wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 06:59 PM EDT

PDB ID	:	1CIC
Title	:	IDIOTOPE-ANTI-IDIOTOPE FAB-FAB COMPLEX; D1.3-E225
Authors	:	Bentley, G.A.
Deposited on	:	1999-03-31
Resolution	:	2.50 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 (1)) were used in the production of this report:

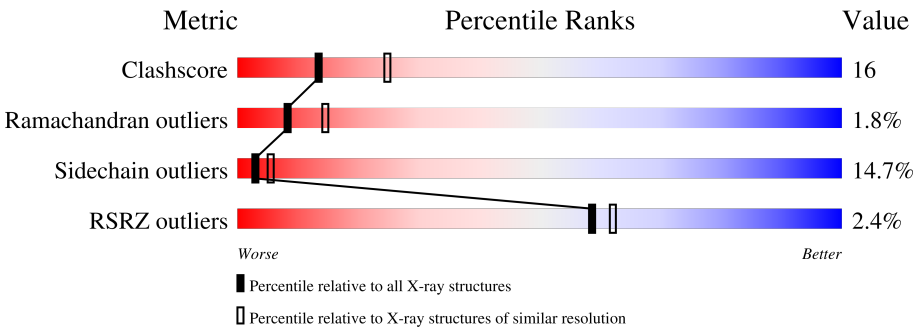
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	214	2%, 48%, 42%, 9% •
2	B	217	3%, 63%, 28%, 9%
3	C	214	2%, 57%, 34%, 8% •
4	D	218	2%, 63%, 28%, 8% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6733 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 PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1668	1038	283	338	9	0	0	0

- Molecule 2 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	217	1629	1030	262	329	8	0	0	0

- Molecule 3 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1665	1037	281	340	7	0	0	0

- Molecule 4 is a protein called PROTEIN (IG HEAVY CHAIN V REGIONS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	218	1643	1030	279	326	8	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	25	25	25	0	0
5	B	33	33	33	0	0
5	C	34	34	34	0	0
5	D	36	36	36	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 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.

• Molecule 1: PROTEIN (IG HEAVY CHAIN V REGIONS)

Chain A: 2% 48% 42% 9%

D1 I2 V3 K9 F10 M11 S12 T13 S14 V15 G16 D17 R18 V19 K24 D28 V29 R30 Y36 Q37 Q38 K39 Q42 S43 P44 K45 L46 L47 I48 Y49 W50 A51 R54 H55 T56 G57 V58 P59 D60 R61 F62 T69 D70 I75 S76 N77 V78 Q79 S80 E81 D82 L83

A84 D85 Q89 H90 C91 G92 S93 F96 S100 G101 T102 E105 I106 K107 R108 A109 D110 A111 A112 P113 T114 V115 S116 S121 S122 E123 Q124 L125 T126 S127 G128 S131 C134 F135 L136 N137 N138 F139 Y140 P141 T144 N145 V146 K147 W148 K149 I150 D151 G152 S153 E154 R155

Q156 V159 L160 D161 T164 D165 S168 K169 D170 S171 S174 M175 S176 S177 T178 L179 T180 L181 T182 K183 D184 E185 Y186 E187 R188 H189 N190 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 S201 T202 I205 V206 K207 S208 R211 N212 E213 C214

• Molecule 2: PROTEIN (IG HEAVY CHAIN V REGIONS)

Chain B: 3% 63% 28% 9%

Q1 V2 Q3 L4 Q5 Q6 S9 E10 L20 K23 Y27 P41 Y52 S55 G56 D57 D61 E62 S66 L70 T71 V72 D73 T74 S75 S76 S77 Y80 L83 L86 D90 S91 A92 Y95 R98 G99 L100 A101 F102 Y103 F104 D105 H106

Q109 G110 T111 T112 L113 T114 V115 L119 P123 Y126 C132 G133 D134 T135 T136 G137 S138 L142 K147 G148 Y149 F150 P151 E152 P153 V154 W158 N159 S160 G161 S162 L163 S164 S165 S166 M181 S182 V187 S194 T198 C199 S200 H203 P204 A205 S206 S207 T208

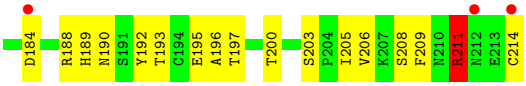
D211 K212 K213 L214 S217

• Molecule 3: PROTEIN (IG HEAVY CHAIN V REGIONS)

