wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 04:43 AM EDT

PDB ID	:	3MSY
Title	:	Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium
Authors	:	Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-04-29
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

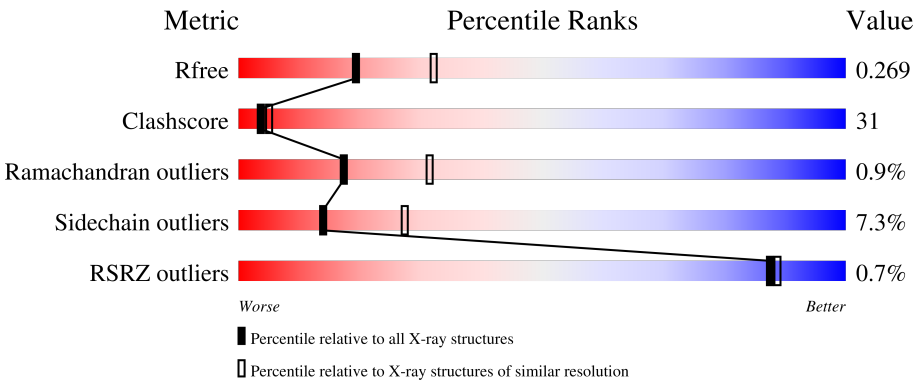
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	379	53% 35% 5% 8%
1	B	379	% 53% 34% 5% 7%
1	C	379	54% 35% • 6%
1	D	379	% 55% 34% • 7%
1	E	379	% 50% 38% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	379	% 53% 36% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16869 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	349	2731	1723	481	512	5	10	0	0	0
1	B	351	2747	1732	485	515	5	10	0	0	0
1	C	355	2786	1757	493	521	5	10	0	0	0
1	D	351	2747	1732	485	515	5	10	0	0	0
1	E	350	2737	1726	482	514	5	10	0	0	0
1	F	351	2747	1732	485	515	5	10	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MSE	-	expression tag	UNP A4AFX2
A	19	SER	-	expression tag	UNP A4AFX2
A	389	GLU	-	expression tag	UNP A4AFX2
A	390	GLY	-	expression tag	UNP A4AFX2
A	391	HIS	-	expression tag	UNP A4AFX2
A	392	HIS	-	expression tag	UNP A4AFX2
A	393	HIS	-	expression tag	UNP A4AFX2
A	394	HIS	-	expression tag	UNP A4AFX2
A	395	HIS	-	expression tag	UNP A4AFX2
A	396	HIS	-	expression tag	UNP A4AFX2
B	18	MSE	-	expression tag	UNP A4AFX2
B	19	SER	-	expression tag	UNP A4AFX2
B	389	GLU	-	expression tag	UNP A4AFX2
B	390	GLY	-	expression tag	UNP A4AFX2
B	391	HIS	-	expression tag	UNP A4AFX2
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	18	MSE	-	expression tag	UNP A4AFX2
C	19	SER	-	expression tag	UNP A4AFX2
C	389	GLU	-	expression tag	UNP A4AFX2
C	390	GLY	-	expression tag	UNP A4AFX2
C	391	HIS	-	expression tag	UNP A4AFX2
C	392	HIS	-	expression tag	UNP A4AFX2
C	393	HIS	-	expression tag	UNP A4AFX2
C	394	HIS	-	expression tag	UNP A4AFX2
C	395	HIS	-	expression tag	UNP A4AFX2
C	396	HIS	-	expression tag	UNP A4AFX2
D	18	MSE	-	expression tag	UNP A4AFX2
D	19	SER	-	expression tag	UNP A4AFX2
D	389	GLU	-	expression tag	UNP A4AFX2
D	390	GLY	-	expression tag	UNP A4AFX2
D	391	HIS	-	expression tag	UNP A4AFX2
D	392	HIS	-	expression tag	UNP A4AFX2
D	393	HIS	-	expression tag	UNP A4AFX2
D	394	HIS	-	expression tag	UNP A4AFX2
D	395	HIS	-	expression tag	UNP A4AFX2
D	396	HIS	-	expression tag	UNP A4AFX2
E	18	MSE	-	expression tag	UNP A4AFX2
E	19	SER	-	expression tag	UNP A4AFX2
E	389	GLU	-	expression tag	UNP A4AFX2
E	390	GLY	-	expression tag	UNP A4AFX2
E	391	HIS	-	expression tag	UNP A4AFX2
E	392	HIS	-	expression tag	UNP A4AFX2
E	393	HIS	-	expression tag	UNP A4AFX2
E	394	HIS	-	expression tag	UNP A4AFX2
E	395	HIS	-	expression tag	UNP A4AFX2
E	396	HIS	-	expression tag	UNP A4AFX2
F	18	MSE	-	expression tag	UNP A4AFX2
F	19	SER	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2
F	390	GLY	-	expression tag	UNP A4AFX2
F	391	HIS	-	expression tag	UNP A4AFX2
F	392	HIS	-	expression tag	UNP A4AFX2
F	393	HIS	-	expression tag	UNP A4AFX2
F	394	HIS	-	expression tag	UNP A4AFX2
F	395	HIS	-	expression tag	UNP A4AFX2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	396	HIS	-	expression tag	UNP A4AFX2

