



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:04 am BST

PDB ID : 3T8Q  
Title : Crystal structure of mandelate racemase/muconate lactonizing enzyme family protein from *Hoeflea phototrophica*  
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-08-01  
Resolution : 2.00 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

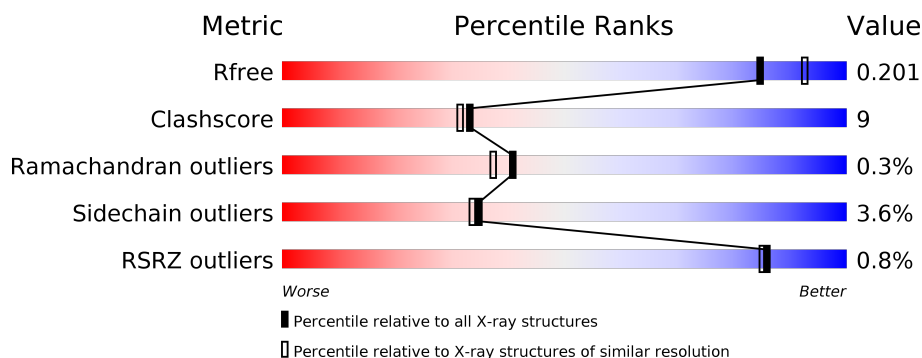
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>84%</span> <span>13%</span> <span>••</span> </div> </div>
1	B	370	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>13%</span> <span>•</span> </div> </div>

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
3	MLI	A	370	-	-	X	-
3	MLI	B	370	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6408 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 Mandelate racemase/muconate lactonizing enzyme family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2876	1824	485	550	17			
1	B	369	Total	C	N	O	S	0	0	0
			2890	1831	488	554	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	EXPRESSION TAG	UNP A9D2J3
A	0	SER	-	EXPRESSION TAG	UNP A9D2J3
B	-1	GLN	-	EXPRESSION TAG	UNP A9D2J3
B	0	SER	-	EXPRESSION TAG	UNP A9D2J3

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

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

- Molecule 3 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	B	1	Total	C	O	0	0
			7	3	4		

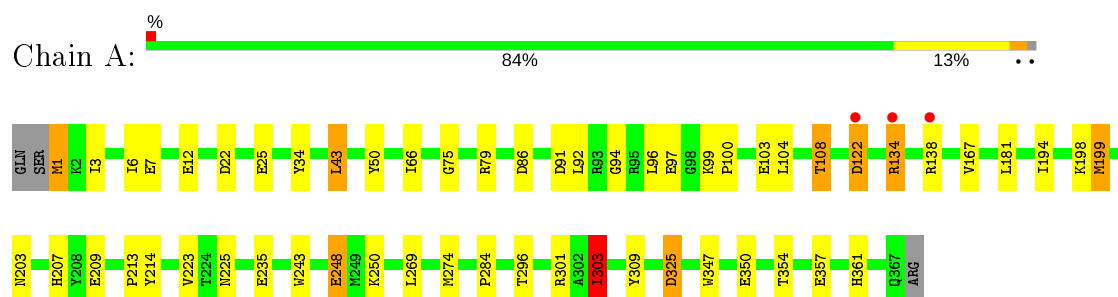
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	308	Total	O	0	0
			308	308		
4	B	318	Total	O	0	0
			318	318		

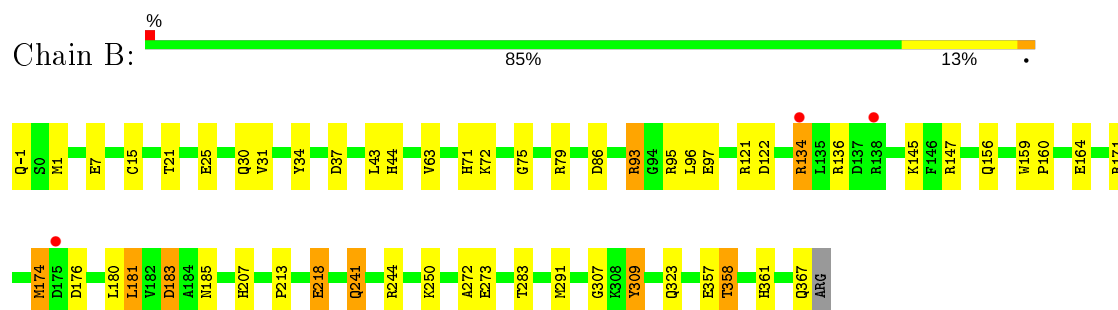
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Mandelate racemase/muconate lactonizing enzyme family protein



