



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2016 – 04:01 PM EDT

PDB ID : 4RAU  
Title : crystal structure of RTOFab in complex with human PF4  
Authors : Cai, Z.; Zhu, Z.; Liu, Q.; Greene, M.I.  
Deposited on : 2014-09-11  
Resolution : 3.74 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

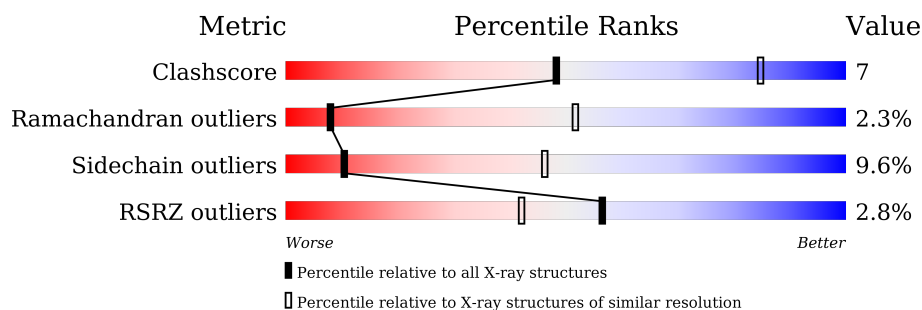
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.74 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))
Clashscore	102246	1279 (3.98-3.50)
Ramachandran outliers	100387	1226 (3.98-3.50)
Sidechain outliers	100360	1224 (3.98-3.50)
RSRZ outliers	91569	1161 (3.98-3.50)

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	212	<div> <div></div> <div>78%20%..</div> </div>
1	D	212	<div> <div></div> <div>78%18%.</div> </div>
1	G	212	<div> <div>%</div> <div>83%15%.</div> </div>
1	J	212	<div> <div>2%</div> <div>83%15%..</div> </div>
1	M	212	<div> <div>5%</div> <div>83%15%.</div> </div>
1	P	212	<div> <div>4%</div> <div>80%17%.</div> </div>
1	S	212	<div> <div>9%</div> <div>81%17%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	V	212	
2	B	219	
2	E	219	
2	H	219	
2	K	219	
2	N	219	
2	Q	219	
2	T	219	
2	W	219	
3	C	70	
3	F	70	
3	I	70	
3	L	70	
3	O	70	
3	R	70	
3	U	70	
3	X	70	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30074 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 RTOFab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	D	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	G	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	J	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	M	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	P	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	S	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			
1	V	212	Total	C	N	O	S	0	0	0
			1635	1020	272	337	6			

- Molecule 2 is a protein called RTOFab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	E	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	H	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	K	219	Total	C	N	O	S	0	0	0
			1620	1021	268	322	9			
2	N	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	Q	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			
2	W	219	Total	C	N	O	S	0	0	0
			1624	1023	268	324	9			

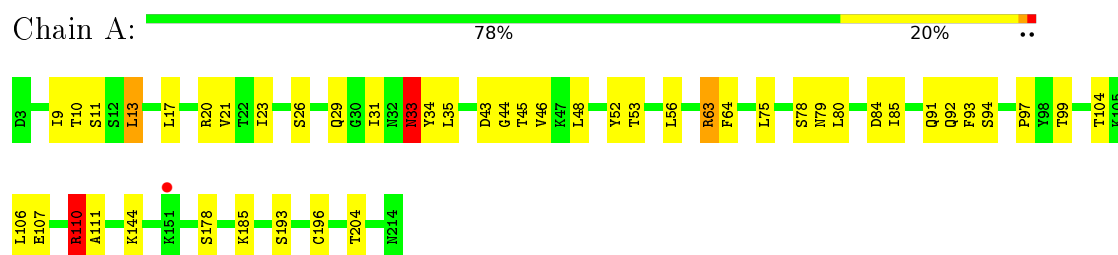
- Molecule 3 is a protein called Platelet factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	F	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	I	66	Total	C	N	O	S	0	0	0
			508	323	92	89	4			
3	L	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	O	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	R	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	U	65	Total	C	N	O	S	0	0	0
			499	318	91	86	4			
3	X	66	Total	C	N	O	S	0	0	0
			504	321	92	87	4			

