



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID : 1YMH  
Title : anti-HCV Fab 19D9D6 complexed with protein L (PpL) mutant A66W  
Authors : Granata, V.; Housden, N.G.; Harrison, S.; Jolivet-Reynaud, C.; Gore, M.G.;  
Stura, E.A.  
Deposited on : 2005-01-21  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

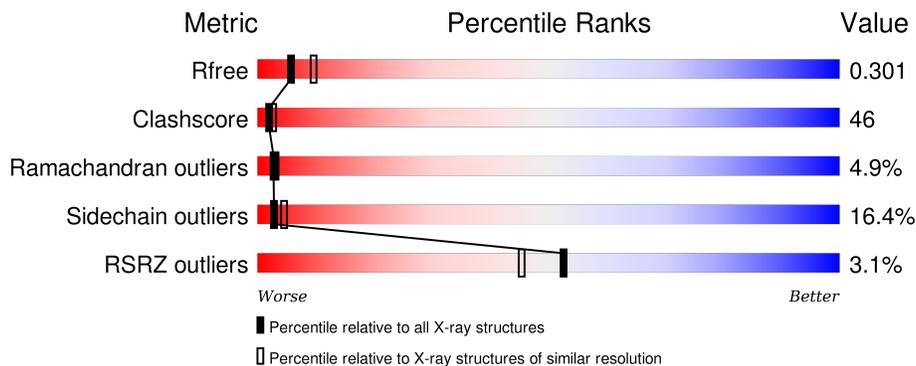
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	
1	C	220	
2	B	218	
2	D	218	
3	E	65	

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Mol	Chain	Length	Quality of chain
3	F	65	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into five segments with the following percentages from left to right: 9% (red), 11% (green), 45% (yellow), 31% (orange), and 14% (red).</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7884 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 Fab 16D9D6, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
1	C	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			

- Molecule 2 is a protein called Fab 16D9D6, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
2	D	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			

- Molecule 3 is a protein called Protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	65	Total	C	N	O	S	0	0	0
			516	329	83	103	1			
3	F	65	Total	C	N	O	S	0	0	0
			516	329	83	103	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	31	Total	O	0	0
			31	31		
4	C	20	Total	O	0	0
			20	20		
4	D	26	Total	O	0	0
			26	26		

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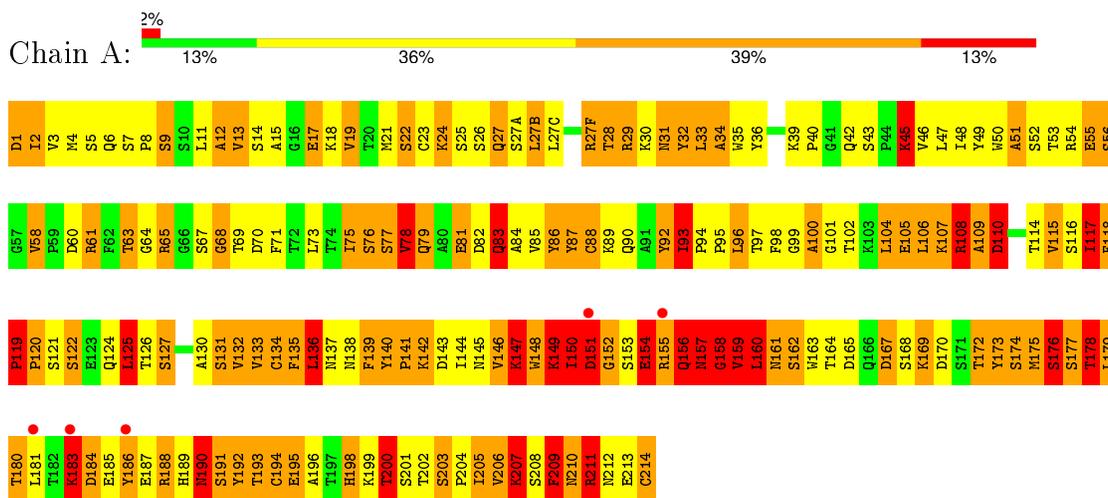
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	E	6	Total	O	0	0
			6	6		
4	F	3	Total	O	0	0
			3	3		

