



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2016 – 03:03 AM EDT

PDB ID : 5EJ8  
Title : EcMenD-ThDP-Mn2+ complex structure soaked with 2-ketoglutarate for 2 min  
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.  
Deposited on : 2015-11-01  
Resolution : 1.34 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027790

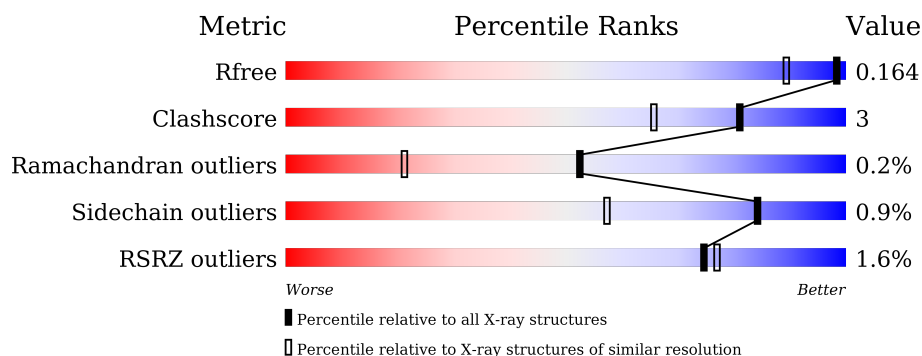
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.34 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))
$R_{free}$	91344	1723 (1.38-1.30)
Clashscore	102246	1806 (1.38-1.30)
Ramachandran outliers	100387	1749 (1.38-1.30)
Sidechain outliers	100360	1749 (1.38-1.30)
RSRZ outliers	91569	1721 (1.38-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	556	<div> <div></div> <div>94%6%</div> </div>
1	B	556	<div> <div></div> <div>95%5%</div> </div>
1	C	556	<div> <div></div> <div>92%8%</div> </div>
1	D	556	<div> <div>3%</div> <div>94%6%</div> </div>
1	E	556	<div> <div></div> <div>94%6%</div> </div>
1	F	556	<div> <div></div> <div>92%8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	556	
1	H	556	

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	MN	F	603[A]	-	-	-	X
4	MG	A	607	-	-	-	X
4	MG	B	607	-	-	-	X
4	MG	E	607	-	-	-	X
4	MG	F	604[B]	-	-	-	X
5	GOL	A	605	-	-	-	X
5	GOL	C	613	-	-	-	X
5	GOL	D	605	-	-	-	X
5	GOL	D	606	-	-	-	X
5	GOL	F	605	-	-	-	X
5	GOL	F	606	-	-	-	X
5	GOL	H	607	-	-	-	X
5	GOL	H	611	-	-	-	X
6	EDO	A	606	-	-	-	X
6	EDO	A	610	-	-	-	X
6	EDO	A	611	-	-	-	X
6	EDO	A	612	-	-	-	X
6	EDO	A	613	-	-	-	X
6	EDO	A	614	-	-	X	X
6	EDO	A	615	-	-	-	X
6	EDO	C	601	-	-	X	X
6	EDO	C	607	-	-	-	X
6	EDO	C	610	-	-	-	X
6	EDO	C	611	-	-	-	X
6	EDO	C	615	-	-	-	X
6	EDO	C	616	-	-	-	X
6	EDO	D	611	-	-	X	X
6	EDO	E	612	-	-	-	X
6	EDO	F	610	-	-	X	X
6	EDO	G	613	-	-	-	X
6	EDO	H	609	-	-	-	X
6	EDO	H	612	-	-	-	X
7	FMT	A	608	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FMT	A	609	-	-	-	X
7	FMT	A	616	-	-	-	X
7	FMT	A	617	-	-	X	X
7	FMT	A	618	-	-	-	X
7	FMT	B	606	-	-	-	X
7	FMT	B	608	-	-	-	X
7	FMT	B	609	-	-	-	X
7	FMT	B	610	-	-	-	X
7	FMT	B	611	-	-	-	X
7	FMT	B	612	-	-	-	X
7	FMT	B	613	-	-	X	X
7	FMT	C	609	-	-	-	X
7	FMT	C	612	-	-	-	X
7	FMT	C	614	-	-	-	X
7	FMT	D	609	-	-	-	X
7	FMT	D	612	-	-	X	X
7	FMT	E	605	-	-	-	X
7	FMT	E	606	-	-	-	X
7	FMT	E	609	-	-	X	X
7	FMT	E	610	-	-	X	X
7	FMT	E	611	-	-	-	X
7	FMT	F	608	-	-	-	X
7	FMT	F	611	-	-	X	X
7	FMT	G	606	-	-	-	X
7	FMT	G	612	-	-	-	X
7	FMT	G	614	-	-	X	X
7	FMT	H	610	-	-	-	X
7	FMT	H	613	-	-	-	X
8	TRS	C	606	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 77229 atoms, of which 35529 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	556	Total	C	H	N	O	S	0	39	0
			8921	2834	4440	818	813	16			
1	B	556	Total	C	H	N	O	S	0	32	0
			8807	2811	4381	798	803	14			
1	C	556	Total	C	H	N	O	S	0	29	0
			8763	2800	4358	793	797	15			
1	D	556	Total	C	H	N	O	S	0	24	0
			8700	2783	4326	784	792	15			
1	E	556	Total	C	H	N	O	S	0	28	0
			8799	2801	4377	802	805	14			
1	F	556	Total	C	H	N	O	S	0	36	0
			8894	2832	4433	811	803	15			
1	G	556	Total	C	H	N	O	S	0	26	0
			8761	2798	4357	795	796	15			
1	H	556	Total	C	H	N	O	S	0	41	0
			8856	2827	4403	802	809	15			

