



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 03:05 am GMT

PDB ID : 4E5T
Title : Crystal structure of a putative Mandelate racemase/Muconate lactonizing enzyme (Target PSI-200750) from *Labrenzia alexandrii* DFL-11
Authors : Kumar, P.R.; Bonanno, J.; Chowdhury, S.; Foti, R.; Gizzi, A.; Glen, S.; Hammonds, J.; Hillerich, B.; Matikainen, B.; Seidel, R.; Toro, R.; Zencheck, W.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2012-03-14
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

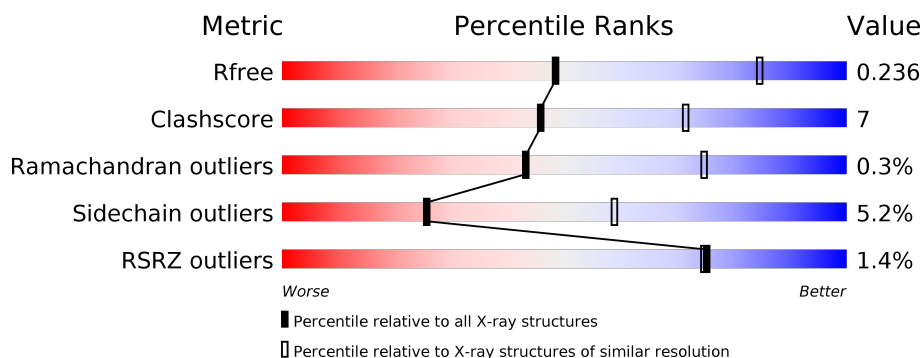
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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 $\leq 5\%$. 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	404	<div> <div></div> <div>76%19% . .</div> </div>
1	B	404	<div> <div></div> <div>78%18% .</div> </div>
1	C	404	<div> <div>%</div> <div>76%18% . .</div> </div>
1	D	404	<div> <div></div> <div>75%19% . .</div> </div>
1	E	404	<div> <div></div> <div>72%18% . 8%</div> </div>
1	F	404	<div> <div>%</div> <div>76%18% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	404	<div><div></div><div>3%</div><div>75%</div><div>16%</div><div>8%</div></div>
1	H	404	<div><div></div><div>4%</div><div>73%</div><div>18%</div><div>8%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23681 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, C-terminal domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3031	1939	513	564	15			
1	B	387	Total	C	N	O	S	0	1	0
			3006	1920	511	560	15			
1	C	386	Total	C	N	O	S	0	0	0
			2988	1910	506	557	15			
1	D	388	Total	C	N	O	S	0	0	0
			3004	1920	509	560	15			
1	E	371	Total	C	N	O	S	0	0	0
			2867	1834	485	533	15			
1	F	386	Total	C	N	O	S	0	0	0
			2991	1911	507	558	15			
1	G	370	Total	C	N	O	S	0	0	0
			2860	1830	484	531	15			
1	H	371	Total	C	N	O	S	0	0	0
			2867	1834	485	533	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP B9R417
B	0	SER	-	EXPRESSION TAG	UNP B9R417
C	0	SER	-	EXPRESSION TAG	UNP B9R417
D	0	SER	-	EXPRESSION TAG	UNP B9R417
E	0	SER	-	EXPRESSION TAG	UNP B9R417
F	0	SER	-	EXPRESSION TAG	UNP B9R417
G	0	SER	-	EXPRESSION TAG	UNP B9R417
H	0	SER	-	EXPRESSION TAG	UNP B9R417