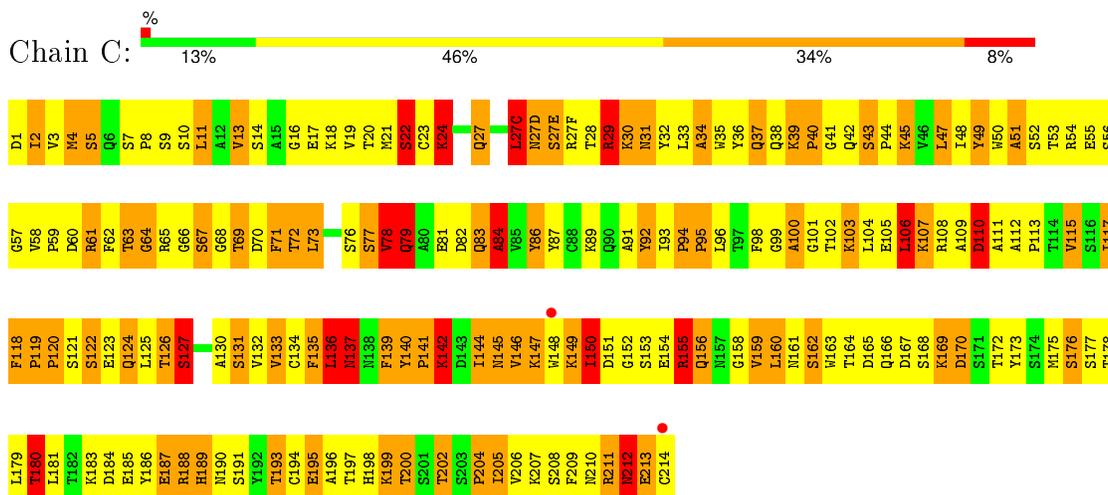
### 3 Residue-property plots

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.

