



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:57 am BST

PDB ID : 4FED  
Title : Crystal Structure of Htt36Q3H  
Authors : Kim, M.  
Deposited on : 2012-05-30  
Resolution : 2.81 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

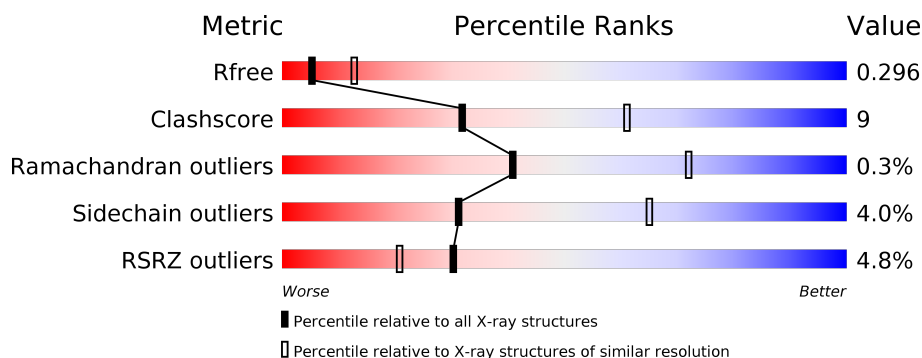
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	452	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	452	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	452	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9446 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
1	A	401	Total	C	N	O	S	0	0	0
			3119	2001	516	594	8			
1	B	402	Total	C	N	O	S	0	0	0
			3128	2006	518	596	8			
1	C	401	Total	C	N	O	S	0	0	0
			3119	2001	516	594	8			

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	14	Total Zn 14 14	0	0
2	A	8	Total Zn 8 8	0	0
2	C	13	Total Zn 13 13	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

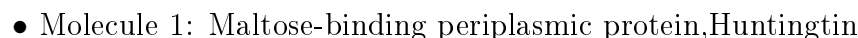
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total 17	O 17	0	0
4	B	13	Total 13	O 13	0	0
4	C	14	Total 14	O 14	0	0



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.18Å 177.36Å 78.35Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	35.00 – 2.81 34.94 – 2.81	Depositor EDS
% Data completeness (in resolution range)	83.5 (35.00-2.81) 83.6 (34.94-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.237 , 0.269 0.275 , 0.296	Depositor DCC
$R_{free}$ test set	2015 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.33	0/3193	0.43	0/4330
1	B	0.35	0/3202	0.44	0/4342
1	C	0.34	0/3193	0.43	0/4330
All	All	0.34	0/9588	0.44	0/13002

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ALA	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	A	3119	0	3084	39	13
1	B	3128	0	3092	51	15
1	C	3119	0	3084	82	15
2	A	8	0	0	0	0
2	B	14	0	0	0	0
2	C	13	0	0	0	0
3	A	1	0	0	0	0
4	A	17	0	0	0	0
4	B	13	0	0	1	0
4	C	14	0	0	0	0
All	All	9446	0	9260	166	28

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 9.

