



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:22 am GMT

PDB ID : 3H0T
Title : Hepcidin-Fab complex
Authors : Syed, R.; Li, V.
Deposited on : 2009-04-10
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

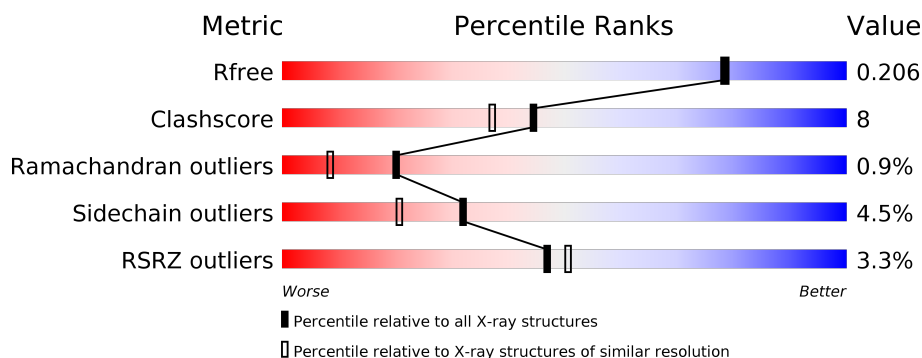
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 $\leq 5\%$. 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	216	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>••</div> </div> </div>
2	B	237	<div> <div></div> <div> <div>74%</div> <div>18%</div> <div>•</div> <div>6%</div> </div> </div>
3	C	25	<div> <div>32%</div> <div> <div>60%</div> <div>24%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3821 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 Fab fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1625	1008	268	343	6			

- Molecule 2 is a protein called Fab fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1681	1059	284	333	5			

- Molecule 3 is a protein called Hepcidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	S	0	0	0
			149	89	28	23	9			

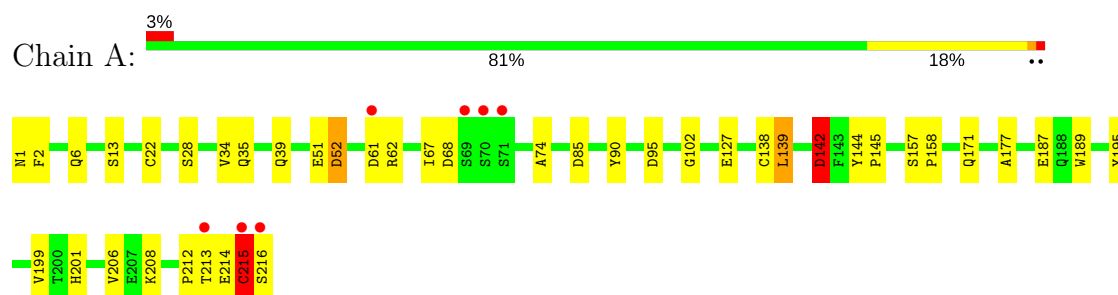
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		
4	B	208	Total	O	0	0
			208	208		
4	C	5	Total	O	0	0
			5	5		

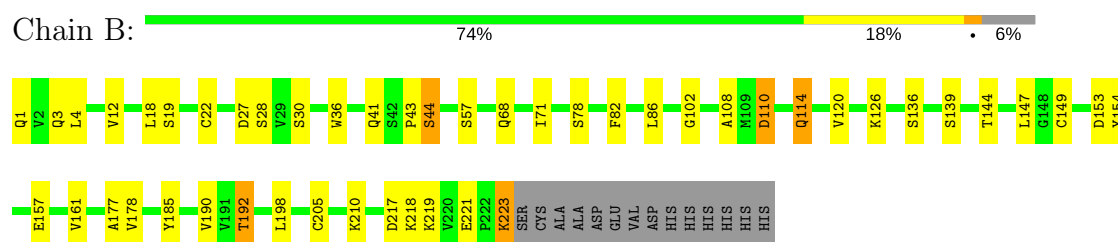
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