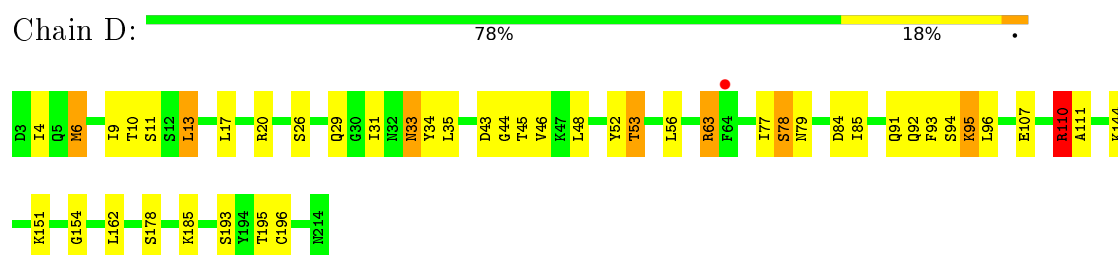
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

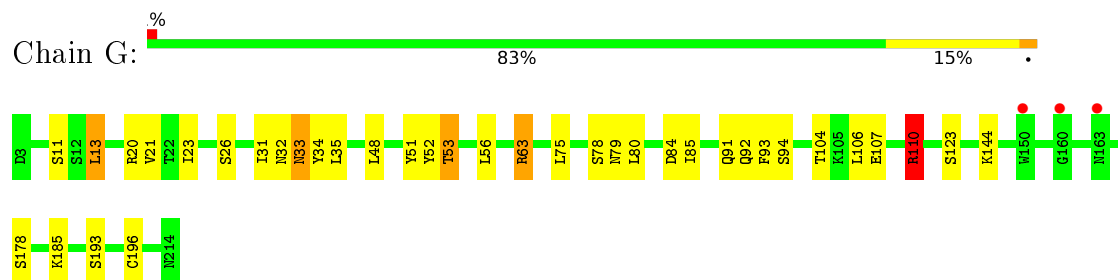
#### • Molecule 1: RTOFab light chain



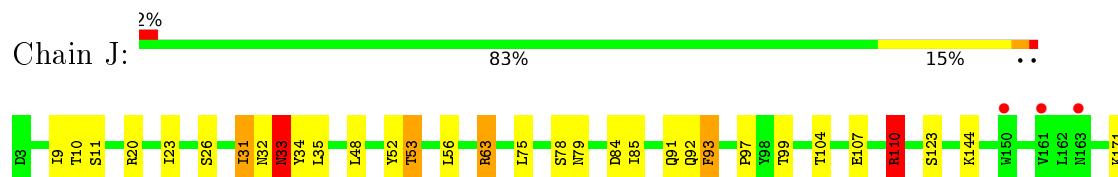
#### • Molecule 1: RTOFab light chain



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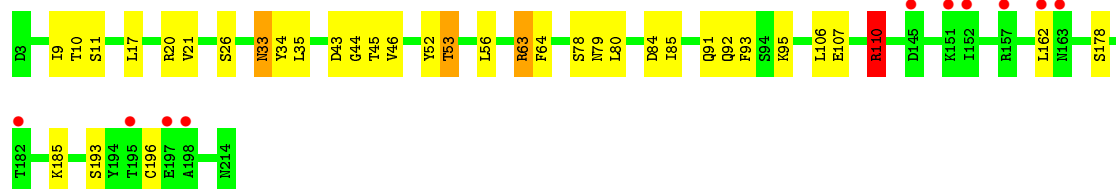
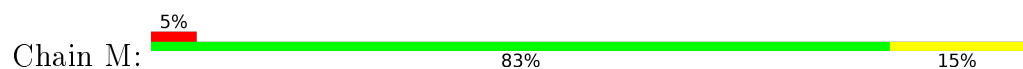


#### • Molecule 1: RTOFab light chain

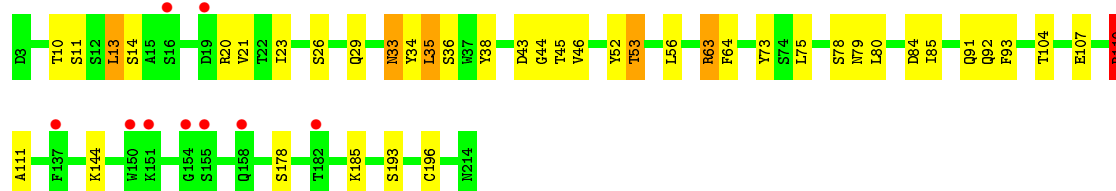
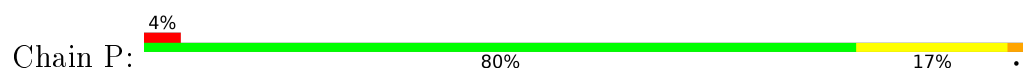




