wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 11:22 AM EDT

PDB ID	:	1P2C
Title	:	crystal structure analysis of an anti-lysozyme antibody
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Deposited on	:	2003-04-15
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
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:

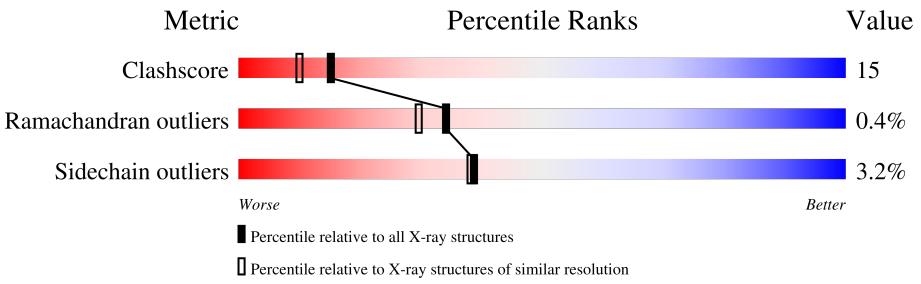
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	212	74% 24% •
1	D	212	76% 23%
2	B	218	69% 24% • •
2	E	218	72% 22% • •
3	C	129	78% 19% •
3	F	129	74% 22% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9350 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 light chain anti-lysozyme antibody F10.6.6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1639	1013	280	340	6	0	0	0
1	D	211	1630	1009	278	337	6	0	0	0

- Molecule 2 is a protein called heavy chain VH+CH1 anti-lysozyme antibody F10.6.6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	210	1592	1016	252	317	7	0	0	0
2	E	211	1600	1020	253	320	7	0	0	0

- Molecule 3 is a protein called Lysozyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	129	1001	613	193	185	10	0	0	0
3	F	129	1001	613	193	185	10	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	209	209	209	0	0
4	B	175	175	175	0	0
4	C	104	104	104	0	0
4	D	157	157	157	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	146	146	146	0	0
			Total	O		
4	F	96	96	96	0	0

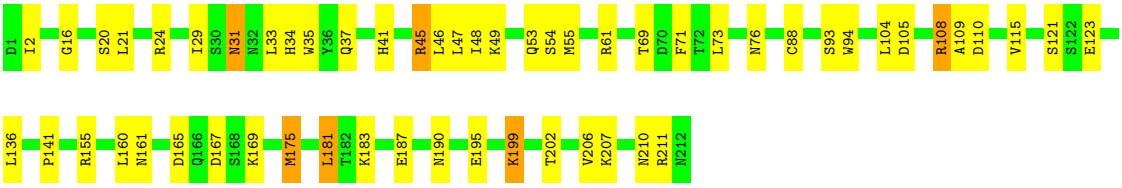
3 Residue-property plots (i)

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: light chain anti-lysozyme antibody F10.6.6

Chain A:

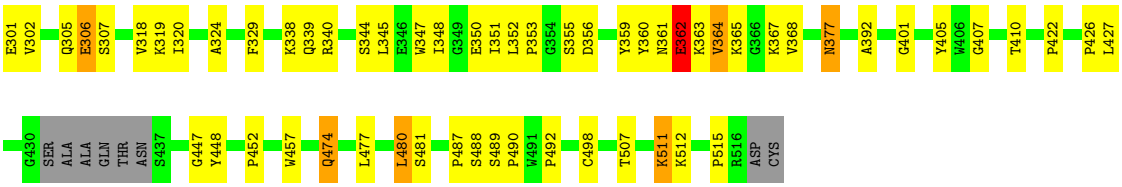


• Molecule 1: light chain anti-lysozyme antibody F10.6.6

Chain D:

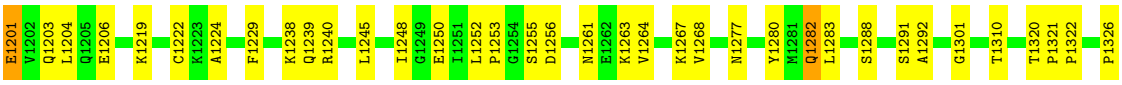
• Molecule 2: heavy chain VH+CH1 anti-lysozyme antibody F10.6.6