All (166) 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:B:402:GLN:CG	1:C:209:ASP:OD2	1.75	1.35
1:C:396:GLN:O	1:C:401:GLN:HB2	1.17	1.30
1:C:396:GLN:O	1:C:401:GLN:CB	1.88	1.20
1:C:397:HIS:O	1:C:400:GLN:O	1.64	1.14
1:B:402:GLN:HG2	1:C:209:ASP:OD2	1.40	1.14
1:B:402:GLN:HG3	1:C:209:ASP:OD2	1.46	1.11
1:C:397:HIS:HA	1:C:401:GLN:HB3	1.10	1.09
1:B:395:HIS:CE1	1:B:396:GLN:CG	2.37	1.07
1:C:388:GLN:O	1:C:392:GLN:CG	2.06	1.04
1:C:1:LYS:N	1:C:55:ASP:OD1	1.89	1.04
1:B:390:GLN:O	1:B:394:GLN:HG3	1.57	1.02
1:B:395:HIS:ND1	1:B:396:GLN:HG3	1.74	1.02
1:A:401:GLN:HG2	1:A:401:GLN:O	1.59	1.01
1:C:397:HIS:CD2	1:C:401:GLN:HG2	1.95	1.00
1:C:2:ILE:HD11	1:C:55:ASP:C	1.87	0.94
1:B:395:HIS:ND1	1:B:396:GLN:CG	2.30	0.94
1:C:397:HIS:CG	1:C:401:GLN:HG2	2.03	0.94
1:C:388:GLN:O	1:C:392:GLN:HG2	1.68	0.93
1:B:397:HIS:O	1:B:398:GLN:HB2	1.67	0.92
1:C:396:GLN:OE1	1:C:396:GLN:HA	1.69	0.92
1:C:397:HIS:HA	1:C:400:GLN:O	1.69	0.92
1:C:400:GLN:O	1:C:401:GLN:HB3	1.73	0.88
1:C:397:HIS:CA	1:C:400:GLN:O	2.22	0.87
1:C:3:GLU:H	1:C:3:GLU:CD	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:HIS:HA	1:A:399:HIS:O	1.73	0.87
1:B:400:GLN:HG3	1:B:401:GLN:N	1.88	0.86
1:C:2:ILE:CD1	1:C:2:ILE:N	2.40	0.85
1:C:397:HIS:C	1:C:400:GLN:O	2.15	0.85
1:B:395:HIS:CE1	1:B:396:GLN:HG2	2.11	0.83
1:B:396:GLN:HB3	1:B:397:HIS:CD2	2.13	0.83
1:B:395:HIS:CE1	1:B:396:GLN:HG3	2.09	0.83
1:C:397:HIS:HA	1:C:401:GLN:CB	2.04	0.83
1:C:1:LYS:H1	1:C:55:ASP:CG	1.81	0.82
1:B:82:ASP:OD2	4:B:605:HOH:O	1.99	0.80
1:A:164:ASP:O	1:A:187:GLY:HA3	1.82	0.79
1:B:401:GLN:HB3	1:B:402:GLN:OE1	1.84	0.78
1:C:397:HIS:CD2	1:C:401:GLN:CG	2.68	0.76
1:B:401:GLN:CB	1:B:402:GLN:OE1	2.34	0.76
1:C:397:HIS:CA	1:C:401:GLN:HB3	2.05	0.76
1:C:389:GLN:O	1:C:393:GLN:HG3	1.85	0.75
1:B:395:HIS:HE1	1:B:396:GLN:NE2	1.84	0.74
1:B:395:HIS:HE1	1:B:396:GLN:CD	1.89	0.74
1:C:2:ILE:HD12	1:C:2:ILE:N	2.01	0.74
1:C:397:HIS:O	1:C:400:GLN:N	2.20	0.74
1:B:395:HIS:ND1	1:B:396:GLN:HG2	2.06	0.70
1:B:400:GLN:HG3	1:B:401:GLN:H	1.57	0.70
1:B:397:HIS:O	1:B:398:GLN:CB	2.40	0.69
1:A:391:GLN:HG3	1:A:395:HIS:CE1	2.29	0.67
1:C:395:HIS:O	1:C:396:GLN:CD	2.32	0.67
1:C:1:LYS:HE2	1:C:3:GLU:OE2	1.95	0.67
1:C:400:GLN:O	1:C:401:GLN:CB	2.44	0.66
1:B:395:HIS:O	1:B:395:HIS:CG	2.48	0.65
1:C:388:GLN:O	1:C:392:GLN:CD	2.35	0.65
1:C:389:GLN:HA	1:C:392:GLN:HG3	1.77	0.65
1:B:395:HIS:O	1:B:395:HIS:ND1	2.30	0.65
1:B:395:HIS:C	1:B:395:HIS:ND1	2.51	0.64
1:B:395:HIS:CE1	1:B:396:GLN:NE2	2.66	0.64
