



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 4FED / pdb\_00004fed  
Title : Crystal Structure of Htt36Q3H  
Authors : Kim, M.  
Deposited on : 2012-05-30  
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

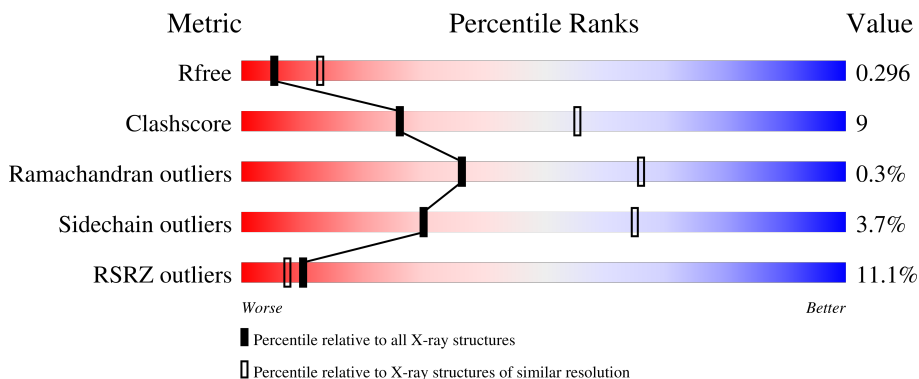
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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	
1	B	452	
1	C	452	

## 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
			Total	C	N	O	S			
1	A	401	Total 3119	C 2001	N 516	O 594	S 8	0	0	0
1	B	402	Total 3128	C 2006	N 518	O 596	S 8	0	0	0
1	C	401	Total 3119	C 2001	N 516	O 594	S 8	0	0	0

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

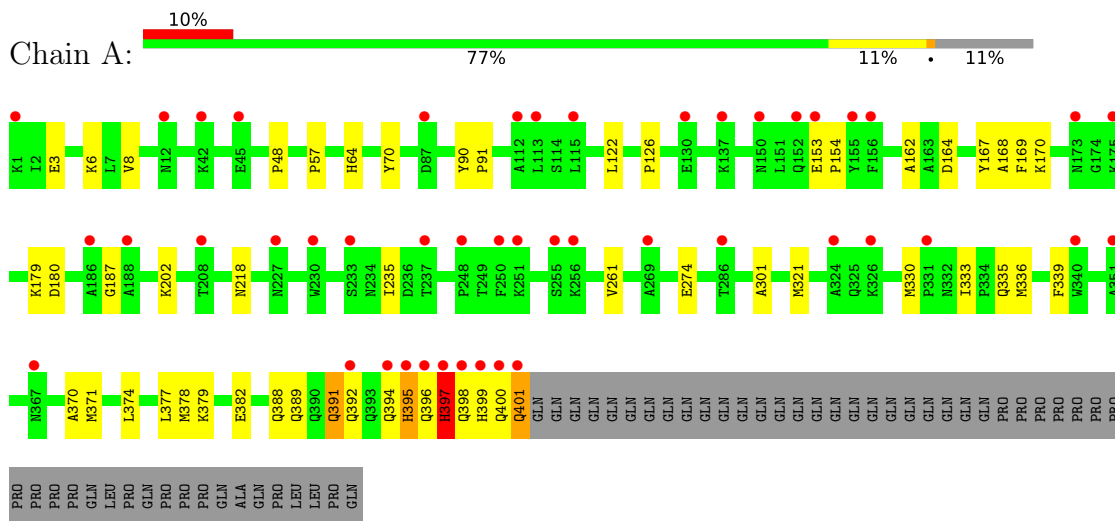
- Molecule 4 is water.

