



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 07:46 AM GMT

PDB ID : 1YUH
Title : FAB FRAGMENT
Authors : Yuhasz, S.C.; Amzel, L.M.; Parry, C.; Strand, M.
Deposited on : 1996-01-30
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

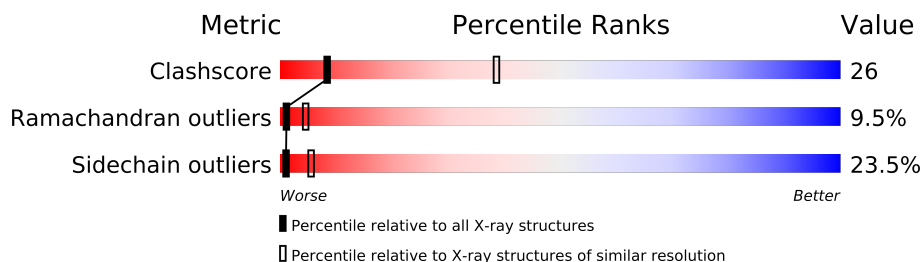
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	
1	L	211	
2	B	218	
2	H	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6530 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 88C6/12 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			
1	A	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	44	ARG	HIS	CONFLICT	GB 387376
L	57	GLY	ALA	CONFLICT	GB 387376
L	160	GLU	GLN	CONFLICT	GB 387376
L	184	SER	THR	CONFLICT	GB 387376
L	192	ALA	SER	CONFLICT	GB 387376
A	44	ARG	HIS	CONFLICT	GB 387376
A	57	GLY	ALA	CONFLICT	GB 387376
A	160	GLU	GLN	CONFLICT	GB 387376
A	184	SER	THR	CONFLICT	GB 387376
A	192	ALA	SER	CONFLICT	GB 387376

- Molecule 2 is a protein called 88C6/12 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			
2	B	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	9	ALA	PRO	CONFLICT	GB 3399661
H	20	LEU	MET	CONFLICT	GB 3399661

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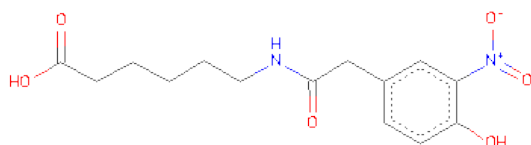
Chain	Residue	Modelled	Actual	Comment	Reference
H	33	LEU	VAL	CONFLICT	GB 3399661
H	37	ILE	VAL	CONFLICT	GB 3399661
H	40	ARG	LYS	CONFLICT	GB 3399661
H	43	ARG	GLN	CONFLICT	GB 3399661
H	50	ARG	TYR	CONFLICT	GB 3399661
H	52	ASP	ASN	CONFLICT	GB 3399661
H	54	ASN	TYR	CONFLICT	GB 3399661
H	56	VAL	ASP	CONFLICT	GB 3399661
H	57	VAL	GLY	CONFLICT	GB 3399661
H	60	PHE	TYR	CONFLICT	GB 3399661
H	66	SER	GLY	CONFLICT	GB 3399661
H	72	VAL	SER	CONFLICT	GB 3399661
H	75	PRO	SER	CONFLICT	GB 3399661
H	97	ALA	VAL	CONFLICT	GB 3399661
H	99	TYR	GLY	CONFLICT	GB 3399661
H	100	ALA	GLY	CONFLICT	GB 3399661
H	102	CYS	-	INSERTION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	TYR	DELETION	GB 3399661
H	?	-	ALA	DELETION	GB 3399661
H	113	THR	SER	CONFLICT	GB 3399661
H	120	ALA	LYS	CONFLICT	GB 3399661
H	163	ALA	SER	CONFLICT	GB 3399661
H	190	ALA	SER	CONFLICT	GB 3399661
H	196	GLY	GLU	CONFLICT	GB 3399661
H	210	ALA	LYS	CONFLICT	GB 3399661
B	9	ALA	PRO	CONFLICT	GB 3399661
B	20	LEU	MET	CONFLICT	GB 3399661
B	33	LEU	VAL	CONFLICT	GB 3399661
B	37	ILE	VAL	CONFLICT	GB 3399661
B	40	ARG	LYS	CONFLICT	GB 3399661
B	43	ARG	GLN	CONFLICT	GB 3399661
B	50	ARG	TYR	CONFLICT	GB 3399661
B	52	ASP	ASN	CONFLICT	GB 3399661
B	54	ASN	TYR	CONFLICT	GB 3399661
B	56	VAL	ASP	CONFLICT	GB 3399661
B	57	VAL	GLY	CONFLICT	GB 3399661
B	60	PHE	TYR	CONFLICT	GB 3399661
B	66	SER	GLY	CONFLICT	GB 3399661
B	72	VAL	SER	CONFLICT	GB 3399661
B	75	PRO	SER	CONFLICT	GB 3399661
B	97	ALA	VAL	CONFLICT	GB 3399661

