



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:09 AM GMT

PDB ID : 2DH3
Title : Crystal Structure of human ED-4F2hc
Authors : Fort, J.; Fita, I.; Palacin, M.
Deposited on : 2006-03-21
Resolution : 2.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

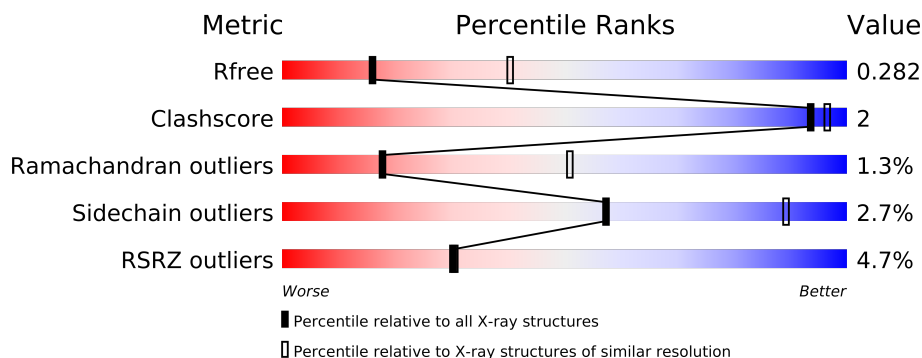
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	424	
1	B	424	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6533 atoms, of which 0 are hydrogen and 0 are deuterium.

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 4F2 cell-surface antigen heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3235	2056	552	622	5			
1	B	421	Total	C	N	O	S	0	0	0
			3269	2077	557	630	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ASP	-	EXPRESSION TAG	UNP P08195
A	107	ARG	-	EXPRESSION TAG	UNP P08195
A	108	TRP	-	EXPRESSION TAG	UNP P08195
A	109	GLY	-	EXPRESSION TAG	UNP P08195
A	110	SER	-	EXPRESSION TAG	UNP P08195
B	106	ASP	-	EXPRESSION TAG	UNP P08195
B	107	ARG	-	EXPRESSION TAG	UNP P08195
B	108	TRP	-	EXPRESSION TAG	UNP P08195
B	109	GLY	-	EXPRESSION TAG	UNP P08195
B	110	SER	-	EXPRESSION TAG	UNP P08195

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

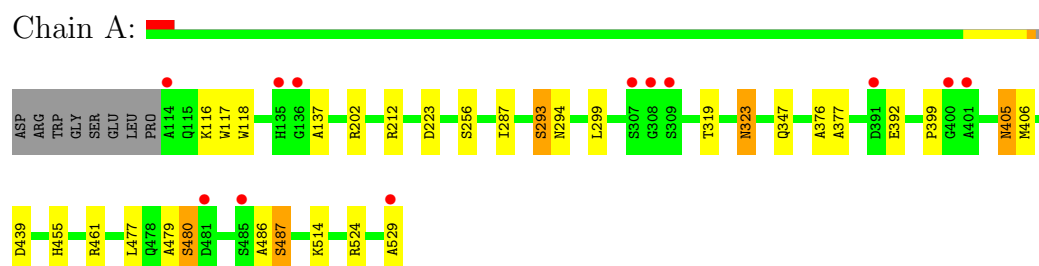
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	13	Total	O	0	0
			13	13		

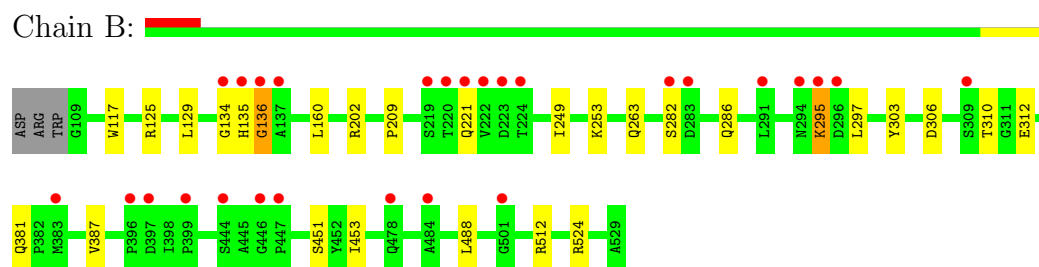
3 Residue-property plots

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.

- Molecule 1: 4F2 cell-surface antigen heavy chain



- Molecule 1: 4F2 cell-surface antigen heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.50Å 101.79Å 121.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 29.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (25.00-2.80) 94.6 (29.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.275 0.221 , 0.282	Depositor DCC
R_{free} test set	1066 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 20740 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0/3307	0.59	1/4484 (0.0%)
1	B	0.34	0/3342	0.51	0/4532
All	All	0.34	0/6649	0.55	1/9016 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	529	ALA	CA-C-O	20.44	163.02	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	LYS	Peptide

