.48
1:A:183:LYS:CG	1:A:184:GLY:N	2.76	0.48
1:A:183:LYS:HG2	1:A:184:GLY:N	2.28	0.48
1:F:67:VAL:HG21	1:F:115:LEU:HD22	1.95	0.48
1:F:24:LYS:CG	1:F:31:ILE:HG13	2.44	0.48
1:B:109:ILE:HD12	1:B:116:ASP:HA	1.96	0.48
1:D:86:THR:HG23	1:D:100:LEU:HD11	1.96	0.47
1:C:7:HIS:HE1	1:C:40:ASN:OD1	1.98	0.47
1:A:174:ILE:HD13	1:A:182:VAL:HG22	1.96	0.47
1:D:58:ASN:OD1	1:D:65:ARG:HD3	2.14	0.46
1:E:75:THR:C	1:E:77:GLY:N	2.73	0.46
1:C:30:TYR:CD1	1:C:177:GLU:HG2	2.51	0.46
1:E:58:ASN:HD21	1:E:60:LEU:HD12	1.79	0.46
1:F:55:ASN:C	1:F:57:ARG:H	2.23	0.46
1:A:184:GLY:CA	1:D:134:ASP:CB	2.94	0.46
1:F:23:VAL:HG13	1:F:27:ASN:ND2	2.31	0.46
1:F:41:ALA:O	1:F:44:ALA:N	2.49	0.46
1:C:76:ASN:HA	1:D:129:LYS:HD3	1.97	0.46
1:E:58:ASN:HB2	1:E:152:ASP:CG	2.41	0.46
1:A:95:MSE:HG3	1:A:99:LEU:HD23	1.98	0.45
1:E:58:ASN:OD1	1:E:65:ARG:HD3	2.15	0.45
1:F:47:THR:O	1:F:51:VAL:HB	2.17	0.45
1:D:93:ILE:HG22	1:D:93:ILE:O	2.15	0.45
1:A:81[A]:CYS:SG	2:A:191:BME:C2	3.05	0.45
1:D:9:ILE:CD1	1:D:21:ARG:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ARG:HG2	1:F:57:ARG:HH21	1.81	0.45
1:F:69:GLN:NE2	1:F:160:ALA:HB2	2.31	0.45
1:B:167:ASN:ND2	1:B:172:THR:OG1	2.45	0.45
1:B:131:ARG:HD2	5:B:223:HOH:O	2.17	0.45
1:C:77:GLY:O	1:D:131:ARG:NH2	2.45	0.45
1:D:20:LEU:CD2	1:D:35:ILE:HG22	2.47	0.45
1:B:142:GLU:O	1:B:142:GLU:HG2	2.16	0.44
1:C:7:HIS:CE1	1:C:40:ASN:OD1	2.70	0.44
1:E:41:ALA:O	1:E:43:THR:N	2.51	0.44
1:D:20:LEU:HD23	1:D:20:LEU:HA	1.78	0.44
1:C:140:PHE:O	1:C:143:VAL:HG12	2.18	0.44
1:C:18:GLU:OE2	1:C:21:ARG:NH1	2.51	0.44
1:B:88:PHE:CE1	1:B:93:ILE:HD11	2.53	0.44
1:B:34[B]:LEU:HD12	2:B:191:BME:H12	2.00	0.43
1:E:47:THR:HG21	1:F:155:LEU:CD1	2.48	0.43
1:A:93:ILE:O	1:A:93:ILE:HG22	2.18	0.43
1:A:146:THR:H	1:A:149:ASN:ND2	2.17	0.43
1:E:123:ILE:O	1:E:124:ALA:C	2.62	0.43
1:F:7:HIS:CE1	1:F:40:ASN:OD1	2.71	0.43
1:A:60:LEU:O	1:A:65:ARG:NH1	2.51	0.43
1:C:145:TYR:HA	1:C:149:ASN:HD22	1.83	0.43
1:D:86:THR:CG2	1:D:181:TYR:HB3	2.49	0.43
1:C:86:THR:HG23	1:C:100:LEU:HD21	2.01	0.43
