



# wwPDB X-ray Structure Validation Summary Report

Aug 25, 2014 – 01:23 PM EDT

PDB ID : 4F37  
Title : Structure of the tethered N-terminus of Alzheimer's disease A peptide  
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Deposited on : 2012-05-09  
Resolution : 2.57 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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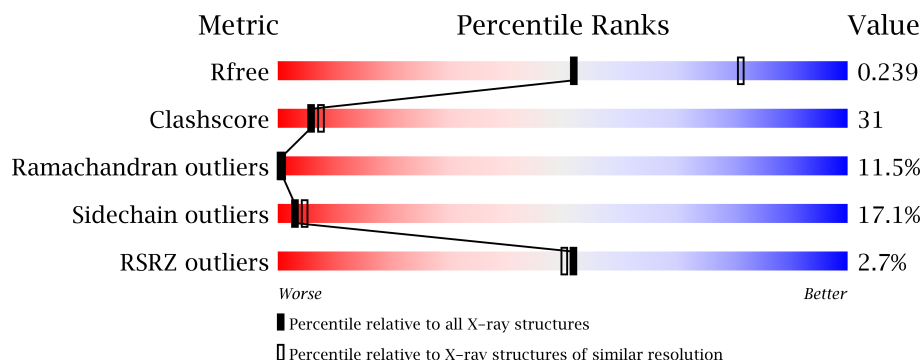
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23489
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.57 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))
$R_{free}$	66092	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	124	
1	B	124	
2	F	228	
2	H	228	
3	K	219	
3	L	219	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8769 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Colicin-E7 immunity protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	0	0	0
			829	520	138	171			
1	B	102	Total	C	N	O	0	0	0
			829	520	138	171			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	-	EXPRESSION TAG	UNP Q03708
A	2	ALA	-	EXPRESSION TAG	UNP Q03708
A	3	GLU	-	EXPRESSION TAG	UNP Q03708
A	4	PHE	-	EXPRESSION TAG	UNP Q03708
A	5	ARG	-	EXPRESSION TAG	UNP Q03708
A	6	HIS	-	EXPRESSION TAG	UNP Q03708
A	7	ASP	-	EXPRESSION TAG	UNP Q03708
A	8	SER	-	EXPRESSION TAG	UNP Q03708
A	9	GLY	-	EXPRESSION TAG	UNP Q03708
A	10	TYR	-	EXPRESSION TAG	UNP Q03708
A	11	GLU	-	EXPRESSION TAG	UNP Q03708
A	12	VAL	-	EXPRESSION TAG	UNP Q03708
A	13	HIS	-	EXPRESSION TAG	UNP Q03708
A	14	HIS	-	EXPRESSION TAG	UNP Q03708
A	15	GLN	-	EXPRESSION TAG	UNP Q03708
A	16	LYS	-	EXPRESSION TAG	UNP Q03708
A	17	SER	-	EXPRESSION TAG	UNP Q03708
A	104	ALA	-	EXPRESSION TAG	UNP Q03708
A	105	ALA	-	EXPRESSION TAG	UNP Q03708
A	106	ALA	-	EXPRESSION TAG	UNP Q03708
A	107	ASP	-	EXPRESSION TAG	UNP Q03708
A	108	TYR	-	EXPRESSION TAG	UNP Q03708
A	109	LYS	-	EXPRESSION TAG	UNP Q03708
A	110	ASP	-	EXPRESSION TAG	UNP Q03708
A	111	ASP	-	EXPRESSION TAG	UNP Q03708

