



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 03:23 PM GMT

PDB ID : 4FE8
Title : Crystal Structure of Htt36Q3H-EX1-X1-C1(Alpha)
Authors : Kim, M.
Deposited on : 2012-05-29
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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>

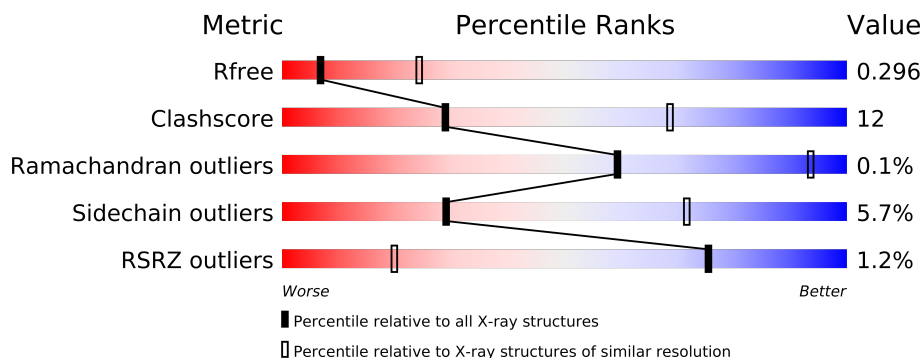
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	452	
1	B	452	
1	C	452	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	B	512	-	X
2	ZN	C	503	-	X
2	ZN	C	511	-	X

2 Entry composition

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

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

There are 90 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 3 is water.

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

Continued on next page...

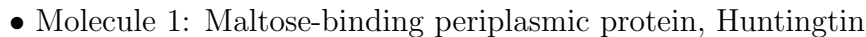
Continued from previous page...

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

i

- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

Age Group	Percentage of Respondents
18-29	90%
30-49	87%
50-64	82%
65+	75%



4 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 34.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (35.00-3.00) 95.9 (34.46-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.227 , 0.275 0.254 , 0.296	Depositor DCC
R_{free} test set	1942 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 38580 reflections	Xtriage
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

Xtriage'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.

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	0.35	0/3220	0.46	1/4366 (0.0%)
1	B	0.38	0/3204	0.47	0/4344
1	C	0.35	0/3283	0.44	0/4450
All	All	0.36	0/9707	0.46	1/13160 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	HIS	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3146	0	276	65	47
1	B	3130	0	270	38	46
1	C	3209	0	342	26	0
2	A	5	0	0	0	0
2	B	13	0	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	0	0	0
3	A	38	0	0	1	0
3	B	61	0	0	0	0
3	C	49	0	0	0	0
All	All	9664	0	888	129	47

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 12.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:394:GLN:HG3	1:A:395:HIS:CE1	1.67	1.28
1:A:397:HIS:CD2	1:A:399:HIS:C	2.16	1.19
1:A:391:GLN:HA	1:A:395:HIS:CE1	1.81	1.14
1:A:394:GLN:CG	1:A:395:HIS:CE1	2.29	1.12
1:A:397:HIS:CD2	1:A:399:HIS:H	1.67	1.12

The worst 5 of 47 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155:TYR:CZ	1:B:398:GLN:NE2[2_556]	0.34	1.86
1:A:155:TYR:CG	1:B:398:GLN:OE1[2_556]	0.43	1.77
1:A:396:GLN:CD	1:B:153:GLU:CD[2_556]	0.49	1.71
1:A:396:GLN:OE1	1:B:153:GLU:OE1[2_556]	0.95	1.25
1:A:396:GLN:NE2	1:B:153:GLU:CB[2_556]	1.05	1.15

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	402/452 (89%)	385 (96%)	17 (4%)	0	100	100
1	B	400/452 (88%)	389 (97%)	10 (2%)	1 (0%)	50	90
1	C	409/452 (90%)	396 (97%)	13 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1211/1356 (89%)	1170 (97%)	40 (3%)	1 (0%)	59 93