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

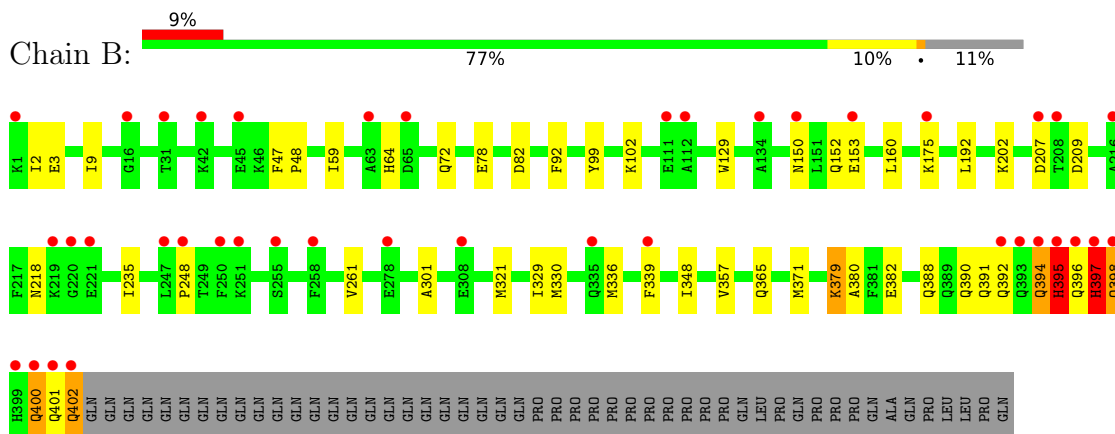
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

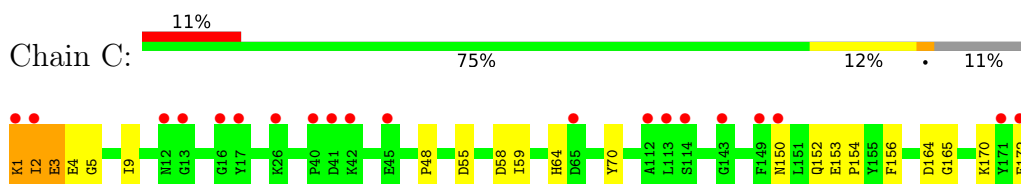
- Molecule 1: Maltose-binding periplasmic protein,Huntingtin

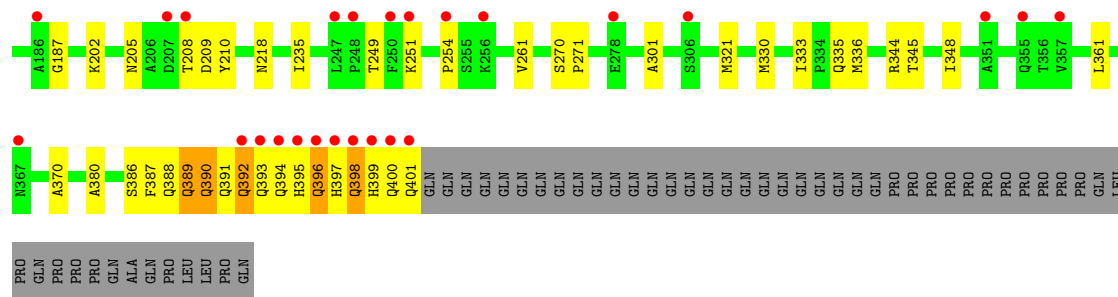


- Molecule 1: Maltose-binding periplasmic protein,Huntingtin



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.18Å 177.36Å 78.35Å 90.00° 108.67° 90.00°	Depositor
Resolution (Å)	35.00 – 2.81 35.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	83.5 (35.00-2.81) 83.5 (35.00-2.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.237 , 0.269 0.275 , 0.296	Depositor DCC
$R_{free}$ test set	2015 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

