



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:04 pm GMT

PDB ID : 4QQF  
Title : Crystal structure of mitochondrial import inner membrane translocase subunit TIM50  
Authors : Li, J.Z.  
Deposited on : 2014-06-27  
Resolution : 2.67 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

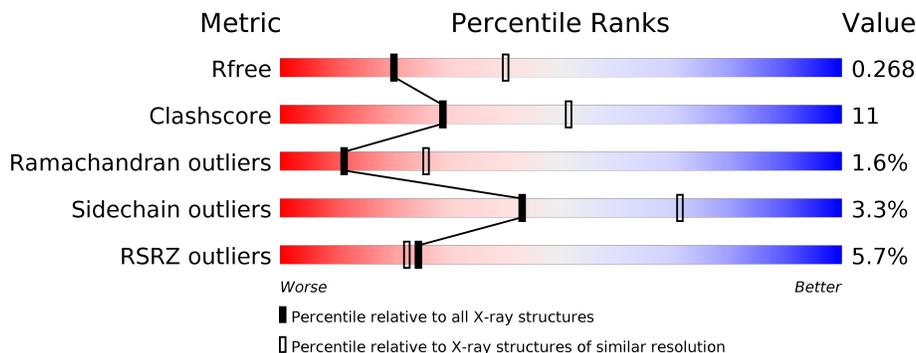
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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))
$R_{free}$	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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. 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	202	
1	B	202	
1	C	202	
1	D	202	
1	E	202	
1	F	202	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	MG	A	401	-	-	-	X
2	MG	B	401	-	-	-	X
2	MG	C	401	-	-	-	X
2	MG	D	401	-	-	-	X
2	MG	E	401	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9432 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 Mitochondrial import inner membrane translocase subunit TIM50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	187	Total 1550	C 1011	N 249	O 286	S 4	0	0	0
1	A	198	Total 1641	C 1070	N 263	O 302	S 6	0	0	0
1	B	181	Total 1496	C 973	N 242	O 277	S 4	0	0	0
1	C	193	Total 1602	C 1045	N 256	O 296	S 5	0	0	0
1	E	182	Total 1504	C 981	N 241	O 278	S 4	0	0	0
1	F	191	Total 1584	C 1035	N 251	O 293	S 5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	160	GLY	-	EXPRESSION TAG	UNP Q02776
D	161	SER	-	EXPRESSION TAG	UNP Q02776
D	162	HIS	-	EXPRESSION TAG	UNP Q02776
D	163	MET	-	EXPRESSION TAG	UNP Q02776
A	160	GLY	-	EXPRESSION TAG	UNP Q02776
A	161	SER	-	EXPRESSION TAG	UNP Q02776
A	162	HIS	-	EXPRESSION TAG	UNP Q02776
A	163	MET	-	EXPRESSION TAG	UNP Q02776
B	160	GLY	-	EXPRESSION TAG	UNP Q02776
B	161	SER	-	EXPRESSION TAG	UNP Q02776
B	162	HIS	-	EXPRESSION TAG	UNP Q02776
B	163	MET	-	EXPRESSION TAG	UNP Q02776
C	160	GLY	-	EXPRESSION TAG	UNP Q02776
C	161	SER	-	EXPRESSION TAG	UNP Q02776
C	162	HIS	-	EXPRESSION TAG	UNP Q02776
C	163	MET	-	EXPRESSION TAG	UNP Q02776

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	GLY	-	EXPRESSION TAG	UNP Q02776
E	161	SER	-	EXPRESSION TAG	UNP Q02776
E	162	HIS	-	EXPRESSION TAG	UNP Q02776
E	163	MET	-	EXPRESSION TAG	UNP Q02776
F	160	GLY	-	EXPRESSION TAG	UNP Q02776
F	161	SER	-	EXPRESSION TAG	UNP Q02776
F	162	HIS	-	EXPRESSION TAG	UNP Q02776
F	163	MET	-	EXPRESSION TAG	UNP Q02776

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

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

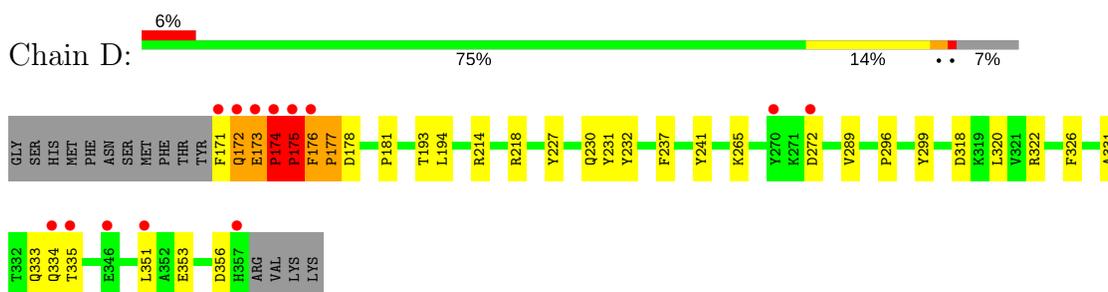
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	12	Total O 12 12	0	0
3	A	17	Total O 17 17	0	0
3	B	6	Total O 6 6	0	0
3	C	6	Total O 6 6	0	0
3	E	6	Total O 6 6	0	0
3	F	2	Total O 2 2	0	0

