



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:17 AM UTC

PDB ID : 4FEB / pdb\_00004feb  
Title : Crystal Structure of Htt36Q3H-EX1-X1-C2(Beta)  
Authors : Kim, M.  
Deposited on : 2012-05-29  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

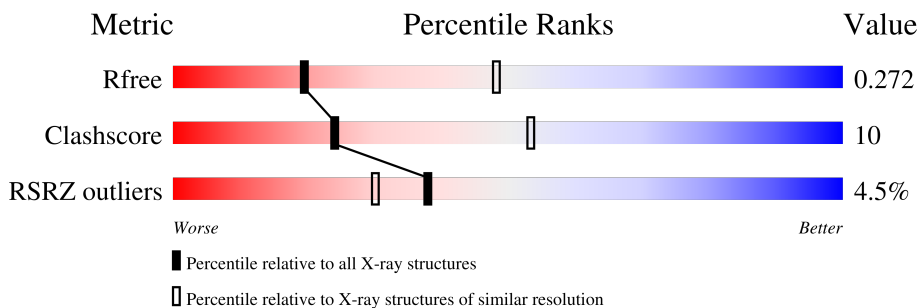
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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	 3% 79% 10% 11%
1	B	452	 4% 74% 14% 11%
1	C	452	 4% 75% 13% 12%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9586 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 3155	C 2021	N 522	O 604	S 8	10	3	0
1	B	402	Total 3146	C 2016	N 520	O 602	S 8	14	2	0
1	C	398	Total 3104	C 1991	N 513	O 592	S 8	22	2	2

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ALA	-	linker	UNP P0AEY0
A	360	ALA	-	linker	UNP P0AEY0
A	361	LEU	-	linker	UNP P0AEY0
A	362	ALA	-	linker	UNP P0AEY0
A	363	ALA	-	linker	UNP P0AEY0
A	364	ALA	-	linker	UNP P0AEY0
A	365	GLN	-	linker	UNP P0AEY0
A	366	THR	-	linker	UNP P0AEY0
A	367	ASN	-	linker	UNP P0AEY0
A	368	ALA	-	linker	UNP P0AEY0
A	369	ALA	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
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 P0AEY0
B	360	ALA	-	linker	UNP P0AEY0
B	361	LEU	-	linker	UNP P0AEY0
B	362	ALA	-	linker	UNP P0AEY0
B	363	ALA	-	linker	UNP P0AEY0
B	364	ALA	-	linker	UNP P0AEY0
B	365	GLN	-	linker	UNP P0AEY0
B	366	THR	-	linker	UNP P0AEY0
B	367	ASN	-	linker	UNP P0AEY0
B	368	ALA	-	linker	UNP P0AEY0
B	369	ALA	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0
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 P0AEY0
C	360	ALA	-	linker	UNP P0AEY0
C	361	LEU	-	linker	UNP P0AEY0
C	362	ALA	-	linker	UNP P0AEY0
C	363	ALA	-	linker	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	-	linker	UNP P0AEY0
C	365	GLN	-	linker	UNP P0AEY0
C	366	THR	-	linker	UNP P0AEY0
C	367	ASN	-	linker	UNP P0AEY0
C	368	ALA	-	linker	UNP P0AEY0
C	369	ALA	-	linker	UNP P0AEY0
C	370	ALA	-	linker	UNP P0AEY0
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	8	Total Zn 8 8	0	0
2	B	19	Total Zn 19 19	0	0
2	C	11	Total Zn 11 11	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Na 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	56	Total 56	O 56	0	0