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

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3193	0.77	0/4330
1	B	0.45	0/3202	0.77	2/4342 (0.0%)
1	C	0.44	0/3193	0.76	0/4330
All	All	0.44	0/9588	0.76	2/13002 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	HIS	N-CA-C	6.48	120.50	112.59
1	B	397	HIS	N-CA-C	5.35	118.96	111.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ALA	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3119	0	3084	43	13
1	B	3128	0	3092	55	15
1	C	3119	0	3084	84	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	176	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 (176) 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:O	1:A:401:GLN:HG2	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	0.99
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:396:GLN:OE1	1.69	0.92
1:C:397:HIS:HA	1:C:400:GLN:O	1.69	0.92
1:C:3:GLU:H	1:C:3:GLU:CD	1.74	0.92
1:C:397:HIS:C	1:C:400:GLN:O	2.15	0.90
1:C:1:LYS:H1	1:C:55:ASP:CG	1.79	0.89
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: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:N	1:C:2:ILE:CD1	2.40	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: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:395:HIS:HE1	1:B:396:GLN:CD	1.89	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:C:2:ILE:N	1:C:2:ILE:HD12	2.01	0.74
1:C:397:HIS:O	1:C:400:GLN:N	2.20	0.74
1:C:395:HIS:O	1:C:396:GLN:CD	2.32	0.72
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:C:388:GLN:O	1:C:392:GLN:CD	2.35	0.70
1:B:397:HIS:O	1:B:398:GLN:CB	2.40	0.69
1:B:395:HIS:ND1	1:B:395:HIS:C	2.51	0.69
1:A:391:GLN:HG3	1:A:395:HIS:CE1	2.29	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:CE1	1:B:396:GLN:CD	2.70	0.65
1:B:395:HIS:O	1:B:395:HIS:CG	2.48	0.65
1:C:389:GLN:HA	1:C:392:GLN:HG3	1.77	0.65
1:B:395:HIS:ND1	1:B:395:HIS:O	2.30	0.65
1:B:395:HIS:CE1	1:B:396:GLN:NE2	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:396:GLN:C	1:A:398:GLN:H	2.07	0.62
1:C:2:ILE:CD1	1:C:55:ASP:HA	2.28	0.62
1:C:395:HIS:O	1:C:396:GLN:NE2	2.32	0.62
1:C:64:HIS:HD2	1:C:261:VAL:H	1.49	0.61
1:A:164:ASP:O	1:A:187:GLY:CA	2.48	0.61
1:C:4:GLU:HG2	1:C:5:GLY:N	2.15	0.61
1:C:396:GLN:O	1:C:401:GLN:HB3	1.95	0.60
1:C:397:HIS:O	1:C:400:GLN:C	2.42	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:B:402:GLN:N	1:B:402:GLN:CD	2.59	0.60
1:C:386:SER:HA	1:C:389:GLN:HG2	1.84	0.59
1:C:1:LYS:O	1:C:1:LYS:HG2	2.01	0.58
1:C:390:GLN:NE2	1:C:394:GLN:OE1	2.37	0.58
1:A:164:ASP:C	1:A:164:ASP:OD1	2.44	0.57
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:B:64:HIS:CD2	1:B:261:VAL:H	2.24	0.56
1:C:64:HIS:CD2	1:C:261:VAL:H	2.22	0.56
1:C:387:PHE:O	1:C:390:GLN:HG3	2.05	0.55
1:B:402:GLN:CD	1:B:402:GLN:H	2.15	0.55
1:A:396:GLN:OE1	1:A:397:HIS:CE1	2.60	0.55
1:C:1:LYS:N	1:C:55:ASP:CG	2.56	0.54
1:A:3:GLU:HB2	1:A:6:LYS:HE2	1.89	0.54
1:A:401:GLN:O	1:A:401:GLN:CG	2.42	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:C:391:GLN:O	1:C:395:HIS:HB3	2.08	0.53
1:A:392:GLN:HB3	1:A:396:GLN:HE21	1.73	0.52
1:C:397:HIS:CE1	1:C:401:GLN:HG2	2.44	0.52
1:B:64:HIS:HE1	1:B:330:MET:O	1.93	0.52
1:C:397:HIS:NE2	1:C:401:GLN:HG2	2.22	0.52
1:A:374:LEU:O	1:A:378:MET:HB2	2.08	0.52
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ALA:HA	1:C:370:ALA:HB1	1.92	0.51
