Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:34 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

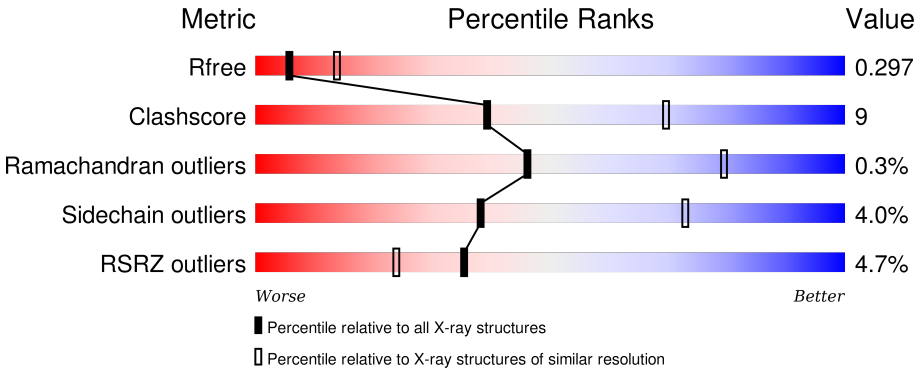
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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% 78% 10% • 11%
1	B	452	4% 78% 9% • 11%
1	C	452	5% 75% 12% • 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	C	510	-	-	-	X

2 Entry composition (i)

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 P42858
A	360	ALA	-	LINKER	UNP P42858
A	361	LEU	-	LINKER	UNP P42858
A	362	ALA	-	LINKER	UNP P42858
A	363	ALA	-	LINKER	UNP P42858
A	364	ALA	-	LINKER	UNP P42858
A	365	GLN	-	LINKER	UNP P42858
A	366	THR	-	LINKER	UNP P42858
A	367	ASN	-	LINKER	UNP P42858
A	368	ALA	-	LINKER	UNP P42858
A	369	ALA	-	LINKER	UNP P42858
A	370	ALA	-	LINKER	UNP P42858
A	388	GLN	-	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 P42858
B	360	ALA	-	LINKER	UNP P42858
B	361	LEU	-	LINKER	UNP P42858
B	362	ALA	-	LINKER	UNP P42858
B	363	ALA	-	LINKER	UNP P42858
B	364	ALA	-	LINKER	UNP P42858
B	365	GLN	-	LINKER	UNP P42858
B	366	THR	-	LINKER	UNP P42858
B	367	ASN	-	LINKER	UNP P42858
B	368	ALA	-	LINKER	UNP P42858
B	369	ALA	-	LINKER	UNP P42858
B	370	ALA	-	LINKER	UNP P42858
B	388	GLN	-	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 P42858
C	360	ALA	-	LINKER	UNP P42858
C	361	LEU	-	LINKER	UNP P42858
C	362	ALA	-	LINKER	UNP P42858
C	363	ALA	-	LINKER	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	-	LINKER	UNP P42858
C	365	GLN	-	LINKER	UNP P42858
C	366	THR	-	LINKER	UNP P42858
C	367	ASN	-	LINKER	UNP P42858
C	368	ALA	-	LINKER	UNP P42858
C	369	ALA	-	LINKER	UNP P42858
C	370	ALA	-	LINKER	UNP P42858
C	388	GLN	-	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.