- Molecule 2 is (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (three-letter code: TD6) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	1
3	C	1	Total 1	Mn 1	0	1
3	A	1	Total 1	Mn 1	0	1
3	F	1	Total 1	Mn 1	0	1

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	Mg 2	0	1
4	D	2	Total 2	Mg 2	0	1
4	E	2	Total 2	Mg 2	0	1
4	H	2	Total 2	Mg 2	0	1
4	B	2	Total 2	Mg 2	0	1
4	C	2	Total 2	Mg 2	0	1
4	A	2	Total 2	Mg 2	0	1
4	F	1	Total 1	Mg 1	0	1

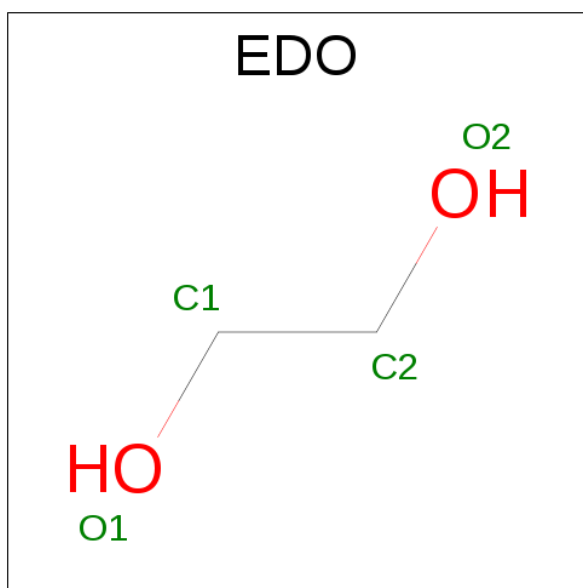
- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		
5	G	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		
5	H	1	Total	C	H	O	0	0
			13	3	7	3		
5	H	1	Total	C	H	O	0	0
			14	3	8	3		



- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



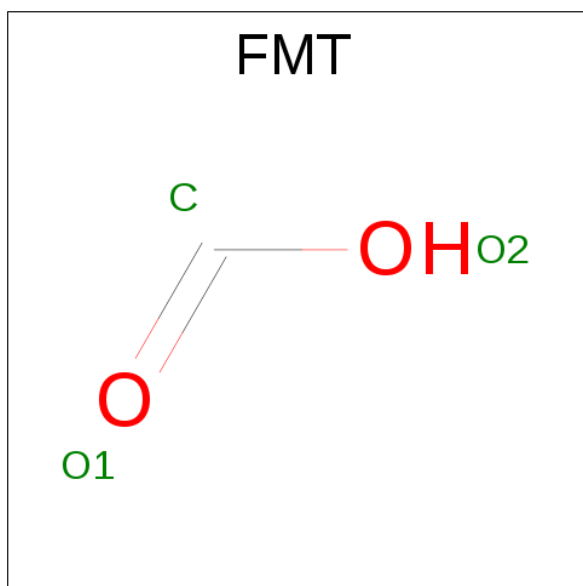
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	F	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		
6	H	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			4	1	1	2		
7	A	1	Total	C	H	O	0	0
			4	1	1	2		
7	A	1	Total	C	H	O	0	0
			4	1	1	2		

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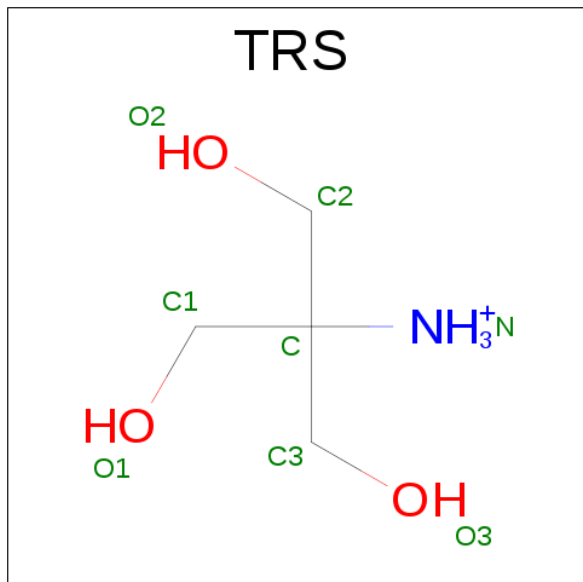
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 4	C 1	H 1	O 2	0	0
7	A	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	B	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	C	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	D	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	E	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	F	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	G	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0
7	H	1	Total 4	C 1	H 1	O 2	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

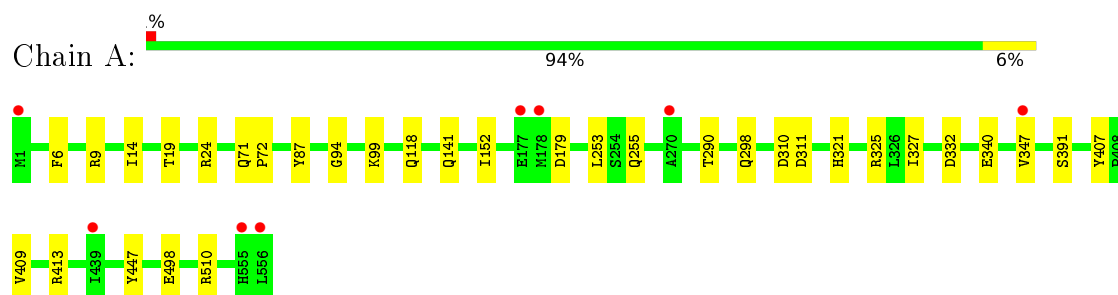
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	743	Total	O	0	0
			743	743		
9	B	757	Total	O	0	0
			757	757		
9	C	701	Total	O	0	0
			701	701		
9	D	604	Total	O	0	0
			604	604		
9	E	756	Total	O	0	0
			756	756		
9	F	735	Total	O	0	0
			735	735		
9	G	643	Total	O	0	0
			643	643		
9	H	737	Total	O	0	0
			737	737		

