



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 11:06 am BST

PDB ID : 1AIF
Title : ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB FROM MOUSE
Authors : Ban, N.; Escobar, C.; Hasel, K.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1994-11-14
Resolution : 2.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (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

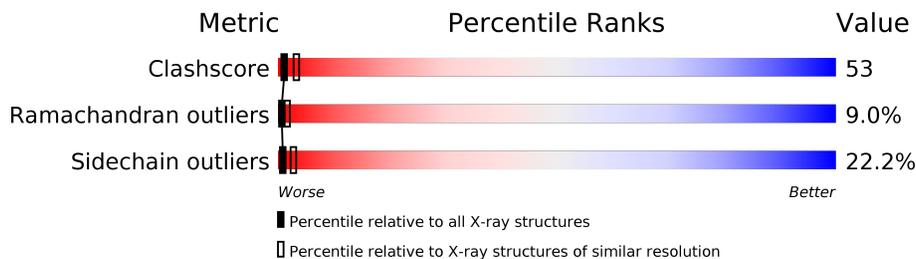
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 ≥ 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	215	
1	L	215	
2	B	218	
2	H	218	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6662 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 ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	215	1655	1029	273	345	8	0	0	0
1	A	215	1655	1029	273	345	8	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ASP	GLN	CONFLICT	UNP P01837
L	3	GLN	VAL	CONFLICT	UNP P01837
L	10	PHE	ILE	CONFLICT	UNP P01837
L	12	ALA	SER	CONFLICT	UNP P01837
L	18	LYS	ARG	CONFLICT	UNP P01837
L	21	ILE	MET	CONFLICT	UNP P01837
L	25	VAL	ALA	CONFLICT	UNP P01837
L	26	SER	ASN	CONFLICT	UNP P01837
L	28	SER	-	INSERTION	UNP P01837
L	29	ILE	-	INSERTION	UNP P01837
L	31	SER	VAL	CONFLICT	UNP P01837
L	33	ASN	TYR	CONFLICT	UNP P01837
L	34	LEU	MET	CONFLICT	UNP P01837
L	42	GLU	GLY	CONFLICT	UNP P01837
L	47	PRO	ARG	CONFLICT	UNP P01837
L	51	GLY	ASP	CONFLICT	UNP P01837
L	54	ASN	LYS	CONFLICT	UNP P01837
L	61	VAL	ALA	CONFLICT	UNP P01837
L	93	ASN	SER	CONFLICT	UNP P01837
L	95	TYR	HIS	CONFLICT	UNP P01837
L	114	PRO	GLN	CONFLICT	UNP P01837
A	1	ASP	GLN	CONFLICT	UNP P01837
A	3	GLN	VAL	CONFLICT	UNP P01837
A	10	PHE	ILE	CONFLICT	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	SER	CONFLICT	UNP P01837
A	18	LYS	ARG	CONFLICT	UNP P01837
A	21	ILE	MET	CONFLICT	UNP P01837
A	25	VAL	ALA	CONFLICT	UNP P01837
A	26	SER	ASN	CONFLICT	UNP P01837
A	28	SER	-	INSERTION	UNP P01837
A	29	ILE	-	INSERTION	UNP P01837
A	31	SER	VAL	CONFLICT	UNP P01837
A	33	ASN	TYR	CONFLICT	UNP P01837
A	34	LEU	MET	CONFLICT	UNP P01837
A	42	GLU	GLY	CONFLICT	UNP P01837
A	47	PRO	ARG	CONFLICT	UNP P01837
A	51	GLY	ASP	CONFLICT	UNP P01837
A	54	ASN	LYS	CONFLICT	UNP P01837
A	61	VAL	ALA	CONFLICT	UNP P01837
A	93	ASN	SER	CONFLICT	UNP P01837
A	95	TYR	HIS	CONFLICT	UNP P01837
A	114	PRO	GLN	CONFLICT	UNP P01837

- Molecule 2 is a protein called ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1676	1066	277	325	8			
2	B	218	Total	C	N	O	S	0	0	0
			1676	1066	277	325	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	GLN	GLU	CONFLICT	GB 1042226
H	20	LEU	VAL	CONFLICT	GB 1042226
H	28	THR	ALA	CONFLICT	GB 1042226
H	30	ASN	SER	CONFLICT	GB 1042226
H	31	ASN	TYR	CONFLICT	GB 1042226
H	35	SER	ASN	CONFLICT	GB 1042226
H	43	LYS	ARG	CONFLICT	GB 1042226
H	48	VAL	ILE	CONFLICT	GB 1042226
H	53	LEU	PHE	CONFLICT	GB 1042226
H	54	ASN	LYS	CONFLICT	GB 1042226
H	56	ASP	-	INSERTION	GB 1042226

