



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:17 PM GMT

PDB ID : 1VF7  
Title : Crystal structure of the membrane fusion protein, MexA of the multidrug transporter  
Authors : Akama, H.; Matsuura, T.; Kashiwagi, S.; Yoneyama, H.; Tsukihara, T.; Nakagawa, A.; Nakae, T.  
Deposited on : 2004-04-09  
Resolution : 2.40 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

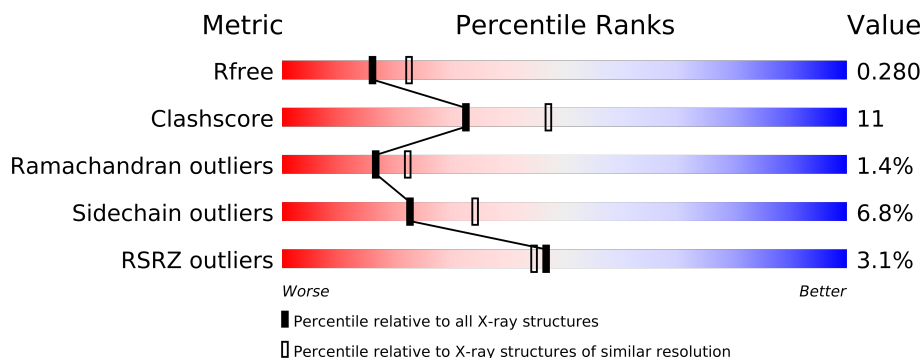
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	369	
1	B	369	
1	C	369	
1	D	369	
1	E	369	
1	F	369	
1	G	369	
1	H	369	
1	I	369	
1	J	369	
1	K	369	
1	L	369	
1	M	369	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23655 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1816	1127	327	360	2			
1	B	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	C	246	Total	C	N	O	S	0	0	0
			1885	1173	339	371	2			
1	D	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	E	252	Total	C	N	O	S	0	0	0
			1928	1198	348	380	2			
1	F	233	Total	C	N	O	S	0	0	0
			1788	1110	323	353	2			
1	G	237	Total	C	N	O	S	0	0	0
			1819	1130	327	360	2			
1	H	241	Total	C	N	O	S	0	0	0
			1846	1146	332	366	2			
1	I	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	J	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	K	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			
1	L	235	Total	C	N	O	S	0	0	0
			1803	1120	325	356	2			
1	M	232	Total	C	N	O	S	0	0	0
			1779	1105	321	351	2			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	CLONING ARTIFACT	UNP P52477
A	-1	GLU	-	CLONING ARTIFACT	UNP P52477
A	0	SER	-	CLONING ARTIFACT	UNP P52477

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	CLONING ARTIFACT	UNP P52477
A	361	HIS	-	EXPRESSION TAG	UNP P52477
A	362	HIS	-	EXPRESSION TAG	UNP P52477
A	363	HIS	-	EXPRESSION TAG	UNP P52477
A	364	HIS	-	EXPRESSION TAG	UNP P52477
A	365	HIS	-	EXPRESSION TAG	UNP P52477
A	366	HIS	-	EXPRESSION TAG	UNP P52477
B	-2	ALA	-	CLONING ARTIFACT	UNP P52477
B	-1	GLU	-	CLONING ARTIFACT	UNP P52477
B	0	SER	-	CLONING ARTIFACT	UNP P52477
B	1	SER	-	CLONING ARTIFACT	UNP P52477
B	361	HIS	-	EXPRESSION TAG	UNP P52477
B	362	HIS	-	EXPRESSION TAG	UNP P52477
B	363	HIS	-	EXPRESSION TAG	UNP P52477
B	364	HIS	-	EXPRESSION TAG	UNP P52477
B	365	HIS	-	EXPRESSION TAG	UNP P52477
B	366	HIS	-	EXPRESSION TAG	UNP P52477
C	-2	ALA	-	CLONING ARTIFACT	UNP P52477
C	-1	GLU	-	CLONING ARTIFACT	UNP P52477
C	0	SER	-	CLONING ARTIFACT	UNP P52477
C	1	SER	-	CLONING ARTIFACT	UNP P52477
C	361	HIS	-	EXPRESSION TAG	UNP P52477
C	362	HIS	-	EXPRESSION TAG	UNP P52477
C	363	HIS	-	EXPRESSION TAG	UNP P52477
C	364	HIS	-	EXPRESSION TAG	UNP P52477
C	365	HIS	-	EXPRESSION TAG	UNP P52477
C	366	HIS	-	EXPRESSION TAG	UNP P52477
D	-2	ALA	-	CLONING ARTIFACT	UNP P52477
D	-1	GLU	-	CLONING ARTIFACT	UNP P52477
D	0	SER	-	CLONING ARTIFACT	UNP P52477
D	1	SER	-	CLONING ARTIFACT	UNP P52477
D	361	HIS	-	EXPRESSION TAG	UNP P52477
D	362	HIS	-	EXPRESSION TAG	UNP P52477
D	363	HIS	-	EXPRESSION TAG	UNP P52477
D	364	HIS	-	EXPRESSION TAG	UNP P52477
D	365	HIS	-	EXPRESSION TAG	UNP P52477
D	366	HIS	-	EXPRESSION TAG	UNP P52477
E	-2	ALA	-	CLONING ARTIFACT	UNP P52477
E	-1	GLU	-	CLONING ARTIFACT	UNP P52477
E	0	SER	-	CLONING ARTIFACT	UNP P52477
E	1	SER	-	CLONING ARTIFACT	UNP P52477
E	361	HIS	-	EXPRESSION TAG	UNP P52477

