wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:37 PM GMT

PDB ID	:	1BOG
Title	:	ANTI-P24 (HIV-1) FAB FRAGMENT CB41 COMPLEXED WITH AN EPITOPE-HOMOLOGOUS PEPTIDE
Authors	:	Keitel, T.; Kramer, A.; Wessner, H.; Scholz, C.; Schneider-Mergener, J.; Hoehne, W.
Deposited on	:	1998-08-04
Resolution	:	2.60 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:

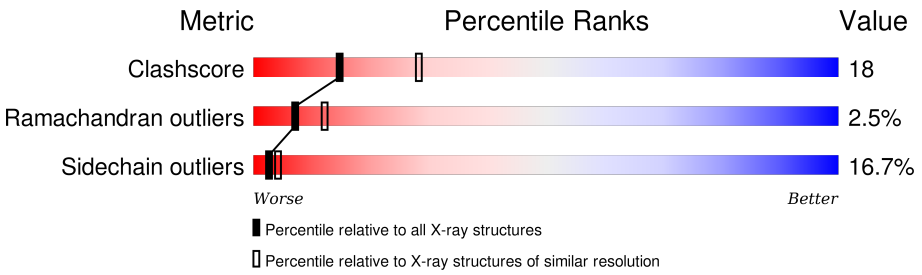
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	58% 32% 8% •
2	B	213	60% 33% 7%
3	C	11	27% 36% 18% 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3404 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 ANTIBODY (CB 4-1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1680	1054	276	340	10	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	THR	ALA	CONFLICT	GB 387371
A	22	THR	SER	CONFLICT	GB 387371
A	32	PHE	TYR	CONFLICT	GB 387371
A	37	LEU	GLN	CONFLICT	GB 387371
A	48	ILE	LEU	CONFLICT	GB 387371
A	55	MET	VAL	CONFLICT	GB 387371
A	56	ILE	ASP	CONFLICT	GB 387371
A	70	THR	ASP	CONFLICT	GB 387371
A	71	TYR	PHE	CONFLICT	GB 387371
A	93	ASP	GLU	CONFLICT	GB 387371
A	105	ASP	GLU	CONFLICT	GB 387371
A	129	THR	GLY	CONFLICT	GB 387371
A	143	GLU	ASP	CONFLICT	GB 387371
A	161	ASP	ASN	CONFLICT	GB 387371
A	165	GLU	ASP	CONFLICT	GB 387371

- Molecule 2 is a protein called ANTIBODY (CB 4-1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	1594	1011	263	314	6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ASP	ILE	CONFLICT	UNP P01864

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	ALA	PRO	CONFLICT	UNP P01864
B	20	LEU	ILE	CONFLICT	UNP P01864
B	25	LEU	SER	CONFLICT	UNP P01864
B	28	ILE	THR	CONFLICT	UNP P01864
B	33	GLU	TYR	CONFLICT	UNP P01864
B	40	THR	ARG	CONFLICT	UNP P01864
B	42	VAL	GLY	CONFLICT	UNP P01864
B	43	HIS	GLU	CONFLICT	UNP P01864
B	50	GLY	TRP	CONFLICT	UNP P01864
B	52	HIS	TYR	CONFLICT	UNP P01864
B	56	SER	GLY	CONFLICT	UNP P01864
B	57	GLY	ASN	CONFLICT	UNP P01864
B	59	ALA	LYS	CONFLICT	UNP P01864
B	62	GLN	GLU	CONFLICT	UNP P01864
B	72	ALA	VAL	CONFLICT	UNP P01864
B	74	LYS	THR	CONFLICT	UNP P01864
B	77	THR	SER	CONFLICT	UNP P01864
B	80	PHE	TYR	CONFLICT	UNP P01864
B	82	GLU	GLN	CONFLICT	UNP P01864
B	95	TYR	PHE	CONFLICT	UNP P01864
B	97	THR	ALA	CONFLICT	UNP P01864
B	?	-	GLY	DELETION	UNP P01864
B	?	-	GLY	DELETION	UNP P01864
B	?	-	LYS	DELETION	UNP P01864
B	?	-	PHE	DELETION	UNP P01864
B	?	-	ALA	DELETION	UNP P01864
B	99	LYS	MET	CONFLICT	UNP P01864
B	107	LEU	SER	CONFLICT	UNP P01864
B	112	ALA	SER	CONFLICT	UNP P01864
B	124	VAL	ALA	CONFLICT	UNP P01864
B	129	GLY	ASP	CONFLICT	UNP P01864
B	168	LEU	VAL	CONFLICT	UNP P01864
B	172	GLY	ASP	CONFLICT	UNP P01864
B	185	ASN	SER	CONFLICT	UNP P01864
B	191	THR	SER	CONFLICT	UNP P01864

- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	82	50	14	18	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	26	26	26	0	0
			Total	O		
4	B	20	20	20	0	0
			Total	O		
4	C	2	2	2	0	0

