



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:36 AM UTC

PDB ID : 3IOR / pdb_00003ior
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C95
Authors : Kim, M.W.
Deposited on : 2009-08-14
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
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

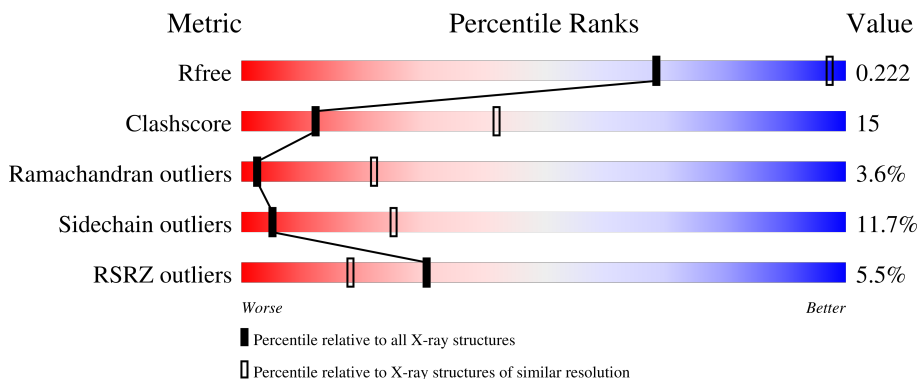
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	449	 3% 57% 24% 5% 13%
1	B	449	 7% 58% 29% • 8%
1	C	449	 5% 52% 31% 5% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	451	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 9166 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 protein, huntingtin fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	Total 2979	C 1918	N 486	O 567	S 8	0	0	0
1	B	412	Total 3124	C 2015	N 510	O 591	S 8	0	0	0
1	C	400	Total 3051	C 1963	N 500	O 580	S 8	0	0	0

There are 105 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	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	431	GLN	-	expression tag	UNP P42858
A	432	SER	-	expression tag	UNP P42858
A	433	TYR	-	expression tag	UNP P42858
A	434	GLN	-	expression tag	UNP P42858
A	435	ILE	-	expression tag	UNP P42858
A	436	THR	-	expression tag	UNP P42858
A	437	ALA	-	expression tag	UNP P42858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP P42858
A	439	LYS	-	expression tag	UNP P42858
A	440	LEU	-	expression tag	UNP P42858
A	441	GLY	-	expression tag	UNP P42858
A	442	THR	-	expression tag	UNP P42858
A	443	GLY	-	expression tag	UNP P42858
A	444	ARG	-	expression tag	UNP P42858
A	445	ARG	-	expression tag	UNP P42858
A	446	PHE	-	expression tag	UNP P42858
A	447	THR	-	expression tag	UNP P42858
A	448	THR	-	expression tag	UNP P42858
A	449	SER	-	expression tag	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	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	431	GLN	-	expression tag	UNP P42858
B	432	SER	-	expression tag	UNP P42858
B	433	TYR	-	expression tag	UNP P42858
B	434	GLN	-	expression tag	UNP P42858
B	435	ILE	-	expression tag	UNP P42858
B	436	THR	-	expression tag	UNP P42858
B	437	ALA	-	expression tag	UNP P42858
B	438	GLY	-	expression tag	UNP P42858
B	439	LYS	-	expression tag	UNP P42858
B	440	LEU	-	expression tag	UNP P42858
B	441	GLY	-	expression tag	UNP P42858
B	442	THR	-	expression tag	UNP P42858
B	443	GLY	-	expression tag	UNP P42858
B	444	ARG	-	expression tag	UNP P42858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	445	ARG	-	expression tag	UNP P42858
B	446	PHE	-	expression tag	UNP P42858
B	447	THR	-	expression tag	UNP P42858
B	448	THR	-	expression tag	UNP P42858
B	449	SER	-	expression tag	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
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	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	431	GLN	-	expression tag	UNP P42858
C	432	SER	-	expression tag	UNP P42858
C	433	TYR	-	expression tag	UNP P42858
C	434	GLN	-	expression tag	UNP P42858
C	435	ILE	-	expression tag	UNP P42858
C	436	THR	-	expression tag	UNP P42858
C	437	ALA	-	expression tag	UNP P42858
C	438	GLY	-	expression tag	UNP P42858
C	439	LYS	-	expression tag	UNP P42858
C	440	LEU	-	expression tag	UNP P42858
C	441	GLY	-	expression tag	UNP P42858
C	442	THR	-	expression tag	UNP P42858
C	443	GLY	-	expression tag	UNP P42858
C	444	ARG	-	expression tag	UNP P42858
C	445	ARG	-	expression tag	UNP P42858
C	446	PHE	-	expression tag	UNP P42858
C	447	THR	-	expression tag	UNP P42858
C	448	THR	-	expression tag	UNP P42858
C	449	SER	-	expression tag	UNP P42858