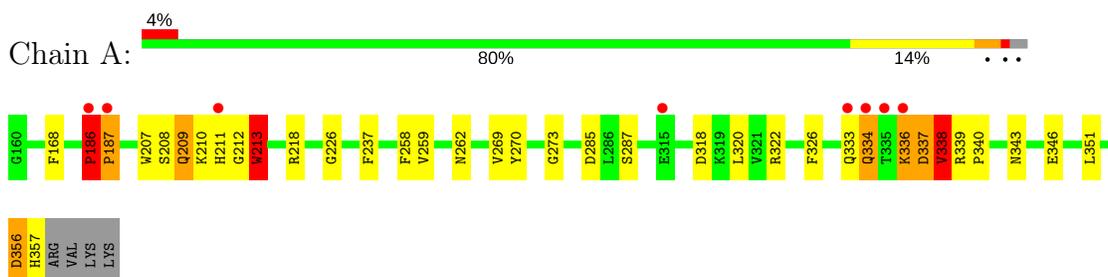
### 3 Residue-property plots [i](#)

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.

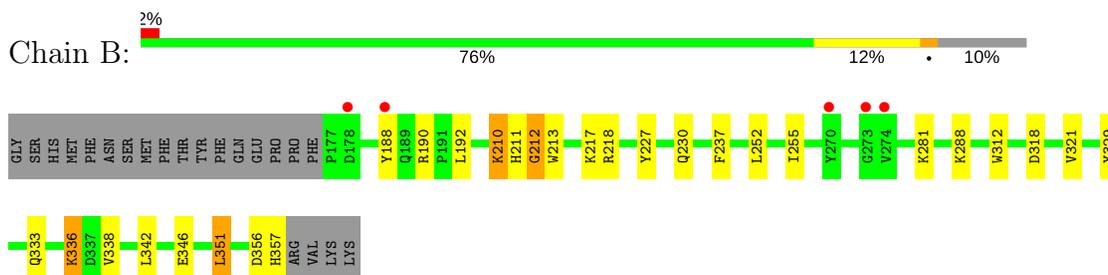
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



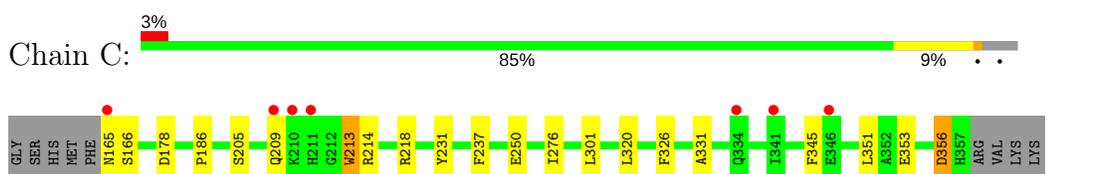
- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



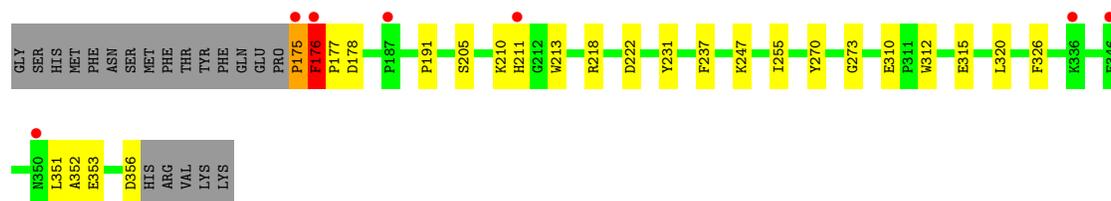
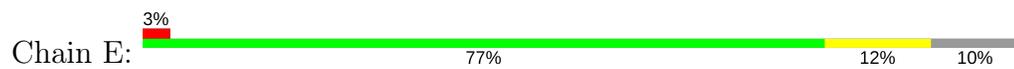
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- Molecule 1: Mitochondrial import inner membrane translocase subunit TIM50