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Chain	Residue	Modelled	Actual	Comment	Reference
H	58	PHE	ASN	CONFLICT	GB 1042226
H	59	ALA	TYR	CONFLICT	GB 1042226
H	69	LYS	ARG	CONFLICT	GB 1042226
H	71	ILE	THR	CONFLICT	GB 1042226
H	80	ARG	SER	CONFLICT	GB 1042226
H	81	LEU	VAL	CONFLICT	GB 1042226
H	87	SER	ASN	CONFLICT	GB 1042226
H	99	VAL	-	INSERTION	GB 1042226
H	100	LEU	THR	CONFLICT	GB 1042226
H	102	PRO	GLU	CONFLICT	GB 1042226
H	103	LEU	GLY	CONFLICT	GB 1042226
H	104	PHE	ILE	CONFLICT	GB 1042226
H	107	ALA	PRO	CONFLICT	GB 1042226
H	108	VAL	PHE	CONFLICT	GB 1042226
H	109	ASP	ALA	CONFLICT	GB 1042226
H	116	SER	LEU	CONFLICT	GB 1042226
H	121	SER	ALA	CONFLICT	GB 1042226
H	?	-	SER	DELETION	GB 1042226
H	196	ARG	-	INSERTION	GB 1042226
B	5	GLN	GLU	CONFLICT	GB 1042226
B	20	LEU	VAL	CONFLICT	GB 1042226
B	28	THR	ALA	CONFLICT	GB 1042226
B	30	ASN	SER	CONFLICT	GB 1042226
B	31	ASN	TYR	CONFLICT	GB 1042226
B	35	SER	ASN	CONFLICT	GB 1042226
B	43	LYS	ARG	CONFLICT	GB 1042226
B	48	VAL	ILE	CONFLICT	GB 1042226
B	53	LEU	PHE	CONFLICT	GB 1042226
B	54	ASN	LYS	CONFLICT	GB 1042226
B	56	ASP	-	INSERTION	GB 1042226
B	58	PHE	ASN	CONFLICT	GB 1042226
B	59	ALA	TYR	CONFLICT	GB 1042226
B	69	LYS	ARG	CONFLICT	GB 1042226
B	71	ILE	THR	CONFLICT	GB 1042226
B	80	ARG	SER	CONFLICT	GB 1042226
B	81	LEU	VAL	CONFLICT	GB 1042226
B	87	SER	ASN	CONFLICT	GB 1042226
B	99	VAL	-	INSERTION	GB 1042226
B	100	LEU	THR	CONFLICT	GB 1042226
B	102	PRO	GLU	CONFLICT	GB 1042226
B	103	LEU	GLY	CONFLICT	GB 1042226
B	104	PHE	ILE	CONFLICT	GB 1042226

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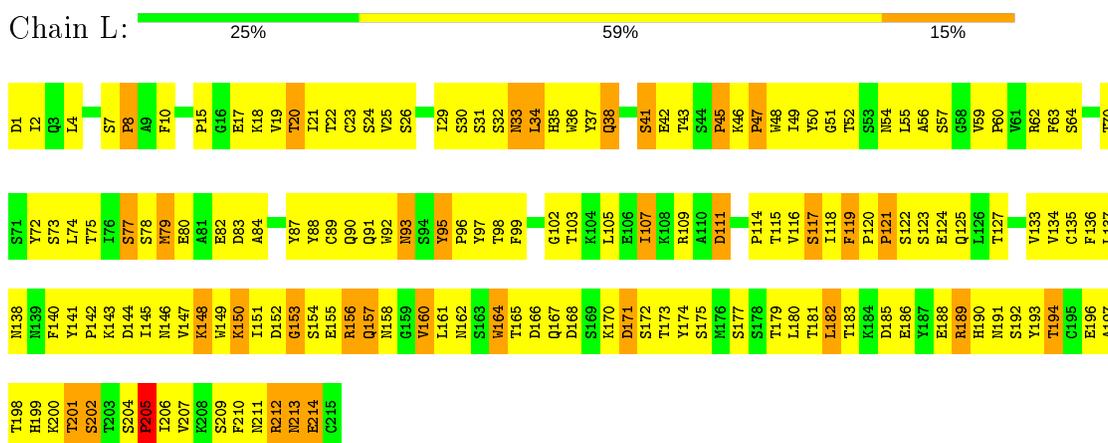
Chain	Residue	Modelled	Actual	Comment	Reference
B	107	ALA	PRO	CONFLICT	GB 1042226
B	108	VAL	PHE	CONFLICT	GB 1042226
B	109	ASP	ALA	CONFLICT	GB 1042226
B	116	SER	LEU	CONFLICT	GB 1042226
B	121	SER	ALA	CONFLICT	GB 1042226
B	?	-	SER	DELETION	GB 1042226
B	196	ARG	-	INSERTION	GB 1042226

