

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

#### Jan 7, 2024 – 12:26 pm GMT

PDB ID	:	6FXN
Title	:	Crystal structure of human BAFF in complex with Fab fragment of anti-BAFF
		antibody belimumab
Authors	:	Lammens, A.; Maskos, K.; Willen, L.; Jiang, X.; Schneider, P.
Deposited on	:	2018-03-09
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	А	164	84%	·	12%
1	В	164	% 85%	•	12%
1	С	164	% 85%	•	12%
1	J	164	86%	•	12%
1	K	164	% 87%	•	12%



Mol	Chain	Length	Quality of chain	
1	L	164	86%	• 12%
2	D	225	92%	•••
2	F	225	95%	•••
2	Н	225	% 92%	•••
2	М	225	93%	••
2	Ο	225	95%	• •
2	Q	225	92%	••
3	Е	214	97%	·
3	G	214	97%	
3	Ι	214	96%	••
3	Ν	214	97%	••
3	Р	214	96%	••
3	R	214	94%	



#### 6FXN

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26179 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	1.4.4	Total	С	Ν	0	$\mathbf{S}$	10	0	0
	A	144	1138	733	182	218	5	19	0	0
1	P	1.4.4	Total	С	Ν	0	S	25	0	0
	D	144	1138	733	182	218	5	2.5	0	0
1	С	144	Total	С	Ν	0	S	- 21	0	0
	U		1138	733	182	218	5	21	0	0
1	т	1.4.4	Total	С	Ν	0	S	20	0	0
	J	144	1138	733	182	218	5	20	0	0
1	K	1.4.4	Total	С	Ν	0	S	18	0	0
	Λ	144	1138	733	182	218	5	10	0	0
1	1 T	144	Total	С	Ν	0	S	20	0	0
		144	1138	733	182	218	5	00	0	U

• Molecule 1 is a protein called Tumor necrosis factor ligand superfamily member 13B.

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	122	MET	-	initiating methionine	UNP Q9Y275
А	123	ARG	-	expression tag	UNP Q9Y275
А	124	GLY	-	expression tag	UNP Q9Y275
А	125	SER	-	expression tag	UNP $Q9Y275$
А	126	HIS	-	expression tag	UNP $Q9Y275$
А	127	HIS	-	expression tag	UNP Q9Y275
А	128	HIS	-	expression tag	UNP Q9Y275
А	129	HIS	-	expression tag	UNP Q9Y275
А	130	HIS	-	expression tag	UNP Q9Y275
А	131	HIS	-	expression tag	UNP Q9Y275
А	132	GLY	-	expression tag	UNP Q9Y275
А	133	SER	-	expression tag	UNP Q9Y275
А	218	ALA	HIS	engineered mutation	UNP Q9Y275
В	122	MET	-	initiating methionine	UNP Q9Y275
В	123	ARG	-	expression tag	UNP Q9Y275
В	124	GLY	-	expression tag	UNP Q9Y275
В	125	SER	-	expression tag	UNP Q9Y275
				Continued	on next page

WORLDWIDE PROTEIN DATA BANK

Comment	Reference
expression tag	UNP Q9Y275
neered mutation	UNP Q9Y275
ating methionine	UNP Q9Y275
expression tag	UNP Q9Y275
expression tag	UNP Q9Y275