4	C	31	Total 31	O 31	0	0





## 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 – 2.80 35.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.00-2.80) 96.4 (35.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.229 , 0.275 (Not available) , 0.272	Depositor DCC
$R_{free}$ test set	2375 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, NA

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	0.46	1/3229 (0.0%)	0.84	4/4379 (0.1%)
1	B	0.48	1/3220 (0.0%)	0.80	4/4366 (0.1%)
1	C	0.50	0/3182	0.80	1/4313 (0.0%)
All	All	0.48	2/9631 (0.0%)	0.81	9/13058 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	GLN	CG-CD	-5.70	1.37	1.52
1	B	4	GLU	N-CA	-5.09	1.40	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	GLN	CG-CD-NE2	14.87	138.70	116.40
1	A	390	GLN	CG-CD-OE1	-12.05	96.69	120.80
1	B	4	GLU	N-CA-C	-9.19	93.42	108.41
1	C	395	HIS	N-CA-C	8.01	120.68	109.31
1	B	399	HIS	N-CA-C	7.95	121.10	111.40
1	A	398	GLN	N-CA-C	-6.33	100.93	110.24
1	A	390	GLN	CB-CG-CD	5.72	122.33	112.60
1	B	228	GLY	CA-C-N	5.18	125.48	119.47
1	B	228	GLY	C-N-CA	5.18	125.48	119.47

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	3155	0	3108	47	0
1	B	3146	0	3102	81	0
1	C	3104	0	3069	64	13
2	A	8	0	0	0	0
2	B	19	0	0	0	0
2	C	11	0	0	0	0
3	A	5	0	0	0	0
3	C	1	0	0	0	0
4	A	50	0	0	0	0
4	B	56	0	0	1	0
4	C	31	0	0	2	0
All	All	9586	0	9279	186	13

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 10.

All (186) 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:398:GLN:OE1	1:B:399:HIS:CD2	1.65	1.47
1:B:398:GLN:CD	1:B:399:HIS:CD2	2.01	1.37
1:B:398:GLN:CD	1:B:399:HIS:HD2	1.30	1.36
1:B:397:HIS:O	1:B:401:GLN:HB2	1.32	1.27
1:B:1:LYS:C	1:B:2:ILE:HD13	1.64	1.23
1:C:1:LYS:H2	1:C:55:ASP:HA	1.13	1.14
1:B:397:HIS:H	1:B:401:GLN:CB	1.64	1.10
1:B:398:GLN:NE2	1:B:399:HIS:CD2	2.23	1.05
1:A:2:ILE:H	1:A:2:ILE:CD1	1.71	1.02
1:A:2:ILE:HD12	1:A:2:ILE:N	1.67	1.01
1:A:2:ILE:H	1:A:2:ILE:HD12	0.87	1.00
1:C:391:GLN:O	1:C:395:HIS:HB2	1.61	1.00
1:B:1:LYS:O	1:B:2:ILE:HD13	1.62	0.98
1:C:397:HIS:HB3	1:C:399:HIS:CE1	2.02	0.94
1:B:395:HIS:O	1:B:401:GLN:CD	2.12	0.93
1:A:401:GLN:C	1:A:401:GLN:HE21	1.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:HIS:H	1:B:401:GLN:HB2	1.35	0.91
1:B:1:LYS:N	1:B:55:ASP:OD1	2.03	0.90