3 Residue-property plots

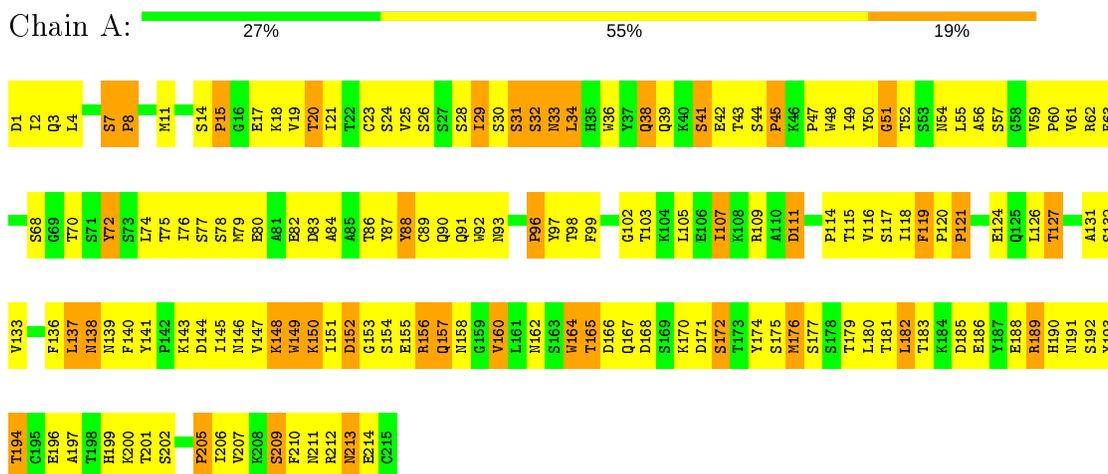
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN)

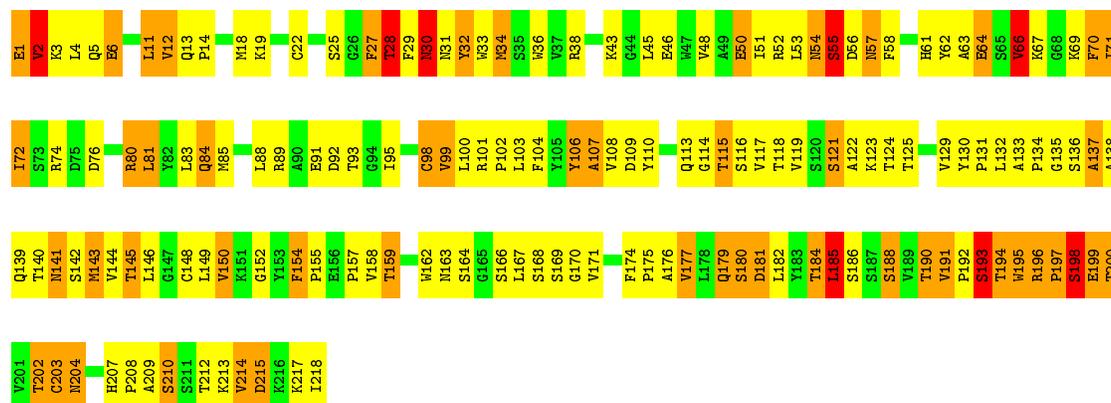


- Molecule 1: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN)