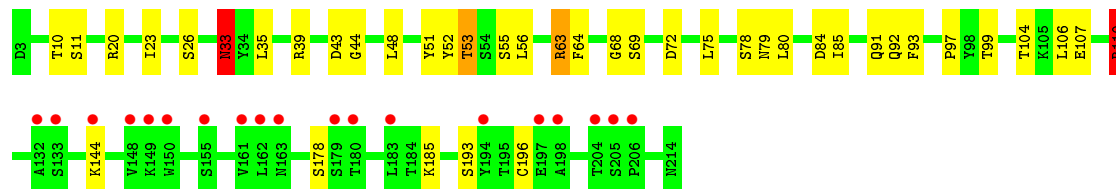
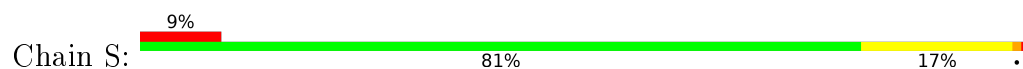
- Molecule 1: RTOFab light chain



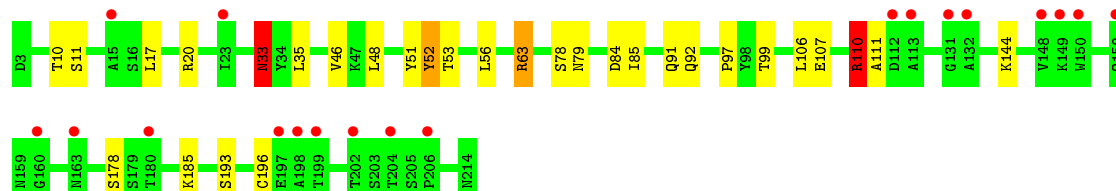
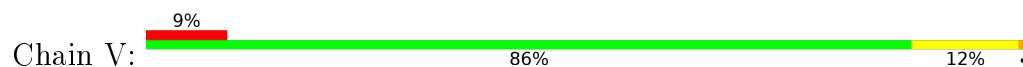
- Molecule 1: RTOFab light chain



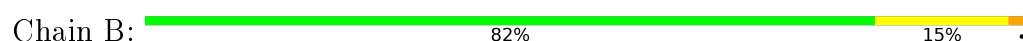
- Molecule 1: RTOFab light chain

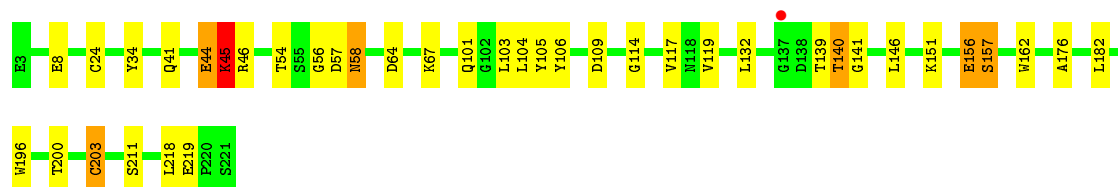


- Molecule 1: RTOFab light chain

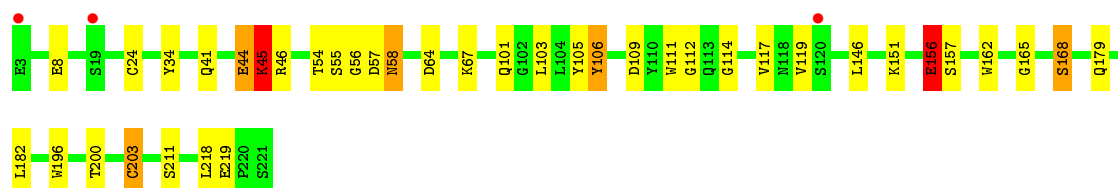
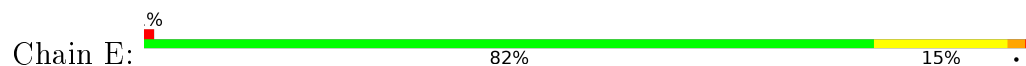


