



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 04:14 AM UTC

PDB ID : 3FA3 / pdb_00003fa3
Title : Crystal structure of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member, trigonal crystal form
Authors : Narayanan, B.C.; Herzberg, O.
Deposited on : 2008-11-14
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

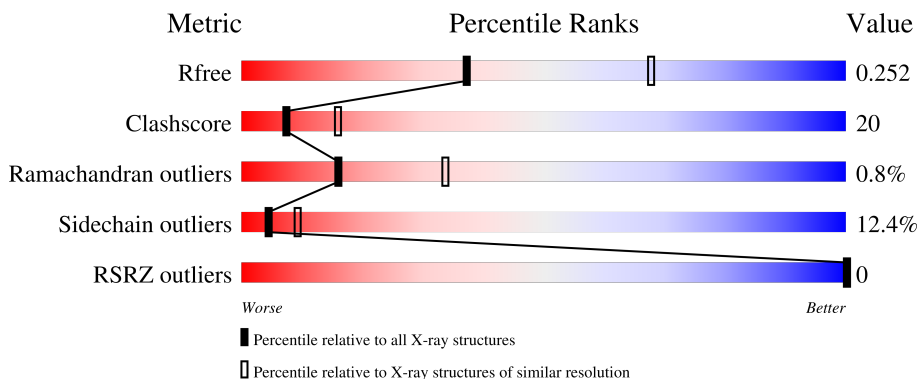
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	 64% 28% 7% .
1	B	302	 62% 32% 6%
1	C	302	 60% 32% 7%
1	D	302	 66% 30% .
1	E	302	 64% 30% 5% .

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Mol	Chain	Length	Quality of chain		
1	F	302	61%	31%	8%
1	G	302	63%	31%	5%
1	H	302	59%	36%	• •
1	I	302	58%	35%	6% •
1	J	302	57%	33%	7% •
1	K	302	58%	35%	6% •
1	L	302	51%	40%	8% •
1	M	302	55%	39%	6% •
1	N	302	54%	36%	6% • •
1	O	302	56%	38%	5% •
1	P	302	50%	42%	7% •

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	G	601	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 36360 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.

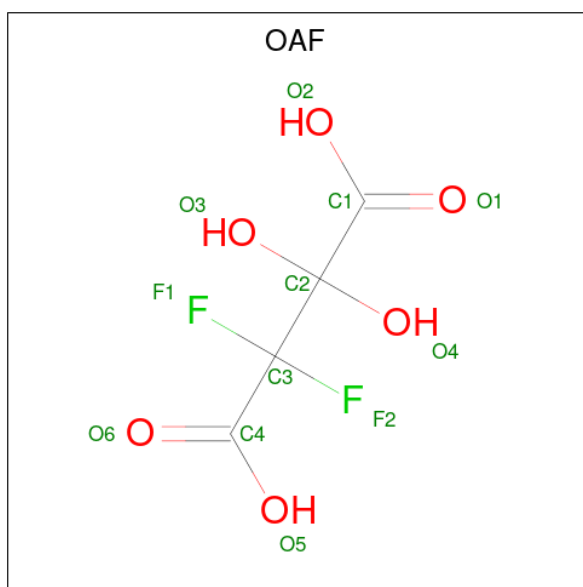
- Molecule 1 is a protein called 2,3-dimethylmalate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2222	1379	397	430	16	0	0	0
1	B	302	2230	1384	399	431	16	0	0	0
1	C	301	2228	1384	398	430	16	0	0	0
1	D	301	2226	1384	398	428	16	0	0	0
1	E	301	2228	1384	398	430	16	0	0	0
1	F	301	2224	1381	397	430	16	0	0	0
1	G	301	2228	1384	398	430	16	0	0	0
1	H	301	2228	1384	398	430	16	0	0	0
1	I	300	2216	1376	397	427	16	0	0	0
1	J	292	2162	1344	383	420	15	0	0	0
1	K	300	2218	1376	397	429	16	0	0	0
1	L	300	2215	1375	396	428	16	0	0	0
1	M	300	2220	1378	397	429	16	0	0	0
1	N	292	2161	1342	383	421	15	0	0	0
1	O	301	2211	1374	397	424	16	0	0	0
1	P	301	2225	1381	398	430	16	0	0	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

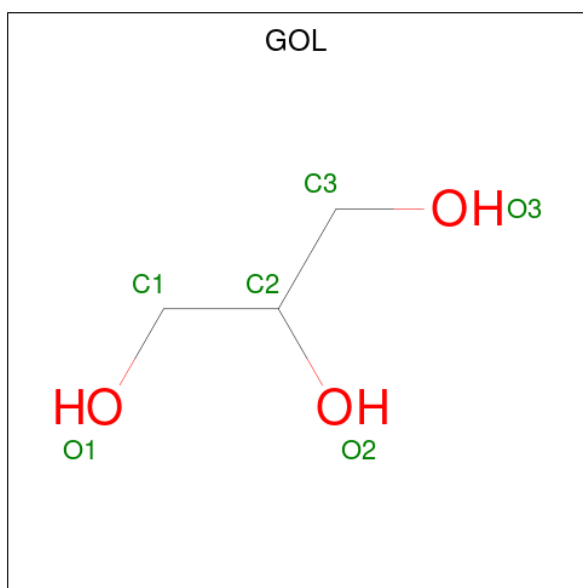
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	E	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	J	1	Total 1	Mn 1	0	0
2	K	1	Total 1	Mn 1	0	0
2	L	1	Total 1	Mn 1	0	0
2	M	1	Total 1	Mn 1	0	0
2	N	1	Total 1	Mn 1	0	0
2	O	1	Total 1	Mn 1	0	0
2	P	1	Total 1	Mn 1	0	0