- Molecule 2 is water.

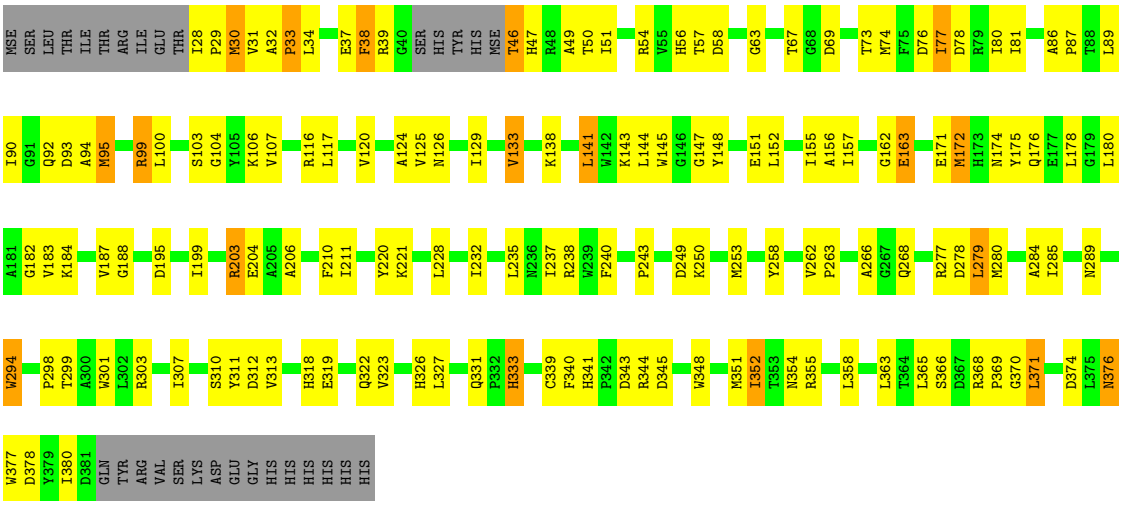
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	65	65	65	0	0
			Total	O		
2	B	62	62	62	0	0
			Total	O		
2	C	63	63	63	0	0
			Total	O		
2	D	72	72	72	0	0
			Total	O		
2	E	55	55	55	0	0
			Total	O		
2	F	57	57	57	0	0

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.