- Molecule 2: RTOFab heavy chain

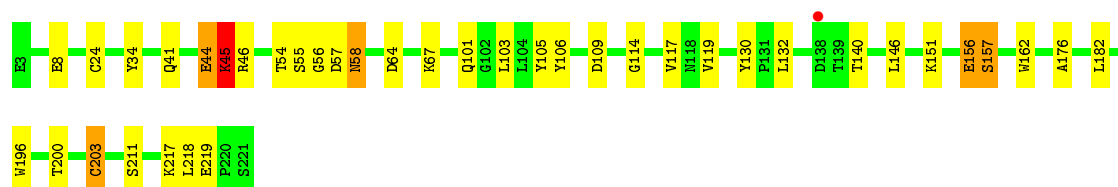
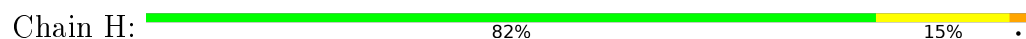




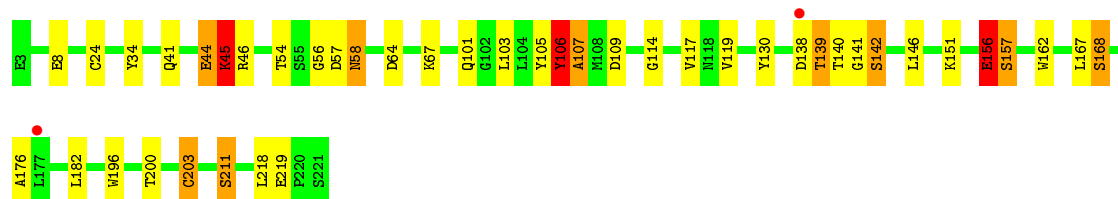
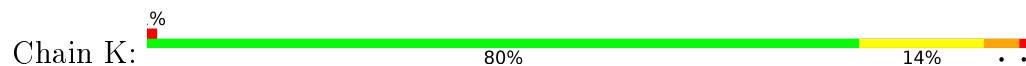
- Molecule 2: RTOFab heavy chain



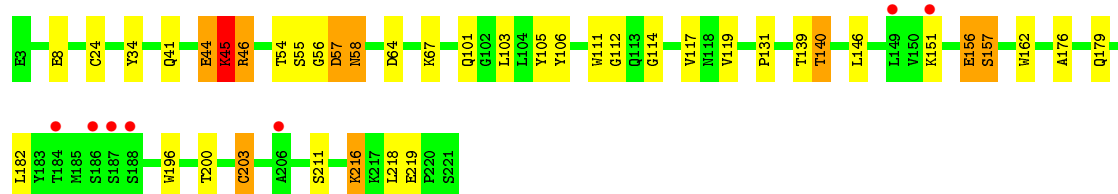
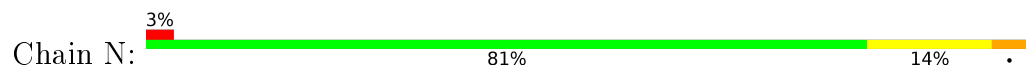
- Molecule 2: RTOFab heavy chain



- Molecule 2: RTOFab heavy chain

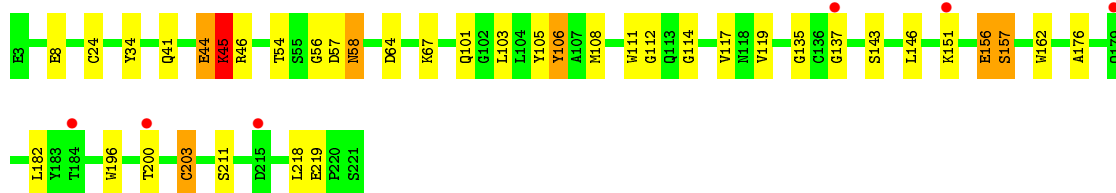
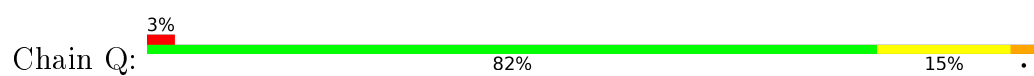