- Molecule 3 is 2,2-difluoro-3,3-dihydroxybutanedioic acid (CCD ID: OAF) (formula: C₄H₄F₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	F			O
3	A	1	12	4	2	6	0	0
3	B	1	12	4	2	6	0	0
3	C	1	12	4	2	6	0	0
3	D	1	12	4	2	6	0	0
3	E	1	12	4	2	6	0	0
3	F	1	12	4	2	6	0	0
3	G	1	12	4	2	6	0	0
3	H	1	12	4	2	6	0	0
3	I	1	12	4	2	6	0	0
3	K	1	12	4	2	6	0	0
3	L	1	12	4	2	6	0	0
3	M	1	12	4	2	6	0	0
3	O	1	12	4	2	6	0	0
3	P	1	12	4	2	6	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	59	Total O 59 59	0	0
5	B	59	Total O 59 59	0	0
5	C	52	Total O 52 52	0	0
5	D	57	Total O 57 57	0	0
5	E	65	Total O 65 65	0	0
5	F	55	Total O 55 55	0	0

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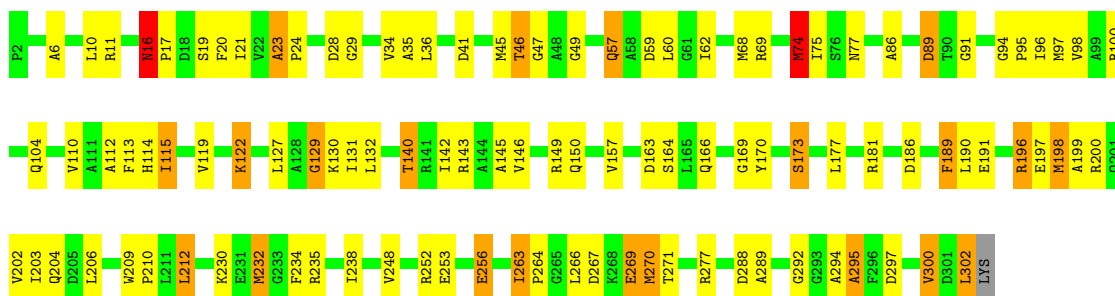
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	66	Total 66	O 66	0	0
5	H	68	Total 68	O 68	0	0
5	I	29	Total 29	O 29	0	0
5	J	29	Total 29	O 29	0	0
5	K	27	Total 27	O 27	0	0
5	L	24	Total 24	O 24	0	0
5	M	38	Total 38	O 38	0	0
5	N	28	Total 28	O 28	0	0
5	O	24	Total 24	O 24	0	0
5	P	24	Total 24	O 24	0	0

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.

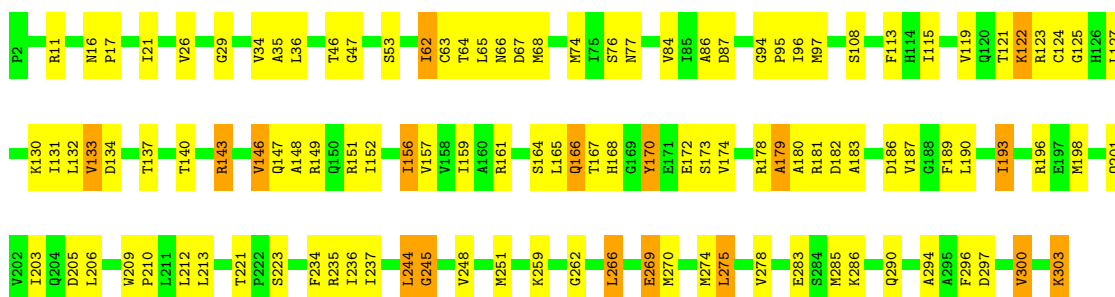
- Molecule 1: 2,3-dimethylmalate lyase

Chain A: 



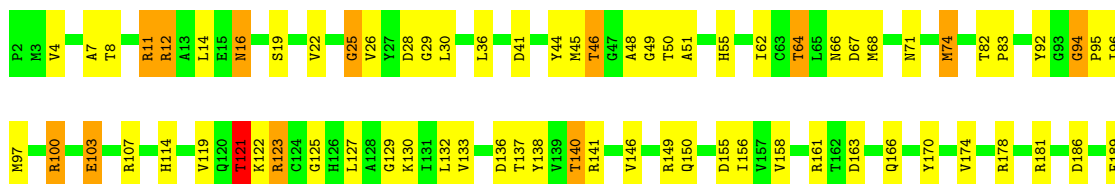
- Molecule 1: 2,3-dimethylmalate lyase

Chain B: 



- Molecule 1: 2,3-dimethylmalate lyase

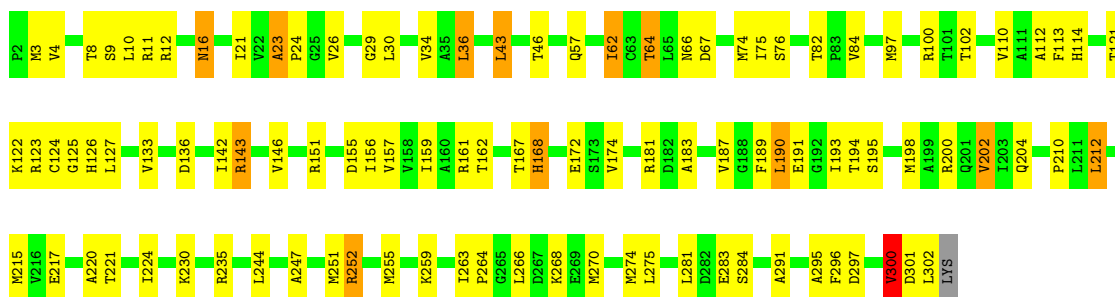
Chain C: 





