wwPDB X-ray Structure Validation Summary Report (i)

Jun 20, 2016 – 07:51 AM EDT

PDB ID	:	5EJ5
Title	:	EcMenD-ThDP-Mn2+ complex soaked with 2-ketoglutarate for 1.5 h
Authors	:	Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.
Deposited on	:	2015-11-01
Resolution	:	2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

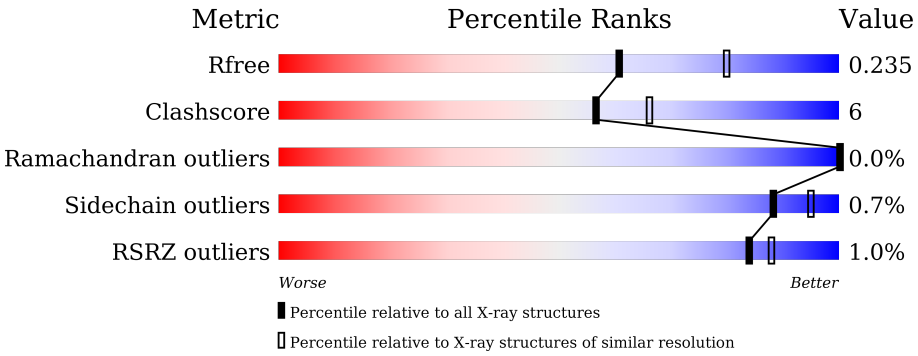
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	89% 11%
1	B	556	89% 11%
1	C	556	88% 12%
1	D	556	86% 14%
1	E	556	87% 13%
1	F	556	87% 13%

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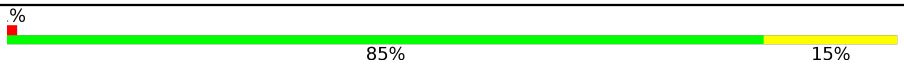
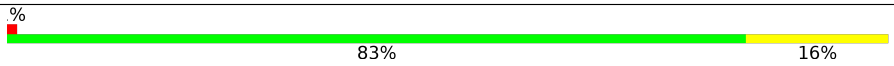
Mol	Chain	Length	Quality of chain
1	G	556	
1	H	556	

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
4	GOL	C	603	-	-	-	X
4	GOL	D	603	-	-	-	X
4	GOL	G	603	-	-	-	X

2 Entry composition

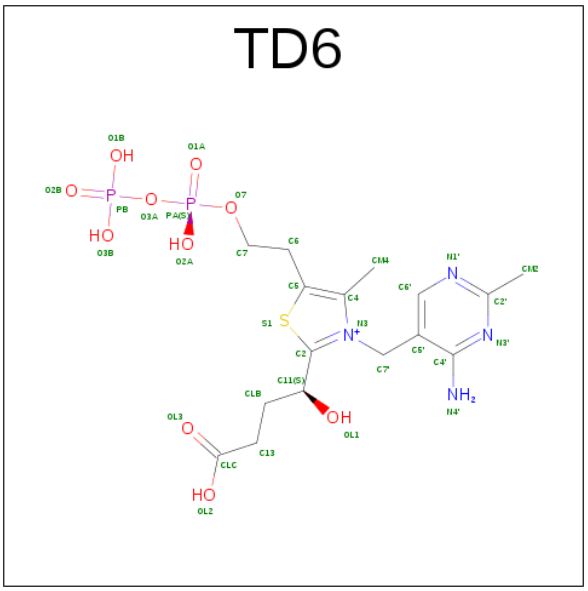
There are 5 unique types of molecules in this entry. The entry contains 36844 atoms, of which 224 are hydrogens and 0 are deuteriums.

