



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 12:01 am BST

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](mailto: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 ⓘ 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

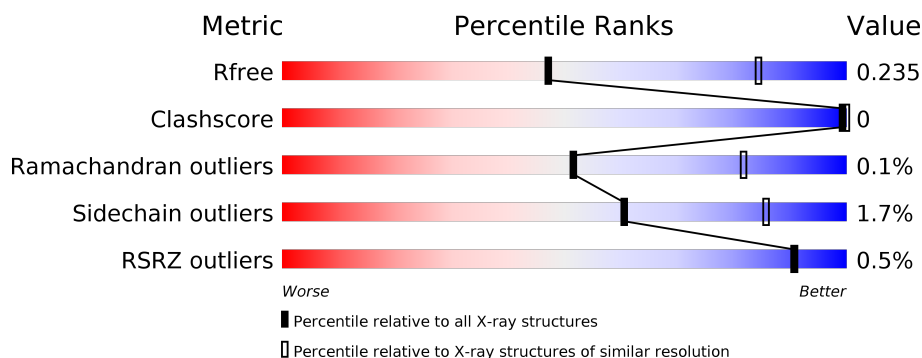
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	164	<div> <div>84%</div> <div>12%</div> </div>
1	B	164	<div> <div>85%</div> <div>12%</div> </div>
1	C	164	<div> <div>85%</div> <div>12%</div> </div>
1	J	164	<div> <div>86%</div> <div>12%</div> </div>
1	K	164	<div> <div>87%</div> <div>12%</div> </div>
1	L	164	<div> <div>86%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	225	<div> <div>%</div> <div> </div> <div>92%</div> <div>..</div> </div>
2	F	225	<div> <div>%</div> <div> </div> <div>95%</div> <div>..</div> </div>
2	H	225	<div> <div>%</div> <div> </div> <div>92%</div> <div>..</div> </div>
2	M	225	<div> <div> </div> <div>93%</div> <div>..</div> </div>
2	O	225	<div> <div> </div> <div>95%</div> <div>..</div> </div>
2	Q	225	<div> <div> </div> <div>92%</div> <div>..</div> </div>
3	E	214	<div> <div> </div> <div>97%</div> <div>.</div> </div>
3	G	214	<div> <div> </div> <div>97%</div> <div>..</div> </div>
3	I	214	<div> <div> </div> <div>96%</div> <div>..</div> </div>
3	N	214	<div> <div> </div> <div>97%</div> <div>..</div> </div>
3	P	214	<div> <div>%</div> <div> </div> <div>96%</div> <div>..</div> </div>
3	R	214	<div> <div> </div> <div>94%</div> <div>..</div> </div>

## 2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	19	0	0
			1138	733	182	218	5			
1	B	144	Total	C	N	O	S	25	0	0
			1138	733	182	218	5			
1	C	144	Total	C	N	O	S	21	0	0
			1138	733	182	218	5			
1	J	144	Total	C	N	O	S	28	0	0
			1138	733	182	218	5			
1	K	144	Total	C	N	O	S	18	0	0
			1138	733	182	218	5			
1	L	144	Total	C	N	O	S	30	0	0
			1138	733	182	218	5			

There are 78 discrepancies between the modelled and reference sequences:

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

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

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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	Atoms					ZeroOcc	AltConf	Trace
2	D	215	Total	C	N	O	S	71	0	0
			1599	1003	277	311	8			
2	F	220	Total	C	N	O	S	35	1	0
			1635	1025	283	318	9			
2	H	216	Total	C	N	O	S	48	1	0
			1614	1014	279	312	9			
2	M	215	Total	C	N	O	S	29	0	0
			1597	1003	276	310	8			
2	O	215	Total	C	N	O	S	49	0	0
			1600	1005	277	310	8			
2	Q	215	Total	C	N	O	S	30	1	0
			1605	1008	277	311	9			

