



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:48 AM UTC

PDB ID : 4FEC / pdb_00004fec
Title : Crystal Structure of Htt36Q3H
Authors : Kim, M.
Deposited on : 2012-05-30
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity : **FAILED**
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

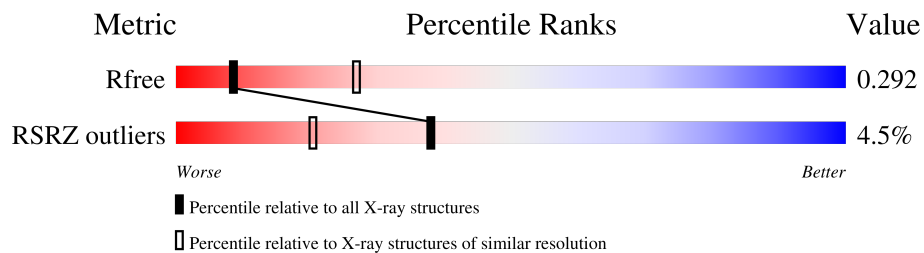
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9664 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 Maltose-binding periplasmic protein,Huntingtin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	Total 3146	C 2016	N 520	O 602	S 8	0	2	0
1	B	401	Total 3130	C 2007	N 520	O 595	S 8	0	1	0
1	C	410	Total 3209	C 2051	N 535	O 615	S 8	0	1	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	linker	UNP P0AEX9
A	360	ALA	-	linker	UNP P0AEX9
A	361	LEU	-	linker	UNP P0AEX9
A	362	ALA	-	linker	UNP P0AEX9
A	363	ALA	-	linker	UNP P0AEX9
A	364	ALA	-	linker	UNP P0AEX9
A	365	GLN	-	linker	UNP P0AEX9
A	366	THR	-	linker	UNP P0AEX9
A	367	ASN	-	linker	UNP P0AEX9
A	368	ALA	-	linker	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	388	GLN	-	insertion	UNP P42858
A	389	GLN	-	insertion	UNP P42858
A	390	GLN	-	insertion	UNP P42858
A	391	GLN	-	insertion	UNP P42858
A	392	GLN	-	insertion	UNP P42858
A	393	GLN	-	insertion	UNP P42858
A	394	GLN	-	insertion	UNP P42858
A	395	HIS	-	insertion	UNP P42858
A	396	GLN	-	insertion	UNP P42858
A	397	HIS	-	insertion	UNP P42858
A	398	GLN	-	insertion	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	399	HIS	-	insertion	UNP P42858
A	400	GLN	-	insertion	UNP P42858
A	401	GLN	-	insertion	UNP P42858
A	402	GLN	-	insertion	UNP P42858
A	403	GLN	-	insertion	UNP P42858
A	404	GLN	-	insertion	UNP P42858
A	405	GLN	-	insertion	UNP P42858
B	359	ALA	-	linker	UNP P0AEX9
B	360	ALA	-	linker	UNP P0AEX9
B	361	LEU	-	linker	UNP P0AEX9
B	362	ALA	-	linker	UNP P0AEX9
B	363	ALA	-	linker	UNP P0AEX9
B	364	ALA	-	linker	UNP P0AEX9
B	365	GLN	-	linker	UNP P0AEX9
B	366	THR	-	linker	UNP P0AEX9
B	367	ASN	-	linker	UNP P0AEX9
B	368	ALA	-	linker	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	388	GLN	-	insertion	UNP P42858
B	389	GLN	-	insertion	UNP P42858
B	390	GLN	-	insertion	UNP P42858
B	391	GLN	-	insertion	UNP P42858
B	392	GLN	-	insertion	UNP P42858
B	393	GLN	-	insertion	UNP P42858
B	394	GLN	-	insertion	UNP P42858
B	395	HIS	-	insertion	UNP P42858
B	396	GLN	-	insertion	UNP P42858
B	397	HIS	-	insertion	UNP P42858
B	398	GLN	-	insertion	UNP P42858
B	399	HIS	-	insertion	UNP P42858
B	400	GLN	-	insertion	UNP P42858
B	401	GLN	-	insertion	UNP P42858
B	402	GLN	-	insertion	UNP P42858
B	403	GLN	-	insertion	UNP P42858
B	404	GLN	-	insertion	UNP P42858
B	405	GLN	-	insertion	UNP P42858
C	359	ALA	-	linker	UNP P0AEX9
C	360	ALA	-	linker	UNP P0AEX9
C	361	LEU	-	linker	UNP P0AEX9
C	362	ALA	-	linker	UNP P0AEX9
C	363	ALA	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	-	linker	UNP P0AEX9
C	365	GLN	-	linker	UNP P0AEX9
C	366	THR	-	linker	UNP P0AEX9
C	367	ASN	-	linker	UNP P0AEX9
C	368	ALA	-	linker	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
C	388	GLN	-	insertion	UNP P42858
C	389	GLN	-	insertion	UNP P42858
C	390	GLN	-	insertion	UNP P42858
C	391	GLN	-	insertion	UNP P42858
C	392	GLN	-	insertion	UNP P42858
C	393	GLN	-	insertion	UNP P42858
C	394	GLN	-	insertion	UNP P42858
C	395	HIS	-	insertion	UNP P42858
C	396	GLN	-	insertion	UNP P42858
C	397	HIS	-	insertion	UNP P42858
C	398	GLN	-	insertion	UNP P42858
C	399	HIS	-	insertion	UNP P42858
C	400	GLN	-	insertion	UNP P42858
C	401	GLN	-	insertion	UNP P42858
C	402	GLN	-	insertion	UNP P42858
C	403	GLN	-	insertion	UNP P42858
C	404	GLN	-	insertion	UNP P42858
C	405	GLN	-	insertion	UNP P42858

