Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 03:13 pm BST

PDB ID	:	6H5I
EMDB ID	:	EMD-0140
Title	:	Single Particle Cryo-EM map of human Transferrin receptor 1 - H-Ferritin complex.
Authors	:	Testi, C.; Montemiglio, L.C.; Vallone, B.; Des Georges, A.; Boffi, A.; Mancia, F.; Baiocco, P.; Savino, C.
Deposited on	:	2018-07-24
Resolution	:	3.90 Å(reported)
Based on initial models	:	3AJO, 3KAS

This is a Full wwPDB EM Validation 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

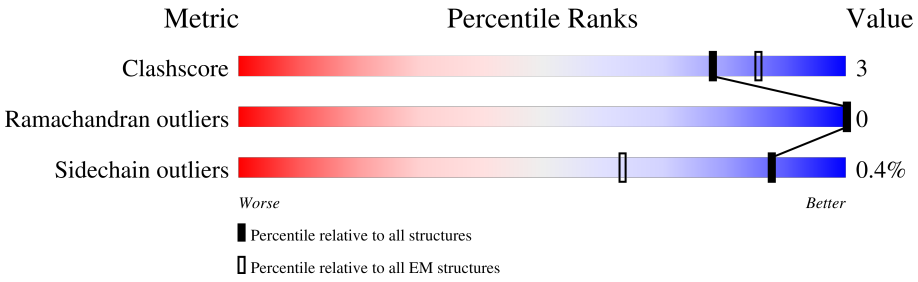
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	Aa	172	99% .
1	Ac	172	99% .
1	Ad	172	100%
1	Ae	172	100%
1	Af	172	100%
1	Ag	172	100%
1	Ah	172	100%
1	Ai	172	99% .
1	Aj	172	99% .

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Mol	Chain	Length	Quality of chain
1	Ak	172	100%
1	Al	172	99% .
1	Am	172	99% .
1	An	172	99% .
1	Ao	172	100%
1	Ap	172	100%
1	Ar	172	99% .
1	As	172	100%
1	At	172	99% .
1	Au	172	100%
1	Av	172	99% .
1	Aw	172	100%
1	Ax	172	100%
1	Ay	172	100%
1	Az	172	100%
2	Ab	640	98% ..
2	Aq	640	98% ..

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 43900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ac	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ad	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ae	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Af	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ag	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ah	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ai	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Aj	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ak	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Al	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Am	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	An	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ao	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ap	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ar	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	As	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	At	171	Total	C	N	O	S	0	0
			1404	880	246	271	7		
1	Au	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Av	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Aw	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ax	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Ay	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		
1	Az	172	Total	C	N	O	S	0	0
			1413	886	248	272	7		

- Molecule 2 is a protein called Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	632	Total	C	N	O	S	0	0
			4993	3204	839	936	14		
2	Aq	633	Total	C	N	O	S	0	0
			5004	3210	843	937	14		

There are 2 discrepancies between the modelled and reference sequences:

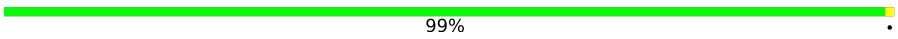
Chain	Residue	Modelled	Actual	Comment	Reference
Ab	142	SER	GLY	variant	UNP P02786
Aq	142	SER	GLY	variant	UNP P02786

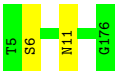
3 Residue-property plots (i)

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: Ferritin heavy chain

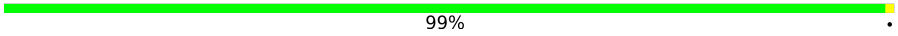
Chain Aa:





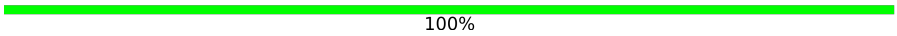
- Molecule 1: Ferritin heavy chain

Chain Ac:



- Molecule 1: Ferritin heavy chain

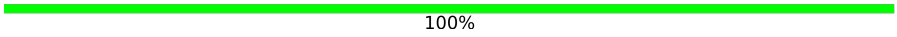
Chain Ad:



There are no outlier residues recorded for this chain.

