wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2021 – 04:25 PM EST

PDB ID	:	3FV9
Title	:	Crystal structure of putative mandelate racemase/muconatelactonizing enzyme from ROSEOVARIUS NUBINHIBENS ISM complexed with magnesium
Authors	:	Malashkevich, V.N.; Rutter, M.; Bain, K.T.; Lau, C.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-01-15
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

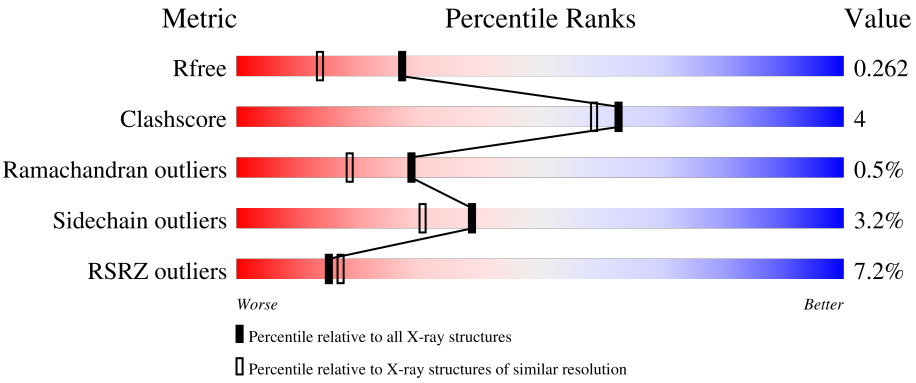
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	386	4% 83% 10% • 6%
1	B	386	3% 85% 9% • 5%
1	C	386	9% 87% 10% • •
1	D	386	4% 88% 9% •
1	E	386	9% 85% 11% • •

