wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:37 AM GMT

PDB ID	:	3FA3
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
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:

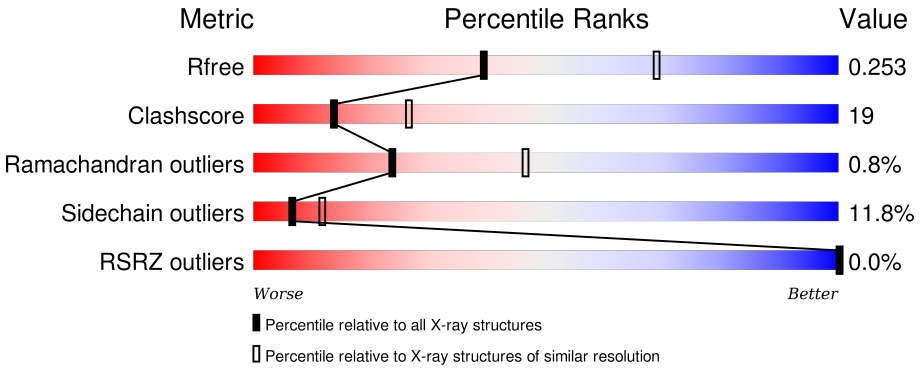
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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	302	69% 26% 5%
1	B	302	65% 30% 5%
1	C	302	64% 30% 5%
1	D	302	67% 28%
1	E	302	70% 25%

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Mol	Chain	Length	Quality of chain
1	F	302	65% 31%
1	G	302	69% 26%
1	H	302	65% 30%
1	I	302	60% 35%
1	J	302	62% 28% 5%
1	K	302	64% 30% 5%
1	L	302	55% 39% 5%
1	M	302	59% 36%
1	N	302	56% 34% 5%
1	O	302	64% 31% 5%
1	P	302	% 55% 38% 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	A	602	-	-	-	X

2 Entry composition

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.

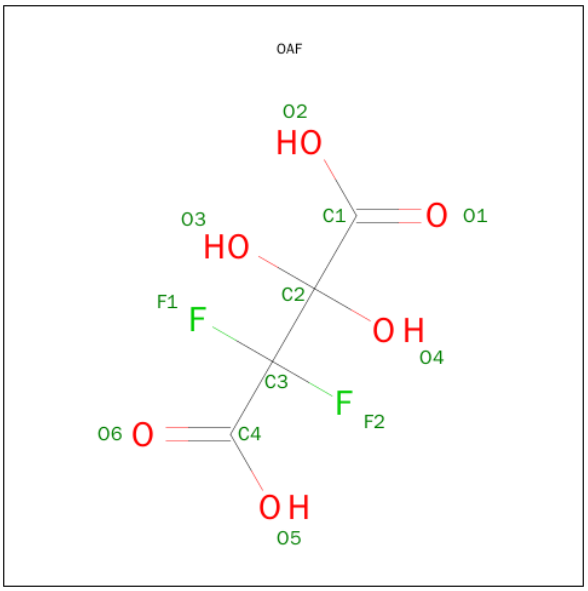
- Molecule 1 is a protein called 2,3-dimethylmalate lyase.

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

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

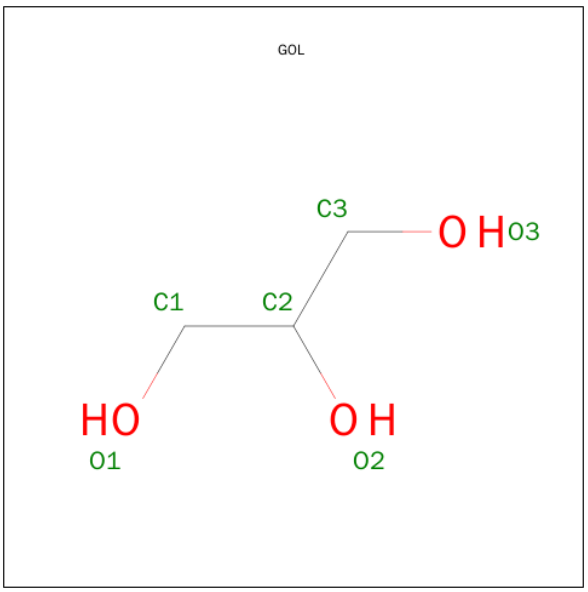
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	K	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	N	1	Total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