- Molecule 1: Ferritin heavy chain

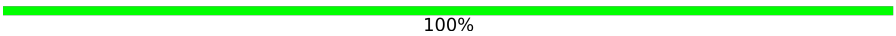
Chain Ae:



There are no outlier residues recorded for this chain.

- Molecule 1: Ferritin heavy chain

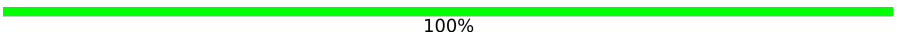
Chain Af:



There are no outlier residues recorded for this chain.

- Molecule 1: Ferritin heavy chain

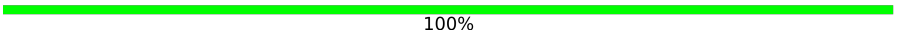
Chain Ag:



There are no outlier residues recorded for this chain.

- Molecule 1: Ferritin heavy chain

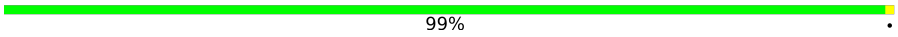
Chain Ah:



There are no outlier residues recorded for this chain.

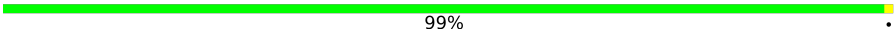
• Molecule 1: Ferritin heavy chain

Chain Ai:



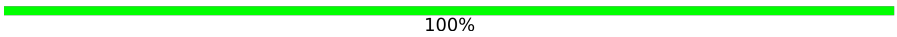
• Molecule 1: Ferritin heavy chain

Chain Aj:



• Molecule 1: Ferritin heavy chain

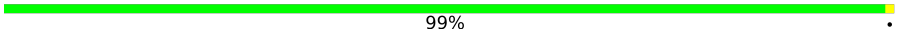
Chain Ak:



There are no outlier residues recorded for this chain.

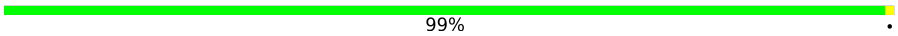
• Molecule 1: Ferritin heavy chain

Chain Al:



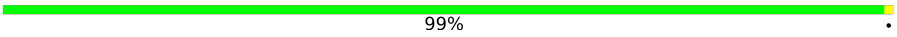
• Molecule 1: Ferritin heavy chain

Chain Am:



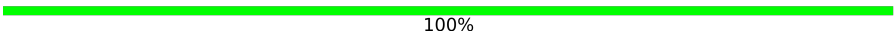
• Molecule 1: Ferritin heavy chain

Chain An:



• Molecule 1: Ferritin heavy chain

Chain Ao:



There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

Chain Ap: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

Chain Ar: 99%

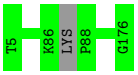
• Molecule 1: Ferritin heavy chain

Chain As: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

Chain At: 99%



• Molecule 1: Ferritin heavy chain

Chain Au: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

Chain Av: 99%

• Molecule 1: Ferritin heavy chain

Chain Aw: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

Chain Ax: 100%

There are no outlier residues recorded for this chain.

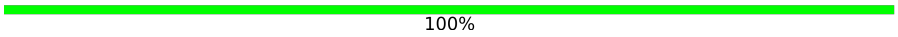
• Molecule 1: Ferritin heavy chain

Chain Ay: 100%

There are no outlier residues recorded for this chain.

• Molecule 1: Ferritin heavy chain

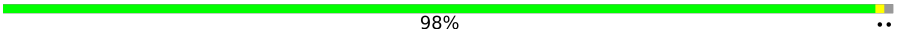
Chain Az:



There are no outlier residues recorded for this chain.