Continued from previous page...ChainResidueModelledActual

B         126         HIS         -         expression tag         UNP Q9Y275           B         127         HIS         -         expression tag         UNP Q9Y275           B         128         HIS         -         expression tag         UNP Q9Y275           B         129         HIS         -         expression tag         UNP Q9Y275           B         130         HIS         -         expression tag         UNP Q9Y275           B         131         HIS         -         expression tag         UNP Q9Y275           B         132         GLY         -         expression tag         UNP Q9Y275           C         122         MET         -         initiating methionine         UNP Q9Y275           C         123         ARG         -         expression tag         UNP Q9Y275           C         124         GLY         -         expression tag         UNP Q9Y275           C         124         GLY         -         expression tag         UNP Q9Y275           C         126         HIS         -         expression tag         UNP Q9Y275           C         126         HIS         -         expression tag						
B         127         IIIS         -         expression tag         UNP Q9Y275           B         128         IIIS         -         expression tag         UNP Q9Y275           B         129         HIS         -         expression tag         UNP Q9Y275           B         130         HIS         -         expression tag         UNP Q9Y275           B         131         HIS         -         expression tag         UNP Q9Y275           B         133         SER         -         expression tag         UNP Q9Y275           B         218         ALA         HIS         engineered mutation         UNP Q9Y275           C         123         ARG         -         expression tag         UNP Q9Y275           C         123         ARG         -         expression tag         UNP Q9Y275           C         124         GLY         -         expression tag         UNP Q9Y275           C         126         HIS         -         expression tag         UNP Q9Y275           C         127         HIS         -         expression tag         UNP Q9Y275           C         128         HIS         -         expression tag	В	126	HIS	-	expression tag	UNP Q9Y275
B         128         HIS         -         expression tag         UNP Q9Y275           B         130         HIS         -         expression tag         UNP Q9Y275           B         130         HIS         -         expression tag         UNP Q9Y275           B         131         HIS         -         expression tag         UNP Q9Y275           B         132         GLY         -         expression tag         UNP Q9Y275           B         133         SER         -         expression tag         UNP Q9Y275           C         122         MET         -         initiating methionine         UNP Q9Y275           C         123         ARG         -         expression tag         UNP Q9Y275           C         124         GLY         -         expression tag         UNP Q9Y275           C         126         HIS         -         expression tag         UNP Q9Y275           C         127         HIS         -         expression tag         UNP Q9Y275           C         128         HIS         -         expression tag         UNP Q9Y275           C         130         HIS         -         expression tag	В	127	HIS	_	expression tag	UNP Q9Y275
B         129         HIS         -         expression tag         UNP Q9Y275           B         130         HIS         -         expression tag         UNP Q9Y275           B         131         HIS         -         expression tag         UNP Q9Y275           B         132         GLY         -         expression tag         UNP Q9Y275           B         133         SER         -         expression tag         UNP Q9Y275           C         122         MET         -         initiating methionine         UNP Q9Y275           C         123         ARG         -         expression tag         UNP Q9Y275           C         124         GLY         -         expression tag         UNP Q9Y275           C         125         SER         -         expression tag         UNP Q9Y275           C         126         HIS         -         expression tag         UNP Q9Y275           C         128         HIS         -         expression tag         UNP Q9Y275           C         130         HIS         -         expression tag         UNP Q9Y275           C         131         HIS         -         expression tag	В	128	HIS	-	expression tag	UNP Q9Y275
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	С	123	ARG	-	expression tag	UNP Q9Y275
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	С	124	GLY	-	expression tag	UNP Q9Y275
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	С	125	SER	-	expression tag	UNP Q9Y275
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	С	126	HIS	-	expression tag	UNP Q9Y275
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J124 $\operatorname{GLY}$ -expression tagUNP Q9Y275J125SER-expression tagUNP Q9Y275J126HIS-expression tagUNP Q9Y275J127HIS-expression tagUNP Q9Y275J128HIS-expression tagUNP Q9Y275J129HIS-expression tagUNP Q9Y275J130HIS-expression tagUNP Q9Y275J131HIS-expression tagUNP Q9Y275J132GLY-expression tagUNP Q9Y275J133SER-expression tagUNP Q9Y275J133SER-expression tagUNP Q9Y275K122MET-initiating methionineUNP Q9Y275K123ARG-expression tagUNP Q9Y275K126HIS-expression tagUNP Q9Y275K126HIS-expression tagUNP Q9Y275K126HIS-expression tagUNP Q9Y275K127HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275K128	J	123	ARG	-	expression tag	UNP Q9Y275
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K124GLY-expression tagUNP Q9Y275K125SER-expression tagUNP Q9Y275K126HIS-expression tagUNP Q9Y275K127HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275	K	123	ARG	-	expression tag	UNP Q9Y275
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K126HIS-expression tagUNP Q9Y275K127HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275	K	125	SER	-	expression tag	UNP Q9Y275
K127HIS-expression tagUNP Q9Y275K128HIS-expression tagUNP Q9Y275	K	126	HIS	-	expression tag	UNP Q9Y275
K     128     HIS     -     expression tag     UNP Q9Y275	K	127	HIS	-	expression tag	UNP Q9Y275
	K	128	HIS	-	expression tag	UNP Q9Y275



