



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 3NO1 / pdb_00003no1
Title : Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium in complex with magnesium
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-06-24
Resolution : 2.16 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

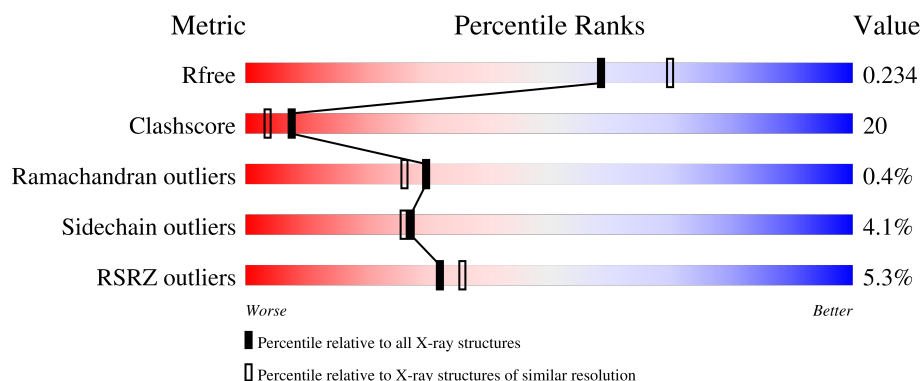
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	398	3% 63% 24% • 11%
1	B	398	5% 56% 27% • 12%
1	C	398	3% 63% 25% • 10%
1	D	398	5% 55% 31% • 12%
1	E	398	5% 54% 29% 5% 11%

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Mol	Chain	Length	Quality of chain
1	F	398	6% 55% 28% 5% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17170 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
1	A	355	Total	C	N	O	S	Se	0	0	0
			2782	1757	488	522	5	10			
1	B	349	Total	C	N	O	S	Se	0	0	0
			2734	1726	477	516	5	10			
1	C	357	Total	C	N	O	S	Se	0	0	0
			2792	1762	490	525	5	10			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2745	1732	481	517	5	10			
1	E	353	Total	C	N	O	S	Se	0	0	0
			2762	1742	484	521	5	10			
1	F	349	Total	C	N	O	S	Se	0	0	0
			2723	1718	476	514	5	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP A4AFX2
A	0	SER	-	expression tag	UNP A4AFX2
A	1	LEU	-	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	-1	MSE	-	expression tag	UNP A4AFX2
B	0	SER	-	expression tag	UNP A4AFX2
B	1	LEU	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	-1	MSE	-	expression tag	UNP A4AFX2
C	0	SER	-	expression tag	UNP A4AFX2
C	1	LEU	-	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	-1	MSE	-	expression tag	UNP A4AFX2
D	0	SER	-	expression tag	UNP A4AFX2
D	1	LEU	-	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	-1	MSE	-	expression tag	UNP A4AFX2
E	0	SER	-	expression tag	UNP A4AFX2
E	1	LEU	-	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	-1	MSE	-	expression tag	UNP A4AFX2
F	0	SER	-	expression tag	UNP A4AFX2
F	1	LEU	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2

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

- Molecule 2 is MAGNESIUM ION (CCD ID: 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
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

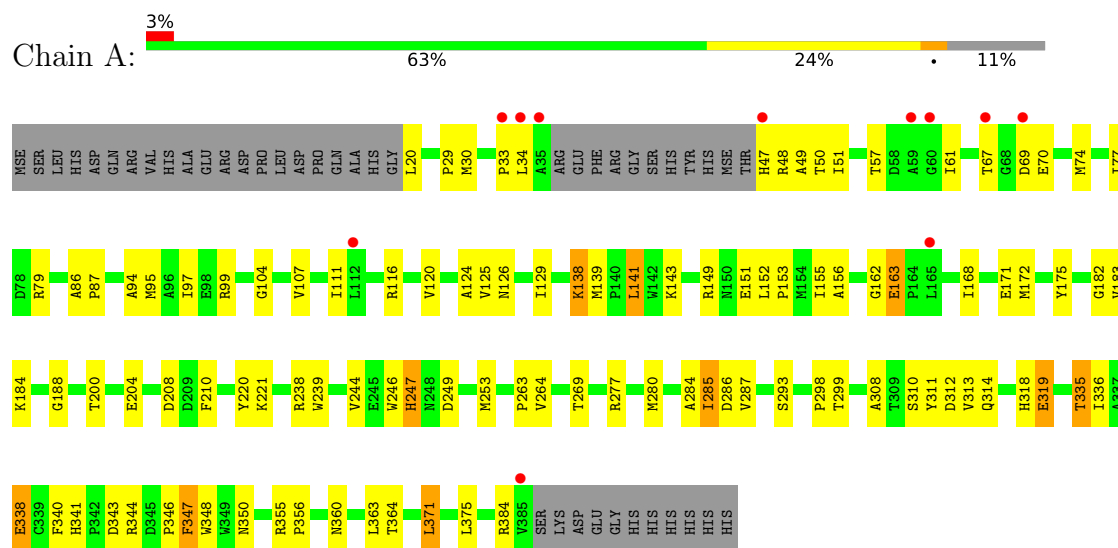
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total 137	O 137	0	0
3	B	84	Total 84	O 84	0	0
3	C	136	Total 136	O 136	0	0
3	D	88	Total 88	O 88	0	0
3	E	80	Total 80	O 80	0	0
3	F	101	Total 101	O 101	0	0