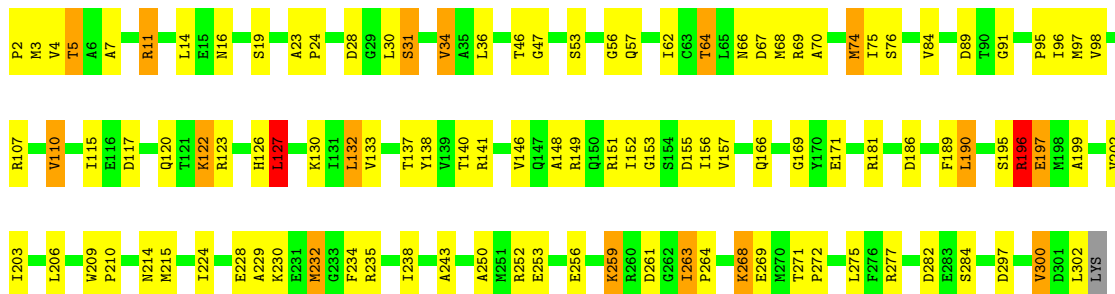
- Molecule 1: 2,3-dimethylmalate lyase

Chain D: 66% 30%



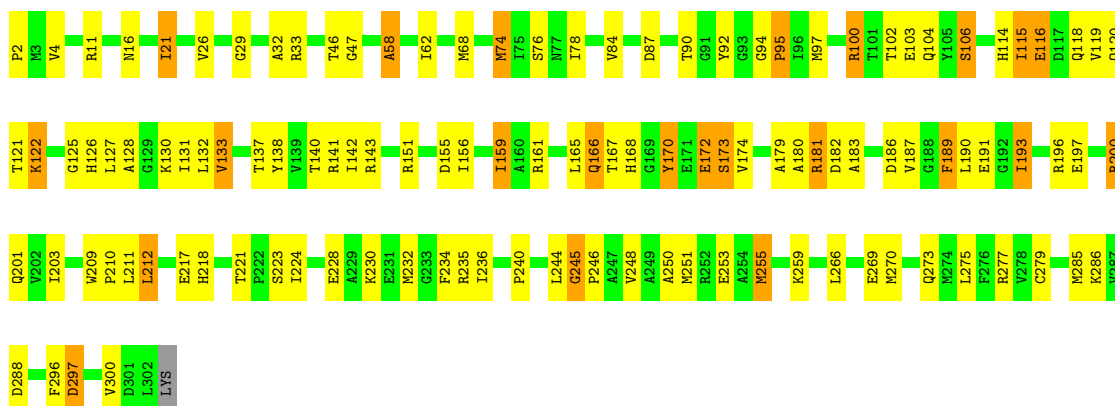
- Molecule 1: 2,3-dimethylmalate lyase

Chain E: 64% 30% 5%



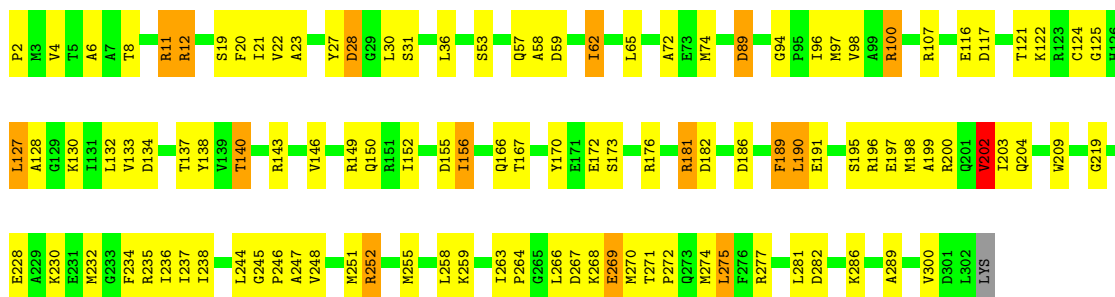
- Molecule 1: 2,3-dimethylmalate lyase

Chain F: 61% 31% 8%



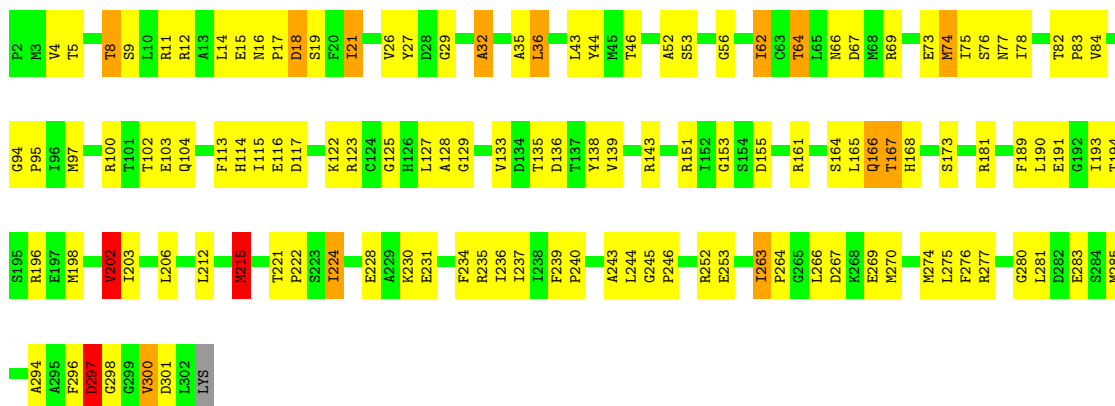
- Molecule 1: 2,3-dimethylmalate lyase

Chain G:  63% 31% 5%



