



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:26 am GMT

PDB ID : 1Z3H  
Title : The exportin Cse1 in its cargo-free, cytoplasmic state  
Authors : Cook, A.; Fernandez, E.; Lindner, D.; Ebert, J.; Schlenstedt, G.; Conti, E.  
Deposited on : 2005-03-12  
Resolution : 3.10 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.

---

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

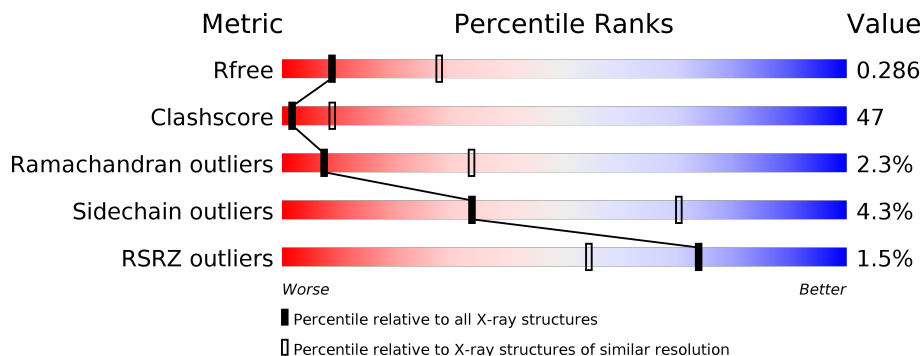
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	968	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 43%; height: 10px; background-color: green;"></div> <div style="width: 48%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	968	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 37%; height: 10px; background-color: green;"></div> <div style="width: 53%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14787 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 Importin alpha re-exporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	925	Total	C	N	O	S	0	0	0
			7435	4818	1208	1391	18			
1	B	914	Total	C	N	O	S	0	0	0
			7351	4774	1189	1370	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	EXPRESSION TAG	UNP P33307
A	962	SER	-	EXPRESSION TAG	UNP P33307
A	963	HIS	-	EXPRESSION TAG	UNP P33307
A	964	HIS	-	EXPRESSION TAG	UNP P33307
A	965	HIS	-	EXPRESSION TAG	UNP P33307
A	966	HIS	-	EXPRESSION TAG	UNP P33307
A	967	HIS	-	EXPRESSION TAG	UNP P33307
A	968	HIS	-	EXPRESSION TAG	UNP P33307
B	961	ARG	-	EXPRESSION TAG	UNP P33307
B	962	SER	-	EXPRESSION TAG	UNP P33307
B	963	HIS	-	EXPRESSION TAG	UNP P33307
B	964	HIS	-	EXPRESSION TAG	UNP P33307
B	965	HIS	-	EXPRESSION TAG	UNP P33307
B	966	HIS	-	EXPRESSION TAG	UNP P33307
B	967	HIS	-	EXPRESSION TAG	UNP P33307
B	968	HIS	-	EXPRESSION TAG	UNP P33307

