



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:45 pm BST

PDB ID : 2CKB  
Title : STRUCTURE OF THE 2C/KB/DEV8 COMPLEX  
Authors : Garcia, K.C.; Degano, M.; Wilson, I.A.  
Deposited on : 1998-01-14  
Resolution : 3.00 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

<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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

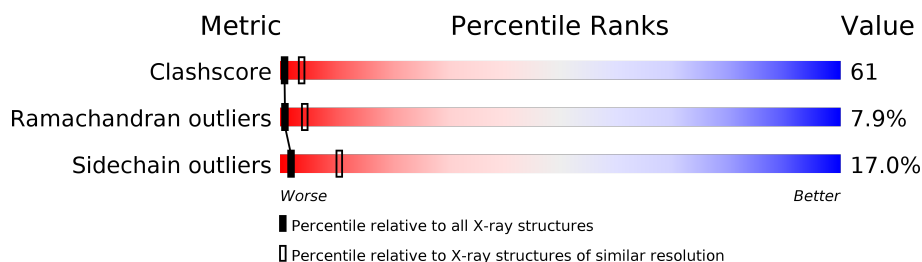
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
1	C	202	
2	B	237	
2	D	237	
3	H	274	
3	I	274	
4	P	8	
4	Q	8	

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Mol	Chain	Length	Quality of chain
5	L	99	<div><div></div><div>31%42%22%</div><div></div></div>
5	M	99	<div><div></div><div>27%45%23%</div><div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13110 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 ALPHA, BETA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			
1	C	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	CONFLICT	EMBL X01134
A	165	ALA	LYS	CONFLICT	EMBL X01134
C	127	ALA	GLN	CONFLICT	EMBL X01134
C	165	ALA	LYS	CONFLICT	EMBL X01134

- Molecule 2 is a protein called ALPHA, BETA T CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			
2	D	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	CONFLICT	GB 1791255
B	?	-	ARG	DELETION	GB 1791255
B	?	-	ALA	DELETION	GB 1791255
B	105	THR	GLU	CONFLICT	GB 1791255
B	106	LEU	GLN	CONFLICT	GB 1791255
B	107	TYR	PHE	CONFLICT	GB 1791255
B	110	ALA	PRO	CONFLICT	GB 1791255
B	115	SER	THR	CONFLICT	GB 1791255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	97	GLY	GLN	CONFLICT	GB 1791255
D	?	-	ARG	DELETION	GB 1791255
D	?	-	ALA	DELETION	GB 1791255
D	105	THR	GLU	CONFLICT	GB 1791255
D	106	LEU	GLN	CONFLICT	GB 1791255
D	107	TYR	PHE	CONFLICT	GB 1791255
D	110	ALA	PRO	CONFLICT	GB 1791255
D	115	SER	THR	CONFLICT	GB 1791255

- Molecule 3 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			
3	I	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

- Molecule 4 is a protein called DEV8 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	8	Total	C	N	O	0	0	0
			76	51	10	15			
4	Q	8	Total	C	N	O	0	0	0
			76	51	10	15			

- Molecule 5 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
5	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 6 is water.

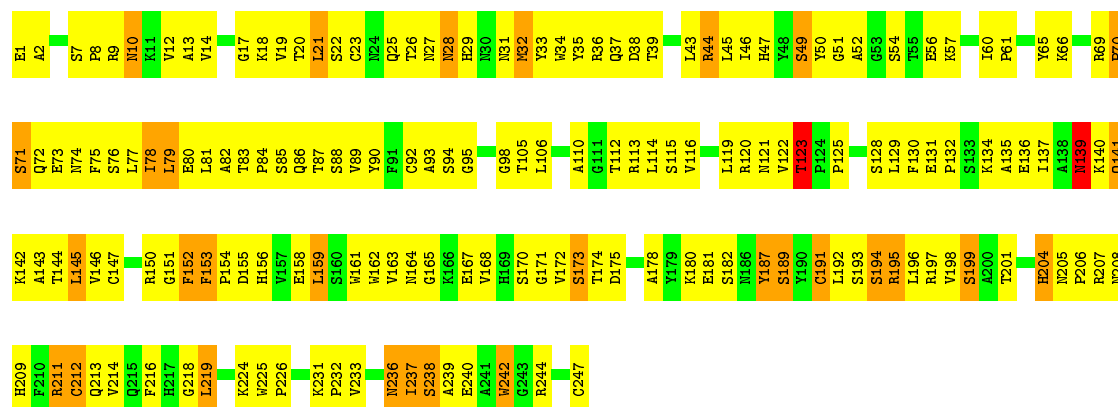
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