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	362	HIS	-	EXPRESSION TAG	UNP P52477
E	363	HIS	-	EXPRESSION TAG	UNP P52477
E	364	HIS	-	EXPRESSION TAG	UNP P52477
E	365	HIS	-	EXPRESSION TAG	UNP P52477
E	366	HIS	-	EXPRESSION TAG	UNP P52477
F	-2	ALA	-	CLONING ARTIFACT	UNP P52477
F	-1	GLU	-	CLONING ARTIFACT	UNP P52477
F	0	SER	-	CLONING ARTIFACT	UNP P52477
F	1	SER	-	CLONING ARTIFACT	UNP P52477
F	361	HIS	-	EXPRESSION TAG	UNP P52477
F	362	HIS	-	EXPRESSION TAG	UNP P52477
F	363	HIS	-	EXPRESSION TAG	UNP P52477
F	364	HIS	-	EXPRESSION TAG	UNP P52477
F	365	HIS	-	EXPRESSION TAG	UNP P52477
F	366	HIS	-	EXPRESSION TAG	UNP P52477
G	-2	ALA	-	CLONING ARTIFACT	UNP P52477
G	-1	GLU	-	CLONING ARTIFACT	UNP P52477
G	0	SER	-	CLONING ARTIFACT	UNP P52477
G	1	SER	-	CLONING ARTIFACT	UNP P52477
G	361	HIS	-	EXPRESSION TAG	UNP P52477
G	362	HIS	-	EXPRESSION TAG	UNP P52477
G	363	HIS	-	EXPRESSION TAG	UNP P52477
G	364	HIS	-	EXPRESSION TAG	UNP P52477
G	365	HIS	-	EXPRESSION TAG	UNP P52477
G	366	HIS	-	EXPRESSION TAG	UNP P52477
H	-2	ALA	-	CLONING ARTIFACT	UNP P52477
H	-1	GLU	-	CLONING ARTIFACT	UNP P52477
H	0	SER	-	CLONING ARTIFACT	UNP P52477
H	1	SER	-	CLONING ARTIFACT	UNP P52477
H	361	HIS	-	EXPRESSION TAG	UNP P52477
H	362	HIS	-	EXPRESSION TAG	UNP P52477
H	363	HIS	-	EXPRESSION TAG	UNP P52477
H	364	HIS	-	EXPRESSION TAG	UNP P52477
H	365	HIS	-	EXPRESSION TAG	UNP P52477
H	366	HIS	-	EXPRESSION TAG	UNP P52477
I	-2	ALA	-	CLONING ARTIFACT	UNP P52477
I	-1	GLU	-	CLONING ARTIFACT	UNP P52477
I	0	SER	-	CLONING ARTIFACT	UNP P52477
I	1	SER	-	CLONING ARTIFACT	UNP P52477
I	361	HIS	-	EXPRESSION TAG	UNP P52477
I	362	HIS	-	EXPRESSION TAG	UNP P52477
I	363	HIS	-	EXPRESSION TAG	UNP P52477

