Full wwPDB X-ray Structure Validation Report (i)

Apr 23, 2024 – 06:21 PM EDT

PDB ID	:	5ESO
Title	:	Crystal Structure of M. tuberculosis MenD with ThDP, Mg2+ and Isochorismate bound
Authors	:	Johnston, J.M.; Jirgis, E.N.M.; Bashiri, G.; Bulloch, E.M.M.; Baker, E.N.
Deposited on	:	2015-11-16
Resolution	:	2.05 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 (i) 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 (i)) were used in the production of this report:

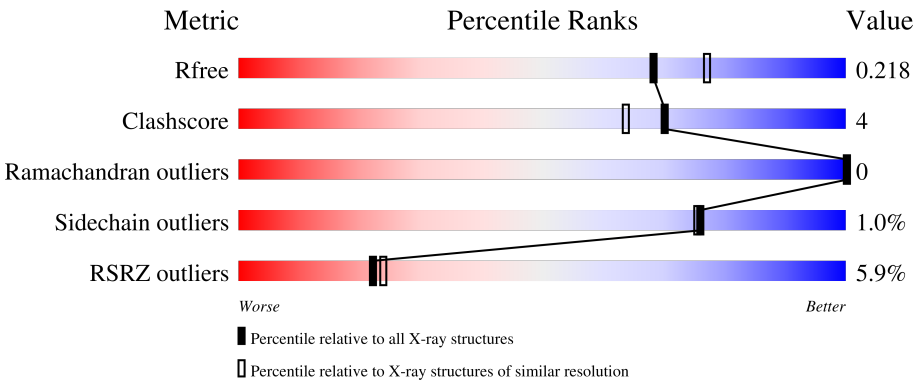
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	574	5% 84% 8% 8%
1	B	574	5% 84% 8% • 7%
1	C	574	5% 88% 6% • 5%
1	D	574	7% 84% 10% • 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16837 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	529	3959	2464	742	741	12	0	8	0
1	B	535	3951	2464	735	741	11	0	5	0
1	C	543	4020	2505	750	754	11	0	3	0
1	D	543	3988	2485	740	753	10	0	3	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11

Continued on next page...

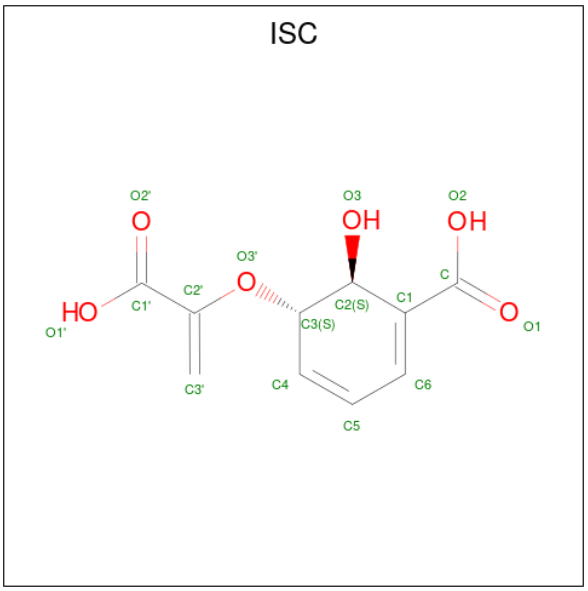
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

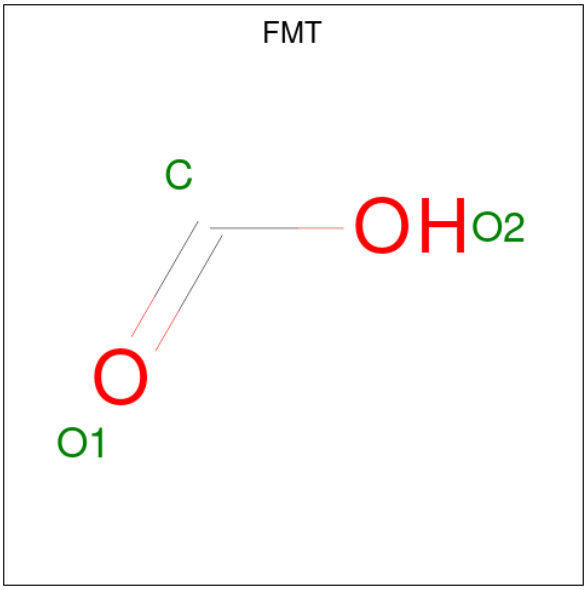
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is (5S,6S)-5-[(1-carboxyethenyl)oxy]-6-hydroxycyclohexa-1,3-diene-1-carboxylic acid (three-letter code: ISC) (formula: $C_{10}H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	16	10	6	0	0
			Total	C	O		
3	B	1	16	10	6	0	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



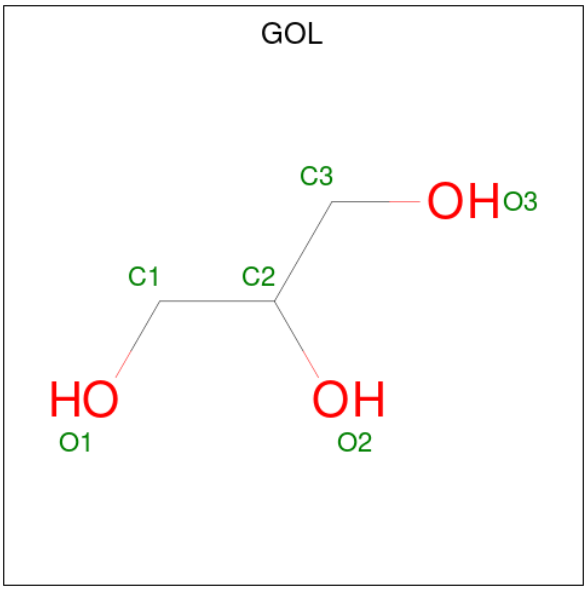
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	3	1	2	0	0
			Total	C	O		
4	B	1	3	1	2	0	0

Continued on next page...

Continued from previous page...

