



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:40 AM GMT

PDB ID : 3BQ4  
Title : Crystal Structure of Ad35 fiber knob  
Authors : Pache, L.; Venkataraman, S.; Nemerow, G.R.; Reddy, V.S.  
Deposited on : 2007-12-19  
Resolution : 2.70 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

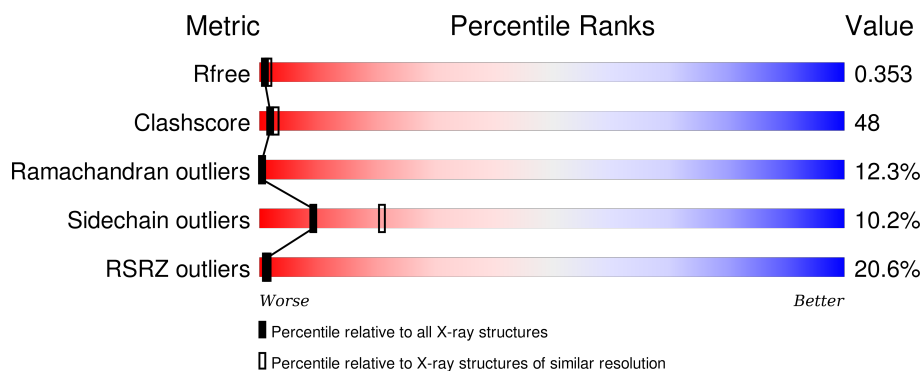
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	220	<div> <div>15%</div> <div>35%</div> <div>39%</div> <div>13%</div> <div>•</div> <div>13%</div> </div>
1	B	220	<div> <div>15%</div> <div>27%</div> <div>45%</div> <div>13%</div> <div>•</div> <div>13%</div> </div>
1	D	220	<div> <div>22%</div> <div>29%</div> <div>44%</div> <div>14%</div> <div>13%</div> </div>
1	E	220	<div> <div>16%</div> <div>32%</div> <div>40%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	F	220	<div> <div>18%</div> <div>34%</div> <div>39%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	220	<div><div></div><div></div><div></div><div></div><div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8976 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	B	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	D	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	E	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	F	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			
1	G	192	Total	C	N	O	S	0	0	0
			1496	944	240	305	7			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	-	EXPRESSION TAG	UNP Q7T925
A	105	SER	-	EXPRESSION TAG	UNP Q7T925
A	106	HIS	-	EXPRESSION TAG	UNP Q7T925
A	107	MET	-	EXPRESSION TAG	UNP Q7T925
A	108	ALA	-	EXPRESSION TAG	UNP Q7T925
A	109	SER	-	EXPRESSION TAG	UNP Q7T925
A	110	MET	-	EXPRESSION TAG	UNP Q7T925
A	111	THR	-	EXPRESSION TAG	UNP Q7T925
A	112	GLY	-	EXPRESSION TAG	UNP Q7T925
A	113	GLY	-	EXPRESSION TAG	UNP Q7T925
A	114	GLN	-	EXPRESSION TAG	UNP Q7T925
A	115	GLN	-	EXPRESSION TAG	UNP Q7T925
A	116	MET	-	EXPRESSION TAG	UNP Q7T925
A	117	GLY	-	EXPRESSION TAG	UNP Q7T925
A	118	ARG	-	EXPRESSION TAG	UNP Q7T925
A	119	GLY	-	EXPRESSION TAG	UNP Q7T925
A	120	SER	-	EXPRESSION TAG	UNP Q7T925