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Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ASP	-	EXPRESSION TAG	UNP Q03708
A	113	ASP	-	EXPRESSION TAG	UNP Q03708
A	114	LYS	-	EXPRESSION TAG	UNP Q03708
A	115	ALA	-	EXPRESSION TAG	UNP Q03708
A	116	ALA	-	EXPRESSION TAG	UNP Q03708
A	117	ASP	-	EXPRESSION TAG	UNP Q03708
A	118	TYR	-	EXPRESSION TAG	UNP Q03708
A	119	LYS	-	EXPRESSION TAG	UNP Q03708
A	120	ASP	-	EXPRESSION TAG	UNP Q03708
A	121	ASP	-	EXPRESSION TAG	UNP Q03708
A	122	ASP	-	EXPRESSION TAG	UNP Q03708
A	123	ASP	-	EXPRESSION TAG	UNP Q03708
A	124	LYS	-	EXPRESSION TAG	UNP Q03708
B	1	ASP	-	EXPRESSION TAG	UNP Q03708
B	2	ALA	-	EXPRESSION TAG	UNP Q03708
B	3	GLU	-	EXPRESSION TAG	UNP Q03708
B	4	PHE	-	EXPRESSION TAG	UNP Q03708
B	5	ARG	-	EXPRESSION TAG	UNP Q03708
B	6	HIS	-	EXPRESSION TAG	UNP Q03708
B	7	ASP	-	EXPRESSION TAG	UNP Q03708
B	8	SER	-	EXPRESSION TAG	UNP Q03708
B	9	GLY	-	EXPRESSION TAG	UNP Q03708
B	10	TYR	-	EXPRESSION TAG	UNP Q03708
B	11	GLU	-	EXPRESSION TAG	UNP Q03708
B	12	VAL	-	EXPRESSION TAG	UNP Q03708
B	13	HIS	-	EXPRESSION TAG	UNP Q03708
B	14	HIS	-	EXPRESSION TAG	UNP Q03708
B	15	GLN	-	EXPRESSION TAG	UNP Q03708
B	16	LYS	-	EXPRESSION TAG	UNP Q03708
B	17	SER	-	EXPRESSION TAG	UNP Q03708
B	104	ALA	-	EXPRESSION TAG	UNP Q03708
B	105	ALA	-	EXPRESSION TAG	UNP Q03708
B	106	ALA	-	EXPRESSION TAG	UNP Q03708
B	107	ASP	-	EXPRESSION TAG	UNP Q03708
B	108	TYR	-	EXPRESSION TAG	UNP Q03708
B	109	LYS	-	EXPRESSION TAG	UNP Q03708
B	110	ASP	-	EXPRESSION TAG	UNP Q03708
B	111	ASP	-	EXPRESSION TAG	UNP Q03708
B	112	ASP	-	EXPRESSION TAG	UNP Q03708
B	113	ASP	-	EXPRESSION TAG	UNP Q03708
B	114	LYS	-	EXPRESSION TAG	UNP Q03708
B	115	ALA	-	EXPRESSION TAG	UNP Q03708

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Chain	Residue	Modelled	Actual	Comment	Reference
B	116	ALA	-	EXPRESSION TAG	UNP Q03708
B	117	ASP	-	EXPRESSION TAG	UNP Q03708
B	118	TYR	-	EXPRESSION TAG	UNP Q03708
B	119	LYS	-	EXPRESSION TAG	UNP Q03708
B	120	ASP	-	EXPRESSION TAG	UNP Q03708
B	121	ASP	-	EXPRESSION TAG	UNP Q03708
B	122	ASP	-	EXPRESSION TAG	UNP Q03708
B	123	ASP	-	EXPRESSION TAG	UNP Q03708
B	124	LYS	-	EXPRESSION TAG	UNP Q03708

- Molecule 2 is a protein called Im7 immunity protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	225	Total	C	N	O	S	0	0	0
			1730	1094	292	339	5			
2	H	225	Total	C	N	O	S	0	0	0
			1730	1094	292	339	5			

- Molecule 3 is a protein called Fab WO2 anti-amyloid-beta antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	218	Total	C	N	O	S	0	0	0
			1693	1059	287	341	6			
3	L	218	Total	C	N	O	S	0	0	0
			1693	1059	287	341	6			

- Molecule 4 is water.