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme family protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.56 Å 189.46 Å 57.99 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 2.00 49.46 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.46-2.00) 98.3 (49.46-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.15 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.151 , 0.193 0.166 , 0.201	Depositor DCC
$R_{free}$ test set	2843 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MLI

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	1.27	7/2947 (0.2%)	0.96	5/4010 (0.1%)
1	B	1.27	8/2961 (0.3%)	0.98	6/4028 (0.1%)
All	All	1.27	15/5908 (0.3%)	0.97	11/8038 (0.1%)

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	A	1	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	VAL	CB-CG1	-5.98	1.40	1.52
1	B	164	GLU	CD-OE1	5.95	1.32	1.25
1	A	325	ASP	CB-CG	5.84	1.64	1.51
1	A	209	GLU	CD-OE2	5.73	1.31	1.25
1	B	244	ARG	C-O	-5.44	1.13	1.23
1	A	214	TYR	CD2-CE2	-5.41	1.31	1.39
1	A	350	GLU	CG-CD	5.29	1.59	1.51
1	B	323	GLN	CB-CG	-5.26	1.38	1.52
1	B	272	ALA	CA-CB	-5.20	1.41	1.52
1	A	97	GLU	CD-OE2	-5.17	1.20	1.25
1	B	44	HIS	C-O	-5.11	1.13	1.23
1	B	145	LYS	CD-CE	-5.09	1.38	1.51
1	A	248	GLU	CG-CD	5.07	1.59	1.51
1	B	71	HIS	C-O	-5.06	1.13	1.23
1	A	250	LYS	CE-NZ	5.01	1.61	1.49



All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	93	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	22	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	303	ILE	CA-CB-CG2	5.84	122.59	110.90
1	B	183	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	358	THR	OG1-CB-CG2	5.35	122.30	110.00
1	B	95	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	43	LEU	CB-CG-CD1	5.23	119.90	111.00
1	B	37	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	134	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	134	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	122	ASP	CB-CG-OD2	5.12	122.91	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	303	ILE	CB

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	2876	0	2788	46	0
1	B	2890	0	2800	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	7	0	2	3	0
3	B	7	0	2	3	0
4	A	308	0	0	8	0
4	B	318	0	0	5	0
All	All	6408	0	5592	98	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 9.