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Zn	0	0
			5	5		
2	B	13	Total	Zn	0	0
			13	13		
2	C	13	Total	Zn	0	0
			13	13		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	61	Total	O	0	0
			61	61		
3	C	49	Total	O	0	0
			49	49		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.05Å 177.28Å 78.87Å 90.00° 109.03° 90.00°	Depositor
Resolution (Å)	35.00 – 3.00 35.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (35.00-3.00) 95.8 (35.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 3.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.227 , 0.275 0.253 , 0.292	Depositor DCC
R_{free} test set	1942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9664	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 31 are 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	402/452 (88%)	0.23	14 (3%) 47 27	24, 84, 120, 155	15 (3%)
1	B	401/452 (88%)	0.22	13 (3%) 50 29	32, 89, 132, 159	13 (3%)
1	C	410/452 (90%)	0.35	28 (6%) 23 12	31, 92, 141, 190	28 (6%)
All	All	1213/1356 (89%)	0.27	55 (4%) 38 20	24, 89, 132, 190	56 (4%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	GLN	7.7
1	A	400	GLN	7.6
1	A	401	GLN	7.3
1	C	171	TYR	6.5
1	C	408	GLN	6.3
1	C	406	GLN	6.1
1	A	395	HIS	5.3
1	B	401	GLN	5.3
1	B	395	HIS	4.9
1	A	1	LYS	4.6
1	A	3	GLU	4.6
1	B	392	GLN	4.3
1	A	394	GLN	4.2
1	A	397	HIS	4.2
1	B	210	TYR	4.1
1	A	396	GLN	4.0
1	C	399	HIS	3.9
1	C	45	GLU	3.9
1	C	410	GLN	3.8
1	B	400	GLN	3.8
1	C	392	GLN	3.6
1	C	407	GLN	3.6
1	B	394	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	396	GLN	3.5
1	B	398	GLN	3.4
1	B	397	HIS	3.4
1	C	401	GLN	3.4
1	C	405	GLN	3.3
1	A	391	GLN	3.1
1	A	398	GLN	3.1
1	C	395	HIS	3.0
1	B	396	GLN	2.9
1	C	174	GLY	2.8
1	B	153	GLU	2.7
1	C	402	GLN	2.7
1	C	283	TYR	2.7
1	B	393	GLN	2.6
1	C	404	GLN	2.6
1	C	393	GLN	2.5
1	C	394	GLN	2.5
1	B	344[A]	ARG	2.5
1	C	367	ASN	2.4
1	A	155	TYR	2.4
1	C	398	GLN	2.4
1	C	400	GLN	2.3
1	C	409	GLN	2.3
1	C	397	HIS	2.3
1	C	14	ASP	2.3
1	A	399	HIS	2.2
1	A	392	GLN	2.1
1	C	366	THR	2.1
1	B	399	HIS	2.1
1	C	100	ASN	2.0
1	C	389	GLN	2.0
1	C	391	GLN	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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	B	513	1/1	0.71	0.20	60,60,60,60	1
2	ZN	B	512	1/1	0.76	0.12	60,60,60,60	1
2	ZN	C	502	1/1	0.78	0.08	60,60,60,60	1
2	ZN	C	503	1/1	0.80	0.14	60,60,60,60	1
2	ZN	A	505	1/1	0.81	0.11	60,60,60,60	1
2	ZN	B	503	1/1	0.85	0.08	60,60,60,60	1
2	ZN	C	501	1/1	0.88	0.32	60,60,60,60	1
2	ZN	C	511	1/1	0.88	0.12	60,60,60,60	1
2	ZN	C	512	1/1	0.88	0.18	60,60,60,60	1
2	ZN	C	513	1/1	0.88	0.14	60,60,60,60	1
2	ZN	B	509	1/1	0.89	0.07	60,60,60,60	1
2	ZN	B	501	1/1	0.89	0.09	60,60,60,60	1
2	ZN	C	505	1/1	0.89	0.12	60,60,60,60	1
2	ZN	B	502	1/1	0.90	0.06	60,60,60,60	1
2	ZN	C	504	1/1	0.90	0.05	60,60,60,60	1
2	ZN	A	504	1/1	0.91	0.07	60,60,60,60	1
2	ZN	A	502	1/1	0.91	0.08	60,60,60,60	1
2	ZN	B	510	1/1	0.92	0.12	55,55,55,55	1
2	ZN	C	506	1/1	0.93	0.11	60,60,60,60	1
2	ZN	A	501	1/1	0.93	0.10	60,60,60,60	1
2	ZN	A	503	1/1	0.94	0.08	60,60,60,60	1
2	ZN	C	507	1/1	0.94	0.14	60,60,60,60	1
2	ZN	C	510	1/1	0.94	0.06	60,60,60,60	1
2	ZN	B	511	1/1	0.95	0.04	60,60,60,60	1
2	ZN	B	504	1/1	0.95	0.09	60,60,60,60	1
2	ZN	B	505	1/1	0.97	0.17	60,60,60,60	1
2	ZN	B	506	1/1	0.97	0.11	59,59,59,59	1
2	ZN	B	507	1/1	0.98	0.05	60,60,60,60	1
2	ZN	B	508	1/1	0.98	0.04	60,60,60,60	1
2	ZN	C	508	1/1	0.98	0.10	60,60,60,60	1
2	ZN	C	509	1/1	0.98	0.05	60,60,60,60	1

5.5 Other polymers [i](#)

There are no such residues in this entry.