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLY	-	EXPRESSION TAG	UNP Q7T925
B	105	SER	-	EXPRESSION TAG	UNP Q7T925
B	106	HIS	-	EXPRESSION TAG	UNP Q7T925
B	107	MET	-	EXPRESSION TAG	UNP Q7T925
B	108	ALA	-	EXPRESSION TAG	UNP Q7T925
B	109	SER	-	EXPRESSION TAG	UNP Q7T925
B	110	MET	-	EXPRESSION TAG	UNP Q7T925
B	111	THR	-	EXPRESSION TAG	UNP Q7T925
B	112	GLY	-	EXPRESSION TAG	UNP Q7T925
B	113	GLY	-	EXPRESSION TAG	UNP Q7T925
B	114	GLN	-	EXPRESSION TAG	UNP Q7T925
B	115	GLN	-	EXPRESSION TAG	UNP Q7T925
B	116	MET	-	EXPRESSION TAG	UNP Q7T925
B	117	GLY	-	EXPRESSION TAG	UNP Q7T925
B	118	ARG	-	EXPRESSION TAG	UNP Q7T925
B	119	GLY	-	EXPRESSION TAG	UNP Q7T925
B	120	SER	-	EXPRESSION TAG	UNP Q7T925
D	104	GLY	-	EXPRESSION TAG	UNP Q7T925
D	105	SER	-	EXPRESSION TAG	UNP Q7T925
D	106	HIS	-	EXPRESSION TAG	UNP Q7T925
D	107	MET	-	EXPRESSION TAG	UNP Q7T925
D	108	ALA	-	EXPRESSION TAG	UNP Q7T925
D	109	SER	-	EXPRESSION TAG	UNP Q7T925
D	110	MET	-	EXPRESSION TAG	UNP Q7T925
D	111	THR	-	EXPRESSION TAG	UNP Q7T925
D	112	GLY	-	EXPRESSION TAG	UNP Q7T925
D	113	GLY	-	EXPRESSION TAG	UNP Q7T925
D	114	GLN	-	EXPRESSION TAG	UNP Q7T925
D	115	GLN	-	EXPRESSION TAG	UNP Q7T925
D	116	MET	-	EXPRESSION TAG	UNP Q7T925
D	117	GLY	-	EXPRESSION TAG	UNP Q7T925
D	118	ARG	-	EXPRESSION TAG	UNP Q7T925
D	119	GLY	-	EXPRESSION TAG	UNP Q7T925
D	120	SER	-	EXPRESSION TAG	UNP Q7T925
E	104	GLY	-	EXPRESSION TAG	UNP Q7T925
E	105	SER	-	EXPRESSION TAG	UNP Q7T925
E	106	HIS	-	EXPRESSION TAG	UNP Q7T925
E	107	MET	-	EXPRESSION TAG	UNP Q7T925
E	108	ALA	-	EXPRESSION TAG	UNP Q7T925
E	109	SER	-	EXPRESSION TAG	UNP Q7T925
E	110	MET	-	EXPRESSION TAG	UNP Q7T925
E	111	THR	-	EXPRESSION TAG	UNP Q7T925

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Chain	Residue	Modelled	Actual	Comment	Reference
E	112	GLY	-	EXPRESSION TAG	UNP Q7T925
E	113	GLY	-	EXPRESSION TAG	UNP Q7T925
E	114	GLN	-	EXPRESSION TAG	UNP Q7T925
E	115	GLN	-	EXPRESSION TAG	UNP Q7T925
E	116	MET	-	EXPRESSION TAG	UNP Q7T925
E	117	GLY	-	EXPRESSION TAG	UNP Q7T925
E	118	ARG	-	EXPRESSION TAG	UNP Q7T925
E	119	GLY	-	EXPRESSION TAG	UNP Q7T925
E	120	SER	-	EXPRESSION TAG	UNP Q7T925
F	104	GLY	-	EXPRESSION TAG	UNP Q7T925
F	105	SER	-	EXPRESSION TAG	UNP Q7T925
F	106	HIS	-	EXPRESSION TAG	UNP Q7T925
F	107	MET	-	EXPRESSION TAG	UNP Q7T925
F	108	ALA	-	EXPRESSION TAG	UNP Q7T925
F	109	SER	-	EXPRESSION TAG	UNP Q7T925
F	110	MET	-	EXPRESSION TAG	UNP Q7T925
F	111	THR	-	EXPRESSION TAG	UNP Q7T925
F	112	GLY	-	EXPRESSION TAG	UNP Q7T925
F	113	GLY	-	EXPRESSION TAG	UNP Q7T925
F	114	GLN	-	EXPRESSION TAG	UNP Q7T925
F	115	GLN	-	EXPRESSION TAG	UNP Q7T925
F	116	MET	-	EXPRESSION TAG	UNP Q7T925
F	117	GLY	-	EXPRESSION TAG	UNP Q7T925
F	118	ARG	-	EXPRESSION TAG	UNP Q7T925
F	119	GLY	-	EXPRESSION TAG	UNP Q7T925
F	120	SER	-	EXPRESSION TAG	UNP Q7T925
G	104	GLY	-	EXPRESSION TAG	UNP Q7T925
G	105	SER	-	EXPRESSION TAG	UNP Q7T925
G	106	HIS	-	EXPRESSION TAG	UNP Q7T925
G	107	MET	-	EXPRESSION TAG	UNP Q7T925
G	108	ALA	-	EXPRESSION TAG	UNP Q7T925
G	109	SER	-	EXPRESSION TAG	UNP Q7T925
G	110	MET	-	EXPRESSION TAG	UNP Q7T925
G	111	THR	-	EXPRESSION TAG	UNP Q7T925
G	112	GLY	-	EXPRESSION TAG	UNP Q7T925
G	113	GLY	-	EXPRESSION TAG	UNP Q7T925
G	114	GLN	-	EXPRESSION TAG	UNP Q7T925
G	115	GLN	-	EXPRESSION TAG	UNP Q7T925
G	116	MET	-	EXPRESSION TAG	UNP Q7T925
G	117	GLY	-	EXPRESSION TAG	UNP Q7T925
G	118	ARG	-	EXPRESSION TAG	UNP Q7T925
G	119	GLY	-	EXPRESSION TAG	UNP Q7T925

