Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:33 PM GMT

PDB ID	:	4FEC
Title	:	Crystal Structure of Htt36Q3H
Authors	:	Kim, M.
Deposited on	:	2012-05-30
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
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:

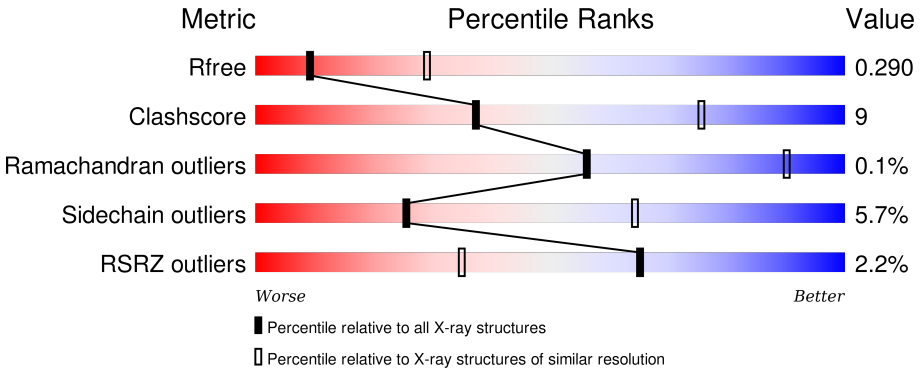
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 >=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	2% 78% 9% • 11%
1	B	452	% 76% 12% • 11%
1	C	452	4% 79% 10% • 9%

2 Entry composition (i)

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 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	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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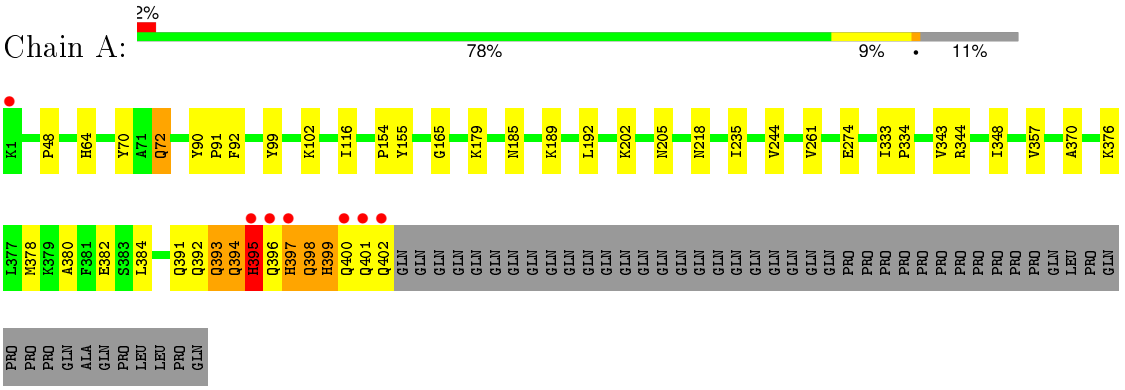
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	61	Total O 61 61	0	0
3	C	49	Total O 49 49	0	0

3 Residue-property plots (i)

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.

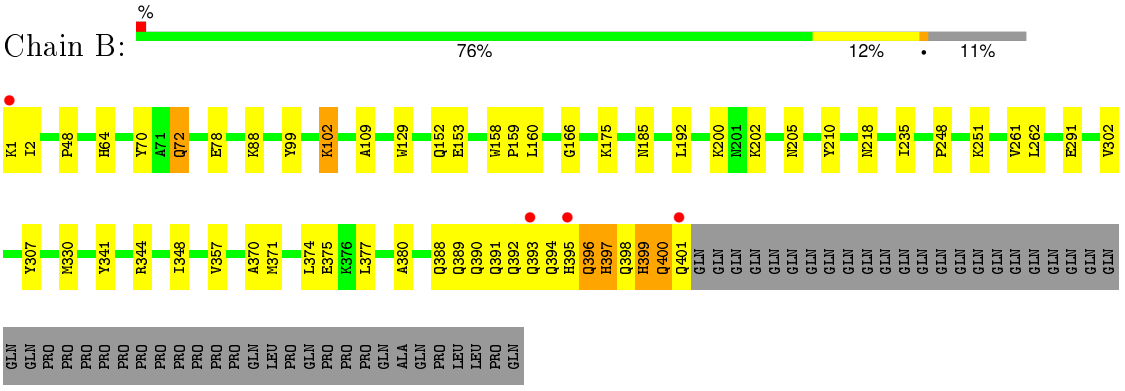
- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