1:C:114:LYS:HA	1:C:143:VAL:HG21	1.99	0.43
1:F:109:ILE:HB	1:F:116:ASP:HB2	2.00	0.43
1:B:88:PHE:CD2	1:B:92[A]:GLN:HG3	2.54	0.42
1:E:51:VAL:HG12	1:E:159:LEU:HD13	2.01	0.42
1:C:174:ILE:HD12	1:C:182:VAL:HG22	2.00	0.42
1:D:61:THR:HB	1:D:62:PRO:HD2	2.00	0.42
1:E:155:LEU:CD1	1:F:47:THR:HG21	2.49	0.42
1:C:9:ILE:O	1:C:17:LYS:HG3	2.18	0.42
1:F:24:LYS:HG3	1:F:31:ILE:HG13	2.01	0.42
1:B:93:ILE:O	1:B:93:ILE:HG22	2.18	0.42
1:B:105:ASN:CB	1:B:107:THR:HG23	2.45	0.42
1:C:31:ILE:O	1:C:32:PRO:C	2.61	0.42
1:E:51:VAL:HG11	1:E:159:LEU:HD13	2.01	0.42
1:D:61:THR:HB	1:D:62:PRO:CD	2.50	0.42
1:E:86:THR:CG2	1:E:104:ARG:HH11	2.33	0.42
1:E:49:ARG:HG3	1:E:49:ARG:HH11	1.84	0.42
1:F:69:GLN:CG	1:F:85:HIS:CE1	3.01	0.41
1:F:107:THR:HG23	1:F:108:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81[A]:CYS:HG	2:A:191:BME:C2	2.33	0.41
1:A:96:ALA:HA	1:A:97:PRO:HD3	1.89	0.41
1:C:120[B]:LYS:N	1:C:120[B]:LYS:HE3	2.35	0.41
1:C:146:THR:HB	1:C:147:PRO:HD2	2.03	0.41
1:E:99:LEU:CD1	1:E:109:ILE:HD13	2.50	0.41
1:D:12:ALA:HB2	1:D:20:LEU:HD12	2.01	0.41
1:F:86:THR:O	1:F:90:ILE:HG13	2.21	0.41
1:C:119:ALA:HB3	1:C:120[B]:LYS:HE3	2.03	0.41
1:D:96:ALA:HA	1:D:97:PRO:HD3	1.91	0.41
1:F:24:LYS:HG2	1:F:31:ILE:HG13	2.02	0.41
1:A:110:ASP:CG	1:D:108:PRO:HG3	2.46	0.41
1:F:140:PHE:CE2	1:F:145:TYR:CB	3.03	0.41
1:D:88:PHE:CD2	1:D:92[B]:GLN:OE1	2.73	0.41
1:E:70:ILE:O	1:E:73:ALA:HB3	2.21	0.41
1:B:78:CYS:O	1:B:82:VAL:HG23	2.21	0.41
1:B:88:PHE:HE1	1:B:93:ILE:HD11	1.86	0.41
1:E:9:ILE:HD13	1:E:9:ILE:HA	1.80	0.41
1:E:109:ILE:H	1:E:109:ILE:HG13	1.60	0.41
1:C:112:ASP:OD1	1:C:115:LEU:HG	2.20	0.40
1:E:102:ALA:HB1	1:E:107:THR:O	2.22	0.40
1:B:129:LYS:HE3	5:B:296:HOH:O	2.20	0.40
1:E:15:ARG:CZ	1:E:15:ARG:HB2	2.51	0.40
1:B:33:ASN:HD22	1:B:33:ASN:HA	1.69	0.40
1:E:19:THR:HG23	1:E:49:ARG:NH1	2.37	0.40
1:E:58:ASN:HA	1:F:43:THR:HG21	2.03	0.40
1:A:131:ARG:NH2	5:A:293:HOH:O	2.54	0.40
1:E:7:HIS:HD2	1:E:11:THR:C	2.29	0.40
1:F:114:LYS:HA	1:F:143:VAL:HG11	2.03	0.40

