W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 01:18 AM EDT

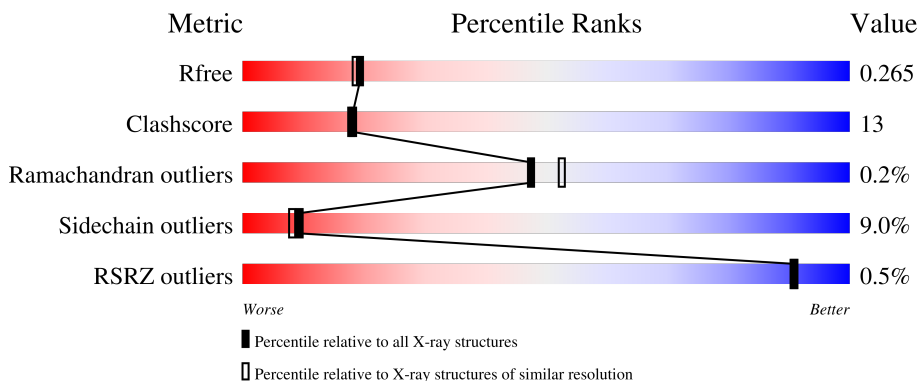|		
PDB ID	:	3FA4
Title	:	Crystal structure of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member, triclinic crystal form
Authors	:	Narayanan, B.C.; Herzberg, O.
Deposited on	:	2008-11-14
Resolution	:	2.18 Å(reported)

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 2.18 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		9.0%
RSRZ outliers		0.5%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	302	70%　21%　·　6%
1	B	302	.% 73%　21%　·　5%
1	C	302	.% 69%　22%　·　6%
1	D	302	.% 72%　19%　·　6%
1	E	302	70%　21%　··　5%

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Mol	Chain	Length	Quality of chain
1	F	302	73% 18% 6%
1	G	302	69% 22% 6%
1	H	302	65% 26% 7%
1	I	302	67% 21% 6% 7%
1	J	302	62% 26% 5% 7%
1	K	302	72% 16% 7%
1	L	302	69% 23% 5%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 26432 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	284	Total 2111	C 1312	N 375	O 409	S 15	0	0	0
1	B	288	Total 2137	C 1330	N 379	O 413	S 15	0	0	0
1	C	284	Total 2112	C 1313	N 375	O 409	S 15	0	0	0
1	D	284	Total 2111	C 1312	N 375	O 409	S 15	0	0	0
1	E	286	Total 2118	C 1316	N 377	O 410	S 15	0	0	0
1	F	285	Total 2116	C 1315	N 376	O 410	S 15	0	0	0
1	G	284	Total 2107	C 1310	N 375	O 407	S 15	0	0	0
1	H	282	Total 2080	C 1293	N 369	O 403	S 15	0	0	0
1	I	282	Total 2100	C 1305	N 373	O 407	S 15	0	0	0
1	J	280	Total 2068	C 1284	N 369	O 400	S 15	0	0	0
1	K	280	Total 2072	C 1287	N 368	O 403	S 14	0	0	0
1	L	288	Total 2126	C 1320	N 384	O 407	S 15	0	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	G	1	Total 1	Mg 1	0	0
2	H	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total 116	O 116	0	0
3	B	115	Total 115	O 115	0	0
3	C	109	Total 109	O 109	0	0
3	D	135	Total 135	O 135	0	0
3	E	104	Total 104	O 104	0	0
3	F	109	Total 109	O 109	0	0
3	G	124	Total 124	O 124	0	0
3	H	104	Total 104	O 104	0	0
3	I	38	Total 38	O 38	0	0