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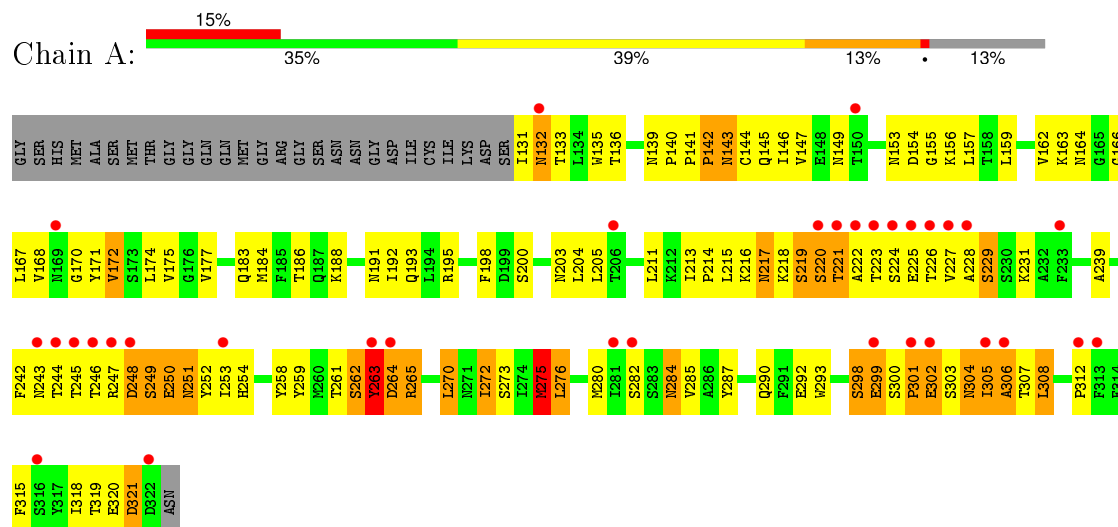
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Chain	Residue	Modelled	Actual	Comment	Reference
G	120	SER	-	EXPRESSION TAG	UNP Q7T925