Chain A:



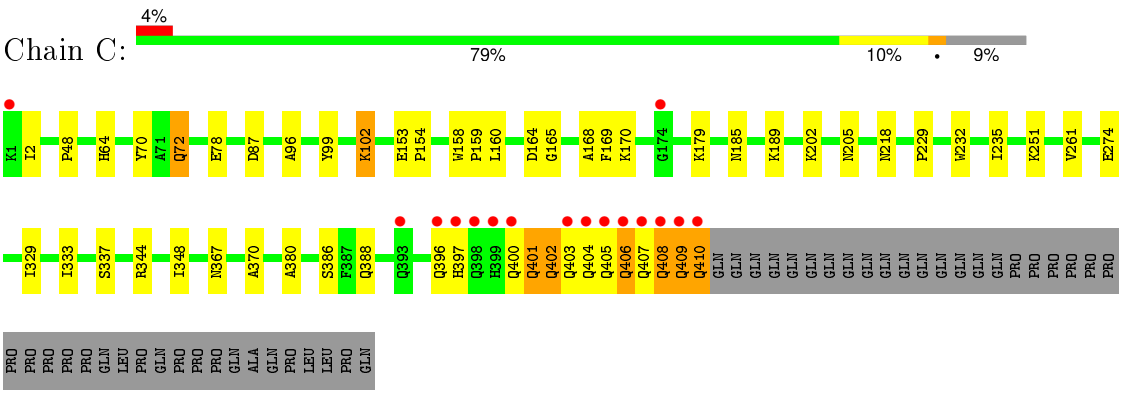
- Molecule 1: Maltose-binding periplasmic protein, Huntingtin

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	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
$< I/\sigma(I) >$ [1]	4.40 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.227 , 0.275 0.252 , 0.290	Depositor DCC
R_{free} test set	1939 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 59.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 38580 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9664	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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

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(^{o})	Ideal(^{o})
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

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:B:398:GLN:O	1:B:399:HIS:CD2	2.48	0.66
1:A:64:HIS:CD2	1:A:261:VAL:H	2.14	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: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:398:GLN:HB2	1:A:399:HIS:HD2	1.59	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:396:GLN:O	1:B:397:HIS:HB2	2.11	0.50
1:B:391:GLN:O	1:B:395:HIS:HB2	2.10	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:B:371:MET:O	1:B:375:GLU:HB2	2.17	0.45
1:A:165:GLY:O	1:A:185:ASN:ND2	2.50	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:HE21	1:A:393:GLN:HB2	1.41	0.43
1:C:406:GLN:C	1:C:410:GLN:HB3	2.37	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:205:ASN:HD22	1:B:205:ASN:HA	1.69	0.43
1:B:396:GLN:HE21	1:B:396:GLN:C	2.22	0.43
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.01	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:B:396:GLN:CB	1:B:401:GLN:C	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ALA:HA	1:B:370:ALA:HB1	2.02	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:394:GLN:HE22	1:A:395:HIS:CD2	2.32	0.41
1:A:154:PRO:HB3	1:A:343:VAL:HG12	2.02	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:A:391:GLN:CG	1:A:392:GLN:N	2.84	0.41
1:C:403:GLN:O	1:C:404:GLN:C	2.59	0.41
1:C:401:GLN:O	1:C:405:GLN:HB2	2.19	0.41
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.94	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:B:166:GLY:HA2	1:B:185:ASN:HD21	1.87	0.40
1:A:102:LYS:HG2	1:A:102:LYS:H	1.78	0.40
1:C:153:GLU:HA	1:C:154:PRO:HD3	1.93	0.40
1:B:302:VAL:HG21	1:B:307:TYR:HD2	1.86	0.40
1:B:109:ALA:HB3	1:B:262:LEU:HB3	2.02	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 (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	402/452 (89%)	385 (96%)	17 (4%)	0	100 100
1	B	400/452 (88%)	389 (97%)	10 (2%)	1 (0%)	46 84
1	C	409/452 (90%)	396 (97%)	13 (3%)	0	100 100
All	All	1211/1356 (89%)	1170 (97%)	40 (3%)	1 (0%)	56 90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	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	323/370 (87%)	307 (95%)	16 (5%)	30 70
1	B	321/370 (87%)	304 (95%)	17 (5%)	28 67
1	C	330/370 (89%)	307 (93%)	23 (7%)	19 55
All	All	974/1110 (88%)	918 (94%)	56 (6%)	25 64