1:B:402:GLN:OE1	1:B:402:GLN:N	2.30	0.64
1:C:390:GLN:O	1:C:394:GLN:HG3	1.97	0.64
1:B:397:HIS:CD2	1:B:397:HIS:N	2.65	0.64
1:A:395:HIS:O	1:A:396:GLN:HG2	1.98	0.63
1:C:2:ILE:CD1	1:C:55:ASP:HA	2.28	0.62
1:C:395:HIS:O	1:C:396:GLN:NE2	2.32	0.62
1:C:64:HIS:HD2	1:C:261:VAL:H	1.49	0.61
1:A:164:ASP:O	1:A:187:GLY:CA	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLU:HG2	1:C:5:GLY:N	2.15	0.61
1:B:395:HIS:CE1	1:B:396:GLN:CD	2.70	0.61
1:C:396:GLN:O	1:C:401:GLN:HB3	1.95	0.60
1:A:169:PHE:CD2	1:A:333:ILE:HD11	2.36	0.60
1:B:64:HIS:HD2	1:B:261:VAL:H	1.50	0.60
1:C:386:SER:HA	1:C:389:GLN:HG2	1.84	0.59
1:C:1:LYS:HG2	1:C:1:LYS:O	2.01	0.58
1:A:396:GLN:C	1:A:398:GLN:H	2.07	0.58
1:C:390:GLN:NE2	1:C:394:GLN:OE1	2.37	0.58
1:C:2:ILE:HD13	1:C:2:ILE:N	2.19	0.57
1:A:64:HIS:CD2	1:A:261:VAL:H	2.23	0.57
1:A:394:GLN:HA	1:A:394:GLN:OE1	2.05	0.56
1:C:388:GLN:O	1:C:392:GLN:OE1	2.23	0.56
1:B:64:HIS:CD2	1:B:261:VAL:H	2.24	0.56
1:C:64:HIS:CD2	1:C:261:VAL:H	2.22	0.56
1:C:397:HIS:O	1:C:400:GLN:C	2.42	0.56
1:C:387:PHE:O	1:C:390:GLN:HG3	2.05	0.55
1:B:402:GLN:N	1:B:402:GLN:CD	2.59	0.55
1:A:396:GLN:OE1	1:A:397:HIS:CE1	2.60	0.55
1:A:401:GLN:O	1:A:401:GLN:CG	2.42	0.54
1:A:3:GLU:HB2	1:A:6:LYS:HE2	1.89	0.54
1:C:2:ILE:HD11	1:C:55:ASP:CA	2.38	0.53
1:A:164:ASP:C	1:A:164:ASP:OD1	2.44	0.53
1:C:398:GLN:O	1:C:399:HIS:HB2	2.08	0.53
1:C:391:GLN:O	1:C:395:HIS:HB3	2.08	0.53
1:A:392:GLN:HB3	1:A:396:GLN:HE21	1.73	0.52
1:C:397:HIS:CE1	1:C:401:GLN:HG2	2.44	0.52
1:B:64:HIS:HE1	1:B:330:MET:O	1.93	0.52
1:C:397:HIS:NE2	1:C:401:GLN:HG2	2.22	0.52
1:A:374:LEU:O	1:A:378:MET:HB2	2.08	0.52
1:A:167:TYR:OH	1:A:180:ASP:OD1	2.28	0.52
1:A:64:HIS:HD2	1:A:261:VAL:H	1.57	0.52
1:C:388:GLN:O	1:C:392:GLN:HG3	2.04	0.52
1:B:380:ALA:HA	1:C:370:ALA:HB1	1.92	0.51
1:B:400:GLN:CG	1:B:401:GLN:N	2.68	0.51
1:A:388:GLN:O	1:A:392:GLN:HG3	2.11	0.51
1:B:402:GLN:H	1:B:402:GLN:CD	2.15	0.51
1:C:2:ILE:HG21	1:C:58:ASP:OD1	2.11	0.51
1:B:395:HIS:HB2	1:B:401:GLN:HA	1.92	0.50
1:A:164:ASP:O	1:A:164:ASP:OD1	2.30	0.50
1:C:64:HIS:HE1	1:C:330:MET:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:LYS:CA	1:C:55:ASP:OD1	2.60	0.50
1:A:64:HIS:HE1	1:A:330:MET:O	1.94	0.50
1:B:398:GLN:OE1	1:B:398:GLN:O	2.30	0.50
1:A:333:ILE:HD12	1:A:335:GLN:HB2	1.94	0.50
1:C:2:ILE:H	1:C:2:ILE:HD13	1.77	0.48
1:A:370:ALA:HB1	1:C:380:ALA:HA	1.95	0.48
1:B:2:ILE:O	1:B:2:ILE:HG22	2.13	0.47
1:A:401:GLN:HE21	1:A:401:GLN:HB3	1.50	0.47
