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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 08:38 am BST

PDB ID	:	3BQU
Title	:	Crystal Structure of the 2F5 Fab'-3H6 Fab Complex
Authors	:	Bryson, S.; Julien, J.-P.; Isenman, D.E.; Kunert, R.; Katinger, H.; Pai, E.F.
Deposited on	:	2007-12-20
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

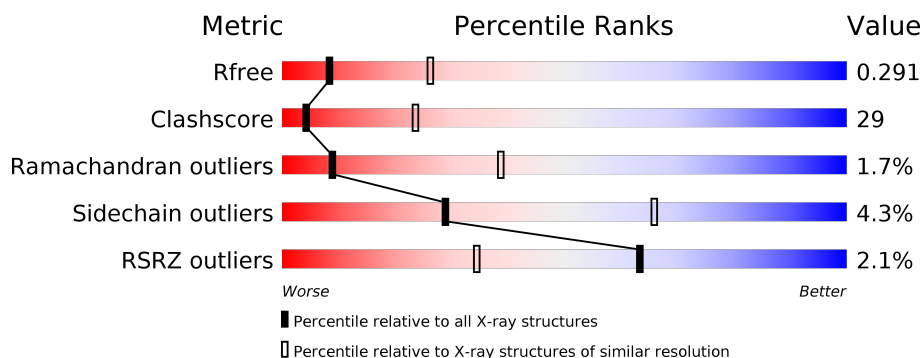|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.291
Clashscore		29
Ramachandran outliers		1.7%
Sidechain outliers		4.3%
RSRZ outliers		2.1%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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 <=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	214	44% / 49% / 6% ·
2	B	235	% / 50% / 39% · / 9%
3	C	233	5% / 38% / 39% · / 20%
4	D	241	% / 51% / 37% · / 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6322 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 2F5 Fab' light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1624	1015	278	327	4			

- Molecule 2 is a protein called 2F5 Fab' heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1612	1028	271	307	6			

- Molecule 3 is a protein called 3H6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	186	Total	C	N	O	S	0	0	0
			1445	903	235	301	6			

- Molecule 4 is a protein called 3H6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	217	Total	C	N	O	S	0	0	0
			1636	1042	265	320	9			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ —— S —— O⁻ O4

S

O

O2

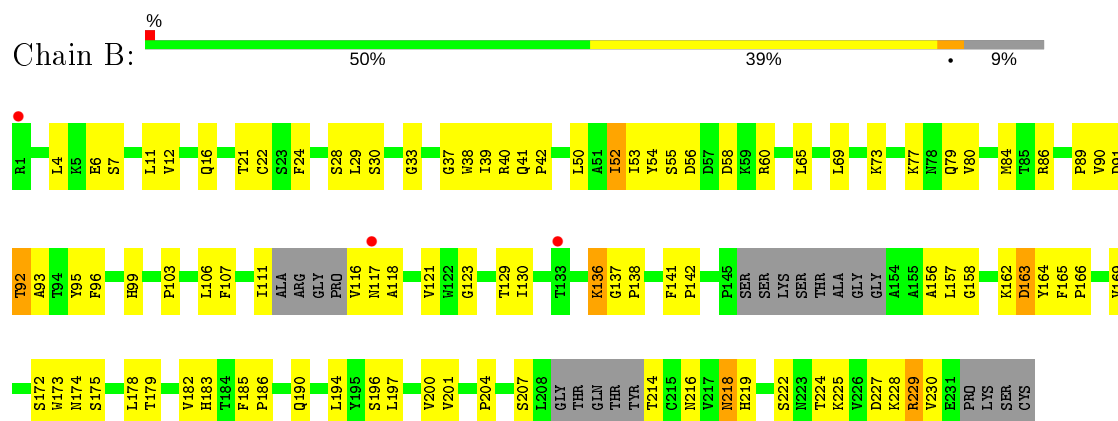| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

