wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 02:03 PM BST

PDB ID	:	2IGF
Title	:	CRYSTAL STRUCTURES OF AN ANTIBODY TO A PEPTIDE AND ITS COMPLEX WITH PEPTIDE ANTIGEN AT 2.8 ANGSTROMS
Authors	:	Stanfield, R.L.; Wilson, I.A.
Deposited on	:	1991-03-21
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
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:

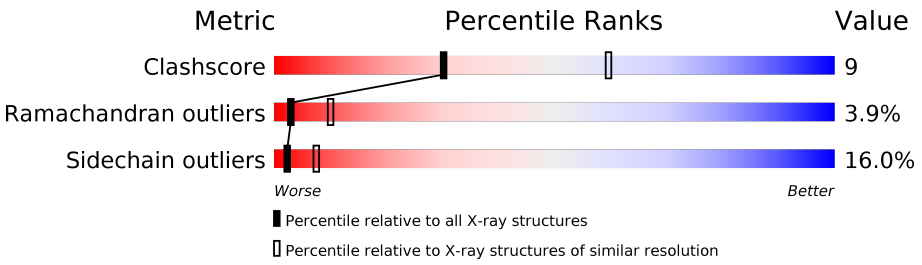
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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	L	219	61% 32% 6% •
2	H	221	53% 34% 10% •
3	P	19	21% 11% 5% 63%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3436 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 IGG1-KAPPA B13I2 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1692	1058	284	343	7	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	ASN	SER	conflict	PIR PC4203
L	27A	THR	SER	conflict	PIR PC4203
L	27C	LEU	VAL	conflict	PIR PC4203
L	27D	LEU	HIS	conflict	PIR PC4203
L	27E	SER	THR	conflict	PIR PC4203
L	28	ASP	ASN	conflict	PIR PC4203
L	30	ASP	ASN	conflict	PIR PC4203
L	96	PRO	ARG	conflict	PIR PC4203

- Molecule 2 is a protein called IGG1-KAPPA B13I2 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	1672	1053	280	330	9	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	GLN	LYS	conflict	PIR S38864
H	5	VAL	LEU	conflict	PIR S38864
H	27	PHE	LEU	conflict	PIR S38864
H	31	ARG	SER	conflict	PIR S38864
H	32	CYS	TYR	conflict	PIR S38864
H	33	ALA	GLY	conflict	PIR S38864
H	40	THR	ILE	conflict	PIR S38864
H	42	GLU	ASP	conflict	PIR S38864

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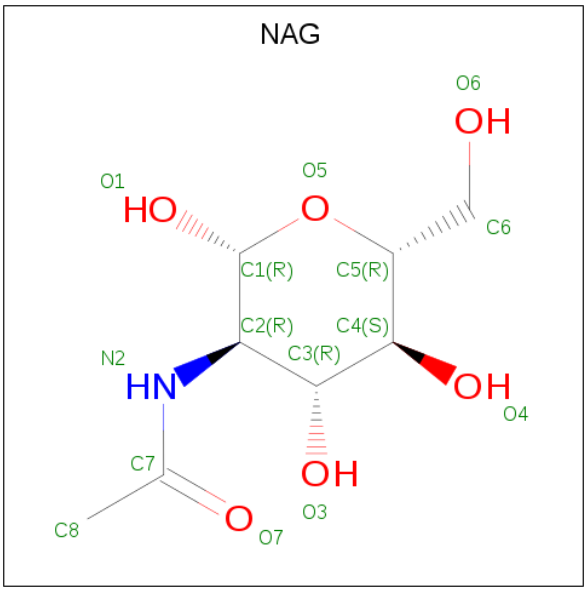
Chain	Residue	Modelled	Actual	Comment	Reference
H	50	GLY	THR	conflict	PIR S38864
H	55	SER	THR	conflict	PIR S38864
H	58	PHE	TYR	conflict	PIR S38864
H	62	THR	SER	conflict	PIR S38864
H	68	ILE	THR	conflict	PIR S38864
H	72	ASN	ASP	conflict	PIR S38864
H	75	ARG	LYS	conflict	PIR S38864
H	79	SER	TYR	conflict	PIR S38864
H	83	ARG	LYS	conflict	PIR S38864
H	89	ILE	MET	conflict	PIR S38864
H	93	THR	ALA	conflict	PIR S38864
H	?	-	GLN	deletion	PIR S38864
H	95	TYR	GLY	conflict	PIR S38864
H	96	SER	VAL	conflict	PIR S38864
H	98	ASP	THR	conflict	PIR S38864
H	99	PRO	MET	conflict	PIR S38864
H	100	PHE	ILE	conflict	PIR S38864
H	100B	TYR	ARG	conflict	PIR S38864
H	101	ASP	ALA	conflict	PIR S38864
H	108	THR	LEU	conflict	PIR S38864
H	109	LEU	VAL	conflict	PIR S38864
H	113	SER	ALA	conflict	PIR S38864
H	114	ALA	GLY	conflict	PIR S38864
H	198	PRO	THR	conflict	PIR S38864
H	199	ARG	TRP	conflict	PIR S38864

- Molecule 3 is a protein called PEPTIDE (RESIDUES 69-87 OF MYOHEMERYTHRIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	7	58	38	11	9	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	L	1	14	8	1	5	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.