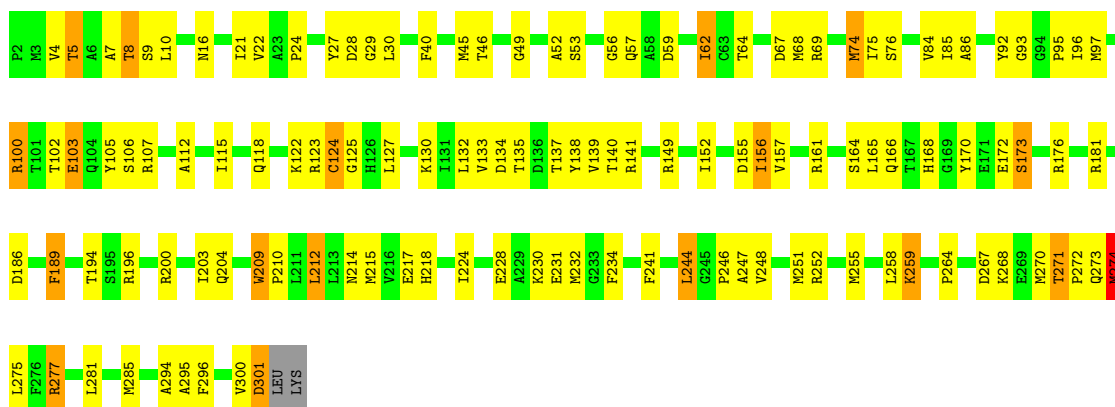
• Molecule 1: 2,3-dimethylmalate lyase

Chain H:  59% 36% 5%



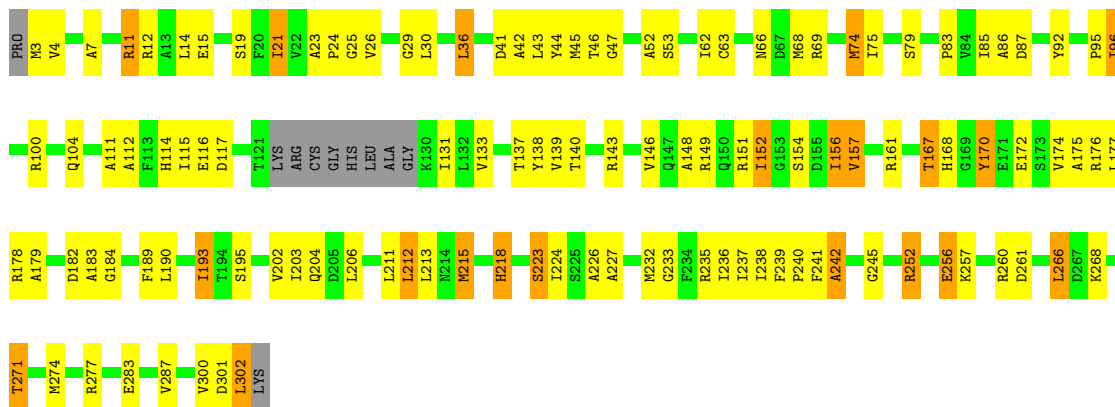
• Molecule 1: 2,3-dimethylmalate lyase

Chain I:  58% 35% 6%



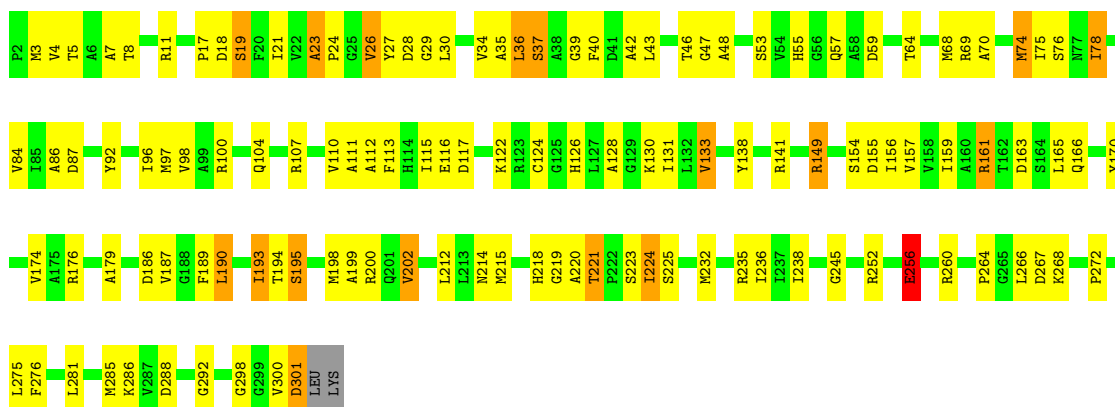
• Molecule 1: 2,3-dimethylmalate lyase

Chain J:  57% 33% 7%



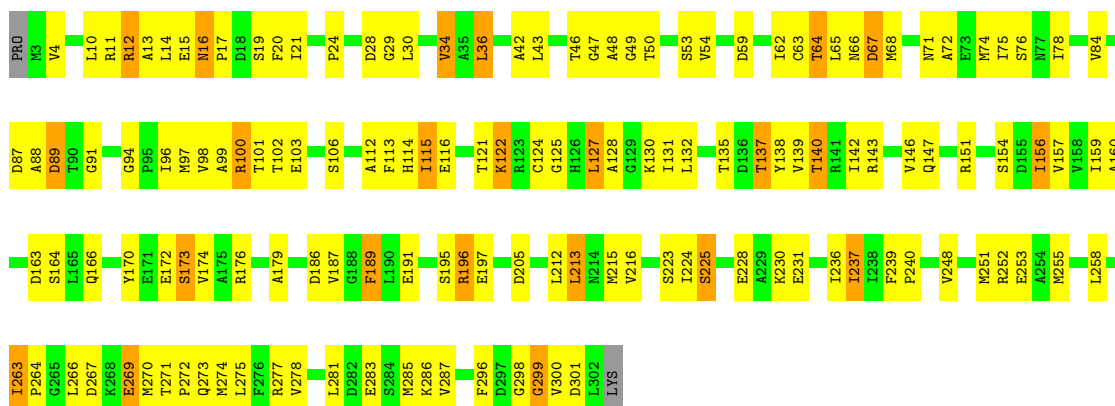
- Molecule 1: 2,3-dimethylmalate lyase

Chain K: 58% 35% 6%