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

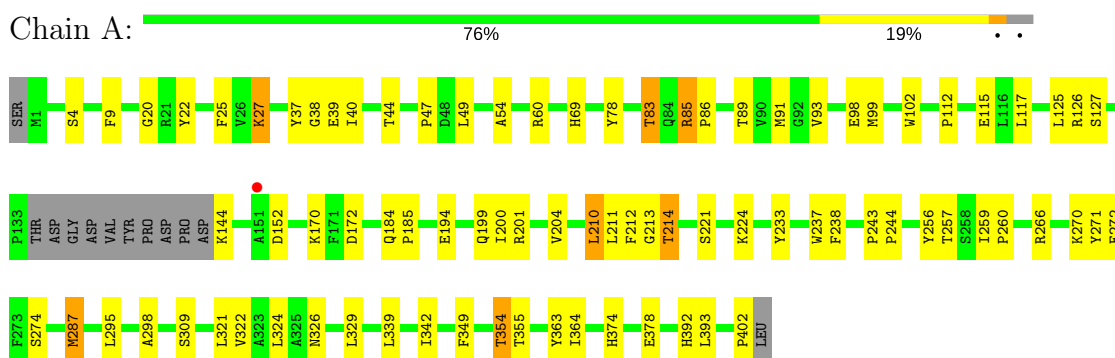
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	8	Total O 8 8	0	0
3	D	10	Total O 10 10	0	0
3	E	9	Total O 9 9	0	0
3	F	5	Total O 5 5	0	0
3	G	6	Total O 6 6	0	0
3	H	4	Total O 4 4	0	0

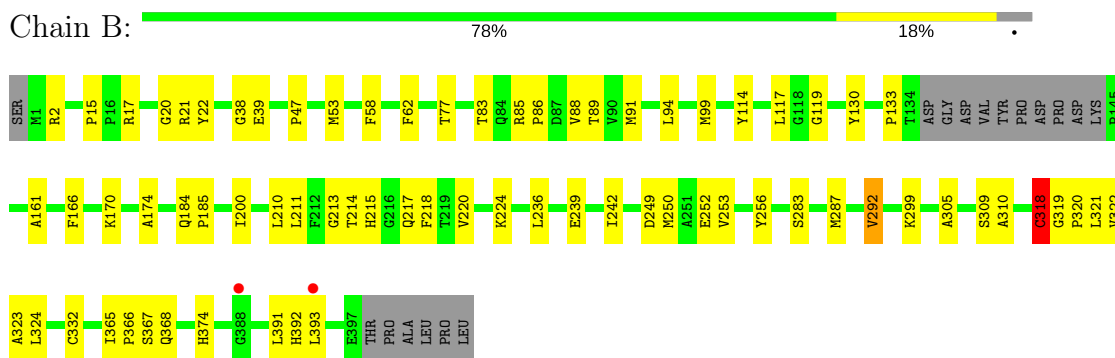
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

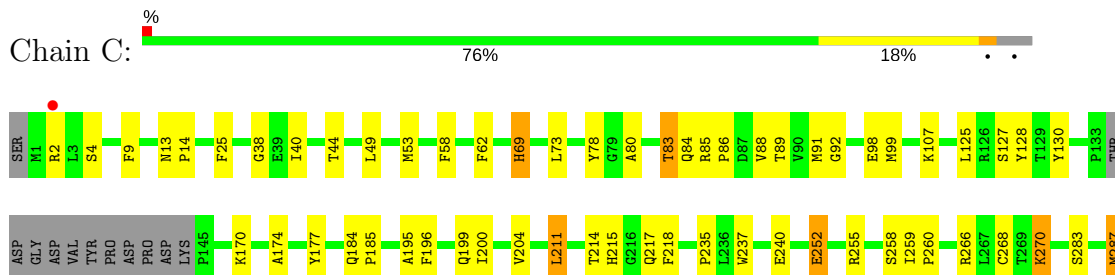
- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein



- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein



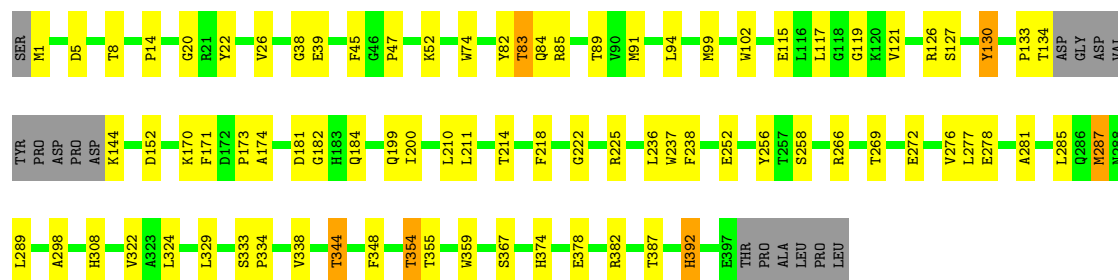
- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein





- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain D: 75% 19% . .



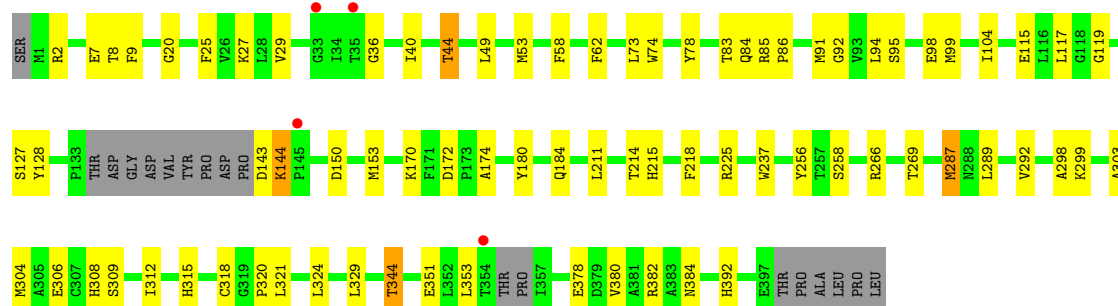
- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain E: 72% 18% . 8%



- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

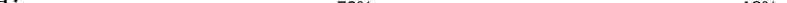
Chain F: 76% 18% . .

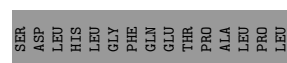
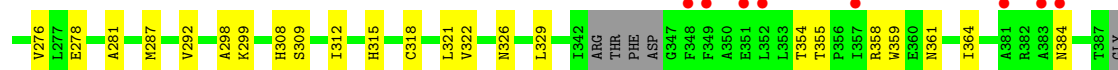


- Molecule 1: Mandelate racemase / muconate lactonizing enzyme, C-terminal domain protein

Chain G: 75% 16% . 8%



- Chain H:  4% 73% 18% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.90Å 156.88Å 218.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.90 49.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.45-2.90) 100.0 (49.45-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.164 , 0.242 0.157 , 0.236	Depositor DCC
R_{free} test set	3817 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23681	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/3110	0.62	0/4227
1	B	0.42	0/3083	0.61	0/4187
1	C	0.41	0/3065	0.58	0/4163
1	D	0.41	0/3081	0.59	0/4185
1	E	0.44	0/2939	0.61	0/3991
1	F	0.37	0/3066	0.54	0/4161
1	G	0.38	0/2932	0.55	0/3982
1	H	0.36	0/2939	0.53	0/3992
All	All	0.41	0/24215	0.58	0/32888

There are no bond length outliers.

There are no bond angle outliers.

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	3031	0	2966	50	0
1	B	3006	0	2936	49	0
1	C	2988	0	2917	48	0
1	D	3004	0	2936	47	0
1	E	2867	0	2809	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2991	0	2918	48	0
1	G	2860	0	2801	41	0
1	H	2867	0	2808	43	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
3	A	8	0	0	0	0
3	B	9	0	0	0	0
3	C	8	0	0	0	0
3	D	10	0	0	0	0
3	E	9	0	0	0	0
3	F	5	0	0	0	0
3	G	6	0	0	0	0
3	H	4	0	0	0	0
All	All	23681	0	23091	321	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 7.