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 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.
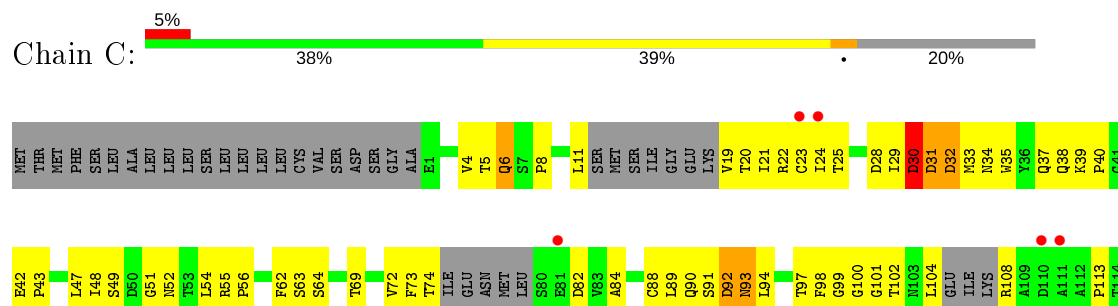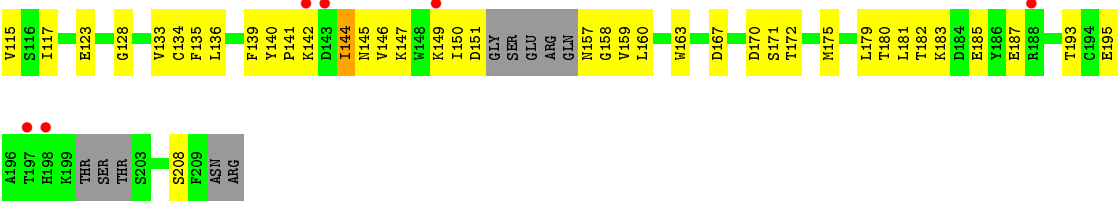
- Molecule 1: 2F5 Fab' light chain
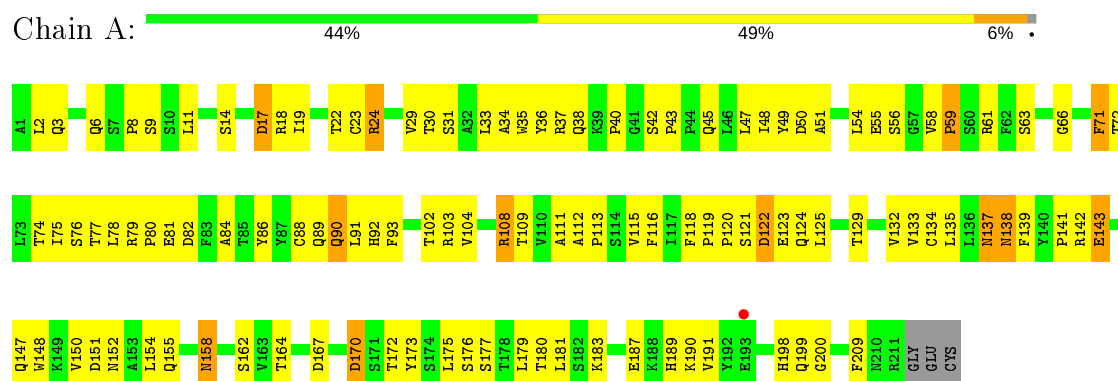
Chain A:
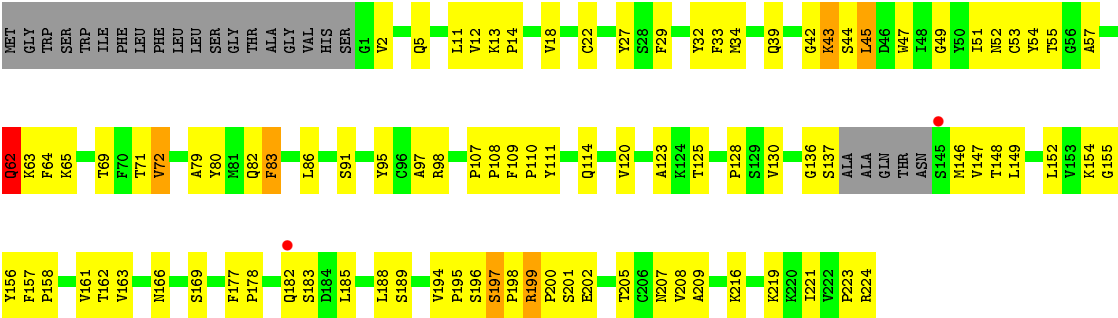

- Molecule 2: 2F5 Fab' heavy chain

Chain B:

- Molecule 3: 3H6 Fab light chain

Chain C:

V115 S116 I117 E123 G128 V133 C134 F135 L136 F139 Y140 P141 K142 D143 I144 N145 V146 K147 W148 K149 I150 D151 GLY SER GLU GLN N157 G158 V159 L160 W163 D167 D170 S171 T172 M175 L179 T180 L181 T182 K183 D184 E185 Y186 E187 R188 T193 C194 E195