Chain	Residue	Modelled	Actual	Comment	Reference
K	129	HIS	-	expression tag	UNP Q9Y275
K	130	HIS	-	expression tag	UNP Q9Y275
K	131	HIS	-	expression tag	UNP Q9Y275
K	132	GLY	-	expression tag	UNP Q9Y275
K	133	SER	-	expression tag	UNP Q9Y275
K	218	ALA	HIS	engineered mutation	UNP Q9Y275
L	122	MET	-	initiating methionine	UNP Q9Y275
L	123	ARG	-	expression tag	UNP Q9Y275
L	124	GLY	-	expression tag	UNP Q9Y275
L	125	SER	-	expression tag	UNP Q9Y275
L	126	HIS	-	expression tag	UNP Q9Y275
L	127	HIS	-	expression tag	UNP Q9Y275
L	128	HIS	-	expression tag	UNP $Q9Y275$
L	129	HIS	-	expression tag	UNP Q9Y275
L	130	HIS	-	expression tag	UNP Q9Y275
L	131	HIS	-	expression tag	UNP Q9Y275
L	132	GLY	-	expression tag	UNP Q9Y275
L	133	SER	-	expression tag	UNP Q9Y275
L	218	ALA	HIS	engineered mutation	UNP Q9Y275

• Molecule 2 is a protein called belimumab heavy chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
9	Л	215	Total	С	Ν	Ο	S	71	0	0
	D	210	1599	1003	277	311	8	11	0	0
9	F	220	Total	С	Ν	0	S	35	1	0
	T,	220	1635	1025	283	318	9		I	0
9	Ц	216	Total	С	Ν	0	S	18	1	0
	11	210	1614	1014	279	312	9	40	I	0
9	М	215	Total	С	Ν	Ο	S	20	0	0
	111	210	1597	1003	276	310	8	29	0	0
0	0	215	Total	С	Ν	0	S	40	0	0
	0	210	1600	1005	277	310	8	49	0	0
0	0	915	Total	С	Ν	0	S	20	1	0
	215	1605	1008	277	311	9	30	1	U	

• Molecule 3 is a protein called belimumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	209	Total 1567	C 975	N 266	0 322	$\frac{S}{4}$	41	0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	С	210	Total	С	Ν	0	S	20	0	0
5	3 G	210	1573	978	267	324	4	20	0	U
2	Т	210	Total	С	Ν	0	S	23	0	0
3	1	210	1573	978	267	324	4	20	0	
2	N	210	Total	С	Ν	0	S	27	0	0
5	11	210	1573	978	267	324	4	21		
2	D	210	Total	С	Ν	0	$\mathbf{S}$	20	0	0
3	1	210	1573	978	267	324	4	59		0
2	В	200	Total	С	Ν	0	S	20	1	0
0	1	209	1572	977	267	324	4	20	1	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	8	Total O 8 8	0	0
4	В	11	Total         O           11         11	0	0
4	С	13	Total O 13 13	0	0
4	D	9	Total O 9 9	0	0
4	Е	4	Total O 4 4	0	0
4	F	25	TotalO2525	0	0
4	G	22	Total O 22 22	0	0
4	Н	19	Total         O           19         19	0	0
4	Ι	20	TotalO2020	0	0
4	J	19	Total O 19 19	0	0
4	K	19	Total         O           19         19	0	0
4	L	8	Total O 8 8	0	0
4	М	17	Total         O           17         17	0	0
4	Ν	19	Total         O           19         19	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	О	9	Total O 9 9	0	0
4	Р	12	Total         O           12         12	0	0
4	Q	20	TotalO2020	0	0
4	R	16	Total         O           16         16	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: Tumor necrosis factor ligand superfamily member 13B