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	3	Total 3	Zn 3	0	0
2	C	1	Total 1	Zn 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	2	Total 2	Ca 2	0	0
3	C	3	Total 3	Ca 3	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.08Å 100.98Å 137.86Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	37.36 – 3.60 37.36 – 3.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (37.36-3.60) 84.6 (37.36-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 3.56Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.258 , 0.267 (Not available) , 0.222	Depositor DCC
R_{free} test set	1591 reflections (7.21%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtrriage
Anisotropy	0.359	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.49	0/3049	0.93	5/4142 (0.1%)
1	B	0.51	0/3205	1.16	16/4367 (0.4%)
1	C	0.50	0/3122	0.96	9/4240 (0.2%)
All	All	0.50	0/9376	1.02	30/12749 (0.2%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	407	PRO	CA-C-N	24.37	145.48	120.38
1	B	407	PRO	C-N-CA	24.37	145.48	120.38
1	B	407	PRO	C-N-CD	-15.85	60.02	125.00
1	B	228	GLY	CA-C-N	9.30	131.46	119.84
1	B	228	GLY	C-N-CA	9.30	131.46	119.84

There are no chirality outliers.

There are no planarity outliers.

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	A	2979	0	2932	85	1
1	B	3124	0	3055	97	1
1	C	3051	0	2988	105	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	1
2	B	3	0	0	0	3
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
All	All	9166	0	8975	281	4

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 15.

The worst 5 of 281 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:C:341:TYR:HE1	1:C:371:MET:HG2	1.17	1.05
1:C:341:TYR:CE1	1:C:371:MET:HG2	1.95	1.02
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.26	0.97
1:B:342:ALA:CB	1:B:368:ALA:HB2	1.96	0.95
1:C:341:TYR:OH	1:C:371:MET:HE3	1.68	0.94

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:OE1	2:A:451:ZN:ZN[3_555]	1.16	1.04
2:B:451:ZN:ZN	2:B:451:ZN:ZN[2_555]	1.43	0.77
1:A:138:GLU:OE1	2:B:450:ZN:ZN[3_455]	1.62	0.58
1:B:310:GLU:OE1	2:B:451:ZN:ZN[2_555]	1.68	0.52

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 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	388/449 (86%)	349 (90%)	31 (8%)	8 (2%)	5	31
1	B	408/449 (91%)	353 (86%)	34 (8%)	21 (5%)	1	15
1	C	398/449 (89%)	356 (89%)	28 (7%)	14 (4%)	3	23
All	All	1194/1347 (89%)	1058 (89%)	93 (8%)	43 (4%)	2	22

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	GLU
1	A	173	ASN
1	A	389	GLN
1	B	354	ARG

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 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	299/363 (82%)	264 (88%)	35 (12%)	5	25
1	B	314/363 (86%)	281 (90%)	33 (10%)	6	29
1	C	304/363 (84%)	265 (87%)	39 (13%)	4	22
All	All	917/1089 (84%)	810 (88%)	107 (12%)	5	25

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	LYS
1	C	38	GLU
1	C	333	ILE
1	B	329	ILE
1	B	416	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	332	ASN
1	C	64	HIS
1	C	49	GLN
1	C	86	GLN
1	A	355	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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.

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	390/449 (86%)	0.21	13 (3%) 49 28	32, 54, 77, 100	20 (5%)
1	B	412/449 (91%)	0.59	32 (7%) 19 13	10, 56, 78, 98	41 (9%)
1	C	400/449 (89%)	0.28	21 (5%) 32 19	10, 56, 83, 94	30 (7%)
All	All	1202/1347 (89%)	0.36	66 (5%) 30 18	10, 55, 80, 100	91 (7%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	PRO	16.1
1	B	404	GLN	16.0
1	B	420	PRO	12.5
1	B	417	LEU	8.3
1	B	412	PRO	6.4

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 oligosaccharides in this entry.

6.4 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(\AA^2)	Q<0.9
2	ZN	B	450	1/1	0.65	0.14	54,54,54,54	0
2	ZN	A	450	1/1	0.71	0.11	108,108,108,108	0
3	CA	B	454	1/1	0.74	0.15	75,75,75,75	0
2	ZN	C	450	1/1	0.80	0.44	16,16,16,16	1
3	CA	C	451	1/1	0.82	0.13	103,103,103,103	0
3	CA	C	453	1/1	0.87	0.06	74,74,74,74	0
3	CA	A	452	1/1	0.91	0.04	69,69,69,69	0
2	ZN	B	452	1/1	0.93	0.07	92,92,92,92	0
3	CA	C	452	1/1	0.95	0.07	78,78,78,78	0
2	ZN	A	451	1/1	0.97	0.05	54,54,54,54	1
3	CA	B	453	1/1	0.97	0.07	64,64,64,64	0
2	ZN	B	451	1/1	0.98	0.03	93,93,93,93	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.