wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:43 PM GMT

PDB ID	:	1LO2
Title	:	Retro-Diels-Alderase Catalytic Antibody
Authors	:	Hugot, M.; Reymond, J.L.; Baumann, U.
Deposited on	:	2002-05-06
Resolution	:	2.00 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
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:

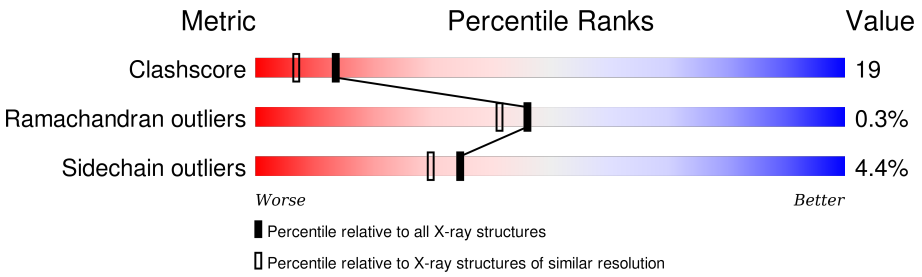
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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	L	219	65% 32% •
1	X	219	65% 32% •
2	H	220	69% 29% •
2	Y	220	66% 33% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6934 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.

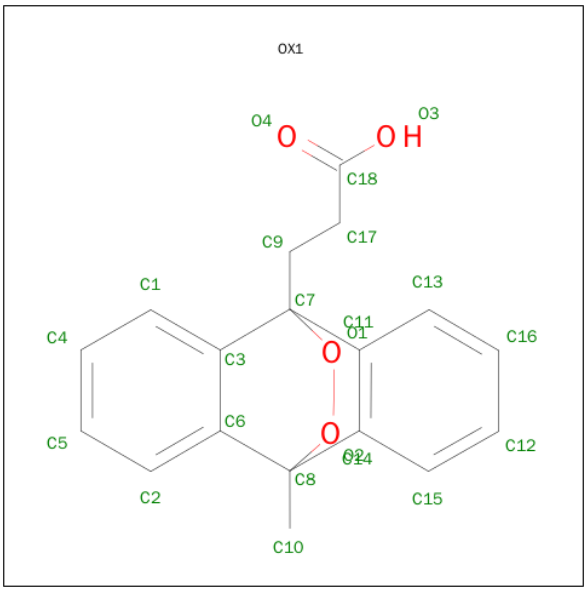
- Molecule 1 is a protein called If kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	219	1707	1073	284	343	7	0	0	0
1	L	219	1707	1073	284	343	7	0	0	0

- Molecule 2 is a protein called Ig gamma 2a heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	Y	220	1668	1063	276	321	8	0	0	0
2	H	220	1668	1063	276	321	8	0	0	0

- Molecule 3 is [2'-CARBOXYLETHYL]-10-METHYL-ANTHRACENE ENDOPEROXIDE (three-letter code: OX1) (formula: $C_{18}H_{16}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	Y	1	22	18	4	0	0
			Total	C	O		
3	H	1	22	18	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	H	27	27	27	0	0
			Total	O		
4	L	34	34	34	0	0
			Total	O		
4	X	39	39	39	0	0
			Total	O		
4	Y	40	40	40	0	0

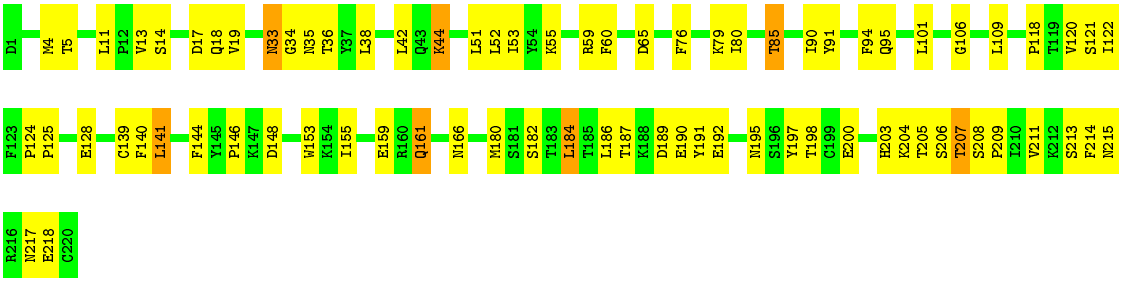
3 Residue-property plots (i)

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.