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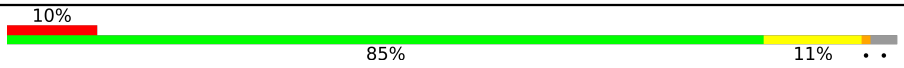
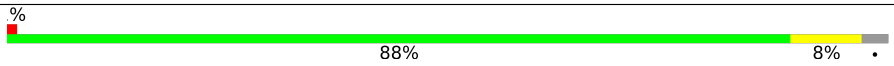
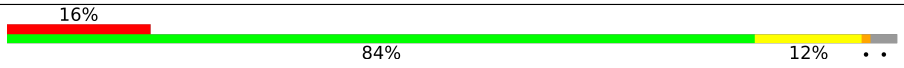
Mol	Chain	Length	Quality of chain
1	F	386	
1	G	386	
1	H	386	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24665 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	G	373	Total	C	N	O	S	0	4	0
			2800	1743	515	526	16			
1	A	363	Total	C	N	O	S	0	0	0
			2687	1667	494	510	16			
1	D	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	E	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	F	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	B	365	Total	C	N	O	S	0	0	0
			2704	1679	496	513	16			
1	H	374	Total	C	N	O	S	0	2	0
			2786	1730	513	527	16			
1	C	374	Total	C	N	O	S	0	1	0
			2782	1727	513	526	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	expression tag	UNP A3SNG0
G	0	SER	-	expression tag	UNP A3SNG0
G	1	LEU	-	expression tag	UNP A3SNG0
G	377	GLU	-	expression tag	UNP A3SNG0
G	378	GLY	-	expression tag	UNP A3SNG0
G	379	HIS	-	expression tag	UNP A3SNG0
G	380	HIS	-	expression tag	UNP A3SNG0
G	381	HIS	-	expression tag	UNP A3SNG0
G	382	HIS	-	expression tag	UNP A3SNG0
G	383	HIS	-	expression tag	UNP A3SNG0
G	384	HIS	-	expression tag	UNP A3SNG0
A	-1	MET	-	expression tag	UNP A3SNG0
A	0	SER	-	expression tag	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	expression tag	UNP A3SNG0
A	377	GLU	-	expression tag	UNP A3SNG0
A	378	GLY	-	expression tag	UNP A3SNG0
A	379	HIS	-	expression tag	UNP A3SNG0
A	380	HIS	-	expression tag	UNP A3SNG0
A	381	HIS	-	expression tag	UNP A3SNG0
A	382	HIS	-	expression tag	UNP A3SNG0
A	383	HIS	-	expression tag	UNP A3SNG0
A	384	HIS	-	expression tag	UNP A3SNG0
D	-1	MET	-	expression tag	UNP A3SNG0
D	0	SER	-	expression tag	UNP A3SNG0
D	1	LEU	-	expression tag	UNP A3SNG0
D	377	GLU	-	expression tag	UNP A3SNG0
D	378	GLY	-	expression tag	UNP A3SNG0
D	379	HIS	-	expression tag	UNP A3SNG0
D	380	HIS	-	expression tag	UNP A3SNG0
D	381	HIS	-	expression tag	UNP A3SNG0
D	382	HIS	-	expression tag	UNP A3SNG0
D	383	HIS	-	expression tag	UNP A3SNG0
D	384	HIS	-	expression tag	UNP A3SNG0
E	-1	MET	-	expression tag	UNP A3SNG0
E	0	SER	-	expression tag	UNP A3SNG0
E	1	LEU	-	expression tag	UNP A3SNG0
E	377	GLU	-	expression tag	UNP A3SNG0
E	378	GLY	-	expression tag	UNP A3SNG0
E	379	HIS	-	expression tag	UNP A3SNG0
E	380	HIS	-	expression tag	UNP A3SNG0
E	381	HIS	-	expression tag	UNP A3SNG0
E	382	HIS	-	expression tag	UNP A3SNG0
E	383	HIS	-	expression tag	UNP A3SNG0
E	384	HIS	-	expression tag	UNP A3SNG0
F	-1	MET	-	expression tag	UNP A3SNG0
F	0	SER	-	expression tag	UNP A3SNG0
F	1	LEU	-	expression tag	UNP A3SNG0
F	377	GLU	-	expression tag	UNP A3SNG0
F	378	GLY	-	expression tag	UNP A3SNG0
F	379	HIS	-	expression tag	UNP A3SNG0
F	380	HIS	-	expression tag	UNP A3SNG0
F	381	HIS	-	expression tag	UNP A3SNG0
F	382	HIS	-	expression tag	UNP A3SNG0
F	383	HIS	-	expression tag	UNP A3SNG0
F	384	HIS	-	expression tag	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP A3SNG0
B	0	SER	-	expression tag	UNP A3SNG0
B	1	LEU	-	expression tag	UNP A3SNG0
B	377	GLU	-	expression tag	UNP A3SNG0
B	378	GLY	-	expression tag	UNP A3SNG0
B	379	HIS	-	expression tag	UNP A3SNG0
B	380	HIS	-	expression tag	UNP A3SNG0
B	381	HIS	-	expression tag	UNP A3SNG0
B	382	HIS	-	expression tag	UNP A3SNG0
B	383	HIS	-	expression tag	UNP A3SNG0
B	384	HIS	-	expression tag	UNP A3SNG0
H	-1	MET	-	expression tag	UNP A3SNG0
H	0	SER	-	expression tag	UNP A3SNG0
H	1	LEU	-	expression tag	UNP A3SNG0
H	377	GLU	-	expression tag	UNP A3SNG0
H	378	GLY	-	expression tag	UNP A3SNG0
H	379	HIS	-	expression tag	UNP A3SNG0
H	380	HIS	-	expression tag	UNP A3SNG0
H	381	HIS	-	expression tag	UNP A3SNG0
H	382	HIS	-	expression tag	UNP A3SNG0
H	383	HIS	-	expression tag	UNP A3SNG0
H	384	HIS	-	expression tag	UNP A3SNG0
C	-1	MET	-	expression tag	UNP A3SNG0
C	0	SER	-	expression tag	UNP A3SNG0
C	1	LEU	-	expression tag	UNP A3SNG0
C	377	GLU	-	expression tag	UNP A3SNG0
C	378	GLY	-	expression tag	UNP A3SNG0
C	379	HIS	-	expression tag	UNP A3SNG0
C	380	HIS	-	expression tag	UNP A3SNG0
C	381	HIS	-	expression tag	UNP A3SNG0
C	382	HIS	-	expression tag	UNP A3SNG0
C	383	HIS	-	expression tag	UNP A3SNG0
C	384	HIS	-	expression tag	UNP A3SNG0

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is water.