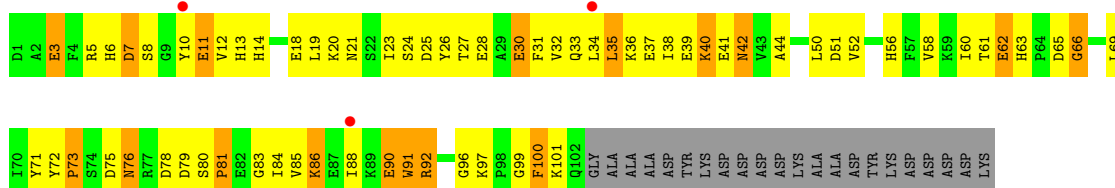
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	34	Total	O	0	0
			34	34		
4	F	53	Total	O	0	0
			53	53		
4	H	50	Total	O	0	0
			50	50		
4	K	42	Total	O	0	0
			42	42		
4	L	54	Total	O	0	0
			54	54		

### 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.

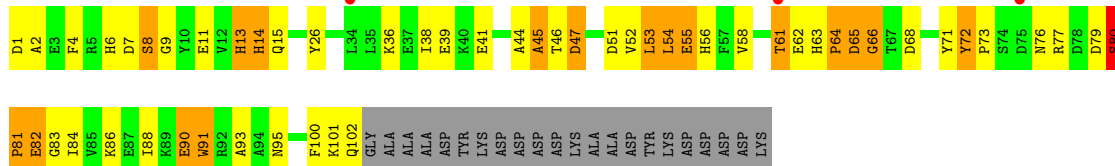
- Molecule 1: Colicin-E7 immunity protein

Chain A: 



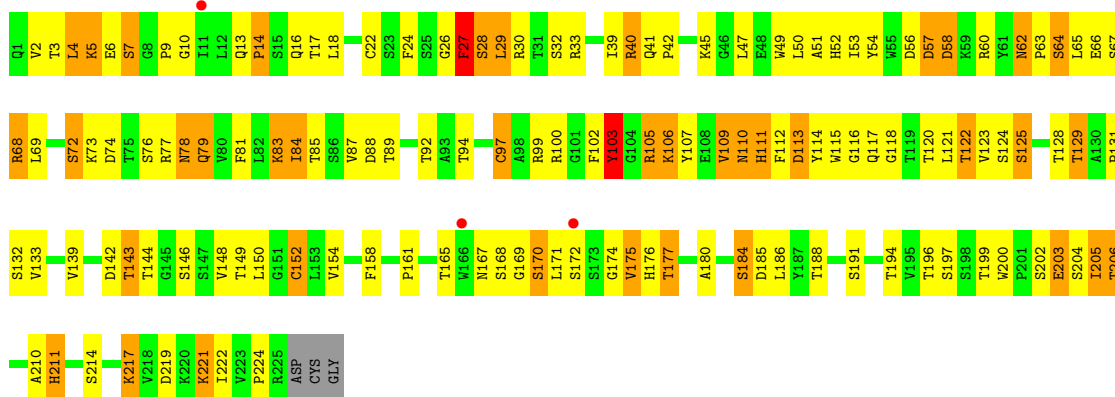
- Molecule 1: Colicin-E7 immunity protein

Chain B: 



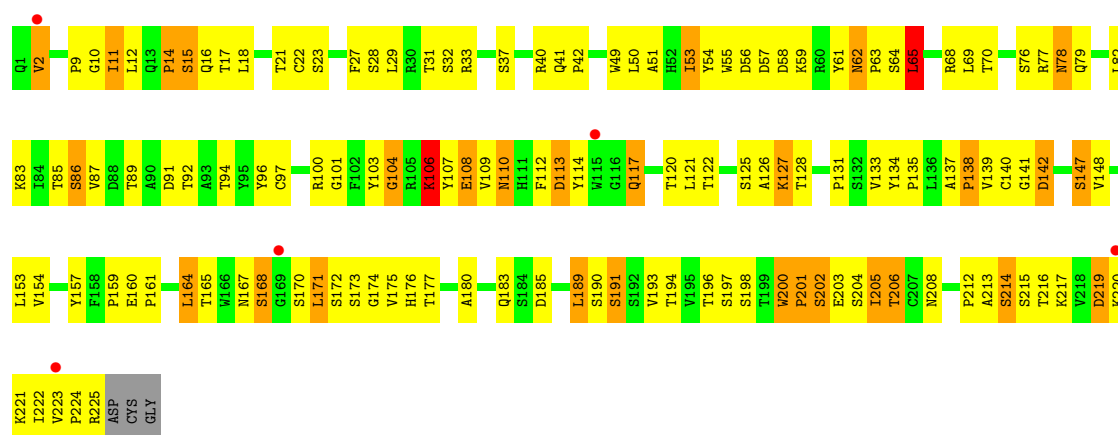
- Molecule 2: Im7 immunity protein

Chain F: 