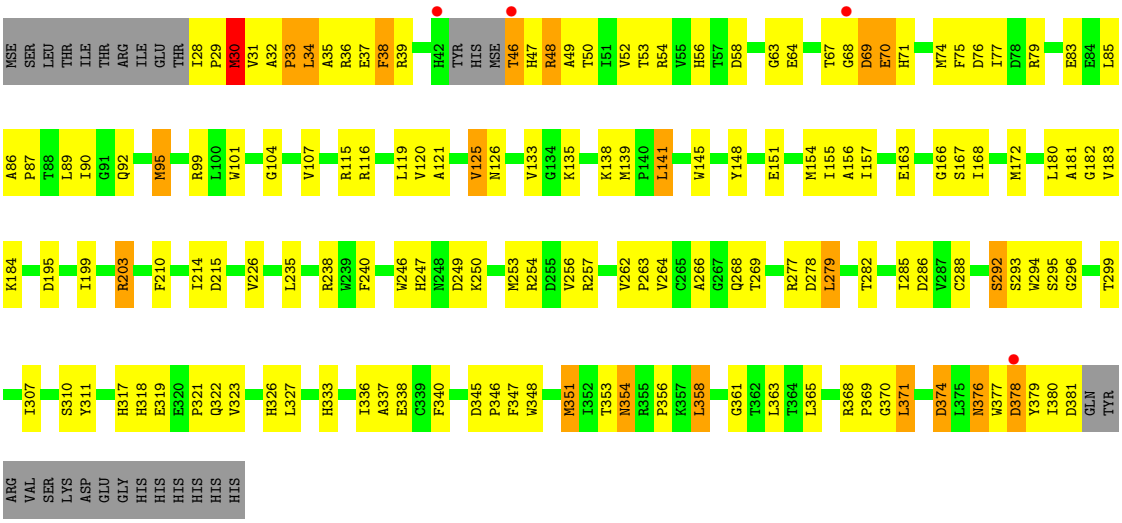
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain A:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain B:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain C: 54% 35% • 6%

MSE SER LEU THR ILE THR ARG ILE GLU THR I28 P29 M30 V31 A32 P33 L34 A35 R36 E37 F38 R39 G40 S41 H42 TYR HIS MSE T46 H47 R48 A49 T50 I51 R54 V55 H56 T57 D58 G63 T67 E70 H71 E72 T73 M74 F75 D76 I77 D78 R79 I80 E83 E84 L85

A86 P87 T88 L89 I90 G91 Q92 D93 A94 M95 A96 I97 S103 G104 V107 I111 L117 V120 V125 N126 T127 A128 I129 W130 V133 L137 K138 M139 P140 L141 W142 K143 R149 N150 E151 L152 P153 A156 I157 Y160 I168 M172 L180 A181 G182 V183

K184 F185 K186 V187 G188 R203 F210 I211 I212 D215 Q218 G219 Y220 K221 I232 I237 F240 V244 E245 W246 H247 N248 D249 K250 R251 S252 M253 R254 D255 V256 R257 Y258 V264 C265 A266 G267 Q268 T269 S274 R277 D278 L279 M280 E281 T282 I285 D286 V287

C288 S293 P298 T299 I307 S310 Y311 D312 V313 Q314 M315 H318 E319 Q322 V323 H333 I336 C339 F340 R344 D345 P346 F347 M351 N354 R355 P356 K357 L358 N359 N360 G361 T362 I363 T364 G370 L371 G372 W373 N376 W377 D378 Y379 I380 D381 Q382

Y383 R384 V385 SER LYS ASP GLU GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain D: % 55% 34% • 7%

MSE SER LEU THR ILE THR ARG ILE GLU THR I28 P29 M30 V31 A32 P33 L34 A35 R36 E37 F38 R39 G40 S41 H42 TYR HIS MSE T46 H47 R48 A49 T50 I51 R54 V55 H56 T57 D58 I61 Y66 T67 G68 D69 E70 H71 E72 T73 M74 F75 D76 I77 D78 R79 E83

A86 P87 T88 L89 I90 G91 Q92 D93 A94 M95 L100 K106 F109 R115 V120 N126 D131 A132 V133 G134 K135 M139 P140 L141 W142 K143 Y148 R149 N150 E151 L152 P153 A156 I157 Y161 G162 E163 G166 S167 E171 M172 H173 N174 Y175 Q176 E177 L178

G179 L180 A181 G182 V183 K184 V187 G188 D195 I199 R203 D209 F210 I211 I212 D215 Y220 I232 L235 N236 I237 F240 E245 W246 H247 N248 D249 K250 M253 R254 D255 Y258 V262 P263 A266 G267 Q268 T269 R277 D278 L279 T282 G283

A284 I285 D286 V287 C288 N289 S293 P298 T299 R303 I307 Y311 D312 H318 E319 E320 P321 Q322 V323 A329 S330 Q331 P332 H333 E338 C339 F340 D345 P346 F347 W348 M351 R355 P356 K357 N360 G361 T362 L363 T364 L365 P369 G370 L371 G372 W373