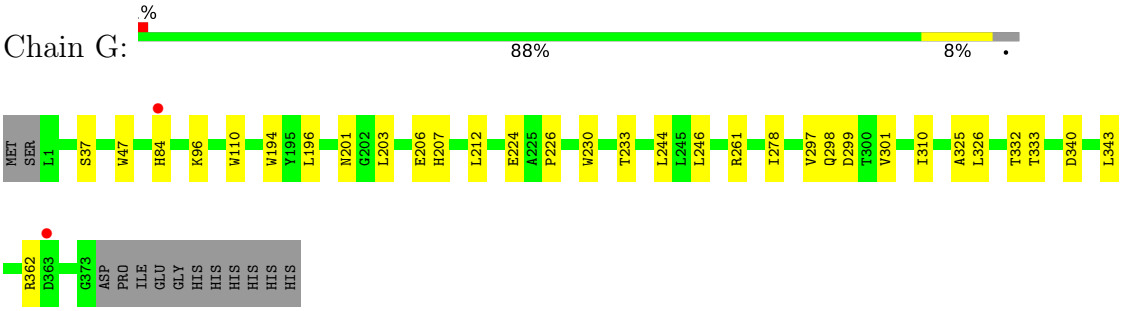
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2600	Total O 2600 2600	0	0

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.

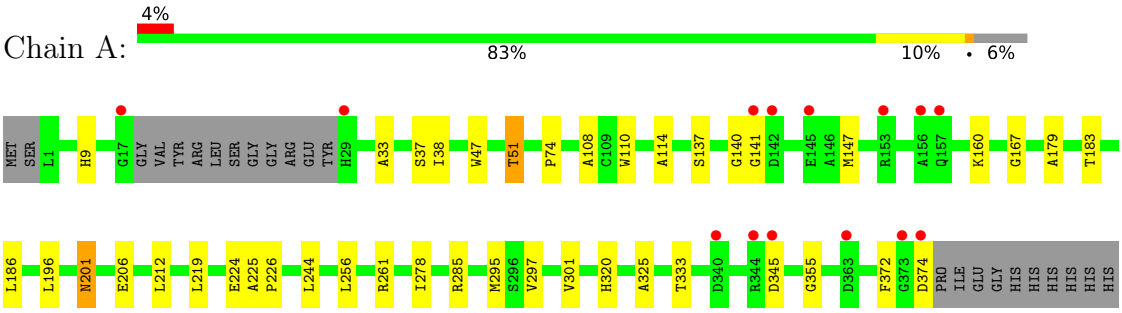
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain G:



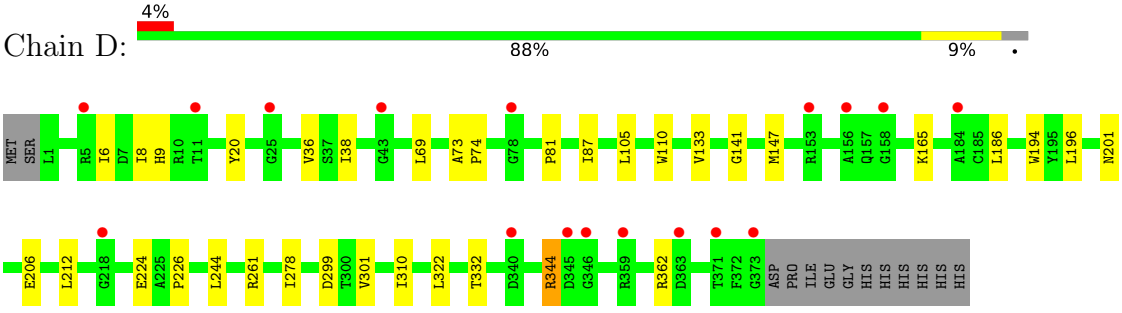
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain A:



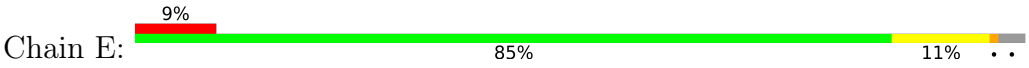
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

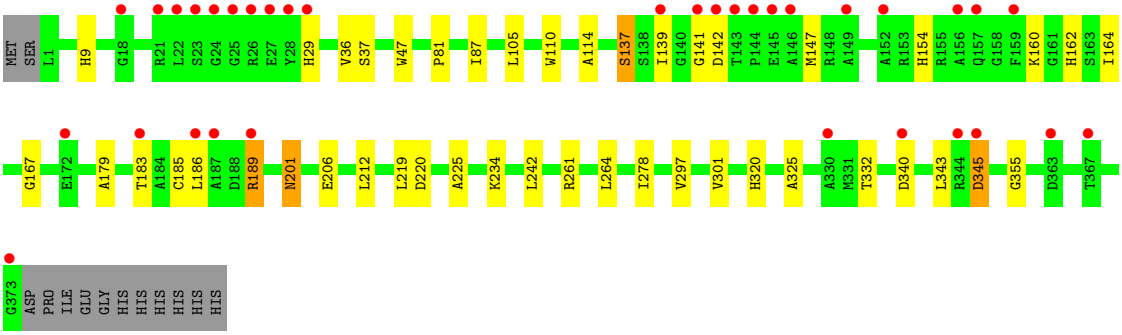
Chain D:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

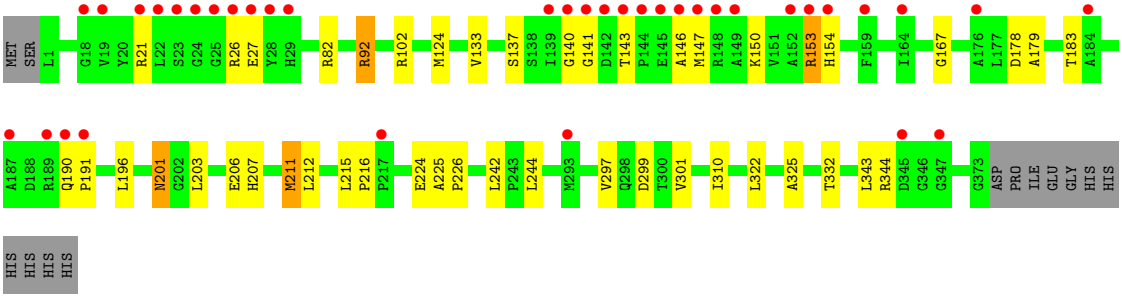
Chain E:





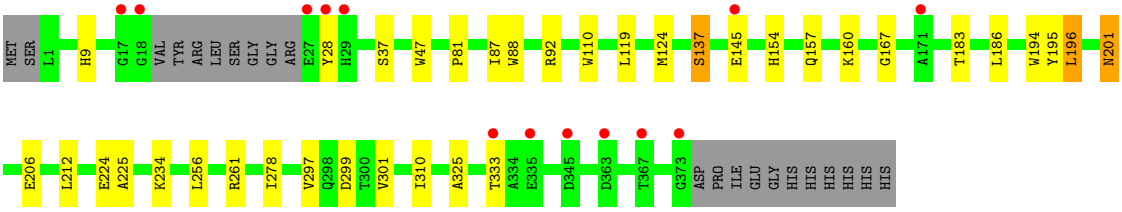
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain F:



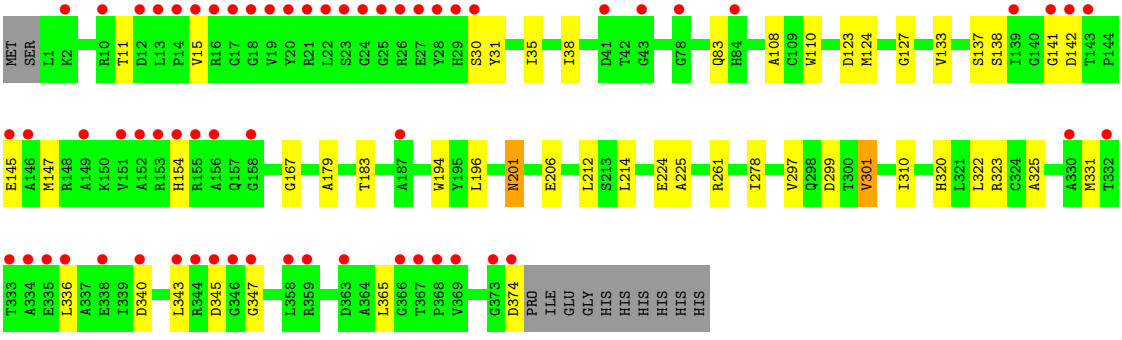
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain B:



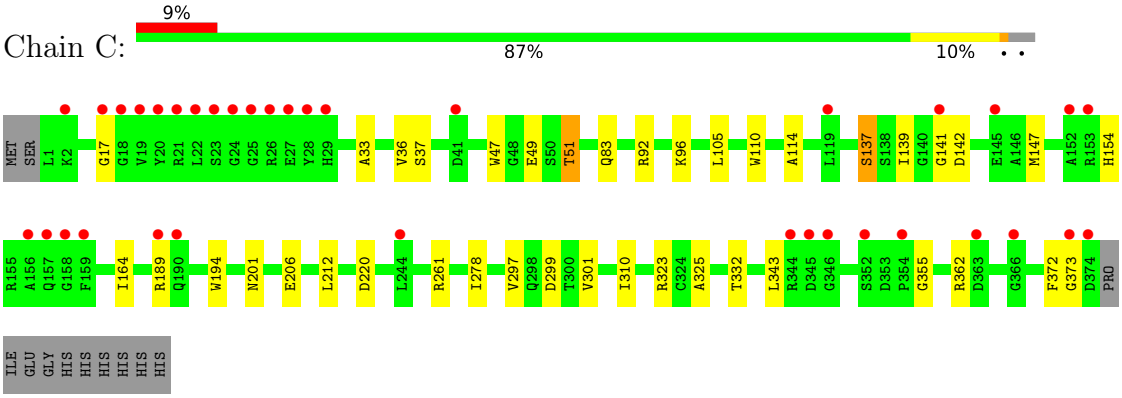
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain H:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme

Chain C:


9%
87%
10%
MET SER L1 K2 G17 G18 V19 Y20 R21 L22 S23 G24 G25 R26 E27 Y28 H29 A33 V36 S37 D41 W47 G48 E49 S50 T51 Q83 R92 K96 L105 W110 A114 L119 S137 S138 I139 G140 G141 D142 E145 A146 M147 A152 R153 H154
R155 A156 Q157 G158 F159 I164 R189 Q190 W194 N201 E206 L212 D220 L244 R261 I278 V297 Q298 D299 T300 V301 I310 R323 C324 A325 T332 L343 R344 D345 G346 S352 D353 P354 G355 R362 D363 G366 F372 G373 D374 PRO
ILE GLU GLY HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	169.08Å 174.57Å 108.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-1.90) 95.7 (20.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.49 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.241 0.229 , 0.262	Depositor DCC
R_{free} test set	12030 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24665	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% 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

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	0.43	0/2732	0.59	0/3711
1	B	0.46	0/2750	0.59	1/3735 (0.0%)
1	C	0.45	0/2834	0.61	0/3849
1	D	0.43	0/2815	0.59	0/3823
1	E	0.43	0/2815	0.60	0/3823
1	F	0.51	0/2815	0.63	2/3823 (0.1%)
1	G	0.45	0/2857	0.60	0/3882
1	H	0.42	0/2841	0.59	0/3859
All	All	0.45	0/22459	0.60	3/30505 (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	211	MET	CG-SD-CE	6.82	111.11	100.20
1	B	196	LEU	CA-CB-CG	5.37	127.66	115.30
1	F	140	GLY	N-CA-C	5.06	125.74	113.10

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	2687	0	2710	21	0
1	B	2704	0	2724	22	0
1	C	2782	0	2802	23	0
1	D	2767	0	2791	20	0
1	E	2767	0	2791	24	0
1	F	2767	0	2791	33	0
1	G	2800	0	2824	18	0
1	H	2786	0	2809	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	G	2600	0	0	32	0
All	All	24665	0	22242	192	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 4.