1:C:3:GLU:N	1:C:3:GLU:CD	2.53	0.47
1:C:164:ASP:OD2	1:C:251:LYS:HD2	2.15	0.47
1:A:164:ASP:O	1:A:164:ASP:CG	2.49	0.46
1:C:397:HIS:O	1:C:398:GLN:C	2.53	0.46
1:C:152:GLN:HA	1:C:348:ILE:HD11	1.98	0.46
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.81	0.46
1:C:1:LYS:C	1:C:2:ILE:HD12	2.35	0.46
1:C:249:THR:HG22	1:C:254:PRO:HA	1.98	0.46
1:A:392:GLN:CB	1:A:396:GLN:HE21	2.28	0.46
1:B:390:GLN:HE22	1:C:345:THR:HG23	1.80	0.46
1:C:218:ASN:HD21	1:C:235:ILE:HG12	1.81	0.46
1:A:379:LYS:HA	1:A:382:GLU:HG2	1.98	0.45
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.98	0.45
1:B:152:GLN:HA	1:B:348:ILE:HD11	1.97	0.45
1:C:390:GLN:HB2	1:C:390:GLN:HE21	1.58	0.45
1:A:122:LEU:HD21	1:A:126:PRO:HD3	1.99	0.44
1:B:388:GLN:HA	1:B:391:GLN:HG2	2.00	0.44
1:C:2:ILE:CG2	1:C:58:ASP:OD1	2.65	0.44
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.82	0.44
1:B:379:LYS:HA	1:B:382:GLU:HG2	2.00	0.44
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.53	0.43
1:C:398:GLN:HG2	1:C:398:GLN:H	1.63	0.43
1:A:396:GLN:C	1:A:398:GLN:N	2.71	0.43
1:A:169:PHE:CE2	1:A:333:ILE:HD11	2.54	0.43
1:C:4:GLU:CG	1:C:5:GLY:N	2.80	0.43
1:B:9:ILE:HG12	1:B:59:ILE:HB	2.00	0.43
1:A:396:GLN:O	1:A:398:GLN:N	2.52	0.43
1:C:390:GLN:O	1:C:394:GLN:CG	2.67	0.42
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.54	0.42
1:B:396:GLN:CB	1:B:397:HIS:CD2	2.95	0.42
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.01	0.42
1:B:396:GLN:HB3	1:B:397:HIS:NE2	2.33	0.42
1:C:333:ILE:HD12	1:C:335:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:LYS:N	1:C:55:ASP:CG	2.56	0.42
1:C:9:ILE:HG12	1:C:59:ILE:HB	2.00	0.42
1:B:72:GLN:HG2	1:B:99:TYR:OH	2.19	0.41
1:A:391:GLN:HG3	1:A:395:HIS:HE1	1.78	0.41
1:A:398:GLN:O	1:A:399:HIS:CD2	2.72	0.41
1:B:47:PHE:HB3	1:B:48:PRO:HD3	2.02	0.41
1:A:168:ALA:HB2	1:A:339:PHE:CE2	2.56	0.41
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.56	0.41
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.85	0.41
1:B:92:PHE:O	1:B:329:ILE:HD11	2.21	0.41
1:C:270:SER:HA	1:C:271:PRO:HD3	1.95	0.41
1:C:2:ILE:CD1	1:C:55:ASP:CA	2.95	0.41
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.94	0.40
1:C:205:ASN:HB3	1:C:208:THR:HG23	2.03	0.40
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.93	0.40
1:B:192:LEU:HD23	1:B:357:VAL:HG13	2.03	0.40
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.04	0.40
1:C:397:HIS:ND1	1:C:401:GLN:HG2	2.33	0.40
1:C:165:GLY:N	1:C:187:GLY:HA3	2.36	0.40