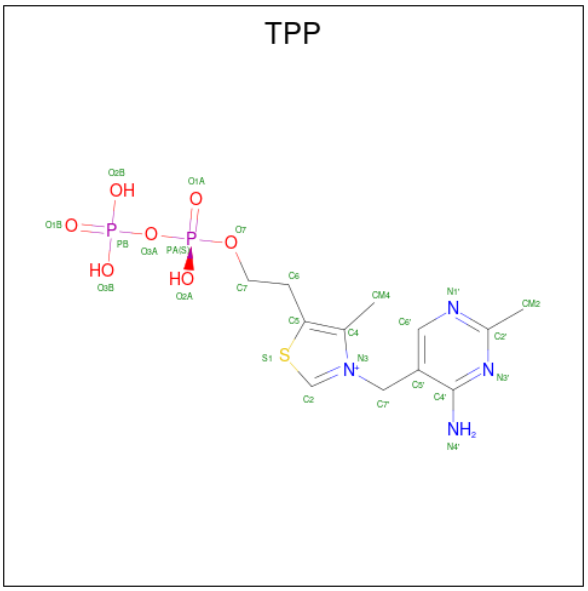
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	B	1	3	1	2		0	0
			Total	C	O			
4	C	1	3	1	2		0	0
			Total	C	O			
4	C	1	3	1	2		0	0
			Total	C	O			
4	C	1	3	1	2		0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



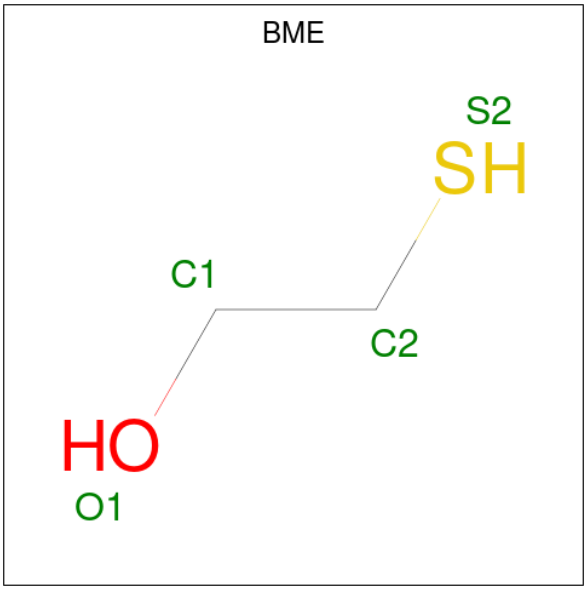
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	B	1	6	3	3		0	0

- Molecule 6 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	C	1	26	12	4	7	2	1	0	0
6	D	1	26	12	4	7	2	1	0	0

- Molecule 7 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	C	1	4	2	1	1	0	0
7	D	1	4	2	1	1	0	0

- Molecule 8 is water.

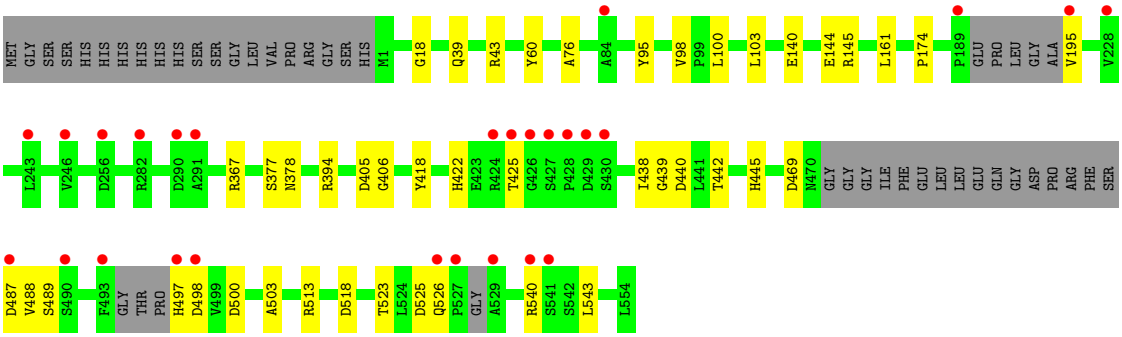
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	230	230	230	0	0
			Total	O		
8	B	200	200	200	0	0
			Total	O		
8	C	246	246	246	0	0
			Total	O		
8	D	111	111	111	0	0

3 Residue-property plots (i)

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

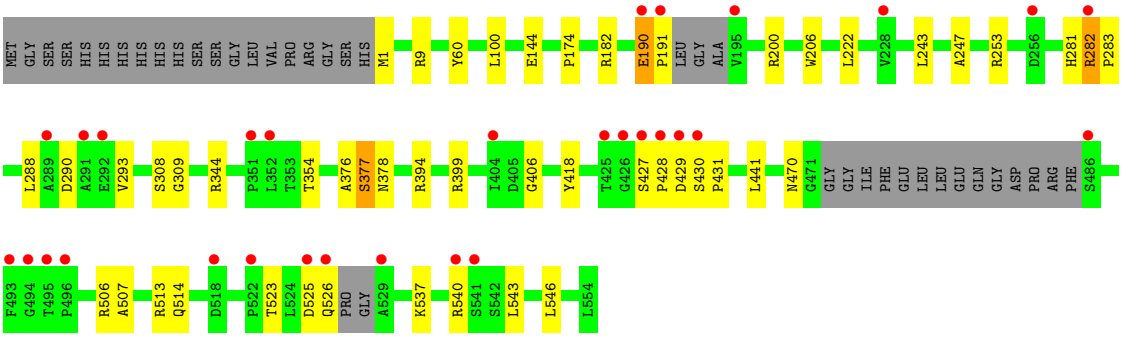
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain A:



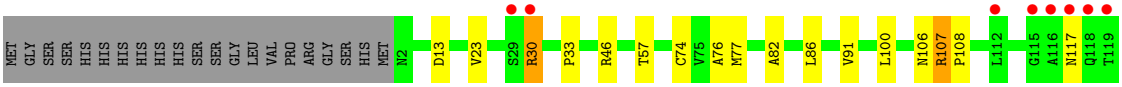
• Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