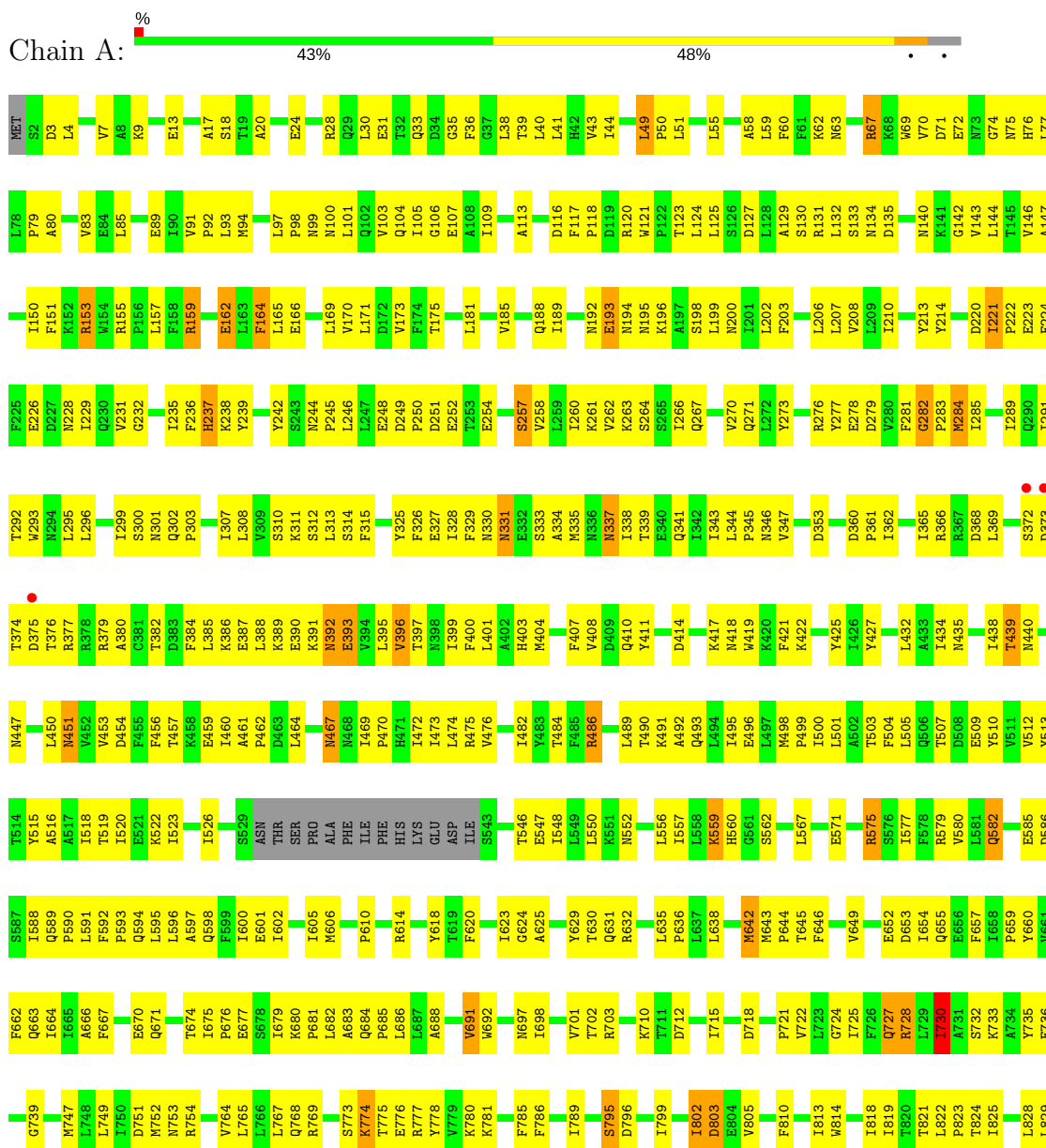
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

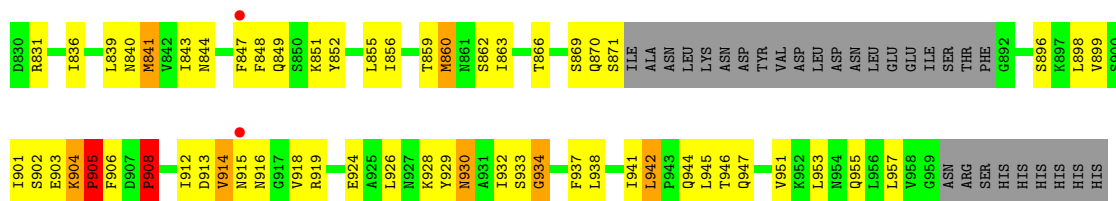
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