All (28) 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:A:400:GLN:NE2	1:B:153:GLU:CG[2_555]	0.73	1.47
1:B:401:GLN:NE2	1:C:395:HIS:NE2[2_555]	0.98	1.22
1:A:400:GLN:CD	1:B:153:GLU:CG[2_555]	1.08	1.12
1:B:401:GLN:NE2	1:C:395:HIS:CE1[2_555]	1.11	1.09
1:C:156:PHE:CE1	1:C:397:HIS:CD2[2_555]	1.11	1.09
1:A:400:GLN:NE2	1:B:153:GLU:CD[2_555]	1.12	1.08
1:A:400:GLN:CD	1:B:153:GLU:CB[2_555]	1.39	0.81
1:A:401:GLN:C	1:B:209:ASP:CB[2_555]	1.49	0.71
1:A:400:GLN:OE1	1:B:153:GLU:CB[2_555]	1.69	0.51
1:C:210:TYR:CE1	1:C:401:GLN:O[2_555]	1.69	0.51
1:C:210:TYR:CZ	1:C:401:GLN:O[2_555]	1.71	0.49
1:C:153:GLU:CG	1:C:397:HIS:CE1[2_555]	1.72	0.48
1:A:400:GLN:NE2	1:B:153:GLU:OE2[2_555]	1.76	0.44
1:C:150:ASN:ND2	1:C:397:HIS:NE2[2_555]	1.80	0.40
1:A:401:GLN:O	1:B:209:ASP:CB[2_555]	1.80	0.40
1:A:400:GLN:CG	1:B:153:GLU:CG[2_555]	1.83	0.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLN:NE2	1:B:153:GLU:CB[2_555]	1.85	0.35
1:A:400:GLN:CB	1:B:150:ASN:ND2[2_555]	1.89	0.31
1:C:153:GLU:CB	1:C:397:HIS:CE1[2_555]	1.90	0.30
1:C:156:PHE:CE1	1:C:397:HIS:NE2[2_555]	2.03	0.17
1:A:400:GLN:CG	1:B:150:ASN:ND2[2_555]	2.04	0.16
1:C:156:PHE:CE1	1:C:397:HIS:CG[2_555]	2.11	0.09
1:C:153:GLU:CG	1:C:397:HIS:ND1[2_555]	2.14	0.06
1:C:156:PHE:CZ	1:C:397:HIS:CD2[2_555]	2.15	0.05
1:C:210:TYR:OH	1:C:401:GLN:O[2_555]	2.16	0.04
1:C:153:GLU:CB	1:C:397:HIS:ND1[2_555]	2.16	0.04
1:C:156:PHE:CD1	1:C:397:HIS:CD2[2_555]	2.18	0.02
1:A:401:GLN:C	1:B:209:ASP:CA[2_555]	2.18	0.02