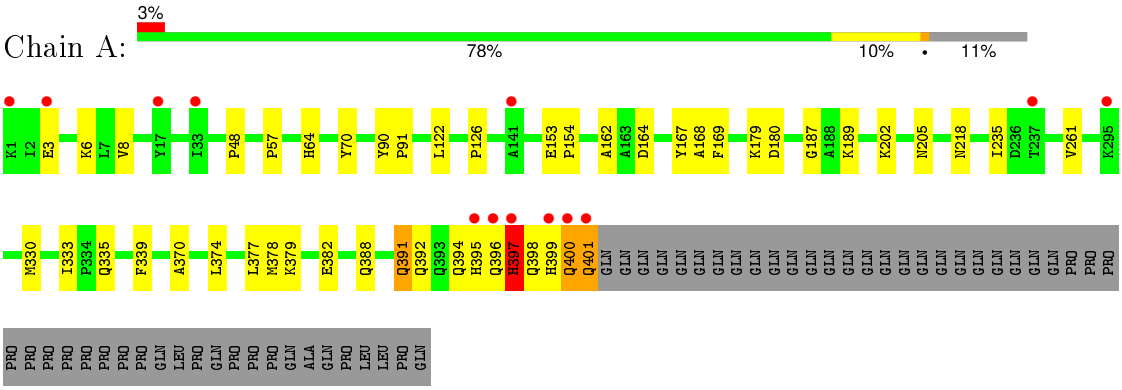
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	13	Total O 13 13	0	0
4	C	14	Total O 14 14	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

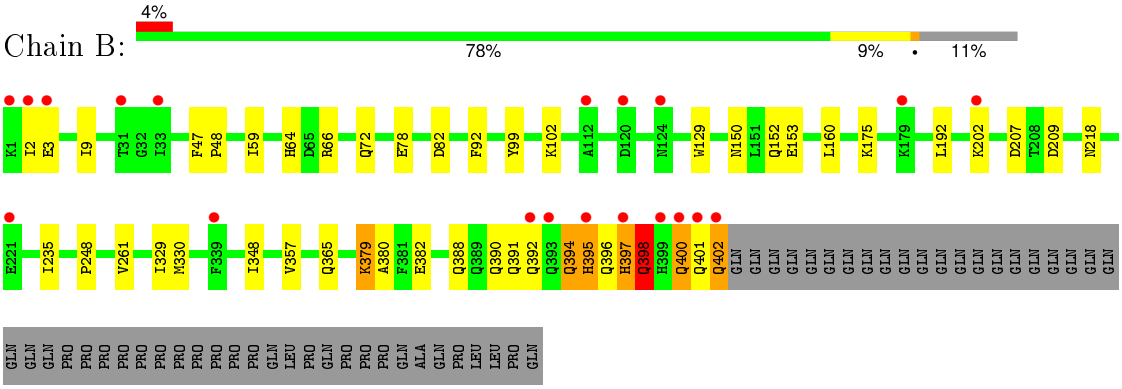
- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

Chain A:



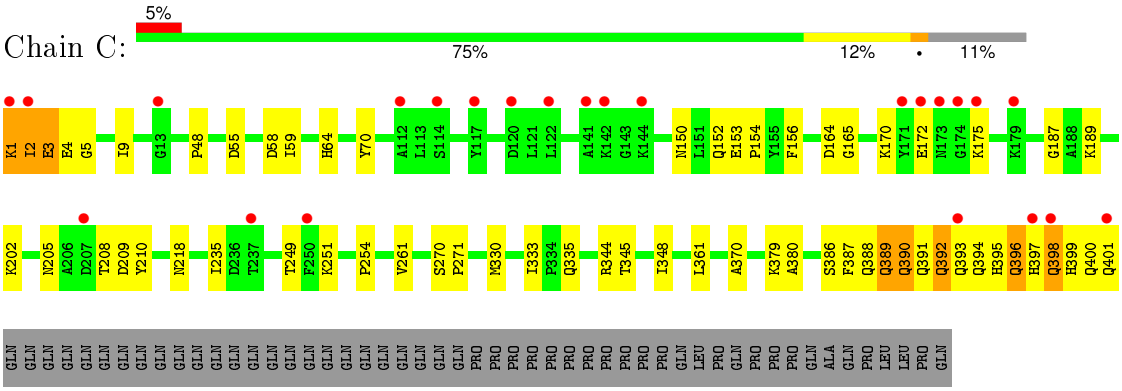
- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

Chain B:



- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.25 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.237 , 0.269 0.274 , 0.297	Depositor DCC
R_{free} test set	2015 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 40310 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9446	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:395:HIS:O	1:C:396:GLN:NE2	2.32	0.62
1:C:2:ILE:CD1	1:C:55:ASP:HA	2.28	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:N	1:C:2:ILE:HD13	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:C:64:HIS:CD2	1:C:261:VAL:H	2.22	0.56
1:B:64:HIS:CD2	1:B:261:VAL:H	2.24	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:C:398:GLN:O	1:C:399:HIS:HB2	2.08	0.53
1:A:164:ASP:C	1:A:164:ASP:OD1	2.44	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:C:397:HIS:NE2	1:C:401:GLN:HG2	2.22	0.52
1:B:64:HIS:HE1	1:B:330:MET:O	1.93	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:400:GLN:CG	1:B:401:GLN:N	2.68	0.51
1:B:380:ALA:HA	1:C:370:ALA:HB1	1.92	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:B:398:GLN:OE1	1:B:398:GLN:O	2.30	0.50
1:A:64:HIS:HE1	1:A:330:MET:O	1.94	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:C:3:GLU:N	1:C:3:GLU:CD	2.53	0.47
1:A:401:GLN:HE21	1:A:401:GLN:HB3	1.50	0.47
1:C:164:ASP:OD2	1:C:251:LYS:HD2	2.15	0.47
1:C:397:HIS:O	1:C:398:GLN:C	2.53	0.46
1:A:164:ASP:CG	1:A:164:ASP:O	2.49	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:B:390:GLN:HE22	1:C:345:THR:HG23	1.80	0.46
1:A:392:GLN:CB	1:A:396:GLN:HE21	2.28	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:396:GLN:CB	1:B:397:HIS:CD2	2.95	0.42
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.54	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:C:205:ASN:HB3	1:C:208:THR:HG23	2.03	0.40
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.94	0.40
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.93	0.40
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.04	0.40
1:B:192:LEU:HD23	1:B:357:VAL:HG13	2.03	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 (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	399/452 (88%)	388 (97%)	10 (2%)	1 (0%)	46 79
1	B	400/452 (88%)	389 (97%)	9 (2%)	2 (0%)	34 69
1	C	399/452 (88%)	384 (96%)	15 (4%)	0	100 100
All	All	1198/1356 (88%)	1161 (97%)	34 (3%)	3 (0%)	46 79

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 (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	320/370 (86%)	311 (97%)	9 (3%)	51 84
1	B	321/370 (87%)	307 (96%)	14 (4%)	35 69
1	C	320/370 (86%)	305 (95%)	15 (5%)	32 67
All	All	961/1110 (87%)	923 (96%)	38 (4%)	38 73

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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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