A196 T197 H198 K199 THR SER THR S203 S208 F209 ASN ARG

• Molecule 4: 3H6 Fab heavy chain

Chain D:

%

51%   37%   •   10%

MET GLY TRP SER TRP ILE PHE LEU PHE LEU SER GLY THR ALA GLY VAL HIS SER G1 V2 Q5 L11 V12 K13 P14 V18 C22 Y27 S28 F29 Y32 F33 M34 Q39 G42 K43 S44 L45 D46 W47 I48 G49 Y50 I51 N52 C53 Y54 T55 G56 A57

Q62 K63 F64 K65 T69 F70 T71 V72 A79 Y80 M81 Q82 F83 L86 S91 Y95 C96 A97 R98 P107 P108 F109 P110 Y111 Q114 V120 A123 K124 T125 P128 S129 V130 G136 S137 ALA ALA GLN THR ASN S145 M146 V147 T148 L149 L152 V153 K154 G155

Y156 F157 P158 V161 T162 V163 N166 S169 F177 P178 Q182 S183 D184 L185 L188 S189 V194 P195 S196 S197 P198 R199 P200 S201 E202 T205 C206 N207 V208 A209 K216 K219 K220 I221 V222 P223 R224

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.44Å 98.33Å 154.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 35.93 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 96.8 (35.93-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	3.78 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.276 , 0.295 0.279 , 0.291	Depositor DCC
R_{free} test set	1061 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	74.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.8	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6322	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.26	0/1661	0.51	0/2259
2	B	0.26	0/1649	0.53	0/2253
3	C	0.27	0/1476	0.51	0/2007
4	D	0.28	0/1684	0.53	0/2299
All	All	0.27	0/6470	0.52	0/8818

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1624	0	1574	107	0
2	B	1612	0	1630	87	0
3	C	1445	0	1355	96	0
4	D	1636	0	1590	88	0
5	D	5	0	0	0	0
All	All	6322	0	6149	365	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 29.

The worst 5 of 365 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)
4:D:199:ARG:HD2	4:D:200:PRO:HA	1.49	0.95
1:A:11:LEU:HD21	1:A:104:VAL:HG22	1.53	0.90
4:D:43:LYS:HE2	4:D:43:LYS:HA	1.54	0.89
1:A:170:ASP:HB3	1:A:172:THR:HG22	1.55	0.88
3:C:6:GLN:HG3	3:C:101:GLY:H	1.42	0.85

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	209/214 (98%)	186 (89%)	19 (9%)	4 (2%)	8	36
2	B	206/235 (88%)	172 (84%)	32 (16%)	2 (1%)	15	53
3	C	174/233 (75%)	148 (85%)	23 (13%)	3 (2%)	9	39
4	D	213/241 (88%)	188 (88%)	20 (9%)	5 (2%)	6	30
All	All	802/923 (87%)	694 (86%)	94 (12%)	14 (2%)	9	39

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	LYS
1	A	122	ASP
1	A	138	ASN
2	B	163	ASP
3	C	30	ASP

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	185/187 (99%)	176 (95%)	9 (5%)	25	61
2	B	188/203 (93%)	178 (95%)	10 (5%)	22	58
3	C	168/210 (80%)	160 (95%)	8 (5%)	25	62
4	D	187/205 (91%)	183 (98%)	4 (2%)	53	82
All	All	728/805 (90%)	697 (96%)	31 (4%)	29	66

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	99	HIS
2	B	227	ASP
4	D	72	VAL
2	B	136	LYS
2	B	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	174	ASN
2	B	216	ASN
4	D	77	ASN
2	B	183	HIS
2	B	218	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)

1 ligand is 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	#$|Z| > 2$
5	SO4	D	225	-	4,4,4	0.27	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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(Å²)	Q<0.9
1	A	211/214 (98%)	0.04	1 (0%)	91	75	43, 68, 84, 109	0
2	B	214/235 (91%)	-0.00	3 (1%)	75	49	37, 60, 83, 97	0
3	C	186/233 (79%)	0.50	11 (5%)	22	7	57, 82, 100, 116	0
4	D	217/241 (90%)	-0.03	2 (0%)	84	63	35, 55, 82, 101	0
All	All	828/923 (89%)	0.11	17 (2%)	63	34	35, 65, 92, 116	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	133	THR	3.9
3	C	23	CYS	3.2
3	C	24	ILE	3.0
3	C	198	HIS	3.0
1	A	193	GLU	2.7

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	SO4	D	225	5/5	0.97	0.14	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.