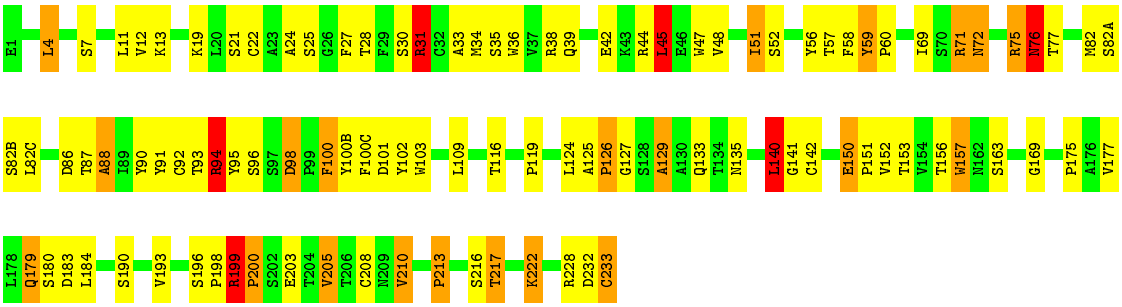
Note EDS was not executed.

- Molecule 1: IGG1-KAPPA B13I2 FAB (LIGHT CHAIN)

Chain L:

- Molecule 2: IGG1-KAPPA B13I2 FAB (HEAVY CHAIN)

Chain H:



- Molecule 3: PEPTIDE (RESIDUES 69-87 OF MYOHEMERYTHRIN)

Chain P:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.50Å 142.50Å 101.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3436	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	wwPDB-VP

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: NAG

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	L	0.99	0/1730	1.87	37/2347 (1.6%)
2	H	1.05	0/1715	1.99	47/2340 (2.0%)
3	P	1.09	0/59	1.54	0/78
All	All	1.02	0/3504	1.93	84/4765 (1.8%)

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	L	0	3
2	H	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	71	ARG	NE-CZ-NH1	15.40	128.00	120.30
2	H	71	ARG	NE-CZ-NH2	-12.65	113.97	120.30
2	H	82	MET	CG-SD-CE	-10.18	83.91	100.20
1	L	148	TRP	CD1-CG-CD2	9.82	114.15	106.30
1	L	83	LEU	CA-CB-CG	8.98	135.97	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	150	GLU	Peptide
2	H	199	ARG	Peptide
1	L	39	LYS	Peptide
1	L	49	TYR	Sidechain
1	L	86	TYR	Sidechain

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	L	1692	0	1633	25	0
2	H	1672	0	1638	39	0
3	P	58	0	63	2	0
4	L	14	0	13	0	0
All	All	3436	0	3347	61	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 9.

The worst 5 of 61 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:140:LEU:HD21	2:H:199:ARG:HG3	1.57	0.87
2:H:72:ASN:HD22	2:H:75:ARG:HH21	1.31	0.78
1:L:160:LEU:HD11	2:H:179:GLN:HG3	1.66	0.76
2:H:198:PRO:HB3	2:H:203:GLU:HB2	1.73	0.71
2:H:198:PRO:HA	2:H:203:GLU:H	1.64	0.62

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	L	217/219 (99%)	186 (86%)	29 (13%)	2 (1%)	17 46
2	H	219/221 (99%)	182 (83%)	22 (10%)	15 (7%)	1 3
3	P	5/19 (26%)	5 (100%)	0	0	100 100
All	All	441/459 (96%)	373 (85%)	51 (12%)	17 (4%)	3 10

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	40	PRO
1	L	211	ARG
2	H	76	ASN
2	H	82(B)	SER
2	H	129	ALA

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	L	195/196 (100%)	164 (84%)	31 (16%)	2 7
2	H	192/192 (100%)	161 (84%)	31 (16%)	2 7
3	P	7/17 (41%)	6 (86%)	1 (14%)	3 10
All	All	394/405 (97%)	331 (84%)	63 (16%)	2 7

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	195	GLU
2	H	25	SER
2	H	208	CYS
1	L	204	PRO
2	H	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	124	GLN
1	L	145	ASN
1	L	161	ASN
1	L	198	HIS

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)

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	$\#\|Z\| > 2$
4	NAG	L	600	1	14,14,15	1.23	2 (14%)	17,19,21	1.54	3 (17%)

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
4	NAG	L	600	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	600	NAG	C1-C2	-2.25	1.49	1.52
4	L	600	NAG	C3-C2	-2.08	1.48	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	600	NAG	C1-O5-C5	3.42	116.82	112.19
4	L	600	NAG	O4-C4-C3	-2.60	104.35	110.35
4	L	600	NAG	C8-C7-N2	-2.18	112.41	116.10

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)

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.