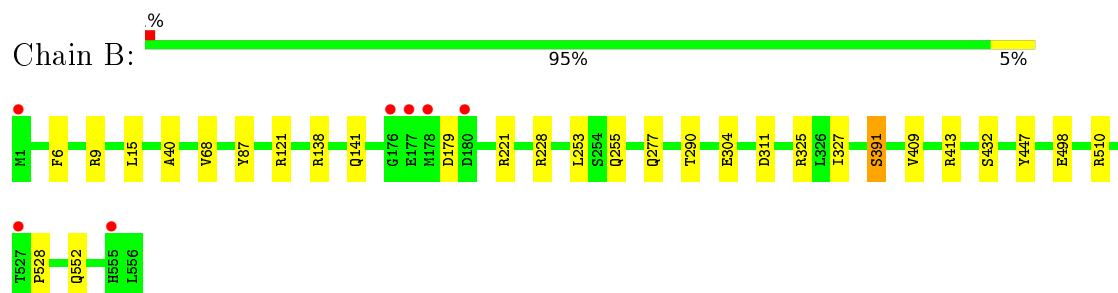
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

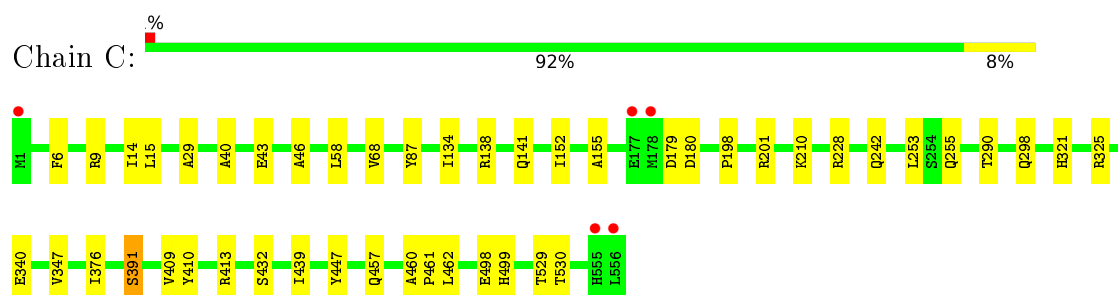
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



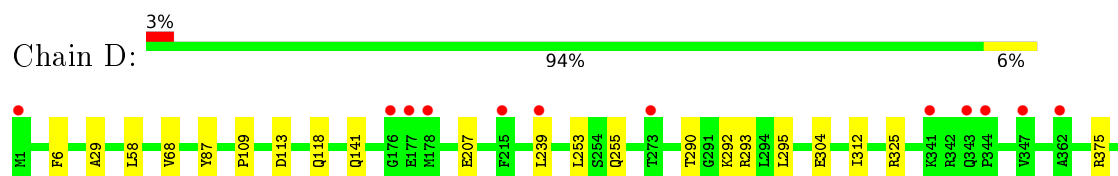
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



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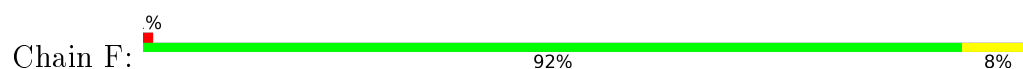




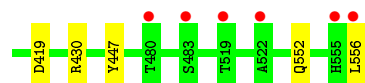
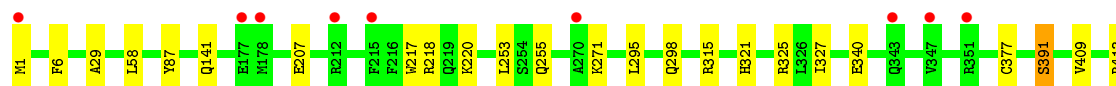
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



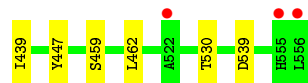
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.66Å 90.76Å 169.34Å 83.25° 76.03° 64.32°	Depositor
Resolution (Å)	27.65 – 1.34 27.65 – 1.34	Depositor EDS
% Data completeness (in resolution range)	94.5 (27.65-1.34) 91.2 (27.65-1.34)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.34Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, $R_{free}$	0.133 , 0.164 0.133 , 0.164	Depositor DCC
$R_{free}$ test set	48790 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	77229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: GOL, MG, FMT, MN, EDO, TRS, TD6