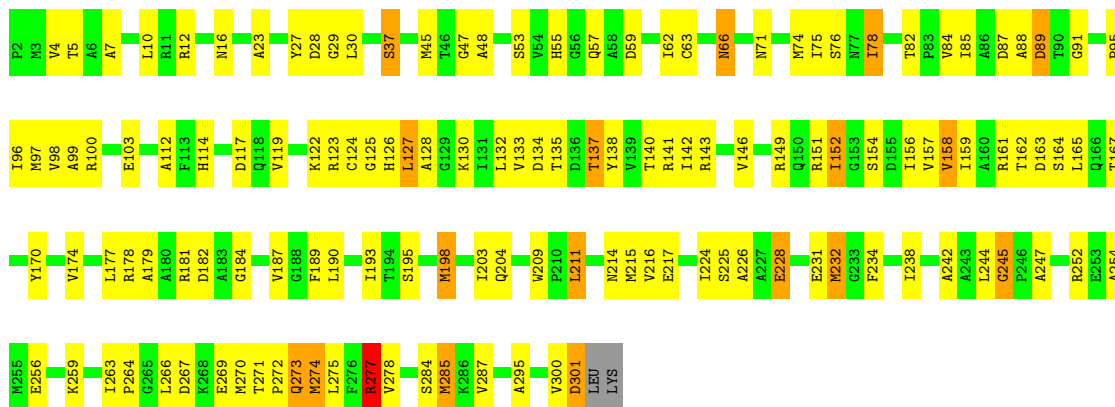
- Molecule 1: 2,3-dimethylmalate lyase

Chain L: 51% 40% 8%



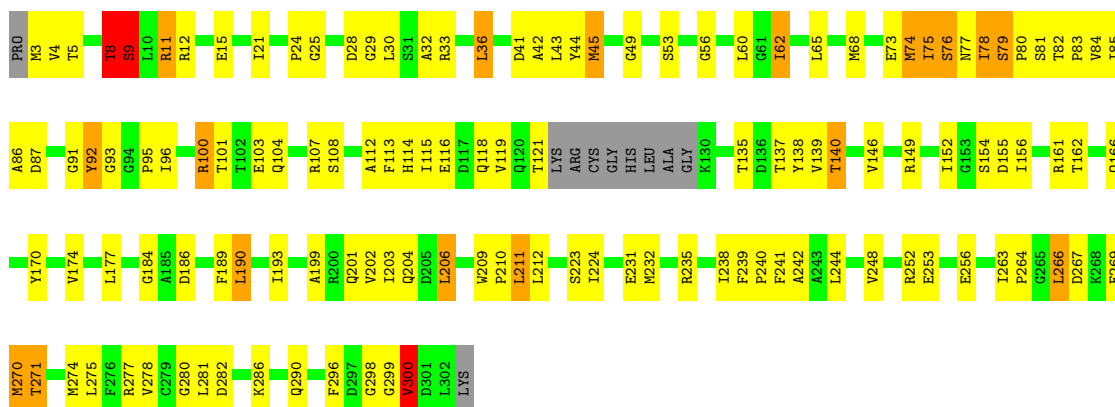
- Molecule 1: 2,3-dimethylmalate lyase

Chain M: 55% 39% 6%



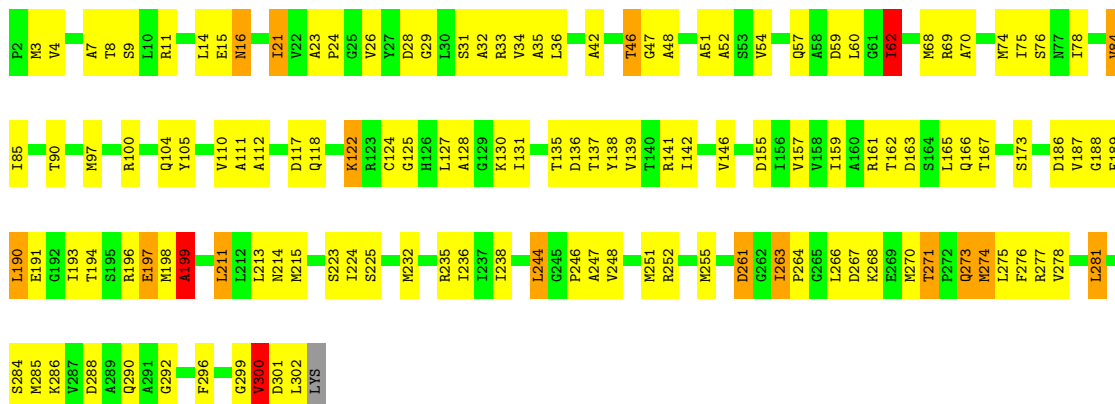
- Molecule 1: 2,3-dimethylmalate lyase

Chain N: 54% 36% 6% ..



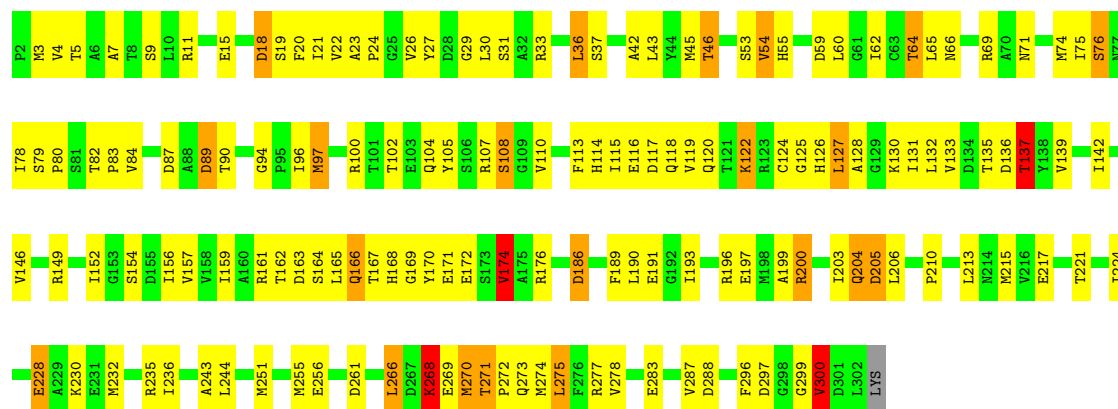
- Molecule 1: 2,3-dimethylmalate lyase

Chain O: 56% 38% 5% .



