

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 - 02:15 pm GMT

PDB ID : 10CW

Title : Free conformation Ab2 of the IgE SPE-7 Authors : James, L.C.; Roversi, P.; Tawfik, D.

Deposited on : 2003-02-11

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 (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

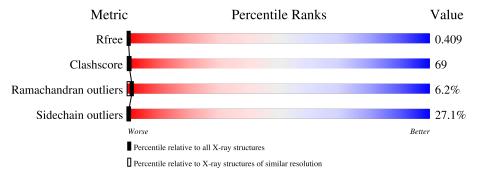
Validation Pipeline (wwPDB-VP) : 2.36

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	8085 (2.00-2.00)
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%

Mol	Chain	Length	Quality of chain				
1	Н	121	12%	51	%	27%	8% •
2	L	120		42%	45%		5% 8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1835 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 IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Н	120	Total 954	C 611	N 156	O 182	S 5	0	0	0

• Molecule 2 is a protein called IMMUNOGLOBULIN E.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	L	110	Total 813	C 510	N 138	O 163	S 2	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	43	Total O 43 43	0	0
3	L	25	Total O 25 25	0	0



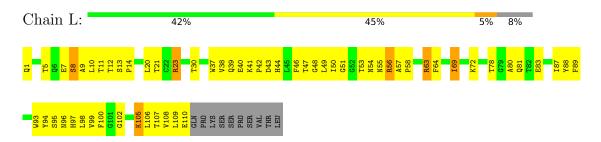
3 Residue-property plots (i)

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.

• Molecule 1: IMMUNOGLOBULIN E



• Molecule 2: IMMUNOGLOBULIN E





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants	79.55Å 79.55Å 67.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.17 - 2.00	Depositor
Resolution (A)	28.12 - 2.02	EDS
% Data completeness	94.4 (28.17-2.00)	Depositor
(in resolution range)	98.1 (28.12-2.02)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.24 (at 2.01Å)	Xtriage
Refinement program	SHELXL-97	Depositor
P.P.	0.267 , 0.290	Depositor
R, R_{free}	0.410 , 0.409	DCC
R_{free} test set	695 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 36.3	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	1835	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.75% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Н	0.35	0/982	1.11	$10/1331 \ (0.8\%)$	
2	L	0.28	0/829	0.80	1/1133 (0.1%)	
All	All	0.32	0/1811	0.98	11/2464 (0.4%)	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Н	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	Н	43	ARG	NE-CZ-NH2	11.60	126.10	120.30
1	Н	101	TYR	C-N-CA	10.74	148.54	121.70
1	Н	100	TRP	CA-CB-CG	6.97	126.95	113.70
1	Н	105	TYR	C-N-CA	6.21	137.24	121.70
1	Н	100	TRP	C-N-CA	5.83	136.27	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Н	41	PRO	Peptide



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	Н	954	0	913	205	75
2	L	813	0	794	118	36
3	Н	43	0	0	24	0
3	L	25	0	0	9	0
All	All	1835	0	1707	238	75

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 69.

The worst 5 of 238 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:H:47:TRP:CZ3	2:L:100:PHE:HB2	1.18	1.64
1:H:110:TRP:CD1	2:L:46:PHE:HB2	1.37	1.58
1:H:110:TRP:CG	2:L:46:PHE:HB2	1.38	1.55
1:H:47:TRP:HZ3	2:L:100:PHE:CB	1.29	1.44
1:H:110:TRP:CD2	2:L:46:PHE:HB3	1.56	1.40

The worst 5 of 75 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	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:H:112:GLN:NE2	2:L:8:SER:OG[3_655]	0.50	1.70
1:H:112:GLN:OE1	2:L:8:SER:C[3_655]	0.52	1.68
1:H:3:GLN:NE2	2:L:10:LEU:CG[3_655]	0.95	1.25
1:H:112:GLN:OE1	2:L:9:ALA:N[3_655]	0.97	1.23
1:H:3:GLN:NE2	2:L:10:LEU:CD1[3_655]	1.08	1.12



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	Perce	ntiles
1	Н	118/121 (98%)	88 (75%)	16 (14%)	14 (12%)	0	0
2	L	108/120~(90%)	99 (92%)	9 (8%)	0	100	100
All	All	$226/241 \; (94\%)$	187 (83%)	25 (11%)	14 (6%)	1	0

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Н	32	TYR
1	Н	33	TRP
1	Н	42	GLY
1	Н	77	SER
1	Н	102	TYR

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	Pe	erce	\mathbf{ntil}	es
1	Н	101/101 (100%)	60 (59%)	41 (41%)		0	0	
2	L	87/97 (90%)	77 (88%)	10 (12%)		5	3	
All	All	188/198 (95%)	137 (73%)	51 (27%)		0	0	

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	96	CYS

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Mol	Chain	Res	Type
1	Н	106	TYR
2	L	105	LYS
1	Н	98	ARG
1	Н	101	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	Н	39	GLN
1	Н	112	GLN
2	L	81	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

