wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1BLN
Title	:	ANTI-P-GLYCOPROTEIN FAB MRK-16
Authors	:	Vasudevan, S.; Tsuruo, T.; Rose, D.R.
Deposited on	:	1998-07-16
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/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:

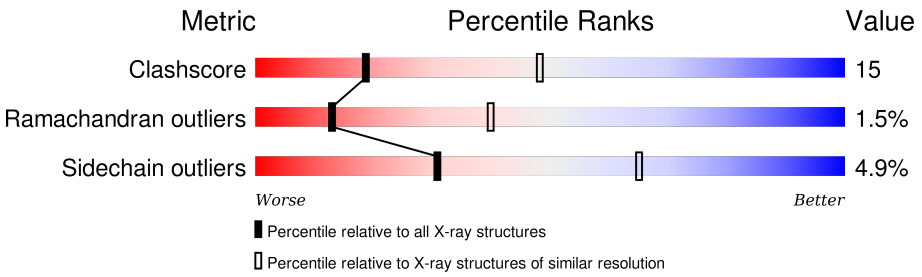
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	66% 30% •
1	C	214	65% 30% •
2	B	218	61% 37% •
2	D	218	65% 33% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6606 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 PROTEIN (MONOCLONAL ANTIBODY MRK-16 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1656	1033	281	335	7	0	0	0
1	C	214	1656	1033	281	335	7	0	0	0

- Molecule 2 is a protein called PROTEIN (MONOCLONAL ANTIBODY MRK-16 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1647	1045	270	325	7	0	0	0
2	D	218	1647	1045	270	325	7	0	0	0

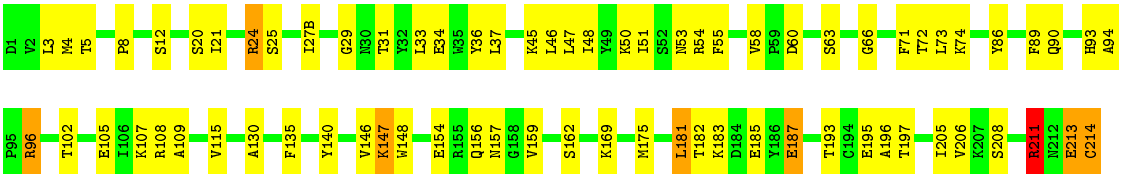
3 Residue-property plots (i)

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.

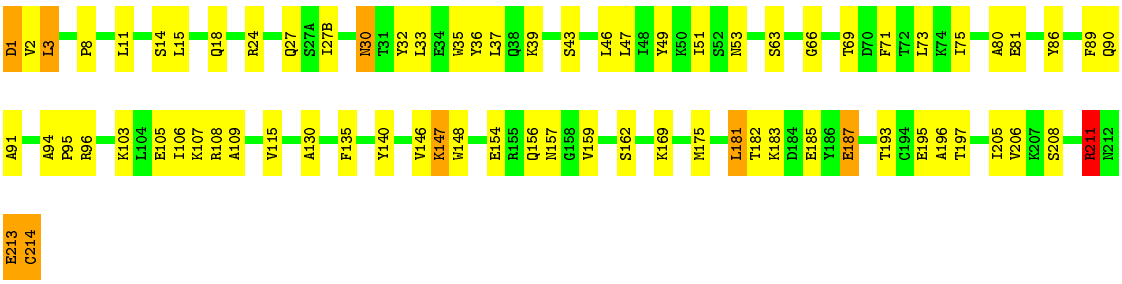
• Molecule 1: PROTEIN (MONOCLONAL ANTIBODY MRK-16 (LIGHT CHAIN))

Chain A:



• Molecule 1: PROTEIN (MONOCLONAL ANTIBODY MRK-16 (LIGHT CHAIN))

Chain C:

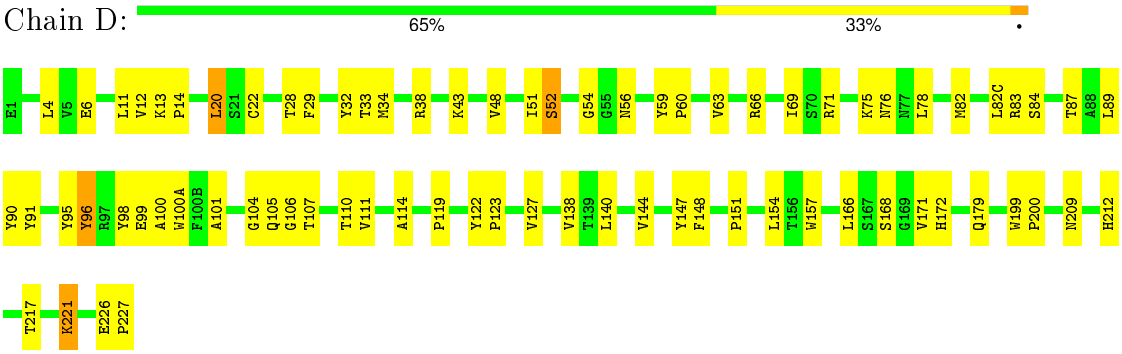


• Molecule 2: PROTEIN (MONOCLONAL ANTIBODY MRK-16 (HEAVY CHAIN))

Chain B:

• Molecule 2: PROTEIN (MONOCLONAL ANTIBODY MRK-16 (HEAVY CHAIN))

Chain D:


65%
33%
E1
L4
V5
E6
L11
V12
K13
P14
L20
S21
C22
T28
F29
Y32
T33
M34
R38
K43
V48
I51
S52
G54
G55
N56
Y59
P60
V63
R66
I69
S70
R71
K75
N76
N77
L78
M82
L82C
R83
S84
T87
A88
L89
Y90
Y91
Y95
Y96
R97
Y98
E99
A100
W100A
F100B
A101
G104
Q105
G106
T107
T110
V111
A114
P119
Y122
P123
V127
V138
T139
L140
V144
Y147
F148
P151
L154
T156
W157
L166
S167
S168
G169
V171
H172
Q179
W199
P200
N209
H212
T217
K221
E226
P227

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.49Å 67.77Å 117.19Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	80.0 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6606	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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	0.35	0/1691	0.64	0/2290
1	C	0.35	0/1691	0.63	0/2290
2	B	0.34	0/1690	0.61	0/2308
2	D	0.35	0/1690	0.64	0/2308
All	All	0.35	0/6762	0.63	0/9196

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	1656	0	1597	49	0
1	C	1656	0	1597	52	0
2	B	1647	0	1609	56	0
2	D	1647	0	1609	49	0
All	All	6606	0	6412	200	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 15.

The worst 5 of 200 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:A:66:GLY:HA2	1:A:71:PHE:HA	1.49	0.90
2:B:9:GLY:HA2	2:B:109:VAL:HG12	1.53	0.89
2:D:82:MET:HB3	2:D:82(C):LEU:HD21	1.61	0.81
2:D:96:TYR:HB2	2:D:101:ALA:HB2	1.63	0.81
1:A:45:LYS:HZ1	1:A:55:PHE:HD2	1.26	0.80

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	210/214 (98%)	189 (90%)	18 (9%)	3 (1%)	14	42
1	C	210/214 (98%)	192 (91%)	14 (7%)	4 (2%)	10	32
2	B	216/218 (99%)	199 (92%)	14 (6%)	3 (1%)	14	42
2	D	216/218 (99%)	195 (90%)	18 (8%)	3 (1%)	14	42
All	All	852/864 (99%)	775 (91%)	64 (8%)	13 (2%)	13	40

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	168	SER
2	D	168	SER
1	A	29	GLY
1	A	154	GLU
1	A	211	ARG

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%)	179 (94%)	11 (6%)	25	57
1	C	190/190 (100%)	178 (94%)	12 (6%)	22	53
2	B	185/185 (100%)	178 (96%)	7 (4%)	40	74
2	D	185/185 (100%)	178 (96%)	7 (4%)	40	74
All	All	750/750 (100%)	713 (95%)	37 (5%)	31	65

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	221	LYS
1	C	24	ARG
2	D	179	GLN
2	B	226	GLU
1	C	1	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	38	GLN
2	D	77	ASN
1	C	53	ASN
1	A	93	HIS
2	D	39	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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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