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	0.42	0/4745	0.67	0/6475
1	B	0.40	0/4652	0.65	1/6350 (0.0%)
1	C	0.39	0/4625	0.65	1/6315 (0.0%)
1	D	0.38	0/4586	0.64	0/6262
1	E	0.38	0/4639	0.66	3/6329 (0.0%)
1	F	0.39	0/4702	0.65	1/6416 (0.0%)
1	G	0.37	0/4614	0.64	1/6296 (0.0%)
1	H	0.39	0/4715	0.65	1/6436 (0.0%)
All	All	0.39	0/37278	0.65	8/50879 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	H	228	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	228	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	C	228	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	F	228	ARG	NE-CZ-NH1	-5.34	117.63	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	4481	4440	4285	22	1
1	B	4426	4381	4268	25	0
1	C	4405	4358	4245	34	0
1	D	4374	4326	4222	24	0
1	E	4422	4377	4268	21	1
1	F	4461	4433	4292	35	1
1	G	4404	4357	4255	20	0
1	H	4453	4403	4241	20	0
2	A	33	20	21	2	0
2	B	33	20	21	2	0
2	C	33	20	21	3	0
2	D	33	20	21	2	0
2	E	33	20	21	3	0
2	F	33	20	21	3	0
2	G	33	20	21	3	0
2	H	33	20	21	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
5	A	12	16	16	0	0
5	B	6	8	8	0	0
5	C	12	16	16	0	0
5	D	12	16	16	0	0
5	E	6	8	8	0	0
5	F	12	16	16	0	0
5	G	6	8	8	0	0
5	H	18	23	23	1	0
6	A	28	42	42	12	0
6	C	24	36	35	13	0
6	D	4	6	6	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	4	6	6	0	0
6	F	8	12	12	5	0
6	G	8	12	12	0	0
6	H	8	12	12	0	0
7	A	15	5	5	2	0
7	B	24	8	8	3	0
7	C	12	4	4	1	0
7	D	15	5	5	2	0
7	E	21	7	7	4	0
7	F	12	4	4	4	0
7	G	24	8	8	5	0
7	H	12	4	4	0	0
8	C	8	12	12	1	0
9	A	743	0	0	10	0
9	B	757	0	0	11	3
9	C	701	0	0	15	3
9	D	604	0	0	8	2
9	E	756	0	0	9	2
9	F	735	0	0	18	0
9	G	643	0	0	10	2
9	H	737	0	0	6	3
All	All	41700	35529	34537	239	9

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 3.

The worst 5 of 239 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)
7:E:610:FMT:O1	9:E:701:HOH:O	1.89	0.90
1:G:1:MET:N	9:G:701:HOH:O	2.03	0.89
1:B:179:ASP:O	9:B:701:HOH:O	1.93	0.86
1:F:379:TYR:OH	9:F:701:HOH:O	1.93	0.85
1:C:347:VAL:O	9:C:702:HOH:O	1.96	0.84

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1405:HOH:O	9:C:714:HOH:O[1_655]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:1410:HOH:O	9:H:728:HOH:O[1_565]	1.87	0.33
9:E:1357:HOH:O	9:H:1046:HOH:O[1_565]	1.88	0.32
9:C:1320:HOH:O	9:G:809:HOH:O[1_554]	1.96	0.24
9:B:1207:HOH:O	9:C:1366:HOH:O[1_655]	2.08	0.12

## 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	593/556 (107%)	580 (98%)	12 (2%)	1 (0%)	52	21
1	B	586/556 (105%)	574 (98%)	11 (2%)	1 (0%)	52	21
1	C	583/556 (105%)	570 (98%)	12 (2%)	1 (0%)	52	21
1	D	578/556 (104%)	566 (98%)	11 (2%)	1 (0%)	52	21
1	E	582/556 (105%)	568 (98%)	13 (2%)	1 (0%)	52	21
1	F	590/556 (106%)	578 (98%)	11 (2%)	1 (0%)	52	21
1	G	580/556 (104%)	566 (98%)	13 (2%)	1 (0%)	52	21
1	H	595/556 (107%)	582 (98%)	10 (2%)	3 (0%)	34	9
All	All	4687/4448 (105%)	4584 (98%)	93 (2%)	10 (0%)	52	21

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	SER
1	B	391	SER
1	C	391	SER
1	D	391	SER
1	E	391	SER

### 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	477/452 (106%)	472 (99%)	5 (1%)	82	53
1	B	464/452 (103%)	460 (99%)	4 (1%)	84	57
1	C	462/452 (102%)	458 (99%)	4 (1%)	84	57
1	D	458/452 (101%)	454 (99%)	4 (1%)	84	57
1	E	466/452 (103%)	463 (99%)	3 (1%)	90	70
1	F	470/452 (104%)	466 (99%)	4 (1%)	84	57
1	G	459/452 (102%)	455 (99%)	4 (1%)	84	57
1	H	471/452 (104%)	467 (99%)	4 (1%)	86	62
All	All	3727/3616 (103%)	3695 (99%)	32 (1%)	84	57