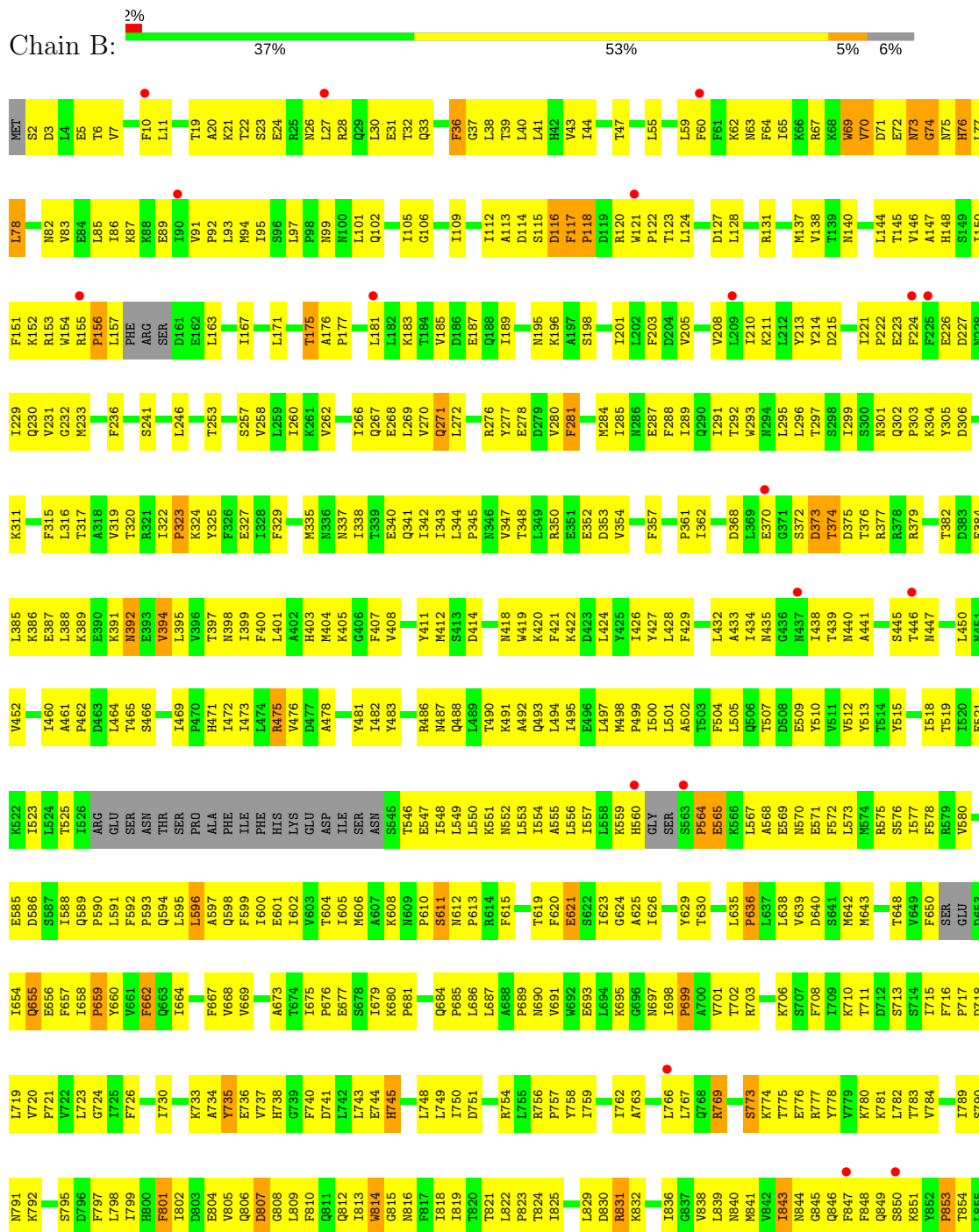
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

