



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:57 am BST

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 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

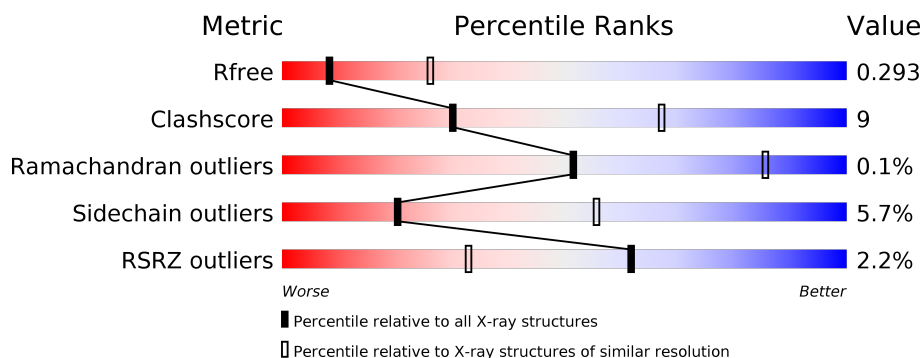
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>11%</div> </div> </div>
1	B	452	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>11%</div> </div> </div>
1	C	452	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>9%</div> </div> </div>

## 2 Entry composition

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
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 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	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

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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		



PRO  
PRO  
PRO  
PRO  
PRO  
GLN  
LEU  
PRO  
GLN  
PRO  
PRO  
PRO  
PRO  
GLN  
ALA  
GLN  
PRO  
LEU  
LEU  
PRO  
GLN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.227 , 0.275 0.253 , 0.293	Depositor DCC
$R_{free}$ test set	1942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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

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 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	3146	0	3100	79	46
1	B	3130	0	3096	55	46
1	C	3209	0	3161	44	0
2	A	5	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	0	0
3	A	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	61	0	0	0	0
3	C	49	0	0	0	0
All	All	9664	0	9357	175	46