- Molecule 3 is 2,2-DIFLUORO-3,3-DIHYDROXYBUTANEDIOIC ACID (three-letter code: OAF) (formula: $C_4H_4F_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 12 4 2 6	0	0
3	B	1	Total C F O 12 4 2 6	0	0
3	C	1	Total C F O 12 4 2 6	0	0
3	D	1	Total C F O 12 4 2 6	0	0
3	E	1	Total C F O 12 4 2 6	0	0
3	F	1	Total C F O 12 4 2 6	0	0
3	G	1	Total C F O 12 4 2 6	0	0
3	H	1	Total C F O 12 4 2 6	0	0
3	I	1	Total C F O 12 4 2 6	0	0
3	K	1	Total C F O 12 4 2 6	0	0
3	L	1	Total C F O 12 4 2 6	0	0
3	M	1	Total C F O 12 4 2 6	0	0
3	O	1	Total C F O 12 4 2 6	0	0
3	P	1	Total C F O 12 4 2 6	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 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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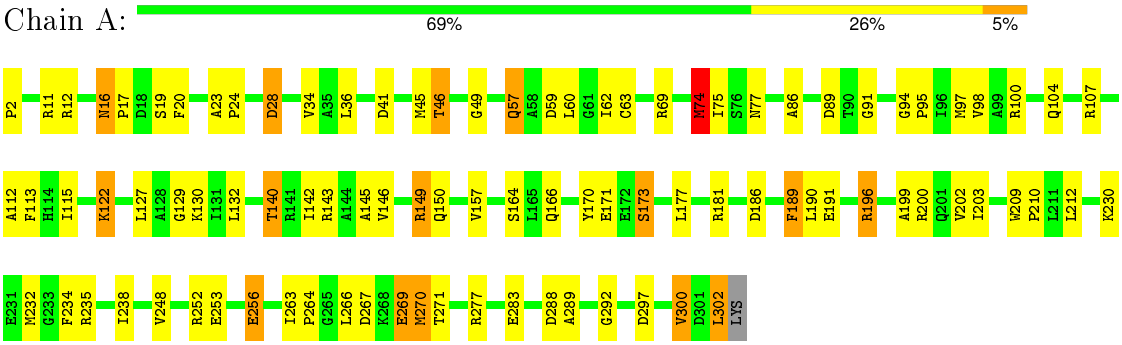
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	66	Total O 66 66	0	0
5	H	68	Total O 68 68	0	0
5	I	29	Total O 29 29	0	0
5	J	29	Total O 29 29	0	0
5	K	27	Total O 27 27	0	0
5	L	24	Total O 24 24	0	0
5	M	38	Total O 38 38	0	0
5	N	28	Total O 28 28	0	0
5	O	24	Total O 24 24	0	0
5	P	24	Total O 24 24	0	0

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.

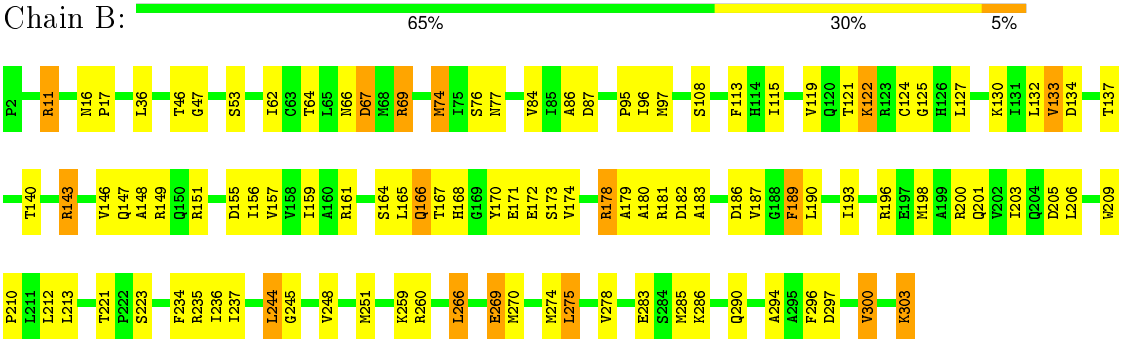
- Molecule 1: 2,3-dimethylmalate lyase

Chain A:



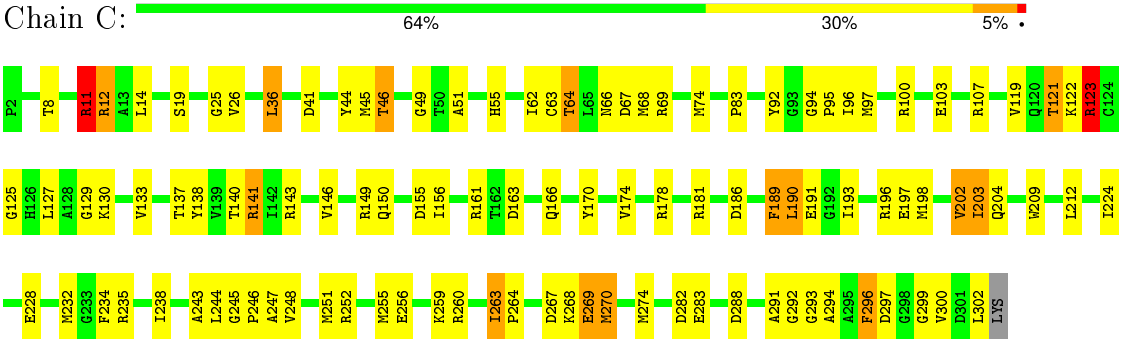
- Molecule 1: 2,3-dimethylmalate lyase

Chain B:



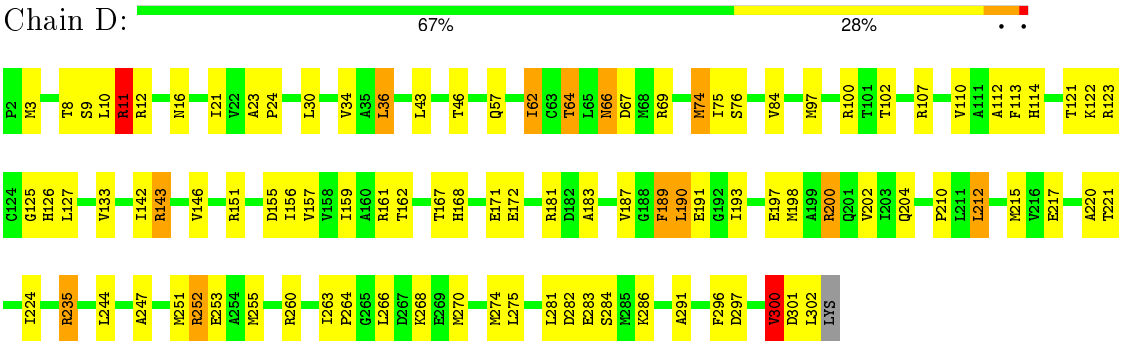
- Molecule 1: 2,3-dimethylmalate lyase

Chain C:



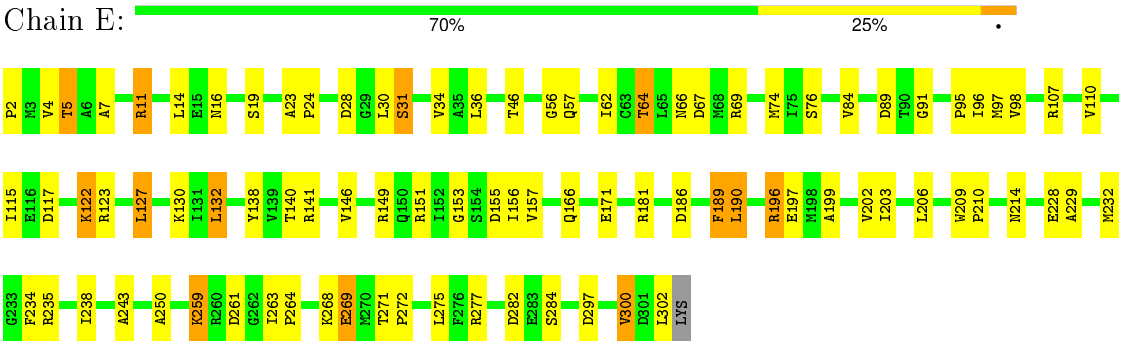
- Molecule 1: 2,3-dimethylmalate lyase

Chain D:



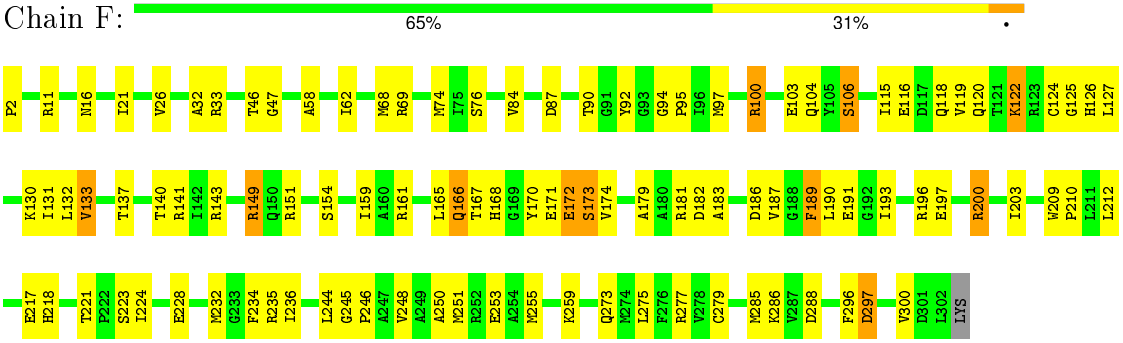
- Molecule 1: 2,3-dimethylmalate lyase

Chain E:



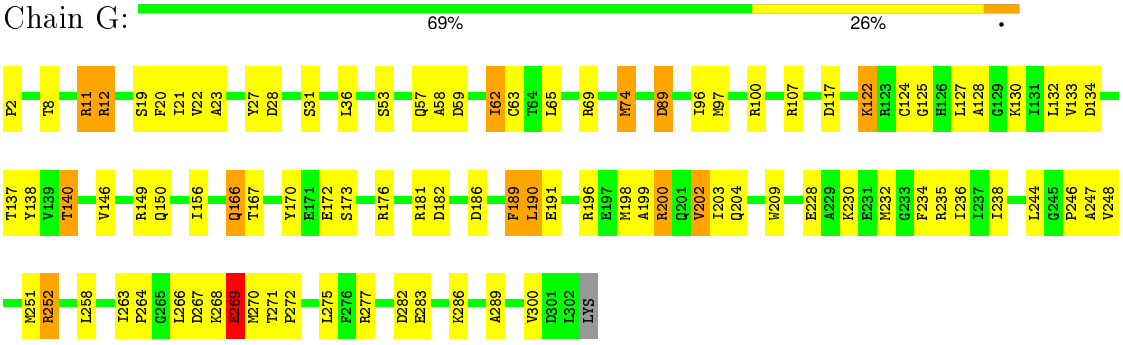
- Molecule 1: 2,3-dimethylmalate lyase

Chain F:



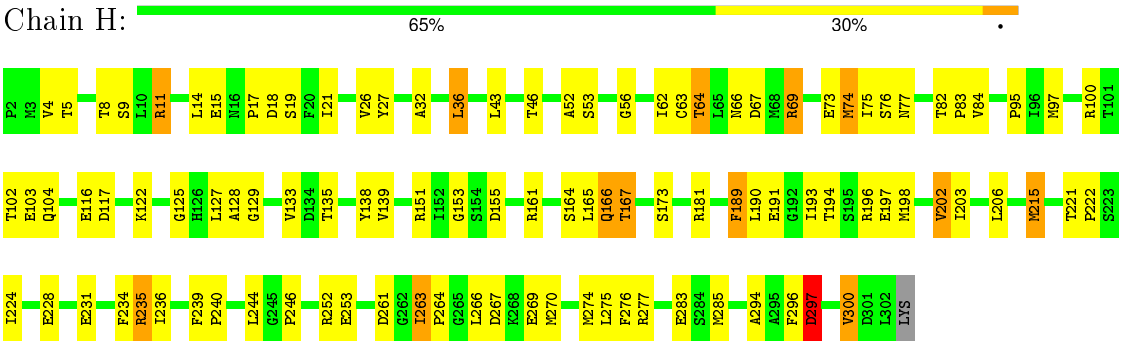
- Molecule 1: 2,3-dimethylmalate lyase

Chain G:



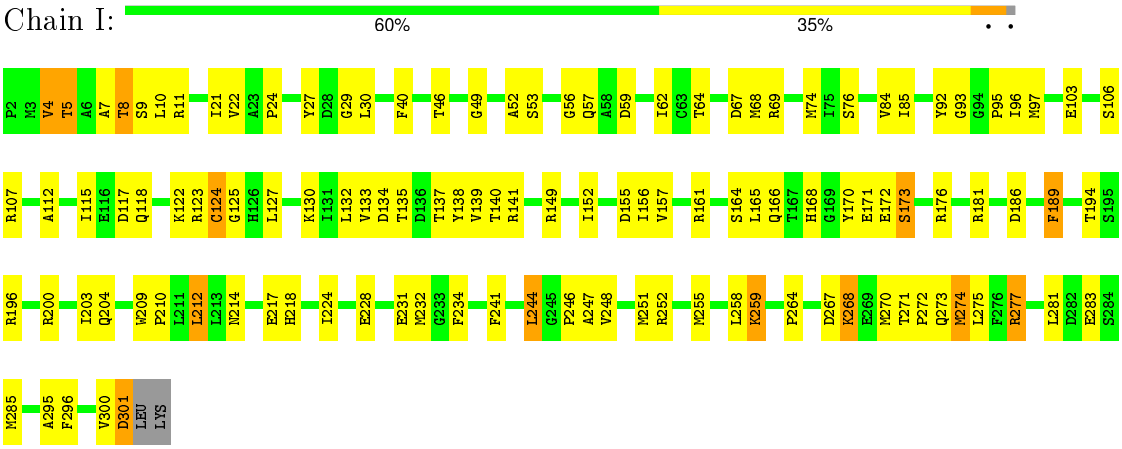
- Molecule 1: 2,3-dimethylmalate lyase

Chain H:



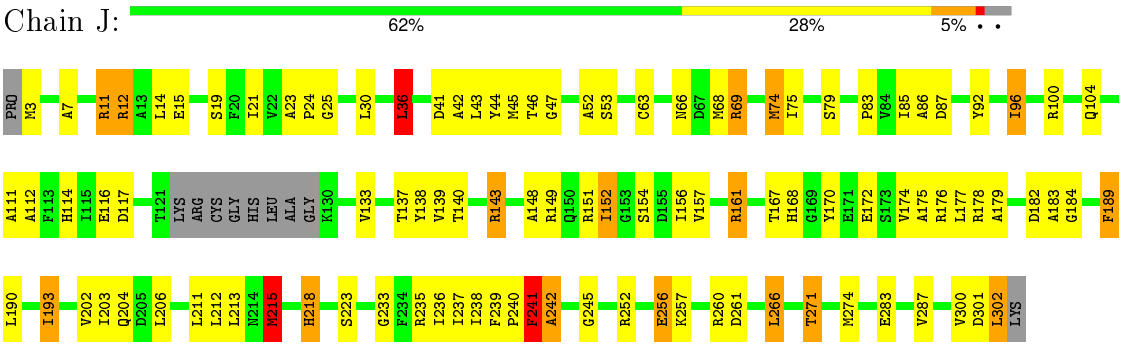
- Molecule 1: 2,3-dimethylmalate lyase

Chain I:



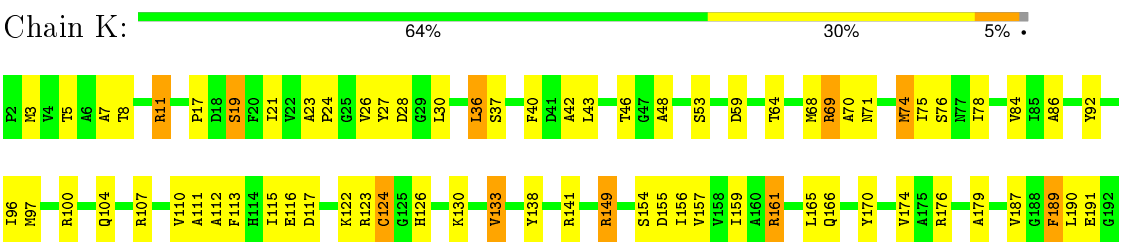
- Molecule 1: 2,3-dimethylmalate lyase

Chain J:



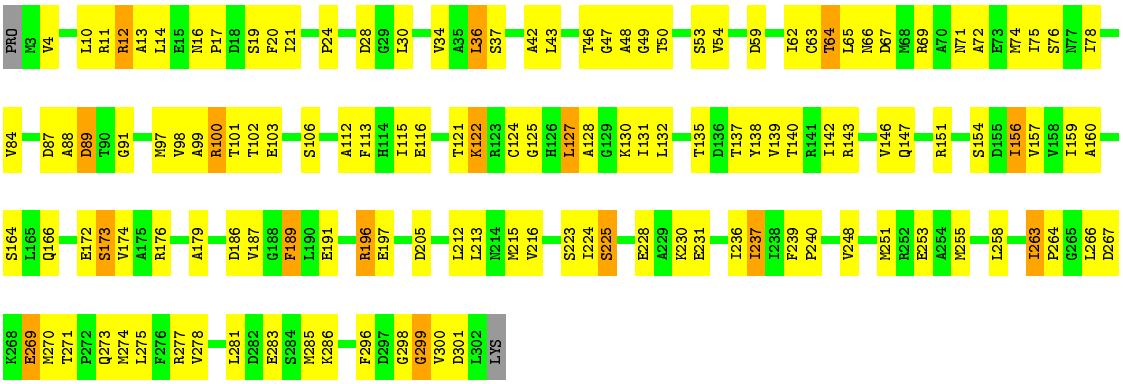
- Molecule 1: 2,3-dimethylmalate lyase

Chain K:



- Molecule 1: 2,3-dimethylmalate lyase

Chain L:

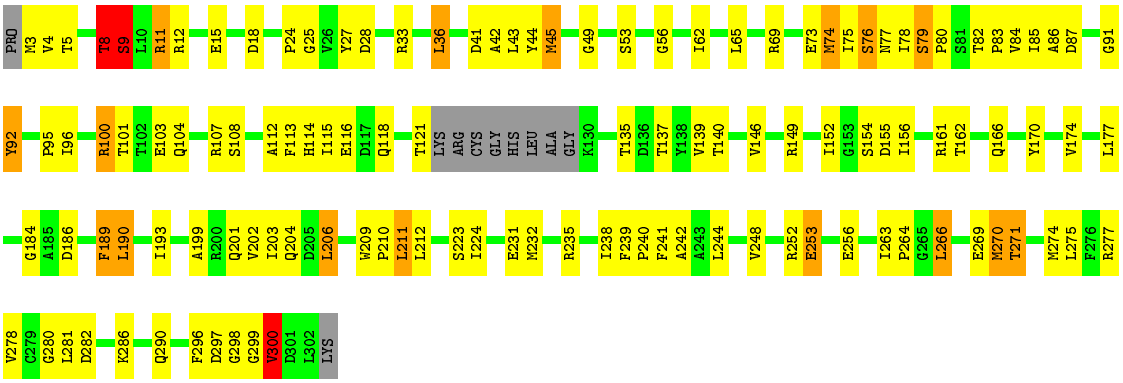


- Molecule 1: 2,3-dimethylmalate lyase

Chain M:

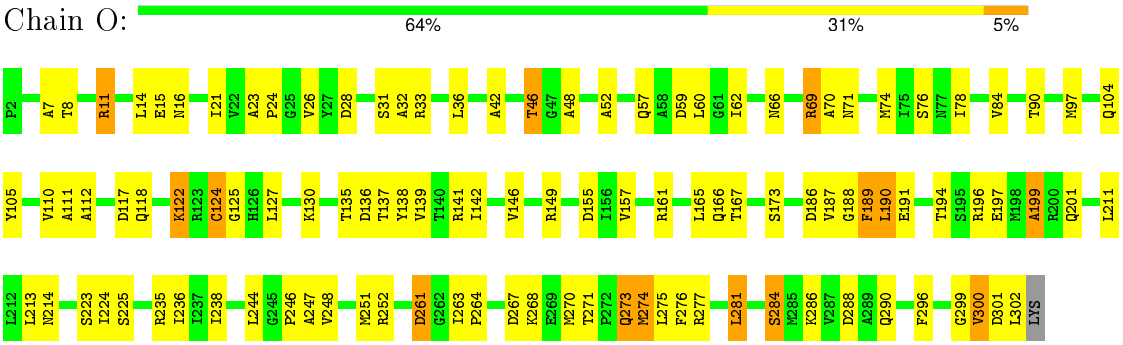
- Molecule 1: 2,3-dimethylmalate lyase

Chain N:



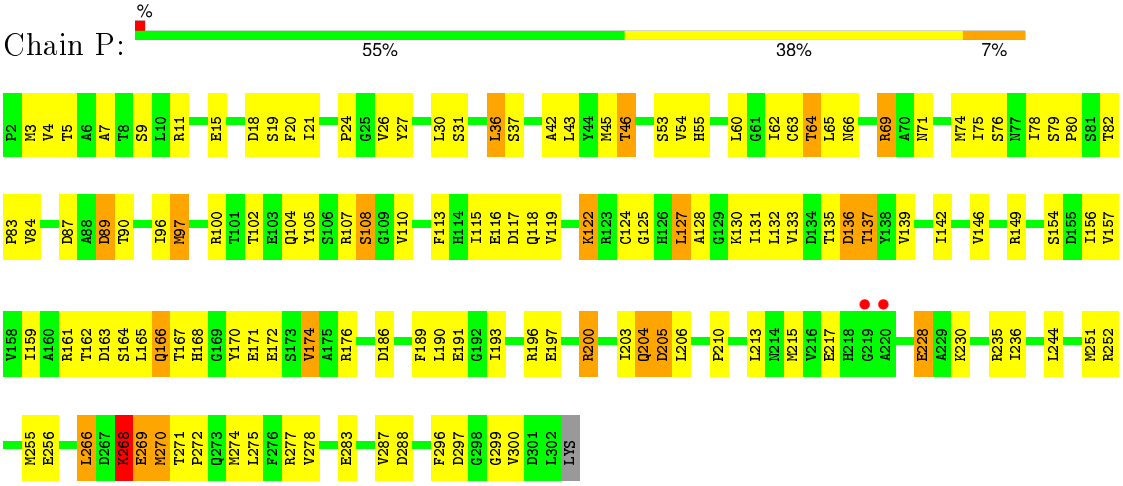
- Molecule 1: 2,3-dimethylmalate lyase

Chain O:



• Molecule 1: 2,3-dimethylmalate lyase

Chain P:



4 Data and refinement statistics (i)

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 49.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-2.60) 94.3 (49.98-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.255 0.190 , 0.253	Depositor DCC
R_{free} test set	6752 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.9	EDS
Estimated twinning fraction	0.447 for -h,-k,l 0.084 for h,-h-k,-l 0.083 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 135026 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36360	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: OAF, MN, GOL

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	1.10	4/2255 (0.2%)	1.07	5/3053 (0.2%)
1	B	1.07	3/2263 (0.1%)	0.98	4/3063 (0.1%)
1	C	1.13	5/2261 (0.2%)	1.05	8/3060 (0.3%)
1	D	1.13	5/2259 (0.2%)	1.11	7/3057 (0.2%)
1	E	1.11	4/2261 (0.2%)	1.04	1/3060 (0.0%)
1	F	1.00	3/2257 (0.1%)	1.03	1/3056 (0.0%)
1	G	1.09	3/2261 (0.1%)	1.03	2/3060 (0.1%)
1	H	1.15	3/2261 (0.1%)	1.09	3/3060 (0.1%)
1	I	0.99	3/2249 (0.1%)	0.98	1/3044 (0.0%)
1	J	0.94	1/2192 (0.0%)	1.01	3/2967 (0.1%)
1	K	0.94	2/2251 (0.1%)	1.00	3/3046 (0.1%)
1	L	0.91	1/2247 (0.0%)	0.87	0/3041
1	M	0.94	0/2253	0.99	2/3049 (0.1%)
1	N	0.99	5/2191 (0.2%)	0.95	0/2966
1	O	0.98	1/2244 (0.0%)	0.94	0/3039
1	P	0.93	2/2258 (0.1%)	0.92	1/3056 (0.0%)
All	All	1.03	45/35963 (0.1%)	1.01	41/48677 (0.1%)

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	283	GLU	CG-CD	-15.69	1.28	1.51
1	P	63	CYS	CB-SG	-8.32	1.68	1.82
1	D	253	GLU	CG-CD	7.75	1.63	1.51
1	N	253	GLU	CG-CD	7.50	1.63	1.51
1	C	197	GLU	CG-CD	7.11	1.62	1.51

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	235	ARG	NE-CZ-NH1	7.42	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	J	161	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	12	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	P	252	ARG	NE-CZ-NH2	-6.34	117.13	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	2222	0	2206	83	0
1	B	2230	0	2217	91	0
1	C	2228	0	2224	97	0
1	D	2226	0	2224	76	0
1	E	2228	0	2224	76	0
1	F	2224	0	2213	92	0
1	G	2228	0	2224	80	0
1	H	2228	0	2224	68	0
1	I	2216	0	2209	94	0
1	J	2162	0	2150	88	0
1	K	2218	0	2206	79	0
1	L	2215	0	2203	116	0
1	M	2220	0	2213	109	0
1	N	2161	0	2146	105	0
1	O	2211	0	2196	97	0
1	P	2225	0	2215	133	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	0	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	6	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	1315	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 19.