1:B:400:GLN:CG	1:B:401:GLN:N	2.68	0.51
1:C:1:LYS:C	1:C:2:ILE:HD12	2.35	0.51
1:A:164:ASP:O	1:A:164:ASP:CG	2.49	0.51
1:C:397:HIS:O	1:C:398:GLN:C	2.53	0.51
1:C:3:GLU:CD	1:C:3:GLU:N	2.53	0.51
1:A:388:GLN:O	1:A:392:GLN:HG3	2.11	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:C:330:MET:HE2	1:C:336:MET:HE2	1.93	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
1:C:1:LYS:CA	1:C:55:ASP:OD1	2.60	0.50
1:B:336:MET:HE3	1:B:339:PHE:CD1	2.47	0.50
1:A:64:HIS:HE1	1:A:330:MET:O	1.94	0.50
1:B:398:GLN:O	1:B:398:GLN:OE1	2.30	0.50
1:B:301:ALA:HB1	1:B:321:MET:HE2	1.93	0.50
1:A:333:ILE:HD12	1:A:335:GLN:HB2	1.94	0.50
1:A:301:ALA:HB1	1:A:321:MET:HE2	1.95	0.48
1:C:2:ILE:HD13	1:C:2:ILE:H	1.77	0.48
1:A:370:ALA:HB1	1:C:380:ALA:HA	1.95	0.48
1:A:330:MET:HE2	1:A:336:MET:HE2	1.95	0.48
1:B:2:ILE:O	1:B:2:ILE:HG22	2.13	0.47
1:A:401:GLN:HE21	1:A:401:GLN:HB3	1.50	0.47
1:C:164:ASP:OD2	1:C:251:LYS:HD2	2.15	0.47
1:B:330:MET:HE2	1:B:336:MET:HE2	1.97	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:249:THR:HG22	1:C:254:PRO:HA	1.98	0.46
1:A:396:GLN:C	1:A:398:GLN:N	2.71	0.46
1:A:392:GLN:CB	1:A:396:GLN:HE21	2.28	0.46
1:B:390:GLN:HE22	1:C:345:THR:HG23	1.80	0.46
1:C:218:ASN:HD21	1:C:235:ILE:HG12	1.81	0.46
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.98	0.45
1:A:379:LYS:HA	1:A:382:GLU:HG2	1.98	0.45
1:B:330:MET:CE	1:B:336:MET:HE2	2.47	0.45
1:B:152:GLN:HA	1:B:348:ILE:HD11	1.97	0.45
1:A:167:TYR:OH	1:A:180:ASP:OD1	2.28	0.45
1:C:390:GLN:HE21	1:C:390:GLN:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:C:398:GLN:HG2	1.63	0.43
1:C:301:ALA:HB1	1:C:321:MET:HE2	2.00	0.43
1:A:169:PHE:CE2	1:A:333:ILE:HD11	2.54	0.43
1:C:4:GLU:CG	1:C:5:GLY:N	2.80	0.43
1:B:9:ILE:HG12	1:B:59:ILE:HB	2.00	0.43
1:A:396:GLN:O	1:A:398:GLN:N	2.52	0.43
1:C:390:GLN:O	1:C:394:GLN:CG	2.67	0.42
1:B:129:TRP:CD1	1:B:248:PRO:HB2	2.54	0.42
1:B:396:GLN:CB	1:B:397:HIS:CD2	2.95	0.42
1:B:78:GLU:HG3	1:B:102:LYS:HB3	2.01	0.42
1:B:396:GLN:HB3	1:B:397:HIS:NE2	2.33	0.42
1:C:333:ILE:HD12	1:C:335:GLN:HB2	2.02	0.42
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:167:TYR:CD1	1:A:167:TYR:C	2.99	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:92:PHE:O	1:B:329:ILE:HD11	2.21	0.41
1:B:218:ASN:HD21	1:B:235:ILE:HG12	1.85	0.41
1:C:270:SER:HA	1:C:271:PRO:HD3	1.95	0.41
1:C:2:ILE:CD1	1:C:55:ASP:CA	2.95	0.41
1:A:153:GLU:HA	1:A:154:PRO:HD3	1.94	0.40
1:C:205:ASN:HB3	1:C:208:THR:HG23	2.03	0.40
1:A:90:TYR:HA	1:A:91:PRO:HD3	1.93	0.40
1:B:192:LEU:HD23	1:B:357:VAL:HG13	2.03	0.40
1:C:154:PRO:HG3	1:C:344:ARG:HA	2.04	0.40
1:C:397:HIS:ND1	1:C:401:GLN:HG2	2.33	0.40
1:A:371:MET:HE3	1:A:374:LEU:HB2	2.03	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:A:401:GLN:O	1:B:209:ASP:CB[2_555]	1.80	0.40
1:C:150:ASN:ND2	1:C:397:HIS:NE2[2_555]	1.80	0.40
1:A:400:GLN:CG	1:B:153:GLU:CG[2_555]	1.83	0.37
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:153:GLU:CB	1:C:397:HIS:ND1[2_555]	2.16	0.04
1:C:210:TYR:OH	1:C:401:GLN:O[2_555]	2.16	0.04
1:A:401:GLN:C	1:B:209:ASP:CA[2_555]	2.18	0.02
1:C:156:PHE:CD1	1:C:397:HIS:CD2[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%)	36 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	400/452 (88%)	389 (97%)	9 (2%)	2 (0%)	24	55
1	C	399/452 (88%)	384 (96%)	15 (4%)	0	100	100
All	All	1198/1356 (88%)	1161 (97%)	34 (3%)	3 (0%)	36	66