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 (175) 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: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
1:A:395:HIS:O	1:A:402:GLN:HG3	1.47	1.12
1:A:397:HIS:CD2	1:A:400:GLN:HG3	1.85	1.10
1:A:397:HIS:HD2	1:A:400:GLN:HG3	1.13	1.07
1:C:408:GLN:HB3	1:C:409:GLN:NE2	1.71	1.06
1:A:394:GLN:HG3	1:A:395:HIS:ND1	1.70	1.05
1:A:397:HIS:CG	1:A:399:HIS:H	1.75	1.04
1:B:398:GLN:C	1:B:399:HIS:CD2	2.30	1.04
1:C:409:GLN:CD	1:C:409:GLN:H	1.57	1.01
1:A:394:GLN:NE2	1:A:395:HIS:CD2	2.30	1.00
1:A:397:HIS:CD2	1:A:399:HIS:N	2.29	1.00
1:A:394:GLN:NE2	1:A:395:HIS:CG	2.30	0.99
1:A:397:HIS:NE2	1:A:399:HIS:CB	2.14	0.99
1:B:391:GLN:HG3	1:B:392:GLN:N	1.77	0.97
1:A:397:HIS:NE2	1:A:399:HIS:CA	2.27	0.96
1:A:397:HIS:NE2	1:A:399:HIS:N	2.14	0.94
1:A:398:GLN:HB2	1:A:399:HIS:CD2	2.01	0.94
1:B:388:GLN:O	1:B:392:GLN:HG3	1.66	0.93
1:A:397:HIS:CD2	1:A:399:HIS:CA	2.50	0.93
1:A:394:GLN:CD	1:A:395:HIS:CE1	2.44	0.91
1:B:389:GLN:O	1:B:393:GLN:N	2.02	0.91
1:A:397:HIS:CE1	1:A:399:HIS:N	2.38	0.91
1:A:395:HIS:O	1:A:402:GLN:CG	2.18	0.91
1:A:397:HIS:HD2	1:A:399:HIS:C	1.69	0.87
1:C:404:GLN:HE22	1:C:407:GLN:CD	1.77	0.87
1:A:399:HIS:N	1:A:399:HIS:CD2	2.42	0.86
1:A:397:HIS:HB3	1:A:400:GLN:HB2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLN:O	1:C:410:GLN:N	2.08	0.85
1:A:393:GLN:HG3	1:A:394:GLN:N	1.91	0.85
1:A:394:GLN:HE21	1:A:395:HIS:CG	1.92	0.84
1:B:390:GLN:HG3	1:B:391:GLN:N	1.92	0.84
1:C:409:GLN:CD	1:C:409:GLN:N	2.30	0.83
1:B:388:GLN:O	1:B:392:GLN:HB2	1.80	0.82
1:C:406:GLN:O	1:C:410:GLN:HB3	1.79	0.82
1:A:398:GLN:C	1:A:399:HIS:CD2	2.52	0.82
1:B:388:GLN:O	1:B:392:GLN:CB	2.29	0.79
1:B:388:GLN:O	1:B:392:GLN:CG	2.30	0.79
1:A:397:HIS:HD2	1:A:400:GLN:CG	1.96	0.78
1:A:395:HIS:N	1:A:395:HIS:ND1	2.31	0.77
1:A:398:GLN:C	1:A:399:HIS:HD2	1.86	0.77
1:A:397:HIS:CE1	1:A:399:HIS:H	2.00	0.76
1:B:399:HIS:N	1:B:399:HIS:CD2	2.54	0.76
1:C:404:GLN:NE2	1:C:407:GLN:OE1	2.18	0.75
1:B:398:GLN:O	1:B:399:HIS:CG	2.39	0.74
1:C:401:GLN:OE1	1:C:405:GLN:OE1	2.05	0.74
1:B:398:GLN:C	1:B:399:HIS:HD2	1.92	0.72
1:C:406:GLN:O	1:C:410:GLN:CA	2.37	0.72
1:A:393:GLN:CG	1:A:394:GLN:N	2.54	0.71
1:C:408:GLN:CB	1:C:409:GLN:NE2	2.53	0.71
1:A:397:HIS:ND1	1:A:398:GLN:N	2.39	0.69
1:B:398:GLN:C	1:B:399:HIS:CG	2.65	0.67
1:A:394:GLN:CD	1:A:395:HIS:NE2	2.48	0.67
1:C:406:GLN:O	1:C:410:GLN:CB	2.43	0.66
1:B:394:GLN:OE1	1:B:394:GLN:HA	1.95	0.66
1:A:397:HIS:CD2	1:A:400:GLN:CG	2.71	0.66
1:A:399:HIS:N	1:A:399:HIS:HD2	1.84	0.66
1:A:397:HIS:NE2	1:A:399:HIS:HB2	2.09	0.66
1:A:64:HIS:CD2	1:A:261:VAL:H	2.14	0.66
1:B:398:GLN:O	1:B:399:HIS:CD2	2.48	0.66
1:A:397:HIS:CD2	1:A:400:GLN:N	2.64	0.65
1:C:404:GLN:HA	1:C:404:GLN:NE2	2.10	0.65
1:B:391:GLN:HG3	1:B:392:GLN:H	1.61	0.65
1:A:391:GLN:HA	1:A:395:HIS:ND1	2.09	0.65
1:C:164:ASP:OD2	1:C:251:LYS:HD2	1.97	0.65
1:A:397:HIS:CD2	1:A:399:HIS:O	2.51	0.64
1:A:394:GLN:CG	1:A:395:HIS:ND1	2.49	0.63
1:A:398:GLN:CB	1:A:399:HIS:CD2	2.81	0.63
1:C:404:GLN:HA	1:C:404:GLN:HE21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLN:HG2	1:C:99:TYR:OH	1.98	0.62
1:B:390:GLN:CG	1:B:391:GLN:N	2.62	0.62
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.65	0.61
1:C:402:GLN:O	1:C:406:GLN:HG3	2.00	0.61
1:A:64:HIS:HD2	1:A:261:VAL:H	1.48	0.61
1:B:396:GLN:HB3	1:B:401:GLN:C	2.22	0.60
1:A:398:GLN:HB2	1:A:399:HIS:HD2	1.59	0.58
1:A:397:HIS:CE1	1:A:398:GLN:HE21	2.21	0.58
1:A:397:HIS:CG	1:A:398:GLN:N	2.70	0.58
1:A:397:HIS:HD2	1:A:399:HIS:O	1.86	0.58
1:B:397:HIS:O	1:B:398:GLN:C	2.41	0.58
1:B:72:GLN:HG2	1:B:99:TYR:OH	2.03	0.58
1:B:64:HIS:HE1	1:B:330:MET:O	1.86	0.58
1:B:399:HIS:N	1:B:399:HIS:HD2	2.01	0.57
1:A:370:ALA:HB1	1:C:380:ALA:HA	1.85	0.57
1:A:398:GLN:HB2	1:A:399:HIS:NE2	2.19	0.56
1:C:404:GLN:NE2	1:C:407:GLN:CD	2.55	0.56
1:B:398:GLN:CB	1:B:399:HIS:CD2	2.88	0.56
1:B:64:HIS:HD2	1:B:261:VAL:H	1.53	0.56