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3235	0	3194	12	0
1	B	3269	0	3226	9	0
2	A	1	0	0	0	0
3	A	15	0	0	0	0
3	B	13	0	0	0	0
All	All	6533	0	6420	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:376:ALA:O	1:A:377:ALA:HB3	2.04	0.57
1:A:287:ILE:HG23	1:A:299:LEU:HD23	1.89	0.55
1:B:129:LEU:HD21	1:B:160:LEU:HD11	1.88	0.55
1:A:319:THR:O	1:A:323:ASN:HB2	2.10	0.52
1:B:282:SER:O	1:B:286:GLN:NE2	2.42	0.51
1:B:286:GLN:HE21	1:B:303:TYR:HD2	1.59	0.50
1:A:433:ARG:HA	1:A:436:LEU:HD12	1.94	0.50
1:B:453:ILE:HD11	1:B:488:LEU:HD11	1.98	0.45
1:A:486:ALA:O	1:A:487:SER:C	2.55	0.45
1:A:439:ASP:HB3	1:A:455:HIS:O	2.16	0.45
1:B:263:GLN:HE21	1:B:295:LYS:HB3	1.82	0.45
1:A:405:ASN:HD22	1:A:406:MET:N	2.16	0.43
1:A:376:ALA:O	1:A:377:ALA:CB	2.65	0.43
1:A:479:ALA:O	1:A:480:SER:C	2.57	0.43
1:A:117:TRP:CD2	1:A:202:ARG:HG3	2.54	0.42
1:B:125:ARG:HB2	1:B:366:SER:HA	2.00	0.42
1:A:256:SER:HB2	1:A:293:SER:HB2	2.02	0.42
1:A:116:LYS:HD3	1:A:118:TRP:CZ2	2.55	0.41
1:B:381:GLN:HE22	1:B:387:VAL:HG23	1.85	0.41
1:B:117:TRP:CD2	1:B:202:ARG:HG3	2.56	0.41
1:B:134:GLY:O	1:B:136:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	414/424 (98%)	379 (92%)	29 (7%)	6 (1%)	16	49
1	B	419/424 (99%)	395 (94%)	19 (4%)	5 (1%)	19	54
All	All	833/848 (98%)	774 (93%)	48 (6%)	11 (1%)	18	51

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	487	SER
1	A	480	SER
1	A	293	SER
1	B	221	GLN
1	A	137	ALA
1	B	135	HIS
1	B	306	ASP
1	B	209	PRO
1	B	136	GLY
1	A	399	PRO

5.3.2 Protein sidechains ⓘ

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	350/357 (98%)	340 (97%)	10 (3%)	55	88
1	B	354/357 (99%)	345 (98%)	9 (2%)	60	90
All	All	704/714 (99%)	685 (97%)	19 (3%)	57	89

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	294	ASN
1	A	323	ASN
1	A	347	GLN
1	A	392	GLU
1	A	405	ASN
1	A	461	ARG
1	A	477	LEU
1	A	514	LYS
1	A	524	ARG
1	B	249	ILE
1	B	253	LYS
1	B	297	LEU
1	B	310	THR
1	B	312	GLU
1	B	347	GLN
1	B	451	SER
1	B	512	ARG
1	B	524	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	194	GLN
1	A	251	ASN
1	A	285	GLN
1	A	294	ASN
1	A	320	GLN
1	A	347	GLN
1	A	405	ASN
1	A	428	GLN
1	B	130	GLN
1	B	194	GLN
1	B	221	GLN
1	B	263	GLN
1	B	320	GLN
1	B	323	ASN
1	B	347	GLN
1	B	459	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	416/424 (98%)	-0.06	12 (2%) 49 50	42, 50, 60, 64	0
1	B	421/424 (99%)	0.17	27 (6%) 19 17	44, 50, 60, 67	0
All	All	837/848 (98%)	0.05	39 (4%) 30 30	42, 50, 60, 67	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	ASP	4.6
1	B	135	HIS	4.3
1	A	307	SER	4.3
1	B	219	SER	4.2
1	B	137	ALA	3.9
1	B	399	PRO	3.7
1	B	295	LYS	3.6
1	A	136	GLY	3.5
1	A	529	ALA	3.4
1	B	309	SER	3.4
1	B	397	ASP	3.4
1	B	447	PRO	3.3
1	A	481	ASP	3.3
1	B	222	VAL	3.2
1	A	308	GLY	3.1
1	B	136	GLY	3.1
1	B	478	GLN	3.0
1	A	309	SER	2.9
1	B	221	GLN	2.8
1	B	220	THR	2.8
1	B	446	GLY	2.7
1	B	224	THR	2.6
1	B	396	PRO	2.5
1	A	114	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	444	SER	2.4
1	B	283	ASP	2.4
1	B	282	SER	2.4
1	A	401	ALA	2.3
1	B	296	ASP	2.3
1	B	291	LEU	2.3
1	B	294	ASN	2.3
1	B	484	ALA	2.3
1	A	135	HIS	2.2
1	B	501	GLY	2.2
1	A	391	ASP	2.2
1	A	400	GLY	2.1
1	A	485	SER	2.1
1	B	383	MET	2.1
1	B	134	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	A	601	1/1	0.07	-2.17	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.