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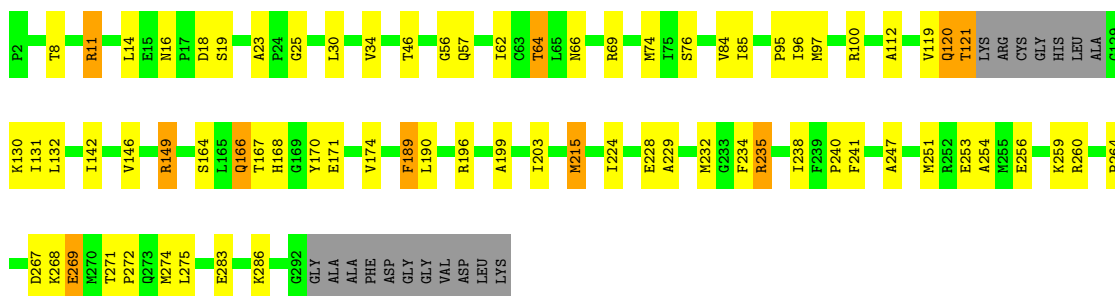
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	83	Total 83	O 83	0	0
3	K	61	Total 61	O 61	0	0
3	L	64	Total 64	O 64	0	0

3 Residue-property plots ⓘ

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.
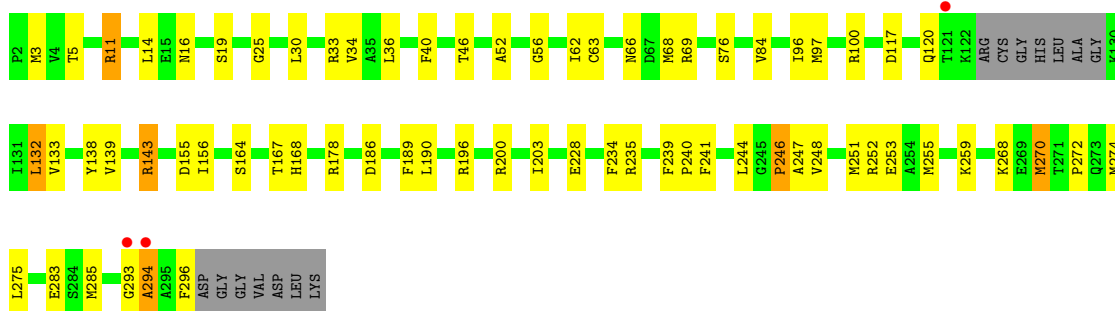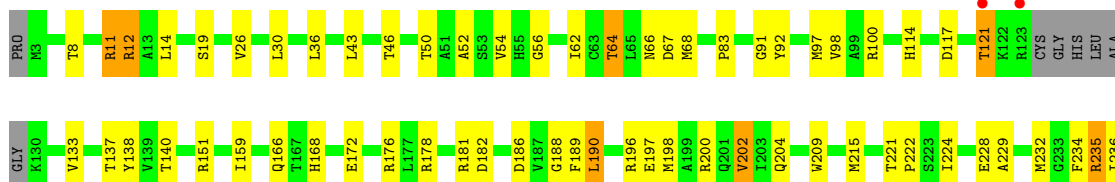
- Molecule 1: 2,3-dimethylmalate lyase

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- Molecule 1: 2,3-dimethylmalate lyase

L244 V248 R252 E256 K259 I263 P264 G265 L266 D267 K268 E269 M274 V278 M285 G292 GLY ALA ALA PHE ASP GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain D:

%

72%   19%   •   6%

P2 R11 R12 A13 L14 E15 D18 S19 L36 D41 A42 L43 T46 Q57 I62 C63 T64 L65 N66 D67 M68 R69 P83 V84 P95 I96 M97 R100 I115 T121 LYS ARG CYS GLY HIS LEU ALA GLY K130 I131 L132 T140 R149 I152 G153

S154 S164 H168 G169 Y170 E171 E172 S173 D186 F189 L190 R196 E197 M198 V202 L213 S223 E228 R235 F241 L244 A247 V248 M251 R252 E253 A254 P264 G265 L266 D267 K268 P272 Q273 M274 E283 S284 M285 K286 G292 G293 ALA

ALA PHE ASP GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain E:

70%   21%   • • 5%

P2 M3 R11 R12 N16 S19 F20 I21 V22 A23 P24 G25 S31 L36 Y44 M45 T50 V54 H55 A58 D59 L60 G61 I62 C63 T64 L65 N66 D67 M68 R69 E73 M74 I78 T90 G91 Y92 P95 I96 M97 R100 S108 F113 H114