The worst 5 of 192 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)
3:G:2043:HOH:O	1:E:340:ASP:HB2	1.58	1.03
1:F:141:GLY:HA2	1:F:147:MET:CE	1.90	1.01
1:F:141:GLY:HA2	1:F:147:MET:HE3	1.40	0.99
1:C:141:GLY:HA2	1:C:147:MET:CE	1.98	0.94
1:F:178:ASP:HB3	1:F:211:MET:HE1	1.48	0.93

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	359/386 (93%)	349 (97%)	8 (2%)	2 (1%)	25 15
1	B	361/386 (94%)	351 (97%)	8 (2%)	2 (1%)	25 15
1	C	373/386 (97%)	363 (97%)	8 (2%)	2 (0%)	29 18
1	D	371/386 (96%)	362 (98%)	8 (2%)	1 (0%)	41 31
1	E	371/386 (96%)	361 (97%)	7 (2%)	3 (1%)	19 9
1	F	371/386 (96%)	358 (96%)	11 (3%)	2 (0%)	29 18
1	G	375/386 (97%)	364 (97%)	10 (3%)	1 (0%)	41 31
1	H	374/386 (97%)	364 (97%)	8 (2%)	2 (0%)	29 18
All	All	2955/3088 (96%)	2872 (97%)	68 (2%)	15 (0%)	29 18

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	GLY
1	A	301	VAL
1	F	301	VAL
1	B	301	VAL
1	C	301	VAL

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	275/294 (94%)	266 (97%)	9 (3%)	38 29
1	B	276/294 (94%)	269 (98%)	7 (2%)	47 41
1	C	284/294 (97%)	274 (96%)	10 (4%)	36 27
1	D	282/294 (96%)	275 (98%)	7 (2%)	47 41
1	E	282/294 (96%)	272 (96%)	10 (4%)	36 27
1	F	282/294 (96%)	269 (95%)	13 (5%)	27 17
1	G	286/294 (97%)	279 (98%)	7 (2%)	49 43
1	H	285/294 (97%)	277 (97%)	8 (3%)	43 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2252/2352 (96%)	2181 (97%)	71 (3%)	39 30

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	345	ASP
1	F	201	ASN
1	C	201	ASN
1	F	92	ARG
1	F	150	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	157	GLN
1	F	154	HIS
1	C	9	HIS
1	E	320	HIS
1	F	201	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)

Of 5 ligands modelled in this entry, 5 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

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, 95^{th} 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	363/386 (94%)	0.31	14 (3%) 39 42	9, 16, 25, 41	0
1	B	365/386 (94%)	0.37	13 (3%) 42 45	8, 16, 24, 51	0
1	C	374/386 (96%)	0.64	36 (9%) 8 9	8, 17, 30, 48	0
1	D	373/386 (96%)	0.47	17 (4%) 32 35	9, 16, 25, 29	0
1	E	373/386 (96%)	0.50	34 (9%) 9 10	10, 17, 29, 46	0
1	F	373/386 (96%)	0.64	37 (9%) 7 8	10, 15, 28, 46	0
1	G	373/386 (96%)	0.23	2 (0%) 91 92	9, 15, 25, 33	0
1	H	374/386 (96%)	0.87	62 (16%) 1 1	8, 16, 31, 49	0
All	All	2968/3088 (96%)	0.51	215 (7%) 15 17	8, 16, 27, 51	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	ASP	10.2
1	H	19	VAL	8.7
1	B	18	GLY	8.2
1	C	24	GLY	7.9
1	H	29	HIS	7.6

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

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

6.3 Carbohydrates

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, 95^{th} 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	F	501	1/1	0.82	0.20	41,41,41,41	0
2	MG	E	501	1/1	0.91	0.11	35,35,35,35	0
2	MG	C	501	1/1	0.94	0.09	37,37,37,37	0
2	MG	B	501	1/1	0.95	0.05	24,24,24,24	0
2	MG	A	501	1/1	0.95	0.09	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.