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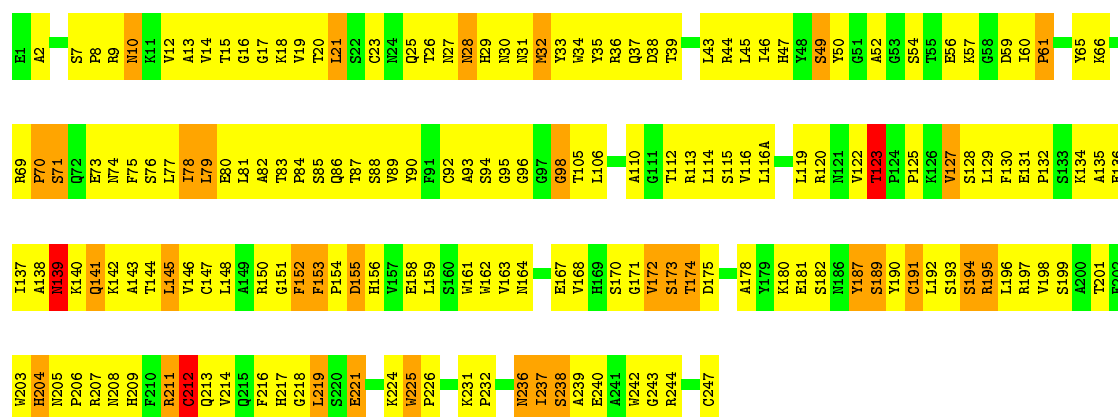
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	I	1	Total 1	O 1	0	0
6	Q	1	Total 1	O 1	0	0





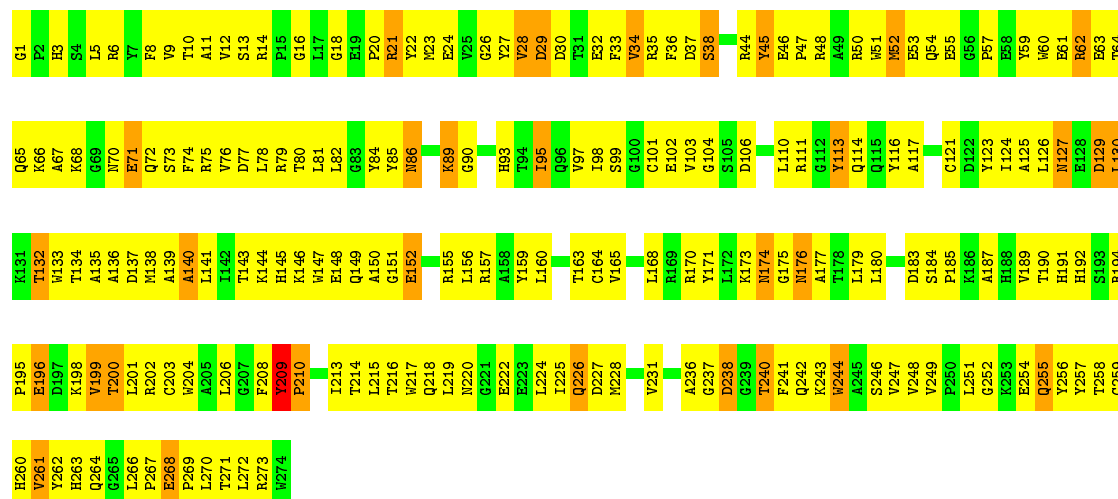
• Molecule 2: ALPHA, BETA T CELL RECEPTOR

Chain D: 25% 59% 14%



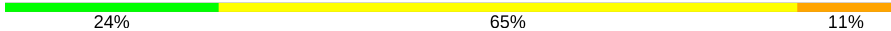
• Molecule 3: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B)