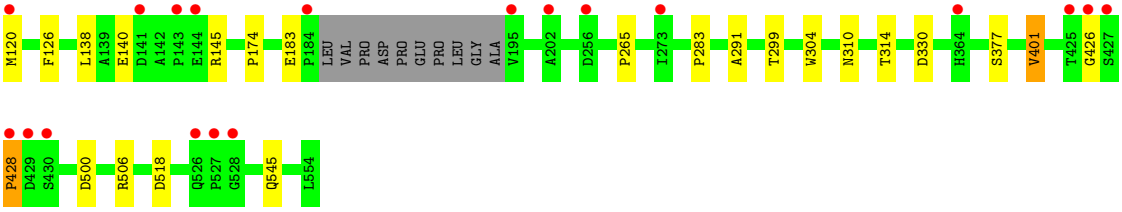
Chain B:



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

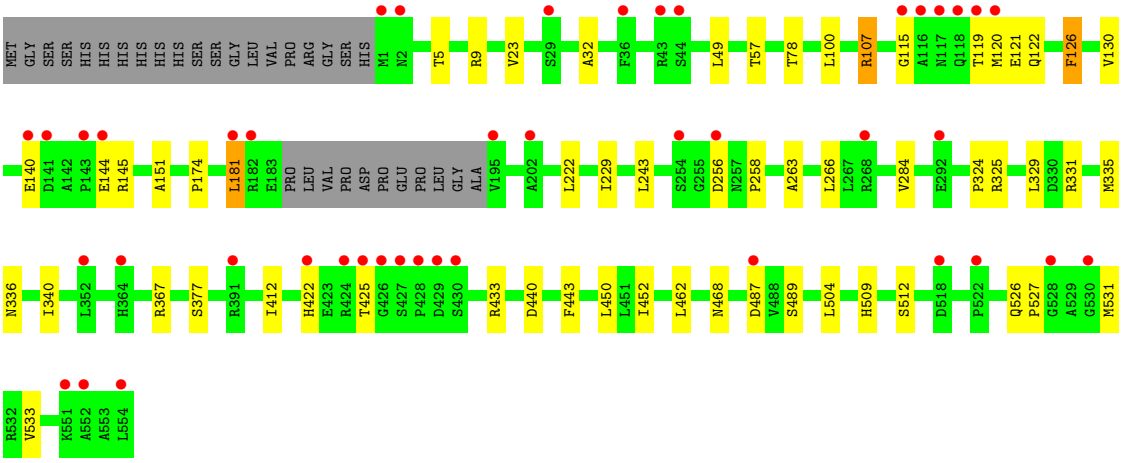
Chain C:





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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.44Å 139.59Å 181.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.05 19.81 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-2.05) 100.0 (19.81-2.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.06Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.219 0.191 , 0.218	Depositor DCC
R_{free} test set	8144 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16837	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BME, TPP, FMT, MG, ISC

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	0.28	1/4043 (0.0%)	0.46	0/5532
1	B	0.26	0/4046	0.49	2/5541 (0.0%)
1	C	0.28	0/4107	0.48	1/5621 (0.0%)
1	D	0.28	0/4073	0.51	1/5580 (0.0%)
All	All	0.27	1/16269 (0.0%)	0.49	4/22274 (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	B	0	2
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	VAL	C-N	5.05	1.43	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	429	ASP	N-CA-C	-5.94	94.97	111.00
1	D	181	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	B	190	GLU	C-N-CD	-5.19	109.18	120.60
1	C	107	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	427	SER	Peptide
1	B	428	PRO	Peptide
1	C	428	PRO	Peptide
1	D	115	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3959	0	4001	30	0
1	B	3951	0	4003	35	1
1	C	4020	0	4048	24	1
1	D	3988	0	3997	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	16	0	8	0	0
3	B	16	0	8	0	0
4	A	3	0	1	0	0
4	B	6	0	2	0	0
4	C	9	0	3	0	0
5	A	12	0	16	0	0
5	B	6	0	8	2	0
6	C	26	0	16	0	0
6	D	26	0	16	0	0
7	C	4	0	5	2	0
7	D	4	0	5	0	0
8	A	230	0	0	1	0
8	B	200	0	0	0	0
8	C	246	0	0	1	0
8	D	111	0	0	0	0
All	All	16837	0	16137	115	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 4.