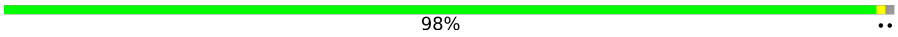
• Molecule 2: Transferrin receptor protein 1

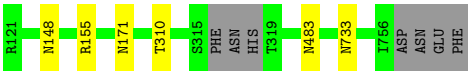
Chain Ab:



• Molecule 2: Transferrin receptor protein 1

Chain Aq:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	53878	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	Aa	0.35	0/1442	0.48	0/1942
1	Ac	0.35	0/1442	0.49	0/1942
1	Ad	0.36	0/1442	0.48	0/1942
1	Ae	0.37	0/1442	0.50	0/1942
1	Af	0.36	0/1442	0.50	0/1942
1	Ag	0.36	0/1442	0.49	0/1942
1	Ah	0.36	0/1442	0.48	0/1942
1	Ai	0.35	0/1442	0.48	0/1942
1	Aj	0.37	0/1442	0.48	0/1942
1	Ak	0.37	0/1442	0.51	0/1942
1	Al	0.35	0/1442	0.50	0/1942
1	Am	0.35	0/1442	0.51	0/1942
1	An	0.35	0/1442	0.50	0/1942
1	Ao	0.36	0/1442	0.51	0/1942
1	Ap	0.36	0/1442	0.49	0/1942
1	Ar	0.35	0/1442	0.48	0/1942
1	As	0.37	0/1442	0.49	0/1942
1	At	0.38	0/1432	0.50	0/1927
1	Au	0.35	0/1442	0.50	0/1942
1	Av	0.36	0/1442	0.50	0/1942
1	Aw	0.35	0/1442	0.48	0/1942
1	Ax	0.36	0/1442	0.48	0/1942
1	Ay	0.36	0/1442	0.49	0/1942
1	Az	0.35	0/1442	0.49	0/1942
2	Ab	0.27	0/5109	0.50	0/6925
2	Aq	0.26	0/5121	0.49	0/6942
All	All	0.34	0/44828	0.49	0/60460

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
2	Ab	0	2
2	Aq	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ab	209	LEU	Peptide
2	Ab	310	THR	Peptide
2	Aq	310	THR	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	Aa	1413	0	1357	0	0
1	Ac	1413	0	1357	0	0
1	Ad	1413	0	1357	0	0
1	Ae	1413	0	1357	0	0
1	Af	1413	0	1357	0	0
1	Ag	1413	0	1357	0	0
1	Ah	1413	0	1357	0	0
1	Ai	1413	0	1357	0	0
1	Aj	1413	0	1357	0	0
1	Ak	1413	0	1357	0	0
1	Al	1413	0	1357	0	0
1	Am	1413	0	1357	0	0
1	An	1413	0	1357	0	0
1	Ao	1413	0	1357	0	0
1	Ap	1413	0	1357	0	0
1	Ar	1413	0	1357	0	0
1	As	1413	0	1357	0	0
1	At	1404	0	1344	0	0
1	Au	1413	0	1357	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Av	1413	0	1357	0	0
1	Aw	1413	0	1357	0	0
1	Ax	1413	0	1357	0	0
1	Ay	1413	0	1357	0	0
1	Az	1413	0	1357	0	0
2	Ab	4993	0	4944	0	0
2	Aq	5004	0	4958	0	0
All	All	43900	0	42457	0	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 3.

There are no clashes within the asymmetric unit.

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 PDB entries followed by that with respect to all EM entries.