- Molecule 3 is a protein called belimumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	209	Total	C	N	O	S	41	0	0
			1567	975	266	322	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	210	Total	C	N	O	S	20	0	0
			1573	978	267	324	4			
3	I	210	Total	C	N	O	S	23	0	0
			1573	978	267	324	4			
3	N	210	Total	C	N	O	S	27	0	0
			1573	978	267	324	4			
3	P	210	Total	C	N	O	S	39	0	0
			1573	978	267	324	4			
3	R	209	Total	C	N	O	S	20	1	0
			1572	977	267	324	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	11	Total	O	0	0
			11	11		
4	C	13	Total	O	0	0
			13	13		
4	D	9	Total	O	0	0
			9	9		
4	E	4	Total	O	0	0
			4	4		
4	F	25	Total	O	0	0
			25	25		
4	G	22	Total	O	0	0
			22	22		
4	H	19	Total	O	0	0
			19	19		
4	I	20	Total	O	0	0
			20	20		
4	J	19	Total	O	0	0
			19	19		
4	K	19	Total	O	0	0
			19	19		
4	L	8	Total	O	0	0
			8	8		
4	M	17	Total	O	0	0
			17	17		
4	N	19	Total	O	0	0
			19	19		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	9	Total 9	O 9	0	0
4	P	12	Total 12	O 12	0	0
4	Q	20	Total 20	O 20	0	0
4	R	16	Total 16	O 16	0	0

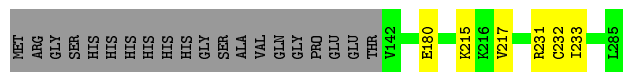


### 3 Residue-property plots [i](#)


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.

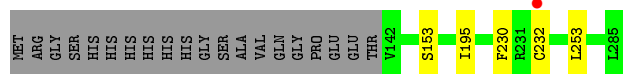
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A: 




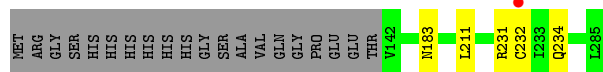
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain B: 




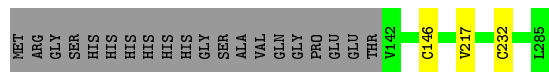
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain C: 




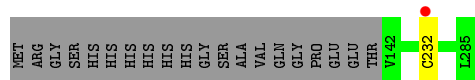
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain J: 




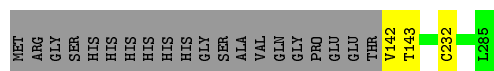
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain K: 




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

Chain L:  86% 12%



• Molecule 2: belimumab heavy chain

Chain D:  92%




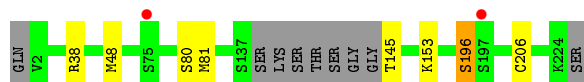
• Molecule 2: belimumab heavy chain

Chain F:  95%



• Molecule 2: belimumab heavy chain

Chain H:  92%



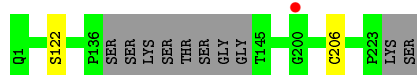
• Molecule 2: belimumab heavy chain

Chain M:  93%



• Molecule 2: belimumab heavy chain

Chain O:  95%



• Molecule 2: belimumab heavy chain

Chain Q:  92%



- Molecule 3: belimumab light chain

Chain E:  97% .



- Molecule 3: belimumab light chain

Chain G:  97% ..



- Molecule 3: belimumab light chain

Chain I:  96% ..



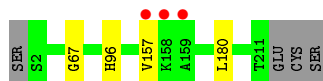
- Molecule 3: belimumab light chain

Chain N:  97% ..



- Molecule 3: belimumab light chain

Chain P:  96% ..



- Molecule 3: belimumab light chain

Chain R:  94% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.69Å 135.50Å 138.18Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	138.11 – 2.90 47.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (138.11-2.90) 99.1 (47.61-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.231 0.195 , 0.235	Depositor DCC
$R_{free}$ test set	654 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	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 0.023 for l,h,k 0.019 for k,l,h 0.013 for -l,-h,k 0.016 for -k,-l,h 0.039 for h,-k,-l 0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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>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