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%)	10	7
1	F	181/207 (87%)	165 (91%)	15 (8%)	1 (1%)	21	18
All	All	1084/1242 (87%)	1045 (96%)	36 (3%)	3 (0%)	36	36

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%)	152 (97%)	4 (3%)	40	46
1	B	158/169 (94%)	149 (94%)	9 (6%)	18	17
1	C	155/169 (92%)	148 (96%)	7 (4%)	24	25
1	D	152/169 (90%)	148 (97%)	4 (3%)	40	46
1	E	145/169 (86%)	132 (91%)	13 (9%)	9	6
1	F	152/169 (90%)	138 (91%)	14 (9%)	8	6
All	All	918/1014 (90%)	867 (94%)	51 (6%)	19	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	43	THR
1	A	92	GLN
1	B	20	LEU
1	B	42	PRO
1	B	43	THR
1	B	94	GLN
1	B	100	LEU
1	B	101	GLU
1	B	142	GLU
1	B	143	VAL
1	B	155	LEU
1	C	9	ILE
1	C	15	ARG
1	C	20	LEU
1	C	43	THR
1	C	56	ARG
1	C	95	MSE
1	C	142	GLU
1	D	19	THR
1	D	93	ILE
1	D	100	LEU
1	D	143	VAL
1	E	9	ILE
1	E	11	THR
1	E	15	ARG
1	E	38	LEU
1	E	51	VAL
1	E	94	GLN
1	E	101	GLU
1	E	109	ILE
1	E	111	ASP
1	E	118	LEU
1	E	135	GLU
1	E	143	VAL
1	E	158	SER
1	F	5	THR
1	F	16	VAL
1	F	20	LEU
1	F	24	LYS
1	F	43	THR
1	F	61	THR
1	F	69	GLN

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Mol	Chain	Res	Type
1	F	91	LYS
1	F	107	THR
1	F	117	THR
1	F	134	ASP
1	F	135	GLU
1	F	143	VAL
1	F	163	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	76	ASN
1	A	92	GLN
1	A	105	ASN
1	A	149	ASN
1	A	164	ASN
1	B	33	ASN
1	B	94	GLN
1	B	105	ASN
1	B	164	ASN
1	C	7	HIS
1	C	33	ASN
1	C	69	GLN
1	C	76	ASN
1	C	149	ASN
1	C	164	ASN
1	C	175	ASN
1	D	7	HIS
1	D	55	ASN
1	D	105	ASN
1	D	149	ASN
1	D	167	ASN
1	E	7	HIS
1	E	27	ASN
1	E	33	ASN
1	E	55	ASN
1	E	149	ASN
1	F	7	HIS
1	F	27	ASN
1	F	69	GLN
1	F	85	HIS

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Mol	Chain	Res	Type
1	F	105	ASN
1	F	149	ASN
1	F	167	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 oligosaccharides 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	$\# Z > 2$
4	SO4	D	191	-	4,4,4	0.22	0	6,6,6	0.09	0
2	BME	A	191	-	3,3,3	0.37	0	2,2,2	0.37	0
2	BME	B	191	-	3,3,3	0.60	0	2,2,2	0.99	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	-
2	BME	B	191	-	-	0/1/1/1	-

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

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	181/207 (87%)	-0.19	2 (1%) 78 80	18, 40, 59, 80	3 (1%)
1	B	180/207 (86%)	-0.23	1 (0%) 85 87	17, 39, 64, 97	5 (2%)
1	C	180/207 (86%)	0.17	2 (1%) 78 80	23, 62, 93, 112	2 (1%)
1	D	177/207 (85%)	0.26	2 (1%) 78 80	38, 65, 107, 127	1 (0%)
1	E	172/207 (83%)	0.85	14 (8%) 18 19	33, 66, 96, 114	166 (96%)
1	F	181/207 (87%)	0.70	10 (5%) 30 32	36, 62, 82, 101	165 (91%)
All	All	1071/1242 (86%)	0.26	31 (2%) 53 56	17, 56, 92, 127	342 (31%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	GLY	5.4
1	E	174	ILE	4.3
1	F	141	LEU	3.7
1	E	88	PHE	3.4
1	E	90	ILE	3.3
1	E	82	VAL	3.1
1	F	117	THR	3.1
1	E	39	ALA	2.9
1	F	136	ALA	2.9
1	A	111	ASP	2.9
1	E	143	VAL	2.8
1	F	150	ALA	2.7
1	B	183	LYS	2.6
1	E	103	LEU	2.6
1	E	172	THR	2.5
1	F	155	LEU	2.5
1	E	130	GLY	2.5
1	F	125	VAL	2.4
1	E	70	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	93	ILE	2.3
1	F	170	ALA	2.3
1	F	16	VAL	2.2
1	E	63	THR	2.2
1	E	173	PRO	2.1
1	E	37	LEU	2.1
1	C	9	ILE	2.1
1	F	82	VAL	2.1
1	D	88	PHE	2.0
1	C	87	ALA	2.0
1	D	178	LEU	2.0
1	E	48	TYR	2.0

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	BME	B	191	4/4	0.68	0.28	44,49,52,140	0
2	BME	A	191	4/4	0.81	0.20	64,67,74,126	0
4	SO4	D	191	5/5	0.85	0.12	107,108,110,111	4
3	CL	A	192	1/1	0.98	0.07	55,55,55,55	0
3	CL	B	192	1/1	0.99	0.08	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.