wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 08:51 PM EDT

PDB ID	:	1BFO
Title	:	CAMPATH-1G IGG2B RAT MONOCLONAL FAB
Authors	:	Cheetham, G.M.T.; Hale, G.; Waldmann, H.; Bloomer, A.C.
Deposited on	:	1998-05-20
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

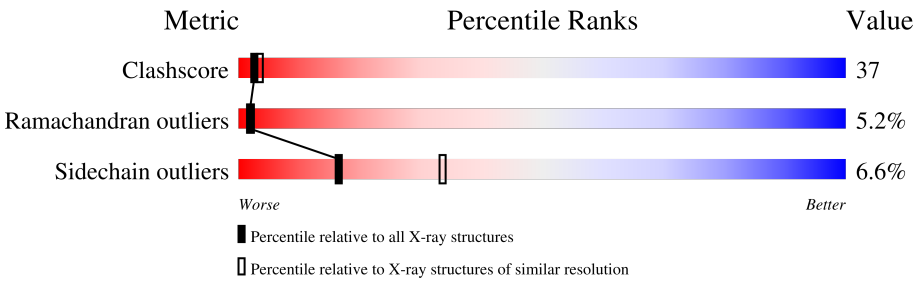
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 of 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	45% 47% 7% •
1	C	214	46% 47% 6% •
1	E	214	42% 50% 7% •
1	G	214	42% 53% 5% •
2	B	216	57% 35% 7%
2	D	216	55% 36% 9%
2	F	216	56% 35% 8%
2	H	216	53% 38% 8% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13523 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 CAMPATH-1G ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1650	1027	284	331	8	0	0	0
1	C	214	1650	1027	284	331	8	0	0	0
1	E	214	1650	1027	284	331	8	0	0	0
1	G	214	1650	1027	284	331	8	0	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	LYS	GLN	conflict	GB 4096754
A	21	LEU	ILE	conflict	GB 4096754
A	30	ASP	ASN	conflict	GB 4096754
A	43	SER	ALA	conflict	GB 4096754
A	46	LEU	ARG	conflict	GB 4096754
A	51	THR	ILE	conflict	GB 4096754
A	71	PHE	TYR	conflict	GB 4096754
A	73	LEU	ILE	conflict	GB 4096754
A	83	VAL	PHE	conflict	GB 4096754
A	92	ILE	ASP	conflict	GB 4096754
A	94	ARG	PHE	conflict	GB 4096754
A	96	ARG	TRP	conflict	GB 4096754
A	100	THR	GLY	conflict	GB 4096754
A	110	ASN	ASP	conflict	GB 4096754
A	122	THR	MET	conflict	GB 4096754
A	126	ALA	THR	conflict	GB 4096754
A	127	THR	SER	conflict	GB 4096754
A	131	SER	THR	conflict	GB 4096754
A	135	LEU	PHE	conflict	GB 4096754
A	136	MET	VAL	conflict	GB 4096754
A	138	LYS	ASN	conflict	GB 4096754