• Molecule 1: Tumor necrosis factor ligand superfamily member 13B



Chain L:	86%	• 12%
MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY GLY GLY CLN CLU CLU CLU CLU CLU CLU CLU CLU CLU	C232	
• Molecule 2: belimumab heav	y chain	
Chain D:	92%	
01 R67 R67 176 183 1887 133 133 104 133 133 104 133 133 133 133 133 133 133 13	GLY GLY 1145 1145 1146 1188 1188 1188 1206 1206 1206 1206 128 222 288 288	
• Molecule 2: belimumab heav	y chain	
Chain F:	95%	
GLM <b>Y2</b> <b>R19</b> M63 M63 M18 M18 M18 M18 M18 M18 M18 M18	8197 K224 SER	
• Molecule 2: belimumab heav	y chain	
Chain H:	92%	• •
CLN V2 N38 N48 N48 N48 N48 N48 N48 SER SER SER SER SER SER SER SER SER SER	SER 4 8196 SER 4 SER 4	
• Molecule 2: belimumab heav	y chain	
Chain M:	93%	• •
GLN V2 R38 R38 R38 88 88 S80 S80 S80 S80 S88 S84 S88 S84 S88 CLY GLY GLY GLY CLY	P229 LYS SER	
• Molecule 2: belimumab heav	y chain	
Chain O:	95%	
01 122 122 122 127 127 127 113 1145 017 1145 017 1145 0206 0206 0206 0206 0208		
• Molecule 2: belimumab heav	y chain	
Chain Q:	92%	• •
GLN V2 N63 N63 N63 N63 N63 N63 S135 S135 S135 S135 S135 S135 S135 S13	8196 206 7206 7219 172 8ER	



• Molecule 3: belimumab light chain Chain E: 97% SER • Molecule 3: belimumab light chain Chain G: •• 97% SER GLU • Molecule 3: belimumab light chain Chain I: 96% • • GLU CYS SER SEI • Molecule 3: belimumab light chain Chain N: •• 97% GLU CYS SER SER • Molecule 3: belimumab light chain Chain P: 96% SER GLU • Molecule 3: belimumab light chain Chain R: 94% . .





## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	135.69Å 135.50Å 138.18Å	Deneriten	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $91.88^{\circ}$ $90.00^{\circ}$	Depositor	
$\mathbf{P}_{\text{acclution}}\left(\hat{\boldsymbol{\lambda}}\right)$	138.11 - 2.90	Depositor	
Resolution (A)	47.61 - 2.90	EDS	
% Data completeness	99.0 (138.11-2.90)	Depositor	
(in resolution range)	$99.1 \ (47.61 - 2.90)$	EDS	
R <sub>merge</sub>	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.15 (at 2.91 \text{\AA})$	Xtriage	
Refinement program	REFMAC	Depositor	
D D	0.191 , 0.231	Depositor	
$\mathbf{n},  \mathbf{n}_{free}$	0.195 , $0.235$	DCC	
$R_{free}$ test set	654 reflections $(0.60%)$	wwPDB-VP	
Wilson B-factor $(Å^2)$	53.9	Xtriage	
Anisotropy	0.085	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 38.6	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage	
	0.003 for l,k,-h		
	0.017 for -h,-l,-k		
	0.005 for -h,l,k		
	0.009 for k,h,-l		
	0.010 for -k,-h,-l		
Estimated twinning fraction	0.023 for l,h,k	Xtriage	
Ŭ	0.019 for k,l,h	Ŭ	
	0.013 for -lh.k		
	0.016 for -kl.h		
	0.039 for hkl		
	0.017 for lk.h		
$F_o, F_c$ correlation	0.93	EDS	
Total number of atoms	26179	wwPDB-VP	
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<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		Bo	nd lengths	Bond angles		
	Ullaili	$\begin{array}{c c c c c c c c c c c c c c c c c c c $		RMSZ	# Z  > 5	
1	А	0.58	1/1159~(0.1%)	0.82	2/1566~(0.1%)	
1	В	0.55	0/1159	0.78	0/1566	
1	С	0.55	0/1159	0.79	1/1566~(0.1%)	
1	J	0.53	0/1159	0.79	0/1566	
1	Κ	0.53	0/1159	0.77	0/1566	
1	L	0.59	1/1159~(0.1%)	0.78	1/1566~(0.1%)	
2	D	0.62	1/1635~(0.1%)	0.81	6/2225~(0.3%)	
2	F	0.54	0/1672	0.79	3/2274~(0.1%)	
2	Н	0.56	1/1651~(0.1%)	0.75	0/2246	
2	М	0.56	0/1634	0.75	0/2225	
2	0	0.59	0/1637	0.75	0/2229	
2	Q	0.54	0/1642	0.74	1/2235~(0.0%)	
3	Е	0.55	0/1605	0.70	0/2193	
3	G	0.56	0/1611	0.72	1/2201~(0.0%)	
3	Ι	0.55	0/1611	0.70	0/2201	
3	Ν	0.56	1/1611~(0.1%)	0.74	0/2201	
3	Р	0.58	0/1611	0.71	0/2201	
3	R	0.55	0/1610	0.75	1/2199~(0.0%)	
All	All	0.56	5/26484~(0.0%)	0.75	$16/\overline{36026}~(0.0\%)$	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	Ν	191	ARG	NE-CZ	6.29	1.41	1.33
2	D	83	LEU	CG-CD1	-5.95	1.29	1.51
1	А	215	LYS	CG-CD	-5.68	1.33	1.52
1	L	142	VAL	CB-CG1	5.51	1.64	1.52
2	Н	153	LYS	CD-CE	5.43	1.64	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	83	LEU	CB-CG-CD1	10.27	128.45	111.00



