wwPDB X-ray Structure Validation Summary Report (i)

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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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

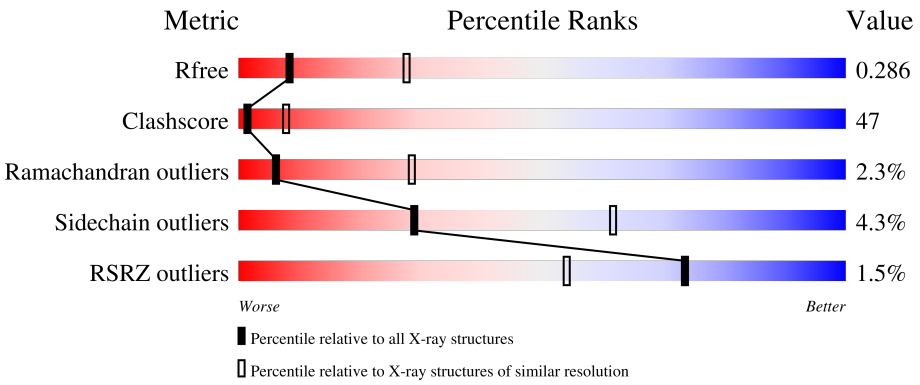
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

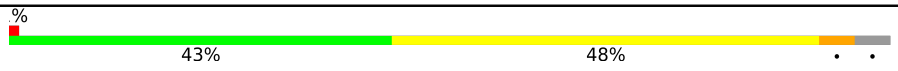
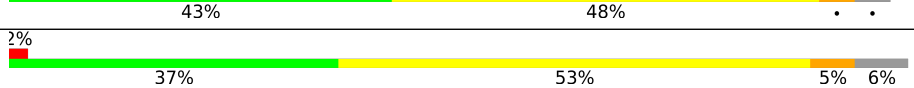
The reported resolution of this entry is 3.10 Å.

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	968	
1	B	968	

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	925	7435	4818	1208	1391	18	0	0	0
1	B	914	7351	4774	1189	1370	18	0	0	0

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).

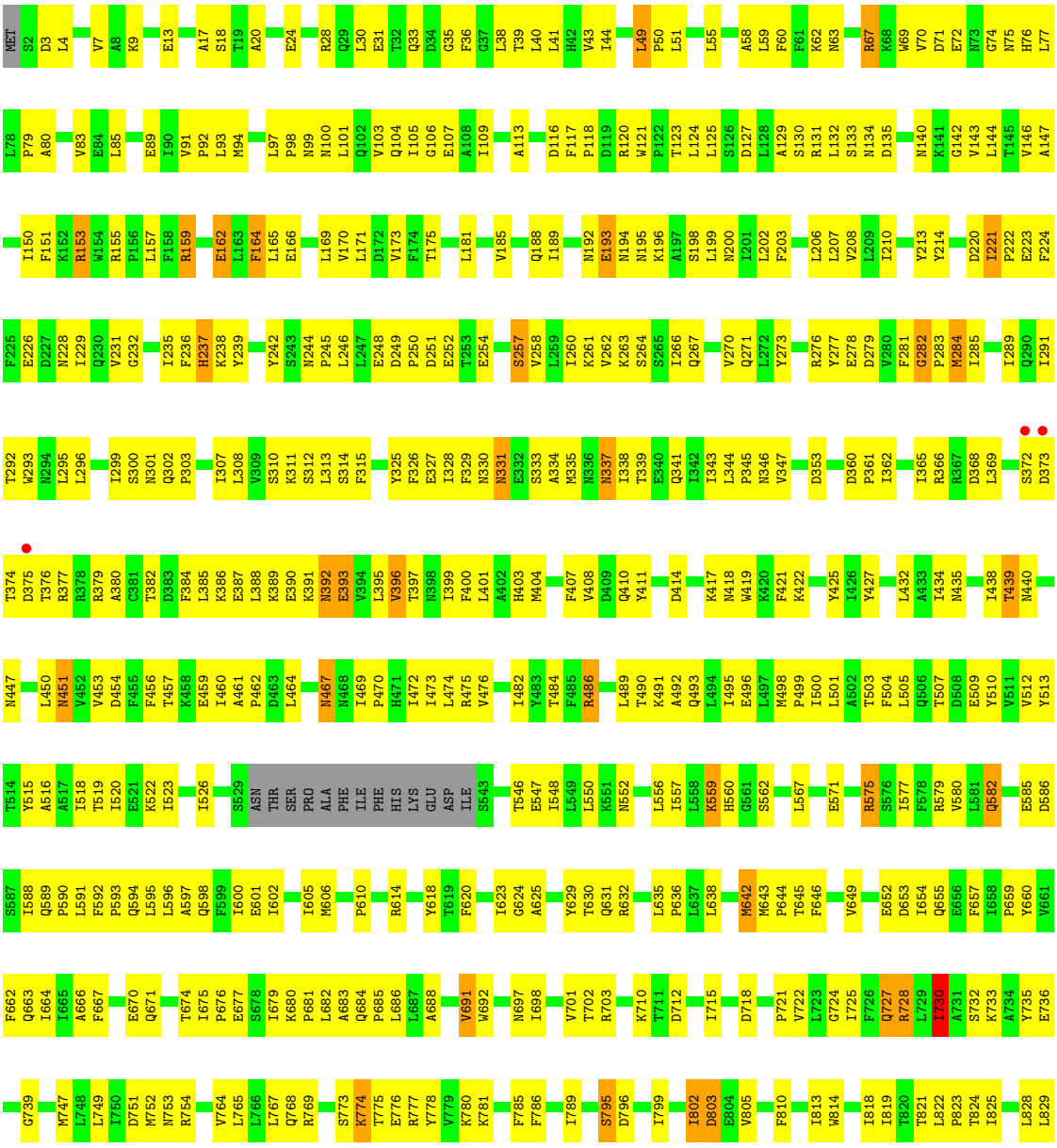
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