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Chain	Residue	Modelled	Actual	Comment	Reference
A	153	THR	SER	conflict	GB 4096754
A	?	-	GLN	deletion	GB 4096754
A	156	ASN	ASP	conflict	GB 4096754
A	160	ASN	ASP	conflict	GB 4096754
A	168	ALA	LYS	conflict	GB 4096754
A	183	ALA	VAL	conflict	GB 4096754
A	184	ASP	GLU	conflict	GB 4096754
A	186	GLN	GLU	conflict	GB 4096754
A	187	SER	ARG	conflict	GB 4096754
A	194	GLN	GLU	conflict	GB 4096754
A	206	ALA	-	insertion	GB 4096754
A	208	ASN	SER	conflict	GB 4096754
C	3	LYS	GLN	conflict	GB 4096754
C	21	LEU	ILE	conflict	GB 4096754
C	30	ASP	ASN	conflict	GB 4096754
C	43	SER	ALA	conflict	GB 4096754
C	46	LEU	ARG	conflict	GB 4096754
C	51	THR	ILE	conflict	GB 4096754
C	71	PHE	TYR	conflict	GB 4096754
C	73	LEU	ILE	conflict	GB 4096754
C	83	VAL	PHE	conflict	GB 4096754
C	92	ILE	ASP	conflict	GB 4096754
C	94	ARG	PHE	conflict	GB 4096754
C	96	ARG	TRP	conflict	GB 4096754
C	100	THR	GLY	conflict	GB 4096754
C	110	ASN	ASP	conflict	GB 4096754
C	122	THR	MET	conflict	GB 4096754
C	126	ALA	THR	conflict	GB 4096754
C	127	THR	SER	conflict	GB 4096754
C	131	SER	THR	conflict	GB 4096754
C	135	LEU	PHE	conflict	GB 4096754
C	136	MET	VAL	conflict	GB 4096754
C	138	LYS	ASN	conflict	GB 4096754
C	153	THR	SER	conflict	GB 4096754
C	?	-	GLN	deletion	GB 4096754
C	156	ASN	ASP	conflict	GB 4096754
C	160	ASN	ASP	conflict	GB 4096754
C	168	ALA	LYS	conflict	GB 4096754
C	183	ALA	VAL	conflict	GB 4096754
C	184	ASP	GLU	conflict	GB 4096754
C	186	GLN	GLU	conflict	GB 4096754
C	187	SER	ARG	conflict	GB 4096754

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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	GLN	GLU	conflict	GB 4096754
C	206	ALA	-	insertion	GB 4096754
C	208	ASN	SER	conflict	GB 4096754
E	3	LYS	GLN	conflict	GB 4096754
E	21	LEU	ILE	conflict	GB 4096754
E	30	ASP	ASN	conflict	GB 4096754
E	43	SER	ALA	conflict	GB 4096754
E	46	LEU	ARG	conflict	GB 4096754
E	51	THR	ILE	conflict	GB 4096754
E	71	PHE	TYR	conflict	GB 4096754
E	73	LEU	ILE	conflict	GB 4096754
E	83	VAL	PHE	conflict	GB 4096754
E	92	ILE	ASP	conflict	GB 4096754
E	94	ARG	PHE	conflict	GB 4096754
E	96	ARG	TRP	conflict	GB 4096754
E	100	THR	GLY	conflict	GB 4096754
E	110	ASN	ASP	conflict	GB 4096754
E	122	THR	MET	conflict	GB 4096754
E	126	ALA	THR	conflict	GB 4096754
E	127	THR	SER	conflict	GB 4096754
E	131	SER	THR	conflict	GB 4096754
E	135	LEU	PHE	conflict	GB 4096754
E	136	MET	VAL	conflict	GB 4096754
E	138	LYS	ASN	conflict	GB 4096754
E	153	THR	SER	conflict	GB 4096754
E	?	-	GLN	deletion	GB 4096754
E	156	ASN	ASP	conflict	GB 4096754
E	160	ASN	ASP	conflict	GB 4096754
E	168	ALA	LYS	conflict	GB 4096754
E	183	ALA	VAL	conflict	GB 4096754
E	184	ASP	GLU	conflict	GB 4096754
E	186	GLN	GLU	conflict	GB 4096754
E	187	SER	ARG	conflict	GB 4096754
E	194	GLN	GLU	conflict	GB 4096754
E	206	ALA	-	insertion	GB 4096754
E	208	ASN	SER	conflict	GB 4096754
G	3	LYS	GLN	conflict	GB 4096754
G	21	LEU	ILE	conflict	GB 4096754
G	30	ASP	ASN	conflict	GB 4096754
G	43	SER	ALA	conflict	GB 4096754
G	46	LEU	ARG	conflict	GB 4096754
G	51	THR	ILE	conflict	GB 4096754