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-carboxyl ate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	4	0
			4348	2756	787	790	15			
1	B	556	Total	C	N	O	S	0	1	0
			4316	2738	776	788	14			
1	C	556	Total	C	N	O	S	0	5	0
			4355	2759	787	794	15			
1	D	556	Total	C	N	O	S	0	1	0
			4312	2738	776	783	15			
1	E	556	Total	C	N	O	S	0	5	0
			4360	2763	788	793	16			
1	F	556	Total	C	N	O	S	0	1	0
			4313	2737	776	786	14			
1	G	556	Total	C	N	O	S	0	5	0
			4350	2757	786	792	15			
1	H	556	Total	C	N	O	S	0	1	0
			4314	2738	777	784	15			

- Molecule 2 is (4S)-4-{3-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-(2-{[(S)-hydroxy(pho sphonooxy)phosphoryl]oxy}ethyl)-4-methyl-1,3lambda 5 -thiazol-2-yl}-4-hydroxybutanoic acid (three-letter code: TD6) (formula: $C_{16}H_{25}N_4O_{10}P_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			53	16	20	4	10	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

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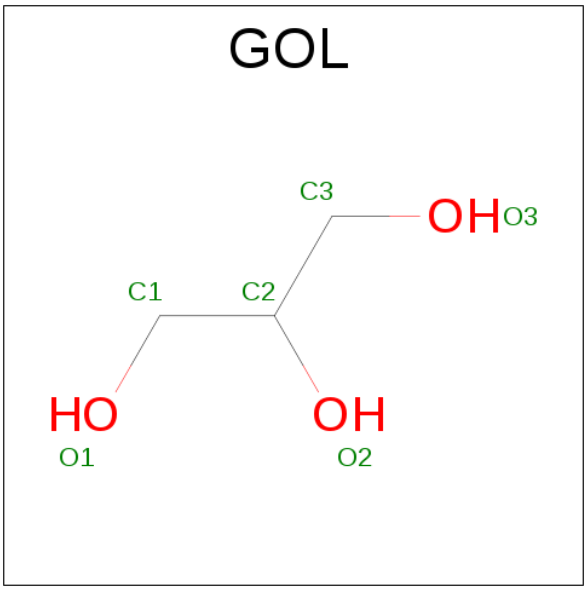
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

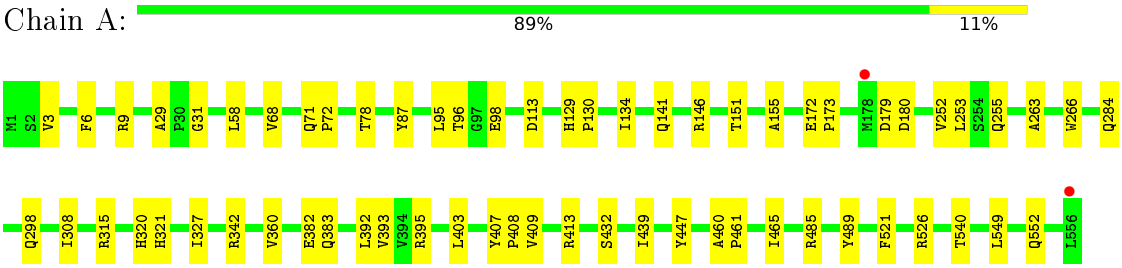
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total	O	0	0
			233	233		
5	B	216	Total	O	0	0
			216	216		
5	C	188	Total	O	0	0
			188	188		
5	D	166	Total	O	0	0
			166	166		
5	E	233	Total	O	0	0
			233	233		
5	F	207	Total	O	0	0
			207	207		
5	G	172	Total	O	0	0
			172	172		
5	H	217	Total	O	0	0
			217	217		

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.

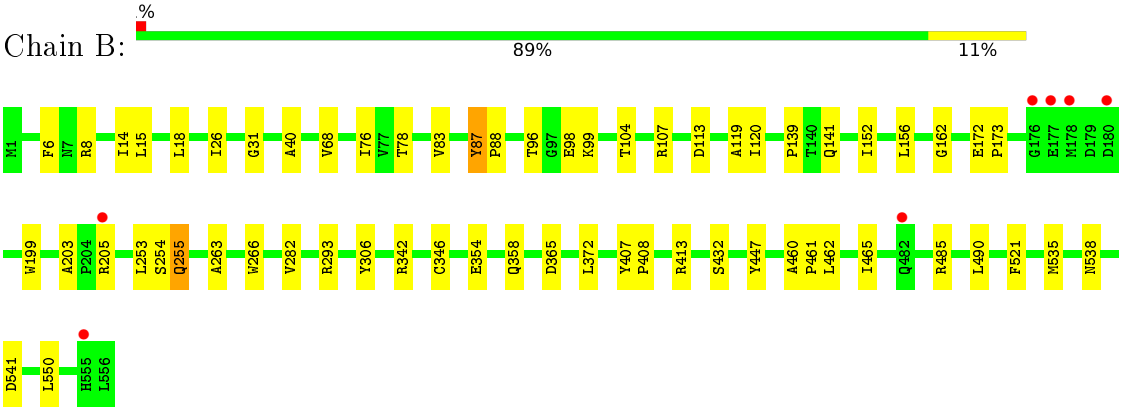
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain A:



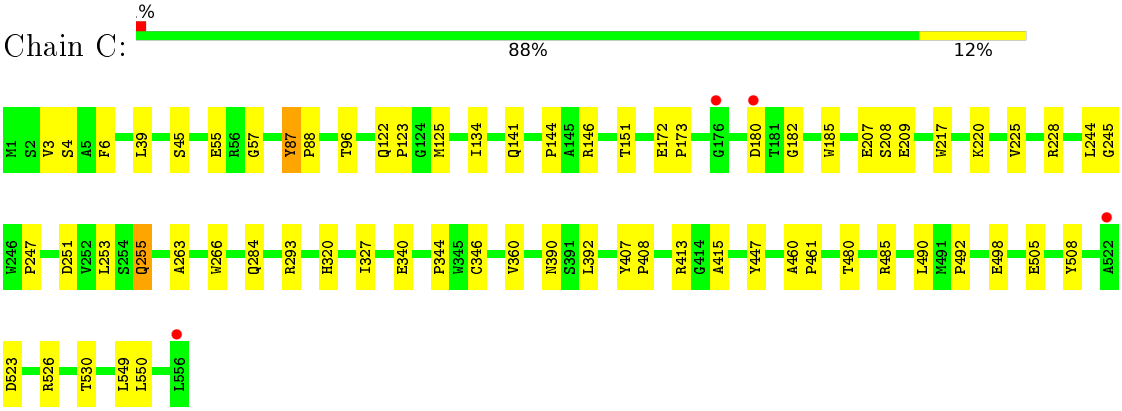
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain B:



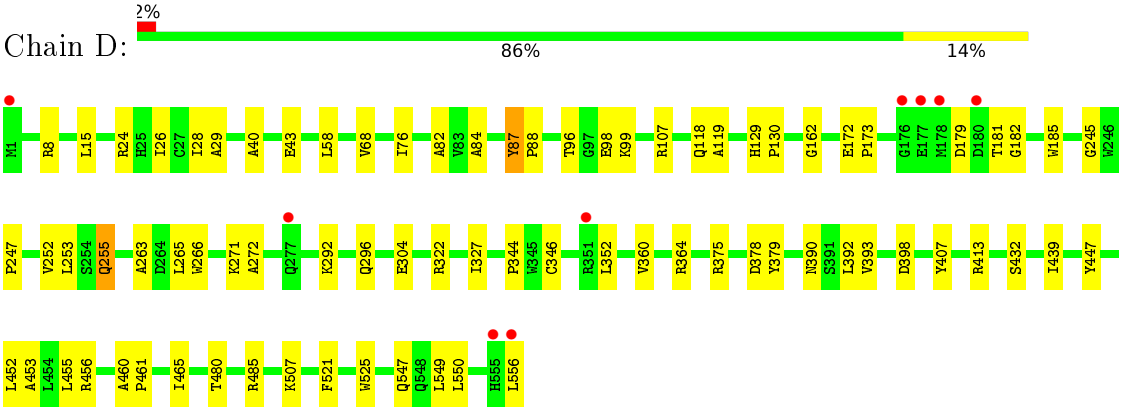
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain C:



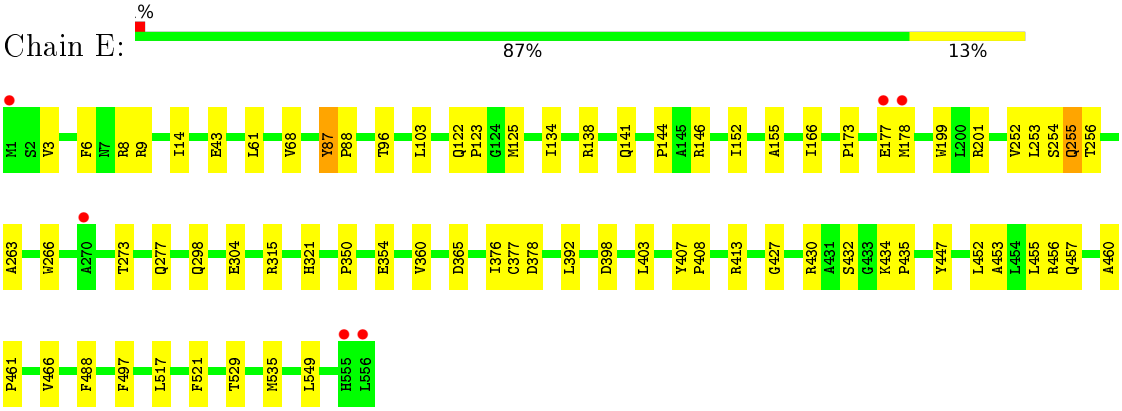
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain D:



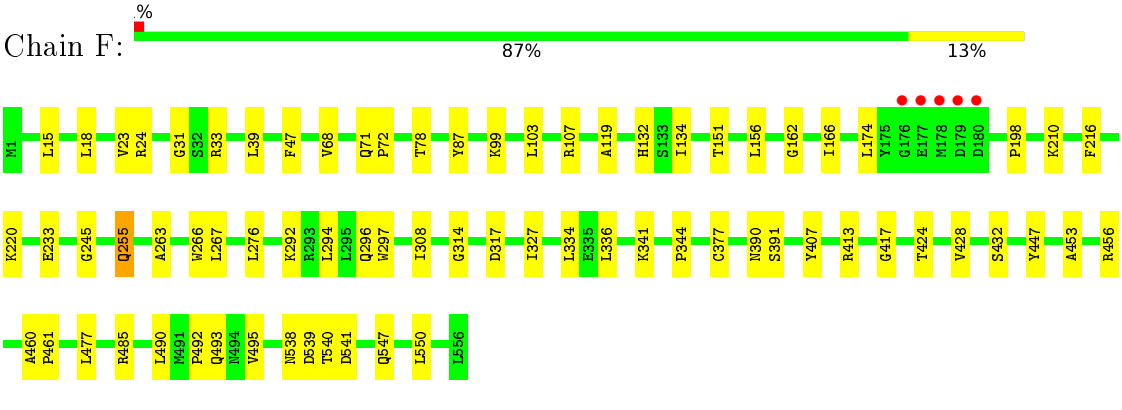
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain E:



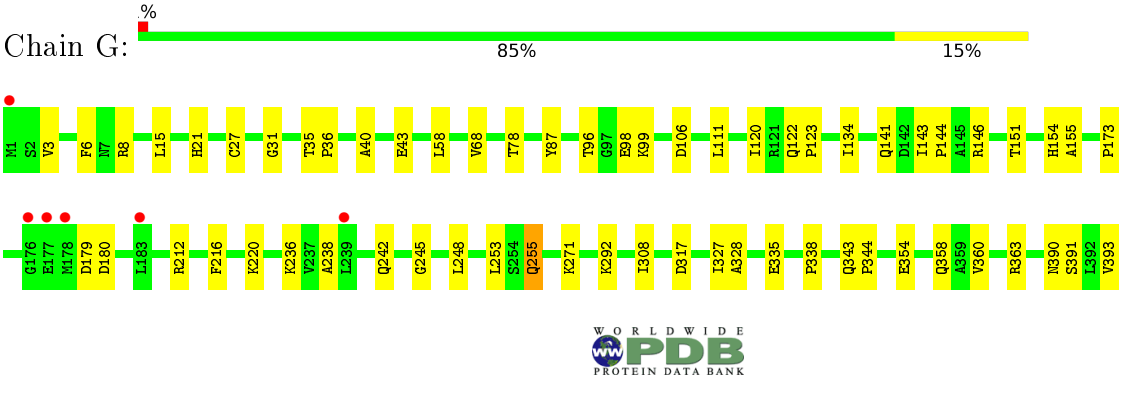
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

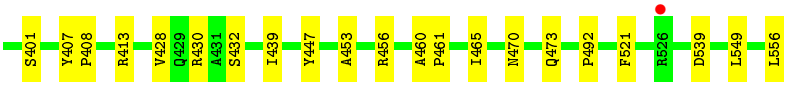
Chain F:



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

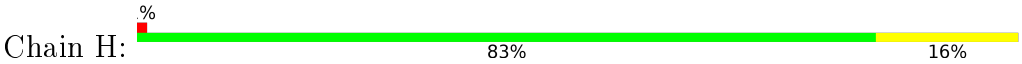
Chain G:

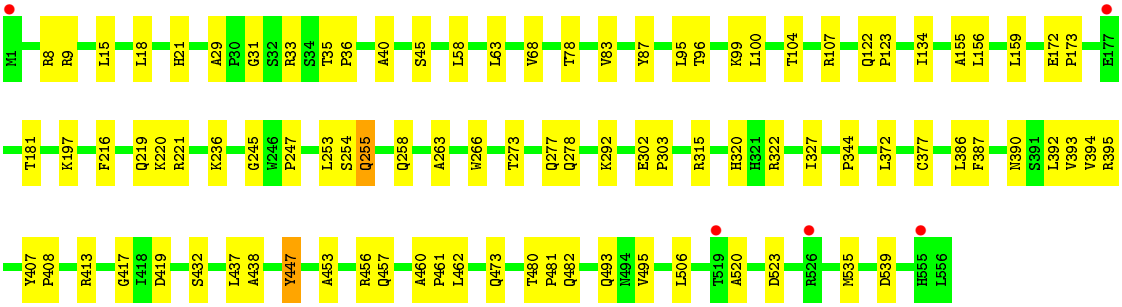




• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.76Å 90.80Å 170.10Å 75.79° 83.29° 64.34°	Depositor
Resolution (Å)	33.76 – 2.30 33.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.4 (33.76-2.30) 82.7 (33.76-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.183 , 0.234 0.183 , 0.235	Depositor DCC
R_{free} test set	9596 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36844	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, 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	0.41	0/4457	0.57	0/6082
1	B	0.47	0/4425	0.57	0/6041
1	C	0.42	0/4464	0.58	0/6092
1	D	0.42	0/4421	0.55	0/6034
1	E	0.42	0/4469	0.59	0/6096
1	F	0.45	0/4422	0.58	1/6037 (0.0%)
1	G	0.38	0/4459	0.55	0/6085
1	H	0.43	0/4423	0.57	0/6037
All	All	0.43	0/35540	0.57	1/48504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	15	LEU	CA-CB-CG	-5.32	103.06	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4348	0	4295	41	0
1	B	4316	0	4253	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4355	0	4294	50	0
1	D	4312	0	4259	54	0
1	E	4360	0	4313	61	0
1	F	4313	0	4251	46	1
1	G	4350	0	4291	55	0
1	H	4314	0	4261	64	1
2	A	33	20	21	4	0
2	B	33	20	21	2	0
2	C	33	20	21	3	0
2	D	33	20	21	3	0
2	E	33	20	21	3	0
2	F	33	20	21	3	0
2	G	33	20	21	2	0
2	H	33	20	21	4	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	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	6	8	8	1	0
4	H	6	8	8	0	0
5	A	233	0	0	10	0
5	B	216	0	0	9	0
5	C	188	0	0	13	0
5	D	166	0	0	8	0
5	E	233	0	0	17	0
5	F	207	0	0	10	0
5	G	172	0	0	12	0
5	H	217	0	0	18	0
All	All	36620	224	34449	420	1

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 6.

The worst 5 of 420 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:VAL:CG2	1:E:398:ASP:HA	1.90	1.01
1:E:252:VAL:HG23	1:E:398:ASP:HA	1.52	0.91
1:B:203:ALA:HB1	1:B:205:ARG:HH12	1.37	0.89
1:H:457:GLN:HG3	5:H:766:HOH:O	1.78	0.82
1:B:365:ASP:O	5:B:701:HOH:O	1.97	0.82

All (1) 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)
1:F:341:LYS:NZ	1:H:45:SER:O[1_545]	2.18	0.02