### 5.1 Standard geometry

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	0.58	1/1159 (0.1%)	0.82	2/1566 (0.1%)
1	B	0.55	0/1159	0.78	0/1566
1	C	0.55	0/1159	0.79	1/1566 (0.1%)
1	J	0.53	0/1159	0.79	0/1566
1	K	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	H	0.56	1/1651 (0.1%)	0.75	0/2246
2	M	0.56	0/1634	0.75	0/2225
2	O	0.59	0/1637	0.75	0/2229
2	Q	0.54	0/1642	0.74	1/2235 (0.0%)
3	E	0.55	0/1605	0.70	0/2193
3	G	0.56	0/1611	0.72	1/2201 (0.0%)
3	I	0.55	0/1611	0.70	0/2201
3	N	0.56	1/1611 (0.1%)	0.74	0/2201
3	P	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	16/36026 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	191	ARG	NE-CZ	6.29	1.41	1.33
2	D	83	LEU	CG-CD1	-5.95	1.29	1.51
1	A	215	LYS	CG-CD	-5.68	1.33	1.52
1	L	142	VAL	CB-CG1	5.51	1.64	1.52
2	H	153	LYS	CD-CE	5.43	1.64	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	83	LEU	CB-CG-CD1	10.27	128.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	A	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	C	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	A	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 ⓘ

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	1138	0	1143	1	0
1	B	1138	0	1143	1	0
1	C	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	H	1614	0	1594	3	0
2	M	1597	0	1573	1	0
2	O	1600	0	1579	0	0
2	Q	1605	0	1581	1	0
3	E	1567	0	1499	0	0
3	G	1573	0	1504	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1573	0	1504	0	0
3	N	1573	0	1504	0	0
3	P	1573	0	1504	1	0
3	R	1572	0	1501	1	0
4	A	8	0	0	0	0
4	B	11	0	0	0	0
4	C	13	0	0	0	0
4	D	9	0	0	0	0
4	E	4	0	0	0	0
4	F	25	0	0	0	0
4	G	22	0	0	0	0
4	H	19	0	0	0	0
4	I	20	0	0	0	0
4	J	19	0	0	0	0
4	K	19	0	0	0	0
4	L	8	0	0	0	0
4	M	17	0	0	0	0
4	N	19	0	0	0	0
4	O	9	0	0	0	0
4	P	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:HB2	2:F:118[A]:MET:HE2	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

### 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	142/164 (87%)	140 (99%)	2 (1%)	0	100	100
1	B	142/164 (87%)	139 (98%)	3 (2%)	0	100	100
1	C	142/164 (87%)	140 (99%)	2 (1%)	0	100	100
1	J	142/164 (87%)	141 (99%)	1 (1%)	0	100	100
1	K	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	H	213/225 (95%)	206 (97%)	7 (3%)	0	100	100
2	M	211/225 (94%)	205 (97%)	6 (3%)	0	100	100
2	O	211/225 (94%)	199 (94%)	12 (6%)	0	100	100
2	Q	212/225 (94%)	204 (96%)	8 (4%)	0	100	100
3	E	207/214 (97%)	197 (95%)	9 (4%)	1 (0%)	29	61
3	G	208/214 (97%)	203 (98%)	5 (2%)	0	100	100
3	I	208/214 (97%)	200 (96%)	7 (3%)	1 (0%)	29	61
3	N	208/214 (97%)	200 (96%)	7 (3%)	1 (0%)	29	61
3	P	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	P	67	GLY

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Mol	Chain	Res	Type
3	E	67	GLY
3	R	67	GLY
3	I	158	LYS
3	N	67	GLY

### 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	125/141 (89%)	122 (98%)	3 (2%)	49	79
1	B	125/141 (89%)	122 (98%)	3 (2%)	49	79
1	C	125/141 (89%)	121 (97%)	4 (3%)	39	73
1	J	125/141 (89%)	122 (98%)	3 (2%)	49	79
1	K	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	H	181/187 (97%)	177 (98%)	4 (2%)	52	81
2	M	179/187 (96%)	176 (98%)	3 (2%)	60	86
2	O	179/187 (96%)	177 (99%)	2 (1%)	73	92
2	Q	180/187 (96%)	174 (97%)	6 (3%)	38	72
3	E	174/179 (97%)	174 (100%)	0	100	100
3	G	175/179 (98%)	174 (99%)	1 (1%)	86	96
3	I	175/179 (98%)	171 (98%)	4 (2%)	50	80
3	N	175/179 (98%)	174 (99%)	1 (1%)	86	96
3	P	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	A	180	GLU
1	A	217	VAL
1	A	232	CYS
1	B	153	SER
1	B	230	PHE
1	B	232	CYS
1	C	183	ASN
1	C	211	LEU
1	C	232	CYS
1	C	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	H	80	SER
2	H	81	MET
2	H	196	SER
2	H	206	CYS
3	I	59	ASP
3	I	124	SER
3	I	147	THR
3	I	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	M	80	SER
2	M	84	SER
2	M	188	LEU
3	N	116	SER
2	O	122	SER
2	O	206	CYS
3	P	96	HIS
2	Q	63	ASN
2	Q	76	THR