## 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	399/452 (88%)	388 (97%)	10 (2%)	1 (0%)	41	72
1	B	400/452 (88%)	389 (97%)	9 (2%)	2 (0%)	29	61
1	C	399/452 (88%)	384 (96%)	15 (4%)	0	100	100
All	All	1198/1356 (88%)	1161 (97%)	34 (3%)	3 (0%)	41	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	B	398	GLN
1	A	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	320/370 (86%)	311 (97%)	9 (3%)	43	77
1	B	321/370 (87%)	307 (96%)	14 (4%)	28	61
1	C	320/370 (86%)	305 (95%)	15 (5%)	26	59
All	All	961/1110 (87%)	923 (96%)	38 (4%)	31	65

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LYS
1	A	189	LYS
1	A	202	LYS
1	A	205	ASN
1	A	377	LEU
1	A	391	GLN
1	A	397	HIS
1	A	400	GLN
1	A	401	GLN
1	B	66	ARG
1	B	160	LEU
1	B	175	LYS
1	B	202	LYS
1	B	207	ASP
1	B	365	GLN
1	B	379	LYS
1	B	392	GLN
1	B	394	GLN
1	B	395	HIS
1	B	397	HIS
1	B	398	GLN
1	B	400	GLN
1	B	402	GLN
1	C	1	LYS
1	C	2	ILE
1	C	3	GLU