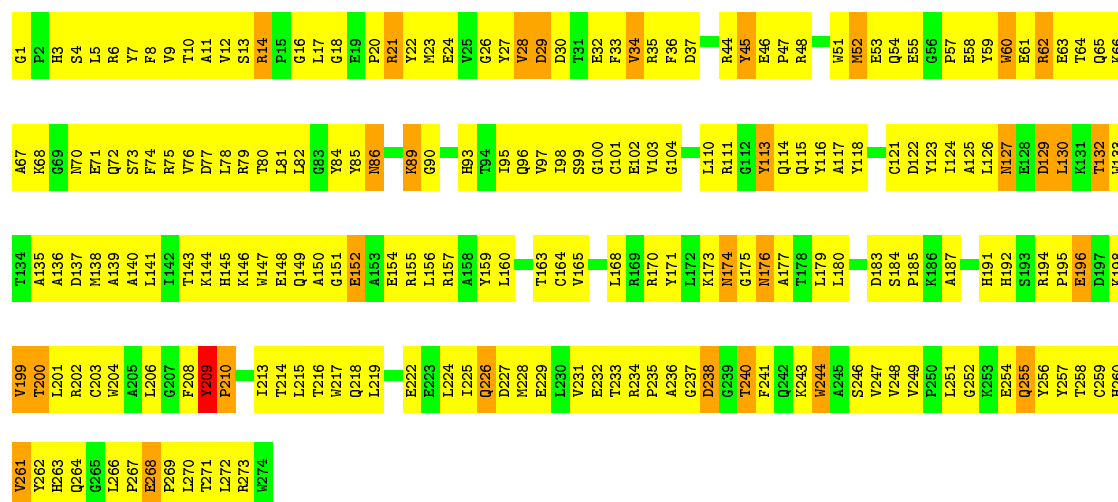
Chain H: 26% 62% 12%



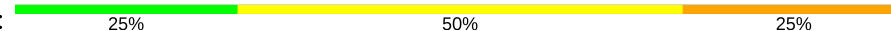
• Molecule 3: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS I MOLECULE K(B)

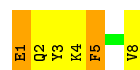


Chain I:  24% 65% 11%

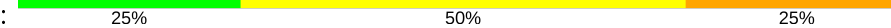


• Molecule 4: DEV8 PEPTIDE

Chain P:  25% 50% 25%




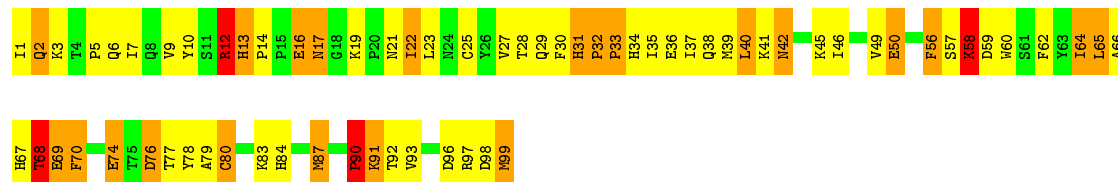
• Molecule 4: DEV8 PEPTIDE

Chain Q:  25% 50% 25%



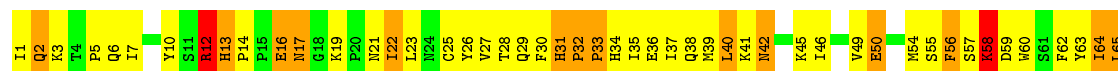
• Molecule 5: BETA-2 MICROGLOBULIN

Chain L:  31% 42% 22% •



• Molecule 5: BETA-2 MICROGLOBULIN

Chain M:  27% 45% 23% •



A66	H67	T68	E69	F70		T73	E74	T75	D76	T77	Y78	A79	C80		K83	H84		M87	A88	E89	P90	K91	T92	V93		D96	R97	D98	M99
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	295.66 Å   89.96 Å   84.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	25.00 – 3.00	Depositor
% Data completeness (in resolution range)	78.7 (25.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.221 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