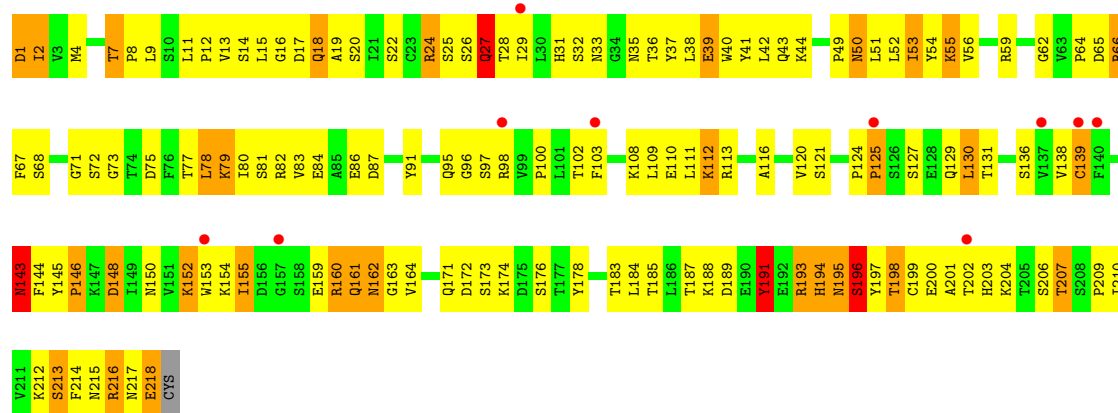
- Molecule 2: Im7 immunity protein

Chain H: 



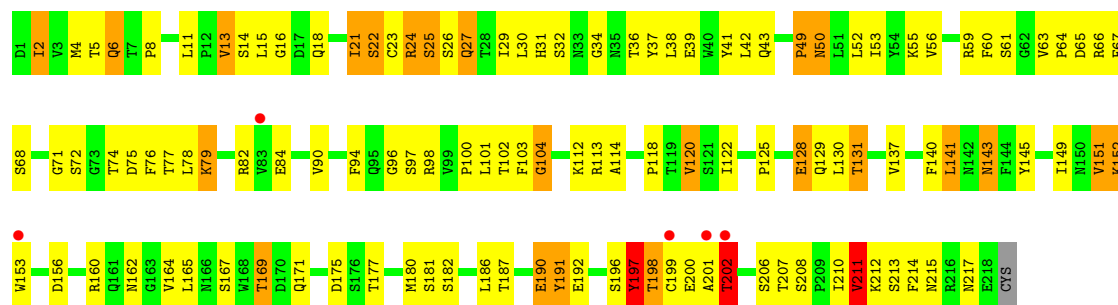
• Molecule 3: Fab WO2 anti-amyloid-beta antibody Fab fragment

Chain K:



• Molecule 3: Fab WO2 anti-amyloid-beta antibody Fab fragment

Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.64Å 82.84Å 89.20Å 90.05° 92.51° 90.00°	Depositor
Resolution (Å)	44.46 – 2.57 44.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	77.9 (44.46-2.57) 85.8 (44.56-2.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.223 , 0.269 0.245 , 0.239	Depositor DCC
$R_{free}$ test set	1542 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 23.9	EDS
Estimated twinning fraction	0.489 for H, K, L 0.391 for -H, K, -L 0.120 for -H, -K, L 0.000 for h,-k,-l 0.168 for -h,k,-l 0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.489 for H, K, L 0.391 for -H, K, -L 0.120 for -H, -K, L	Depositor
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 31156 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.47	0/847	0.70	0/1145
1	B	0.48	0/847	0.80	2/1145 (0.2%)
2	F	0.52	0/1775	0.72	0/2425
2	H	0.52	0/1775	0.71	0/2425
3	K	0.53	0/1730	0.76	0/2347
3	L	0.55	0/1730	0.75	0/2347
All	All	0.52	0/8704	0.74	2/11834 (0.0%)