6FXN
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	19	ARG	NE-CZ-NH2	7.01	123.81	120.30
2	D	87	ARG	NE-CZ-NH2	6.63	123.61	120.30
2	D	83	LEU	CB-CG-CD2	-6.25	100.37	111.00
1	L	142	VAL	CA-CB-CG2	6.07	120.00	110.90
2	F	19	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	А	215	LYS	CB-CG-CD	5.62	126.22	111.60
2	D	67	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	D	87	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	D	188	LEU	CA-CB-CG	5.53	128.01	115.30
3	G	211	THR	CA-CB-CG2	-5.49	104.71	112.40
1	С	231	ARG	NE-CZ-NH1	5.41	123.00	120.30
2	Q	67	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	А	231	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	F	19	ARG	CD-NE-CZ	5.03	130.64	123.60
3	R	91	ASP	CB-CG-OD1	5.02	122.82	118.30

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	А	1138	0	1143	1	0
1	В	1138	0	1143	1	0
1	С	1138	0	1143	0	0
1	J	1138	0	1143	0	0
1	K	1138	0	1143	0	0
1	L	1138	0	1143	0	0
2	D	1599	0	1577	2	0
2	F	1635	0	1612	1	0
2	Н	1614	0	1594	3	0
2	М	1597	0	1573	1	0
2	0	1600	0	1579	0	0
2	Q	1605	0	1581	1	0
3	Е	1567	0	1499	0	0
3	G	1573	0	1504	0	0



6FXN
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Ι	1573	0	1504	0	0
3	Ν	1573	0	1504	0	0
3	Р	1573	0	1504	1	0
3	R	1572	0	1501	1	0
4	А	8	0	0	0	0
4	В	11	0	0	0	0
4	С	13	0	0	0	0
4	D	9	0	0	0	0
4	Ε	4	0	0	0	0
4	F	25	0	0	0	0
4	G	22	0	0	0	0
4	Н	19	0	0	0	0
4	Ι	20	0	0	0	0
4	J	19	0	0	0	0
4	Κ	19	0	0	0	0
4	L	8	0	0	0	0
4	М	17	0	0	0	0
4	Ν	19	0	0	0	0
4	0	9	0	0	0	0
4	Р	12	0	0	0	0
4	Q	20	0	0	0	0
4	R	16	0	0	0	0
All	All	26179	0	25390	11	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 0.