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	GLY	CONFLICT	GB 3399661
B	100	ALA	GLY	CONFLICT	GB 3399661
B	102	CYS	-	INSERTION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	TYR	DELETION	GB 3399661
B	?	-	ALA	DELETION	GB 3399661
B	113	THR	SER	CONFLICT	GB 3399661
B	120	ALA	LYS	CONFLICT	GB 3399661
B	163	ALA	SER	CONFLICT	GB 3399661
B	190	ALA	SER	CONFLICT	GB 3399661
B	196	GLY	GLU	CONFLICT	GB 3399661
B	210	ALA	LYS	CONFLICT	GB 3399661

- Molecule 3 is 4-HYDROXY-3-NITROPHENYLACETYL-EPSILON-AMINOCAPROIC ACID (three-letter code: NP) (formula: C₁₄H₁₈N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			22	14	2	6		
3	B	1	Total	C	N	O	0	0
			22	14	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

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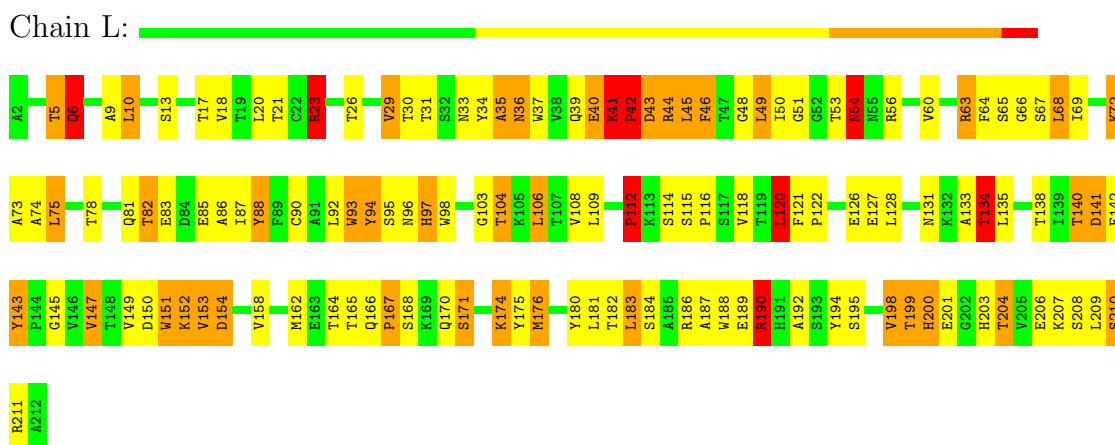
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	3	Total	O	0	0
			3	3		

3 Residue-property plots

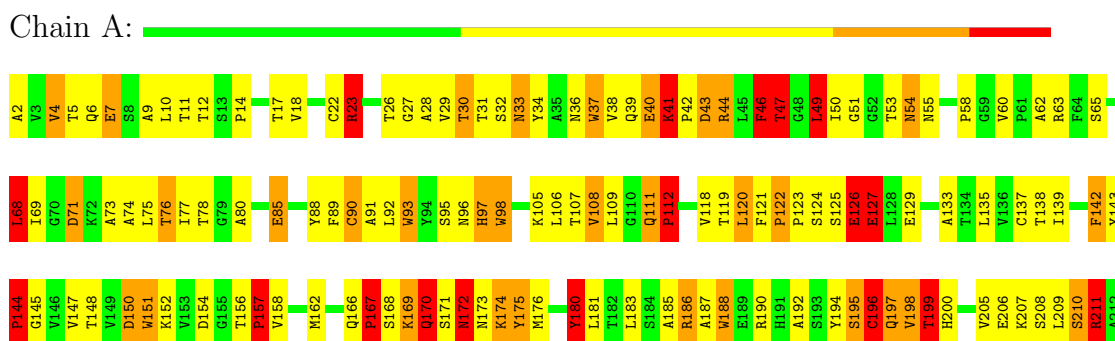
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

