

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:25 pm GMT

PDB ID : 2WST

Title: Head domain of porcine adenovirus type 4 NADC-1 isolate fibre

Authors: Guardado-Calvo, P.; Munoz, E.M.; Llamas-Saiz, A.L.; Fox, G.C.; Glasgow,

J.N.; van Raaij, M.J.

Deposited on : 2009-09-09

Resolution : 3.20 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)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

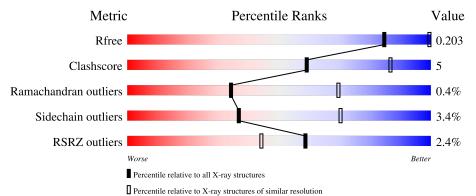
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 3.20 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	208	74%	11%	15%
1	В	208	71%	13%	15%
1	С	208	73%	12%	15%
1	D	208	79%	5% •	15%
1	Е	208	75%	8% •	15%



N	Mol	Chain	Length	Quality of chain		
	1	F	208	75%	9%	15%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7984 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 PUTATIVE FIBER PROTEIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	176	Total	С	N	О	S	0	0	0
1	A	170	1330	839	219	267	5	0	0	0
1	В	176	Total	С	N	О	S	0	0	0
1	Ъ	170	1330	839	219	267	5	0	0	
1	С	176	Total	С	N	О	S	0	0	0
1		170	1330	839	219	267	5	0		
1	D	176	Total	С	N	О	S	0	0	0
1	D	170	1330	839	219	267	5	U		
1	Е	176	Total	С	N	О	S	0	0	0
1	l Li	170	1330	839	219	267	5	0	0	
1	F	176	Total	С	N	О	S	0	0	0
1	I.	170	1330	839	219	267	5	U	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	expression tag	UNP Q83467
A	85	GLY	-	expression tag	UNP Q83467
A	86	SER	-	expression tag	UNP Q83467
A	87	SER	-	expression tag	UNP Q83467
A	88	HIS	-	expression tag	UNP Q83467
A	89	HIS	-	expression tag	UNP Q83467
A	90	HIS	-	expression tag	UNP Q83467
A	91	HIS	-	expression tag	UNP Q83467
A	92	HIS	-	expression tag	UNP Q83467
A	93	HIS	-	expression tag	UNP Q83467
A	94	SER	-	expression tag	UNP Q83467
A	95	SER	-	expression tag	UNP Q83467
A	96	GLY	-	expression tag	UNP Q83467
A	97	LEU		expression tag	UNP Q83467
A	98	VAL	=	expression tag	UNP Q83467
A	99	PRO	-	expression tag	UNP Q83467
A	100	ARG	-	expression tag	UNP Q83467



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
A	101	GLY	_	expression tag	UNP Q83467
A	102	SER	-	expression tag	UNP Q83467
A	103	HIS	-	expression tag	UNP Q83467
A	104	MET	-	expression tag	UNP Q83467
A	105	ALA	-	expression tag	UNP Q83467
A	106	SER	_	expression tag	UNP Q83467
A	107	MET	-	expression tag	UNP Q83467
A	108	THR	-	expression tag	UNP Q83467
A	109	GLY	-	expression tag	UNP Q83467
A	110	GLY	-	expression tag	UNP Q83467
A	111	GLN	-	expression tag	UNP Q83467
A	112	GLN	-	expression tag	UNP Q83467
A	113	GLY	-	expression tag	UNP Q83467
A	114	ARG	-	expression tag	UNP Q83467
A	115	ILE	-	expression tag	UNP Q83467
В	84	MET	-	expression tag	UNP Q83467
В	85	GLY	-	expression tag	UNP Q83467
В	86	SER	_	expression tag	UNP Q83467
В	87	SER	-	expression tag	UNP Q83467
В	88	HIS	-	expression tag	UNP Q83467
В	89	HIS	-	expression tag	UNP Q83467
В	90	HIS	-	expression tag	UNP Q83467
В	91	HIS	-	expression tag	UNP Q83467
В	92	HIS	-	expression tag	UNP Q83467
В	93	HIS	-	expression tag	UNP Q83467
В	94	SER	-	expression tag	UNP Q83467
В	95	SER	-	expression tag	UNP Q83467
В	96	GLY	-	expression tag	UNP Q83467
В	97	LEU	-	expression tag	UNP Q83467
В	98	VAL	-	expression tag	UNP Q83467
В	99	PRO	-	expression tag	UNP Q83467
В	100	ARG	-	expression tag	UNP Q83467
В	101	GLY	-	expression tag	UNP Q83467
В	102	SER	-	expression tag	UNP Q83467
В	103	HIS	-	expression tag	UNP Q83467
В	104	MET	-	expression tag	UNP Q83467
В	105	ALA	-	expression tag	UNP Q83467
В	106	SER	-	expression tag	UNP Q83467
В	107	MET	-	expression tag	UNP Q83467
В	108	THR	-	expression tag	UNP Q83467
В	109	GLY	-	expression tag	UNP Q83467
В	110	GLY	-	expression tag	UNP Q83467