All (115) 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:367:ARG:NH2	1:A:525:ASP:OD1	2.00	0.93
1:A:140:GLU:OE1	1:A:145:ARG:NH1	2.07	0.88
1:D:120:MET:SD	1:D:122:GLN:NE2	2.50	0.84
1:D:526:GLN:NE2	1:D:527:PRO:O	2.13	0.81
1:C:140:GLU:OE2	1:C:145:ARG:NH2	2.13	0.81
1:B:506:ARG:HE	1:C:506:ARG:HH12	1.31	0.79
1:A:39[B]:GLN:OE1	1:A:43[B]:ARG:NH1	2.17	0.76
1:B:377:SER:OG	1:B:378:ASN:N	2.15	0.75
1:C:77:MET:HE3	1:C:86:LEU:HD12	1.70	0.73
1:C:117:ASN:OD1	1:C:120:MET:N	2.16	0.73
1:A:422:HIS:O	1:A:425:THR:OG1	2.07	0.70
1:C:30[B]:ARG:NH1	1:C:183:GLU:OE1	2.27	0.67
1:D:422:HIS:O	1:D:425:THR:OG1	2.12	0.65
1:B:247:ALA:HB3	5:B:605:GOL:H31	1.78	0.65
1:B:282[B]:ARG:HG2	1:B:283:PRO:HD3	1.78	0.65
1:C:33:PRO:HD2	1:C:76:ALA:HB1	1.79	0.63
1:B:470:ASN:O	1:B:540:ARG:NH1	2.32	0.63
1:B:543:LEU:HD12	1:B:546:LEU:HB3	1.82	0.61
1:D:140:GLU:OE1	1:D:145:ARG:NH1	2.34	0.60
1:B:282[A]:ARG:HG2	1:B:283:PRO:HD3	1.84	0.59
1:A:145:ARG:NH1	1:B:182:ARG:HH12	2.01	0.58
1:C:30[B]:ARG:NH1	1:C:107:ARG:HE	2.00	0.58
1:A:500:ASP:OD2	1:A:503:ALA:N	2.34	0.58
1:B:523:THR:O	1:B:526:GLN:HG2	2.04	0.58
1:A:487:ASP:OD1	1:A:489:SER:N	2.26	0.57
1:D:107[B]:ARG:NH1	1:D:119:THR:HG21	2.19	0.57
1:D:336:ASN:O	1:D:340:ILE:HG13	2.05	0.57
1:B:1:MET:SD	1:B:9:ARG:NH1	2.77	0.57
1:D:256:ASP:O	1:D:258:PRO:HD3	2.06	0.56
1:A:498:ASP:O	1:D:509:HIS:NE2	2.26	0.56
1:A:377:SER:OG	1:A:378:ASN:N	2.39	0.55
1:D:412:ILE:HD13	1:D:452:ILE:HD11	1.89	0.55
1:A:440:ASP:OD2	1:A:497:HIS:NE2	2.35	0.54
1:C:426:GLY:O	1:C:428:PRO:HD3	2.08	0.54
1:B:376:ALA:O	1:B:399:ARG:NH1	2.41	0.54
1:A:469:ASP:O	1:A:540:ARG:NH1	2.42	0.53
1:B:354:THR:HG21	1:B:543:LEU:HD13	1.90	0.53
1:B:281:HIS:HB3	1:B:283:PRO:HD2	1.89	0.53
1:D:440:ASP:HB3	1:D:468:ASN:HA	1.91	0.53
1:C:304:TRP:CG	1:C:314:THR:HG21	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:CD	1:A:145:ARG:HH12	2.11	0.52
1:D:487:ASP:OD1	1:D:487:ASP:N	2.40	0.51
1:A:377:SER:OG	8:A:701:HOH:O	2.18	0.51
1:D:229:ILE:HD13	1:D:284:VAL:HG13	1.92	0.50
1:C:106:ASN:OD1	1:C:120:MET:HE1	2.11	0.50
1:B:513:ARG:NH1	1:B:526:GLN:OE1	2.46	0.48
1:A:18:GLY:HA3	1:A:161:LEU:HD13	1.96	0.48
1:B:514:GLN:OE1	1:B:537:LYS:HE3	2.14	0.48
1:D:23:VAL:HB	1:D:49:LEU:HD23	1.95	0.48
1:B:394:ARG:HD3	1:B:418:TYR:CE1	2.48	0.48
1:D:324:PRO:HG2	1:D:329:LEU:HD11	1.95	0.48
1:A:487:ASP:OD1	1:A:488:VAL:N	2.47	0.48
1:C:108:PRO:HG2	1:C:138:LEU:HD22	1.95	0.47
1:B:100:LEU:O	1:B:174:PRO:HA	2.15	0.47
1:D:107[B]:ARG:NH2	1:D:181:LEU:HD21	2.29	0.47
1:C:100:LEU:O	1:C:174:PRO:HA	2.14	0.47
1:D:462:LEU:HD23	1:D:531:MET:HG2	1.96	0.47
1:B:282[A]:ARG:HG3	1:B:282[A]:ARG:HH11	1.80	0.46
1:A:438:ILE:HG22	1:A:439:GLY:O	2.14	0.46
1:A:405:ASP:OD1	1:A:445:HIS:NE2	2.34	0.46
1:B:60:TYR:CG	1:B:406:GLY:HA3	2.51	0.46
1:A:144:GLU:OE1	1:A:144:GLU:N	2.36	0.46
1:B:288:LEU:HB3	1:B:308:SER:HB2	1.98	0.46
1:B:430:SER:HB2	1:B:431:PRO:HD2	1.97	0.46
1:C:91:VAL:HG12	1:C:401:VAL:HG21	1.97	0.46
1:A:60:TYR:CG	1:A:406:GLY:HA3	2.51	0.46
1:C:76:ALA:O	7:C:606:BME:H21	2.16	0.46
1:C:265:PRO:HG3	1:C:283:PRO:HB3	1.97	0.46
1:B:253:ARG:CZ	5:B:605:GOL:H32	2.46	0.45
1:D:450:LEU:O	1:D:452:ILE:HG13	2.16	0.45
1:A:523:THR:O	1:A:526:GLN:HG2	2.16	0.45
1:B:506:ARG:HE	1:C:506:ARG:NH1	2.08	0.45
1:B:282[A]:ARG:HG2	1:B:283:PRO:CD	2.46	0.45
1:B:190:GLU:HA	1:B:191:PRO:C	2.36	0.45
1:D:32:ALA:HA	1:D:78:THR:HG22	1.98	0.45
1:A:394:ARG:NE	1:A:418:TYR:HE1	2.15	0.45
1:C:13:ASP:OD1	1:C:46:ARG:NH1	2.42	0.45
1:A:394:ARG:NE	1:A:418:TYR:CE1	2.85	0.44
1:D:126:PHE:O	1:D:130:VAL:HG22	2.18	0.44
1:A:438:ILE:HG23	1:A:442:THR:HB	1.99	0.44
1:B:290:ASP:OD1	1:B:293:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107[B]:ARG:HH22	1:D:181:LEU:HD21	1.82	0.44
1:D:512:SER:HA	1:D:533:VAL:O	2.18	0.44
1:C:77:MET:HB2	1:C:82:ALA:HB1	1.99	0.44
1:A:144:GLU:H	1:A:144:GLU:CD	2.18	0.44
1:B:144:GLU:OE1	1:B:144:GLU:N	2.28	0.44
1:B:200:ARG:HG2	1:B:206:TRP:HA	2.00	0.44
1:B:222:LEU:HD22	1:B:243:LEU:HD11	1.99	0.43
1:D:263:ALA:HA	1:D:266:LEU:HD12	1.99	0.43
1:D:367:ARG:NE	1:D:433:ARG:HH22	2.15	0.43
1:A:76:ALA:HA	1:A:103:LEU:O	2.18	0.43
1:B:282[A]:ARG:HH11	1:B:282[A]:ARG:CG	2.32	0.43
1:C:291:ALA:HA	1:C:310:ASN:OD1	2.19	0.43
1:C:86:LEU:HD11	7:C:606:BME:H11	2.01	0.42
1:A:543:LEU:HD23	1:A:543:LEU:HA	1.81	0.42
1:C:107:ARG:HG2	1:C:107:ARG:HH11	1.83	0.42
1:D:222:LEU:HD22	1:D:243:LEU:HD11	2.01	0.42
1:D:331:ARG:O	1:D:335:MET:HG2	2.19	0.42
1:D:325:ARG:O	1:D:329:LEU:HD12	2.19	0.42
1:D:526:GLN:HA	1:D:527:PRO:HD3	1.83	0.42
1:A:95:TYR:OH	1:D:121:GLU:OE2	2.35	0.42
1:B:309:GLY:O	1:D:151:ALA:HB1	2.19	0.42
1:C:299:THR:HG23	8:C:708:HOH:O	2.19	0.42
1:D:144:GLU:OE1	1:D:144:GLU:N	2.37	0.42
1:A:195:VAL:O	1:A:195:VAL:HG13	2.20	0.42
1:A:100:LEU:O	1:A:174:PRO:HA	2.20	0.41
1:B:282[B]:ARG:HG2	1:B:283:PRO:CD	2.48	0.41
1:B:507:ALA:HA	1:C:500:ASP:HB3	2.00	0.41
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.78	0.41
1:D:5:THR:HG22	1:D:9:ARG:NH2	2.36	0.41
1:C:23:VAL:HG22	1:C:74:CYS:HB2	2.03	0.41
1:A:513:ARG:HE	1:A:513:ARG:HB2	1.65	0.40
1:B:200:ARG:CG	1:B:206:TRP:HA	2.51	0.40
1:D:100:LEU:O	1:D:174:PRO:HA	2.21	0.40
1:D:443:PHE:HE2	1:D:504:LEU:HD23	1.86	0.40