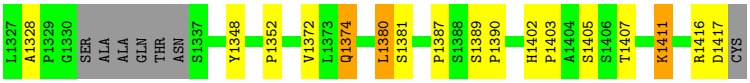
Chain B:



• Molecule 2: heavy chain VH+CH1 anti-lysozyme antibody F10.6.6

Chain E:





• Molecule 3: Lysozyme C

Chain C:

• Molecule 3: Lysozyme C

Chain F:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.66Å 73.75Å 83.78Å 66.59° 74.74° 85.44°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9350	wwPDB-VP
Average B, all atoms ($Å^2$)	21.0	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	0.34	0/1676	0.63	0/2273
1	D	0.34	0/1667	0.61	0/2262
2	B	0.40	1/1637 (0.1%)	0.68	2/2241 (0.1%)
2	E	0.35	0/1645	0.66	1/2252 (0.0%)
3	C	0.33	0/1021	0.62	1/1379 (0.1%)
3	F	0.33	0/1021	0.62	1/1379 (0.1%)
All	All	0.35	1/8667 (0.0%)	0.64	5/11786 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	306	GLU	CD-OE2	7.15	1.33	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1301	GLY	N-CA-C	-5.57	99.18	113.10
3	C	654	GLY	N-CA-C	5.18	126.06	113.10
2	B	401	GLY	N-CA-C	-5.17	100.18	113.10
3	F	1554	GLY	N-CA-C	5.11	125.87	113.10
2	B	407	GLY	N-CA-C	-5.01	100.57	113.10

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	1639	0	1558	44	0
1	D	1630	0	1549	44	0
2	B	1592	0	1542	58	0
2	E	1600	0	1546	46	0
3	C	1001	0	956	28	0
3	F	1001	0	956	35	0
4	A	209	0	0	9	0
4	B	175	0	0	4	0
4	C	104	0	0	2	0
4	D	157	0	0	7	1
4	E	146	0	0	5	1
4	F	96	0	0	2	0
All	All	9350	0	8107	248	1

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 248 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:31:ASN:H	1:A:31:ASN:HD22	1.11	0.99
2:E:1387:PRO:O	2:E:1390:PRO:HD2	1.72	0.88
2:E:1263:LYS:HB2	4:E:2280:HOH:O	1.75	0.85
2:B:487:PRO:O	2:B:490:PRO:HD2	1.78	0.83
1:D:956:SER:HB2	4:D:2876:HOH:O	1.77	0.83

All (1) 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:D:2551:HOH:O	4:E:2270:HOH:O[1_455]	2.02	0.18

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	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
1	D	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
2	B	206/218 (94%)	196 (95%)	8 (4%)	2 (1%)	15	9
2	E	207/218 (95%)	200 (97%)	6 (3%)	1 (0%)	29	23
3	C	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	F	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	13
All	All	1086/1118 (97%)	1042 (96%)	40 (4%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	362	GLU
3	F	1628	ARG
2	E	1416	ARG
2	B	364	VAL

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%)	183 (96%)	8 (4%)	30	27
1	D	190/191 (100%)	187 (98%)	3 (2%)	62	67
2	B	181/187 (97%)	173 (96%)	8 (4%)	28	25
2	E	182/187 (97%)	176 (97%)	6 (3%)	38	37
3	C	105/105 (100%)	102 (97%)	3 (3%)	42	43
3	F	105/105 (100%)	102 (97%)	3 (3%)	42	43
All	All	954/966 (99%)	923 (97%)	31 (3%)	39	38

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	488	SER
2	E	1411	LYS
3	C	662	TRP
3	F	1568	ARG
2	E	1352	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	976	ASN
2	E	1282	GLN
1	D	1110	ASN
3	F	1527	ASN
2	B	305	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 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.