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%)	310 (97%)	10 (3%)	35	70
1	B	321/370 (87%)	308 (96%)	13 (4%)	28	63
1	C	320/370 (86%)	307 (96%)	13 (4%)	27	62
All	All	961/1110 (87%)	925 (96%)	36 (4%)	30	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	179	LYS
1	A	202	LYS
1	A	274	GLU
1	A	377	LEU
1	A	389	GLN
1	A	391	GLN
1	A	395	HIS
1	A	397	HIS
1	A	401	GLN
1	B	160	LEU

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Mol	Chain	Res	Type
1	B	175	LYS
1	B	202	LYS
1	B	207	ASP
1	B	365	GLN
1	B	371	MET
1	B	379	LYS
1	B	392	GLN
1	B	394	GLN
1	B	395	HIS
1	B	397	HIS
1	B	400	GLN
1	B	402	GLN
1	C	1	LYS
1	C	2	ILE
1	C	3	GLU
1	C	170	LYS
1	C	172	GLU
1	C	175	LYS
1	C	202	LYS
1	C	361	LEU
1	C	389	GLN
1	C	390	GLN
1	C	392	GLN
1	C	396	GLN
1	C	398	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	49	GLN
1	A	64	HIS
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	388	GLN
1	A	389	GLN
1	A	390	GLN

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Mol	Chain	Res	Type
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	86	GLN
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	398	GLN
1	B	399	HIS
1	B	400	GLN
1	C	18	ASN
1	C	49	GLN
1	C	64	HIS
1	C	72	GLN
1	C	86	GLN
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	393	GLN
1	C	397	HIS