Chain C: 2% 57% 34% 8%

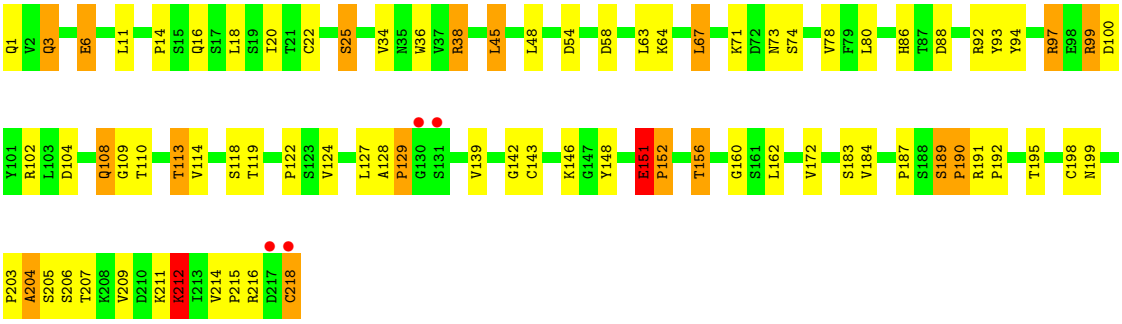
D1 M4 S10 L11 S12 T18 V19 T22 C23 R24 W35 Y36 Q40 S43 P44 Q45 V48 Y49 L54 A55 D56 R61 F62 S63 S67 Q70 K74 I75 L78 E81 D82 F83 G84 S85 Y86 Y87 C88 Q89 H90 F91 W92 S93 R96 T97

T102 K103 L106 D110 P113 T114 V115 S116 P119 P120 S121 L125 C134 F135 L136 N137 N138 I144 N145 V146 K147 W148 K149 I150 D151 G152 S153 E154 R155 Q156 V159 L160 D161 T164 D165 Q166 D167 S168 K169 D170 S171 T172 M175 S176 S177 T178 L179 T180 L181



• Molecule 4: PROTEIN (IG HEAVY CHAIN V REGIONS)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.11Å 77.65Å 96.75Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50 7.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 81.2 (7.00-2.53)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	203.33 (at 2.51Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.179 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 71.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6733	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.92	0/1707	1.71	28/2315 (1.2%)
2	B	1.01	0/1676	1.76	19/2294 (0.8%)
3	C	1.01	0/1705	1.77	25/2315 (1.1%)
4	D	1.03	0/1684	1.72	22/2300 (1.0%)
All	All	0.99	0/6772	1.74	94/9224 (1.0%)

There are no bond length outliers.

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	98	ARG	NE-CZ-NH2	-13.24	113.68	120.30
3	C	61	ARG	NE-CZ-NH2	11.06	125.83	120.30
4	D	99	ARG	NE-CZ-NH2	-10.81	114.89	120.30
4	D	6	GLU	CA-CB-CG	10.63	136.79	113.40
4	D	58	ASP	CB-CG-OD2	10.38	127.64	118.30

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	1668	0	1589	71	0
2	B	1629	0	1562	44	0
3	C	1665	0	1582	58	0
4	D	1643	0	1612	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	25	0	0	0	0
5	B	33	0	0	1	0
5	C	34	0	0	0	0
5	D	36	0	0	0	0
All	All	6733	0	6345	206	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 16.

The worst 5 of 206 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:C:4:MET:HG2	3:C:97:THR:HG22	1.24	1.15
4:D:195:THR:HG23	4:D:212:LYS:HE3	1.21	1.09
4:D:187:PRO:O	4:D:190:PRO:HD2	1.57	1.05
1:A:193:THR:HG22	1:A:208:SER:HB3	1.47	0.96
2:B:119:LEU:HD12	2:B:119:LEU:H	1.33	0.94

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%)	192 (91%)	15 (7%)	5 (2%)	6 9
2	B	215/217 (99%)	199 (93%)	11 (5%)	5 (2%)	6 10
3	C	212/214 (99%)	199 (94%)	11 (5%)	2 (1%)	17 31
4	D	216/218 (99%)	204 (94%)	9 (4%)	3 (1%)	11 20
All	All	855/863 (99%)	794 (93%)	46 (5%)	15 (2%)	8 14

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
2	B	134	ASP
2	B	159	ASN
3	C	211	ARG
4	D	129	PRO

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%)	167 (87%)	24 (13%)	4 8
2	B	186/186 (100%)	154 (83%)	32 (17%)	2 3
3	C	189/189 (100%)	161 (85%)	28 (15%)	3 5
4	D	190/190 (100%)	163 (86%)	27 (14%)	3 6
All	All	756/756 (100%)	645 (85%)	111 (15%)	3 5

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	11	LEU
4	D	218	CYS
3	C	114	THR
4	D	212	LYS
4	D	143	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	40	GLN
3	C	45	GLN
4	D	83	ASN
3	C	156	GLN
4	D	73	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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	214/214 (100%)	-0.42	5 (2%)	60	63	11, 42, 83, 112	0
2	B	217/217 (100%)	-0.70	7 (3%)	47	51	10, 31, 64, 80	0
3	C	214/214 (100%)	-0.60	5 (2%)	60	63	9, 30, 83, 112	0
4	D	218/218 (100%)	-0.81	4 (1%)	68	71	7, 27, 63, 99	0
All	All	863/863 (100%)	-0.63	21 (2%)	59	62	7, 33, 77, 112	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	CYS	5.2
2	B	134	ASP	5.0
1	A	213	GLU	4.6
3	C	212	ASN	4.5
3	C	214	CYS	4.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.