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Mol	Chain	Res	Type
2	Q	80	SER
2	Q	196	SER
2	Q	206	CYS
2	Q	219	LYS
3	R	11	SER
3	R	12	VAL
3	R	59	ASP
3	R	116	SER

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

Mol	Chain	Res	Type
1	A	234	GLN
1	K	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 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

### 6.1 Protein, DNA and RNA chains

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	144/164 (87%)	-0.19	0 <span>100</span> <span>100</span>	30, 43, 69, 114	9 (6%)
1	B	144/164 (87%)	-0.16	1 (0%) <span>87</span> <span>87</span>	29, 45, 72, 94	10 (6%)
1	C	144/164 (87%)	-0.20	1 (0%) <span>87</span> <span>87</span>	29, 44, 68, 101	9 (6%)
1	J	144/164 (87%)	-0.27	0 <span>100</span> <span>100</span>	29, 43, 66, 85	11 (7%)
1	K	144/164 (87%)	-0.25	1 (0%) <span>87</span> <span>87</span>	30, 42, 67, 86	9 (6%)
1	L	144/164 (87%)	-0.19	0 <span>100</span> <span>100</span>	32, 47, 77, 115	13 (9%)
2	D	215/225 (95%)	-0.00	3 (1%) <span>75</span> <span>75</span>	40, 81, 108, 119	33 (15%)
2	F	220/225 (97%)	-0.17	3 (1%) <span>75</span> <span>75</span>	35, 53, 104, 127	16 (7%)
2	H	216/225 (96%)	-0.12	2 (0%) <span>84</span> <span>84</span>	34, 63, 107, 117	18 (8%)
2	M	215/225 (95%)	-0.27	0 <span>100</span> <span>100</span>	34, 57, 87, 106	11 (5%)
2	O	215/225 (95%)	-0.01	1 (0%) <span>91</span> <span>91</span>	41, 78, 106, 125	22 (10%)
2	Q	215/225 (95%)	-0.20	1 (0%) <span>91</span> <span>91</span>	30, 56, 91, 112	14 (6%)
3	E	209/214 (97%)	-0.06	1 (0%) <span>91</span> <span>91</span>	42, 69, 102, 127	16 (7%)
3	G	210/214 (98%)	-0.25	0 <span>100</span> <span>100</span>	33, 52, 77, 98	8 (3%)
3	I	210/214 (98%)	-0.12	0 <span>100</span> <span>100</span>	36, 55, 74, 103	9 (4%)
3	N	210/214 (98%)	-0.24	0 <span>100</span> <span>100</span>	36, 53, 72, 87	11 (5%)
3	P	210/214 (98%)	0.00	3 (1%) <span>75</span> <span>75</span>	42, 69, 99, 130	15 (7%)
3	R	209/214 (97%)	-0.24	0 <span>100</span> <span>100</span>	33, 56, 77, 87	7 (3%)
All	All	3418/3618 (94%)	-0.16	17 (0%) <span>91</span> <span>91</span>	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	K	232	CYS	2.8
2	H	75	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	143	GLY	2.6
3	P	159	ALA	2.5
2	F	197	SER	2.5
3	P	157	VAL	2.5
3	P	158	LYS	2.4
2	H	197	SER	2.3
2	O	200	GLY	2.3
2	D	131	VAL	2.2
1	C	232	CYS	2.2
1	B	232	CYS	2.2
3	E	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.