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Chain	Residue	Modelled	Actual	Comment	Reference
В	111	GLN	-	expression tag	UNP Q83467
В	112	GLN	-	expression tag	UNP Q83467
В	113	GLY	-	expression tag	UNP Q83467
В	114	ARG	-	expression tag	UNP Q83467
В	115	ILE	-	expression tag	UNP Q83467
С	84	MET	-	expression tag	UNP Q83467
С	85	GLY	-	expression tag	UNP Q83467
С	86	SER	-	expression tag	UNP Q83467
С	87	SER	-	expression tag	UNP Q83467
С	88	HIS	-	expression tag	UNP Q83467
С	89	HIS	-	expression tag	UNP Q83467
С	90	HIS	-	expression tag	UNP Q83467
С	91	HIS	-	expression tag	UNP Q83467
С	92	HIS	-	expression tag	UNP Q83467
С	93	HIS	-	expression tag	UNP Q83467
С	94	SER	-	expression tag	UNP Q83467
С	95	SER	-	expression tag	UNP Q83467
С	96	GLY	-	expression tag	UNP Q83467
С	97	LEU	-	expression tag	UNP Q83467
С	98	VAL	-	expression tag	UNP Q83467
С	99	PRO	-	expression tag	UNP Q83467
С	100	ARG	-	expression tag	UNP Q83467
С	101	GLY	-	expression tag	UNP Q83467
С	102	SER	-	expression tag	UNP Q83467
С	103	HIS	-	expression tag	UNP Q83467
С	104	MET	-	expression tag	UNP Q83467
С	105	ALA	-	expression tag	UNP Q83467
С	106	SER	-	expression tag	UNP Q83467
С	107	MET	-	expression tag	UNP Q83467
С	108	THR	-	expression tag	UNP Q83467
С	109	GLY	-	expression tag	UNP Q83467
С	110	GLY	-	expression tag	UNP Q83467
С	111	GLN	-	expression tag	UNP Q83467
С	112	GLN	-	expression tag	UNP Q83467
С	113	GLY	-	expression tag	UNP Q83467
С	114	ARG	-	expression tag	UNP Q83467
С	115	ILE	-	expression tag	UNP Q83467
D	84	MET	_	expression tag	UNP Q83467
D	85	GLY	-	expression tag	UNP Q83467
D	86	SER	-	expression tag	UNP Q83467
D	87	SER	-	expression tag	UNP Q83467
D	88	HIS	-	expression tag	UNP Q83467



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
D	89	HIS	-	expression tag	UNP Q83467
D	90	HIS	-	expression tag	UNP Q83467
D	91	HIS	-	expression tag	UNP Q83467
D	92	HIS	-	expression tag	UNP Q83467
D	93	HIS	-	expression tag	UNP Q83467
D	94	SER	-	expression tag	UNP Q83467
D	95	SER	-	expression tag	UNP Q83467
D	96	GLY	-	expression tag	UNP Q83467
D	97	LEU	-	expression tag	UNP Q83467
D	98	VAL	-	expression tag	UNP Q83467
D	99	PRO	-	expression tag	UNP Q83467
D	100	ARG	-	expression tag	UNP Q83467
D	101	GLY	-	expression tag	UNP Q83467
D	102	SER	-	expression tag	UNP Q83467
D	103	HIS	-	expression tag	UNP Q83467
D	104	MET	-	expression tag	UNP Q83467
D	105	ALA	-	expression tag	UNP Q83467
D	106	SER	-	expression tag	UNP Q83467
D	107	MET	-	expression tag	UNP Q83467
D	108	THR	-	expression tag	UNP Q83467
D	109	GLY	-	expression tag	UNP Q83467
D	110	GLY	-	expression tag	UNP Q83467
D	111	GLN	-	expression tag	UNP Q83467
D	112	GLN	-	expression tag	UNP Q83467
D	113	GLY	-	expression tag	UNP Q83467
D	114	ARG	-	expression tag	UNP Q83467
D	115	ILE	-	expression tag	UNP Q83467
Е	84	MET	-	expression tag	UNP Q83467
Е	85	GLY	-	expression tag	UNP Q83467
Е	86	SER	_	expression tag	UNP Q83467
Е	87	SER	_	expression tag	UNP Q83467
Е	88	HIS	-	expression tag	UNP Q83467
Е	89	HIS	-	expression tag	UNP Q83467
Е	90	HIS	-	expression tag	UNP Q83467
Е	91	HIS	_	expression tag	UNP Q83467
Е	92	HIS	-	expression tag	UNP Q83467
Е	93	HIS		expression tag	UNP Q83467
Е	94	SER	-	expression tag	UNP Q83467
Е	95	SER	_	expression tag	UNP Q83467
Е	96	GLY	-	expression tag	UNP Q83467
Е	97	LEU	-	expression tag	UNP Q83467
Е	98	VAL	-	expression tag	UNP Q83467