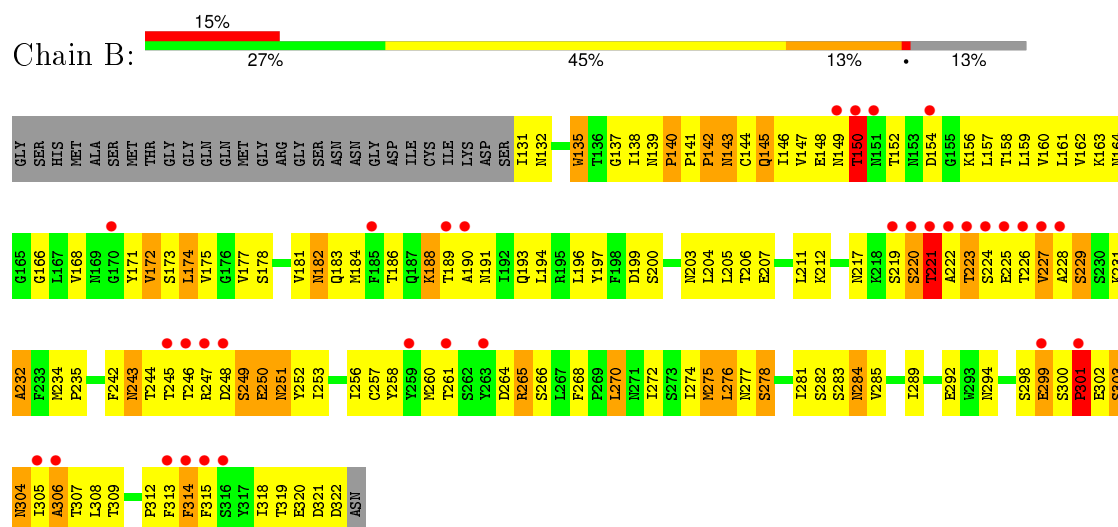
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Fiber