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	558/556 (100%)	547 (98%)	11 (2%)	0	100	100
1	B	555/556 (100%)	544 (98%)	11 (2%)	0	100	100
1	C	559/556 (100%)	548 (98%)	11 (2%)	0	100	100
1	D	555/556 (100%)	543 (98%)	12 (2%)	0	100	100
1	E	559/556 (100%)	548 (98%)	11 (2%)	0	100	100
1	F	555/556 (100%)	544 (98%)	11 (2%)	0	100	100
1	G	559/556 (100%)	547 (98%)	11 (2%)	1 (0%)	52	64
1	H	555/556 (100%)	545 (98%)	10 (2%)	0	100	100
All	All	4455/4448 (100%)	4366 (98%)	88 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	391	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/452 (100%)	449 (100%)	2 (0%)	93	97
1	B	447/452 (99%)	444 (99%)	3 (1%)	88	95
1	C	452/452 (100%)	449 (99%)	3 (1%)	88	95
1	D	446/452 (99%)	443 (99%)	3 (1%)	88	95
1	E	454/452 (100%)	451 (99%)	3 (1%)	88	95
1	F	446/452 (99%)	441 (99%)	5 (1%)	80	90
1	G	451/452 (100%)	448 (99%)	3 (1%)	88	95
1	H	447/452 (99%)	443 (99%)	4 (1%)	84	93
All	All	3594/3616 (99%)	3568 (99%)	26 (1%)	88	95

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	87	TYR
1	F	24	ARG
1	H	377	CYS
1	E	255	GLN
1	E	447	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	24,34,34	1.42	5 (20%)	32,50,50	1.88	8 (25%)
4	GOL	A	603	-	5,5,5	0.27	0	5,5,5	0.22	0
2	TD6	B	601	3	24,34,34	1.43	4 (16%)	32,50,50	1.91	8 (25%)
4	GOL	B	603	-	5,5,5	0.28	0	5,5,5	0.37	0
2	TD6	C	601	3	24,34,34	1.39	4 (16%)	32,50,50	1.89	9 (28%)
4	GOL	C	603	-	5,5,5	0.34	0	5,5,5	0.20	0
2	TD6	D	601	3	24,34,34	1.34	4 (16%)	32,50,50	1.87	8 (25%)
4	GOL	D	603	-	5,5,5	0.38	0	5,5,5	0.46	0
2	TD6	E	601	3	24,34,34	1.35	3 (12%)	32,50,50	1.71	7 (21%)
4	GOL	E	603	-	5,5,5	0.36	0	5,5,5	0.22	0
2	TD6	F	601	3	24,34,34	1.35	5 (20%)	32,50,50	1.87	9 (28%)
4	GOL	F	603	-	5,5,5	0.27	0	5,5,5	0.32	0
2	TD6	G	601	3	24,34,34	1.39	4 (16%)	32,50,50	1.81	7 (21%)
4	GOL	G	603	-	5,5,5	0.28	0	5,5,5	0.37	0
2	TD6	H	601	3	24,34,34	1.37	4 (16%)	32,50,50	1.83	8 (25%)
4	GOL	H	603	-	5,5,5	0.34	0	5,5,5	0.23	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	TD6	A	601	3	-	0/19/26/26	0/2/2/2
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0
2	TD6	B	601	3	-	0/19/26/26	0/2/2/2
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0
2	TD6	C	601	3	-	0/19/26/26	0/2/2/2
4	GOL	C	603	-	-	0/4/4/4	0/0/0/0
2	TD6	D	601	3	-	0/19/26/26	0/2/2/2
4	GOL	D	603	-	-	0/4/4/4	0/0/0/0
2	TD6	E	601	3	-	0/19/26/26	0/2/2/2
4	GOL	E	603	-	-	0/4/4/4	0/0/0/0
2	TD6	F	601	3	-	0/19/26/26	0/2/2/2
4	GOL	F	603	-	-	0/4/4/4	0/0/0/0
2	TD6	G	601	3	-	0/19/26/26	0/2/2/2
4	GOL	G	603	-	-	0/4/4/4	0/0/0/0
2	TD6	H	601	3	-	0/19/26/26	0/2/2/2
4	GOL	H	603	-	-	0/4/4/4	0/0/0/0