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
Е	99	PRO	_	expression tag	UNP Q83467
Е	100	ARG	-	expression tag	UNP Q83467
Е	101	GLY	-	expression tag	UNP Q83467
Е	102	SER	-	expression tag	UNP Q83467
Е	103	HIS	-	expression tag	UNP Q83467
Е	104	MET	-	expression tag	UNP Q83467
Е	105	ALA	-	expression tag	UNP Q83467
Е	106	SER	-	expression tag	UNP Q83467
Е	107	MET	-	expression tag	UNP Q83467
Е	108	THR	-	expression tag	UNP Q83467
Е	109	GLY	-	expression tag	UNP Q83467
Е	110	GLY	-	expression tag	UNP Q83467
Е	111	GLN	-	expression tag	UNP Q83467
Е	112	GLN	-	expression tag	UNP Q83467
Е	113	GLY	-	expression tag	UNP Q83467
Е	114	ARG	-	expression tag	UNP Q83467
Е	115	ILE	-	expression tag	UNP Q83467
F	84	MET	-	expression tag	UNP Q83467
F	85	GLY	-	expression tag	UNP Q83467
F	86	SER	-	expression tag	UNP Q83467
F	87	SER	-	expression tag	UNP Q83467
F	88	HIS	-	expression tag	UNP Q83467
F	89	HIS	-	expression tag	UNP Q83467
F	90	HIS	-	expression tag	UNP Q83467
F	91	HIS	-	expression tag	UNP Q83467
F	92	HIS	-	expression tag	UNP Q83467
F	93	HIS	-	expression tag	UNP Q83467
F	94	SER	-	expression tag	UNP Q83467
F	95	SER	-	expression tag	UNP Q83467
F	96	GLY	-	expression tag	UNP Q83467
F	97	LEU	-	expression tag	UNP Q83467
F	98	VAL	-	expression tag	UNP Q83467
F	99	PRO	-	expression tag	UNP Q83467
F	100	ARG	-	expression tag	UNP Q83467
F	101	GLY	-	expression tag	UNP Q83467
F	102	SER	-	expression tag	UNP Q83467
F	103	HIS	-	expression tag	UNP Q83467
F	104	MET	-	expression tag	UNP Q83467
F	105	ALA	-	expression tag	UNP Q83467
F	106	SER	-	expression tag	UNP Q83467
F	107	MET	-	expression tag	UNP Q83467
F	108	THR	-	expression tag	UNP Q83467



Chain	Residue	Modelled	Actual	Comment	Reference
F	109	GLY	-	expression tag	UNP Q83467
F	110	GLY	-	expression tag	UNP Q83467
F	111	GLN	-	expression tag	UNP Q83467
F	112	GLN	-	expression tag	UNP Q83467
F	113	GLY	-	expression tag	UNP Q83467
F	114	ARG	-	expression tag	UNP Q83467
F	115	ILE	-	expression tag	UNP Q83467

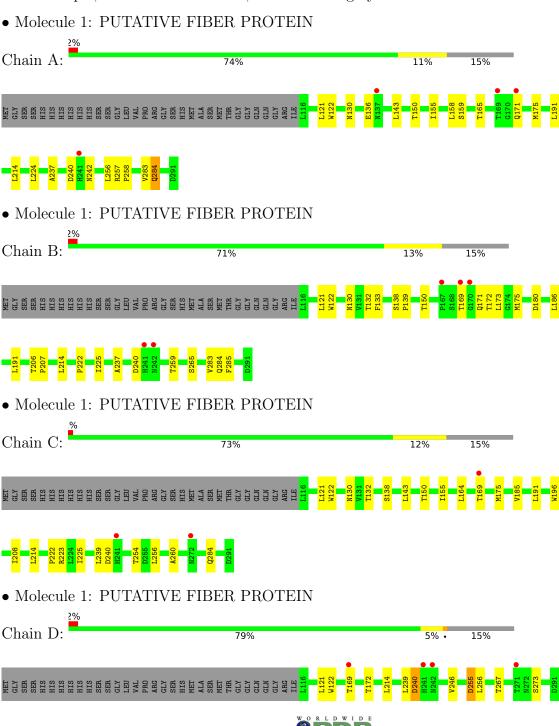
## • Molecule 2 is water.