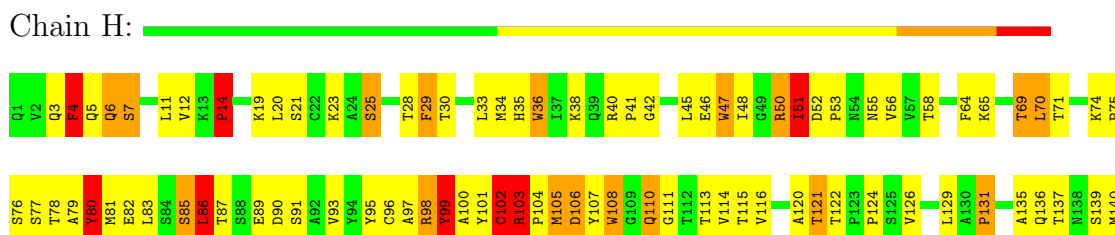
• Molecule 1: 88C6/12 FAB (LIGHT CHAIN)



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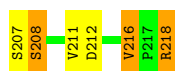


• Molecule 2: 88C6/12 FAB (HEAVY CHAIN)





Chain B:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.20Å 86.90Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NP

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	0.93	0/1630	2.06	55/2224 (2.5%)
1	L	0.93	0/1630	2.03	59/2224 (2.7%)
2	B	0.92	0/1691	2.10	64/2311 (2.8%)
2	H	0.92	0/1691	2.06	54/2311 (2.3%)
All	All	0.92	0/6642	2.06	232/9070 (2.6%)

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	6
2	B	0	6
2	H	0	2
All	All	0	14

There are no bond length outliers.

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	TYR	CB-CG-CD2	-12.10	113.74	121.00
1	L	190	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	B	98	ARG	NE-CZ-NH2	-10.58	115.01	120.30
2	H	99	TYR	CB-CG-CD1	-10.56	114.66	121.00
2	B	36	TRP	CD1-CG-CD2	10.53	114.72	106.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	A	143	TYR	Peptide
1	A	41	LYS	Peptide
2	H	193	TRP	Peptide
2	H	99	TYR	Sidechain

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	1594	0	1538	96	0
1	L	1594	0	1538	80	0
2	B	1647	0	1622	98	0
2	H	1647	0	1622	107	0
3	B	22	0	16	2	0
3	H	22	0	16	1	0
4	H	1	0	0	0	0
4	L	3	0	0	0	0
All	All	6530	0	6352	337	0

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 26.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:ASP:HB2	1:A:197:GLN:HB3	1.38	1.02
2:H:105:MET:HG2	2:H:108:TRP:HE1	1.32	0.94
2:B:39:GLN:HB3	2:B:93:VAL:HB	1.55	0.88
2:H:19:LYS:HD2	2:H:80:TYR:HB3	1.57	0.86
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.58	0.86

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	207/211 (98%)	149 (72%)	41 (20%)	17 (8%)	1	6
1	L	207/211 (98%)	164 (79%)	28 (14%)	15 (7%)	2	8
2	B	214/218 (98%)	155 (72%)	35 (16%)	24 (11%)	1	3
2	H	214/218 (98%)	167 (78%)	23 (11%)	24 (11%)	1	3
All	All	842/858 (98%)	635 (75%)	127 (15%)	80 (10%)	1	4

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	112	PRO
1	L	154	ASP
1	L	167	PRO
1	L	171	SER
2	H	7	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	177/177 (100%)	133 (75%)	44 (25%)	1	4
1	L	177/177 (100%)	127 (72%)	50 (28%)	0	3
2	B	185/185 (100%)	143 (77%)	42 (23%)	1	6
2	H	185/185 (100%)	151 (82%)	34 (18%)	2	13
All	All	724/724 (100%)	554 (76%)	170 (24%)	1	5

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	158	THR
1	A	71	ASP
2	B	175	LEU
2	H	164	LEU
1	A	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	54	ASN
2	B	3	GLN
2	H	54	ASN
1	A	197	GLN

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NP	B	996	-	22,22,22	2.03	2 (9%)	28,28,28	4.28	8 (28%)
3	NP	H	995	-	22,22,22	1.93	3 (13%)	28,28,28	7.86	10 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NP	B	996	-	-	0/17/17/17	0/1/1/1
3	NP	H	995	-	-	0/17/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	996	NP	C5'-N5'	-8.03	1.34	1.46
3	H	995	NP	C5'-N5'	-6.94	1.35	1.46
3	H	995	NP	ON2-N5'	3.56	1.29	1.23
3	B	996	NP	ON2-N5'	3.03	1.28	1.23
3	H	995	NP	ON1-N5'	2.42	1.30	1.25

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	995	NP	C1-C2-N3	28.27	158.28	116.21
3	H	995	NP	O2-C2-N3	-25.44	72.51	122.94
3	B	996	NP	O2-C2-C1	-14.55	79.46	121.91
3	H	995	NP	O2-C2-C1	-12.38	85.79	121.91
3	B	996	NP	C6'-C5'-N5'	9.78	125.63	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.