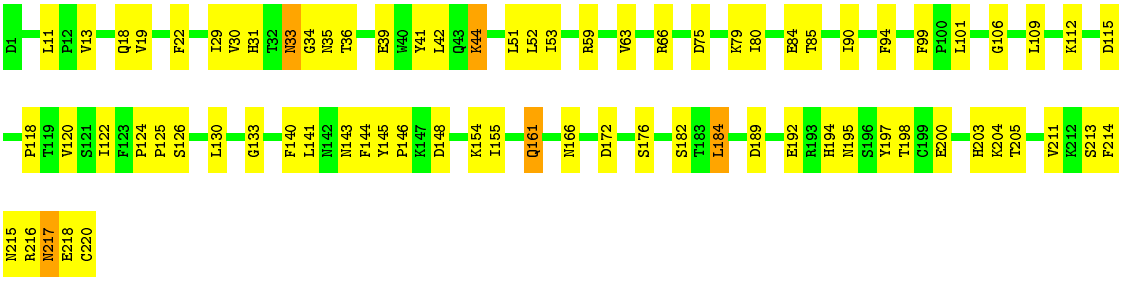
- Molecule 1: If kappa light chain

Chain X:



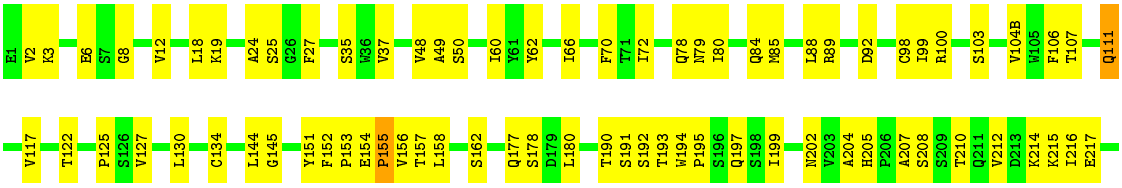
- Molecule 1: If kappa light chain

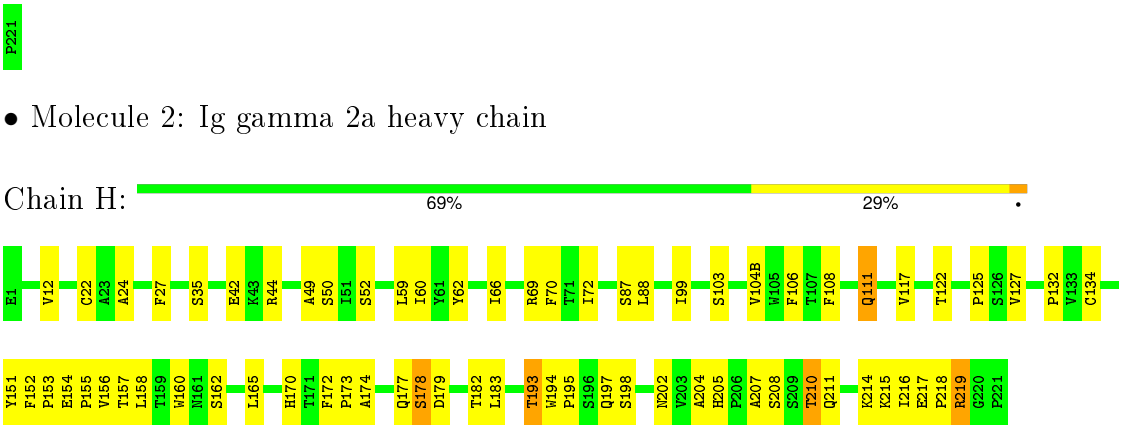
Chain L:



- Molecule 2: Ig gamma 2a heavy chain

Chain Y:




P221
• Molecule 2: Ig gamma 2a heavy chain
Chain H:
69%
29%
E1 V12 C22 A23 A24 F27 S35 E42 K43 R44 A49 S50 I51 S52 L59 I60 Y61 Y62 I66 R69 F70 T71 I72 S87 L88 I99 S103 V104B W105 F106 T107 F108 Q111 V117 T122 P125 S126 V127 P132 V133 C134
Y151 F152 P153 E154 P155 V156 T157 L158 T159 W160 N161 S162 L165 H170 T171 F172 P173 A174 Q177 S178 D179 T182 L183 T193 W194 P195 S196 Q197 S198 N202 V203 A204 H205 P206 A207 S208 S209 T210 Q211 K214 K215 I216 E217 P218 R219 G220 P221

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	40.53Å 140.09Å 85.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.80 – 2.00	Depositor
% Data completeness (in resolution range)	1.0 (30.80-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6934	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	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: OX1

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	0.43	0/1747	0.68	0/2371
1	X	0.43	0/1747	0.68	0/2371
2	H	0.44	0/1712	0.69	0/2334
2	Y	0.43	0/1712	0.67	0/2334
All	All	0.43	0/6918	0.68	0/9410

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	L	1707	0	1647	60	0
1	X	1707	0	1647	66	0
2	H	1668	0	1644	61	0
2	Y	1668	0	1644	64	0
3	H	22	0	15	4	0
3	Y	22	0	15	6	0
4	H	27	0	0	1	0
4	L	34	0	0	1	0
4	X	39	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	40	0	0	0	0
All	All	6934	0	6612	249	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 19.

The worst 5 of 249 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)
3:Y:500:OX1:O2	3:Y:500:OX1:O1	1.63	1.17
3:H:501:OX1:O2	3:H:501:OX1:O1	1.63	1.13
2:H:162:SER:H	2:H:202:ASN:HD21	1.10	0.98
1:X:200:GLU:HG2	1:X:211:VAL:HG22	1.45	0.96
2:Y:162:SER:H	2:Y:202:ASN:HD21	1.09	0.93

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%)	207 (95%)	10 (5%)	0	100	100
1	X	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	34	26
2	H	218/220 (99%)	203 (93%)	14 (6%)	1 (0%)	34	26
2	Y	218/220 (99%)	209 (96%)	8 (4%)	1 (0%)	34	26
All	All	870/878 (99%)	826 (95%)	41 (5%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	178	SER

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Mol	Chain	Res	Type
2	H	178	SER
1	X	207	THR

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	197/197 (100%)	187 (95%)	10 (5%)	29	23
1	X	197/197 (100%)	186 (94%)	11 (6%)	26	20
2	H	188/188 (100%)	179 (95%)	9 (5%)	31	26
2	Y	188/188 (100%)	184 (98%)	4 (2%)	61	63
All	All	770/770 (100%)	736 (96%)	34 (4%)	35	30

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	33	ASN
1	L	161	GLN
2	H	193	THR
1	L	85	THR
1	X	161	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	197	GLN
1	L	33	ASN
2	H	170	HIS
2	Y	202	ASN
2	Y	205	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	$\#\|Z\| > 2$
3	OX1	H	501	-	20,25,25	3.71	11 (55%)	21,39,39	0.52	0
3	OX1	Y	500	-	20,25,25	3.69	11 (55%)	21,39,39	0.52	0

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
3	OX1	H	501	-	-	0/4/37/37	0/2/4/4
3	OX1	Y	500	-	-	0/4/37/37	0/2/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	500	OX1	C2-C6	2.06	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	OX1	C2-C6	2.34	1.42	1.39
3	Y	500	OX1	C15-C14	2.50	1.42	1.39
3	H	501	OX1	C15-C14	2.50	1.42	1.39
3	Y	500	OX1	C1-C3	2.51	1.42	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	501	OX1	4	0
3	Y	500	OX1	6	0

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.