I115 Q120 T121 LYS ARG CYS GLY HIS LEU ALA G129 K130 I131 L132 V133 T140 R141 I142 R143 V146 R149 D155 I159 S164 T167 V187 G188 F189 L190 T194 S195 R196 R200 Q201 V202 P210 L211 L212 M215 V216 R235 I238 F239 P240 F241

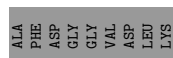E253 I263 P264 G265 L266 D267 K268 E269 M270 L275 F276 R277 S284 D288 A291 G292 G293 A294 ALA PHE ASP GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain F:

%

73%   18%   • • 6%

P2 R11 R12 S19 V26 A32 L36 D41 V54 Q57 I62 D67 M68 R69 M74 I78 I85 A86 G94 P95 I96 M97 V98 A99 R100 A112 F113 H114 I115 T121 K122 ARG CYS GLY HIS LEU ALA G129 V133 T140 R149

I156 R161 T162 L165 Q166 T167 H168 E172 S173 D186 F189 L190 T194 V202 I203 Q204 D205 L206 W209 L213 N214 M215 V216 E217 I224 M232 F234 R235 P240 F241 L244 V248 A249 A250 M251 R252 E253 I263 P264 M274 G292
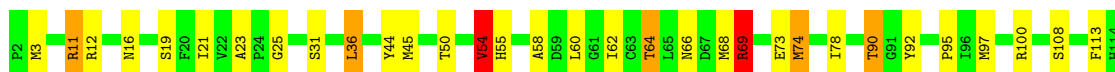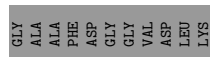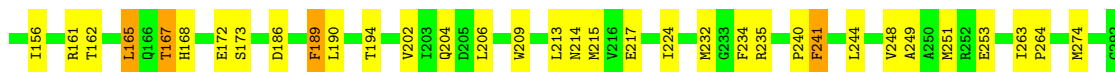
GLY ALA ALA PHE ASP GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain G:

69%   22%   • • 6%

P2 R11 N16 I21 D28 G29 L30 R33 L36 T46 T50 A51 A52 S53 V54 H55 G56 Q57 I62 R69 A70 N71 M74 I75 S76 V84 D89 G94 P95 I96 M97 V98 A99 R100 Q104 H114 D117 T121 LYS ARG CYS GLY

HIS LEU ALA G129 K130 I131 L132 V133 D136 T137 Y138 V139 T140 R141 I142 R143 V146 I152 D155 I159 A160 R161 T162 D163 S164 T167 Y170 S173 R176 R181 F189 L190 A199 R200 I203 L213 N214 M215 V216 R235 P240 F241 M255

R260 D261 P264 K268 E269 M270 T271 P272 Q273 M274 L275 E283 S284 M285 G292 GLY ALA ALA PHE ASP GLY GLY VAL ASP LEU LYS
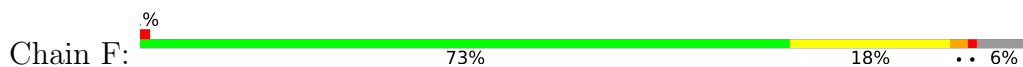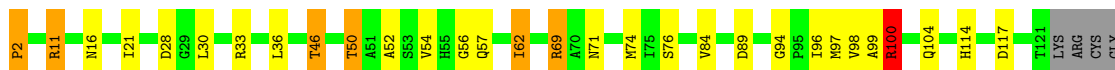
• Molecule 1: 2,3-dimethylmalate lyase

Chain H: 65% 26% 7%

P2 M3 V4 T5 T8 R11 R12 S19 A23 L30 L36 S37 T46 G49 T50 V54 H55 G56 Q57 A58 I62 N66 D67 M68 R69 M74 I85 A86 D89 M97 A112 F113 H114 I115 E116 Q120 THR LYS ARG CYS GLY HIS LEU

ALA GLY K130 I131 L132 V133 D134 T135 D136 T137 Y138 V146 Q147 A148 R149 Q150 R151 I152 G153 I159 R176 L177 R178 A179 A180 R181 V187 G188 F189 L190 I193 R196 A199 V202 I203 Q204 D205 W209 P210 L211 L212 L213 N214 M215 I224 E228