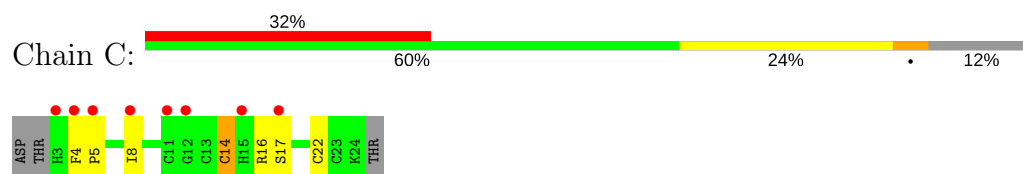
- Molecule 1: Fab fragment, Light chain



- Molecule 2: Fab fragment, Heavy chain



- Molecule 3: Hepcidin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.08Å 52.17Å 65.63Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	86.07 – 1.89 38.57 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.5 (86.07-1.89) 91.7 (38.57-1.89)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.36 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.251 0.204 , 0.206	Depositor DCC
R_{free} test set	3465 reflections (8.84%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3821	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 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	1.14	4/1664 (0.2%)	1.02	5/2270 (0.2%)
2	B	1.35	8/1723 (0.5%)	1.12	5/2356 (0.2%)
3	C	0.97	1/151 (0.7%)	1.06	0/200
All	All	1.24	13/3538 (0.4%)	1.07	10/4826 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	139	SER	CA-CB	7.96	1.64	1.52
2	B	185	TYR	CD2-CE2	7.46	1.50	1.39
1	A	199	VAL	CB-CG2	7.18	1.68	1.52
2	B	177	ALA	CA-CB	6.60	1.66	1.52
1	A	138	CYS	CB-SG	6.19	1.92	1.82
2	B	178	VAL	CB-CG1	5.87	1.65	1.52
2	B	149	CYS	CB-SG	-5.83	1.72	1.81
1	A	195	TYR	CD2-CE2	-5.53	1.31	1.39
3	C	22	CYS	CB-SG	-5.52	1.72	1.81
2	B	161	VAL	CB-CG2	5.46	1.64	1.52
2	B	110	ASP	CB-CG	-5.17	1.40	1.51
1	A	144	TYR	CG-CD2	5.13	1.45	1.39
2	B	154	TYR	CD1-CE1	5.00	1.46	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	VAL	CB-CA-C	-7.93	96.33	111.40
1	A	139	LEU	CB-CG-CD2	7.77	124.20	111.00
1	A	142	ASP	CB-CG-OD1	6.02	123.72	118.30
2	B	19	SER	N-CA-CB	-5.81	101.78	110.50
2	B	217	ASP	CB-CG-OD2	5.78	123.50	118.30
2	B	86	LEU	CA-CB-CG	5.75	128.52	115.30
2	B	205	CYS	CA-CB-SG	5.67	124.20	114.00
1	A	95	ASP	CB-CG-OD1	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	215	CYS	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1625	0	1553	25	0
2	B	1681	0	1650	24	0
3	C	149	0	128	6	0
4	A	153	0	0	4	0
4	B	208	0	0	4	0
4	C	5	0	0	1	0
All	All	3821	0	3331	51	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 8.