- Molecule 1: 2,3-dimethylmalate lyase

Chain P: 50% 42% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	160.57Å 160.57Å 161.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.60) 94.3 (50.00-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.255 0.190 , 0.252	Depositor DCC
R_{free} test set	6752 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.447 for -h,-k,l 0.084 for h,-h-k,-l 0.083 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36360	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5454e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OAF, GOL, MN

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	1.38	7/2255 (0.3%)	1.42	13/3053 (0.4%)
1	B	1.32	3/2263 (0.1%)	1.32	5/3063 (0.2%)
1	C	1.41	7/2261 (0.3%)	1.38	17/3060 (0.6%)
1	D	1.38	6/2259 (0.3%)	1.40	11/3057 (0.4%)
1	E	1.39	5/2261 (0.2%)	1.37	12/3060 (0.4%)
1	F	1.26	6/2257 (0.3%)	1.37	14/3056 (0.5%)
1	G	1.38	9/2261 (0.4%)	1.36	13/3060 (0.4%)
1	H	1.40	6/2261 (0.3%)	1.39	19/3060 (0.6%)
1	I	1.25	3/2249 (0.1%)	1.34	10/3044 (0.3%)
1	J	1.18	2/2192 (0.1%)	1.34	7/2967 (0.2%)
1	K	1.18	2/2251 (0.1%)	1.34	17/3046 (0.6%)
1	L	1.14	0/2247	1.26	10/3041 (0.3%)
1	M	1.17	4/2253 (0.2%)	1.36	16/3049 (0.5%)
1	N	1.21	2/2191 (0.1%)	1.31	5/2966 (0.2%)
1	O	1.21	5/2244 (0.2%)	1.31	15/3039 (0.5%)
1	P	1.17	4/2258 (0.2%)	1.29	14/3056 (0.5%)
All	All	1.28	71/35963 (0.2%)	1.35	198/48677 (0.4%)

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	300	VAL	CA-CB	-9.99	1.44	1.54
1	D	283	GLU	CG-CD	-9.45	1.28	1.52
1	E	196	ARG	C-N	-7.74	1.23	1.33
1	E	4	VAL	CA-CB	7.74	1.66	1.54
1	C	158	VAL	CA-CB	7.69	1.62	1.53

The worst 5 of 198 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	300	VAL	N-CA-C	-9.37	104.01	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ILE	CA-C-N	9.31	128.92	119.24
1	A	263	ILE	C-N-CA	9.31	128.92	119.24
1	I	271	THR	CA-C-N	8.59	129.12	119.32
1	I	271	THR	C-N-CA	8.59	129.12	119.32

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	2222	0	2206	91	0
1	B	2230	0	2217	98	0
1	C	2228	0	2224	103	0
1	D	2226	0	2224	79	0
1	E	2228	0	2224	82	0
1	F	2224	0	2213	96	0
1	G	2228	0	2224	85	0
1	H	2228	0	2224	79	0
1	I	2216	0	2209	105	0
1	J	2162	0	2150	95	0
1	K	2218	0	2206	89	0
1	L	2215	0	2203	127	0
1	M	2220	0	2213	115	0
1	N	2161	0	2146	116	0
1	O	2211	0	2196	115	0
1	P	2225	0	2215	147	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	12	0	1	0	0
3	B	12	0	1	0	0
3	C	12	0	1	0	0
3	D	12	0	1	2	0
3	E	12	0	1	0	0
3	F	12	0	1	1	0
3	G	12	0	1	0	0
3	H	12	0	1	1	0
3	I	12	0	1	2	0
3	K	12	0	1	1	0
3	L	12	0	1	1	0
3	M	12	0	1	1	0
3	O	12	0	1	1	0
3	P	12	0	1	1	0
4	A	12	0	16	6	0
4	E	6	0	8	0	0
4	G	6	0	8	2	0
4	M	6	0	8	1	0
5	A	59	0	0	4	0
5	B	59	0	0	3	0
5	C	52	0	0	7	0
5	D	57	0	0	4	0
5	E	65	0	0	7	0
5	F	55	0	0	3	0
5	G	66	0	0	5	0
5	H	68	0	0	2	0
5	I	29	0	0	1	0
5	J	29	0	0	1	0
5	K	27	0	0	0	0
5	L	24	0	0	1	0
5	M	38	0	0	6	0
5	N	28	0	0	4	0
5	O	24	0	0	3	0
5	P	24	0	0	4	0
All	All	36360	0	35348	1446	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1446 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:N:210:PRO:C	1:N:211:LEU:HD12	1.49	1.33
1:N:210:PRO:O	1:N:211:LEU:HD12	1.23	1.27
1:C:8:THR:HG22	1:C:155:ASP:OD2	1.38	1.19
1:L:10:LEU:O	1:L:14:LEU:HD12	1.41	1.18
1:N:210:PRO:C	1:N:211:LEU:CD1	2.17	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/302 (99%)	278 (93%)	20 (7%)	1 (0%)	36	58
1	B	300/302 (99%)	284 (95%)	15 (5%)	1 (0%)	36	58
1	C	299/302 (99%)	286 (96%)	11 (4%)	2 (1%)	18	38
1	D	299/302 (99%)	289 (97%)	8 (3%)	2 (1%)	18	38
1	E	299/302 (99%)	279 (93%)	20 (7%)	0	100	100
1	F	299/302 (99%)	279 (93%)	19 (6%)	1 (0%)	36	58
1	G	299/302 (99%)	282 (94%)	15 (5%)	2 (1%)	18	38
1	H	299/302 (99%)	284 (95%)	14 (5%)	1 (0%)	36	58
1	I	298/302 (99%)	271 (91%)	24 (8%)	3 (1%)	12	28
1	J	288/302 (95%)	260 (90%)	27 (9%)	1 (0%)	36	58
1	K	298/302 (99%)	275 (92%)	20 (7%)	3 (1%)	12	28
1	L	298/302 (99%)	268 (90%)	22 (7%)	8 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	298/302 (99%)	270 (91%)	26 (9%)	2 (1%)	18	38
1	N	288/302 (95%)	266 (92%)	18 (6%)	4 (1%)	9	19
1	O	299/302 (99%)	268 (90%)	28 (9%)	3 (1%)	12	28
1	P	299/302 (99%)	262 (88%)	32 (11%)	5 (2%)	7	15
All	All	4759/4832 (98%)	4401 (92%)	319 (7%)	39 (1%)	16	34