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

Mol	Chain	Res	Type
1	D	109	PRO
1	E	87	TYR
1	H	325	ARG
1	D	447	TYR
1	E	325	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	255	GLN
1	F	219	GLN
1	G	358	GLN
1	D	255	GLN
1	G	255	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 112 ligands modelled in this entry, 23 are monoatomic - leaving 89 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	TD6	A	601	3,4	24,34,34	1.23	4 (16%)	32,50,50	1.86	9 (28%)
5	GOL	A	604	-	5,5,5	0.45	0	5,5,5	0.90	0
5	GOL	A	605	-	5,5,5	0.32	0	5,5,5	0.31	0
6	EDO	A	606	-	3,3,3	0.47	0	2,2,2	0.48	0
7	FMT	A	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	A	610	-	3,3,3	0.46	0	2,2,2	0.17	0
6	EDO	A	611	-	3,3,3	0.55	0	2,2,2	0.09	0
6	EDO	A	612	-	3,3,3	0.48	0	2,2,2	0.19	0
6	EDO	A	613	-	3,3,3	0.55	0	2,2,2	0.66	0
6	EDO	A	614	-	3,3,3	0.43	0	2,2,2	0.28	0
6	EDO	A	615	-	3,3,3	0.46	0	2,2,2	0.73	0
7	FMT	A	616	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	617	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	618	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	B	602	3,4	24,34,34	1.14	2 (8%)	32,50,50	1.80	8 (25%)
5	GOL	B	605	-	5,5,5	0.33	0	5,5,5	1.00	0
7	FMT	B	606	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	609	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	610	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	FMT	B	611	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	612	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	613	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	601	-	3,3,3	0.33	0	2,2,2	0.03	0
2	TD6	C	602	3,4	24,34,34	1.28	3 (12%)	32,50,50	2.16	9 (28%)
5	GOL	C	605	-	5,5,5	0.30	0	5,5,5	0.99	0
8	TRS	C	606	-	7,7,7	1.21	1 (14%)	9,9,9	1.58	2 (22%)
6	EDO	C	607	4	3,3,3	0.47	0	2,2,2	0.21	0
7	FMT	C	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	610	-	3,3,3	0.24	0	2,2,2	0.68	0
6	EDO	C	611	-	3,3,3	0.38	0	2,2,2	0.50	0
7	FMT	C	612	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	C	613	-	5,5,5	0.39	0	5,5,5	0.50	0
7	FMT	C	614	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	C	615	-	3,3,3	0.42	0	2,2,2	0.57	0
6	EDO	C	616	-	3,3,3	0.69	0	2,2,2	1.02	0
7	FMT	C	617	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	D	602	3,4	24,34,34	1.22	3 (12%)	32,50,50	1.92	8 (25%)
5	GOL	D	605	-	5,5,5	0.40	0	5,5,5	0.60	0
5	GOL	D	606	-	5,5,5	0.38	0	5,5,5	0.43	0
7	FMT	D	607	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	609	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	610	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	D	611	-	3,3,3	0.45	0	2,2,2	0.32	0
7	FMT	D	612	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	E	601	3,4	24,34,34	1.25	4 (16%)	32,50,50	1.90	9 (28%)
5	GOL	E	604	-	5,5,5	0.39	0	5,5,5	1.09	0
7	FMT	E	605	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	606	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	609	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	610	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	611	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	E	612	-	3,3,3	0.47	0	2,2,2	0.34	0
7	FMT	E	613	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	F	602	3,4	24,34,34	1.22	3 (12%)	32,50,50	2.23	8 (25%)
5	GOL	F	605	-	5,5,5	0.39	0	5,5,5	1.06	0
5	GOL	F	606	-	5,5,5	0.38	0	5,5,5	0.39	0
7	FMT	F	607	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	608	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	F	609	-	3,3,3	0.50	0	2,2,2	0.31	0
6	EDO	F	610	-	3,3,3	0.29	0	2,2,2	1.34	0
7	FMT	F	611	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	G	601	3,4	24,34,34	1.18	4 (16%)	32,50,50	2.06	10 (31%)
5	GOL	G	604	-	5,5,5	0.43	0	5,5,5	0.69	0