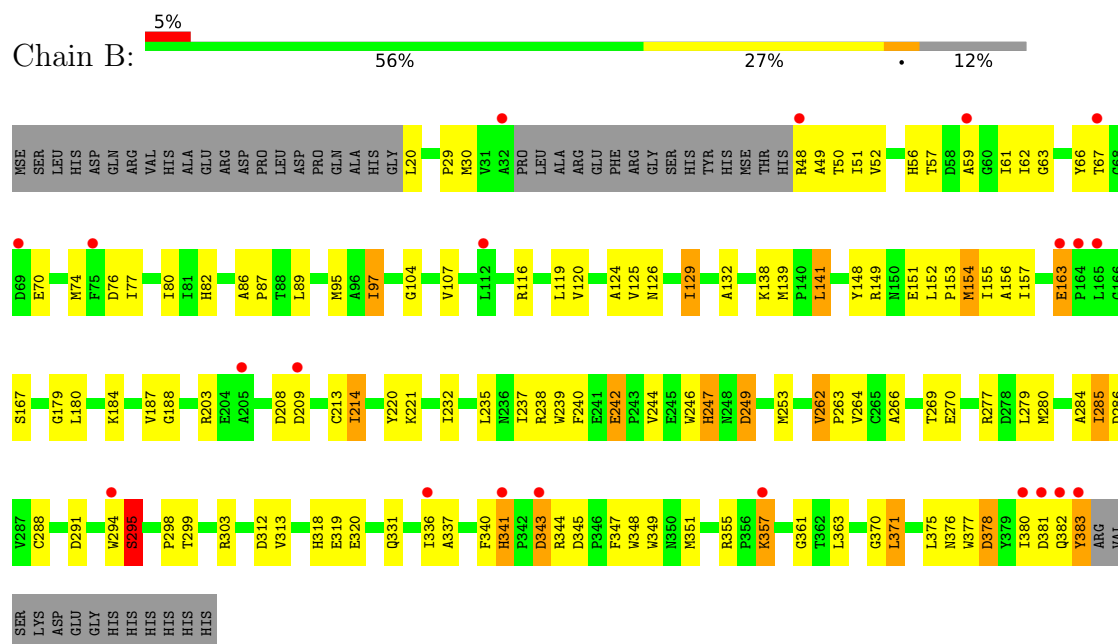
3 Residue-property plots

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: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



Chain C:

Chain D:

Chain E:

Amino Acid	Count	Category
MSE	1	Grey
SER	1	Green
LEU	1	Green
HIS	1	Green
ASP	1	Green
GLN	1	Green
ARG	1	Green
VAL	1	Green
HIS	1	Green
LEU	1	Green
ALA	1	Green
GLU	1	Green
ARG	1	Green
ASP	1	Green
PRO	1	Green
LEU	1	Green
ASP	1	Green
PRO	1	Green
GLN	1	Green
ALA	1	Green
HIS	1	Green
G19	1	Green
T27	1	Yellow
M30	1	Yellow
V31	1	Yellow
A32	1	Yellow
PRO	1	Yellow
LEU	1	Yellow
ALA	1	Yellow
ARG	1	Yellow
GLU	1	Yellow
PHE	1	Yellow
ARG	1	Yellow
GLY	1	Yellow
SER	1	Yellow
HIS	1	Yellow
TYR	1	Yellow
HIS	1	Yellow
MSE	1	Yellow
THR	1	Yellow
HIS	1	Yellow
R48	1	Yellow
A49	1	Yellow
T50	1	Yellow
I51	1	Yellow
R54	1	Orange
V55	1	Orange
H56	1	Orange
A59	1	Orange
G60	1	Orange
I61	1	Orange
I62	1	Orange
G63	1	Orange
T67	1	Orange
G68	1	Orange
T69	1	Orange
E70	1	Green
M74	1	Green
F75	1	Green
D76	1	Green
I77	1	Green
D78	1	Green
R79	1	Green
I80	1	Green
I81	1	Green
H82	1	Green
A86	1	Green
P87	1	Green
T88	1	Green
L89	1	Green
I90	1	Green
M95	1	Orange
A96	1	Orange
I97	1	Orange
E98	1	Orange
R99	1	Orange
S103	1	Yellow
I104	1	Yellow
I105	1	Yellow
K106	1	Yellow
V107	1	Yellow
I111	1	Yellow
D114	1	Yellow
R115	1	Yellow
R116	1	Yellow
L117	1	Yellow
V120	1	Yellow
A124	1	Yellow
V125	1	Yellow
M126	1	Yellow
I129	1	Yellow
V133	1	Yellow
K138	1	Orange
L141	1	Orange
V145	1	Orange
Y148	1	Orange
L149	1	Orange
M150	1	Orange
E151	1	Orange
L152	1	Orange
P153	1	Orange
L154	1	Orange