All (11) 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)
2:Q:145:THR:N	2:Q:196:SER:HG	1.99	0.59
2:H:38:ARG:HB3	2:H:48:MET:CE	2.32	0.58
1:A:233:ILE:HD13	2:D:104:LEU:HD23	1.87	0.57
2:H:145:THR:N	2:H:196:SER:HG	2.08	0.52
2:H:38:ARG:HB3	2:H:48:MET:HE1	1.93	0.49
2:M:38:ARG:HB3	2:M:48:MET:HE1	1.94	0.48
3:R:12:VAL:CG2	3:R:105:LEU:HD11	2.48	0.43
2:F:118[A]:MET:HE2	2:F:118[A]:MET:HB2	1.85	0.42
1:B:195:ILE:HD11	1:B:253:LEU:HD11	2.02	0.41
2:D:73:ASP:HB3	2:D:76:THR:HG22	2.01	0.41
3:P:157:VAL:HG11	3:P:180:LEU:HD11	2.04	0.40



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	А	142/164~(87%)	140 (99%)	2(1%)	0	100	100
1	В	142/164~(87%)	139~(98%)	3~(2%)	0	100	100
1	С	142/164~(87%)	140 (99%)	2(1%)	0	100	100
1	J	142/164~(87%)	141 (99%)	1 (1%)	0	100	100
1	К	142/164 (87%)	140 (99%)	2 (1%)	0	100	100
1	L	142/164~(87%)	139 (98%)	3 (2%)	0	100	100
2	D	211/225 (94%)	200 (95%)	11 (5%)	0	100	100
2	F	217/225~(96%)	207~(95%)	10 (5%)	0	100	100
2	Н	213/225~(95%)	206 (97%)	7 (3%)	0	100	100
2	М	211/225 (94%)	205 (97%)	6 (3%)	0	100	100
2	Ο	211/225 (94%)	199 (94%)	12 (6%)	0	100	100
2	Q	212/225~(94%)	204 (96%)	8 (4%)	0	100	100
3	Е	207/214~(97%)	197 (95%)	9 (4%)	1 (0%)	29	61
3	G	208/214~(97%)	203 (98%)	5 (2%)	0	100	100
3	Ι	208/214~(97%)	200 (96%)	7 (3%)	1 (0%)	29	61
3	Ν	208/214~(97%)	200 (96%)	7 (3%)	1 (0%)	29	61
3	Р	208/214 (97%)	202 (97%)	5 (2%)	1 (0%)	29	61
3	R	208/214 (97%)	203 (98%)	4 (2%)	1 (0%)	29	61
All	All	3374/3618~(93%)	3265 (97%)	104 (3%)	5 (0%)	51	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type		
3	Р	67	GLY		
Continued on next nage					



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	U	1	1 0
Mol	Chain	$\mathbf{Res}$	Type
3	Е	67	GLY
3	R	67	GLY
3	Ι	158	LYS
3	Ν	67	GLY

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	125/141~(89%)	122~(98%)	3~(2%)	49	79
1	В	125/141~(89%)	122 (98%)	3 (2%)	49	79
1	С	125/141~(89%)	121~(97%)	4(3%)	39	73
1	J	125/141~(89%)	122 (98%)	3~(2%)	49	79
1	Κ	125/141~(89%)	124~(99%)	1 (1%)	81	94
1	L	125/141~(89%)	123~(98%)	2(2%)	62	86
2	D	179/187~(96%)	176~(98%)	3(2%)	60	86
2	F	183/187~(98%)	177 (97%)	6 (3%)	38	72
2	Н	181/187~(97%)	177 (98%)	4 (2%)	52	81
2	М	179/187~(96%)	176 (98%)	3 (2%)	60	86
2	Ο	179/187~(96%)	177~(99%)	2(1%)	73	92
2	Q	180/187~(96%)	174 (97%)	6 (3%)	38	72
3	Ε	174/179~(97%)	174 (100%)	0	100	100
3	G	175/179~(98%)	174 (99%)	1 (1%)	86	96
3	Ι	175/179~(98%)	171 (98%)	4 (2%)	50	80
3	Ν	175/179~(98%)	174 (99%)	1 (1%)	86	96
3	Р	175/179~(98%)	174 (99%)	1 (1%)	86	96
3	R	175/179~(98%)	171 (98%)	4 (2%)	50	80
All	All	2880/3042~(95%)	2829 (98%)	51 (2%)	60	85