1:A:401:GLN:C	1:A:401:GLN:NE2	2.30	0.89
1:C:2:ILE:HG12	1:C:56:GLY:O	1.72	0.89
1:B:397:HIS:O	1:B:401:GLN:CB	2.22	0.87
1:B:397:HIS:H	1:B:401:GLN:HB3	1.38	0.87
1:B:390:GLN:HA	1:B:394:GLN:HB2	1.55	0.86
1:C:2:ILE:CG1	1:C:56:GLY:O	2.25	0.85
1:C:1:LYS:C	1:C:2:ILE:HD12	2.03	0.83
1:C:1:LYS:N	1:C:55:ASP:HA	1.93	0.83
1:A:392:GLN:O	1:A:396:GLN:O	1.98	0.81
1:C:1:LYS:N	1:C:55:ASP:OD1	2.13	0.81
1:B:397:HIS:CD2	1:B:398:GLN:H	1.98	0.80
1:B:1:LYS:C	1:B:2:ILE:CD1	2.54	0.79
1:B:397:HIS:HD2	1:B:398:GLN:H	1.28	0.79
1:B:397:HIS:N	1:B:401:GLN:CB	2.46	0.77
1:B:398:GLN:NE2	1:B:399:HIS:NE2	2.31	0.77
1:A:64:HIS:HD2	1:A:261:VAL:H	1.33	0.76
1:B:328[B]:GLU:HA	1:B:328[B]:GLU:OE2	1.83	0.76
1:B:2:ILE:HA	4:B:610:HOH:O	1.86	0.75
1:B:397:HIS:C	1:B:401:GLN:HB2	2.11	0.75
1:B:398:GLN:OE1	1:B:399:HIS:NE2	2.22	0.72
1:C:171[B]:TYR:O	1:C:171[B]:TYR:CG	2.42	0.70
1:A:395:HIS:HE1	1:B:152:GLN:OE1	1.74	0.69
1:A:274[A]:GLU:H	1:A:274[A]:GLU:CD	1.98	0.69
1:B:371:MET:O	1:B:375:GLU:HB2	1.92	0.69
1:C:2:ILE:O	4:C:602:HOH:O	2.12	0.68
1:A:395:HIS:CE1	1:B:152:GLN:OE1	2.46	0.68
1:C:64:HIS:HD2	1:C:261:VAL:H	1.43	0.67
1:A:2:ILE:HD11	1:A:54:GLY:O	1.94	0.67
1:C:2:ILE:HD12	1:C:2:ILE:N	2.10	0.67
1:C:72:GLN:HG2	1:C:99:TYR:OH	1.94	0.67
1:C:2:ILE:CG2	1:C:8:VAL:CG1	2.73	0.66
1:B:388:GLN:O	1:B:392:GLN:HB3	1.96	0.66
1:B:397:HIS:N	1:B:401:GLN:HB2	2.07	0.66
1:B:1:LYS:H1	1:B:55:ASP:CG	2.01	0.66
1:B:72:GLN:HG2	1:B:99:TYR:OH	1.96	0.66
1:C:1:LYS:H2	1:C:55:ASP:CA	2.02	0.65
1:C:2:ILE:CG2	1:C:8:VAL:HG11	2.27	0.65
1:C:400:GLN:HG2	1:C:401:GLN:N	2.10	0.65
1:B:395:HIS:O	1:B:401:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLN:HG2	1:A:99:TYR:OH	1.98	0.64
1:A:401:GLN:NE2	1:A:401:GLN:O	2.30	0.64
1:C:288[A]:GLU:OE2	1:C:288[A]:GLU:HA	1.98	0.63
1:A:64:HIS:CD2	1:A:261:VAL:H	2.15	0.63
1:C:400:GLN:CG	1:C:401:GLN:N	2.61	0.63
1:C:396:GLN:HA	1:C:401:GLN:HA	1.78	0.63
1:B:2:ILE:HD11	1:B:55:ASP:HA	1.80	0.62
1:C:1:LYS:N	1:C:54:GLY:O	2.32	0.62
1:C:369:ALA:O	1:C:373:THR:HG22	1.99	0.62
1:A:398:GLN:O	1:A:399:HIS:CB	2.47	0.61
1:B:398:GLN:CD	1:B:399:HIS:NE2	2.57	0.61
1:A:390:GLN:O	1:A:394:GLN:HB3	2.01	0.61
1:C:401:GLN:O	1:C:402:GLN:C	2.43	0.61
1:B:96:ALA:HB2	1:B:329:ILE:HD13	1.82	0.61
1:A:2:ILE:HG23	1:A:56:GLY:O	2.00	0.61
1:B:6:LYS:CG	1:B:7:LEU:N	2.64	0.60