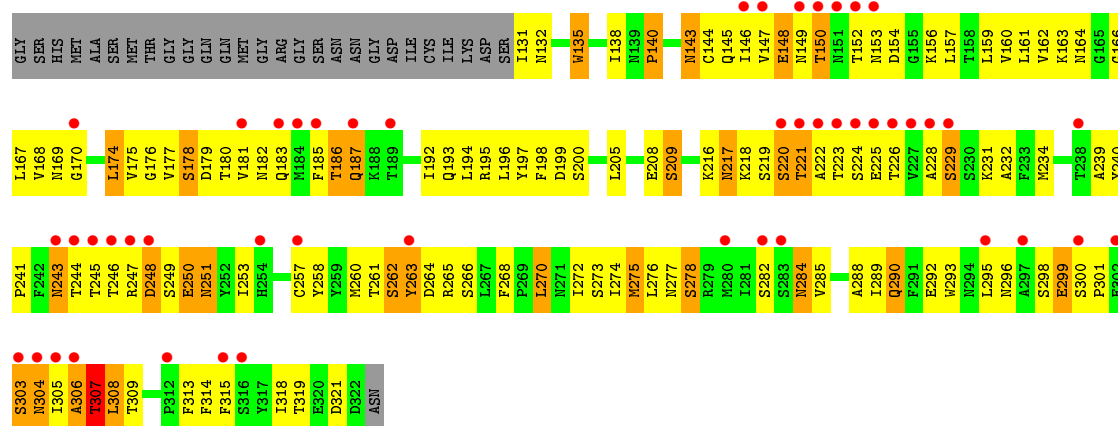
#### • Molecule 1: Fiber



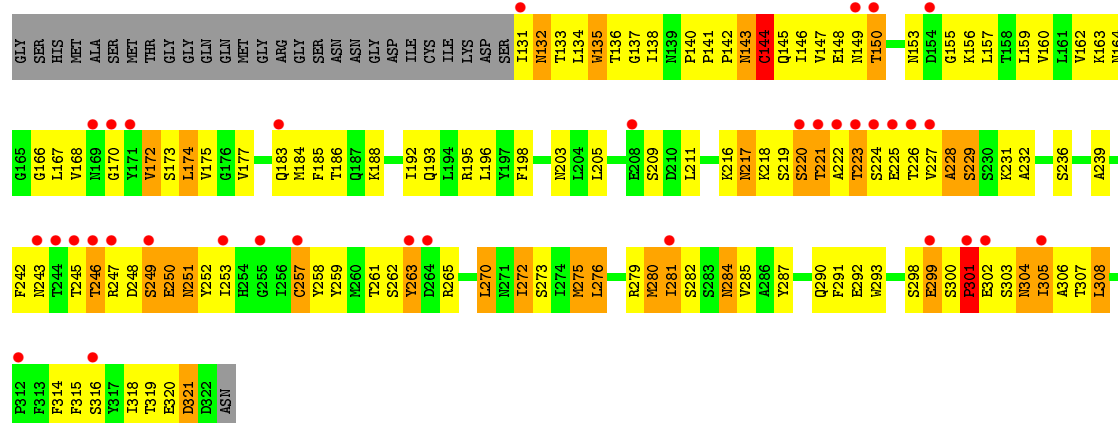
#### • Molecule 1: Fiber



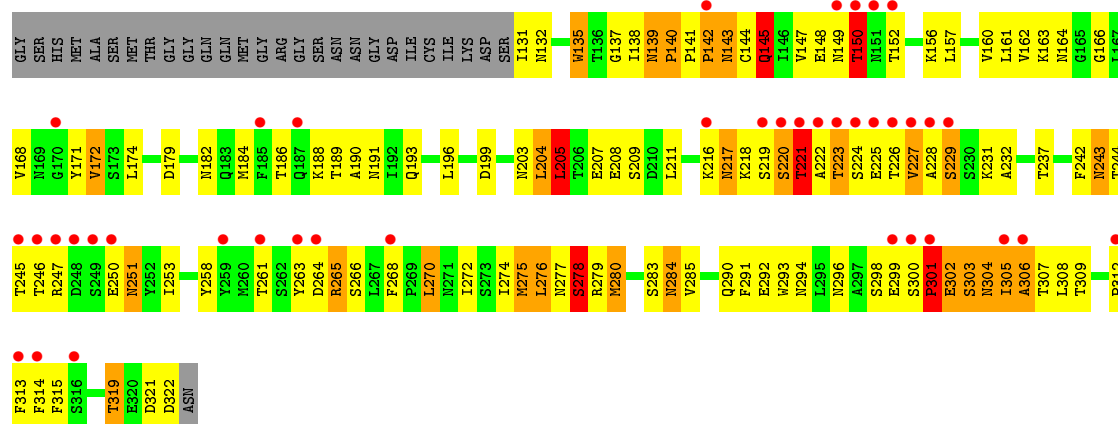




• Molecule 1: Fiber



• Molecule 1: Fiber



• Molecule 1: Fiber



T309	N243	G185	GLY
P312	T244	G166	SER
F313	T245	L167	HIS
F314	T246	V168	MET
F315	R247	N169	ALA
S316	D248	G170	SER
Y317	S249	Y171	MET
I318	E250	V172	THR
T319	N251	S173	GLY
E320	Y252	L174	GLY
E321	I253	V175	GLN
D321	H254	G176	GLN
D322	Y258	V177	MET
ASN	Y258	G177	GLY
	T261	V181	ARG
	S262	N182	GLY
	Y263	Q183	SER
	D264	M184	ASN
	R265	F185	ASN
	S266	T186	GLY
	L267	Q187	ASP
	F268	K188	ILE
	P269	T189	ILE
	L270		CYS
		Q193	ILE
		L194	LYS
		R195	ASP
	S273	L196	ASP
	I274	Y197	SER
	M275	F198	I131
	L276	D199	N132
	N277	S200	
	R279		W135
	M280		T136
	I281	L205	G137
	S282	T206	I138
	S283	E207	N139
	N284	F208	P140
	V285	S209	P141
			P142
			N143
	A288	K216	C144
	I289	N217	Q145
	Q290	K218	I146
	F291	S219	V147
	E292	S220	E148
		T221	N149
		A222	T150
	L295	T223	N151
	N296	S224	T152
	A297	E225	N153
	S298	T226	D154
	E299	V227	G155
	S300	A228	K156
	P301	S229	L157
	E302		T158
	S303	A232	L159
	N304		V160
	I305	A239	L161
	A306	Y240	V162
	T307	P241	K163
	L308	F242	N164

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.91Å 173.91Å 154.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.70 46.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (46.03-2.70) 91.5 (46.03-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.332 , 0.352 0.332 , 0.353	Depositor DCC
$R_{free}$ test set	2911 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 69.9	EDS
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57497 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/1527	0.80	1/2084 (0.0%)
1	B	0.48	0/1527	0.82	1/2084 (0.0%)
1	D	0.47	0/1527	0.75	1/2084 (0.0%)
1	E	0.50	1/1527 (0.1%)	0.80	1/2084 (0.0%)
1	F	0.49	0/1527	0.82	1/2084 (0.0%)
1	G	0.48	0/1527	0.75	1/2084 (0.0%)
All	All	0.49	1/9162 (0.0%)	0.79	6/12504 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	144	CYS	CB-SG	-6.08	1.72	1.82