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
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	SER	C-N-CD	-9.61	99.45	120.60
1	B	80	SER	C-N-CA	5.46	144.93	122.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	80	SER	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	829	0	782	50	0
1	B	829	0	782	39	1
2	F	1730	0	1699	132	1
2	H	1730	0	1699	114	0
3	K	1693	0	1645	114	0
3	L	1693	0	1645	111	0
4	A	32	0	0	2	0
4	B	34	0	0	1	0
4	F	53	0	0	2	0
4	H	50	0	0	4	0
4	K	42	0	0	1	0
4	L	54	0	0	1	1
All	All	8769	0	8252	525	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

The worst 5 of 525 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:201:ALA:HB2	3:L:210:ILE:HB	1.28	1.14
2:H:205:ILE:HG23	2:H:221:LYS:HB2	1.16	1.11
2:H:109:VAL:HG23	3:L:55:LYS:HE3	1.24	1.10
2:F:205:ILE:HG21	2:F:222:ILE:HG12	1.32	1.07
2:H:103:TYR:HB2	2:H:109:VAL:HG11	1.36	1.07

All (2) 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	Distance(Å)	Clash(Å)
4:L:321:HOH:O	4:L:354:HOH:O[1_655]	1.90	0.30
1:B:45:ALA:O	2:F:114:TYR:OH[1_655]	2.08	0.12

## 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	100/124 (81%)	53 (53%)	26 (26%)	21 (21%)	0	0
1	B	100/124 (81%)	62 (62%)	20 (20%)	18 (18%)	0	0
2	F	223/228 (98%)	145 (65%)	55 (25%)	23 (10%)	1	0
2	H	223/228 (98%)	155 (70%)	43 (19%)	25 (11%)	1	0
3	K	216/219 (99%)	153 (71%)	42 (19%)	21 (10%)	1	1
3	L	216/219 (99%)	163 (76%)	37 (17%)	16 (7%)	2	1
All	All	1078/1142 (94%)	731 (68%)	223 (21%)	124 (12%)	1	0

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	HIS
1	A	40	LYS
1	A	42	ASN
1	A	73	PRO

### 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	91/107 (85%)	82 (90%)	9 (10%)	11	20
1	B	91/107 (85%)	82 (90%)	9 (10%)	11	20
2	F	199/201 (99%)	161 (81%)	38 (19%)	2	3
2	H	199/201 (99%)	167 (84%)	32 (16%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	195/196 (100%)	156 (80%)	39 (20%)	2	3
3	L	195/196 (100%)	156 (80%)	39 (20%)	2	3
All	All	970/1008 (96%)	804 (83%)	166 (17%)	3	5

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	168	SER
3	K	24	ARG
3	L	165	LEU
2	H	185	ASP
2	H	205	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	62	ASN
3	K	27	GLN
3	L	161	GLN
2	H	176	HIS
2	H	208	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	102/124 (82%)	0.09	3 (2%) 49 47	22, 28, 31, 32	0
1	B	102/124 (82%)	0.22	3 (2%) 49 47	23, 29, 30, 31	0
2	F	225/228 (98%)	0.13	3 (1%) 74 75	18, 22, 29, 34	0
2	H	225/228 (98%)	0.17	5 (2%) 59 57	17, 23, 29, 31	0
3	K	218/219 (99%)	0.14	10 (4%) 31 29	16, 20, 30, 32	0
3	L	218/219 (99%)	0.14	5 (2%) 57 56	15, 18, 30, 33	0
All	All	1090/1142 (95%)	0.14	29 (2%) 52 50	15, 24, 30, 34	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	199	CYS	5.2
3	L	153	TRP	4.8
2	H	2	VAL	4.1
2	H	223	VAL	4.1
3	L	202	THR	4.0

### 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.