A229 M232 G233 F234 R235 I238 F239 A243 L244 V248 A249 M251 M255 R260 I263 P264 D267 K268 E269 R277 E283 S284 G292 GLY ALA ALA PHE ASP GLY GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain I: % 67% 21% 6% 7%

PRO M3 V4 R11 R12 S19 P24 G25 V26 Y27 L30 S31 A32 L36 S37 F40 M45 T46 G47 T50 A51 A52 S53 V54 H55 G56 I62 C63 T64 L65 N66 D67 M68 R69 M74 I75 Y92 I96 M97 R107 E116 D117 V118 V119 Q120 T121

LYS ARG CYS GLY HIS LEU ALA GLY K130 I131 L132 T135 D136 T137 Y138 V139 T140 R141 I142 R161 H168 G169 Y170 E171 E172 S173 R181 A185 D186 F189 L190 T194 S195 R196 E197 M198 A199 V202 I203 L211 L212 L213 N214 M215 S223 I224 M232 R235

I238 F239 P240 F241 A242 A250 M251 R252 E253 P264 K268 M274 R277 E283 S284 V287 G292 GLY ALA ALA PHE ASP GLY GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase

Chain J: 62% 26% 5% 7%

PRO M3 V4 T5 A6 R12 A13 S19 F20 I21 V22 A23 P24 L30 V34 A35 L36 S37 D41 A42 L43 T46 G47 T50 A51 A52 S53 V54 H55 G56 Q57 A58 D59 L60 G61 I62 C63 M68 R69 A70 N71 M74 P83 V84 D87 G91 I96

M97 V98 A99 R100 A112 I115 E116 D117 Q118 V119 Q120 THR LYS ARG CYS GLY HIS LEU ALA GLY LYS I131 L132 V133 Y138 R141 I142 R143 Q147 V157 S164 L165 Q166 T167 H168 E172 A180 R181 A185 D186 V187 G188 F189 L190 I193 T194 E197

L206 W209 P210 L213 N214 M215 H218 T221 I224 M232 I236 I237 I238 F239 P240 F241 L244 R252 M255 I263 P264 G265 L266 E269 M270 M274 L275 F276 R277 L281 D282 E283 S284 M285 K286 V287 Q290 A291 G292 GLY ALA ALA PHE ASP GLY

GLY VAL ASP LEU LYS

• Molecule 1: 2,3-dimethylmalate lyase
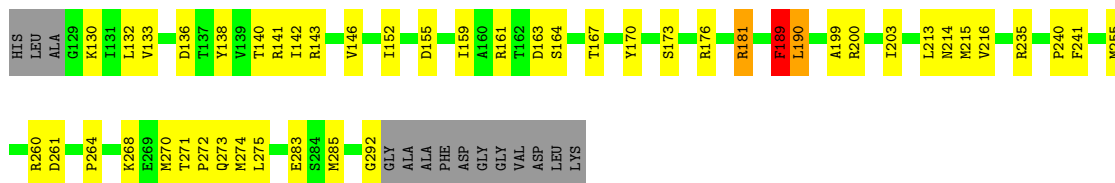
Chain K:

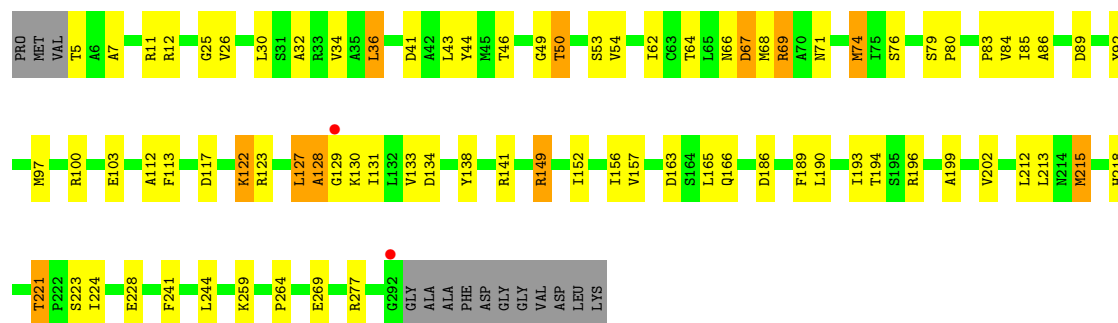

• Molecule 1: 2,3-dimethylmalate lyase

Chain L:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	79.09Å 115.47Å 115.75Å 119.66° 90.71° 96.28°	Depositor
Resolution (Å)	46.83 – 2.18 46.81 – 2.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (46.83-2.18) 91.8 (46.81-2.18)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.33 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.265 0.202 , 0.265	Depositor DCC
R_{free} test set	8603 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.6	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.159 for -h,-k-l,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26432	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG

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	1.09	1/2141 (0.0%)	1.04	5/2898 (0.2%)
1	B	1.11	1/2168 (0.0%)	1.03	2/2935 (0.1%)
1	C	1.08	2/2141 (0.1%)	1.08	8/2898 (0.3%)
1	D	1.12	2/2141 (0.1%)	1.06	5/2898 (0.2%)
1	E	1.07	4/2148 (0.2%)	1.08	8/2907 (0.3%)
1	F	1.02	0/2146	1.03	4/2905 (0.1%)
1	G	1.16	4/2137 (0.2%)	1.08	8/2893 (0.3%)
1	H	1.09	2/2110 (0.1%)	1.06	4/2861 (0.1%)
1	I	0.93	1/2129 (0.0%)	0.96	1/2882 (0.0%)
1	J	0.97	1/2097 (0.0%)	0.95	3/2841 (0.1%)
1	K	0.96	1/2101 (0.0%)	0.94	3/2846 (0.1%)
1	L	0.92	1/2157 (0.0%)	0.96	4/2922 (0.1%)
All	All	1.05	20/25616 (0.1%)	1.02	55/34686 (0.2%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	GLU	CG-CD	5.95	1.60	1.51
1	J	63	CYS	CB-SG	-5.88	1.72	1.81
1	G	283	GLU	CG-CD	5.88	1.60	1.51
1	E	54	VAL	CB-CG2	-5.87	1.40	1.52
1	B	283	GLU	CG-CD	5.77	1.60	1.51

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	C	235	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	C	235	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	235	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	L	149	ARG	NE-CZ-NH2	-8.01	116.30	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	2111	0	2110	71	0
1	B	2137	0	2131	79	0
1	C	2112	0	2107	61	0
1	D	2111	0	2110	53	0
1	E	2118	0	2113	68	0
1	F	2116	0	2112	64	0
1	G	2107	0	2106	53	0
1	H	2080	0	2057	72	0
1	I	2100	0	2099	72	0
1	J	2068	0	2046	85	0
1	K	2072	0	2053	48	0
1	L	2126	0	2119	74	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
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	116	0	0	3	0
3	B	115	0	0	4	0
3	C	109	0	0	3	0
3	D	135	0	0	2	0
3	E	104	0	0	3	0
3	F	109	0	0	6	0
3	G	124	0	0	6	0
3	H	104	0	0	7	0
3	I	38	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	83	0	0	10	0
3	K	61	0	0	2	0
3	L	64	0	0	4	0
All	All	26432	0	25163	678	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 13.

The worst 5 of 678 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:97:MET:CE	1:A:100:ARG:HD3	1.65	1.25
1:E:74:MET:CE	1:E:78:ILE:HD11	1.72	1.19
1:A:97:MET:HE2	1:A:100:ARG:HD3	1.19	1.18
1:A:62:ILE:HG22	1:D:97:MET:HE3	1.30	1.12
1:B:97:MET:HE1	1:B:100:ARG:HD3	1.34	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	280/302 (93%)	273 (98%)	7 (2%)	0	100	100
1	B	284/302 (94%)	270 (95%)	13 (5%)	1 (0%)	34	35
1	C	280/302 (93%)	273 (98%)	7 (2%)	0	100	100
1	D	280/302 (93%)	267 (95%)	13 (5%)	0	100	100
1	E	282/302 (93%)	276 (98%)	6 (2%)	0	100	100
1	F	281/302 (93%)	273 (97%)	8 (3%)	0	100	100
1	G	280/302 (93%)	274 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	278/302 (92%)	265 (95%)	11 (4%)	2 (1%)	22	20
1	I	278/302 (92%)	268 (96%)	10 (4%)	0	100	100
1	J	276/302 (91%)	263 (95%)	12 (4%)	1 (0%)	34	35
1	K	276/302 (91%)	268 (97%)	6 (2%)	2 (1%)	22	20
1	L	286/302 (95%)	276 (96%)	10 (4%)	0	100	100
All	All	3361/3624 (93%)	3246 (97%)	109 (3%)	6 (0%)	47	52