### 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 36 ligands modelled in this entry, 36 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	401/452 (88%)	0.97	46 (11%) <b>9</b> <b>7</b>	34, 86, 121, 156	8 (1%)
1	B	402/452 (88%)	0.90	40 (9%) <b>12</b> <b>9</b>	39, 83, 112, 154	12 (2%)
1	C	401/452 (88%)	0.94	48 (11%) <b>9</b> <b>6</b>	45, 86, 114, 160	9 (2%)
All	All	1204/1356 (88%)	0.94	134 (11%) <b>10</b> <b>7</b>	34, 85, 118, 160	29 (2%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	HIS	9.5
1	C	398	GLN	6.4
1	C	395	HIS	6.3
1	A	400	GLN	6.2
1	A	401	GLN	6.2
1	B	400	GLN	5.9
1	A	395	HIS	5.8
1	B	1	LYS	5.8
1	C	396	GLN	5.5
1	C	401	GLN	5.3
1	A	1	LYS	5.3
1	B	397	HIS	5.1
1	C	399	HIS	4.9
1	B	398	GLN	4.8
1	A	397	HIS	4.7
1	A	112	ALA	4.6
1	A	396	GLN	4.4
1	C	174	GLY	4.3
1	A	150	ASN	4.2
1	B	112	ALA	4.1
1	C	250	PHE	4.1
1	C	112	ALA	4.0
1	C	397	HIS	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	367	ASN	3.9
1	A	250	PHE	3.8
1	B	392	GLN	3.8
1	A	42	LYS	3.8
1	A	113	LEU	3.8
1	A	155	TYR	3.7
1	B	395	HIS	3.6
1	C	113	LEU	3.6
1	B	339	PHE	3.5
1	A	398	GLN	3.5
1	B	251	LYS	3.5
1	C	171	TYR	3.5
1	A	394	GLN	3.4
1	B	394	GLN	3.4
1	C	173	ASN	3.4
1	A	399	HIS	3.4
1	B	250	PHE	3.3
1	B	401	GLN	3.3
1	C	393	GLN	3.2
1	C	150	ASN	3.1
1	B	258	PHE	3.1
1	B	150	ASN	3.1
1	B	207	ASP	3.0
1	C	186	ALA	3.0
1	A	173	ASN	2.9
1	B	134	ALA	2.8
1	A	156	PHE	2.8
1	B	16	GLY	2.8
1	B	153	GLU	2.8
1	A	227	ASN	2.8
1	A	251	LYS	2.8
1	A	286	THR	2.8
1	C	392	GLN	2.8
1	B	221	GLU	2.7
1	A	186	ALA	2.7
1	B	335	GLN	2.7
1	B	216	ALA	2.7
1	B	220	GLY	2.7
1	C	172	GLU	2.7
1	C	45	GLU	2.6
1	C	40	PRO	2.6
1	C	1	LYS	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	402	GLN	2.6
1	B	65	ASP	2.6
1	B	278	GLU	2.5
1	B	396	GLN	2.5
1	A	188	ALA	2.5
1	A	230	TRP	2.5
1	B	45	GLU	2.5
1	C	400	GLN	2.5
1	C	2	ILE	2.5
1	C	16	GLY	2.4
1	B	42	LYS	2.4
1	A	152	GLN	2.4
1	A	12	ASN	2.4
1	C	179	LYS	2.4
1	A	45	GLU	2.4
1	B	31	THR	2.4
1	A	248	PRO	2.4
1	C	13	GLY	2.3
1	B	393	GLN	2.3
1	C	247	LEU	2.3
1	A	331	PRO	2.3
1	C	248	PRO	2.3
1	A	351	ALA	2.3
1	B	247	LEU	2.3
1	A	367	ASN	2.3
1	A	392	GLN	2.3
1	C	42	LYS	2.3
1	A	324	ALA	2.2
1	C	26	LYS	2.2
1	C	41	ASP	2.2
1	B	255	SER	2.2
1	C	149	PHE	2.2
1	A	137	LYS	2.2
1	A	175	LYS	2.2
1	C	12	ASN	2.2
1	A	208	THR	2.2
1	A	237	THR	2.2