- Molecule 2: RTOFab heavy chain

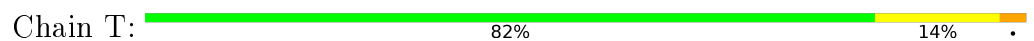


- Molecule 2: RTOFab heavy chain

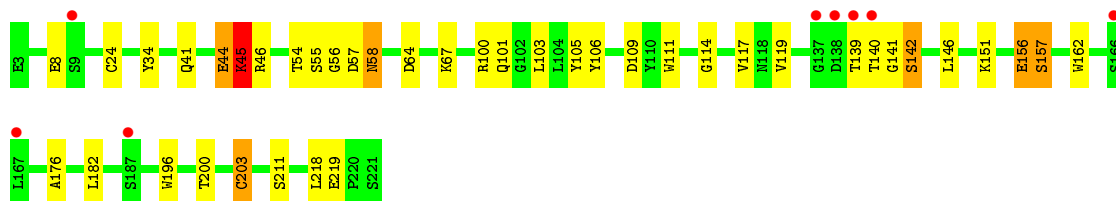
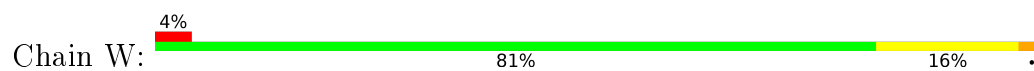




- Molecule 2: RTOFab heavy chain



- Molecule 2: RTOFab heavy chain



- Molecule 3: Platelet factor 4



- Molecule 3: Platelet factor 4

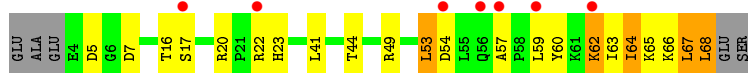


- Molecule 3: Platelet factor 4



- Molecule 3: Platelet factor 4

Chain L: 



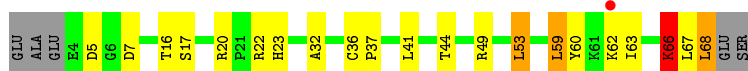
- Molecule 3: Platelet factor 4

Chain O: 



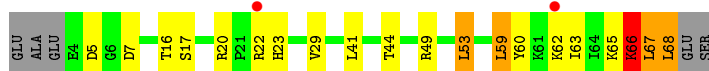
- Molecule 3: Platelet factor 4

Chain R: 



- Molecule 3: Platelet factor 4

Chain U: 



- Molecule 3: Platelet factor 4

Chain X: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.42Å 171.87Å 208.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 49.81 – 3.74	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.74) 99.2 (49.81-3.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.243 , 0.284 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	118.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 75.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 60076 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	30074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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 ⓘ

### 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	0.34	0/1671	0.63	1/2270 (0.0%)
1	D	0.35	0/1671	0.65	2/2270 (0.1%)
1	G	0.35	0/1671	0.63	1/2270 (0.0%)
1	J	0.37	0/1671	0.64	2/2270 (0.1%)
1	M	0.35	0/1671	0.63	1/2270 (0.0%)
1	P	0.36	0/1671	0.68	4/2270 (0.2%)
1	S	0.35	0/1671	0.65	1/2270 (0.0%)
1	V	0.39	0/1671	0.64	1/2270 (0.0%)
2	B	0.35	0/1666	0.57	0/2274
2	E	0.36	0/1666	0.64	2/2274 (0.1%)
2	H	0.34	0/1666	0.57	0/2274
2	K	0.40	0/1662	0.67	4/2268 (0.2%)
2	N	0.38	0/1666	0.66	4/2274 (0.2%)
2	Q	0.39	0/1666	0.62	3/2274 (0.1%)
2	T	0.40	0/1666	0.64	1/2274 (0.0%)
2	W	0.38	0/1666	0.58	0/2274
3	C	0.38	0/505	0.71	1/681 (0.1%)
3	F	0.39	0/505	0.72	1/681 (0.1%)
3	I	0.42	0/514	0.93	4/693 (0.6%)
3	L	0.44	0/505	0.78	1/681 (0.1%)
3	O	0.39	0/505	0.74	1/681 (0.1%)
3	R	0.40	0/505	0.95	3/681 (0.4%)
3	U	0.41	0/505	0.81	3/681 (0.4%)
3	X	0.41	0/510	0.75	1/688 (0.1%)
All	All	0.37	0/30746	0.66	42/41813 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	H	0	1
2	K	0	1
2	N	0	1
2	Q	0	1
2	T	0	1
2	W	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	7	ASP	CB-CG-OD1	11.69	128.82	118.30
3	R	7	ASP	CB-CG-OD2	-11.61	107.85	118.30
2	T	56	GLY	N-CA-C	-10.88	85.89	113.10
2	K	106	TYR	CB-CA-C	10.40	131.21	110.40
2	N	57	ASP	CB-CG-OD2	10.34	127.60	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	101	GLN	Peptide
2	E	101	GLN	Peptide
2	H	101	GLN	Peptide
2	K	101	GLN	Peptide
2	N	101	GLN	Peptide