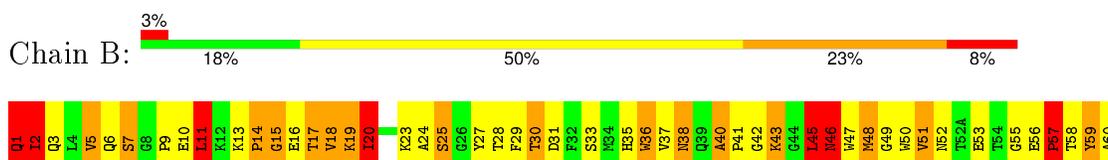
- Molecule 1: Fab 16D9D6, light chain

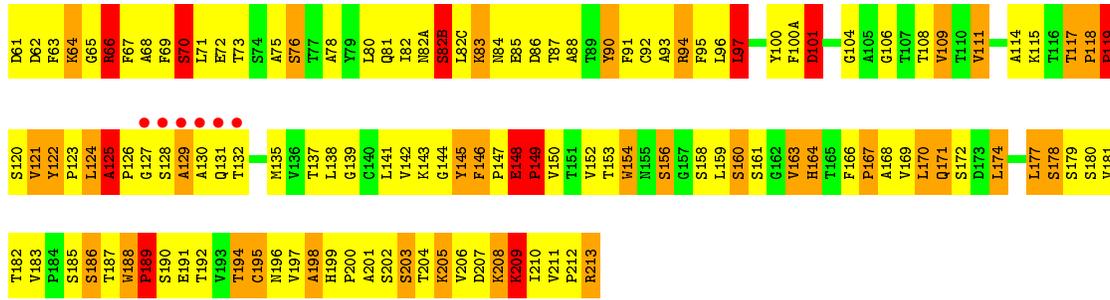


- Molecule 1: Fab 16D9D6, light chain

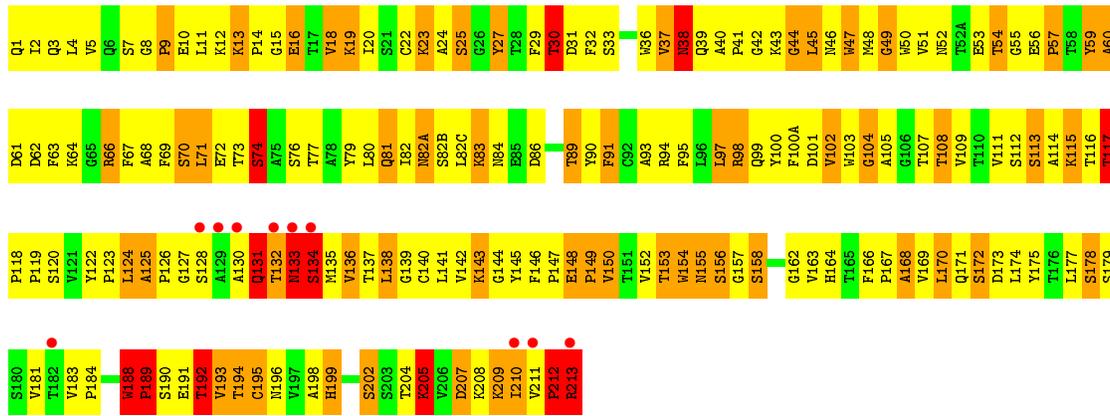
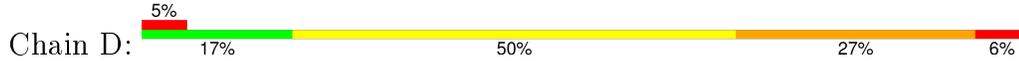


- Molecule 2: Fab 16D9D6, heavy chain

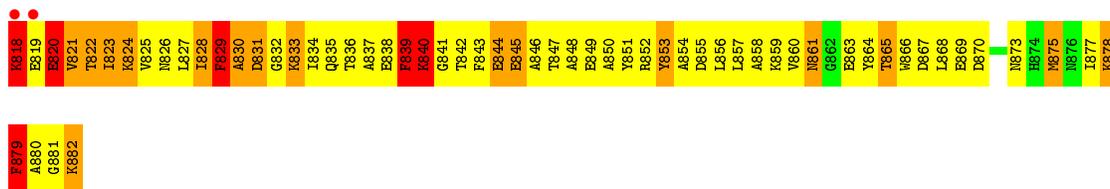




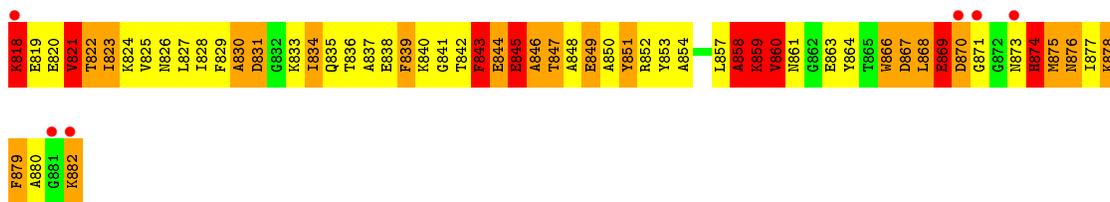
• Molecule 2: Fab 16D9D6, heavy chain



• Molecule 3: Protein L



• Molecule 3: Protein L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.14Å 111.47Å 148.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.60 89.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (87.71-2.60) 97.5 (89.19-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.68 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.224 , 0.302 0.230 , 0.301	Depositor DCC
$R_{free}$ test set	2008 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 40049 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	3.19	192/1745 (11.0%)	2.31	98/2366 (4.1%)
1	C	3.03	173/1745 (9.9%)	2.02	48/2366 (2.0%)
2	B	2.90	134/1707 (7.9%)	2.23	68/2335 (2.9%)
2	D	2.88	151/1707 (8.8%)	2.15	67/2335 (2.9%)
3	E	3.37	73/525 (13.9%)	2.25	29/704 (4.1%)
3	F	2.81	34/525 (6.5%)	2.18	16/704 (2.3%)
All	All	3.02	757/7954 (9.5%)	2.18	326/10810 (3.0%)

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	A	1	19
1	C	0	4
2	B	1	14
2	D	3	13
3	E	2	4
3	F	1	3
All	All	8	57

The worst 5 of 757 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	TYR	CD2-CE2	19.94	1.69	1.39
1	A	50	TRP	CE3-CZ3	15.38	1.64	1.38
1	C	103	LYS	CD-CE	15.16	1.89	1.51
1	A	43	SER	CB-OG	-15.14	1.22	1.42
3	F	849	GLU	CD-OE2	14.76	1.41	1.25