All (98) 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:B:30:GLN:HB2	1:B:291:MET:CE	1.55	1.34
1:B:136:ARG:HH11	1:B:174:MET:CE	1.66	1.07
1:A:108:THR:HG22	1:A:301:ARG:HH21	1.15	1.07
1:B:30:GLN:HB2	1:B:291:MET:HE2	1.42	1.01
1:B:121:ARG:HH22	1:B:185:ASN:HD22	1.04	0.98
1:B:1:MET:HE3	1:B:25:GLU:OE1	1.65	0.96
1:B:136:ARG:NH1	1:B:174:MET:CE	2.28	0.96
1:B:30:GLN:HB2	1:B:291:MET:HE3	1.45	0.96
1:A:325:ASP:HB2	4:A:604:HOH:O	1.64	0.96
1:B:30:GLN:CB	1:B:291:MET:CE	2.46	0.93
1:A:167:VAL:HG11	1:A:199:MET:HE1	1.50	0.93
1:B:147:ARG:HH11	1:B:185:ASN:HD21	1.19	0.89
1:A:79:ARG:HH21	3:A:370:MLI:H12	1.41	0.85
1:A:269:LEU:CD2	1:A:303:ILE:HD11	2.07	0.85
1:A:199:MET:HE2	1:A:203:ASN:OD1	1.79	0.82
1:A:167:VAL:HG11	1:A:199:MET:CE	2.10	0.81
1:B:30:GLN:CB	1:B:291:MET:HE3	2.10	0.81
1:B:218:GLU:H	1:B:218:GLU:CD	1.85	0.79
1:B:121:ARG:NH2	1:B:185:ASN:HD22	1.80	0.79
1:A:361:HIS:HD2	4:A:494:HOH:O	1.66	0.78
1:A:243:TRP:HB3	1:A:274:MET:HE1	1.67	0.77
1:B:241:GLN:H	1:B:241:GLN:HE21	1.34	0.75
1:B:136:ARG:HH11	1:B:174:MET:HE2	1.49	0.75
1:B:79:ARG:HH21	3:B:370:MLI:H12	1.52	0.74
1:B:361:HIS:HD2	4:B:428:HOH:O	1.71	0.73
1:A:269:LEU:HD23	1:A:303:ILE:HD11	1.71	0.72
1:B:367:GLN:HA	1:B:367:GLN:OE1	1.89	0.72
1:B:136:ARG:NH1	1:B:174:MET:HE1	2.05	0.71
1:A:108:THR:HG22	1:A:301:ARG:NH2	1.99	0.71
1:A:248:GLU:HG3	4:A:575:HOH:O	1.92	0.70
1:B:121:ARG:HH22	1:B:185:ASN:ND2	1.86	0.69
1:B:181:LEU:HD12	1:B:181:LEU:N	2.08	0.68
1:B:-1:GLN:N	4:B:746:HOH:O	2.28	0.67
1:A:92:LEU:HD12	4:A:622:HOH:O	1.95	0.64
1:A:50:TYR:HB2	1:A:66:ILE:HD13	1.80	0.64
1:A:325:ASP:CG	1:A:325:ASP:O	2.36	0.63
1:A:79:ARG:NH2	3:A:370:MLI:H12	2.11	0.63
1:A:134:ARG:HH22	1:A:138:ARG:NH1	1.98	0.62
1:A:108:THR:CG2	1:A:301:ARG:HH21	2.01	0.62
1:B:1:MET:CE	1:B:25:GLU:OE1	2.43	0.62
1:B:136:ARG:NH1	1:B:174:MET:HE3	2.12	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLN:H	1:B:241:GLN:NE2	1.98	0.61
1:B:30:GLN:HB2	1:B:291:MET:HE1	1.72	0.60
1:A:167:VAL:CG1	1:A:199:MET:CE	2.78	0.60
1:A:194:ILE:HD11	1:A:223:VAL:HA	1.85	0.59
1:A:1:MET:HE1	1:A:96:LEU:HD11	1.86	0.58
1:B:1:MET:HE3	1:B:25:GLU:CD	2.23	0.57
1:B:180:LEU:C	1:B:181:LEU:HD12	2.24	0.57
1:A:199:MET:O	1:A:199:MET:HE2	2.06	0.55
1:A:1:MET:CE	1:A:96:LEU:HD11	2.37	0.54
1:B:93:ARG:NH1	1:B:97:GLU:OE2	2.42	0.53
1:A:167:VAL:CG1	1:A:199:MET:HE3	2.38	0.53
1:B:171:ARG:O	1:B:171:ARG:HD3	2.10	0.52
1:A:199:MET:CE	1:A:203:ASN:OD1	2.54	0.51
1:A:91:ASP:HB2	1:A:347:TRP:CD1	2.45	0.51
1:B:207:HIS:HD2	4:B:381:HOH:O	1.92	0.51
1:B:181:LEU:HG	1:B:207:HIS:HB3	1.93	0.51
1:A:243:TRP:HB3	1:A:274:MET:CE	2.39	0.50
1:B:79:ARG:NH2	3:B:370:MLI:H12	2.24	0.49
1:A:7:GLU:OE1	1:A:361:HIS:HE1	1.95	0.49
3:A:370:MLI:O6	3:A:370:MLI:O8	2.28	0.49
1:B:43:LEU:HD23	1:B:43:LEU:O	2.13	0.49
1:A:12:GLU:HG2	4:A:506:HOH:O	2.12	0.49
1:B:134:ARG:HD3	4:B:614:HOH:O	2.13	0.48
1:A:25:GLU:HG2	1:A:96:LEU:HD21	1.95	0.48
1:A:100:PRO:HG2	1:A:103:GLU:HG3	1.95	0.48
1:B:30:GLN:CB	1:B:291:MET:HE2	2.26	0.48
1:A:99:LYS:HE3	4:A:406:HOH:O	2.13	0.47
1:B:181:LEU:CD1	1:B:181:LEU:N	2.77	0.47
1:B:25:GLU:HG2	1:B:96:LEU:HD21	1.97	0.47
1:B:7:GLU:OE1	1:B:361:HIS:HE1	1.98	0.47
1:A:194:ILE:CD1	1:A:223:VAL:HA	2.43	0.46
1:B:250:LYS:HD3	4:B:509:HOH:O	2.16	0.46
1:B:283:THR:OG1	1:B:307:GLY:HA3	2.16	0.46
1:B:181:LEU:HD21	1:B:309:TYR:CZ	2.51	0.46
1:A:181:LEU:HG	1:A:207:HIS:HB3	1.97	0.46
1:A:75:GLY:HA3	1:B:75:GLY:HA3	1.97	0.45
1:B:159:TRP:HB2	1:B:160:PRO:HD2	1.98	0.45
1:A:3:ILE:HG21	1:A:6:ILE:HD11	1.97	0.45
1:A:303:ILE:HA	1:A:303:ILE:HD12	1.81	0.44
1:A:99:LYS:CE	4:A:406:HOH:O	2.64	0.44
1:B:147:ARG:NH1	1:B:183:ASP:OD2	2.51	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:O	1:A:198:LYS:HG2	2.18	0.43
1:A:235:GLU:OE2	1:B:72:LYS:NZ	2.52	0.43
1:A:269:LEU:HD22	1:A:303:ILE:HD11	1.99	0.43
3:B:370:MLI:O6	3:B:370:MLI:O8	2.36	0.42
1:A:243:TRP:CB	1:A:274:MET:HE1	2.42	0.42
1:B:367:GLN:CA	1:B:367:GLN:OE1	2.63	0.42
1:B:1:MET:HE1	1:B:21:THR:HG21	2.01	0.42
1:A:225:ASN:HB3	4:A:442:HOH:O	2.20	0.42
1:A:284:PRO:HB2	1:A:296:THR:HG23	2.01	0.42
1:B:43:LEU:HD23	1:B:43:LEU:C	2.40	0.41
1:B:136:ARG:HD3	1:B:174:MET:CE	2.50	0.41
1:B:171:ARG:HD3	1:B:171:ARG:HA	1.88	0.41
1:B:15:CYS:HB3	1:B:31:VAL:HG22	2.02	0.41
1:B:136:ARG:HD3	1:B:174:MET:HE1	2.03	0.40
1:A:94:GLY:HA2	1:A:104:LEU:HD11	2.04	0.40
1:A:354:THR:O	1:A:357:GLU:HG2	2.21	0.40