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	Aa	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
1	Ac	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
1	Ad	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
1	Ae	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
1	Af	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
1	Ag	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
1	Ah	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
1	Ai	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
1	Aj	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
1	Ak	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
1	Al	170/172 (99%)	164 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Am	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
1	An	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
1	Ao	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
1	Ap	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
1	Ar	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
1	As	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
1	At	167/172 (97%)	156 (93%)	11 (7%)	0	100	100
1	Au	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
1	Av	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
1	Aw	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
1	Ax	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
1	Ay	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
1	Az	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	Ab	626/640 (98%)	585 (94%)	41 (6%)	0	100	100
2	Aq	629/640 (98%)	600 (95%)	29 (5%)	0	100	100
All	All	5332/5408 (99%)	5102 (96%)	230 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	Aa	153/153 (100%)	151 (99%)	2 (1%)	65	76
1	Ac	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Ad	153/153 (100%)	153 (100%)	0	100	100
1	Ae	153/153 (100%)	153 (100%)	0	100	100
1	Af	153/153 (100%)	153 (100%)	0	100	100
1	Ag	153/153 (100%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ah	153/153 (100%)	153 (100%)	0	100	100
1	Ai	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Aj	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Ak	153/153 (100%)	153 (100%)	0	100	100
1	Al	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Am	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	An	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Ao	153/153 (100%)	153 (100%)	0	100	100
1	Ap	153/153 (100%)	153 (100%)	0	100	100
1	Ar	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	As	153/153 (100%)	153 (100%)	0	100	100
1	At	152/153 (99%)	152 (100%)	0	100	100
1	Au	153/153 (100%)	153 (100%)	0	100	100
1	Av	153/153 (100%)	152 (99%)	1 (1%)	81	86
1	Aw	153/153 (100%)	153 (100%)	0	100	100
1	Ax	153/153 (100%)	153 (100%)	0	100	100
1	Ay	153/153 (100%)	153 (100%)	0	100	100
1	Az	153/153 (100%)	153 (100%)	0	100	100
2	Ab	541/549 (98%)	536 (99%)	5 (1%)	75	83
2	Aq	542/549 (99%)	537 (99%)	5 (1%)	75	83
All	All	4754/4770 (100%)	4734 (100%)	20 (0%)	88	91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	6	SER
1	Aa	11	ASN
2	Ab	148	ASN
2	Ab	155	ARG
2	Ab	171	ASN
2	Ab	483	ASN
2	Ab	733	ASN
1	Ac	6	SER
1	Ai	36	SER
1	Aj	6	SER

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Mol	Chain	Res	Type
1	Al	98	ASN
1	Am	22	ARG
1	An	87	LYS
2	Aq	148	ASN
2	Aq	155	ARG
2	Aq	171	ASN
2	Aq	483	ASN
2	Aq	733	ASN
1	Ar	84	ASP
1	Av	44	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ab	164	ASN
2	Ab	171	ASN
2	Ab	197	GLN
2	Ab	335	GLN
2	Ab	408	GLN
2	Ab	483	ASN
2	Ab	493	ASN
2	Ab	626	ASN
2	Ab	684	HIS
2	Ab	733	ASN
2	Ab	747	ASN
1	Ac	11	ASN
1	Ac	105	HIS
1	Ac	112	GLN
1	Ac	173	HIS
1	Ad	7	GLN
1	Ad	21	ASN
1	Ad	25	ASN
1	Af	11	ASN
1	Af	65	HIS
1	Ag	173	HIS
1	Ah	112	GLN
1	Aj	151	HIS
1	Ak	112	GLN
1	Al	11	ASN
1	Al	98	ASN
1	Am	11	ASN
1	Am	25	ASN

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Mol	Chain	Res	Type
1	Am	57	HIS
1	Am	83	GLN
1	An	173	HIS
1	Ao	11	ASN
1	Ap	11	ASN
2	Aq	171	ASN
2	Aq	300	HIS
2	Aq	483	ASN
2	Aq	733	ASN
2	Aq	747	ASN
1	Ar	173	HIS
1	As	11	ASN
1	As	173	HIS
1	At	11	ASN
1	Au	11	ASN
1	Av	11	ASN
1	Aw	11	ASN
1	Aw	173	HIS
1	Ax	11	ASN
1	Ay	11	ASN
1	Az	10	GLN
1	Az	21	ASN
1	Az	173	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-0140. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.