The worst 5 of 326 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	94	ARG	NE-CZ-NH2	-15.19	112.71	120.30
1	A	61	ARG	NE-CZ-NH1	-14.70	112.95	120.30
1	C	60	ASP	CB-CG-OD1	-13.37	106.27	118.30
2	B	149	PRO	CA-N-CD	-13.29	92.89	111.50
1	C	60	ASP	CB-CG-OD2	13.14	130.12	118.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	83	GLN	CA
2	B	177	LEU	CA
3	E	820	GLU	CA
3	E	828	ILE	CB
2	D	132	THR	CA

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PRO	Mainchain
1	A	125	LEU	Peptide
1	A	152	GLY	Peptide
1	A	2	ILE	Mainchain
1	A	76	SER	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1708	0	1657	196	1
1	C	1708	0	1658	177	0
2	B	1660	0	1615	137	0
2	D	1660	0	1614	140	1
3	E	516	0	495	36	0
3	F	516	0	496	55	0
4	A	30	0	0	4	0
4	B	31	0	0	5	0
4	C	20	0	0	2	0
4	D	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	6	0	0	1	0
4	F	3	0	0	1	0
All	All	7884	0	7535	708	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 708 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:C:147:LYS:CG	1:C:147:LYS:CD	1.75	1.65
1:A:45:LYS:CG	1:A:45:LYS:CD	1.75	1.65
1:C:79:GLN:CB	1:C:79:GLN:CG	1.75	1.65
2:B:43:LYS:CD	2:B:43:LYS:CG	1.76	1.64
2:D:97:LEU:CD2	2:D:97:LEU:CG	1.75	1.62

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27(F):ARG:NH1	2:D:127:GLY:O[2_555]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	218/220 (99%)	182 (84%)	24 (11%)	12 (6%)	<a href="#">2</a> <a href="#">2</a>
1	C	218/220 (99%)	184 (84%)	23 (11%)	11 (5%)	<a href="#">3</a> <a href="#">3</a>
2	B	216/218 (99%)	185 (86%)	20 (9%)	11 (5%)	<a href="#">2</a> <a href="#">3</a>
2	D	216/218 (99%)	180 (83%)	30 (14%)	6 (3%)	<a href="#">6</a> <a href="#">10</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	12	24
3	F	63/65 (97%)	39 (62%)	16 (25%)	8 (13%)	0	0
All	All	994/1006 (99%)	826 (83%)	119 (12%)	49 (5%)	3	3

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	A	154	GLU
1	A	190	ASN
2	B	189	PRO
1	C	126	THR

### 5.3.2 Protein sidechains [i](#)

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	195/195 (100%)	156 (80%)	39 (20%)	1	2
1	C	195/195 (100%)	165 (85%)	30 (15%)	3	5
2	B	187/187 (100%)	157 (84%)	30 (16%)	3	5
2	D	187/187 (100%)	163 (87%)	24 (13%)	5	10
3	E	51/51 (100%)	40 (78%)	11 (22%)	1	2
3	F	51/51 (100%)	43 (84%)	8 (16%)	3	5
All	All	866/866 (100%)	724 (84%)	142 (16%)	3	4

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	186	SER
3	E	882	LYS
2	D	205	LYS
2	B	205	LYS
3	E	822	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	124	GLN
1	C	190	ASN
3	F	874	HIS
1	C	137	ASN
1	C	156	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	220/220 (100%)	-0.17	5 (2%) 64 57	28, 58, 108, 123	3 (1%)
1	C	220/220 (100%)	-0.33	2 (0%) 85 83	33, 66, 103, 122	3 (1%)
2	B	218/218 (100%)	-0.14	6 (2%) 56 49	29, 60, 100, 136	2 (0%)
2	D	218/218 (100%)	-0.12	10 (4%) 36 29	32, 68, 110, 137	2 (0%)
3	E	65/65 (100%)	-0.20	2 (3%) 52 45	43, 67, 94, 124	1 (1%)
3	F	65/65 (100%)	0.10	6 (9%) 11 7	56, 84, 115, 123	1 (1%)
All	All	1006/1006 (100%)	-0.17	31 (3%) 52 45	28, 66, 107, 137	12 (1%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	132	THR	6.5
2	B	128	SER	6.3
2	D	129	ALA	6.0
2	D	128	SER	5.3
2	D	210	ILE	5.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.