The worst 5 of 1315 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	1.29
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:I:62:ILE:HG23	1:L:97:MET:HE3	1.14	1.13

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%)	46 72
1	B	300/302 (99%)	284 (95%)	15 (5%)	1 (0%)	46 72
1	C	299/302 (99%)	286 (96%)	11 (4%)	2 (1%)	26 51
1	D	299/302 (99%)	289 (97%)	8 (3%)	2 (1%)	26 51
1	E	299/302 (99%)	279 (93%)	20 (7%)	0	100 100
1	F	299/302 (99%)	279 (93%)	19 (6%)	1 (0%)	46 72
1	G	299/302 (99%)	282 (94%)	15 (5%)	2 (1%)	26 51
1	H	299/302 (99%)	284 (95%)	14 (5%)	1 (0%)	46 72
1	I	298/302 (99%)	271 (91%)	24 (8%)	3 (1%)	19 39
1	J	288/302 (95%)	260 (90%)	27 (9%)	1 (0%)	46 72
1	K	298/302 (99%)	275 (92%)	20 (7%)	3 (1%)	19 39
1	L	298/302 (99%)	268 (90%)	22 (7%)	8 (3%)	6 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	298/302 (99%)	270 (91%)	26 (9%)	2 (1%)	26 51
1	N	288/302 (95%)	266 (92%)	18 (6%)	4 (1%)	14 28
1	O	299/302 (99%)	268 (90%)	28 (9%)	3 (1%)	19 39
1	P	299/302 (99%)	262 (88%)	32 (11%)	5 (2%)	11 22
All	All	4759/4832 (98%)	4401 (92%)	319 (7%)	39 (1%)	24 46

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%)	206 (92%)	19 (8%)	14 26
1	B	226/228 (99%)	201 (89%)	25 (11%)	8 13
1	C	227/228 (100%)	204 (90%)	23 (10%)	9 17
1	D	226/228 (99%)	196 (87%)	30 (13%)	5 8
1	E	227/228 (100%)	202 (89%)	25 (11%)	8 14
1	F	226/228 (99%)	203 (90%)	23 (10%)	9 17
1	G	227/228 (100%)	204 (90%)	23 (10%)	9 17
1	H	227/228 (100%)	199 (88%)	28 (12%)	6 11
1	I	225/228 (99%)	199 (88%)	26 (12%)	7 12
1	J	220/228 (96%)	194 (88%)	26 (12%)	6 12
1	K	225/228 (99%)	202 (90%)	23 (10%)	9 17
1	L	224/228 (98%)	196 (88%)	28 (12%)	6 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	226/228 (99%)	197 (87%)	29 (13%)	5 10
1	N	220/228 (96%)	181 (82%)	39 (18%)	2 3
1	O	222/228 (97%)	194 (87%)	28 (13%)	5 10
1	P	226/228 (99%)	197 (87%)	29 (13%)	5 10
All	All	3599/3648 (99%)	3175 (88%)	424 (12%)	6 12

5 of 424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	275	LEU
1	J	204	GLN
1	O	281	LEU
1	I	8	THR
1	I	252	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	168	HIS
1	H	166	GLN
1	L	166	GLN
1	F	166	GLN
1	K	166	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 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	A	501	2	2,11,11	1.25	0	1,18,18	1.14	0
4	GOL	A	602	-	5,5,5	0.87	0	5,5,5	1.64	1 (20%)
4	GOL	A	605	-	5,5,5	0.44	0	5,5,5	0.98	0
3	OAF	B	501	2	2,11,11	0.80	0	1,18,18	3.20	1 (100%)
3	OAF	C	501	2	2,11,11	1.51	0	1,18,18	0.11	0
3	OAF	D	501	2	2,11,11	0.86	0	1,18,18	3.11	1 (100%)
3	OAF	E	501	2	2,11,11	1.77	1 (50%)	1,18,18	2.73	1 (100%)
4	GOL	E	604	-	5,5,5	0.64	0	5,5,5	0.76	0
3	OAF	F	501	2	2,11,11	1.21	0	1,18,18	0.15	0
3	OAF	G	501	2	2,11,11	1.47	0	1,18,18	0.47	0
4	GOL	G	601	-	5,5,5	0.87	0	5,5,5	1.69	2 (40%)
3	OAF	H	501	2	2,11,11	0.61	0	1,18,18	2.17	1 (100%)
3	OAF	I	501	2	2,11,11	0.33	0	1,18,18	1.87	0
3	OAF	K	501	2	2,11,11	1.47	0	1,18,18	0.70	0
3	OAF	L	501	2	2,11,11	0.64	0	1,18,18	2.03	1 (100%)
3	OAF	M	501	2	2,11,11	0.36	0	1,18,18	2.21	1 (100%)
4	GOL	M	606	-	5,5,5	0.45	0	5,5,5	0.95	0
3	OAF	O	501	2	2,11,11	1.10	0	1,18,18	3.45	1 (100%)
3	OAF	P	501	2	2,11,11	1.04	0	1,18,18	4.28	1 (100%)

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	A	501	2	-	0/0/21/21	0/0/0/0
4	GOL	A	602	-	-	0/4/4/4	0/0/0/0
4	GOL	A	605	-	-	0/4/4/4	0/0/0/0

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	OAF	F2-C3	-2.08	1.28	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	OAF	F1-C3-F2	-2.73	100.14	106.40
4	G	601	GOL	O3-C3-C2	-2.04	100.30	110.18
3	L	501	OAF	F1-C3-F2	2.03	111.06	106.40
3	H	501	OAF	F1-C3-F2	2.17	111.38	106.40
3	M	501	OAF	F1-C3-F2	2.21	111.48	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	GOL	3	0
4	A	605	GOL	3	0
3	D	501	OAF	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	OAF	1	0
4	G	601	GOL	2	0
3	H	501	OAF	1	0
3	I	501	OAF	2	0
3	L	501	OAF	1	0
3	M	501	OAF	1	0
4	M	606	GOL	1	0
3	O	501	OAF	1	0
3	P	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