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Chain	Residue	Modelled	Actual	Comment	Reference
G	71	PHE	TYR	conflict	GB 4096754
G	73	LEU	ILE	conflict	GB 4096754
G	83	VAL	PHE	conflict	GB 4096754
G	92	ILE	ASP	conflict	GB 4096754
G	94	ARG	PHE	conflict	GB 4096754
G	96	ARG	TRP	conflict	GB 4096754
G	100	THR	GLY	conflict	GB 4096754
G	110	ASN	ASP	conflict	GB 4096754
G	122	THR	MET	conflict	GB 4096754
G	126	ALA	THR	conflict	GB 4096754
G	127	THR	SER	conflict	GB 4096754
G	131	SER	THR	conflict	GB 4096754
G	135	LEU	PHE	conflict	GB 4096754
G	136	MET	VAL	conflict	GB 4096754
G	138	LYS	ASN	conflict	GB 4096754
G	153	THR	SER	conflict	GB 4096754
G	?	-	GLN	deletion	GB 4096754
G	156	ASN	ASP	conflict	GB 4096754
G	160	ASN	ASP	conflict	GB 4096754
G	168	ALA	LYS	conflict	GB 4096754
G	183	ALA	VAL	conflict	GB 4096754
G	184	ASP	GLU	conflict	GB 4096754
G	186	GLN	GLU	conflict	GB 4096754
G	187	SER	ARG	conflict	GB 4096754
G	194	GLN	GLU	conflict	GB 4096754
G	206	ALA	-	insertion	GB 4096754
G	208	ASN	SER	conflict	GB 4096754

- Molecule 2 is a protein called CAMPATH-1G ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	1634	1031	272	321	10	0	0	0
			Total	C	N	O	S			
2	D	216	1634	1031	272	321	10	0	0	0
			Total	C	N	O	S			
2	F	216	1634	1031	272	321	10	0	0	0
			Total	C	N	O	S			
2	H	216	1634	1031	272	321	10	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	GLY	ALA	conflict	GB 1220486
B	53	ASP	ASN	conflict	GB 1220486
B	56	LYS	ASN	conflict	GB 1220486
B	?	-	GLY	deletion	GB 1220486
B	?	-	ASP	deletion	GB 1220486
B	?	-	TYR	deletion	GB 1220486
B	?	-	PHE	deletion	GB 1220486
B	?	-	ASN	deletion	GB 1220486
B	101	GLU	ASN	conflict	GB 1220486
B	102	GLY	TYR	conflict	GB 1220486
B	103	HIS	MET	conflict	GB 1220486
B	104	THR	PHE	conflict	GB 1220486
B	105	ALA	PRO	conflict	GB 1220486
B	106	ALA	TYR	conflict	GB 1220486
B	107	PRO	VAL	conflict	GB 1220486
B	108	PHE	MET	conflict	GB 1220486
B	110	TYR	ALA	conflict	GB 1220486
B	115	VAL	GLY	conflict	GB 1220486
B	116	MET	SER	conflict	GB 1220486
B	123	GLN	GLU	conflict	GB 1220486
B	136	CYS	THR	conflict	GB 1220486
B	137	GLY	ALA	conflict	GB 1220486
B	138	ASP	LEU	conflict	GB 1220486
B	139	THR	LYS	conflict	GB 1220486
B	140	THR	SER	conflict	GB 1220486
B	141	SER	ASN	conflict	GB 1220486
B	143	THR	MET	conflict	GB 1220486
B	170	ASP	GLY	conflict	GB 1220486
B	?	-	VAL	deletion	GB 1220486
B	?	-	PRO	deletion	GB 1220486
B	195	PRO	SER	conflict	GB 1220486
B	198	THR	ALA	conflict	GB 1220486
D	24	GLY	ALA	conflict	GB 1220486
D	53	ASP	ASN	conflict	GB 1220486
D	56	LYS	ASN	conflict	GB 1220486
D	?	-	GLY	deletion	GB 1220486
D	?	-	ASP	deletion	GB 1220486
D	?	-	TYR	deletion	GB 1220486
D	?	-	PHE	deletion	GB 1220486
D	?	-	ASN	deletion	GB 1220486
D	101	GLU	ASN	conflict	GB 1220486
D	102	GLY	TYR	conflict	GB 1220486
D	103	HIS	MET	conflict	GB 1220486