1:B:64:HIS:HD2	1:B:261:VAL:H	1.49	0.59
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.67	0.59
1:A:398:GLN:O	1:A:399:HIS:HB3	2.00	0.59
1:B:48:PRO:HG3	1:B:70:TYR:CE1	2.37	0.59
1:B:395:HIS:O	1:B:401:GLN:OE1	2.20	0.59
1:B:6:LYS:HG2	1:B:7:LEU:N	2.15	0.59
1:C:2:ILE:O	1:C:3:GLU:CB	2.51	0.59
1:C:2:ILE:HG13	1:C:56:GLY:O	1.99	0.59
1:A:2:ILE:CD1	1:A:54:GLY:O	2.51	0.58
1:B:274[A]:GLU:H	1:B:274[A]:GLU:CD	2.11	0.58
1:C:218:ASN:HD21	1:C:235:ILE:HG12	1.68	0.57
1:A:397:HIS:O	1:A:398:GLN:C	2.46	0.57
1:C:400:GLN:CG	1:C:401:GLN:H	2.18	0.57
1:B:336:MET:HE3	1:B:339:PHE:CD1	2.40	0.57
1:B:1:LYS:O	1:B:2:ILE:CD1	2.46	0.56
1:C:205:ASN:HD22	1:C:207:ASP:H	1.53	0.56
1:A:397:HIS:O	1:A:400:GLN:N	2.35	0.56
1:B:396:GLN:HB3	1:B:402:GLN:HB3	1.87	0.56
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.71	0.56
1:B:64:HIS:HE1	1:B:330:MET:O	1.88	0.56
1:B:398:GLN:HE22	1:B:399:HIS:CD2	2.06	0.55
1:C:64:HIS:CD2	1:C:261:VAL:H	2.23	0.55
1:A:4:GLU:HG3	1:A:5:GLY:H	1.72	0.55
1:A:116:ILE:HG12	1:A:244:VAL:HG22	1.90	0.54
1:A:64:HIS:HE1	1:A:330:MET:O	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:GLN:O	1:C:398:GLN:HG3	2.08	0.54
1:B:192:LEU:HD23	1:B:357:VAL:HG13	1.90	0.53
1:C:397:HIS:CB	1:C:399:HIS:CE1	2.86	0.53
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.44	0.53
1:C:395:HIS:CG	1:C:396:GLN:H	2.27	0.51
1:B:330:MET:HE1	1:B:340:TRP:CZ2	2.46	0.51
1:C:2:ILE:HG23	1:C:8:VAL:HG11	1.93	0.51
1:B:371:MET:HA	1:B:374:LEU:HD22	1.92	0.50
1:A:370:ALA:HB1	1:C:380:ALA:HA	1.92	0.50
1:C:1:LYS:N	1:C:55:ASP:CA	2.69	0.50
1:C:397:HIS:O	1:C:400:GLN:O	2.30	0.50
1:B:152:GLN:HA	1:B:348:ILE:HD11	1.94	0.50
1:C:181:VAL:HG12	1:C:183:VAL:HG23	1.95	0.49
1:C:3:GLU:O	1:C:271:PRO:HG2	2.12	0.49
1:B:398:GLN:O	1:B:398:GLN:HG2	2.11	0.49
1:B:301:ALA:HB1	1:B:321:MET:HE2	1.95	0.49
1:B:392:GLN:O	1:B:396:GLN:O	2.30	0.49
1:A:301:ALA:HB1	1:A:321:MET:HE2	1.96	0.48
1:B:397:HIS:N	1:B:401:GLN:HB3	2.16	0.48
1:A:1:LYS:CG	1:A:55:ASP:OD1	2.51	0.48
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.94	0.48
1:C:51:ALA:HA	1:C:55:ASP:O	2.14	0.48
1:B:48:PRO:HG3	1:B:70:TYR:HE1	1.79	0.48
1:C:2:ILE:C	4:C:602:HOH:O	2.56	0.48
1:A:4:GLU:CG	1:A:5:GLY:N	2.76	0.48
1:B:116:ILE:HG12	1:B:244:VAL:HG22	1.96	0.47
1:C:1:LYS:C	1:C:2:ILE:CD1	2.83	0.47
1:B:328[B]:GLU:OE2	1:B:328[B]:GLU:CA	2.58	0.47