1:A:72:GLN:HG2	1:A:99:TYR:OH	2.05	0.56
1:C:401:GLN:O	1:C:405:GLN:CB	2.53	0.55
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.71	0.55
1:A:400:GLN:O	1:A:401:GLN:HG3	2.07	0.55
1:C:218:ASN:HD21	1:C:235:ILE:HG12	1.71	0.55
1:B:48:PRO:HG3	1:B:70:TYR:CE1	2.42	0.54
1:B:380:ALA:HA	1:C:370:ALA:HB1	1.90	0.54
1:A:391:GLN:HG3	1:A:392:GLN:N	2.23	0.53
1:A:399:HIS:O	1:A:400:GLN:HG3	2.09	0.53
1:C:401:GLN:O	1:C:405:GLN:HB3	2.09	0.52
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.92	0.52
1:B:398:GLN:HB3	1:B:399:HIS:CD2	2.45	0.52
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.45	0.52
1:C:403:GLN:O	1:C:406:GLN:N	2.30	0.51
1:C:405:GLN:O	1:C:405:GLN:HG2	2.09	0.51
1:A:394:GLN:NE2	1:A:395:HIS:ND1	2.59	0.51
1:C:408:GLN:CB	1:C:409:GLN:HE22	2.19	0.51
1:B:393:GLN:CG	1:B:394:GLN:N	2.73	0.51
1:A:398:GLN:CA	1:A:399:HIS:HD2	2.24	0.50
1:B:391:GLN:O	1:B:395:HIS:HB2	2.10	0.50
1:B:396:GLN:O	1:B:397:HIS:HB2	2.11	0.50
1:C:164:ASP:O	1:C:164:ASP:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLN:HE21	1:B:392:GLN:HG2	1.76	0.50
1:B:393:GLN:HG3	1:B:394:GLN:N	2.25	0.50
1:A:116:ILE:HG12	1:A:244:VAL:HG22	1.94	0.49
1:A:274[A]:GLU:N	1:A:274[A]:GLU:OE1	2.31	0.49
1:A:398:GLN:CB	1:A:399:HIS:HD2	2.22	0.49
1:B:397:HIS:O	1:B:400:GLN:N	2.46	0.48
1:A:397:HIS:HD1	1:A:398:GLN:NE2	2.12	0.48
1:A:397:HIS:HD2	1:A:400:GLN:N	2.08	0.48
1:B:399:HIS:O	1:B:400:GLN:NE2	2.47	0.47
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.49	0.47
1:B:398:GLN:O	1:B:399:HIS:CB	2.61	0.47
1:C:64:HIS:CD2	1:C:261:VAL:H	2.33	0.47
1:B:192:LEU:HD23	1:B:357:VAL:HG13	1.96	0.47
1:B:398:GLN:HB3	1:B:399:HIS:HD2	1.80	0.46
1:C:169:PHE:CD2	1:C:333:ILE:HD11	2.50	0.46
1:A:344:ARG:O	1:A:348:ILE:HG12	2.16	0.46
1:B:341:TYR:CD1	1:B:371:MET:HB2	2.50	0.46
1:B:397:HIS:CG	1:B:398:GLN:H	2.33	0.46
1:A:397:HIS:HD1	1:A:398:GLN:H	1.62	0.46
1:B:158:TRP:N	1:B:159:PRO:HD2	2.30	0.46
1:C:158:TRP:N	1:C:159:PRO:HD2	2.31	0.45
1:B:2:ILE:O	1:B:2:ILE:HG22	2.17	0.45
1:A:165:GLY:O	1:A:185:ASN:ND2	2.50	0.45
1:B:371:MET:O	1:B:375:GLU:HB2	2.17	0.45
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.52	0.44
1:C:78:GLU:HG3	1:C:102:LYS:HB3	2.00	0.44
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.82	0.44
1:C:165:GLY:O	1:C:185:ASN:ND2	2.50	0.44
1:A:192:LEU:HD23	1:A:357:VAL:HG13	2.00	0.44
1:B:401:GLN:CD	1:B:401:GLN:C	2.77	0.44
1:A:393:GLN:HB2	1:A:393:GLN:HE21	1.41	0.43
1:C:406:GLN:C	1:C:410:GLN:HB3	2.37	0.43
1:B:205:ASN:HD22	1:B:205:ASN:HA	1.69	0.43
1:B:64:HIS:CE1	1:B:330:MET:O	2.68	0.43
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.54	0.43
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.01	0.43
1:B:396:GLN:HE21	1:B:396:GLN:C	2.22	0.43
1:A:394:GLN:O	1:A:400:GLN:OE1	2.36	0.43
1:A:333:ILE:HB	1:A:334:PRO:HD2	2.01	0.43
1:B:152:GLN:HA	1:B:348:ILE:HD11	2.01	0.42
1:A:380:ALA:HA	1:B:370:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLN:CB	1:B:401:GLN:C	2.86	0.42
1:C:96:ALA:HB2	1:C:329:ILE:HD13	2.02	0.42
1:A:394:GLN:NE2	1:A:395:HIS:CE1	2.78	0.42
1:A:154:PRO:HB3	1:A:343:VAL:HG12	2.02	0.41
1:A:394:GLN:HE22	1:A:395:HIS:CD2	2.32	0.41
1:C:64:HIS:HD2	1:C:261:VAL:H	1.69	0.41
1:C:2:ILE:O	1:C:2:ILE:HG22	2.20	0.41
1:C:401:GLN:O	1:C:405:GLN:HB2	2.19	0.41
1:A:391:GLN:CG	1:A:392:GLN:N	2.84	0.41
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.94	0.41
1:C:403:GLN:O	1:C:404:GLN:C	2.59	0.41
1:C:168:ALA:O	1:C:169:PHE:CD1	2.74	0.40
1:B:394:GLN:OE1	1:B:394:GLN:CA	2.61	0.40
1:C:344:ARG:O	1:C:348:ILE:HG12	2.20	0.40
1:A:102:LYS:HG2	1:A:102:LYS:H	1.78	0.40
1:B:166:GLY:HA2	1:B:185:ASN:HD21	1.87	0.40
1:B:109:ALA:HB3	1:B:262:LEU:HB3	2.02	0.40
1:B:302:VAL:HG21	1:B:307:TYR:HD2	1.86	0.40
1:C:153:GLU:HA	1:C:154:PRO:HD3	1.93	0.40
1:A:394:GLN:NE2	1:A:395:HIS:NE2	2.61	0.40
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.04	0.40