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	364	HIS	-	EXPRESSION TAG	UNP P52477
I	365	HIS	-	EXPRESSION TAG	UNP P52477
I	366	HIS	-	EXPRESSION TAG	UNP P52477
J	-2	ALA	-	CLONING ARTIFACT	UNP P52477
J	-1	GLU	-	CLONING ARTIFACT	UNP P52477
J	0	SER	-	CLONING ARTIFACT	UNP P52477
J	1	SER	-	CLONING ARTIFACT	UNP P52477
J	361	HIS	-	EXPRESSION TAG	UNP P52477
J	362	HIS	-	EXPRESSION TAG	UNP P52477
J	363	HIS	-	EXPRESSION TAG	UNP P52477
J	364	HIS	-	EXPRESSION TAG	UNP P52477
J	365	HIS	-	EXPRESSION TAG	UNP P52477
J	366	HIS	-	EXPRESSION TAG	UNP P52477
K	-2	ALA	-	CLONING ARTIFACT	UNP P52477
K	-1	GLU	-	CLONING ARTIFACT	UNP P52477
K	0	SER	-	CLONING ARTIFACT	UNP P52477
K	1	SER	-	CLONING ARTIFACT	UNP P52477
K	361	HIS	-	EXPRESSION TAG	UNP P52477
K	362	HIS	-	EXPRESSION TAG	UNP P52477
K	363	HIS	-	EXPRESSION TAG	UNP P52477
K	364	HIS	-	EXPRESSION TAG	UNP P52477
K	365	HIS	-	EXPRESSION TAG	UNP P52477
K	366	HIS	-	EXPRESSION TAG	UNP P52477
L	-2	ALA	-	CLONING ARTIFACT	UNP P52477
L	-1	GLU	-	CLONING ARTIFACT	UNP P52477
L	0	SER	-	CLONING ARTIFACT	UNP P52477
L	1	SER	-	CLONING ARTIFACT	UNP P52477
L	361	HIS	-	EXPRESSION TAG	UNP P52477
L	362	HIS	-	EXPRESSION TAG	UNP P52477
L	363	HIS	-	EXPRESSION TAG	UNP P52477
L	364	HIS	-	EXPRESSION TAG	UNP P52477
L	365	HIS	-	EXPRESSION TAG	UNP P52477
L	366	HIS	-	EXPRESSION TAG	UNP P52477
M	-2	ALA	-	CLONING ARTIFACT	UNP P52477
M	-1	GLU	-	CLONING ARTIFACT	UNP P52477
M	0	SER	-	CLONING ARTIFACT	UNP P52477
M	1	SER	-	CLONING ARTIFACT	UNP P52477
M	361	HIS	-	EXPRESSION TAG	UNP P52477
M	362	HIS	-	EXPRESSION TAG	UNP P52477
M	363	HIS	-	EXPRESSION TAG	UNP P52477
M	364	HIS	-	EXPRESSION TAG	UNP P52477
M	365	HIS	-	EXPRESSION TAG	UNP P52477

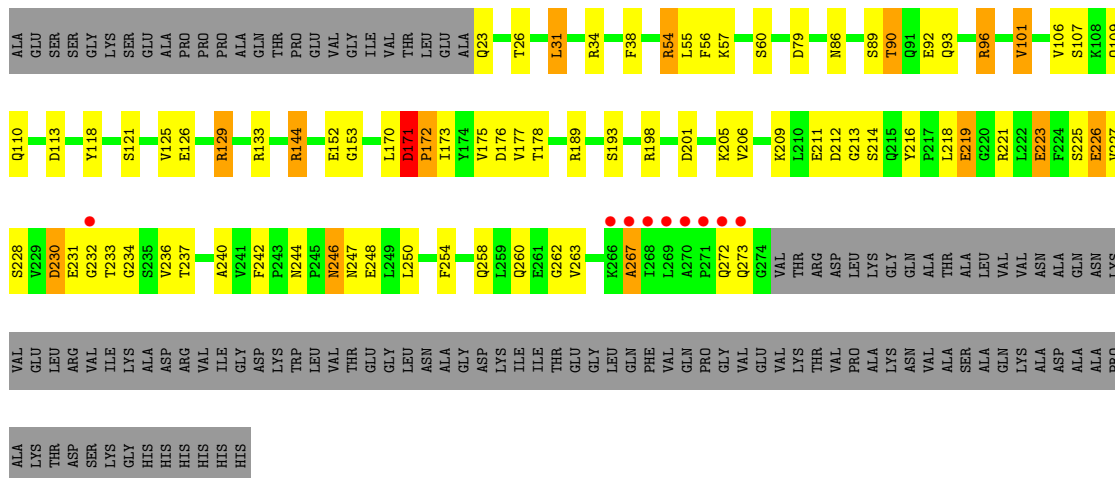
*Continued on next page...*

*Continued from previous page...*

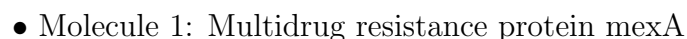
Chain	Residue	Modelled	Actual	Comment	Reference
M	366	HIS	-	EXPRESSION TAG	UNP P52477