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^{th} 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	401/452 (88%)	0.30	13 (3%)	51	39	62, 87, 121, 156	8 (1%)
1	B	402/452 (88%)	0.39	20 (4%)	32	21	54, 83, 112, 154	12 (2%)
1	C	401/452 (88%)	0.43	24 (5%)	25	15	53, 87, 114, 160	9 (2%)
All	All	1204/1356 (88%)	0.37	57 (4%)	35	24	53, 86, 118, 160	29 (2%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	HIS	7.2
1	C	173	ASN	6.6
1	A	400	GLN	5.2
1	B	1	LYS	5.1
1	A	401	GLN	4.8
1	C	174	GLY	4.5
1	C	398	GLN	4.5
1	C	171	TYR	4.5
1	B	393	GLN	4.4
1	C	179	LYS	4.1
1	B	401	GLN	4.0
1	C	1	LYS	3.9
1	B	402	GLN	3.8
1	B	2	ILE	3.7
1	C	141	ALA	3.7
1	C	172	GLU	3.6
1	A	1	LYS	3.6
1	A	33	ILE	3.4
1	C	237	THR	3.1
1	B	124	ASN	3.1
1	C	122	LEU	3.1
1	A	17	TYR	3.0
1	A	397	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	2.8
1	C	144	LYS	2.8
1	B	400	GLN	2.6
1	B	120	ASP	2.6
1	C	207	ASP	2.6
1	C	13	GLY	2.6
1	C	401	GLN	2.6
1	B	179	LYS	2.6
1	C	393	GLN	2.5
1	C	142	LYS	2.5
1	B	339	PHE	2.5
1	C	114	SER	2.4
1	C	397	HIS	2.4
1	B	395	HIS	2.4
1	C	120	ASP	2.4
1	C	112	ALA	2.4
1	C	2	ILE	2.3
1	B	221	GLU	2.3
1	A	141	ALA	2.2
1	B	112	ALA	2.2
1	A	237	THR	2.2
1	B	31	THR	2.2
1	B	392	GLN	2.2
1	B	202	LYS	2.2
1	C	117	TYR	2.2
1	A	396	GLN	2.2
1	A	399	HIS	2.2
1	C	250	PHE	2.1
1	B	399	HIS	2.1
1	A	295	LYS	2.1
1	B	3	GLU	2.1
1	B	33	ILE	2.1
1	B	397	HIS	2.0
1	C	175	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	C	510	1/1	0.93	0.37	2.40	56,56,56,56	1
2	ZN	C	511	1/1	0.93	0.34	1.77	47,47,47,47	1
2	ZN	B	508	1/1	0.91	0.24	0.52	155,155,155,155	0
2	ZN	C	513	1/1	0.99	0.36	0.00	30,30,30,30	0
2	ZN	B	501	1/1	0.96	0.21	-0.20	105,105,105,105	0
2	ZN	C	503	1/1	0.83	0.13	-1.25	145,145,145,145	0
2	ZN	B	504	1/1	0.85	0.13	-	87,87,87,87	1
2	ZN	A	504	1/1	0.69	0.10	-	113,113,113,113	1
2	ZN	C	507	1/1	0.98	0.20	-	95,95,95,95	0
2	ZN	A	506	1/1	-0.23	0.29	-	196,196,196,196	0
2	ZN	C	501	1/1	0.89	0.37	-	64,64,64,64	1
2	ZN	A	508	1/1	0.66	0.19	-	137,137,137,137	0
2	ZN	B	511	1/1	0.86	0.06	-	145,145,145,145	0
2	ZN	C	512	1/1	0.92	0.33	-	162,162,162,162	1
2	ZN	A	505	1/1	0.91	0.36	-	85,85,85,85	1
2	ZN	A	502	1/1	0.84	0.05	-	113,113,113,113	0
2	ZN	A	503	1/1	0.63	0.14	-	101,101,101,101	1
2	ZN	B	505	1/1	0.97	0.06	-	129,129,129,129	0
2	ZN	B	509	1/1	0.63	0.26	-	166,166,166,166	0
2	ZN	B	502	1/1	0.87	0.12	-	155,155,155,155	0
2	ZN	B	507	1/1	0.50	0.14	-	171,171,171,171	0
2	ZN	B	513	1/1	0.68	0.19	-	93,93,93,93	1
2	ZN	C	508	1/1	0.93	0.32	-	60,60,60,60	1
2	ZN	A	507	1/1	0.92	0.13	-	148,148,148,148	0
3	CA	A	509	1/1	0.91	0.23	-	114,114,114,114	0
2	ZN	C	502	1/1	0.94	0.05	-	136,136,136,136	0
2	ZN	C	506	1/1	0.79	0.08	-	130,130,130,130	0
2	ZN	B	514	1/1	0.98	0.06	-	98,98,98,98	0
2	ZN	B	506	1/1	0.72	0.08	-	121,121,121,121	0
2	ZN	C	505	1/1	0.87	0.10	-	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	503	1/1	0.84	0.09	-	124,124,124,124	0
2	ZN	A	501	1/1	0.96	0.04	-	115,115,115,115	0
2	ZN	C	504	1/1	0.94	0.10	-	133,133,133,133	0
2	ZN	B	510	1/1	0.92	0.13	-	101,101,101,101	0
2	ZN	B	512	1/1	0.89	0.16	-	70,70,70,70	1
2	ZN	C	509	1/1	0.38	0.36	-	135,135,135,135	1

6.5 Other polymers

There are no such residues in this entry.