All (51) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	180	GLU
1	А	217	VAL
1	А	232	CYS
1	В	153	SER
1	В	230	PHE
1	В	232	CYS
1	С	183	ASN
1	С	211	LEU
1	С	232	CYS
1	С	234	GLN
2	D	76	THR
2	D	188	LEU
2	D	206	CYS
2	F	63	ASN
2	F	80	SER
2	F	118[A]	MET
2	F	118[B]	MET
2	F	126	THR
2	F	163	SER
3	G	89	SER
2	Н	80	SER
2	Н	81	MET
2	Н	196	SER
2	Н	206	CYS
3	Ι	59	ASP
3	Ι	124	SER
3	Ι	147	THR
3	Ι	192	SER
1	J	146	CYS
1	J	217	VAL
1	J	232	CYS
1	K	232	CYS
1	L	143	THR
1	L	232	CYS
2	М	80	SER
2	М	84	SER
2	М	188	LEU
3	N	116	SER
2	Ο	122	SER
2	0	206	CYS
3	Р	96	HIS
2	Q	63	ASN
2	Q	76	THR



3

3

3

Continued from previous page						
Mol	Chain	Res	Type			
2	Q	80	SER			
2	Q	196	SER			
2	Q	206	CYS			
2	Q	219	LYS			
3	R	11	SER			

12

59

116

VAL

ASP

SER

R

R

R

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	234	GLN
1	Κ	234	GLN

#### 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	$Q{<}0.9$
1	А	144/164~(87%)	-0.19	0 100 100	30, 43, 69, 114	9~(6%)
1	В	144/164~(87%)	-0.16	1 (0%) 87 87	29,  45,  72,  94	10 (6%)
1	С	144/164~(87%)	-0.20	1 (0%) 87 87	29, 44, 68, 101	9~(6%)
1	J	144/164~(87%)	-0.27	0 100 100	29,  43,  66,  85	11 (7%)
1	Κ	144/164~(87%)	-0.25	1 (0%) 87 87	30, 42, 67, 86	9~(6%)
1	L	144/164~(87%)	-0.19	0 100 100	32, 47, 77, 115	13 (9%)
2	D	215/225~(95%)	-0.00	3 (1%) 75 75	40, 81, 108, 119	33 (15%)
2	F	220/225~(97%)	-0.17	3 (1%) 75 75	35, 53, 104, 127	16 (7%)
2	Н	216/225~(96%)	-0.12	2 (0%) 84 84	34, 63, 107, 117	18 (8%)
2	М	215/225~(95%)	-0.27	0 100 100	34, 57, 87, 106	11 (5%)
2	Ο	215/225~(95%)	-0.01	1 (0%) 91 91	41, 78, 106, 125	22 (10%)
2	Q	215/225~(95%)	-0.20	1 (0%) 91 91	30, 56, 91, 112	14 (6%)
3	Е	209/214~(97%)	-0.06	1 (0%) 91 91	42, 69, 102, 127	16 (7%)
3	G	210/214~(98%)	-0.25	0 100 100	33, 52, 77, 98	8 (3%)
3	Ι	210/214~(98%)	-0.12	0 100 100	36, 55, 74, 103	9 (4%)
3	N	210/214~(98%)	-0.24	0 100 100	36, 53, 72, 87	11 (5%)
3	Р	210/214 (98%)	0.00	3 (1%) 75 75	42, 69, 99, 130	15 (7%)
3	R	209/214~(97%)	-0.24	0 100 100	33, 56, 77, 87	7 (3%)
All	All	3418/3618 (94%)	-0.16	17 (0%) 91 91	29, 56, 96, 130	241 (7%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	141	THR	4.2
1	Κ	232	CYS	2.8
2	Н	75	SER	2.6



Mol	Chain	Res	Type	RSRZ
2	F	143	GLY	2.6
3	Р	159	ALA	2.5
2	F	197	SER	2.5
3	Р	157	VAL	2.5
3	Р	158	LYS	2.4
2	Н	197	SER	2.3
2	0	200	GLY	2.3
2	D	131	VAL	2.2
1	С	232	CYS	2.2
1	В	232	CYS	2.2
3	Ε	154	SER	2.1
2	D	171	SER	2.1
2	D	132	PHE	2.1
2	Q	135	ALA	2.0

## 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.