1:C:43:LEU:O	1:C:46:LYS:N	2.47	0.47
1:C:397:HIS:CD2	1:C:398:GLN:H	2.32	0.47
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.97	0.47
1:A:398:GLN:O	1:A:399:HIS:CD2	2.68	0.47
1:B:302:VAL:HG21	1:B:307:TYR:HD2	1.80	0.47
1:C:154:PRO:HG3	1:C:344:ARG:HA	1.96	0.47
1:B:3:GLU:O	1:B:271:PRO:HG2	2.14	0.46
1:B:64:HIS:CD2	1:B:261:VAL:H	2.32	0.46
1:B:402:GLN:H	1:B:402:GLN:CD	2.22	0.46
1:B:371:MET:SD	1:B:374:LEU:HD21	2.56	0.46
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.51	0.46
1:B:1:LYS:N	1:B:55:ASP:CG	2.68	0.46
1:C:371:MET:O	1:C:371:MET:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ILE:HG12	1:C:244:VAL:HG22	1.98	0.45
1:B:330:MET:HE2	1:B:336:MET:HE2	1.99	0.45
1:B:333:ILE:HD12	1:B:335:GLN:HB2	1.99	0.44
1:A:52:ALA:O	1:B:355:GLN:HA	2.17	0.44
1:C:41:ASP:OD2	1:C:42:LYS:HE3	2.17	0.44
1:C:64:HIS:HE1	1:C:330:MET:O	2.01	0.44
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.83	0.44
1:C:374:LEU:O	1:C:378:MET:HG3	2.18	0.44
1:B:396:GLN:HA	1:B:401:GLN:HB3	1.99	0.44
1:C:397:HIS:HB3	1:C:399:HIS:NE2	2.30	0.43
1:B:380:ALA:HB1	1:C:374:LEU:HD13	2.01	0.43
1:C:96:ALA:HB2	1:C:329:ILE:HD12	2.01	0.43
1:A:85:PHE:O	1:A:88:LYS:HB2	2.19	0.43
1:A:77:ALA:HB2	1:A:268:ALA:HA	2.01	0.43
1:A:390:GLN:O	1:A:394:GLN:CB	2.66	0.43
1:A:392:GLN:HG3	1:A:393:GLN:N	2.34	0.43
1:A:398:GLN:O	1:A:399:HIS:CG	2.72	0.43
1:B:397:HIS:CA	1:B:401:GLN:HB2	2.49	0.43
1:B:158:TRP:N	1:B:159:PRO:HD2	2.33	0.43
1:A:28:GLU:HG2	1:A:34:LYS:HA	2.01	0.43
1:B:181:VAL:HG12	1:B:183:VAL:HG23	2.00	0.43
1:C:400:GLN:HG3	1:C:401:GLN:H	1.83	0.43
1:A:154:PRO:HB3	1:A:343:VAL:HG12	2.01	0.42
1:B:6:LYS:HB3	1:B:6:LYS:HE3	1.55	0.42
1:B:8:VAL:HG13	1:B:57:PRO:HA	2.02	0.42
1:B:395:HIS:CG	1:B:396:GLN:N	2.81	0.42
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.81	0.42
1:C:171[B]:TYR:O	1:C:171[B]:TYR:CD1	2.71	0.42
1:A:4:GLU:HG3	1:A:5:GLY:N	2.35	0.42
1:A:153[A]:GLU:HA	1:A:154:PRO:HD3	1.90	0.42
1:A:1:LYS:HG3	1:A:55:ASP:OD1	2.18	0.42
1:A:40:PRO:HG2	1:A:43:LEU:HB3	2.02	0.42
1:C:43:LEU:O	1:C:45:GLU:N	2.53	0.41
1:C:2:ILE:O	1:C:3:GLU:HB2	2.21	0.41
1:A:401:GLN:C	1:A:401:GLN:CD	2.81	0.41
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.55	0.41
1:A:2:ILE:CD1	1:A:2:ILE:N	2.42	0.41
1:B:7:LEU:HD23	1:B:58:ASP:HB2	2.03	0.41