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Mol	Chain	Res	Type
1	C	170	LYS
1	C	172	GLU
1	C	175	LYS
1	C	189	LYS
1	C	202	LYS
1	C	361	LEU
1	C	379	LYS
1	C	389	GLN
1	C	390	GLN
1	C	392	GLN
1	C	396	GLN
1	C	398	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	64	HIS
1	A	201	ASN
1	A	203	HIS
1	A	205	ASN
1	A	218	ASN
1	A	234	ASN
1	A	388	GLN
1	A	389	GLN
1	A	396	GLN
1	A	397	HIS
1	A	399	HIS
1	A	401	GLN
1	B	49	GLN
1	B	64	HIS
1	B	201	ASN
1	B	218	ASN
1	B	234	ASN
1	B	390	GLN
1	B	392	GLN
1	B	393	GLN
1	B	397	HIS
1	B	400	GLN
1	C	49	GLN
1	C	64	HIS
1	C	72	GLN

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Mol	Chain	Res	Type
1	C	201	ASN
1	C	203	HIS
1	C	205	ASN
1	C	218	ASN
1	C	234	ASN
1	C	365	GLN
1	C	389	GLN
1	C	390	GLN
1	C	391	GLN
1	C	392	GLN
1	C	393	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 36 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	401/452 (88%)	0.30	12 (2%)	50 40	62, 87, 121, 156	8 (1%)
1	B	402/452 (88%)	0.40	21 (5%)	27 18	54, 83, 112, 154	12 (2%)
1	C	401/452 (88%)	0.44	25 (6%)	20 13	53, 87, 114, 160	9 (2%)
All	All	1204/1356 (88%)	0.38	58 (4%)	30 21	53, 86, 118, 160	29 (2%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	HIS	7.1
1	C	173	ASN	6.6
1	B	1	LYS	4.9
1	A	400	GLN	4.9
1	A	401	GLN	4.6
1	C	171	TYR	4.6
1	C	174	GLY	4.6
1	B	393	GLN	4.3
1	C	398	GLN	4.3
1	C	179	LYS	3.9
1	B	2	ILE	3.9
1	B	401	GLN	3.8
1	C	141	ALA	3.8
1	B	402	GLN	3.7
1	C	1	LYS	3.7
1	C	172	GLU	3.7
1	A	1	LYS	3.4
1	C	122	LEU	3.3
1	A	33	ILE	3.3
1	A	17	TYR	3.2
1	B	124	ASN	3.1
1	C	237	THR	2.9
1	A	397	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	2.7
1	C	144	LYS	2.7
1	B	400	GLN	2.6
1	C	142	LYS	2.5
1	C	120	ASP	2.5
1	B	339	PHE	2.5
1	C	401	GLN	2.5
1	B	179	LYS	2.4
1	C	117	TYR	2.4
1	C	13	GLY	2.4
1	B	395	HIS	2.4
1	C	114	SER	2.4
1	C	207	ASP	2.4
1	B	31	THR	2.4
1	B	120	ASP	2.4
1	C	112	ALA	2.4
1	C	393	GLN	2.3
1	C	397	HIS	2.3
1	C	250	PHE	2.3
1	A	141	ALA	2.3
1	B	112	ALA	2.3
1	B	202	LYS	2.3
1	C	2	ILE	2.2
1	B	392	GLN	2.2
1	B	33	ILE	2.2
1	C	121	LEU	2.2
1	B	221	GLU	2.2
1	A	237	THR	2.2
1	A	396	GLN	2.1
1	C	175	LYS	2.1
1	B	3	GLU	2.1
1	B	125	PRO	2.1
1	B	397	HIS	2.1
1	A	399	HIS	2.1
1	B	399	HIS	2.0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	A	506	1/1	-0.23	0.28	196,196,196,196	0
2	ZN	C	509	1/1	0.37	0.36	135,135,135,135	1
2	ZN	B	507	1/1	0.49	0.14	171,171,171,171	0
2	ZN	B	509	1/1	0.60	0.26	166,166,166,166	0
2	ZN	A	503	1/1	0.63	0.14	101,101,101,101	1
2	ZN	A	508	1/1	0.66	0.20	137,137,137,137	0
2	ZN	B	513	1/1	0.68	0.19	93,93,93,93	1
2	ZN	A	504	1/1	0.70	0.10	113,113,113,113	1
2	ZN	B	506	1/1	0.72	0.08	121,121,121,121	0
2	ZN	C	506	1/1	0.77	0.08	130,130,130,130	0
2	ZN	C	503	1/1	0.82	0.13	145,145,145,145	0
2	ZN	A	502	1/1	0.84	0.05	113,113,113,113	0
2	ZN	B	503	1/1	0.84	0.09	124,124,124,124	0
2	ZN	B	504	1/1	0.85	0.12	87,87,87,87	1
2	ZN	B	502	1/1	0.86	0.12	155,155,155,155	0
2	ZN	C	505	1/1	0.87	0.09	158,158,158,158	0
2	ZN	B	511	1/1	0.87	0.06	145,145,145,145	0
2	ZN	B	512	1/1	0.89	0.16	70,70,70,70	1
3	CA	A	509	1/1	0.90	0.24	114,114,114,114	0
2	ZN	C	501	1/1	0.90	0.37	64,64,64,64	1
2	ZN	A	505	1/1	0.91	0.37	85,85,85,85	1
2	ZN	B	508	1/1	0.91	0.25	155,155,155,155	0
2	ZN	A	507	1/1	0.92	0.14	148,148,148,148	0
2	ZN	C	512	1/1	0.92	0.31	162,162,162,162	1
2	ZN	B	510	1/1	0.92	0.13	101,101,101,101	0
2	ZN	C	510	1/1	0.93	0.37	56,56,56,56	1
2	ZN	C	502	1/1	0.93	0.05	136,136,136,136	0
2	ZN	C	508	1/1	0.93	0.32	60,60,60,60	1
2	ZN	C	504	1/1	0.94	0.10	133,133,133,133	0
2	ZN	C	511	1/1	0.94	0.34	47,47,47,47	1
2	ZN	A	501	1/1	0.95	0.04	115,115,115,115	0
2	ZN	B	501	1/1	0.96	0.21	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	505	1/1	0.97	0.05	129,129,129,129	0
2	ZN	B	514	1/1	0.97	0.06	98,98,98,98	0
2	ZN	C	507	1/1	0.98	0.20	95,95,95,95	0
2	ZN	C	513	1/1	0.99	0.35	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.