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	ALA
1	H	268	LYS
1	J	119	VAL
1	K	268	LYS
1	H	89	ASP

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/228 (95%)	201 (93%)	16 (7%)	13	13
1	B	218/228 (96%)	203 (93%)	15 (7%)	15	15
1	C	216/228 (95%)	198 (92%)	18 (8%)	11	10
1	D	217/228 (95%)	202 (93%)	15 (7%)	15	15
1	E	216/228 (95%)	196 (91%)	20 (9%)	9	7
1	F	217/228 (95%)	200 (92%)	17 (8%)	12	11
1	G	216/228 (95%)	196 (91%)	20 (9%)	9	7
1	H	211/228 (92%)	193 (92%)	18 (8%)	10	9
1	I	216/228 (95%)	189 (88%)	27 (12%)	4	3
1	J	209/228 (92%)	181 (87%)	28 (13%)	4	2
1	K	210/228 (92%)	193 (92%)	17 (8%)	11	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	215/228 (94%)	193 (90%)	22 (10%)	7 6
All	All	2578/2736 (94%)	2345 (91%)	233 (9%)	9 8

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	189	PHE
1	L	133	VAL
1	I	36	LEU
1	L	123	ARG
1	K	74	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	G	273	GLN
1	H	118	GLN
1	L	71	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	284/302 (94%)	-0.39	0	100	100	30, 36, 43, 54	0
1	B	288/302 (95%)	-0.37	3 (1%)	82	82	29, 36, 44, 53	0
1	C	284/302 (94%)	-0.37	2 (0%)	87	88	30, 36, 43, 50	0
1	D	284/302 (94%)	-0.41	2 (0%)	87	88	31, 36, 43, 50	0
1	E	286/302 (94%)	-0.34	1 (0%)	94	94	31, 36, 43, 52	0
1	F	285/302 (94%)	-0.38	2 (0%)	87	88	28, 36, 44, 52	0
1	G	284/302 (94%)	-0.43	0	100	100	27, 36, 43, 49	0
1	H	282/302 (93%)	-0.40	0	100	100	29, 36, 43, 48	0
1	I	282/302 (93%)	-0.20	3 (1%)	80	80	30, 37, 43, 49	0
1	J	280/302 (92%)	-0.27	1 (0%)	92	92	29, 36, 42, 49	0
1	K	280/302 (92%)	-0.31	1 (0%)	92	92	31, 36, 42, 46	0
1	L	288/302 (95%)	-0.25	2 (0%)	87	88	30, 36, 43, 52	0
All	All	3407/3624 (94%)	-0.34	17 (0%)	91	91	27, 36, 43, 54	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	4	VAL	5.1
1	L	129	GLY	4.9
1	E	129	GLY	4.6
1	C	123	ARG	3.2
1	I	4	VAL	3.1

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

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

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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
2	MG	A	401	1/1	0.90	0.07	51,51,51,51	0
2	MG	L	401	1/1	0.90	0.07	48,48,48,48	0
2	MG	J	401	1/1	0.92	0.06	47,47,47,47	0
2	MG	D	401	1/1	0.94	0.05	40,40,40,40	0
2	MG	F	401	1/1	0.94	0.06	44,44,44,44	0
2	MG	B	401	1/1	0.95	0.05	35,35,35,35	0
2	MG	I	401	1/1	0.97	0.05	42,42,42,42	0
2	MG	E	401	1/1	0.98	0.05	40,40,40,40	0
2	MG	C	401	1/1	0.98	0.04	46,46,46,46	0
2	MG	K	401	1/1	0.98	0.11	46,46,46,46	0
2	MG	H	401	1/1	0.98	0.09	43,43,43,43	0
2	MG	G	401	1/1	1.00	0.03	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.