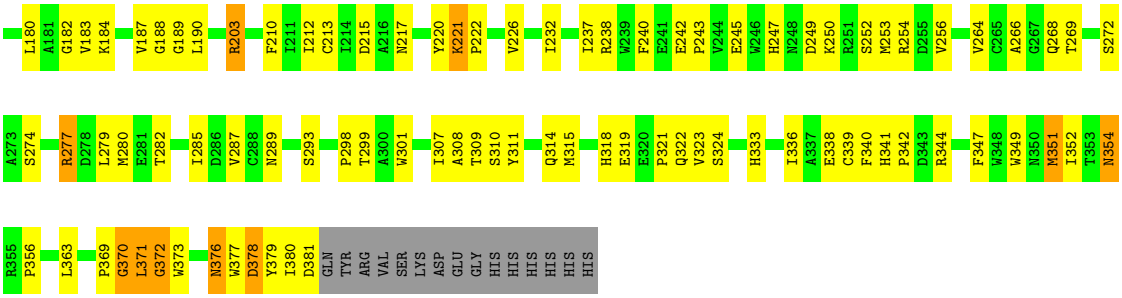
N376 W377 D378 Y379 I380 D381 GLN TYR ARG VAL SER LYS ASP GLU GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain E: % 50% 38% 5% 8%

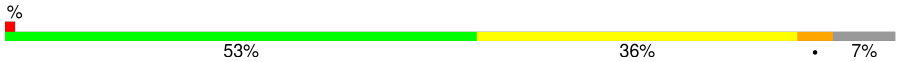
MSE SER LEU THR ILE THR ARG ILE GLU THR I28 P29 M30 V31 A32 P33 L34 A35 R36 E37 F38 R39 G40 S41 HIS TYR HIS MSE T46 H47 R48 A49 T50 I51 R54 V55 H56 T57 D58 A59 G63 E64 A65 Y66 T67 G68 D69 E70 H71 M74 F75 D76 I77 D78 R79 I80

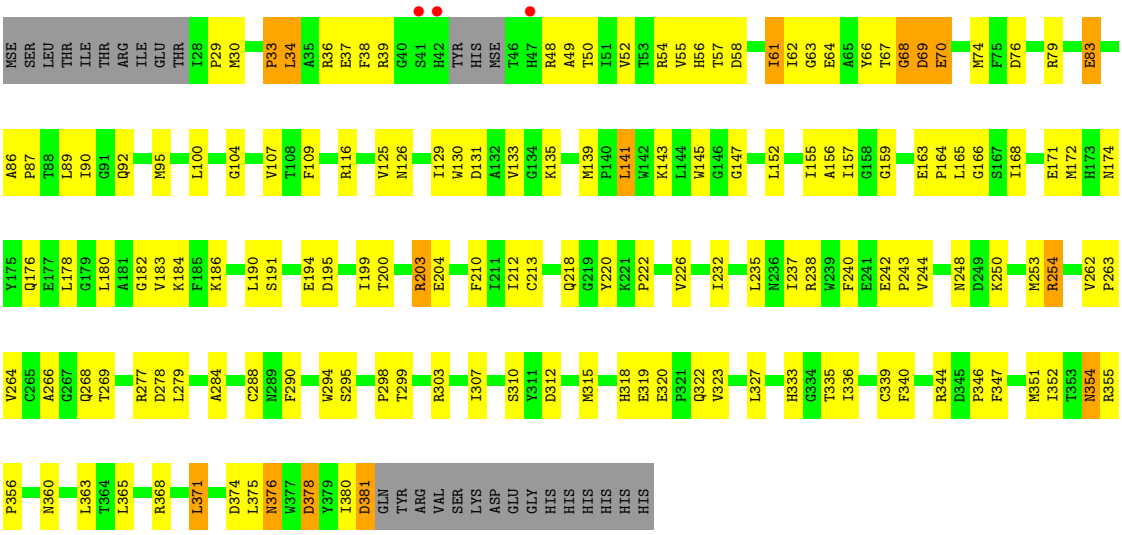
A86 P87 T88 L89 I90 G91 Q92 M95 A96 L100 S103 G104 Y105 K106 V107 I111 R115 V125 N126 I129 W130 D131 A132 V133 G134 M139 P140 L141 W145 R149 N150 E151 L152 I155 A156 I157 E163 S167 I168 E171 M172 H173 N174 Y175 Q176 E177