7	FMT	G	606	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	G	607	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	G	608	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	G	609	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	G	610	-	3,3,3	0.43	0	2,2,2	0.40	0
7	FMT	G	611	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	G	612	-	0,2,2	0.00	-	0,1,1	0.00	-
6	EDO	G	613	-	3,3,3	0.48	0	2,2,2	0.27	0
7	FMT	G	614	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	G	615	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	H	601	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TD6	H	602	3,4	24,34,34	1.13	2 (8%)	32,50,50	1.83	9 (28%)
5	GOL	H	605	-	5,5,5	0.32	0	5,5,5	1.04	0
7	FMT	H	606	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	H	607	4	5,5,5	0.39	0	5,5,5	0.25	0
6	EDO	H	609	-	3,3,3	0.58	0	2,2,2	0.68	0
7	FMT	H	610	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	H	611	-	5,5,5	0.45	0	5,5,5	0.27	0
6	EDO	H	612	-	3,3,3	0.51	0	2,2,2	0.21	0
7	FMT	H	613	-	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TD6	A	601	3,4	-	0/19/26/26	0/2/2/2
5	GOL	A	604	-	-	0/4/4/4	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
6	EDO	A	606	-	-	0/1/1/1	0/0/0/0
7	FMT	A	608	-	-	0/0/0/0	0/0/0/0
7	FMT	A	609	-	-	0/0/0/0	0/0/0/0
6	EDO	A	610	-	-	0/1/1/1	0/0/0/0
6	EDO	A	611	-	-	0/1/1/1	0/0/0/0
6	EDO	A	612	-	-	0/1/1/1	0/0/0/0
6	EDO	A	613	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	614	-	-	0/1/1/1	0/0/0/0
6	EDO	A	615	-	-	0/1/1/1	0/0/0/0
7	FMT	A	616	-	-	0/0/0/0	0/0/0/0
7	FMT	A	617	-	-	0/0/0/0	0/0/0/0
7	FMT	A	618	-	-	0/0/0/0	0/0/0/0
7	FMT	B	601	-	-	0/0/0/0	0/0/0/0
2	TD6	B	602	3,4	-	0/19/26/26	0/2/2/2
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0
7	FMT	B	606	-	-	0/0/0/0	0/0/0/0
7	FMT	B	608	-	-	0/0/0/0	0/0/0/0
7	FMT	B	609	-	-	0/0/0/0	0/0/0/0
7	FMT	B	610	-	-	0/0/0/0	0/0/0/0
7	FMT	B	611	-	-	0/0/0/0	0/0/0/0
7	FMT	B	612	-	-	0/0/0/0	0/0/0/0
7	FMT	B	613	-	-	0/0/0/0	0/0/0/0
6	EDO	C	601	-	-	0/1/1/1	0/0/0/0
2	TD6	C	602	3,4	-	0/19/26/26	0/2/2/2
5	GOL	C	605	-	-	0/4/4/4	0/0/0/0
8	TRS	C	606	-	-	0/9/9/9	0/0/0/0
6	EDO	C	607	4	-	0/1/1/1	0/0/0/0
7	FMT	C	609	-	-	0/0/0/0	0/0/0/0
6	EDO	C	610	-	-	0/1/1/1	0/0/0/0
6	EDO	C	611	-	-	0/1/1/1	0/0/0/0
7	FMT	C	612	-	-	0/0/0/0	0/0/0/0
5	GOL	C	613	-	-	0/4/4/4	0/0/0/0
7	FMT	C	614	-	-	0/0/0/0	0/0/0/0
6	EDO	C	615	-	-	0/1/1/1	0/0/0/0
6	EDO	C	616	-	-	0/1/1/1	0/0/0/0
7	FMT	C	617	-	-	0/0/0/0	0/0/0/0
7	FMT	D	601	-	-	0/0/0/0	0/0/0/0
2	TD6	D	602	3,4	-	0/19/26/26	0/2/2/2
5	GOL	D	605	-	-	0/4/4/4	0/0/0/0
5	GOL	D	606	-	-	0/4/4/4	0/0/0/0
7	FMT	D	607	-	-	0/0/0/0	0/0/0/0
7	FMT	D	609	-	-	0/0/0/0	0/0/0/0
7	FMT	D	610	-	-	0/0/0/0	0/0/0/0
6	EDO	D	611	-	-	0/1/1/1	0/0/0/0
7	FMT	D	612	-	-	0/0/0/0	0/0/0/0
2	TD6	E	601	3,4	-	0/19/26/26	0/2/2/2
5	GOL	E	604	-	-	0/4/4/4	0/0/0/0
7	FMT	E	605	-	-	0/0/0/0	0/0/0/0
7	FMT	E	606	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FMT	E	608	-	-	0/0/0/0	0/0/0/0
7	FMT	E	609	-	-	0/0/0/0	0/0/0/0
7	FMT	E	610	-	-	0/0/0/0	0/0/0/0
7	FMT	E	611	-	-	0/0/0/0	0/0/0/0
6	EDO	E	612	-	-	0/1/1/1	0/0/0/0
7	FMT	E	613	-	-	0/0/0/0	0/0/0/0
7	FMT	F	601	-	-	0/0/0/0	0/0/0/0
2	TD6	F	602	3,4	-	0/19/26/26	0/2/2/2
5	GOL	F	605	-	-	0/4/4/4	0/0/0/0
5	GOL	F	606	-	-	0/4/4/4	0/0/0/0
7	FMT	F	607	-	-	0/0/0/0	0/0/0/0
7	FMT	F	608	-	-	0/0/0/0	0/0/0/0
6	EDO	F	609	-	-	0/1/1/1	0/0/0/0
6	EDO	F	610	-	-	0/1/1/1	0/0/0/0
7	FMT	F	611	-	-	0/0/0/0	0/0/0/0
2	TD6	G	601	3,4	-	0/19/26/26	0/2/2/2
5	GOL	G	604	-	-	0/4/4/4	0/0/0/0
7	FMT	G	606	-	-	0/0/0/0	0/0/0/0
7	FMT	G	607	-	-	0/0/0/0	0/0/0/0
7	FMT	G	608	-	-	0/0/0/0	0/0/0/0
7	FMT	G	609	-	-	0/0/0/0	0/0/0/0
6	EDO	G	610	-	-	0/1/1/1	0/0/0/0
7	FMT	G	611	-	-	0/0/0/0	0/0/0/0
7	FMT	G	612	-	-	0/0/0/0	0/0/0/0
6	EDO	G	613	-	-	0/1/1/1	0/0/0/0
7	FMT	G	614	-	-	0/0/0/0	0/0/0/0
7	FMT	G	615	-	-	0/0/0/0	0/0/0/0
7	FMT	H	601	-	-	0/0/0/0	0/0/0/0
2	TD6	H	602	3,4	-	0/19/26/26	0/2/2/2