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	397	HIS

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	323/370 (87%)	307 (95%)	16 (5%)	34 77
1	B	321/370 (87%)	304 (95%)	17 (5%)	32 74
1	C	330/370 (89%)	307 (93%)	23 (7%)	21 62
All	All	974/1110 (88%)	918 (94%)	56 (6%)	29 71

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	291	GLU
1	B	399	HIS
1	C	402	GLN
1	B	344[A]	ARG
1	B	374	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	391	GLN
1	B	393	GLN
1	B	400	GLN
1	A	399	HIS
1	B	399	HIS

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 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.

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	402/452 (88%)	-0.23	4 (0%)	79 22	24, 84, 120, 155	13 (3%)
1	B	401/452 (88%)	-0.20	1 (0%)	93 54	38, 89, 132, 159	12 (2%)
1	C	410/452 (90%)	-0.12	7 (1%)	67 15	58, 92, 141, 190	27 (6%)
All	All	1213/1356 (89%)	-0.18	12 (0%)	75 22	24, 89, 133, 190	52 (4%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	410	GLN	4.6
1	B	395	HIS	4.3
1	C	408	GLN	3.4
1	C	407	GLN	3.2
1	A	395	HIS	3.0

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(\AA^2)	Q<0.9
2	ZN	C	503	1/1	0.28	74.33	60,60,60,60	1
2	ZN	B	512	1/1	0.39	7.29	60,60,60,60	1
2	ZN	C	511	1/1	0.24	4.77	60,60,60,60	1
2	ZN	A	505	1/1	0.33	1.79	60,60,60,60	1
2	ZN	A	502	1/1	0.31	1.26	60,60,60,60	1
2	ZN	C	507	1/1	0.26	1.13	60,60,60,60	1
2	ZN	A	503	1/1	0.19	0.68	60,60,60,60	1
2	ZN	C	502	1/1	0.19	0.61	60,60,60,60	1
2	ZN	B	504	1/1	0.22	0.07	60,60,60,60	1
2	ZN	C	506	1/1	0.24	0.04	60,60,60,60	1
2	ZN	B	503	1/1	0.25	-0.11	60,60,60,60	1
2	ZN	C	513	1/1	0.26	-0.16	60,60,60,60	1
2	ZN	C	501	1/1	0.29	-0.17	60,60,60,60	1
2	ZN	C	512	1/1	0.28	-0.50	60,60,60,60	1
2	ZN	B	506	1/1	0.15	-0.77	59,59,59,59	1
2	ZN	C	509	1/1	0.14	-0.97	60,60,60,60	1
2	ZN	A	501	1/1	0.21	-1.08	60,60,60,60	1
2	ZN	C	508	1/1	0.17	-1.11	60,60,60,60	1
2	ZN	B	505	1/1	0.19	-1.19	60,60,60,60	1
2	ZN	B	502	1/1	0.12	-1.56	60,60,60,60	1
2	ZN	A	504	1/1	0.07	-1.84	60,60,60,60	1
2	ZN	B	507	1/1	0.15	-1.86	60,60,60,60	1
2	ZN	B	510	1/1	0.19	-2.06	55,55,55,55	1
2	ZN	B	509	1/1	0.13	-2.07	60,60,60,60	1
2	ZN	B	508	1/1	0.14	-2.10	60,60,60,60	1
2	ZN	B	501	1/1	0.08	-2.42	60,60,60,60	1
2	ZN	C	510	1/1	0.08	-2.78	60,60,60,60	1
2	ZN	C	505	1/1	0.11	-4.88	60,60,60,60	1
2	ZN	C	504	1/1	0.08	-15.09	60,60,60,60	1
2	ZN	B	513	1/1	0.19	-	60,60,60,60	1
2	ZN	B	511	1/1	0.09	-	60,60,60,60	1

6.5 Other polymers ⓘ

There are no such residues in this entry.