All (46) 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: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
1:A:401:GLN:CD	1:B:210:TYR:CD1[2_556]	1.06	1.14
1:A:155:TYR:CD2	1:B:398:GLN:OE1[2_556]	1.09	1.11
1:A:396:GLN:CD	1:B:153:GLU:CG[2_556]	1.12	1.08
1:A:155:TYR:CE2	1:B:398:GLN:NE2[2_556]	1.15	1.05
1:A:396:GLN:CG	1:B:153:GLU:CD[2_556]	1.17	1.03
1:A:401:GLN:OE1	1:B:210:TYR:CG[2_556]	1.24	0.96
1:A:396:GLN:NE2	1:B:153:GLU:CG[2_556]	1.25	0.95
1:A:396:GLN:CG	1:B:153:GLU:OE2[2_556]	1.37	0.83
1:A:396:GLN:OE1	1:B:153:GLU:CD[2_556]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLN:OE1	1:B:210:TYR:CD1[2_556]	1.41	0.79
1:A:155:TYR:CD1	1:B:398:GLN:OE1[2_556]	1.41	0.79
1:A:396:GLN:CD	1:B:153:GLU:OE1[2_556]	1.42	0.78
1:A:155:TYR:CE1	1:B:398:GLN:CD[2_556]	1.48	0.72
1:A:155:TYR:CD1	1:B:398:GLN:CD[2_556]	1.49	0.71
1:A:155:TYR:CE1	1:B:398:GLN:NE2[2_556]	1.50	0.70
1:A:396:GLN:NE2	1:B:153:GLU:CA[2_556]	1.51	0.69
1:A:155:TYR:CZ	1:B:398:GLN:CD[2_556]	1.55	0.65
1:A:155:TYR:OH	1:B:398:GLN:NE2[2_556]	1.58	0.62
1:A:155:TYR:CG	1:B:398:GLN:CD[2_556]	1.59	0.61
1:A:396:GLN:CD	1:B:153:GLU:OE2[2_556]	1.62	0.58
1:A:155:TYR:CE2	1:B:398:GLN:CD[2_556]	1.63	0.57
1:A:155:TYR:CD2	1:B:398:GLN:CD[2_556]	1.63	0.57
1:A:401:GLN:CB	1:B:210:TYR:CB[2_556]	1.65	0.55
1:A:396:GLN:NE2	1:B:153:GLU:CD[2_556]	1.65	0.55
1:A:401:GLN:CG	1:B:210:TYR:CD1[2_556]	1.69	0.51
1:A:401:GLN:CD	1:B:210:TYR:CG[2_556]	1.74	0.46
1:A:401:GLN:OE1	1:B:210:TYR:CB[2_556]	1.83	0.37
1:A:155:TYR:CB	1:B:398:GLN:OE1[2_556]	1.91	0.29
1:A:396:GLN:OE1	1:B:153:GLU:CG[2_556]	1.92	0.28
1:A:396:GLN:CG	1:B:153:GLU:OE1[2_556]	1.95	0.25
1:A:401:GLN:CB	1:B:210:TYR:CG[2_556]	1.97	0.23
1:A:396:GLN:CG	1:B:153:GLU:CG[2_556]	2.01	0.19
1:A:155:TYR:CE2	1:B:398:GLN:OE1[2_556]	2.01	0.19
1:A:401:GLN:CG	1:B:210:TYR:CG[2_556]	2.01	0.19
1:A:401:GLN:NE2	1:B:210:TYR:CD1[2_556]	2.03	0.17
1:A:396:GLN:NE2	1:B:153:GLU:OE2[2_556]	2.05	0.15
1:A:396:GLN:CB	1:B:153:GLU:OE1[2_556]	2.06	0.14
1:A:401:GLN:OE1	1:B:210:TYR:CA[2_556]	2.08	0.12
1:A:155:TYR:CD2	1:B:398:GLN:NE2[2_556]	2.16	0.04
1:A:401:GLN:CD	1:B:210:TYR:CB[2_556]	2.18	0.02
1:A:396:GLN:CD	1:B:153:GLU:CB[2_556]	2.19	0.01