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	365/370 (99%)	360 (99%)	4 (1%)	1 (0%)	41	37
1	B	367/370 (99%)	361 (98%)	5 (1%)	1 (0%)	41	37
All	All	732/740 (99%)	721 (98%)	9 (1%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	TYR
1	B	34	TYR

### 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	303/307 (99%)	294 (97%)	9 (3%)	41	41
1	B	305/307 (99%)	292 (96%)	13 (4%)	29	26
All	All	608/614 (99%)	586 (96%)	22 (4%)	35	34

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	43	LEU
1	A	86	ASP
1	A	108	THR
1	A	122	ASP
1	A	199	MET
1	A	213	PRO
1	A	303	ILE
1	A	309	TYR
1	B	86	ASP
1	B	122	ASP
1	B	156	GLN
1	B	174	MET
1	B	176	ASP
1	B	181	LEU
1	B	213	PRO
1	B	218	GLU
1	B	241	GLN
1	B	273	GLU
1	B	309	TYR
1	B	357	GLU
1	B	358	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	361	HIS
1	A	362	GLN
1	B	185	ASN
1	B	207	HIS
1	B	222	GLN
1	B	236	GLN
1	B	241	GLN
1	B	361	HIS

### 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	MLI	A	370	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLI	B	370	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLI	A	370	-	-	0/0/4/4	-
3	MLI	B	370	-	-	0/0/4/4	-

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	370	MLI	3	0
3	B	370	MLI	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/370 (99%)	-0.28	3 (0%) 86 85	6, 10, 17, 25	0
1	B	369/370 (99%)	-0.28	3 (0%) 86 85	5, 10, 18, 26	0
All	All	736/740 (99%)	-0.28	6 (0%) 86 85	5, 10, 18, 26	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	ARG	2.9
1	A	134	ARG	2.8
1	A	122	ASP	2.8
1	B	175	ASP	2.5
1	B	138	ARG	2.0
1	A	138	ARG	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 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MLI	A	370	7/7	0.84	0.15	31,37,38,39	0
3	MLI	B	370	7/7	0.87	0.13	29,34,36,38	0
2	MG	A	369	1/1	0.93	0.26	12,12,12,12	1
2	MG	B	369	1/1	0.97	0.10	14,14,14,14	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.