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	MET
1	C	299	GLY
1	I	295	ALA
1	J	242	ALA
1	L	151	ARG

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	225/228 (99%)	201 (89%)	24 (11%)	6	14
1	B	226/228 (99%)	202 (89%)	24 (11%)	6	14
1	C	227/228 (100%)	201 (88%)	26 (12%)	5	11
1	D	226/228 (99%)	199 (88%)	27 (12%)	5	10
1	E	227/228 (100%)	197 (87%)	30 (13%)	4	8
1	F	226/228 (99%)	197 (87%)	29 (13%)	4	8
1	G	227/228 (100%)	201 (88%)	26 (12%)	5	11
1	H	227/228 (100%)	196 (86%)	31 (14%)	3	7
1	I	225/228 (99%)	200 (89%)	25 (11%)	6	12
1	J	220/228 (96%)	192 (87%)	28 (13%)	4	9
1	K	225/228 (99%)	202 (90%)	23 (10%)	7	15
1	L	224/228 (98%)	193 (86%)	31 (14%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	226/228 (99%)	199 (88%)	27 (12%)	5	10
1	N	220/228 (96%)	181 (82%)	39 (18%)	2	3
1	O	222/228 (97%)	196 (88%)	26 (12%)	5	11
1	P	226/228 (99%)	196 (87%)	30 (13%)	4	8
All	All	3599/3648 (99%)	3153 (88%)	446 (12%)	4	9

5 of 446 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	189	PHE
1	P	275	LEU
1	K	202	VAL
1	P	228	GLU
1	O	131	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	168	HIS
1	O	290	GLN
1	K	204	GLN
1	N	71	ASN
1	P	273	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 16 are monoatomic - leaving 19 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
3	OAF	G	501	2	10,11,11	1.91	2 (20%)	13,18,18	1.15	1 (7%)
3	OAF	F	501	2	10,11,11	1.41	1 (10%)	13,18,18	2.49	6 (46%)
3	OAF	D	501	2	10,11,11	2.46	3 (30%)	13,18,18	3.26	5 (38%)
4	GOL	A	602	-	5,5,5	0.95	0	5,5,5	1.70	2 (40%)
3	OAF	K	501	2	10,11,11	1.29	1 (10%)	13,18,18	1.43	3 (23%)
3	OAF	B	501	2	10,11,11	1.12	0	13,18,18	2.10	5 (38%)
3	OAF	C	501	2	10,11,11	1.76	3 (30%)	13,18,18	1.40	3 (23%)
4	GOL	A	605	-	5,5,5	0.52	0	5,5,5	1.08	0
4	GOL	M	606	-	5,5,5	0.52	0	5,5,5	0.98	0
3	OAF	E	501	2	10,11,11	1.80	2 (20%)	13,18,18	1.76	6 (46%)
3	OAF	P	501	2	10,11,11	2.54	3 (30%)	13,18,18	3.28	6 (46%)
4	GOL	G	601	-	5,5,5	0.91	0	5,5,5	1.85	2 (40%)
3	OAF	O	501	2	10,11,11	1.58	2 (20%)	13,18,18	2.38	6 (46%)
3	OAF	I	501	2	10,11,11	1.22	2 (20%)	13,18,18	1.59	4 (30%)
4	GOL	E	604	-	5,5,5	0.72	0	5,5,5	0.77	0
3	OAF	A	501	2	10,11,11	1.80	2 (20%)	13,18,18	1.79	3 (23%)
3	OAF	M	501	2	10,11,11	1.47	1 (10%)	13,18,18	1.68	3 (23%)
3	OAF	H	501	2	10,11,11	1.71	1 (10%)	13,18,18	1.83	4 (30%)
3	OAF	L	501	2	10,11,11	1.83	3 (30%)	13,18,18	3.14	3 (23%)

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
3	OAF	G	501	2	-	6/14/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAF	F	501	2	-	5/14/21/21	-
3	OAF	D	501	2	-	3/14/21/21	-
4	GOL	A	602	-	-	2/4/4/4	-
3	OAF	K	501	2	-	7/14/21/21	-
3	OAF	B	501	2	-	5/14/21/21	-
3	OAF	C	501	2	-	4/14/21/21	-
4	GOL	A	605	-	-	3/4/4/4	-
4	GOL	M	606	-	-	2/4/4/4	-
3	OAF	E	501	2	-	5/14/21/21	-
3	OAF	P	501	2	-	6/14/21/21	-
4	GOL	G	601	-	-	4/4/4/4	-
3	OAF	O	501	2	-	6/14/21/21	-
3	OAF	I	501	2	-	5/14/21/21	-
4	GOL	E	604	-	-	0/4/4/4	-
3	OAF	A	501	2	-	3/14/21/21	-
3	OAF	M	501	2	-	1/14/21/21	-
3	OAF	H	501	2	-	4/14/21/21	-
3	OAF	L	501	2	-	1/14/21/21	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	OAF	C3-C4	-6.62	1.45	1.54
3	P	501	OAF	C3-C4	5.01	1.62	1.54
3	P	501	OAF	O3-C2	4.65	1.46	1.39
3	H	501	OAF	C3-C4	-4.37	1.48	1.54
3	G	501	OAF	C3-C2	-4.29	1.50	1.54