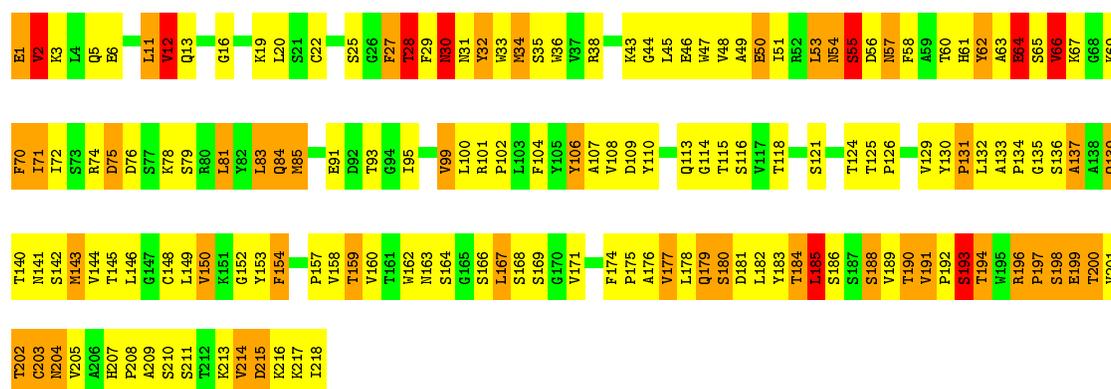
- Molecule 2: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN)





● Molecule 2: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN)

Chain B: 28% 48% 21%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.20 Å 71.20 Å 75.80 Å 85.30° 121.40° 116.50°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.0 (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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	0.91	1/1696 (0.1%)	1.04	2/2306 (0.1%)
1	L	0.97	1/1696 (0.1%)	1.06	4/2306 (0.2%)
2	B	1.05	2/1721 (0.1%)	1.21	14/2347 (0.6%)
2	H	1.05	6/1721 (0.3%)	1.23	12/2347 (0.5%)
All	All	1.00	10/6834 (0.1%)	1.14	32/9306 (0.3%)

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	0	1
2	B	0	2
2	H	0	2
All	All	0	5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	64	GLU	CB-CG	7.54	1.66	1.52
2	H	64	GLU	CB-CG	6.52	1.64	1.52
1	A	149	TRP	CB-CG	-6.15	1.39	1.50
2	H	194	THR	CA-CB	6.04	1.69	1.53
2	H	64	GLU	CG-CD	5.61	1.60	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	212	ARG	NE-CZ-NH2	-8.39	116.11	120.30
2	H	134	PRO	N-CA-C	8.38	133.89	112.10
2	B	28	THR	N-CA-C	-8.20	88.87	111.00
2	B	197	PRO	N-CA-C	-7.90	91.57	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	197	PRO	N-CA-C	-7.78	91.88	112.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TYR	Sidechain
2	B	28	THR	Mainchain
2	B	32	TYR	Sidechain
2	H	196	ARG	Mainchain
2	H	32	TYR	Sidechain

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	1655	0	1562	174	0
1	L	1655	0	1562	185	0
2	B	1676	0	1637	193	0
2	H	1676	0	1637	187	0
All	All	6662	0	6398	695	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 53.

The worst 5 of 695 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:H:48:VAL:HG13	2:H:66:VAL:HG11	1.34	1.08
2:B:48:VAL:HG13	2:B:66:VAL:HG11	1.34	1.05
2:B:53:LEU:HG	2:B:53:LEU:O	1.58	1.00
1:L:15:PRO:HG3	1:L:107:ILE:HD11	1.41	0.98
2:B:142:SER:HB2	2:B:193:SER:HB3	1.47	0.94

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	213/215 (99%)	160 (75%)	34 (16%)	19 (9%)	1	1
1	L	213/215 (99%)	164 (77%)	34 (16%)	15 (7%)	1	3
2	B	216/218 (99%)	161 (74%)	36 (17%)	19 (9%)	1	2
2	H	216/218 (99%)	161 (74%)	31 (14%)	24 (11%)	0	1
All	All	858/866 (99%)	646 (75%)	135 (16%)	77 (9%)	1	1

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	200	LYS
1	L	202	SER
1	L	205	PRO
2	H	30	ASN
2	H	54	ASN

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	190/190 (100%)	148 (78%)	42 (22%)	1	3
1	L	190/190 (100%)	153 (80%)	37 (20%)	1	4
2	B	189/189 (100%)	143 (76%)	46 (24%)	0	2
2	H	189/189 (100%)	146 (77%)	43 (23%)	1	2
All	All	758/758 (100%)	590 (78%)	168 (22%)	1	3

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	200	THR
1	A	96	PRO
2	B	179	GLN
2	H	204	ASN
1	A	33	ASN

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	179	GLN
1	A	35	HIS
2	B	172	HIS
2	H	204	ASN
1	A	33	ASN

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

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.