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.29Å 164.29Å 150.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.52 – 2.67 47.99 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.52-2.67) 95.7 (47.99-2.67)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.212 , 0.252 0.238 , 0.268	Depositor DCC
$R_{free}$ test set	2937 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.60	2/1696 (0.1%)	0.78	1/2309 (0.0%)
1	B	0.51	0/1543	0.75	2/2101 (0.1%)
1	C	0.50	0/1655	0.71	1/2255 (0.0%)
1	D	0.56	2/1601 (0.1%)	0.79	3/2182 (0.1%)
1	E	0.53	1/1552 (0.1%)	0.68	1/2114 (0.0%)
1	F	0.50	2/1636 (0.1%)	0.72	2/2229 (0.1%)
All	All	0.54	7/9683 (0.1%)	0.74	10/13190 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	177	PRO	N-CD	5.82	1.55	1.47
1	A	338	VAL	CB-CG2	-5.70	1.40	1.52
1	D	174	PRO	N-CD	5.54	1.55	1.47
1	F	174	PRO	N-CD	5.27	1.55	1.47
1	A	213	TRP	CB-CG	5.16	1.59	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	TRP	CA-CB-CG	6.43	125.91	113.70
1	D	176	PHE	N-CA-C	6.29	127.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	TRP	CA-CB-CG	6.27	125.61	113.70
1	B	351	LEU	CA-CB-CG	6.23	129.63	115.30
1	D	174	PRO	C-N-CD	6.12	141.25	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	212	GLY	Peptide
1	B	356	ASP	Peptide

## 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	1641	0	1590	40	0
1	B	1496	0	1467	15	0
1	C	1602	0	1557	11	0
1	D	1550	0	1512	47	0
1	E	1504	0	1476	28	0
1	F	1584	0	1544	71	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	17	0	0	0	1
3	B	6	0	0	3	0
3	C	6	0	0	0	0
3	D	12	0	0	1	0
3	E	6	0	0	0	0
3	F	2	0	0	0	0
All	All	9432	0	9146	202	1

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 11.

The worst 5 of 202 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:F:207:TRP:CD1	1:F:213:TRP:HZ3	1.48	1.31
1:F:207:TRP:CE2	1:F:213:TRP:CH2	2.20	1.30
1:F:207:TRP:CD1	1:F:213:TRP:CZ3	2.20	1.30
1:A:337:ASP:OD1	1:A:339:ARG:NE	1.72	1.20
1:F:207:TRP:CE2	1:F:213:TRP:CZ3	2.36	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:511:HOH:O	3:A:511:HOH:O[8_554]	2.15	0.05

## 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	196/202 (97%)	183 (93%)	8 (4%)	5 (3%)	6	14
1	B	179/202 (89%)	176 (98%)	2 (1%)	1 (1%)	28	54
1	C	191/202 (95%)	181 (95%)	8 (4%)	2 (1%)	18	40
1	D	185/202 (92%)	177 (96%)	6 (3%)	2 (1%)	17	37
1	E	180/202 (89%)	176 (98%)	3 (2%)	1 (1%)	28	54
1	F	189/202 (94%)	171 (90%)	11 (6%)	7 (4%)	4	8
All	All	1120/1212 (92%)	1064 (95%)	38 (3%)	18 (2%)	11	26

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	GLN

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Mol	Chain	Res	Type
1	A	186	PRO
1	A	187	PRO
1	A	337	ASP
1	A	338	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	184/188 (98%)	176 (96%)	8 (4%)	33	61
1	B	168/188 (89%)	161 (96%)	7 (4%)	34	62
1	C	180/188 (96%)	175 (97%)	5 (3%)	49	77
1	D	174/188 (93%)	169 (97%)	5 (3%)	48	75
1	E	169/188 (90%)	165 (98%)	4 (2%)	54	81
1	F	178/188 (95%)	172 (97%)	6 (3%)	42	70
All	All	1053/1128 (93%)	1018 (97%)	35 (3%)	43	71

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	321	VAL
1	B	351	LEU
1	F	237	PHE
1	B	336	LYS
1	B	338	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	211	HIS
1	B	262	ASN
1	B	357	HIS
1	F	211	HIS

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Mol	Chain	Res	Type
1	F	275	HIS

### 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 carbohydrates 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, 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	198/202 (98%)	0.34	8 (4%) 39 37	46, 60, 111, 192	0
1	B	181/202 (89%)	0.26	5 (2%) 53 52	48, 69, 104, 167	0
1	C	193/202 (95%)	0.29	7 (3%) 43 42	48, 69, 118, 141	0
1	D	187/202 (92%)	0.49	13 (6%) 17 15	24, 71, 117, 156	0
1	E	182/202 (90%)	0.32	7 (3%) 41 39	24, 68, 107, 131	0
1	F	191/202 (94%)	0.78	24 (12%) 4 3	57, 92, 148, 263	0
All	All	1132/1212 (93%)	0.41	64 (5%) 24 22	24, 70, 121, 263	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	PHE	6.5
1	D	175	PRO	5.9
1	D	174	PRO	5.8
1	E	176	PHE	5.8
1	A	335	THR	5.2

### 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	401	1/1	0.88	0.73	25.46	68,68,68,68	0
2	MG	B	401	1/1	0.94	0.62	17.21	47,47,47,47	0
2	MG	E	401	1/1	0.97	0.53	13.76	39,39,39,39	0
2	MG	C	401	1/1	0.98	0.55	7.88	41,41,41,41	0
2	MG	A	401	1/1	0.97	0.49	6.98	41,41,41,41	0
2	MG	F	401	1/1	0.88	0.26	0.73	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.