WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:49 PM EST

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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)

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 2.80 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.
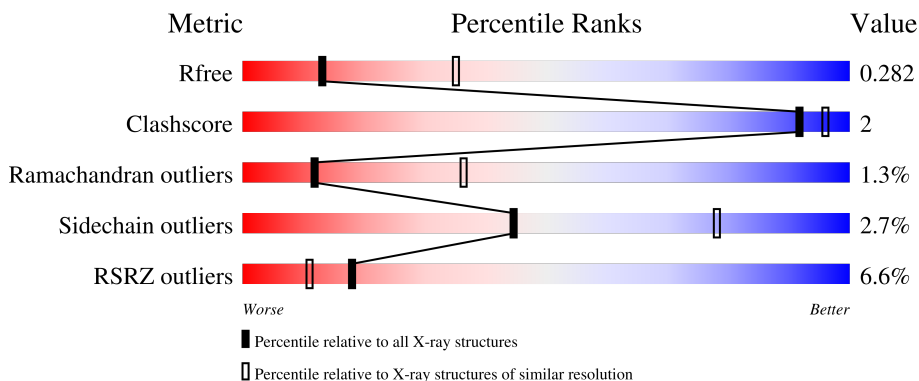
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	424	4% / 90% / 7% ··
1	B	424	9% / 92% / 7% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6533 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 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, 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: 4F2 cell-surface antigen heavy chain
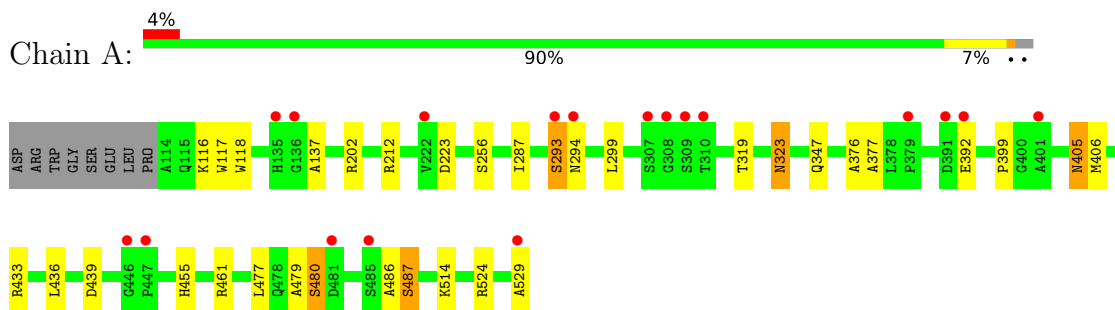
Chain A:

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

Chain B:
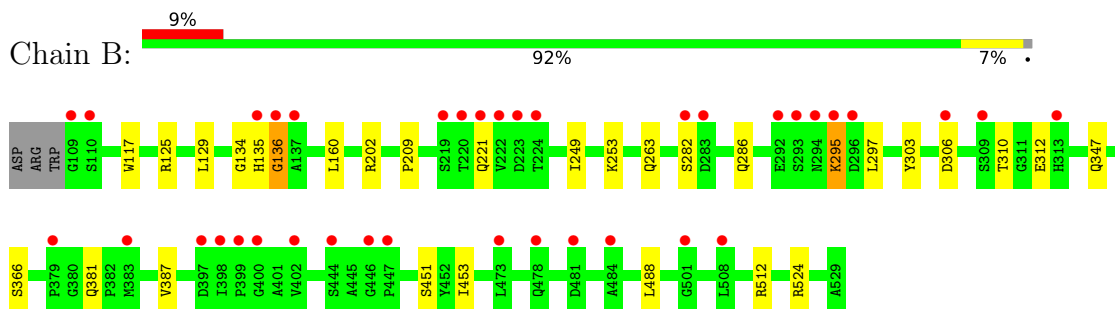
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.14%)	wwPDB-VP
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 , 55.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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[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 ⓘ

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(^{o})	Ideal(^{o})
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 Too-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 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	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

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 2.

All (21) 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: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:117:TRP:CD2	1:B:202:ARG:HG3	2.56	0.41
1:B:381:GLN:HE22	1:B:387:VAL:HG23	1.85	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%)	11	34
1	B	419/424 (99%)	395 (94%)	19 (4%)	5 (1%)	13	39
All	All	833/848 (98%)	774 (93%)	48 (6%)	11 (1%)	12	36

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%)	42	76
1	B	354/357 (99%)	345 (98%)	9 (2%)	47	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	704/714 (99%)	685 (97%)	19 (3%)	44 78

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

Sometimes 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

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	323	ASN
1	B	347	GLN
1	B	459	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides 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.

No monomer is involved in short contacts.

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%)	0.14	18 (4%)	35	25	42, 50, 60, 64	0
1	B	421/424 (99%)	0.37	37 (8%)	10	5	44, 50, 60, 67	0
All	All	837/848 (98%)	0.26	55 (6%)	18	11	42, 50, 60, 67	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	SER	5.3
1	B	135	HIS	5.3
1	A	307	SER	5.1
1	B	484	ALA	4.9
1	B	220	THR	4.8
1	B	399	PRO	4.6
1	B	223	ASP	4.4
1	A	481	ASP	3.7
1	B	397	ASP	3.7
1	B	444	SER	3.7
1	B	447	PRO	3.7
1	B	282	SER	3.6
1	A	529	ALA	3.6
1	A	309	SER	3.6
1	B	137	ALA	3.5
1	A	293	SER	3.5
1	B	222	VAL	3.5
1	A	308	GLY	3.1
1	B	224	THR	3.1
1	B	501	GLY	3.0
1	B	309	SER	3.0
1	B	313	HIS	2.9
1	A	446	GLY	2.9
1	B	295	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	296	ASP	2.8
1	A	294	ASN	2.8
1	A	485	SER	2.8
1	B	478	GLN	2.8
1	B	221	GLN	2.7
1	B	136	GLY	2.7
1	A	136	GLY	2.7
1	B	383	MET	2.5
1	A	401	ALA	2.5
1	B	109	GLY	2.5
1	A	310	THR	2.4
1	A	379	PRO	2.4
1	B	293	SER	2.4
1	B	400	GLY	2.3
1	B	402	VAL	2.3
1	B	446	GLY	2.3
1	B	379	PRO	2.3
1	A	135	HIS	2.2
1	B	283	ASP	2.2
1	B	473	LEU	2.2
1	A	447	PRO	2.2
1	A	392	GLU	2.2
1	B	398	ILE	2.1
1	B	110	SER	2.1
1	B	508	LEU	2.1
1	B	481	ASP	2.1
1	B	294	ASN	2.1
1	B	292	GLU	2.1
1	A	222	VAL	2.0
1	A	391	ASP	2.0
1	B	306	ASP	2.0

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 ⓘ

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. 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	601	1/1	0.99	0.09	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.