1	A	340	TRP	2.2
1	B	248	PRO	2.2
1	C	208	THR	2.2
1	A	233	SER	2.2
1	C	306	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	LYS	2.2
1	C	17	TYR	2.2
1	B	219	LYS	2.2
1	A	87	ASP	2.2
1	C	65	ASP	2.2
1	A	115	LEU	2.2
1	C	114	SER	2.1
1	C	351	ALA	2.1
1	C	278	GLU	2.1
1	A	326	LYS	2.1
1	A	269	ALA	2.1
1	A	255	SER	2.1
1	C	394	GLN	2.1
1	C	256	LYS	2.1
1	C	254	PRO	2.1
1	C	143	GLY	2.1
1	C	355	GLN	2.0
1	C	357	VAL	2.0
1	B	63	ALA	2.0
1	C	207	ASP	2.0
1	A	153	GLU	2.0
1	B	111	GLU	2.0
1	B	308	GLU	2.0
1	A	256	LYS	2.0
1	B	208	THR	2.0
1	A	130	GLU	2.0
1	B	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	ZN	C	509	1/1	0.48	0.09	135,135,135,135	1
2	ZN	B	507	1/1	0.50	0.09	171,171,171,171	0
2	ZN	A	503	1/1	0.65	0.18	101,101,101,101	1
2	ZN	B	513	1/1	0.66	0.27	93,93,93,93	1
2	ZN	A	506	1/1	0.66	0.16	196,196,196,196	0
2	ZN	A	504	1/1	0.70	0.34	113,113,113,113	1
2	ZN	C	512	1/1	0.75	0.12	162,162,162,162	1
3	CA	A	509	1/1	0.81	0.08	114,114,114,114	0
2	ZN	B	509	1/1	0.82	0.20	166,166,166,166	0
2	ZN	A	508	1/1	0.84	0.11	137,137,137,137	0
2	ZN	A	507	1/1	0.85	0.09	148,148,148,148	0
2	ZN	A	505	1/1	0.85	0.08	85,85,85,85	1
2	ZN	C	505	1/1	0.86	0.07	158,158,158,158	0
2	ZN	C	503	1/1	0.86	0.13	145,145,145,145	0
2	ZN	C	506	1/1	0.88	0.06	130,130,130,130	0
2	ZN	B	511	1/1	0.88	0.07	145,145,145,145	0
2	ZN	B	503	1/1	0.89	0.12	124,124,124,124	0
2	ZN	C	501	1/1	0.89	0.25	64,64,64,64	1
2	ZN	B	504	1/1	0.90	0.20	87,87,87,87	1
2	ZN	B	508	1/1	0.90	0.17	155,155,155,155	0
2	ZN	B	502	1/1	0.92	0.06	155,155,155,155	0
2	ZN	B	506	1/1	0.92	0.06	121,121,121,121	0
2	ZN	A	501	1/1	0.93	0.11	115,115,115,115	0
2	ZN	B	505	1/1	0.94	0.04	129,129,129,129	0
2	ZN	B	512	1/1	0.94	0.08	70,70,70,70	1
2	ZN	C	504	1/1	0.94	0.17	133,133,133,133	0
2	ZN	B	510	1/1	0.94	0.07	101,101,101,101	0
2	ZN	C	508	1/1	0.95	0.19	60,60,60,60	1
2	ZN	B	501	1/1	0.95	0.10	105,105,105,105	0
2	ZN	C	510	1/1	0.96	0.22	56,56,56,56	1
2	ZN	A	502	1/1	0.96	0.04	113,113,113,113	0
2	ZN	C	502	1/1	0.96	0.06	136,136,136,136	0
2	ZN	B	514	1/1	0.97	0.04	98,98,98,98	0
2	ZN	C	507	1/1	0.98	0.07	95,95,95,95	0
2	ZN	C	513	1/1	0.98	0.43	30,30,30,30	0
2	ZN	C	511	1/1	0.98	0.21	47,47,47,47	1

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

There are no such residues in this entry.