## 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	0.55	0/1611	0.83	1/2193 (0.0%)
1	C	0.58	1/1611 (0.1%)	0.83	0/2193
2	B	0.52	1/1904 (0.1%)	0.77	1/2586 (0.0%)
2	D	0.66	1/1904 (0.1%)	0.81	1/2586 (0.0%)
3	H	0.51	0/2293	0.75	0/3113
3	I	0.52	0/2293	0.75	0/3113
4	P	0.61	0/78	0.84	0/102
4	Q	0.68	0/78	0.81	0/102
5	L	0.49	0/847	0.79	1/1148 (0.1%)
5	M	0.51	0/847	0.80	1/1148 (0.1%)
All	All	0.55	3/13466 (0.0%)	0.79	5/18284 (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	C	0	1
2	B	0	1
2	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	212	CYS	CB-SG	-6.18	1.71	1.82
2	B	212	CYS	CB-SG	-5.91	1.72	1.81
1	C	90	CYS	CB-SG	-5.24	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	175	ASP	N-CA-C	-5.99	94.82	111.00
1	A	140	LEU	CA-CB-CG	5.72	128.46	115.30
2	B	175	ASP	N-CA-C	-5.18	97.02	111.00
5	L	90	PRO	N-CA-C	5.07	125.29	112.10
5	M	90	PRO	N-CA-C	5.05	125.24	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	187	TYR	Sidechain
1	C	35	TYR	Sidechain
2	D	187	TYR	Sidechain

## 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	1570	0	1508	185	0
1	C	1570	0	1508	200	0
2	B	1853	0	1767	248	0
2	D	1853	0	1767	260	0
3	H	2232	0	2127	270	0
3	I	2232	0	2127	275	0
4	P	76	0	70	15	0
4	Q	76	0	70	17	0
5	L	821	0	798	98	0
5	M	821	0	798	103	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	2	0
6	H	1	0	0	1	0
6	I	1	0	0	1	0
6	Q	1	0	0	0	0
All	All	13110	0	12540	1558	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 61.

The worst 5 of 1558 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:B:153:PHE:CD1	2:B:154:PRO:HD3	1.82	1.14
1:A:146:PHE:HD2	1:A:150:ILE:HD11	1.03	1.14
3:H:138:MET:HA	3:H:141:LEU:HD12	1.31	1.13
3:H:215:LEU:HD21	3:H:261:VAL:HG13	1.33	1.10
2:D:181:GLU:HB3	2:D:189:SER:O	1.52	1.08

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	Percentiles	
1	A	200/202 (99%)	144 (72%)	35 (18%)	21 (10%)	0	2
1	C	200/202 (99%)	146 (73%)	32 (16%)	22 (11%)	0	2
2	B	235/237 (99%)	181 (77%)	43 (18%)	11 (5%)	2	14
2	D	235/237 (99%)	181 (77%)	44 (19%)	10 (4%)	2	15
3	H	272/274 (99%)	205 (75%)	50 (18%)	17 (6%)	1	7
3	I	272/274 (99%)	203 (75%)	53 (20%)	16 (6%)	1	9
4	P	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
4	Q	6/8 (75%)	3 (50%)	2 (33%)	1 (17%)	0	0
5	L	97/99 (98%)	65 (67%)	18 (19%)	14 (14%)	0	1
5	M	97/99 (98%)	65 (67%)	17 (18%)	15 (16%)	0	1
All	All	1620/1640 (99%)	1196 (74%)	296 (18%)	128 (8%)	1	4

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ALA

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Mol	Chain	Res	Type
1	A	71	SER
1	A	101	ALA
1	A	102	SER
1	A	137	ASP

### 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	176/176 (100%)	143 (81%)	33 (19%)	1	8
1	C	176/176 (100%)	146 (83%)	30 (17%)	2	10
2	B	200/200 (100%)	161 (80%)	39 (20%)	1	7
2	D	200/200 (100%)	158 (79%)	42 (21%)	1	5
3	H	232/232 (100%)	203 (88%)	29 (12%)	4	20
3	I	232/232 (100%)	203 (88%)	29 (12%)	4	20
4	P	8/8 (100%)	7 (88%)	1 (12%)	4	20
4	Q	8/8 (100%)	7 (88%)	1 (12%)	4	20
5	L	94/94 (100%)	76 (81%)	18 (19%)	1	8
5	M	94/94 (100%)	75 (80%)	19 (20%)	1	6
All	All	1420/1420 (100%)	1179 (83%)	241 (17%)	2	10

5 of 241 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	56	PHE
1	C	93	SER
5	M	2	GLN
5	L	65	LEU
1	C	19	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
4	P	2	GLN
1	C	192	GLN
3	I	260	HIS
1	C	74	HIS
2	D	25	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.