## 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%)	41	76
1	C	409/452 (90%)	396 (97%)	13 (3%)	0	100	100
All	All	1211/1356 (89%)	1170 (97%)	40 (3%)	1 (0%)	51	85

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%)	24	60
1	B	321/370 (87%)	304 (95%)	17 (5%)	22	58
1	C	330/370 (89%)	307 (93%)	23 (7%)	15	47
All	All	974/1110 (88%)	918 (94%)	56 (6%)	20	56

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	92	PHE
1	A	179	LYS
1	A	189	LYS
1	A	202	LYS
1	A	205	ASN
1	A	376	LYS
1	A	378	MET
1	A	382	GLU
1	A	384	LEU

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Mol	Chain	Res	Type
1	A	393	GLN
1	A	394	GLN
1	A	395	HIS
1	A	397	HIS
1	A	398	GLN
1	A	399	HIS
1	B	1	LYS
1	B	72	GLN
1	B	88	LYS
1	B	102	LYS
1	B	160	LEU
1	B	175	LYS
1	B	200	LYS
1	B	202	LYS
1	B	251	LYS
1	B	291	GLU
1	B	344[A]	ARG
1	B	344[B]	ARG
1	B	374	LEU
1	B	377	LEU
1	B	396	GLN
1	B	399	HIS
1	B	400	GLN
1	C	72	GLN
1	C	87	ASP
1	C	102	LYS
1	C	160	LEU
1	C	170	LYS
1	C	179	LYS
1	C	189	LYS
1	C	202	LYS
1	C	205	ASN
1	C	274	GLU
1	C	337	SER
1	C	367	ASN
1	C	386	SER
1	C	388	GLN
1	C	396	GLN
1	C	397	HIS
1	C	400	GLN
1	C	401	GLN
1	C	402	GLN

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Mol	Chain	Res	Type
1	C	406	GLN
1	C	408	GLN
1	C	409	GLN
1	C	410	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	64	HIS
1	A	72	GLN
1	A	86	GLN
1	A	201	ASN
1	A	203	HIS
1	A	205	ASN
1	A	218	ASN
1	A	234	ASN
1	A	365	GLN
1	A	393	GLN
1	A	394	GLN
1	A	397	HIS
1	A	398	GLN
1	A	399	HIS
1	B	64	HIS
1	B	201	ASN
1	B	205	ASN
1	B	218	ASN
1	B	234	ASN
1	B	365	GLN
1	B	391	GLN
1	B	393	GLN
1	B	396	GLN
1	B	399	HIS
1	B	400	GLN
1	C	64	HIS
1	C	201	ASN
1	C	203	HIS
1	C	205	ASN
1	C	218	ASN
1	C	234	ASN
1	C	367	ASN
1	C	404	GLN

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Mol	Chain	Res	Type
1	C	406	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 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.