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	TD6	C5'-C4'	-2.19	1.39	1.42
2	F	601	TD6	C5'-C4'	-2.13	1.39	1.42
2	A	601	TD6	C5'-C4'	-2.12	1.39	1.42
2	H	601	TD6	C5'-C4'	-2.01	1.39	1.42
2	F	601	TD6	C7'-C5'	2.07	1.55	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	TD6	CM4-C4-C5	-4.04	120.36	128.91
2	A	601	TD6	CM4-C4-C5	-4.01	120.43	128.91
2	G	601	TD6	CM4-C4-C5	-3.87	120.71	128.91
2	B	601	TD6	CM4-C4-C5	-3.80	120.85	128.91
2	H	601	TD6	CM4-C4-C5	-3.74	120.99	128.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TD6	4	0
2	B	601	TD6	2	0
2	C	601	TD6	3	0
2	D	601	TD6	3	0
2	E	601	TD6	3	0
2	F	601	TD6	3	0
2	G	601	TD6	2	0
4	G	603	GOL	1	0
2	H	601	TD6	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	556/556 (100%)	-0.29	2 (0%)	93	95	13, 22, 38, 61	0
1	B	556/556 (100%)	-0.27	7 (1%)	79	84	13, 22, 35, 55	2 (0%)
1	C	556/556 (100%)	-0.32	4 (0%)	89	92	16, 23, 38, 57	1 (0%)
1	D	556/556 (100%)	-0.17	9 (1%)	74	80	14, 27, 46, 63	2 (0%)
1	E	556/556 (100%)	-0.31	6 (1%)	82	86	14, 22, 36, 72	2 (0%)
1	F	556/556 (100%)	-0.33	5 (0%)	85	89	15, 23, 35, 65	1 (0%)
1	G	556/556 (100%)	-0.14	7 (1%)	79	84	15, 28, 45, 74	2 (0%)
1	H	556/556 (100%)	-0.31	5 (0%)	85	89	14, 23, 38, 63	0
All	All	4448/4448 (100%)	-0.27	45 (1%)	84	88	13, 24, 40, 74	10 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	MET	6.2
1	D	178	MET	4.8
1	G	177	GLU	4.7
1	A	556	LEU	4.6
1	F	176	GLY	4.4

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	G	603	6/6	0.91	0.20	3.74	37,46,55,55	0
4	GOL	C	603	6/6	0.86	0.18	2.39	31,47,61,61	0
4	GOL	D	603	6/6	0.96	0.18	2.21	31,38,44,46	0
4	GOL	A	603	6/6	0.91	0.15	1.09	23,31,38,38	0
4	GOL	E	603	6/6	0.96	0.13	0.30	23,29,34,40	0
2	TD6	E	601	33/33	0.97	0.13	0.13	12,23,42,46	0
4	GOL	H	603	6/6	0.96	0.13	0.04	26,39,47,48	0
4	GOL	B	603	6/6	0.94	0.11	-0.27	23,33,39,43	0
2	TD6	F	601	33/33	0.97	0.12	-0.28	15,28,45,49	0
2	TD6	H	601	33/33	0.97	0.11	-0.48	16,26,40,48	0
2	TD6	D	601	33/33	0.97	0.11	-0.60	18,27,45,56	0
2	TD6	A	601	33/33	0.97	0.12	-0.61	16,28,42,50	0
2	TD6	C	601	33/33	0.97	0.11	-0.65	13,28,37,42	0
2	TD6	B	601	33/33	0.97	0.11	-0.71	17,26,39,58	0
2	TD6	G	601	33/33	0.97	0.10	-1.02	15,29,46,50	0
3	MN	C	602	1/1	0.98	0.03	-2.40	39,39,39,39	0
3	MN	E	602	1/1	0.97	0.03	-2.49	30,30,30,30	0
3	MN	G	602	1/1	0.98	0.04	-2.61	34,34,34,34	0
3	MN	D	602	1/1	0.98	0.05	-2.64	34,34,34,34	0
3	MN	F	602	1/1	0.99	0.04	-2.65	34,34,34,34	0
3	MN	A	602	1/1	0.99	0.03	-2.69	34,34,34,34	0
3	MN	B	602	1/1	0.98	0.04	-3.15	31,31,31,31	0
3	MN	H	602	1/1	0.99	0.02	-3.31	30,30,30,30	0
4	GOL	F	603	6/6	0.97	0.06	-3.63	17,29,33,35	0

6.5 Other polymers

There are no such residues in this entry.