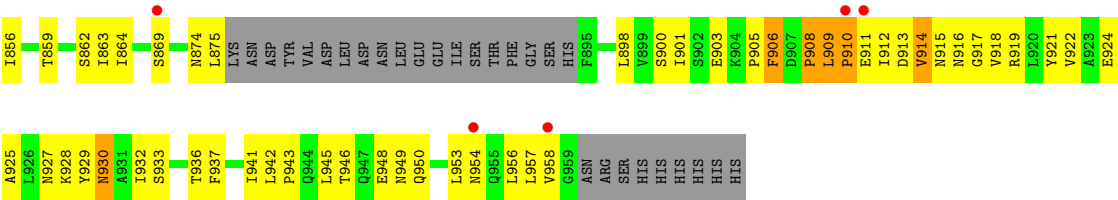
#### • Molecule 1: Importin alpha re-exporter





## ● Molecule 1: Importin alpha re-exporter





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.52Å 113.04Å 122.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.00 – 3.10 98.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (122.00-3.10) 99.6 (98.06-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.288 0.239 , 0.286	Depositor DCC
$R_{free}$ test set	2096 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.7	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 73.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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	0.50	0/7584	0.74	2/10306 (0.0%)
1	B	0.54	7/7495 (0.1%)	0.75	12/10185 (0.1%)
All	All	0.52	7/15079 (0.0%)	0.74	14/20491 (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	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	807	ASP	C-O	-20.19	0.84	1.23
1	B	807	ASP	C-N	8.88	1.49	1.33
1	B	808	GLY	N-CA	6.85	1.56	1.46
1	B	73	ASN	C-O	-6.20	1.11	1.23
1	B	74	GLY	N-CA	5.75	1.54	1.46

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASN	O-C-N	-17.55	93.36	123.20
1	A	908	PRO	CA-N-CD	-11.49	95.41	111.50
1	B	807	ASP	CA-C-N	-9.48	97.24	116.20
1	B	807	ASP	CA-C-O	9.33	139.69	120.10
1	B	807	ASP	C-N-CA	-9.19	103.00	122.30



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	73	ASN	Mainchain,Peptide
1	B	910	PRO	Mainchain

## 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	7435	0	7576	598	0
1	B	7351	0	7510	805	0
2	A	1	0	0	0	0
All	All	14787	0	15086	1403	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 47.

The worst 5 of 1403 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:546:THR:CG2	1:B:588:ILE:HD11	1.38	1.53
1:B:6:THR:HG22	1:B:10:PHE:CE1	1.51	1.44
1:B:791:ASN:ND2	1:B:909:LEU:CD1	1.78	1.43
1:B:69:TRP:CD1	1:B:70:VAL:CG2	2.04	1.39
1:B:6:THR:CG2	1:B:10:PHE:HE1	1.37	1.36

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	919/968 (95%)	814 (89%)	83 (9%)	22 (2%)	7	32
1	B	902/968 (93%)	800 (89%)	82 (9%)	20 (2%)	8	35
All	All	1821/1936 (94%)	1614 (89%)	165 (9%)	42 (2%)	7	33

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	653	ASP
1	A	905	PRO
1	A	908	PRO
1	B	99	ASN

### 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	849/890 (95%)	804 (95%)	45 (5%)	26	63
1	B	839/890 (94%)	811 (97%)	28 (3%)	43	77
All	All	1688/1780 (95%)	1615 (96%)	73 (4%)	33	70

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	795	SER
1	A	906	PHE
1	B	801	PHE
1	A	860	MET
1	A	914	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	GLN
1	A	870	GLN
1	B	791	ASN
1	A	655	GLN
1	A	927	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	925/968 (95%)	-0.11	5 (0%) 90 80	22, 55, 114, 154	0
1	B	914/968 (94%)	0.22	23 (2%) 58 35	37, 89, 150, 172	0
All	All	1839/1936 (94%)	0.05	28 (1%) 74 54	22, 70, 141, 172	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	910	PRO	4.2
1	B	911	GLU	4.1
1	B	958	VAL	3.4
1	A	847	PHE	3.1
1	B	27	LEU	3.1

### 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( $\text{\AA}^2$ )	Q<0.9
2	MG	A	969	1/1	0.97	0.17	-0.59	1,1,1,1	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.