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.00Å 103.39Å 234.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.50 47.31 – 2.22	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.31-2.50) 96.0 (47.31-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.76	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.268 0.225 , 0.269	Depositor DCC
R_{free} test set	5679 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16869	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/2790	0.67	0/3779
1	B	0.38	0/2807	0.67	1/3802 (0.0%)
1	C	0.38	0/2847	0.67	1/3856 (0.0%)
1	D	0.38	0/2807	0.68	0/3802
1	E	0.37	0/2796	0.69	0/3787
1	F	0.36	0/2807	0.65	1/3802 (0.0%)
All	All	0.37	0/16854	0.67	3/22828 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	68	GLY	N-CA-C	6.79	130.08	113.10
1	B	30	MSE	CB-CG-SE	-5.69	95.63	112.70
1	C	363	LEU	CA-CB-CG	5.17	127.19	115.30

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	2731	0	2624	170	0
1	B	2747	0	2636	183	0
1	C	2786	0	2675	200	0
1	D	2747	0	2636	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2737	0	2629	208	0
1	F	2747	0	2636	151	0
2	A	65	0	0	19	0
2	B	62	0	0	14	0
2	C	63	0	0	16	0
2	D	72	0	0	6	0
2	E	55	0	0	30	0
2	F	57	0	0	9	0
All	All	16869	0	15836	1015	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 31.

The worst 5 of 1015 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:E:376:ASN:HD21	1:E:378:ASP:HB2	1.16	1.06
1:D:67:THR:HG23	1:D:293:SER:HB2	1.36	1.05
1:E:30:MSE:HE2	1:E:89:LEU:HB3	1.35	1.03
1:C:253:MSE:HE3	1:C:264:VAL:HG12	1.42	1.00
1:C:37:GLU:H	1:C:37:GLU:CD	1.66	0.99

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	345/379 (91%)	326 (94%)	16 (5%)	3 (1%)	17 31
1	B	347/379 (92%)	323 (93%)	22 (6%)	2 (1%)	25 43
1	C	351/379 (93%)	332 (95%)	17 (5%)	2 (1%)	25 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	347/379 (92%)	325 (94%)	18 (5%)	4 (1%)	13	24
1	E	346/379 (91%)	315 (91%)	26 (8%)	5 (1%)	11	20
1	F	347/379 (92%)	327 (94%)	18 (5%)	2 (1%)	25	43
All	All	2083/2274 (92%)	1948 (94%)	117 (6%)	18 (1%)	17	31

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	B	69	ASP
1	D	61	ILE
1	E	69	ASP
1	C	33	PRO

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	280/297 (94%)	255 (91%)	25 (9%)	9	19
1	B	282/297 (95%)	259 (92%)	23 (8%)	11	22
1	C	286/297 (96%)	263 (92%)	23 (8%)	12	23
1	D	282/297 (95%)	265 (94%)	17 (6%)	19	37
1	E	281/297 (95%)	265 (94%)	16 (6%)	20	39
1	F	282/297 (95%)	262 (93%)	20 (7%)	14	28
All	All	1693/1782 (95%)	1569 (93%)	124 (7%)	14	27

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	184	LYS
1	F	141	LEU
1	D	34	LEU
1	F	83	GLU

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Mol	Chain	Res	Type
1	F	360	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	HIS
1	D	376	ASN
1	F	268	GLN
1	D	126	ASN
1	D	350	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	339/379 (89%)	-0.27	0	100	100	10, 22, 37, 49	0
1	B	341/379 (89%)	-0.26	4 (1%)	79	80	10, 22, 37, 52	0
1	C	345/379 (91%)	-0.23	1 (0%)	94	94	10, 23, 38, 52	0
1	D	341/379 (89%)	-0.21	3 (0%)	84	86	10, 21, 36, 57	0
1	E	340/379 (89%)	0.04	4 (1%)	79	80	12, 27, 44, 61	0
1	F	341/379 (89%)	-0.06	3 (0%)	84	86	12, 26, 43, 57	0
All	All	2047/2274 (90%)	-0.17	15 (0%)	87	89	10, 23, 40, 61	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	68	GLY	3.3
1	B	42	HIS	3.0
1	F	42	HIS	2.9
1	B	46	THR	2.8
1	F	41	SER	2.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.