All (51) 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)
2:B:1:GLN:HE21	2:B:3:GLN:HE21	1.13	0.96
3:C:14:CYS:SG	3:C:14:CYS:O	2.30	0.88
1:A:39:GLN:HE22	2:B:41:GLN:HE22	1.21	0.86
1:A:215:CYS:HA	1:A:216:SER:HB2	1.57	0.84
1:A:215:CYS:CA	1:A:216:SER:HB2	2.17	0.73
1:A:214:GLU:HA	1:A:215:CYS:O	1.88	0.72
1:A:201:HIS:HD2	4:A:269:HOH:O	1.72	0.71
2:B:27:ASP:OD1	2:B:28:SER:N	2.23	0.68
2:B:126:LYS:NZ	4:B:357:HOH:O	2.28	0.66
2:B:1:GLN:NE2	2:B:3:GLN:HE21	1.91	0.66
1:A:171:GLN:HE21	1:A:177:ALA:HB2	1.63	0.62
2:B:43:PRO:O	2:B:44:SER:CB	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLN:OE1	4:B:420:HOH:O	2.16	0.61
1:A:6:GLN:HE21	1:A:102:GLY:HA3	1.65	0.61
2:B:157:GLU:OE1	4:B:386:HOH:O	2.16	0.59
2:B:219:LYS:NZ	2:B:221:GLU:OE2	2.36	0.57
1:A:139:LEU:HD22	2:B:190:VAL:HG21	1.86	0.57
1:A:189:TRP:CZ2	1:A:212:PRO:HA	2.42	0.54
1:A:62:ARG:NH1	1:A:85:ASP:OD2	2.39	0.52
2:B:43:PRO:O	2:B:44:SER:OG	2.27	0.51
1:A:213:THR:O	1:A:215:CYS:HB2	2.10	0.51
1:A:34:VAL:HG11	1:A:74:ALA:CB	2.43	0.49
2:B:114:GLN:HG2	2:B:114:GLN:O	2.12	0.49
1:A:6:GLN:HE22	1:A:90:TYR:HA	1.78	0.49
2:B:4:LEU:HD22	2:B:22:CYS:SG	2.54	0.48
2:B:136:SER:HB3	2:B:223:LYS:HD3	1.95	0.47
3:C:16:ARG:NH1	4:C:34:HOH:O	2.38	0.47
1:A:142:ASP:H	1:A:171:GLN:HE22	1.63	0.46
1:A:68:ASP:HA	4:A:331:HOH:O	2.14	0.46
1:A:215:CYS:HA	1:A:216:SER:CB	2.30	0.46
2:B:102:GLY:HA3	2:B:108:ALA:O	2.16	0.46
1:A:35:GLN:NE2	1:A:51:GLU:H	2.13	0.45
1:A:157:SER:HA	1:A:158:PRO:HD3	1.85	0.45
1:A:142:ASP:H	1:A:171:GLN:NE2	2.14	0.45
3:C:4:PHE:HA	3:C:5:PRO:HD3	1.73	0.44
2:B:36:TRP:HB3	2:B:82:PHE:CZ	2.53	0.44
2:B:68:GLN:HA	2:B:71:ILE:HG22	2.00	0.44
2:B:1:GLN:O	2:B:1:GLN:HG3	2.19	0.43
1:A:208:LYS:HE3	4:B:412:HOH:O	2.18	0.43
1:A:215:CYS:CB	1:A:216:SER:HB2	2.49	0.42
4:A:340:HOH:O	3:C:16:ARG:NH2	2.52	0.42
1:A:35:GLN:HE21	1:A:51:GLU:H	1.67	0.42
2:B:57:SER:HB2	3:C:5:PRO:HB3	2.02	0.42
2:B:12:VAL:O	2:B:120:VAL:HA	2.20	0.42
2:B:144:THR:HG23	2:B:192:THR:HG23	2.02	0.41
4:A:340:HOH:O	3:C:16:ARG:HG2	2.19	0.41
2:B:18:LEU:HD23	2:B:18:LEU:C	2.41	0.41
1:A:145:PRO:O	1:A:201:HIS:HE1	2.04	0.41
1:A:52:ASP:OD2	1:A:67:ILE:HG13	2.21	0.40
1:A:127:GLU:OE1	2:B:218:LYS:NZ	2.53	0.40
2:B:102:GLY:HA2	2:B:110:ASP:HB2	2.03	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	214/216 (99%)	201 (94%)	11 (5%)	2 (1%)	20	8
2	B	221/237 (93%)	212 (96%)	8 (4%)	1 (0%)	32	20
3	C	20/25 (80%)	16 (80%)	3 (15%)	1 (5%)	2	0
All	All	455/478 (95%)	429 (94%)	22 (5%)	4 (1%)	20	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	CYS
2	B	44	SER
3	C	14	CYS
1	A	2	PHE

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	189/189 (100%)	181 (96%)	8 (4%)	34	23
2	B	194/206 (94%)	186 (96%)	8 (4%)	35	24
3	C	17/23 (74%)	15 (88%)	2 (12%)	6	2
All	All	400/418 (96%)	382 (96%)	18 (4%)	32	21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	13	SER
1	A	22	CYS
1	A	28	SER
1	A	52	ASP
1	A	61	ASP
1	A	142	ASP
1	A	187	GLU
2	B	30	SER
2	B	78	SER
2	B	114	GLN
2	B	147	LEU
2	B	192	THR
2	B	198	LEU
2	B	210	LYS
2	B	223	LYS
3	C	8	ILE
3	C	17	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	6	GLN
1	A	35	GLN
1	A	39	GLN
1	A	171	GLN
1	A	174	ASN
1	A	198	GLN
1	A	201	HIS
2	B	1	GLN
2	B	81	GLN

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 [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](#)

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	216/216 (100%)	0.14	7 (3%) 48 51	18, 36, 60, 76	0
2	B	223/237 (94%)	-0.15	0 100 100	17, 29, 42, 58	0
3	C	22/25 (88%)	1.64	8 (36%) 0 0	56, 68, 74, 77	0
All	All	461/478 (96%)	0.07	15 (3%) 47 50	17, 32, 63, 77	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	CYS	5.3
3	C	5	PRO	4.0
1	A	216	SER	3.9
1	A	71	SER	3.5
3	C	4	PHE	3.3
3	C	3	HIS	3.3
1	A	213	THR	3.1
3	C	17	SER	3.1
1	A	69	SER	2.9
3	C	8	ILE	2.9
3	C	12	GLY	2.7
1	A	70	SER	2.7
1	A	61	ASP	2.3
3	C	15	HIS	2.3
3	C	11	CYS	2.2

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 carbohydrates 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.