5	GOL	H	605	-	-	0/4/4/4	0/0/0/0
7	FMT	H	606	-	-	0/0/0/0	0/0/0/0
5	GOL	H	607	4	-	0/4/4/4	0/0/0/0
6	EDO	H	609	-	-	0/1/1/1	0/0/0/0
7	FMT	H	610	-	-	0/0/0/0	0/0/0/0
5	GOL	H	611	-	-	0/4/4/4	0/0/0/0
6	EDO	H	612	-	-	0/1/1/1	0/0/0/0
7	FMT	H	613	-	-	0/0/0/0	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TD6	C4-N3	-2.46	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	606	TRS	C-N	-2.46	1.47	1.50
2	H	602	TD6	C4-N3	-2.16	1.34	1.39
2	G	601	TD6	C4-N3	-2.13	1.34	1.39
2	F	602	TD6	C4-N3	-2.11	1.34	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	TD6	C13-CLB-C11	-7.02	106.47	114.74
2	G	601	TD6	C13-CLB-C11	-6.67	106.88	114.74
2	F	602	TD6	C13-CLB-C11	-6.19	107.44	114.74
2	H	602	TD6	C13-CLB-C11	-4.79	109.09	114.74
2	B	602	TD6	OL1-C11-CLB	-4.63	98.42	109.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	2	0
6	A	606	EDO	1	0
6	A	611	EDO	3	0
6	A	612	EDO	1	0
6	A	613	EDO	2	0
6	A	614	EDO	5	0
6	A	615	EDO	1	0
7	A	617	FMT	2	0
2	B	602	TD6	2	0
7	B	613	FMT	3	0
6	C	601	EDO	5	0
2	C	602	TD6	3	0
8	C	606	TRS	1	0
6	C	607	EDO	1	0
6	C	610	EDO	2	0
6	C	611	EDO	1	0
7	C	612	FMT	1	0
6	C	615	EDO	3	0
6	C	616	EDO	2	0
2	D	602	TD6	2	0
6	D	611	EDO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	612	FMT	2	0
2	E	601	TD6	3	0
7	E	609	FMT	2	0
7	E	610	FMT	2	0
2	F	602	TD6	3	0
6	F	610	EDO	5	0
7	F	611	FMT	4	0
2	G	601	TD6	3	0
7	G	608	FMT	1	0
7	G	609	FMT	1	0
7	G	614	FMT	3	0
2	H	602	TD6	3	0
5	H	611	GOL	1	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, 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	556/556 (100%)	-0.15	8 (1%) 78 80	8, 12, 28, 43	0
1	B	556/556 (100%)	-0.16	7 (1%) 79 82	8, 13, 24, 43	0
1	C	556/556 (100%)	-0.16	5 (0%) 85 88	8, 13, 28, 48	0
1	D	556/556 (100%)	-0.01	18 (3%) 51 53	9, 16, 33, 50	0
1	E	556/556 (100%)	-0.16	7 (1%) 79 82	8, 13, 27, 41	0
1	F	556/556 (100%)	-0.16	4 (0%) 89 90	7, 12, 27, 43	0
1	G	556/556 (100%)	-0.07	15 (2%) 58 60	9, 14, 31, 46	0
1	H	556/556 (100%)	-0.15	6 (1%) 82 85	8, 13, 26, 41	0
All	All	4448/4448 (100%)	-0.13	70 (1%) 74 77	7, 13, 28, 50	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	VAL	6.3
1	C	1	MET	5.5
1	B	1	MET	4.4
1	F	347	VAL	3.9
1	E	176	GLY	3.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
7	FMT	A	617	3/3	0.80	0.25	25.73	21,21,26,26	0
7	FMT	E	609	3/3	0.77	0.25	23.60	22,23,23,28	0
6	EDO	A	613	4/4	0.83	0.24	20.51	19,23,26,27	0
6	EDO	A	614	4/4	0.76	0.31	20.14	31,37,41,42	0
7	FMT	G	612	3/3	0.90	0.25	16.98	33,34,34,41	0
7	FMT	G	614	3/3	0.80	0.23	16.39	30,31,33,37	0
6	EDO	F	610	4/4	0.73	0.22	16.07	29,34,37,41	0
6	EDO	A	606	4/4	0.82	0.21	15.79	33,42,47,51	0
6	EDO	C	616	4/4	0.83	0.21	14.77	17,20,23,26	0
6	EDO	A	611	4/4	0.87	0.18	14.66	27,35,37,42	0
7	FMT	E	605	3/3	0.93	0.19	13.69	27,31,34,38	0
7	FMT	A	618	3/3	0.90	0.17	13.59	18,19,21,23	0
5	GOL	C	613	6/6	0.80	0.19	13.05	37,45,50,50	0
6	EDO	C	615	4/4	0.92	0.17	12.50	26,31,35,35	0
6	EDO	A	610	4/4	0.83	0.29	12.20	41,49,51,53	0
7	FMT	B	613	3/3	0.87	0.14	12.15	29,31,34,37	0
7	FMT	E	610	3/3	0.83	0.17	12.06	31,32,33,37	0
5	GOL	H	611	6/6	0.92	0.22	11.97	30,36,41,41	0
7	FMT	F	608	3/3	0.76	0.19	11.62	21,23,24,27	0
8	TRS	C	606	8/8	0.83	0.25	11.59	25,35,41,45	0
7	FMT	C	609	3/3	0.70	0.18	11.08	29,31,31,37	0
7	FMT	B	610	3/3	0.76	0.24	10.79	26,26,30,32	0
4	MG	B	607	1/1	0.98	0.24	10.61	26,26,26,26	0
7	FMT	A	608	3/3	0.74	0.18	10.13	23,24,24,29	0
7	FMT	F	611	3/3	0.88	0.19	9.99	25,26,28,30	0
7	FMT	E	611	3/3	0.80	0.23	9.48	42,44,45,53	0
7	FMT	D	609	3/3	0.89	0.16	9.30	28,30,32,36	0
7	FMT	B	608	3/3	0.73	0.17	9.25	28,30,30,37	0
7	FMT	D	612	3/3	0.82	0.20	9.24	30,32,34,36	0
6	EDO	H	612	4/4	0.93	0.12	9.08	20,28,32,33	0
4	MG	A	607	1/1	0.98	0.24	9.03	29,29,29,29	0
6	EDO	H	609	4/4	0.84	0.18	8.12	17,21,26,27	0
6	EDO	C	610	4/4	0.92	0.23	7.98	21,27,32,32	0