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:B:344:ARG:NH1	1:C:330:ASP:OD2[2_654]	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	527/574 (92%)	519 (98%)	8 (2%)	0	100	100
1	B	532/574 (93%)	520 (98%)	12 (2%)	0	100	100
1	C	542/574 (94%)	530 (98%)	12 (2%)	0	100	100
1	D	542/574 (94%)	527 (97%)	15 (3%)	0	100	100
All	All	2143/2296 (93%)	2096 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/445 (94%)	418 (100%)	1 (0%)	93	94
1	B	418/445 (94%)	414 (99%)	4 (1%)	76	75
1	C	422/445 (95%)	414 (98%)	8 (2%)	57	53
1	D	416/445 (94%)	410 (99%)	6 (1%)	67	65
All	All	1675/1780 (94%)	1656 (99%)	19 (1%)	76	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	ASP
1	B	282[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	282[B]	ARG
1	B	377	SER
1	B	525	ASP
1	C	30[A]	ARG
1	C	30[B]	ARG
1	C	57	THR
1	C	126	PHE
1	C	377	SER
1	C	401	VAL
1	C	518	ASP
1	C	545	GLN
1	D	57	THR
1	D	107[A]	ARG
1	D	107[B]	ARG
1	D	126	PHE
1	D	377	SER
1	D	489	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	FMT	A	603	-	2,2,2	0.67	0	1,1,1	0.66	0
7	BME	C	606	1	3,3,3	0.80	0	1,2,2	1.05	0
4	FMT	C	603	-	2,2,2	0.68	0	1,1,1	0.62	0
4	FMT	C	604	-	2,2,2	0.67	0	1,1,1	0.67	0
7	BME	D	603	1	3,3,3	0.79	0	1,2,2	0.91	0
6	TPP	D	602	2	22,27,27	1.45	3 (13%)	29,40,40	2.04	7 (24%)
4	FMT	C	602	-	2,2,2	0.66	0	1,1,1	0.69	0
3	ISC	A	602	-	15,16,16	1.60	2 (13%)	15,22,22	1.12	1 (6%)
4	FMT	B	603	-	2,2,2	0.68	0	1,1,1	0.62	0
5	GOL	B	605	-	5,5,5	0.39	0	5,5,5	0.40	0
5	GOL	A	605	-	5,5,5	0.35	0	5,5,5	0.44	0
3	ISC	B	602	-	15,16,16	1.57	2 (13%)	15,22,22	1.30	1 (6%)
5	GOL	A	604	-	5,5,5	0.40	0	5,5,5	0.37	0
6	TPP	C	605	2	22,27,27	1.46	2 (9%)	29,40,40	2.09	7 (24%)
4	FMT	B	604	2	2,2,2	0.69	0	1,1,1	0.63	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
7	BME	C	606	1	-	1/1/1/1	-
7	BME	D	603	1	-	1/1/1/1	-
6	TPP	D	602	2	-	2/16/17/17	0/2/2/2
3	ISC	A	602	-	-	0/10/26/26	0/1/1/1
5	GOL	B	605	-	-	2/4/4/4	-
5	GOL	A	605	-	-	0/4/4/4	-
5	GOL	A	604	-	-	0/4/4/4	-
3	ISC	B	602	-	-	2/10/26/26	0/1/1/1
6	TPP	C	605	2	-	1/16/17/17	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	TPP	C4-N3	-5.00	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	602	TPP	C4-N3	-4.78	1.35	1.39
6	C	605	TPP	C5'-C4'	3.47	1.48	1.42
6	D	602	TPP	C5'-C4'	3.37	1.48	1.42
3	A	602	ISC	C2'-C1'	-2.97	1.46	1.49
3	A	602	ISC	O3'-C2'	2.93	1.46	1.36
3	B	602	ISC	C2'-C1'	-2.91	1.46	1.49
3	B	602	ISC	O3'-C2'	2.91	1.46	1.36
6	D	602	TPP	C6-C5	2.29	1.51	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	605	TPP	C6-C5-C4	7.41	133.38	127.43
6	D	602	TPP	C6-C5-C4	6.69	132.80	127.43
6	D	602	TPP	C6'-N1'-C2'	3.99	122.75	115.96
6	C	605	TPP	C6'-N1'-C2'	3.90	122.60	115.96
3	B	602	ISC	O1'-C1'-C2'	2.93	118.91	113.91
6	D	602	TPP	C5'-C6'-N1'	-2.83	119.11	123.82
3	A	602	ISC	O1'-C1'-C2'	2.72	118.54	113.91
6	C	605	TPP	C5'-C6'-N1'	-2.71	119.31	123.82
6	C	605	TPP	N4'-C4'-N3'	2.50	120.56	117.03
6	D	602	TPP	N4'-C4'-N3'	2.47	120.53	117.03
6	D	602	TPP	N1'-C2'-N3'	-2.38	121.45	125.54
6	C	605	TPP	N1'-C2'-N3'	-2.38	121.45	125.54
6	D	602	TPP	PA-O3A-PB	-2.22	125.22	132.83
6	D	602	TPP	CM4-C4-N3	2.19	125.33	122.53
6	C	605	TPP	PA-O3A-PB	-2.16	125.42	132.83
6	C	605	TPP	CM4-C4-N3	2.07	125.17	122.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	605	GOL	C1-C2-C3-O3
6	C	605	TPP	PA-O3A-PB-O2B
6	D	602	TPP	PA-O3A-PB-O2B
7	C	606	BME	O1-C1-C2-S2
7	D	603	BME	O1-C1-C2-S2
5	B	605	GOL	O2-C2-C3-O3
3	B	602	ISC	O2-C-C1-C6
3	B	602	ISC	O2-C-C1-C2
6	D	602	TPP	PA-O3A-PB-O1B