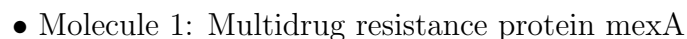




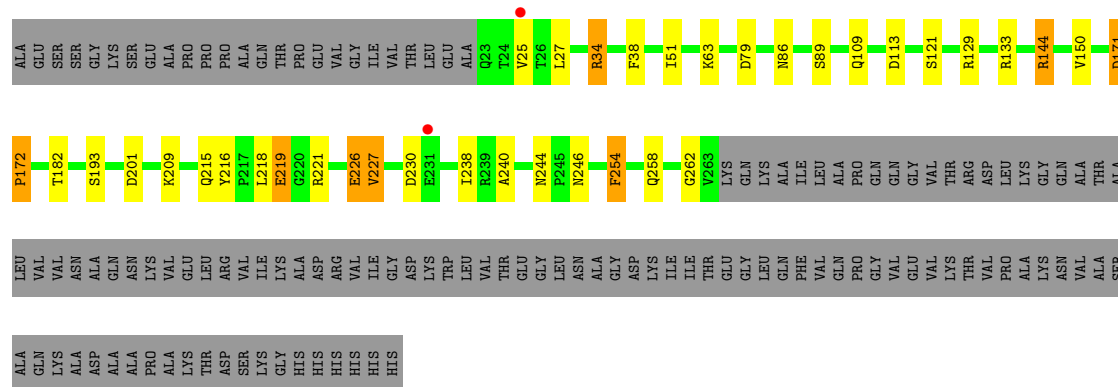
Chain F:



Chain G:



## Chain H:



- Molecule 1: Multidrug resistance protein mexA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.03Å 180.35Å 214.23Å 90.00° 106.99° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.40) 99.8 (40.00-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.258 , 0.282 0.255 , 0.280	Depositor DCC
$R_{free}$ test set	18428 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.9	EDS
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 365653 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.77	0/1840	0.92	7/2495 (0.3%)
1	B	1.17	3/1827 (0.2%)	1.18	16/2478 (0.6%)
1	C	1.09	4/1909 (0.2%)	1.13	13/2588 (0.5%)
1	D	1.22	5/1827 (0.3%)	1.33	23/2478 (0.9%)
1	E	1.05	1/1953 (0.1%)	1.11	14/2648 (0.5%)
1	F	1.05	2/1812 (0.1%)	1.08	12/2457 (0.5%)
1	G	0.77	1/1843 (0.1%)	0.92	6/2500 (0.2%)
1	H	0.89	0/1870	0.98	9/2537 (0.4%)
1	I	1.04	2/1827 (0.1%)	1.11	15/2478 (0.6%)
1	J	0.88	1/1827 (0.1%)	0.99	11/2478 (0.4%)
1	K	0.86	1/1803 (0.1%)	0.93	7/2445 (0.3%)
1	L	0.85	0/1827	0.97	8/2478 (0.3%)
1	M	0.62	0/1803	0.78	3/2445 (0.1%)
All	All	0.96	20/23968 (0.1%)	1.04	144/32505 (0.4%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	246	ASN	C-O	11.84	1.45	1.23
1	B	248	GLU	CD-OE1	7.55	1.33	1.25
1	C	77	GLU	CD-OE2	6.76	1.33	1.25
1	G	129	ARG	CZ-NH1	6.44	1.41	1.33
1	B	55	LEU	N-CA	5.91	1.58	1.46

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	C	96	ARG	NE-CZ-NH2	-14.83	112.88	120.30
1	G	133	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	E	54	ARG	NE-CZ-NH2	-13.33	113.64	120.30
1	D	54	ARG	NE-CZ-NH2	-13.06	113.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1816	54	0
1	B	1803	0	1807	48	0
1	C	1885	0	1902	53	0
1	D	1803	0	1807	42	0
1	E	1928	0	1941	53	0
1	F	1788	0	1789	43	0
1	G	1819	0	1822	39	0
1	H	1846	0	1849	25	0
1	I	1803	0	1807	39	0
1	J	1803	0	1807	43	0
1	K	1779	0	1781	50	0
1	L	1803	0	1807	51	0
1	M	1779	0	1781	43	0
All	All	23655	0	23716	536	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 536 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:54:ARG:HG3	1:C:54:ARG:HH11	1.20	1.05
1:H:34:ARG:HH11	1:H:34:ARG:HG2	1.15	1.04
1:I:178:THR:HG22	1:I:237:THR:OG1	1.58	1.02
1:B:90:THR:HG23	1:B:118:TYR:HA	1.41	0.99
1:A:189:ARG:HH11	1:A:189:ARG:HG3	1.28	0.99