### 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

### 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	402/452 (88%)	-0.34	7 (1%)	70 41	24, 84, 120, 155	13 (3%)
1	B	401/452 (88%)	-0.26	4 (0%)	82 59	38, 89, 132, 159	12 (2%)
1	C	410/452 (90%)	-0.15	16 (3%)	39 15	58, 92, 141, 190	27 (6%)
All	All	1213/1356 (89%)	-0.25	27 (2%)	62 33	24, 89, 133, 190	52 (4%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	410	GLN	6.0
1	C	407	GLN	5.9
1	B	395	HIS	5.2
1	C	408	GLN	5.2
1	A	402	GLN	4.3
1	C	400	GLN	4.3
1	C	406	GLN	3.7
1	C	409	GLN	3.6
1	A	395	HIS	3.4
1	C	1	LYS	3.2
1	A	400	GLN	3.1
1	C	396	GLN	3.0
1	C	398	GLN	3.0
1	C	405	GLN	3.0
1	C	404	GLN	2.9
1	A	401	GLN	2.6
1	A	1	LYS	2.5
1	C	393	GLN	2.5
1	B	393	GLN	2.4
1	C	397	HIS	2.4
1	C	403	GLN	2.4
1	B	401	GLN	2.4
1	C	174	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	396	GLN	2.2
1	A	397	HIS	2.2
1	B	1	LYS	2.2
1	C	399	HIS	2.0

## 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 carbohydrates 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, 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( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	501	1/1	0.61	0.28	60,60,60,60	1
2	ZN	C	512	1/1	0.63	0.40	60,60,60,60	1
2	ZN	C	513	1/1	0.66	0.28	60,60,60,60	1
2	ZN	C	503	1/1	0.69	0.28	60,60,60,60	1
2	ZN	C	505	1/1	0.75	0.10	60,60,60,60	1
2	ZN	B	503	1/1	0.82	0.25	60,60,60,60	1
2	ZN	B	512	1/1	0.83	0.38	60,60,60,60	1
2	ZN	A	505	1/1	0.87	0.33	60,60,60,60	1
2	ZN	C	511	1/1	0.87	0.29	60,60,60,60	1
2	ZN	C	502	1/1	0.88	0.17	60,60,60,60	1
2	ZN	B	501	1/1	0.88	0.07	60,60,60,60	1
2	ZN	A	504	1/1	0.88	0.06	60,60,60,60	1
2	ZN	B	513	1/1	0.89	0.15	60,60,60,60	1
2	ZN	A	501	1/1	0.91	0.17	60,60,60,60	1
2	ZN	B	502	1/1	0.91	0.13	60,60,60,60	1
2	ZN	B	509	1/1	0.91	0.11	60,60,60,60	1
2	ZN	B	510	1/1	0.92	0.17	55,55,55,55	1
2	ZN	B	504	1/1	0.94	0.25	60,60,60,60	1
2	ZN	A	503	1/1	0.94	0.18	60,60,60,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	504	1/1	0.94	0.07	60,60,60,60	1
2	ZN	A	502	1/1	0.95	0.23	60,60,60,60	1
2	ZN	C	507	1/1	0.95	0.27	60,60,60,60	1
2	ZN	B	508	1/1	0.96	0.15	60,60,60,60	1
2	ZN	C	509	1/1	0.97	0.16	60,60,60,60	1
2	ZN	C	510	1/1	0.97	0.09	60,60,60,60	1
2	ZN	B	511	1/1	0.97	0.06	60,60,60,60	1
2	ZN	B	506	1/1	0.97	0.15	59,59,59,59	1
2	ZN	C	506	1/1	0.97	0.27	60,60,60,60	1
2	ZN	B	507	1/1	0.98	0.15	60,60,60,60	1
2	ZN	B	505	1/1	0.98	0.21	60,60,60,60	1
2	ZN	C	508	1/1	0.99	0.19	60,60,60,60	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.