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	501	OAF	F2-C3-C2	-9.78	97.81	109.32
3	P	501	OAF	F2-C3-C2	-9.26	98.42	109.32
3	D	501	OAF	F1-C3-C2	7.48	118.12	109.32
3	D	501	OAF	F2-C3-C2	-7.06	101.01	109.32
3	F	501	OAF	F1-C3-C2	6.18	116.60	109.32

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	501	OAF	O3-C2-C3-F1
3	G	501	OAF	O4-C2-C3-F1
3	G	501	OAF	O4-C2-C3-F2
3	G	501	OAF	O3-C2-C3-F1
3	I	501	OAF	O2-C1-C2-O3

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	OAF	1	0
3	D	501	OAF	2	0
4	A	602	GOL	3	0
3	K	501	OAF	1	0
4	A	605	GOL	3	0
4	M	606	GOL	1	0
3	P	501	OAF	1	0
4	G	601	GOL	2	0
3	O	501	OAF	1	0
3	I	501	OAF	2	0
3	M	501	OAF	1	0
3	H	501	OAF	1	0
3	L	501	OAF	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 [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	301/302 (99%)	-1.73	0 100 100	33, 37, 40, 44	0
1	B	302/302 (100%)	-1.72	0 100 100	33, 37, 42, 44	0
1	C	301/302 (99%)	-1.74	0 100 100	31, 37, 41, 44	0
1	D	301/302 (99%)	-1.75	0 100 100	33, 37, 41, 45	0
1	E	301/302 (99%)	-1.74	0 100 100	33, 37, 41, 44	0
1	F	301/302 (99%)	-1.72	0 100 100	32, 37, 41, 45	0
1	G	301/302 (99%)	-1.72	0 100 100	33, 37, 40, 45	0
1	H	301/302 (99%)	-1.73	0 100 100	32, 37, 41, 44	0
1	I	300/302 (99%)	-1.71	0 100 100	32, 38, 41, 46	0
1	J	292/302 (96%)	-1.70	0 100 100	33, 38, 42, 46	0
1	K	300/302 (99%)	-1.73	0 100 100	33, 38, 42, 48	0
1	L	300/302 (99%)	-1.65	0 100 100	33, 38, 44, 48	0
1	M	300/302 (99%)	-1.72	0 100 100	32, 37, 42, 47	0
1	N	292/302 (96%)	-1.69	0 100 100	32, 38, 42, 48	0
1	O	301/302 (99%)	-1.72	0 100 100	33, 38, 42, 46	0
1	P	301/302 (99%)	-1.68	0 100 100	34, 38, 43, 47	0
All	All	4795/4832 (99%)	-1.72	0 100 100	31, 37, 42, 48	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OAF	B	501	12/12	0.99	0.03	28,32,36,36	0
3	OAF	I	501	12/12	0.99	0.03	35,36,38,41	0
3	OAF	L	501	12/12	0.99	0.04	38,41,43,44	0
3	OAF	P	501	12/12	0.99	0.03	37,40,42,42	0
4	GOL	A	602	6/6	0.99	0.04	33,35,39,40	0
4	GOL	A	605	6/6	0.99	0.03	36,39,41,42	0
4	GOL	E	604	6/6	0.99	0.04	37,40,41,43	0
4	GOL	M	606	6/6	0.99	0.04	35,38,39,41	0
2	MN	I	401	1/1	1.00	0.02	39,39,39,39	0
2	MN	J	401	1/1	1.00	0.02	43,43,43,43	0
2	MN	K	401	1/1	1.00	0.02	38,38,38,38	0
2	MN	L	401	1/1	1.00	0.03	41,41,41,41	0
2	MN	M	401	1/1	1.00	0.02	38,38,38,38	0
2	MN	N	401	1/1	1.00	0.02	43,43,43,43	0
2	MN	O	401	1/1	1.00	0.02	39,39,39,39	0
2	MN	P	401	1/1	1.00	0.03	42,42,42,42	0
3	OAF	A	501	12/12	1.00	0.04	33,35,36,37	0
2	MN	A	401	1/1	1.00	0.02	33,33,33,33	0
3	OAF	C	501	12/12	1.00	0.03	32,34,35,36	0
3	OAF	D	501	12/12	1.00	0.02	30,31,33,34	0
3	OAF	E	501	12/12	1.00	0.02	28,32,34,34	0
3	OAF	F	501	12/12	1.00	0.03	32,33,35,35	0
3	OAF	G	501	12/12	1.00	0.02	31,34,37,38	0
3	OAF	H	501	12/12	1.00	0.02	33,36,36,39	0
2	MN	B	401	1/1	1.00	0.02	37,37,37,37	0
3	OAF	K	501	12/12	1.00	0.03	33,36,38,39	0
2	MN	C	401	1/1	1.00	0.02	35,35,35,35	0
3	OAF	M	501	12/12	1.00	0.02	29,34,36,37	0
3	OAF	O	501	12/12	1.00	0.02	30,35,37,38	0
2	MN	D	401	1/1	1.00	0.01	36,36,36,36	0
2	MN	E	401	1/1	1.00	0.03	36,36,36,36	0
2	MN	F	401	1/1	1.00	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	G	401	1/1	1.00	0.02	34,34,34,34	0
4	GOL	G	601	6/6	1.00	0.03	31,35,37,38	0
2	MN	H	401	1/1	1.00	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.