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	THR	N-CA-C	-7.55	90.62	111.00
1	A	221	THR	N-CA-C	-7.17	91.64	111.00
1	G	221	THR	N-CA-C	-6.30	94.00	111.00
1	D	221	THR	N-CA-C	-6.18	94.31	111.00
1	B	221	THR	N-CA-C	-5.64	95.76	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1496	0	1453	153	1
1	B	1496	0	1453	154	0
1	D	1496	0	1453	160	0
1	E	1496	0	1453	149	1
1	F	1496	0	1453	133	0
1	G	1496	0	1453	150	0
All	All	8976	0	8718	840	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 48.

The worst 5 of 840 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:E:217:ASN:ND2	1:E:224:SER:H	1.57	1.00
1:D:261:THR:HG22	1:D:301:PRO:HG3	1.45	0.98
1:A:143:ASN:HD21	1:A:157:LEU:H	1.09	0.96
1:B:268:PHE:HE1	1:B:300:SER:HA	1.27	0.96
1:F:242:PHE:CE1	1:F:277:ASN:ND2	2.38	0.92

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)
1:A:186:THR:O	1:E:302:GLU:OE1[7_444]	2.08	0.12

## 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	190/220 (86%)	139 (73%)	29 (15%)	22 (12%)	0	0
1	B	190/220 (86%)	132 (70%)	31 (16%)	27 (14%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	190/220 (86%)	139 (73%)	30 (16%)	21 (11%)	0	0
1	E	190/220 (86%)	135 (71%)	32 (17%)	23 (12%)	0	0
1	F	190/220 (86%)	139 (73%)	28 (15%)	23 (12%)	0	0
1	G	190/220 (86%)	136 (72%)	30 (16%)	24 (13%)	0	0
All	All	1140/1320 (86%)	820 (72%)	180 (16%)	140 (12%)	0	0

5 of 140 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	SER
1	A	221	THR
1	A	248	ASP
1	A	250	GLU
1	A	304	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	175/196 (89%)	159 (91%)	16 (9%)	12	26
1	B	175/196 (89%)	159 (91%)	16 (9%)	12	26
1	D	175/196 (89%)	155 (89%)	20 (11%)	7	16
1	E	175/196 (89%)	156 (89%)	19 (11%)	8	18
1	F	175/196 (89%)	153 (87%)	22 (13%)	5	13
1	G	175/196 (89%)	161 (92%)	14 (8%)	15	33
All	All	1050/1176 (89%)	943 (90%)	107 (10%)	9	21

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	275	MET
1	E	188	LYS

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Mol	Chain	Res	Type
1	G	174	LEU
1	D	284	ASN
1	E	144	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	243	ASN
1	E	143	ASN
1	G	243	ASN
1	D	290	GLN
1	E	164	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](#)

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<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	192/220 (87%)	1.22	34 (17%)	2 1	34, 79, 108, 113	72 (37%)
1	B	192/220 (87%)	1.17	33 (17%)	2 1	41, 83, 108, 113	77 (40%)
1	D	192/220 (87%)	1.39	48 (25%)	1 1	51, 90, 108, 113	62 (32%)
1	E	192/220 (87%)	1.14	35 (18%)	2 1	42, 79, 108, 113	70 (36%)
1	F	192/220 (87%)	1.19	40 (20%)	1 1	42, 80, 108, 113	69 (35%)
1	G	192/220 (87%)	1.31	47 (24%)	1 1	55, 89, 108, 113	69 (35%)
All	All	1152/1320 (87%)	1.24	237 (20%)	1 1	34, 83, 108, 113	419 (36%)

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	GLU	22.0
1	F	246	THR	18.2
1	A	224	SER	14.0
1	E	225	GLU	13.3
1	D	228	ALA	12.8

### 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](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.