## 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	1635	0	1559	32	0
1	D	1635	0	1559	44	0
1	G	1635	0	1559	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1635	0	1559	39	0
1	M	1635	0	1559	22	0
1	P	1635	0	1559	37	0
1	S	1635	0	1559	36	0
1	V	1635	0	1559	17	0
2	B	1624	0	1525	25	0
2	E	1624	0	1525	26	0
2	H	1624	0	1525	21	0
2	K	1620	0	1515	24	0
2	N	1624	0	1525	23	0
2	Q	1624	0	1525	22	0
2	T	1624	0	1525	20	0
2	W	1624	0	1525	19	0
3	C	499	0	544	10	0
3	F	499	0	544	14	0
3	I	508	0	550	5	0
3	L	499	0	544	10	0
3	O	499	0	544	14	0
3	R	499	0	544	13	0
3	U	499	0	544	9	0
3	X	504	0	546	8	0
All	All	30074	0	29022	434	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 7.

The worst 5 of 434 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:D:154:GLY:O	1:S:68:GLY:HA2	1.51	1.09
1:D:6:MET:HE2	1:D:92:GLN:HG2	1.34	1.07
2:N:55:SER:OG	3:O:31:LYS:NZ	1.92	1.01
1:D:6:MET:CE	1:D:92:GLN:HG2	1.97	0.94
1:D:6:MET:HE3	1:D:92:GLN:HB3	1.53	0.91

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	210/212 (99%)	197 (94%)	11 (5%)	2 (1%)	19	66
1	D	210/212 (99%)	193 (92%)	14 (7%)	3 (1%)	14	59
1	G	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	19	66
1	J	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	19	66
1	M	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	19	66
1	P	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	19	66
1	S	210/212 (99%)	195 (93%)	13 (6%)	2 (1%)	19	66
1	V	210/212 (99%)	196 (93%)	12 (6%)	2 (1%)	19	66
2	B	217/219 (99%)	196 (90%)	14 (6%)	7 (3%)	5	44
2	E	217/219 (99%)	197 (91%)	14 (6%)	6 (3%)	6	47
2	H	217/219 (99%)	196 (90%)	15 (7%)	6 (3%)	6	47
2	K	217/219 (99%)	190 (88%)	15 (7%)	12 (6%)	2	29
2	N	217/219 (99%)	197 (91%)	14 (6%)	6 (3%)	6	47
2	Q	217/219 (99%)	195 (90%)	15 (7%)	7 (3%)	5	44
2	T	217/219 (99%)	193 (89%)	16 (7%)	8 (4%)	4	40
2	W	217/219 (99%)	194 (89%)	15 (7%)	8 (4%)	4	40
3	C	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	44
3	F	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	44
3	I	64/70 (91%)	55 (86%)	8 (12%)	1 (2%)	12	58
3	L	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	44
3	O	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	44
3	R	63/70 (90%)	55 (87%)	6 (10%)	2 (3%)	5	44
3	U	63/70 (90%)	55 (87%)	8 (13%)	0	100	100
3	X	64/70 (91%)	55 (86%)	7 (11%)	2 (3%)	5	45
All	All	3922/4008 (98%)	3561 (91%)	271 (7%)	90 (2%)	8	52

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	46	ARG
2	B	57	ASP
2	B	58	ASN
2	B	157	SER
1	D	78	SER