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Chain	Residue	Modelled	Actual	Comment	Reference
D	104	THR	PHE	conflict	GB 1220486
D	105	ALA	PRO	conflict	GB 1220486
D	106	ALA	TYR	conflict	GB 1220486
D	107	PRO	VAL	conflict	GB 1220486
D	108	PHE	MET	conflict	GB 1220486
D	110	TYR	ALA	conflict	GB 1220486
D	115	VAL	GLY	conflict	GB 1220486
D	116	MET	SER	conflict	GB 1220486
D	123	GLN	GLU	conflict	GB 1220486
D	136	CYS	THR	conflict	GB 1220486
D	137	GLY	ALA	conflict	GB 1220486
D	138	ASP	LEU	conflict	GB 1220486
D	139	THR	LYS	conflict	GB 1220486
D	140	THR	SER	conflict	GB 1220486
D	141	SER	ASN	conflict	GB 1220486
D	143	THR	MET	conflict	GB 1220486
D	170	ASP	GLY	conflict	GB 1220486
D	?	-	VAL	deletion	GB 1220486
D	?	-	PRO	deletion	GB 1220486
D	195	PRO	SER	conflict	GB 1220486
D	198	THR	ALA	conflict	GB 1220486
F	24	GLY	ALA	conflict	GB 1220486
F	53	ASP	ASN	conflict	GB 1220486
F	56	LYS	ASN	conflict	GB 1220486
F	?	-	GLY	deletion	GB 1220486
F	?	-	ASP	deletion	GB 1220486
F	?	-	TYR	deletion	GB 1220486
F	?	-	PHE	deletion	GB 1220486
F	?	-	ASN	deletion	GB 1220486
F	101	GLU	ASN	conflict	GB 1220486
F	102	GLY	TYR	conflict	GB 1220486
F	103	HIS	MET	conflict	GB 1220486
F	104	THR	PHE	conflict	GB 1220486
F	105	ALA	PRO	conflict	GB 1220486
F	106	ALA	TYR	conflict	GB 1220486
F	107	PRO	VAL	conflict	GB 1220486
F	108	PHE	MET	conflict	GB 1220486
F	110	TYR	ALA	conflict	GB 1220486
F	115	VAL	GLY	conflict	GB 1220486
F	116	MET	SER	conflict	GB 1220486
F	123	GLN	GLU	conflict	GB 1220486
F	136	CYS	THR	conflict	GB 1220486

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Chain	Residue	Modelled	Actual	Comment	Reference
F	137	GLY	ALA	conflict	GB 1220486
F	138	ASP	LEU	conflict	GB 1220486
F	139	THR	LYS	conflict	GB 1220486
F	140	THR	SER	conflict	GB 1220486
F	141	SER	ASN	conflict	GB 1220486
F	143	THR	MET	conflict	GB 1220486
F	170	ASP	GLY	conflict	GB 1220486
F	?	-	VAL	deletion	GB 1220486
F	?	-	PRO	deletion	GB 1220486
F	195	PRO	SER	conflict	GB 1220486
F	198	THR	ALA	conflict	GB 1220486
H	24	GLY	ALA	conflict	GB 1220486
H	53	ASP	ASN	conflict	GB 1220486
H	56	LYS	ASN	conflict	GB 1220486
H	?	-	GLY	deletion	GB 1220486
H	?	-	ASP	deletion	GB 1220486
H	?	-	TYR	deletion	GB 1220486
H	?	-	PHE	deletion	GB 1220486
H	?	-	ASN	deletion	GB 1220486
H	101	GLU	ASN	conflict	GB 1220486
H	102	GLY	TYR	conflict	GB 1220486
H	103	HIS	MET	conflict	GB 1220486
H	104	THR	PHE	conflict	GB 1220486
H	105	ALA	PRO	conflict	GB 1220486
H	106	ALA	TYR	conflict	GB 1220486
H	107	PRO	VAL	conflict	GB 1220486
H	108	PHE	MET	conflict	GB 1220486
H	110	TYR	ALA	conflict	GB 1220486
H	115	VAL	GLY	conflict	GB 1220486
H	116	MET	SER	conflict	GB 1220486
H	123	GLN	GLU	conflict	GB 1220486
H	136	CYS	THR	conflict	GB 1220486
H	137	GLY	ALA	conflict	GB 1220486
H	138	ASP	LEU	conflict	GB 1220486
H	139	THR	LYS	conflict	GB 1220486
H	140	THR	SER	conflict	GB 1220486
H	141	SER	ASN	conflict	GB 1220486
H	143	THR	MET	conflict	GB 1220486
H	170	ASP	GLY	conflict	GB 1220486
H	?	-	VAL	deletion	GB 1220486
H	?	-	PRO	deletion	GB 1220486
H	195	PRO	SER	conflict	GB 1220486