1:B:397:HIS:CD2	1:B:398:GLN:N	2.78	0.41
1:C:397:HIS:C	1:C:399:HIS:H	2.28	0.41
1:B:401:GLN:HA	1:B:402:GLN:HA	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:C	1:B:389:GLN:N	2.79	0.40
1:C:158:TRP:N	1:C:159:PRO:HD2	2.36	0.40
1:C:301:ALA:HB1	1:C:321:MET:HE2	2.03	0.40
1:A:380:ALA:HA	1:B:370:ALA:HB1	2.03	0.40
1:B:341:TYR:CD1	1:B:371:MET:HB2	2.56	0.40
1:C:2:ILE:O	1:C:2:ILE:HG22	2.20	0.40

All (13) 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:153:GLU:CG	1:C:396:GLN:NE2[2_556]	0.19	2.01
1:C:153:GLU:CD	1:C:396:GLN:CD[2_556]	0.70	1.50
1:C:153:GLU:CD	1:C:396:GLN:OE1[2_556]	0.72	1.48
1:C:153:GLU:OE1	1:C:396:GLN:OE1[2_556]	1.02	1.18
1:C:153:GLU:OE2	1:C:396:GLN:OE1[2_556]	1.19	1.01
1:C:153:GLU:CG	1:C:396:GLN:CD[2_556]	1.32	0.88
1:C:153:GLU:OE2	1:C:396:GLN:CD[2_556]	1.35	0.85
1:C:153:GLU:CB	1:C:396:GLN:NE2[2_556]	1.35	0.85
1:C:153:GLU:CD	1:C:396:GLN:NE2[2_556]	1.52	0.68
1:C:153:GLU:OE1	1:C:396:GLN:CD[2_556]	1.77	0.43
1:C:344:ARG:NH2	1:C:395:HIS:NE2[2_556]	1.98	0.22
1:C:153:GLU:OE2	1:C:396:GLN:CG[2_556]	2.13	0.07
1:C:153:GLU:CD	1:C:396:GLN:CG[2_556]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 44 ligands modelled in this entry, 44 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, 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%)	0.30	15 (3%) 45 36	18, 85, 121, 149	21 (5%)
1	B	402/452 (88%)	0.39	20 (4%) 34 26	22, 89, 131, 157	17 (4%)
1	C	396/452 (87%)	0.42	19 (4%) 35 28	16, 93, 147, 183	19 (4%)
All	All	1200/1356 (88%)	0.37	54 (4%) 38 30	16, 89, 132, 183	57 (4%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171[A]	TYR	10.3
1	A	1	LYS	7.4
1	C	398	GLN	7.1
1	A	402	GLN	7.0
1	A	396	GLN	6.8
1	C	400	GLN	6.2
1	B	2	ILE	6.2
1	A	397	HIS	5.2
1	C	1	LYS	5.1
1	A	3	GLU	4.9
1	B	397	HIS	4.9
1	C	397	HIS	4.7
1	B	328[A]	GLU	4.7
1	B	398	GLN	4.3
1	A	399	HIS	4.3
1	C	402	GLN	4.2
1	B	392	GLN	4.1
1	B	396	GLN	4.1
1	B	1	LYS	3.8
1	C	393	GLN	3.8
1	A	137	LYS	3.7
1	C	401	GLN	3.5
1	B	273	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	ASP	3.3
1	B	274[A]	GLU	3.2
1	B	395	HIS	3.1
1	B	402	GLN	3.1
1	A	173	ASN	3.0
1	B	393	GLN	3.0
1	C	174	GLY	2.9
1	A	395	HIS	2.9
1	B	399	HIS	2.8
1	B	394	GLN	2.8
1	A	398	GLN	2.7
1	C	283	TYR	2.7
1	B	400	GLN	2.7
1	A	365[A]	GLN	2.6
1	B	3	GLU	2.6