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

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 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

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	402/452 (88%)	-0.33	7 (1%)	73	45	24, 84, 120, 155	13 (3%)
1	B	401/452 (88%)	-0.25	4 (0%)	84	60	38, 89, 132, 159	12 (2%)
1	C	410/452 (90%)	-0.13	16 (3%)	43	18	58, 92, 141, 190	27 (6%)
All	All	1213/1356 (89%)	-0.23	27 (2%)	65	35	24, 89, 133, 190	52 (4%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	410	GLN	6.1
1	C	407	GLN	6.0
1	C	408	GLN	5.3
1	B	395	HIS	5.3
1	A	402	GLN	4.4
1	C	400	GLN	4.3
1	C	406	GLN	3.8
1	C	409	GLN	3.7
1	A	395	HIS	3.5
1	C	1	LYS	3.3
1	A	400	GLN	3.2
1	C	396	GLN	3.1
1	C	398	GLN	3.1
1	C	405	GLN	3.0
1	C	404	GLN	2.9
1	A	1	LYS	2.6
1	A	401	GLN	2.6
1	C	393	GLN	2.5
1	B	393	GLN	2.4
1	B	401	GLN	2.4
1	C	397	HIS	2.4
1	C	174	GLY	2.4
1	C	403	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	396	GLN	2.3
1	B	1	LYS	2.2
1	A	397	HIS	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. 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	507	1/1	0.95	0.27	1.14	60,60,60,60	1
2	ZN	C	508	1/1	0.99	0.19	-0.53	60,60,60,60	1
2	ZN	A	504	1/1	0.88	0.06	-	60,60,60,60	1
2	ZN	B	509	1/1	0.91	0.11	-	60,60,60,60	1
2	ZN	B	503	1/1	0.82	0.25	-	60,60,60,60	1
2	ZN	C	513	1/1	0.66	0.28	-	60,60,60,60	1
2	ZN	A	505	1/1	0.86	0.33	-	60,60,60,60	1
2	ZN	C	501	1/1	0.60	0.28	-	60,60,60,60	1
2	ZN	A	502	1/1	0.95	0.24	-	60,60,60,60	1
2	ZN	B	511	1/1	0.97	0.06	-	60,60,60,60	1
2	ZN	C	503	1/1	0.70	0.28	-	60,60,60,60	1
2	ZN	B	513	1/1	0.89	0.14	-	60,60,60,60	1
2	ZN	B	507	1/1	0.98	0.15	-	60,60,60,60	1
2	ZN	C	505	1/1	0.75	0.10	-	60,60,60,60	1
2	ZN	C	511	1/1	0.87	0.29	-	60,60,60,60	1
2	ZN	C	510	1/1	0.97	0.09	-	60,60,60,60	1
2	ZN	C	509	1/1	0.97	0.16	-	60,60,60,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	512	1/1	0.83	0.38	-	60,60,60,60	1
2	ZN	B	505	1/1	0.98	0.21	-	60,60,60,60	1
2	ZN	C	504	1/1	0.94	0.07	-	60,60,60,60	1
2	ZN	B	502	1/1	0.91	0.13	-	60,60,60,60	1
2	ZN	B	506	1/1	0.97	0.15	-	59,59,59,59	1
2	ZN	B	501	1/1	0.88	0.07	-	60,60,60,60	1
2	ZN	B	504	1/1	0.94	0.24	-	60,60,60,60	1
2	ZN	B	508	1/1	0.96	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	510	1/1	0.92	0.17	-	55,55,55,55	1
2	ZN	C	512	1/1	0.64	0.39	-	60,60,60,60	1
2	ZN	C	502	1/1	0.88	0.17	-	60,60,60,60	1
2	ZN	C	506	1/1	0.97	0.27	-	60,60,60,60	1
2	ZN	A	503	1/1	0.94	0.17	-	60,60,60,60	1

6.5 Other polymers (i)

There are no such residues in this entry.