7	FMT	B	612	3/3	0.83	0.26	7.35	37,38,39,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	A	612	4/4	0.85	0.22	6.52	37,44,46,48	0
5	GOL	D	606	6/6	0.79	0.23	6.19	28,35,43,45	0
5	GOL	H	607	6/6	0.94	0.14	6.03	15,20,25,30	0
6	EDO	D	611	4/4	0.90	0.17	5.85	25,30,34,38	0
6	EDO	C	601	4/4	0.84	0.14	5.68	30,37,38,40	0
7	FMT	A	609	3/3	0.80	0.19	5.51	17,26,28,31	0
6	EDO	C	611	4/4	0.96	0.12	5.37	16,20,25,25	0
7	FMT	G	606	3/3	0.89	0.24	5.29	29,29,29,35	0
6	EDO	A	615	4/4	0.71	0.21	5.05	40,48,49,49	0
7	FMT	H	610	3/3	0.84	0.13	4.78	34,34,35,41	0
6	EDO	C	607	4/4	0.95	0.10	4.68	16,20,25,25	0
7	FMT	B	609	3/3	0.62	0.16	4.42	43,46,47,56	0
4	MG	E	607	1/1	0.99	0.21	4.32	29,29,29,29	0
7	FMT	C	612	3/3	0.89	0.17	4.08	24,26,26,31	0
5	GOL	F	606	6/6	0.89	0.18	4.03	24,31,36,41	0
7	FMT	B	606	3/3	0.74	0.19	3.81	33,38,38,45	0
6	EDO	E	612	4/4	0.79	0.12	3.41	41,49,50,51	0
7	FMT	B	611	3/3	0.94	0.12	3.36	20,21,21,25	0
6	EDO	G	613	4/4	0.68	0.14	3.28	42,50,51,54	0
5	GOL	A	605	6/6	0.91	0.16	3.15	22,32,38,40	0
5	GOL	D	605	6/6	0.94	0.10	2.57	16,24,29,29	0
7	FMT	C	614	3/3	0.90	0.11	2.54	21,26,31,32	0
7	FMT	E	606	3/3	0.95	0.14	2.53	24,25,26,31	0
5	GOL	F	605	6/6	0.97	0.11	2.46	12,20,24,24	0
7	FMT	H	613	3/3	0.68	0.15	2.41	42,43,43,52	0
3	MN	F	603[A]	1/1	0.99	0.08	2.16	11,11,11,11	1
4	MG	F	604[B]	1/1	0.99	0.08	2.16	10,10,10,10	1
7	FMT	A	616	3/3	0.95	0.09	2.00	20,20,20,25	0
3	MN	C	603[A]	1/1	0.99	0.08	1.97	15,15,15,15	1
6	EDO	F	609	4/4	0.80	0.12	1.64	39,47,50,50	0
5	GOL	G	604	6/6	0.96	0.09	1.63	15,22,26,27	0
7	FMT	H	601	3/3	0.98	0.07	1.26	21,21,22,26	0
7	FMT	B	601	3/3	0.97	0.07	1.25	20,22,22,26	0
5	GOL	C	605	6/6	0.96	0.09	1.05	16,24,28,28	0
3	MN	G	602[A]	1/1	1.00	0.07	1.00	14,14,14,14	1
4	MG	G	603[B]	1/1	1.00	0.07	1.00	6,6,6,6	1
7	FMT	D	607	3/3	0.95	0.11	0.84	23,26,27,32	0
3	MN	E	602[A]	1/1	1.00	0.07	0.53	11,11,11,11	1
6	EDO	G	610	4/4	0.95	0.10	0.42	23,28,31,32	0
2	TD6	B	602	33/33	0.98	0.07	0.39	8,12,22,30	0
7	FMT	F	601	3/3	0.98	0.07	0.31	21,21,22,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	C	604[B]	1/1	1.00	0.07	0.30	5,5,5,5	1
5	GOL	H	605	6/6	0.97	0.07	0.27	15,22,25,26	0
2	TD6	E	601	33/33	0.99	0.07	0.21	8,12,22,26	0
2	TD6	A	601	33/33	0.99	0.07	0.13	8,12,22,26	0
5	GOL	B	605	6/6	0.96	0.07	0.06	13,17,24,24	0
4	MG	E	603[B]	1/1	1.00	0.07	0.05	8,8,8,8	1
7	FMT	G	615	3/3	0.98	0.06	0.00	19,20,21,24	0
2	TD6	D	602	33/33	0.98	0.06	-0.01	10,14,23,27	0
2	TD6	G	601	33/33	0.99	0.06	-0.05	9,13,22,27	0
5	GOL	E	604	6/6	0.97	0.06	-0.08	14,19,23,23	0
7	FMT	C	617	3/3	0.98	0.06	-0.26	21,21,22,25	0
7	FMT	E	613	3/3	0.98	0.06	-0.27	22,22,22,27	0
2	TD6	F	602	33/33	0.99	0.06	-0.28	8,12,25,30	0
5	GOL	A	604	6/6	0.98	0.07	-0.34	12,18,23,23	0
4	MG	B	604[B]	1/1	0.99	0.06	-0.45	2,2,2,2	1
3	MN	B	603[A]	1/1	0.99	0.06	-0.45	16,16,16,16	1
7	FMT	G	609	3/3	0.90	0.07	-0.61	43,44,44,52	0
2	TD6	H	602	33/33	0.99	0.06	-0.74	9,12,22,27	0
7	FMT	D	610	3/3	0.98	0.05	-0.78	21,21,22,26	0
2	TD6	C	602	33/33	0.99	0.06	-0.80	9,12,22,29	0
4	MG	D	604[B]	1/1	1.00	0.05	-0.96	7,7,7,7	1
3	MN	D	603[A]	1/1	1.00	0.05	-1.17	16,16,16,16	1
3	MN	A	602[A]	1/1	1.00	0.04	-1.25	11,11,11,11	1
4	MG	A	603[B]	1/1	1.00	0.04	-1.25	6,6,6,6	1
3	MN	H	603[A]	1/1	1.00	0.04	-1.36	13,13,13,13	1
4	MG	H	604[B]	1/1	1.00	0.04	-1.36	6,6,6,6	1
4	MG	D	608	1/1	0.99	0.10	-	23,23,23,23	0
7	FMT	D	601	3/3	0.82	0.12	-	26,28,29,35	0
4	MG	C	608	1/1	0.99	0.10	-	15,15,15,15	0
7	FMT	F	607	3/3	0.93	0.14	-	42,43,44,51	0
4	MG	G	605	1/1	0.98	0.15	-	24,24,24,24	0
7	FMT	G	608	3/3	0.59	0.23	-	34,36,36,44	0
7	FMT	E	608	3/3	0.70	0.17	-	34,35,36,43	0
7	FMT	G	607	3/3	0.95	0.13	-	23,26,28,31	0
7	FMT	G	611	3/3	0.60	0.24	-	35,37,38,45	0
7	FMT	H	606	3/3	0.96	0.07	-	23,28,31,33	0
4	MG	H	608	1/1	1.00	0.07	-	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.