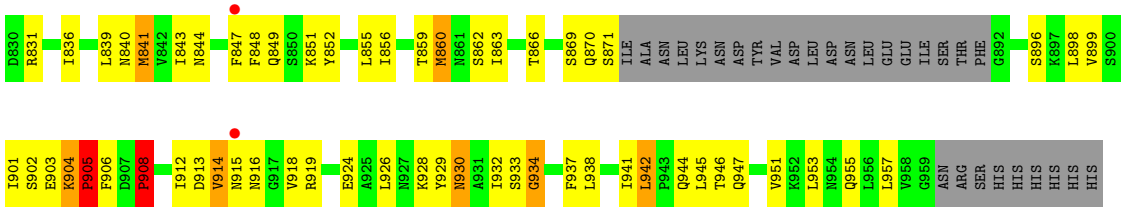
3 Residue-property plots (i)

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: Importin alpha re-exporter

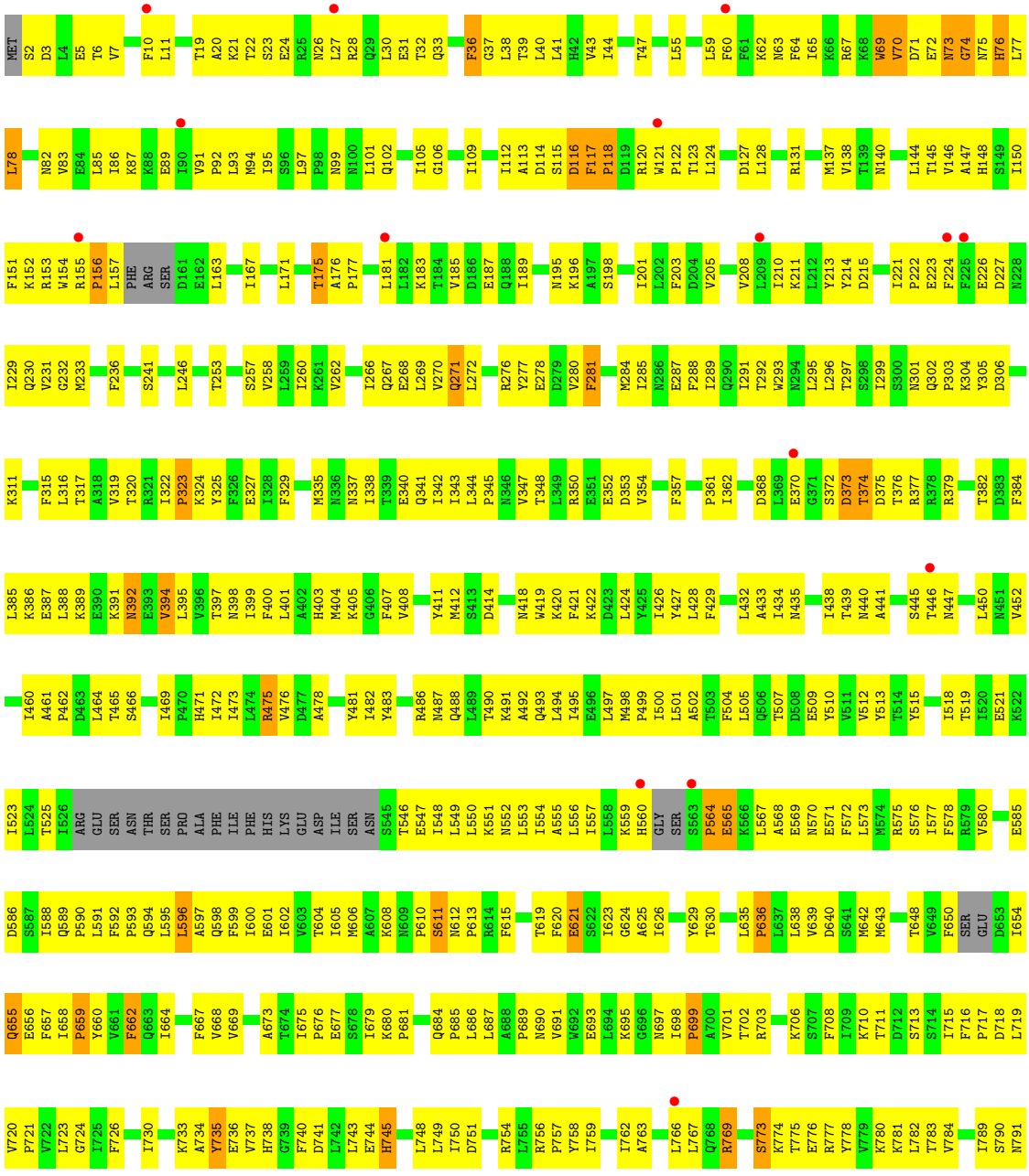
Chain A:

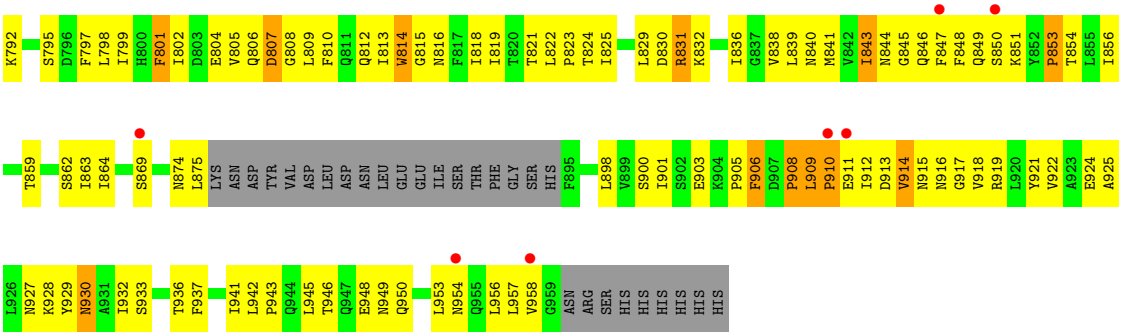




• Molecule 1: Importin alpha re-exporter

Chain B: 2% 37% 53% 5% 6%




K792 S795 D796 F797 L798 I799 H800 F801 I802 D803 E804 V805 Q806 D807 G808 L809 F810 Q811 Q812 I813 W814 G815 N816 F817 I818 I819 T820 T821 L822 P823 T824 I825 L829 D830 R831 K832 I836 G837 V838 L839 N840 M841 V842 I843 N844 G845 Q846 F847 F848 Q849 S850 K851 Y852 P853 T854 L855 I856
T859 S862 I863 I864 S869 N874 L875 LYS ASN ASP TYR VAL ASP LEU ASP ASN LEU GLU GLU ILE SER THR PHE GLY SER HIS F895 L898 V899 S900 I901 S902 E903 K904 P905 F906 D907 P908 L909 P910 E911 I912 D913 V914 N915 N916 G917 V918 R919 L920 Y921 V922 A923 E924 A925
L926 N927 K928 Y929 N930 A931 I932 S933 T936 F937 I941 L942 P943 Q944 L945 T946 Q947 E948 N949 Q950 L953 N954 Q955 L956 L957 V958 G959 ASN ARG SER HIS 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	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
$< I/\sigma(I) >$ [1]	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	2291 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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^2)	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.*

[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 (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(^{o})	Ideal(^{o})
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 (i)

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 (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	919/968 (95%)	814 (89%)	83 (9%)	22 (2%)	6	27
1	B	902/968 (93%)	800 (89%)	82 (9%)	20 (2%)	6	29
All	All	1821/1936 (94%)	1614 (89%)	165 (9%)	42 (2%)	6	28

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 (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	849/890 (95%)	804 (95%)	45 (5%)	22	54
1	B	839/890 (94%)	811 (97%)	28 (3%)	38	69
All	All	1688/1780 (95%)	1615 (96%)	73 (4%)	29	62

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

Mol	Chain	Res	Type
1	B	621	GLU
1	B	862	SER
1	B	659	PRO
1	B	773	SER
1	A	486	ARG

Sometimes 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	949	ASN
1	B	398	ASN
1	A	955	GLN
1	B	148	HIS
1	B	437	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 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, 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	925/968 (95%)	-0.11	5 (0%)	91	81	22, 55, 114, 154	0
1	B	914/968 (94%)	0.22	22 (2%)	59	37	37, 89, 150, 172	0
All	All	1839/1936 (94%)	0.05	27 (1%)	73	54	22, 70, 141, 172	0

The worst 5 of 27 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 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, 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(Å^2)	Q<0.9
2	MG	A	969	1/1	0.97	0.17	1,1,1,1	0

6.5 Other polymers (i)

There are no such residues in this entry.