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 90.10Å 94.66Å 115.80° 109.75° 97.58°	Depositor
Resolution (Å)	42.51 – 2.16 42.51 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.51-2.16) 96.1 (42.51-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.240 0.202 , 0.234	Depositor DCC
R_{free} test set	4670 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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

5.1 Standard geometry

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	0.42	0/2841	0.96	12/3851 (0.3%)
1	B	0.41	0/2791	0.98	17/3782 (0.4%)
1	C	0.43	0/2851	0.97	14/3864 (0.4%)
1	D	0.41	0/2802	0.97	13/3796 (0.3%)
1	E	0.40	0/2819	0.98	16/3819 (0.4%)
1	F	0.44	0/2779	1.01	17/3765 (0.5%)
All	All	0.42	0/16883	0.98	89/22877 (0.4%)

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	246	TRP	N-CA-C	11.72	123.61	111.07
1	F	246	TRP	N-CA-C	11.54	123.86	111.28
1	E	246	TRP	N-CA-C	11.05	122.89	111.07
1	A	246	TRP	N-CA-C	11.04	122.88	111.07
1	B	246	TRP	N-CA-C	10.85	122.68	111.07

There are no chirality outliers.

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	2782	0	2685	108	0
1	B	2734	0	2632	130	0
1	C	2792	0	2692	85	0
1	D	2745	0	2645	110	0
1	E	2762	0	2662	130	0
1	F	2723	0	2622	120	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
3	A	137	0	0	5	0
3	B	84	0	0	8	0
3	C	136	0	0	5	0
3	D	88	0	0	8	0
3	E	80	0	0	4	0
3	F	101	0	0	3	0
All	All	17170	0	15938	656	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 20.

The worst 5 of 656 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:253:MSE:HE3	1:A:264:VAL:HG12	1.32	1.07
1:F:30:MSE:HE1	1:F:380:ILE:HG23	1.34	1.05
1:A:253:MSE:HE3	1:A:264:VAL:CG1	1.86	1.05
1:A:280:MSE:HE2	1:A:311:TYR:HB2	1.40	1.04
1:F:253:MSE:HE3	1:F:264:VAL:CG1	1.90	1.01

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	351/398 (88%)	340 (97%)	10 (3%)	1 (0%)	36	34
1	B	345/398 (87%)	328 (95%)	16 (5%)	1 (0%)	36	34
1	C	353/398 (89%)	344 (98%)	8 (2%)	1 (0%)	36	34
1	D	346/398 (87%)	331 (96%)	14 (4%)	1 (0%)	36	34
1	E	349/398 (88%)	333 (95%)	14 (4%)	2 (1%)	21	15
1	F	345/398 (87%)	325 (94%)	18 (5%)	2 (1%)	21	15
All	All	2089/2388 (88%)	2001 (96%)	80 (4%)	8 (0%)	30	26

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	319	GLU
1	A	319	GLU
1	F	319	GLU
1	B	187	VAL
1	C	319	GLU

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	287/313 (92%)	280 (98%)	7 (2%)	43	47
1	B	282/313 (90%)	267 (95%)	15 (5%)	20	17
1	C	288/313 (92%)	281 (98%)	7 (2%)	43	47
1	D	283/313 (90%)	273 (96%)	10 (4%)	32	32
1	E	285/313 (91%)	267 (94%)	18 (6%)	16	11
1	F	280/313 (90%)	267 (95%)	13 (5%)	24	22
All	All	1705/1878 (91%)	1635 (96%)	70 (4%)	27	26

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	95	MSE
1	F	117	LEU
1	F	262	VAL
1	C	152	LEU
1	C	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	92	GLN
1	D	376	ASN
1	F	247	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [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	345/398 (86%)	-0.01	11 (3%)	50	54	7, 16, 31, 41	0
1	B	339/398 (85%)	0.38	21 (6%)	26	30	8, 21, 38, 43	0
1	C	347/398 (87%)	-0.01	10 (2%)	53	57	7, 16, 31, 40	0
1	D	340/398 (85%)	0.32	21 (6%)	26	30	8, 21, 37, 44	0
1	E	343/398 (86%)	0.42	21 (6%)	27	31	10, 22, 37, 43	0
1	F	339/398 (85%)	0.41	25 (7%)	20	23	7, 22, 38, 48	0
All	All	2053/2388 (85%)	0.25	109 (5%)	32	36	7, 20, 36, 48	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	ASP	5.8
1	F	163	GLU	5.3
1	A	35	ALA	4.6
1	E	164	PRO	4.4
1	F	162	GLY	4.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	MG	A	397	1/1	0.93	0.06	19,19,19,19	0
2	MG	F	397	1/1	0.94	0.12	26,26,26,26	0
2	MG	E	397	1/1	0.96	0.07	29,29,29,29	0
2	MG	D	397	1/1	0.97	0.12	24,24,24,24	0
2	MG	B	397	1/1	0.97	0.12	25,25,25,25	0
2	MG	C	397	1/1	0.97	0.08	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.