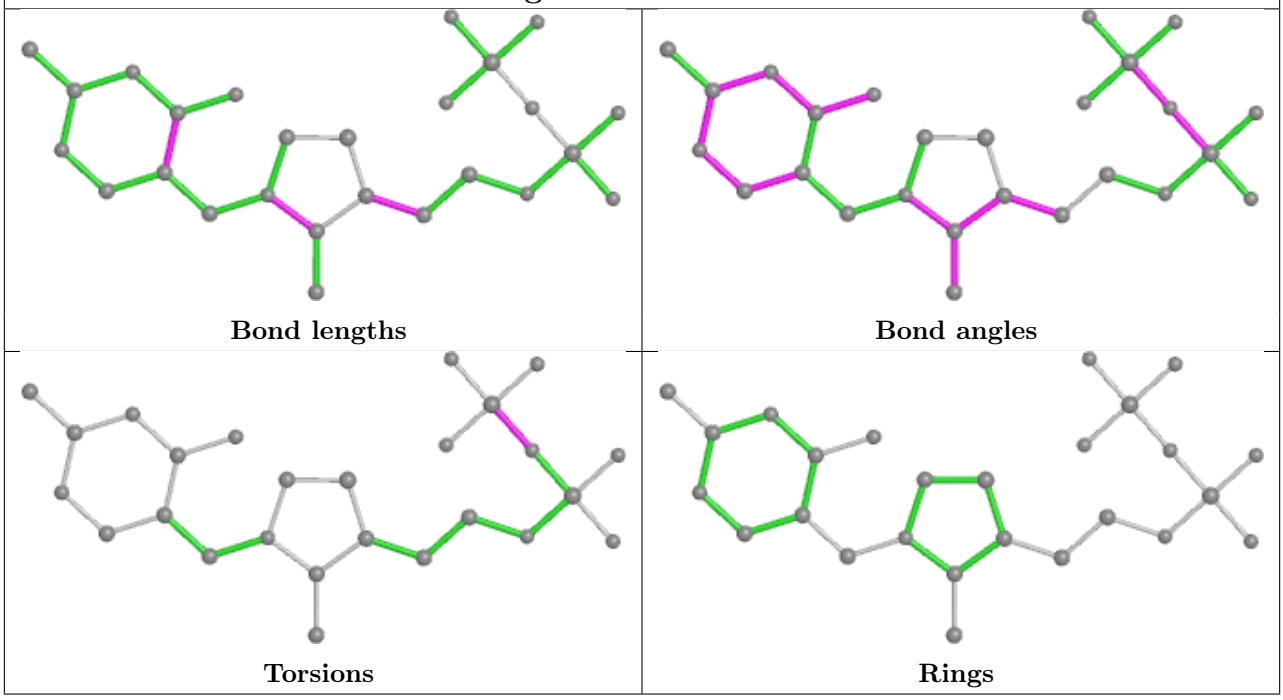
There are no ring outliers.

2 monomers are involved in 4 short contacts:

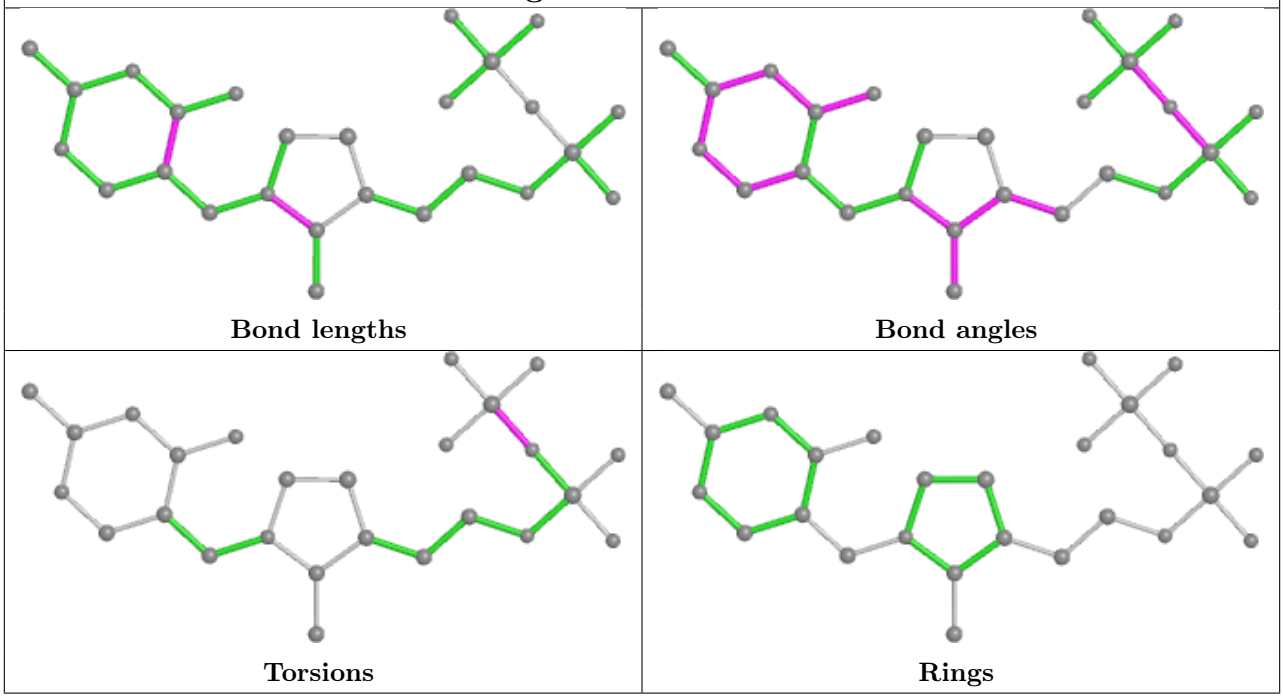
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	606	BME	2	0
5	B	605	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TPP D 602



Ligand TPP C 605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	529/574 (92%)	-0.02	27 (5%)	28	30	27, 42, 69, 102	0
1	B	535/574 (93%)	0.11	30 (5%)	24	26	26, 44, 73, 110	0
1	C	543/574 (94%)	-0.03	27 (4%)	28	31	26, 41, 69, 96	0
1	D	543/574 (94%)	0.25	43 (7%)	12	13	32, 52, 77, 111	0
All	All	2150/2296 (93%)	0.08	127 (5%)	22	24	26, 45, 74, 111	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	PRO	7.4
1	C	195	VAL	6.7
1	B	428	PRO	6.7
1	D	195	VAL	6.0
1	B	429	ASP	6.0
1	A	428	PRO	5.8
1	A	493	PHE	5.7
1	D	119	THR	5.6
1	B	425	THR	5.5
1	D	426	GLY	5.2
1	C	119	THR	5.0
1	D	117	ASN	5.0
1	D	118	GLN	4.9
1	A	426	GLY	4.9
1	D	116	ALA	4.8
1	D	1	MET	4.8
1	C	184	PRO	4.8
1	B	496	PRO	4.7
1	C	118	GLN	4.7
1	B	291	ALA	4.5
1	D	29	SER	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	425	THR	4.4
1	C	428	PRO	4.4
1	D	430	SER	4.4
1	C	116	ALA	4.3
1	B	195	VAL	4.3
1	A	425	THR	4.3
1	B	494	GLY	4.3
1	D	429	ASP	4.2
1	B	191	PRO	4.1
1	A	430	SER	4.1
1	D	120	MET	4.0
1	B	493	PHE	4.0
1	C	427	SER	3.9
1	D	36	PHE	3.9
1	C	426	GLY	3.9
1	B	426	GLY	3.9
1	A	429	ASP	3.8
1	B	430	SER	3.8
1	D	425	THR	3.8
1	A	424	ARG	3.7
1	C	429	ASP	3.7
1	C	117	ASN	3.7
1	A	527	PRO	3.6
1	C	120	MET	3.6
1	C	527	PRO	3.6
1	B	427	SER	3.5
1	B	495	THR	3.5
1	A	498	ASP	3.5
1	A	195	VAL	3.5
1	B	529	ALA	3.5
1	B	289	ALA	3.4
1	B	282[A]	ARG	3.4
1	C	115	GLY	3.4
1	B	351	PRO	3.4
1	D	256	ASP	3.2
1	D	554	LEU	3.2
1	B	541	SER	3.2
1	D	427	SER	3.1
1	D	352	LEU	3.1
1	D	115	GLY	3.0
1	B	486	SER	3.0
1	D	552	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	30[A]	ARG	2.9
1	A	526	GLN	2.9
1	C	430	SER	2.9
1	D	2	ASN	2.9
1	B	190	GLU	2.9
1	A	282[A]	ARG	2.8
1	D	530	GLY	2.8
1	B	256	ASP	2.8
1	A	497	HIS	2.8
1	D	528	GLY	2.8
1	D	487	ASP	2.7
1	B	540	ARG	2.7
1	A	490	SER	2.7
1	D	43	ARG	2.7
1	C	141	ASP	2.6
1	C	144	GLU	2.6
1	D	143	PRO	2.6
1	C	526	GLN	2.6
1	A	256	ASP	2.6
1	B	518	ASP	2.5
1	A	291	ALA	2.5
1	D	202	ALA	2.5
1	B	525	ASP	2.5
1	A	228	VAL	2.5
1	B	522	PRO	2.5
1	B	404	ILE	2.5
1	A	84	ALA	2.5
1	B	526	GLN	2.4
1	C	29	SER	2.4
1	D	424	ARG	2.4
1	A	427	SER	2.4
1	D	391	ARG	2.4
1	D	364	HIS	2.4
1	A	246	VAL	2.3
1	A	540	ARG	2.3
1	A	541	SER	2.3
1	D	292	GLU	2.3
1	C	143	PRO	2.3
1	D	268	ARG	2.3
1	D	551	LYS	2.3
1	B	352	LEU	2.3
1	A	529	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	181	LEU	2.2
1	D	518	ASP	2.2
1	A	189	PRO	2.2
1	C	256	ASP	2.2
1	C	528	GLY	2.2
1	D	522	PRO	2.2
1	D	422	HIS	2.2
1	D	141	ASP	2.2
1	A	487	ASP	2.2
1	D	182	ARG	2.2
1	C	112	LEU	2.1
1	B	228	VAL	2.1
1	B	292	GLU	2.1
1	D	144	GLU	2.1
1	A	290	ASP	2.1
1	C	202	ALA	2.1
1	A	243	LEU	2.1
1	D	140	GLU	2.1
1	D	44	SER	2.0
1	C	273	ILE	2.0
1	D	254	SER	2.0
1	C	364[A]	HIS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	BME	C	606	4/4	0.72	0.28	48,54,56,73	0

Continued on next page...

