WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:28 PM GMT

PDB ID	:	1P2C
Title	:	crystal structure analysis of an anti-lysozyme antibody
Authors	:	Cauerhff, A.; Goldbaum, F.A.; Braden, B.C.
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

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:

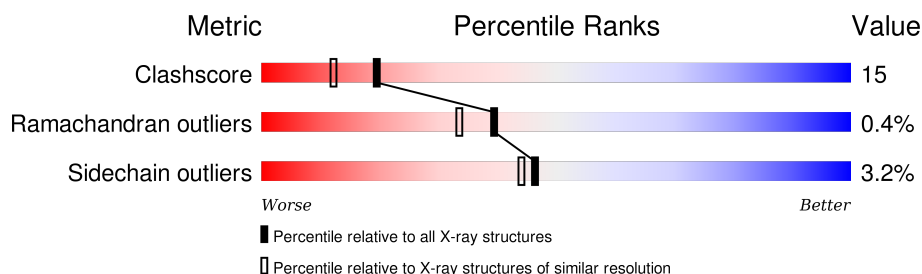|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		3.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	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
1	A	212	Total 1639	C 1013	N 280	O 340	S 6	0	0	0
1	D	211	Total 1630	C 1009	N 278	O 337	S 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
2	B	210	Total 1592	C 1016	N 252	O 317	S 7	0	0	0
2	E	211	Total 1600	C 1020	N 253	O 320	S 7	0	0	0

- Molecule 3 is a protein called Lysozyme C.

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

- Molecule 4 is water.

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

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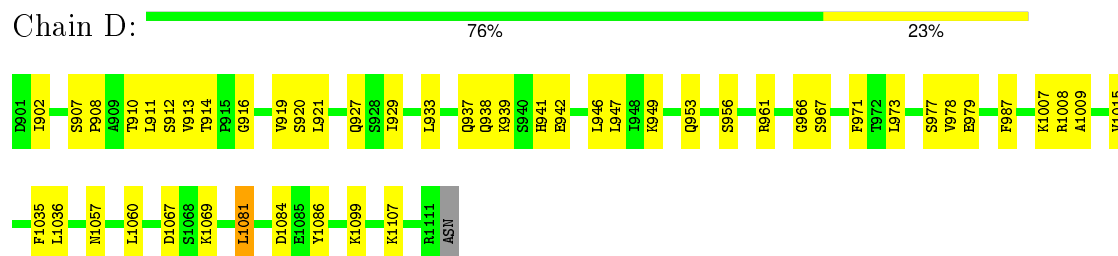| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	146	Total O 146 146	0	0
4	F	96	Total O 96 96	0	0

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.
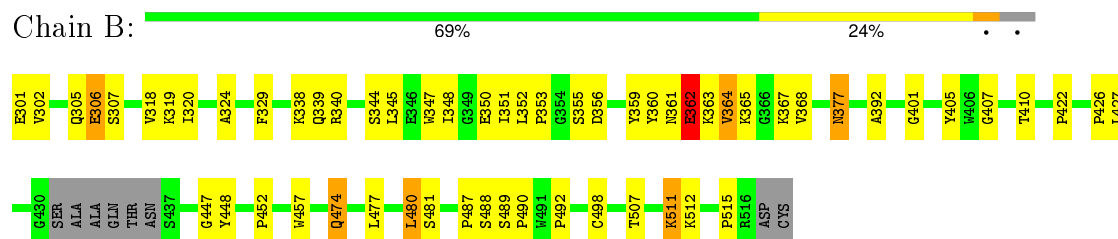
Note EDS was not executed.

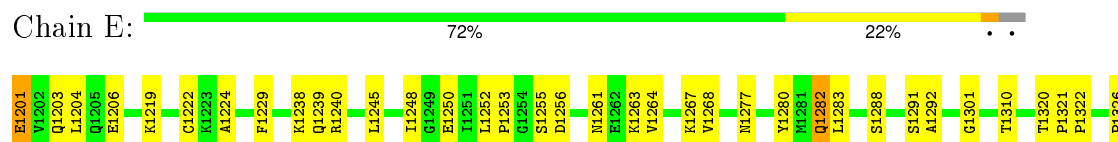- Molecule 1: light chain anti-lysozyme antibody F10.6.6