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	235/369 (64%)	213 (91%)	19 (8%)	3 (1%)	18	24
1	B	233/369 (63%)	216 (93%)	13 (6%)	4 (2%)	14	17
1	C	244/369 (66%)	236 (97%)	5 (2%)	3 (1%)	19	26
1	D	233/369 (63%)	222 (95%)	9 (4%)	2 (1%)	25	35
1	E	250/369 (68%)	232 (93%)	10 (4%)	8 (3%)	6	5
1	F	231/369 (63%)	211 (91%)	17 (7%)	3 (1%)	18	24
1	G	235/369 (64%)	226 (96%)	7 (3%)	2 (1%)	25	35
1	H	239/369 (65%)	228 (95%)	9 (4%)	2 (1%)	27	39
1	I	233/369 (63%)	228 (98%)	2 (1%)	3 (1%)	18	24
1	J	233/369 (63%)	225 (97%)	6 (3%)	2 (1%)	25	35
1	K	230/369 (62%)	208 (90%)	18 (8%)	4 (2%)	14	17
1	L	233/369 (63%)	216 (93%)	16 (7%)	1 (0%)	43	61
1	M	230/369 (62%)	204 (89%)	19 (8%)	7 (3%)	7	5
All	All	3059/4797 (64%)	2865 (94%)	150 (5%)	44 (1%)	16	22

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	VAL
1	E	267	ALA
1	F	29	THR
1	K	194	GLY
1	A	176	ASP

### 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	191/295 (65%)	174 (91%)	17 (9%)	14	21
1	B	190/295 (64%)	178 (94%)	12 (6%)	25	38
1	C	199/295 (68%)	190 (96%)	9 (4%)	38	57
1	D	190/295 (64%)	179 (94%)	11 (6%)	28	43
1	E	203/295 (69%)	184 (91%)	19 (9%)	13	18
1	F	188/295 (64%)	178 (95%)	10 (5%)	32	48
1	G	192/295 (65%)	174 (91%)	18 (9%)	13	18
1	H	195/295 (66%)	184 (94%)	11 (6%)	30	45
1	I	190/295 (64%)	176 (93%)	14 (7%)	20	30
1	J	190/295 (64%)	183 (96%)	7 (4%)	45	66
1	K	187/295 (63%)	174 (93%)	13 (7%)	21	33
1	L	190/295 (64%)	175 (92%)	15 (8%)	18	26
1	M	187/295 (63%)	173 (92%)	14 (8%)	19	29
All	All	2492/3835 (65%)	2322 (93%)	170 (7%)	22	34

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	239	ARG
1	G	261	GLU
1	M	52	LEU
1	G	35	THR
1	G	150	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	131	ASN
1	H	36	ASN
1	L	162	ASN
1	F	162	ASN
1	G	110	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

### 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<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	237/369 (64%)	0.34	15 (6%) 19 18	41, 73, 122, 134	0
1	B	235/369 (63%)	0.10	3 (1%) 74 73	30, 51, 97, 109	0
1	C	246/369 (66%)	0.15	8 (3%) 44 42	29, 51, 92, 110	0
1	D	235/369 (63%)	0.09	1 (0%) 90 90	32, 46, 90, 101	0
1	E	252/369 (68%)	0.24	9 (3%) 41 39	35, 56, 112, 139	0
1	F	233/369 (63%)	0.14	5 (2%) 60 58	36, 56, 99, 106	0
1	G	237/369 (64%)	0.23	8 (3%) 43 41	46, 77, 118, 139	0
1	H	241/369 (65%)	0.07	2 (0%) 83 82	50, 68, 97, 114	0
1	I	235/369 (63%)	0.13	5 (2%) 60 58	35, 52, 95, 105	0
1	J	235/369 (63%)	0.14	4 (1%) 67 65	39, 58, 120, 125	0
1	K	232/369 (62%)	0.17	3 (1%) 74 73	41, 68, 116, 128	0
1	L	235/369 (63%)	0.14	6 (2%) 53 51	45, 69, 113, 120	0
1	M	232/369 (62%)	0.58	28 (12%) 5 4	56, 88, 150, 157	0
All	All	3085/4797 (64%)	0.19	97 (3%) 47 44	29, 64, 118, 157	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	VAL	11.3
1	C	268	ILE	7.2
1	E	270	ALA	5.6
1	E	272	GLN	5.5
1	J	232	GLY	5.0

### 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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.