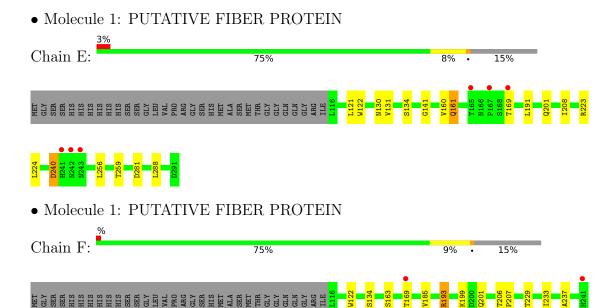
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	С	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0



# 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.









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	125.73Å 145.44Å 147.60Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	29.21 - 3.20	Depositor
Resolution (A)	28.93 - 3.19	EDS
% Data completeness	95.4 (29.21-3.20)	Depositor
(in resolution range)	93.7 (28.93-3.19)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.86 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
D.D.	0.173 , 0.201	Depositor
$R, R_{free}$	0.178 , $0.203$	DCC
$R_{free}$ test set	2026  reflections  (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.28 , 37.6	EDS
L-test for twinning <sup>2</sup>	$< L >=0.53, < L^2>=0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

## 5.1 Standard geometry (i)

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.46	0/1360	0.66	0/1861	
1	В	0.45	0/1360	0.65	0/1861	
1	С	0.45	0/1360	0.65	0/1861	
1	D	0.44	0/1360	0.62	0/1861	
1	Е	0.45	0/1360	0.64	0/1861	
1	F	0.48	0/1360	0.68	0/1861	
All	All	0.45	0/8160	0.65	0/11166	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ASN	Peptide

## 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	1330	0	1295	20	0
1	В	1330	0	1295	25	0
1	С	1330	0	1295	14	0
1	D	1330	0	1295	6	0
1	Е	1330	0	1295	11	0
1	F	1330	0	1295	10	0
2	A	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
All	All	7984	0	7770	74	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 5.

The worst 5 of 74 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:150:THR:CG2	1:B:150:THR:HG21	1.45	1.43
1:A:150:THR:HG23	1:B:150:THR:CG2	1.82	1.10
1:A:150:THR:CG2	1:B:150:THR:CG2	2.34	1.05
1:A:150:THR:HG23	1:B:150:THR:HG21	0.92	0.90
1:A:150:THR:HG21	1:C:150:THR:HB	1.64	0.77

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	Perce	ntiles
1	A	174/208~(84%)	163 (94%)	10 (6%)	1 (1%)	25	64
1	В	174/208 (84%)	158 (91%)	16 (9%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	С	174/208 (84%)	160 (92%)	13 (8%)	1 (1%)	25	64
1	D	174/208 (84%)	164 (94%)	9 (5%)	1 (1%)	25	64
1	E	174/208 (84%)	161 (92%)	12 (7%)	1 (1%)	25	64
1	F	174/208 (84%)	159 (91%)	15 (9%)	0	100	100
All	All	1044/1248 (84%)	965 (92%)	75 (7%)	4 (0%)	34	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	240	ASP
1	Е	240	ASP
1	A	240	ASP
1	С	240	ASP

#### 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	Rotameric Outliers	
1	A	150/175~(86%)	146 (97%)	4 (3%)	44 75
1	В	150/175 (86%)	144 (96%)	6 (4%)	31 66
1	С	150/175 (86%)	143 (95%)	7 (5%)	26 62
1	D	150/175 (86%)	145 (97%)	5 (3%)	38 71
1	E	150/175~(86%)	145 (97%)	5 (3%)	38 71
1	F	150/175 (86%)	146 (97%)	4 (3%)	44 75
All	All	900/1050 (86%)	869 (97%)	31 (3%)	37 70

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	222	PRO
1	F	122	TRP
1	D	122	TRP



Mol	Chain	Res	Type
1	F	193	ARG
1	Е	161	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

There are no ligands in this entry.

## 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,  $95^{th}$  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>	#RSF	RZ>	2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	176/208 (84%)	-0.49	4 (2%)	60	47	37, 57, 103, 119	0
1	В	176/208 (84%)	-0.39	5 (2%) 5	53	37	40, 67, 121, 142	0
1	С	176/208 (84%)	-0.56	3 (1%) 7	70	57	37, 56, 107, 123	0
1	D	176/208 (84%)	-0.43	4 (2%)	60	47	40, 67, 125, 144	0
1	E	176/208 (84%)	-0.45	6 (3%)	45	29	40, 60, 121, 141	0
1	F	176/208 (84%)	-0.62	3 (1%) 7	70	57	36, 53, 99, 112	0
All	All	1056/1248 (84%)	-0.49	25 (2%)	59	44	36, 59, 112, 144	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	169	THR	4.5
1	D	169	THR	3.8
1	Е	242	ASN	3.4
1	С	169	THR	3.4
1	Е	167	PRO	3.0

## 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)

There are no ligands in this entry.



# 6.5 Other polymers (i)

There are no such residues in this entry.