Chain A: 74%   24%

Chain A residues: D1 I2 G16 S20 L21 R24 I29 S30 N31 N32 L33 H34 W35 Y36 Q37 H41 R45 L46 L47 I48 K49 Q53 S54 M55 R61 T69 D70 F71 T72 L73 N76 C88 S93 W94 L104 D105 R108 A109 D110 V115 S121 S122 E123

L136 P141 R155 L160 N161 D165 Q166 D167 S168 K169 M175 L181 T182 K183 E187 N190 E195 K199 T202 V206 K207 N210 R211 N212

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

Chain D: 76%   23%

Chain D residues: D901 I902 S907 P908 A909 T910 L911 S912 V913 T914 P915 G916 V919 S920 L921 Q927 S928 I929 L933 Q937 Q938 K939 S940 H941 E942 L946 L947 I948 K949 Q953 S956 R961 G966 S967 F971 T972 L973 S977 V978 E979 F987 K1007 R1008 A1009 V1015

F1035 L1036 N1057 L1060 D1067 S1068 K1069 L1081 D1084 E1085 Y1086 K1099 K1107 R1111 ASN

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

Chain B: 69%   24%

Chain B residues: E301 V302 Q305 E306 S307 V318 K319 I320 A324 F329 K338 Q339 R340 S344 L345 E346 W347 I348 G349 E350 I351 L352 P353 G354 S355 D356 Y359 V360 N361 E362 K363 V364 K365 G366 K367 V368 N377 A392 G401 Y405 W406 G407 T410 P422 P426 L427

G430 SER ALA ALA GLN THR ASN S437 G447 Y448 P452 W457 Q474 L477 L480 S481 P487 S488 S489 P490 W491 P492 C498 T507 K511 K512 P515 R516 ASP CYS

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

Chain E: 72%   22%

Chain E residues: E1201 V1202 Q1203 L1204 Q1205 E1206 K1219 C1222 K1223 A1224 F1229 K1238 Q1239 R1240 L1245 I1248 Q1249 E1250 I1251 L1252 P1253 G1254 S1255 D1256 N1261 E1262 K1263 V1264 K1267 V1268 N1277 Y1280 M1281 Q1282 L1283 S1288 S1291 A1292 G1301 T1310 T1320 P1321 P1322 P1326

L1327 A1328 P1329 G1330 SER ALA ALA GLN THR ASN S1337 Y1348 P1352 V1372 L1373 Q1374 L1380 S1381 P1387 S1388 S1389 P1390 H1402 P1403 A1404 S1405 S1406 T1407 K1411 R1416 D1417 CYS

• Molecule 3: Lysozyme C

Chain C:

78%   19%   ·

K601 L608 M612 L617 N627 K633 N644 R645 D652 Y653 G654 I658 R661 W662 R668 S672 N677 I678 S681 A682 L683 I688 V692 W711 C715 D719 V720 Q721 A722 W723 I724 R725 L729

• Molecule 3: Lysozyme C

Chain F:

74%   22%   ·

K1501 L1508 M1512 H1515 N1527 C1530 F1534 N1537 F1538 G1554 I1555 L1556 Q1557 I1558 R1561 R1568 S1572 S1581 V1592 I1598 N1606 V1609 A1610 W1611 R1612 N1613 R1614 C1615 K1616 D1619 V1620 Q1621 A1622 W1623 I1624 R1625 G1626 C1627 R1628 L1629

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	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(°)	Ideal(°)
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%)	19	11
2	E	207/218 (95%)	200 (97%)	6 (3%)	1 (0%)	34	26
3	C	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	F	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	24	15
All	All	1086/1118 (97%)	1042 (96%)	40 (4%)	4 (0%)	39	33

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%)	36	31
1	D	190/191 (100%)	187 (98%)	3 (2%)	70	73
2	B	181/187 (97%)	173 (96%)	8 (4%)	35	30
2	E	182/187 (97%)	176 (97%)	6 (3%)	45	43
3	C	105/105 (100%)	102 (97%)	3 (3%)	50	49
3	F	105/105 (100%)	102 (97%)	3 (3%)	50	49
All	All	954/966 (99%)	923 (97%)	31 (3%)	46	44

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

Mol	Chain	Res	Type
2	B	488	SER
3	C	662	TRP
3	F	1508	LEU
2	B	511	LYS
3	C	668	ARG

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

Mol	Chain	Res	Type
2	B	382	GLN
3	C	677	ASN
3	F	1606	ASN
3	C	627	ASN
3	C	646	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 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.