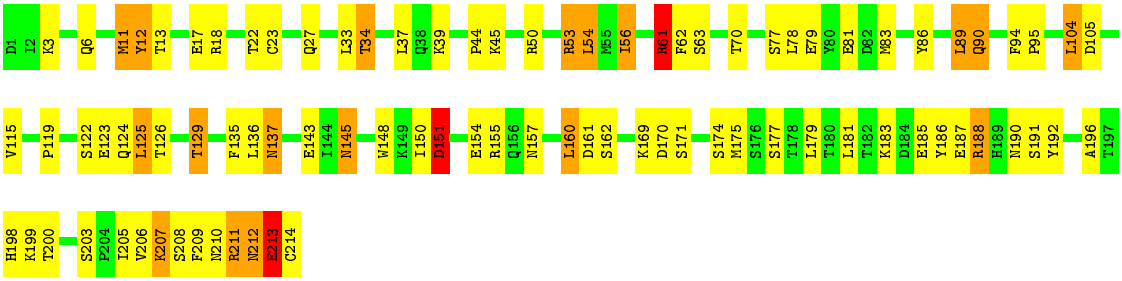
3 Residue-property plots (i)

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.

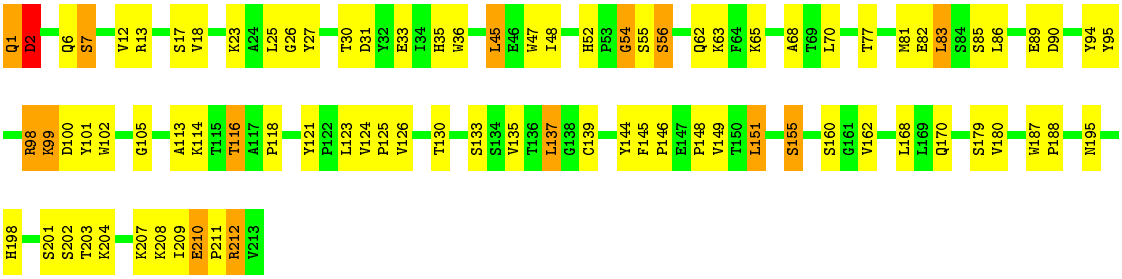
- Molecule 1: ANTIBODY (CB 4-1)

Chain A:



- Molecule 2: ANTIBODY (CB 4-1)

Chain B:



- Molecule 3: PEPTIDE

Chain C:

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 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	104.43Å 104.43Å 295.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	91.00 – 2.60	Depositor
% Data completeness (in resolution range)	96.0 (91.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.307	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3404	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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	0.62	0/1717	1.56	12/2326 (0.5%)
2	B	0.59	0/1634	1.36	11/2233 (0.5%)
3	C	0.76	0/82	2.36	3/110 (2.7%)
All	All	0.61	0/3433	1.49	26/4669 (0.6%)

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	4
2	B	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH2	24.50	132.55	120.30
1	A	61	ARG	NE-CZ-NH1	-15.38	112.61	120.30
3	C	5	GLU	O-C-N	-14.80	99.01	122.70
1	A	11	MET	CA-CB-CG	9.63	129.68	113.30
1	A	53	ARG	NE-CZ-NH1	9.18	124.89	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Mainchain
1	A	125	LEU	Mainchain
1	A	188	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	77	SER	Mainchain
2	B	89	GLU	Mainchain

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	1680	0	1628	60	1
2	B	1594	0	1576	64	0
3	C	82	0	83	10	0
4	A	26	0	0	1	3
4	B	20	0	0	1	2
4	C	2	0	0	0	0
All	All	3404	0	3287	118	3

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 18.

The worst 5 of 118 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:162:VAL:HG22	2:B:180:VAL:HG12	1.47	0.94
1:A:210:ASN:HD22	1:A:214:CYS:HA	1.31	0.93
2:B:30:THR:HG23	2:B:54:GLY:HA2	1.52	0.90
2:B:155:SER:H	2:B:195:ASN:HD21	1.17	0.90
2:B:155:SER:H	2:B:195:ASN:ND2	1.76	0.83

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:236:HOH:O	4:B:230:HOH:O[7_556]	1.68	0.52
4:A:234:HOH:O	4:B:232:HOH:O[5_564]	1.79	0.41
1:A:81:GLU:CD	4:A:238:HOH:O[7_556]	1.97	0.23

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	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	21 42
2	B	211/213 (99%)	192 (91%)	14 (7%)	5 (2%)	7 13
3	C	9/11 (82%)	5 (56%)	0	4 (44%)	0 0
All	All	432/438 (99%)	398 (92%)	23 (5%)	11 (2%)	7 12

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	5	GLU
2	B	130	THR
3	C	7	LEU
1	A	213	GLU
2	B	99	LYS

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	194/194 (100%)	156 (80%)	38 (20%)	1 2
2	B	180/180 (100%)	157 (87%)	23 (13%)	5 10
3	C	9/9 (100%)	6 (67%)	3 (33%)	0 0
All	All	383/383 (100%)	319 (83%)	64 (17%)	3 4

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	MET
1	A	208	SER
2	B	208	LYS
1	A	177	SER
1	A	203	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1	GLN
2	B	6	GLN
2	B	195	ASN
1	A	210	ASN
2	B	170	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.