### 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	188/190 (99%)	171 (91%)	17 (9%)	12	50
1	D	188/190 (99%)	170 (90%)	18 (10%)	10	46
1	G	188/190 (99%)	175 (93%)	13 (7%)	19	60
1	J	188/190 (99%)	172 (92%)	16 (8%)	13	52
1	M	188/190 (99%)	175 (93%)	13 (7%)	19	60
1	P	188/190 (99%)	174 (93%)	14 (7%)	17	57
1	S	188/190 (99%)	174 (93%)	14 (7%)	17	57
1	V	188/190 (99%)	173 (92%)	15 (8%)	15	54
2	B	179/189 (95%)	163 (91%)	16 (9%)	12	50
2	E	179/189 (95%)	164 (92%)	15 (8%)	14	53
2	H	179/189 (95%)	163 (91%)	16 (9%)	12	50
2	K	177/189 (94%)	162 (92%)	15 (8%)	13	52
2	N	179/189 (95%)	163 (91%)	16 (9%)	12	50
2	Q	179/189 (95%)	165 (92%)	14 (8%)	16	55
2	T	179/189 (95%)	164 (92%)	15 (8%)	14	53
2	W	179/189 (95%)	164 (92%)	15 (8%)	14	53
3	C	57/62 (92%)	47 (82%)	10 (18%)	2	17
3	F	57/62 (92%)	46 (81%)	11 (19%)	2	13
3	I	58/62 (94%)	47 (81%)	11 (19%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	57/62 (92%)	45 (79%)	12 (21%)	1	10
3	O	57/62 (92%)	47 (82%)	10 (18%)	2	17
3	R	57/62 (92%)	48 (84%)	9 (16%)	3	23
3	U	57/62 (92%)	47 (82%)	10 (18%)	2	17
3	X	57/62 (92%)	46 (81%)	11 (19%)	2	13
All	All	3391/3528 (96%)	3065 (90%)	326 (10%)	10	46

5 of 326 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	64	ASP
1	M	196	CYS
2	W	44	GLU
2	K	156	GLU
3	L	60	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	79	ASN
1	M	79	ASN
2	W	41	GLN
2	K	41	GLN
3	L	9	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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	212/212 (100%)	0.01	1 (0%) 91 86	78, 118, 159, 182	0
1	D	212/212 (100%)	-0.07	1 (0%) 91 86	88, 122, 157, 182	0
1	G	212/212 (100%)	0.05	3 (1%) 78 65	80, 141, 202, 235	0
1	J	212/212 (100%)	0.20	5 (2%) 62 48	96, 144, 187, 212	0
1	M	212/212 (100%)	0.22	10 (4%) 35 24	85, 123, 179, 198	0
1	P	212/212 (100%)	0.30	9 (4%) 40 28	97, 141, 177, 193	0
1	S	212/212 (100%)	0.51	19 (8%) 12 7	90, 154, 210, 229	0
1	V	212/212 (100%)	0.41	19 (8%) 12 7	91, 160, 211, 229	0
2	B	219/219 (100%)	-0.07	1 (0%) 91 86	87, 124, 169, 206	0
2	E	219/219 (100%)	-0.05	3 (1%) 78 65	93, 132, 170, 211	0
2	H	219/219 (100%)	-0.07	1 (0%) 91 86	76, 127, 184, 230	0
2	K	219/219 (100%)	-0.04	2 (0%) 85 76	95, 136, 181, 196	0
2	N	219/219 (100%)	0.14	7 (3%) 51 37	90, 145, 195, 254	0
2	Q	219/219 (100%)	0.20	6 (2%) 58 43	94, 152, 204, 231	0
2	T	219/219 (100%)	-0.07	1 (0%) 91 86	87, 144, 192, 249	0
2	W	219/219 (100%)	0.06	8 (3%) 45 32	90, 145, 207, 244	0
3	C	65/70 (92%)	0.10	0 100 100	75, 117, 187, 196	0
3	F	65/70 (92%)	0.07	2 (3%) 52 38	89, 120, 204, 230	0
3	I	66/70 (94%)	0.12	0 100 100	95, 128, 197, 203	0
3	L	65/70 (92%)	0.36	7 (10%) 8 5	104, 141, 232, 265	0
3	O	65/70 (92%)	-0.00	1 (1%) 76 63	81, 122, 184, 220	0
3	R	65/70 (92%)	-0.03	1 (1%) 76 63	82, 116, 189, 237	0
3	U	65/70 (92%)	0.19	2 (3%) 52 38	105, 138, 202, 219	0
3	X	66/70 (94%)	0.19	2 (3%) 54 38	95, 132, 204, 211	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3970/4008 (99%)	0.11	111 (2%) 56 42	75, 136, 196, 265	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	204	THR	5.1
1	S	197	GLU	4.5
1	S	206	PRO	4.4
1	S	162	LEU	4.4
1	M	163	ASN	4.4

## 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.