The worst 5 of 321 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:287:MET:HG2	1:B:292:VAL:HG21	1.56	0.86
1:B:85:ARG:NH1	1:B:86:PRO:O	2.12	0.83
1:E:85:ARG:NH1	1:E:86:PRO:O	2.14	0.80
1:B:38:GLY:HA2	1:B:99:MET:HE2	1.65	0.78
1:H:213:GLY:HA2	1:H:239:GLU:HB3	1.71	0.71

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	388/404 (96%)	372 (96%)	16 (4%)	0	100	100
1	B	384/404 (95%)	360 (94%)	22 (6%)	2 (0%)	31	65
1	C	382/404 (95%)	359 (94%)	22 (6%)	1 (0%)	43	75
1	D	384/404 (95%)	355 (92%)	26 (7%)	3 (1%)	21	54
1	E	365/404 (90%)	339 (93%)	26 (7%)	0	100	100
1	F	380/404 (94%)	359 (94%)	19 (5%)	2 (0%)	31	65
1	G	364/404 (90%)	341 (94%)	22 (6%)	1 (0%)	43	75
1	H	365/404 (90%)	345 (94%)	19 (5%)	1 (0%)	43	75
All	All	3012/3232 (93%)	2830 (94%)	172 (6%)	10 (0%)	43	75

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	269	THR
1	C	69	HIS
1	B	133	PRO
1	D	392	HIS
1	F	144	LYS

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	311/322 (97%)	294 (94%)	17 (6%)	24	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	308/322 (96%)	301 (98%)	7 (2%)	53 83
1	C	306/322 (95%)	287 (94%)	19 (6%)	20 51
1	D	308/322 (96%)	288 (94%)	20 (6%)	19 48
1	E	293/322 (91%)	273 (93%)	20 (7%)	17 45
1	F	306/322 (95%)	291 (95%)	15 (5%)	27 61
1	G	292/322 (91%)	280 (96%)	12 (4%)	33 68
1	H	293/322 (91%)	277 (94%)	16 (6%)	24 56
All	All	2417/2576 (94%)	2291 (95%)	126 (5%)	25 59

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	252	GLU
1	E	237	TRP
1	H	130	TYR
1	D	289	LEU
1	E	41	TYR

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

Mol	Chain	Res	Type
1	A	368	GLN
1	D	311	GLN
1	F	184	GLN
1	H	384	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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 [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	392/404 (97%)	-0.53	1 (0%) 93 94	23, 42, 64, 97	0
1	B	387/404 (95%)	-0.46	2 (0%) 90 90	24, 45, 80, 113	0
1	C	386/404 (95%)	-0.51	4 (1%) 82 81	30, 49, 80, 127	0
1	D	388/404 (96%)	-0.50	0 100 100	25, 52, 74, 101	0
1	E	371/404 (91%)	-0.50	1 (0%) 93 94	24, 44, 78, 117	0
1	F	386/404 (95%)	-0.21	4 (1%) 82 81	34, 64, 94, 116	0
1	G	370/404 (91%)	-0.10	13 (3%) 44 38	35, 66, 97, 119	0
1	H	371/404 (91%)	-0.07	17 (4%) 32 28	37, 68, 104, 119	0
All	All	3051/3232 (94%)	-0.36	42 (1%) 75 75	23, 53, 91, 127	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	390	ASP	4.1
1	H	16	PRO	4.0
1	H	349	PHE	3.9
1	H	15	PRO	3.7
1	G	16	PRO	3.3

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, 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	B	501	1/1	0.92	0.26	69,69,69,69	0
2	MG	G	501	1/1	0.92	0.23	93,93,93,93	0
2	MG	D	501	1/1	0.93	0.34	68,68,68,68	0
2	MG	E	501	1/1	0.95	0.34	90,90,90,90	0
2	MG	A	501	1/1	0.96	0.32	73,73,73,73	0
2	MG	H	501	1/1	0.96	0.17	75,75,75,75	0
2	MG	C	501	1/1	0.97	0.35	67,67,67,67	0
2	MG	F	501	1/1	0.97	0.24	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.