1	C	394	GLN	2.6
1	C	370	ALA	2.6
1	C	399	HIS	2.5
1	A	2	ILE	2.5
1	A	390	GLN	2.4
1	A	393	GLN	2.4
1	B	401	GLN	2.4
1	C	2	ILE	2.4
1	C	288[A]	GLU	2.3
1	C	395	HIS	2.3
1	C	175	LYS	2.2
1	B	134	ALA	2.1
1	A	400	GLN	2.1
1	C	173	ASN	2.0
1	B	283	TYR	2.0
1	B	74	GLY	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 oligosaccharides 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	505	1/1	0.75	0.09	60,60,60,60	1
2	ZN	C	501	1/1	0.76	0.15	60,60,60,60	1
2	ZN	A	504	1/1	0.77	0.24	60,60,60,60	1
2	ZN	C	506	1/1	0.78	0.13	60,60,60,60	1
2	ZN	B	514	1/1	0.80	0.31	60,60,60,60	1
2	ZN	C	508	1/1	0.81	0.10	60,60,60,60	1
2	ZN	B	518	1/1	0.82	0.15	60,60,60,60	1
2	ZN	A	508	1/1	0.82	0.08	60,60,60,60	1
2	ZN	B	509	1/1	0.84	0.08	60,60,60,60	1
2	ZN	A	507	1/1	0.84	0.09	60,60,60,60	1
3	NA	A	512	1/1	0.84	0.11	60,60,60,60	0
2	ZN	B	510	1/1	0.85	0.07	60,60,60,60	1
2	ZN	C	510	1/1	0.86	0.09	60,60,60,60	1
2	ZN	C	502	1/1	0.86	0.14	60,60,60,60	1
2	ZN	B	516	1/1	0.87	0.09	60,60,60,60	1
2	ZN	C	511	1/1	0.87	0.23	55,55,55,55	1
2	ZN	B	513	1/1	0.87	0.08	60,60,60,60	1
2	ZN	C	505	1/1	0.89	0.07	60,60,60,60	1
2	ZN	B	511	1/1	0.89	0.10	60,60,60,60	1
2	ZN	A	502	1/1	0.90	0.06	60,60,60,60	1
2	ZN	B	519	1/1	0.90	0.07	60,60,60,60	1
2	ZN	C	509	1/1	0.91	0.08	60,60,60,60	1
3	NA	A	510	1/1	0.91	0.06	60,60,60,60	0
2	ZN	A	506	1/1	0.91	0.07	60,60,60,60	1
3	NA	A	513	1/1	0.91	0.08	60,60,60,60	0
3	NA	A	509	1/1	0.92	0.15	60,60,60,60	0
2	ZN	C	507	1/1	0.92	0.06	60,60,60,60	1
3	NA	C	512	1/1	0.93	0.07	60,60,60,60	0
3	NA	A	511	1/1	0.94	0.05	60,60,60,60	0
2	ZN	B	508	1/1	0.94	0.04	60,60,60,60	1
2	ZN	B	517	1/1	0.95	0.17	45,45,45,45	1
2	ZN	B	515	1/1	0.95	0.09	56,56,56,56	1
2	ZN	B	506	1/1	0.95	0.08	60,60,60,60	1
2	ZN	C	503	1/1	0.97	0.12	60,60,60,60	1
2	ZN	A	501	1/1	0.97	0.05	60,60,60,60	1
2	ZN	B	507	1/1	0.98	0.02	60,60,60,60	1
2	ZN	B	501	1/1	0.98	0.04	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	0.98	0.06	60,60,60,60	1
2	ZN	B	502	1/1	0.98	0.05	60,60,60,60	1
2	ZN	B	504	1/1	0.98	0.04	60,60,60,60	1
2	ZN	B	505	1/1	0.98	0.05	60,60,60,60	1
2	ZN	B	512	1/1	0.98	0.05	60,60,60,60	1
2	ZN	A	503	1/1	0.98	0.08	60,60,60,60	1
2	ZN	B	503	1/1	0.99	0.05	60,60,60,60	1

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

There are no such residues in this entry.