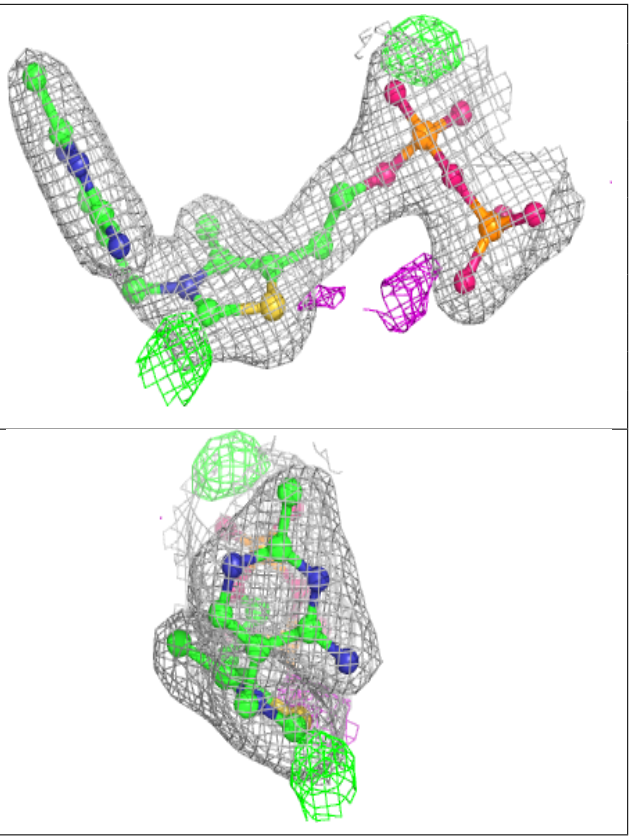
Continued from previous page...

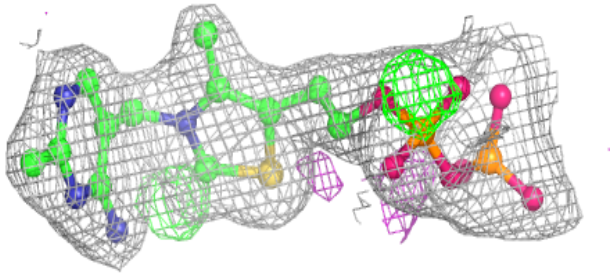
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ISC	A	602	16/16	0.76	0.26	48,66,72,74	0
5	GOL	B	605	6/6	0.81	0.17	50,55,59,62	0
2	MG	B	601	1/1	0.87	0.10	52,52,52,52	0
5	GOL	A	604	6/6	0.87	0.12	44,51,52,57	0
3	ISC	B	602	16/16	0.91	0.12	38,51,59,63	0
4	FMT	B	603	3/3	0.91	0.10	51,51,55,57	0
4	FMT	C	602	3/3	0.91	0.11	38,38,46,48	0
4	FMT	A	603	3/3	0.92	0.10	45,45,46,46	0
4	FMT	B	604	3/3	0.94	0.07	51,51,55,61	0
5	GOL	A	605	6/6	0.94	0.21	48,56,62,66	0
2	MG	C	601	1/1	0.94	0.09	32,32,32,32	0
4	FMT	C	604	3/3	0.94	0.08	43,43,54,57	0
4	FMT	C	603	3/3	0.96	0.11	56,56,60,71	0
7	BME	D	603	4/4	0.96	0.08	56,57,61,61	0
6	TPP	D	602	26/26	0.97	0.07	39,46,52,56	0
2	MG	D	601	1/1	0.98	0.08	42,42,42,42	0
6	TPP	C	605	26/26	0.99	0.08	25,33,35,35	0
2	MG	A	601	1/1	0.99	0.05	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TPP D 602:

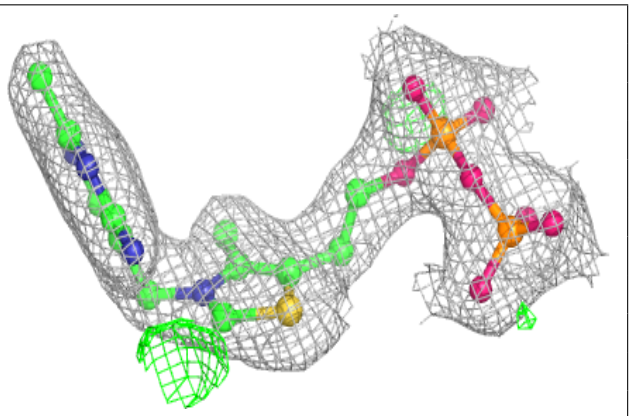
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

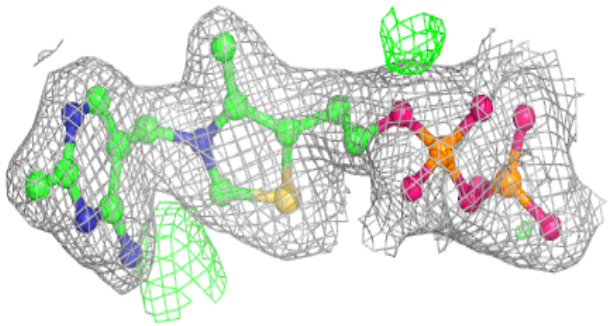


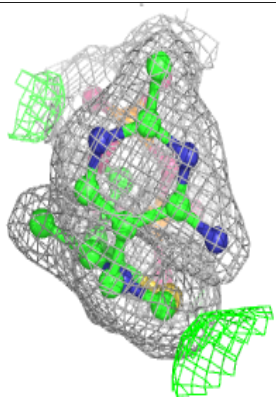


Electron density around TPP C 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.