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Chain	Residue	Modelled	Actual	Comment	Reference
H	198	THR	ALA	conflict	GB 1220486

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	51	51	51	0	0
			Total	O		
3	B	48	48	48	0	0
			Total	O		
3	C	49	49	49	0	0
			Total	O		
3	D	43	43	43	0	0
			Total	O		
3	E	37	37	37	0	0
			Total	O		
3	F	44	44	44	0	0
			Total	O		
3	G	56	56	56	0	0
			Total	O		
3	H	59	59	59	0	0

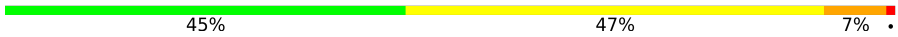
3 Residue-property plots (i)

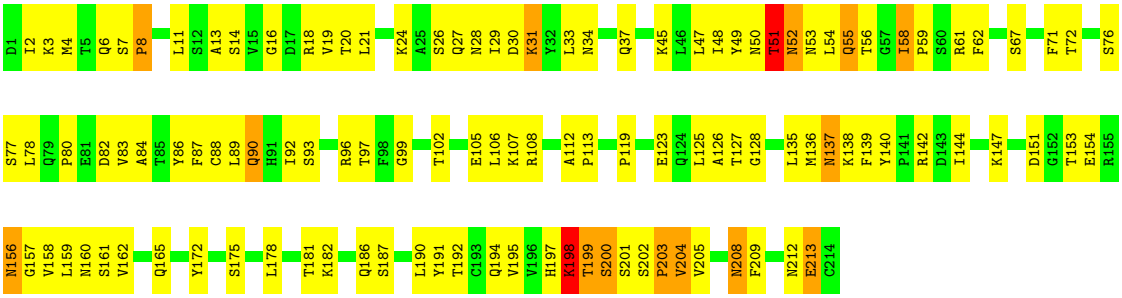
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CAMPATH-1G ANTIBODY

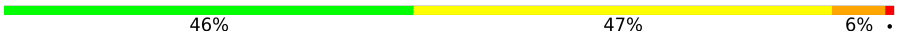
Chain A:

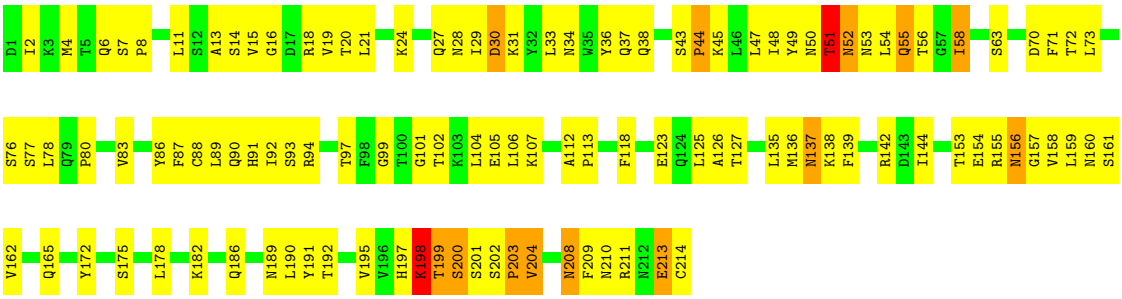




• Molecule 1: CAMPATH-1G ANTIBODY

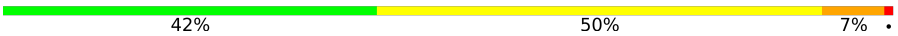
Chain C:

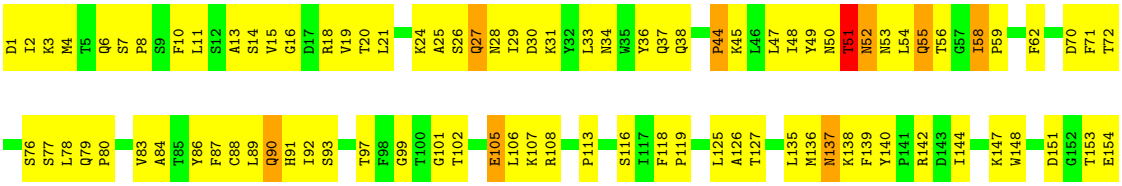




• Molecule 1: CAMPATH-1G ANTIBODY

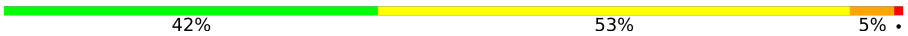
Chain E:

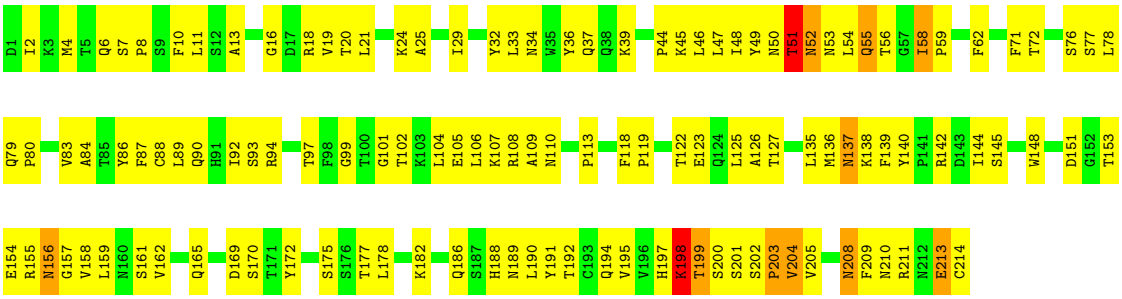




• Molecule 1: CAMPATH-1G ANTIBODY

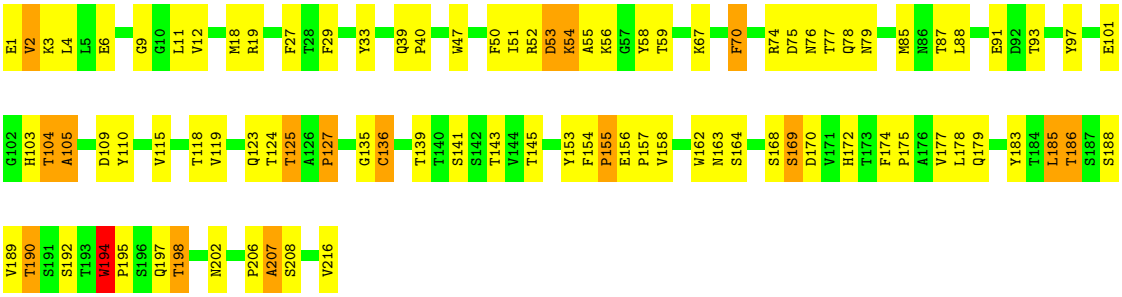
Chain G:





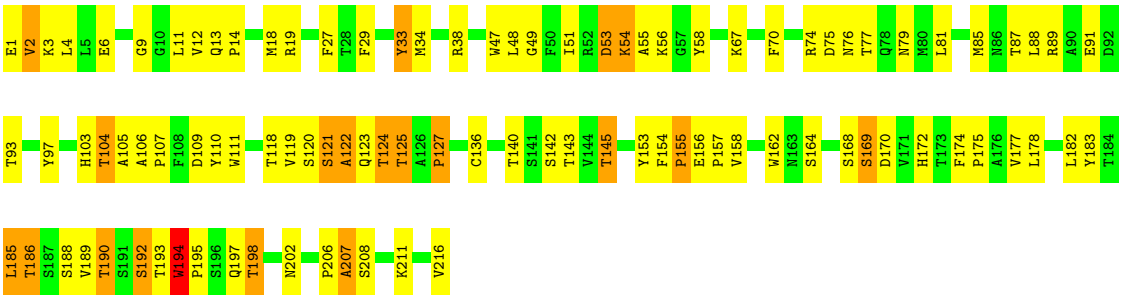
• Molecule 2: CAMPATH-1G ANTIBODY

Chain B:



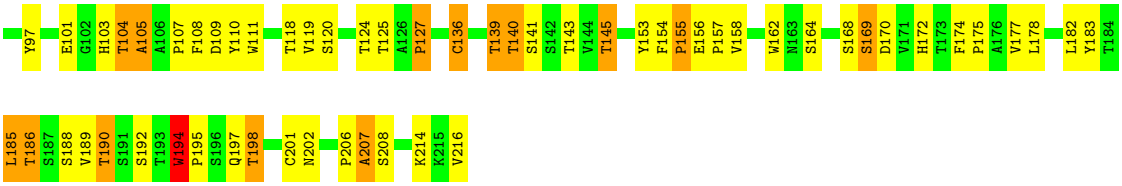
• Molecule 2: CAMPATH-1G ANTIBODY

Chain D:



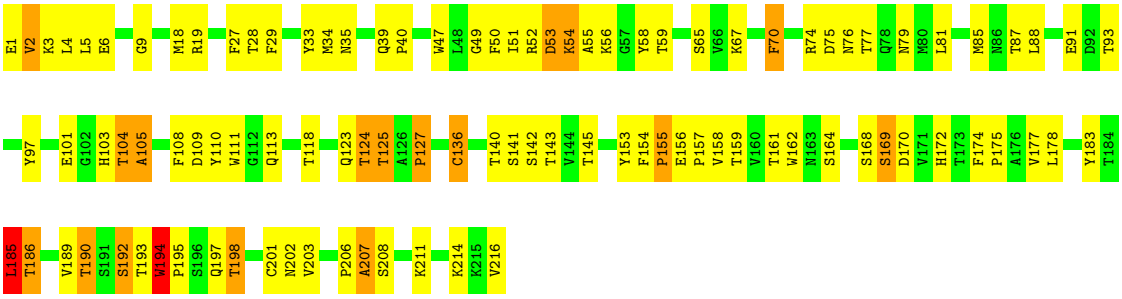
• Molecule 2: CAMPATH-1G ANTIBODY

Chain F:



• Molecule 2: CAMPATH-1G ANTIBODY

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.28Å 108.15Å 166.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	90.5 (20.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 0.3, X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13523	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	0.77	0/1682	0.98	3/2282 (0.1%)
1	C	0.77	0/1682	0.98	3/2282 (0.1%)
1	E	0.75	0/1682	1.01	3/2282 (0.1%)
1	G	0.79	0/1682	0.99	3/2282 (0.1%)
2	B	0.79	1/1677 (0.1%)	0.99	4/2289 (0.2%)
2	D	0.85	1/1677 (0.1%)	0.99	4/2289 (0.2%)
2	F	0.82	1/1677 (0.1%)	0.98	3/2289 (0.1%)
2	H	0.80	1/1677 (0.1%)	0.98	3/2289 (0.1%)
All	All	0.79	4/13436 (0.0%)	0.99	26/18284 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	194	TRP	CB-CG	7.80	1.64	1.50
2	F	194	TRP	CB-CG	7.72	1.64	1.50
2	B	194	TRP	CB-CG	7.55	1.63	1.50
2	D	194	TRP	CB-CG	6.96	1.62	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	185	LEU	CB-CG-CD2	-7.08	98.96	111.00
2	H	185	LEU	CB-CG-CD2	-6.66	99.68	111.00
2	H	185	LEU	CA-CB-CG	6.39	130.00	115.30
2	H	192	SER	N-CA-C	-6.29	94.02	111.00
2	B	192	SER	N-CA-C	-6.13	94.45	111.00

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	1650	0	1622	134	0
1	C	1650	0	1622	143	0
1	E	1650	0	1622	156	0
1	G	1650	0	1622	161	0
2	B	1634	0	1579	100	0
2	D	1634	0	1579	96	0
2	F	1634	0	1579	98	0
2	H	1634	0	1579	105	0
3	A	51	0	0	13	0
3	B	48	0	0	4	0
3	C	49	0	0	4	0
3	D	43	0	0	6	0
3	E	37	0	0	7	0
3	F	44	0	0	1	0
3	G	56	0	0	9	0
3	H	59	0	0	5	0
All	All	13523	0	12804	949	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 37.

The worst 5 of 949 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:51:ILE:HD13	2:H:74:ARG:HG3	1.29	1.15
2:F:51:ILE:HD13	2:F:74:ARG:HG3	1.27	1.14
2:B:51:ILE:HD13	2:B:74:ARG:HG3	1.26	1.11
2:D:51:ILE:HD13	2:D:74:ARG:HG3	1.27	1.09
2:B:194:TRP:HB3	2:B:195:PRO:HD3	1.27	1.08

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	212/214 (99%)	188 (89%)	16 (8%)	8 (4%)	3	4
1	C	212/214 (99%)	187 (88%)	16 (8%)	9 (4%)	3	3
1	E	212/214 (99%)	187 (88%)	17 (8%)	8 (4%)	3	4
1	G	212/214 (99%)	188 (89%)	16 (8%)	8 (4%)	3	4
2	B	214/216 (99%)	180 (84%)	21 (10%)	13 (6%)	1	1
2	D	214/216 (99%)	181 (85%)	18 (8%)	15 (7%)	1	1
2	F	214/216 (99%)	183 (86%)	17 (8%)	14 (6%)	1	1
2	H	214/216 (99%)	182 (85%)	18 (8%)	14 (6%)	1	1
All	All	1704/1720 (99%)	1476 (87%)	139 (8%)	89 (5%)	2	2

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	126	ALA
1	A	198	LYS
1	A	199	THR
1	A	200	SER

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	191/191 (100%)	180 (94%)	11 (6%)	20	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	191/191 (100%)	181 (95%)	10 (5%)	23	46
1	E	191/191 (100%)	177 (93%)	14 (7%)	14	28
1	G	191/191 (100%)	181 (95%)	10 (5%)	23	46
2	B	180/180 (100%)	167 (93%)	13 (7%)	14	29
2	D	180/180 (100%)	169 (94%)	11 (6%)	18	38
2	F	180/180 (100%)	166 (92%)	14 (8%)	12	25
2	H	180/180 (100%)	165 (92%)	15 (8%)	11	22
All	All	1484/1484 (100%)	1386 (93%)	98 (7%)	16	33

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	198	LYS
2	F	194	TRP
2	F	4	LEU
2	F	145	THR
1	G	52	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	202	ASN
2	H	197	GLN
1	E	137	ASN
2	H	172	HIS
1	G	160	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 monosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.