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	301/302 (99%)	-0.72	0 100 100	33, 37, 40, 44	0
1	B	302/302 (100%)	-0.66	0 100 100	33, 37, 42, 44	0
1	C	301/302 (99%)	-0.71	0 100 100	31, 37, 41, 44	0
1	D	301/302 (99%)	-0.75	0 100 100	33, 37, 41, 45	0
1	E	301/302 (99%)	-0.71	0 100 100	33, 37, 41, 44	0
1	F	301/302 (99%)	-0.66	0 100 100	32, 37, 41, 45	0
1	G	301/302 (99%)	-0.73	0 100 100	33, 37, 40, 45	0
1	H	301/302 (99%)	-0.72	0 100 100	32, 37, 41, 44	0
1	I	300/302 (99%)	-0.56	0 100 100	32, 38, 41, 46	0
1	J	292/302 (96%)	-0.51	0 100 100	33, 38, 42, 46	0
1	K	300/302 (99%)	-0.55	0 100 100	33, 38, 42, 48	0
1	L	300/302 (99%)	-0.37	0 100 100	33, 38, 44, 48	0
1	M	300/302 (99%)	-0.52	0 100 100	32, 37, 42, 47	0
1	N	292/302 (96%)	-0.53	0 100 100	32, 38, 42, 48	0
1	O	301/302 (99%)	-0.62	0 100 100	33, 38, 42, 46	0
1	P	301/302 (99%)	-0.34	2 (0%) 89 87	34, 38, 43, 47	0
All	All	4795/4832 (99%)	-0.60	2 (0%) 100 100	31, 37, 42, 48	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	220	ALA	2.3
1	P	219	GLY	2.2

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 carbohydrates 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. 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	A	602	6/6	0.95	0.17	4.21	33,35,39,40	0
4	GOL	G	601	6/6	0.96	0.13	0.65	31,35,37,38	0
4	GOL	M	606	6/6	0.97	0.14	0.15	35,38,39,41	0
4	GOL	A	605	6/6	0.96	0.12	-0.36	36,39,41,42	0
3	OAF	L	501	12/12	0.98	0.12	-0.61	38,41,43,44	0
3	OAF	A	501	12/12	0.99	0.10	-0.72	33,35,36,37	0
4	GOL	E	604	6/6	0.95	0.11	-0.89	37,40,41,43	0
3	OAF	B	501	12/12	0.98	0.08	-1.20	28,32,36,36	0
3	OAF	O	501	12/12	0.98	0.09	-1.29	30,35,37,38	0
3	OAF	G	501	12/12	0.99	0.08	-1.43	31,34,37,38	0
3	OAF	F	501	12/12	0.99	0.08	-1.50	32,33,35,35	0
3	OAF	C	501	12/12	0.99	0.08	-1.52	32,34,35,36	0
3	OAF	P	501	12/12	0.97	0.10	-1.54	37,40,42,42	0
3	OAF	E	501	12/12	0.99	0.08	-1.59	28,32,34,34	0
3	OAF	I	501	12/12	0.99	0.07	-1.72	35,36,38,41	0
3	OAF	K	501	12/12	0.98	0.09	-1.74	33,36,38,39	0
3	OAF	D	501	12/12	0.99	0.07	-1.97	30,31,33,34	0
3	OAF	H	501	12/12	0.99	0.08	-2.16	33,36,36,39	0
3	OAF	M	501	12/12	0.99	0.07	-2.38	29,34,36,37	0
2	MN	N	401	1/1	0.97	0.04	-3.47	43,43,43,43	0
2	MN	D	401	1/1	1.00	0.04	-3.56	36,36,36,36	0
2	MN	P	401	1/1	0.97	0.03	-4.21	42,42,42,42	0
2	MN	A	401	1/1	1.00	0.04	-4.94	33,33,33,33	0
2	MN	B	401	1/1	1.00	0.03	-5.44	37,37,37,37	0
2	MN	C	401	1/1	1.00	0.03	-5.46	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	O	401	1/1	0.99	0.03	-5.84	39,39,39,39	0
2	MN	F	401	1/1	1.00	0.03	-5.90	36,36,36,36	0
2	MN	J	401	1/1	0.99	0.03	-5.91	43,43,43,43	0
2	MN	I	401	1/1	1.00	0.03	-6.20	39,39,39,39	0
2	MN	H	401	1/1	1.00	0.03	-6.22	35,35,35,35	0
2	MN	E	401	1/1	1.00	0.02	-6.48	36,36,36,36	0
2	MN	G	401	1/1	0.99	0.05	-6.78	34,34,34,34	0
2	MN	L	401	1/1	0.99	0.02	-7.04	41,41,41,41	0
2	MN	K	401	1/1	0.99	0.03	-7.36	38,38,38,38	0
2	MN	M	401	1/1	1.00	0.01	-10.59	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.