



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2017 – 11:55 AM EDT

PDB ID : 3IOW  
Title : Huntingtin amino-terminal region with 17 Gln residues - crystal C99-Hg  
Authors : Kim, M.W.  
Deposited on : 2009-08-14  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029077

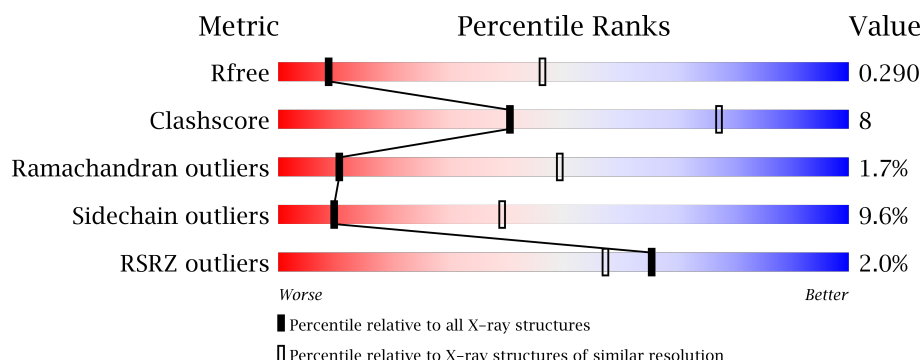
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	449	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	449	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>10%</div> </div> </div>
1	C	449	<div> <div></div> <div> <div></div> <div>72%</div> <div>12%</div> <div>12%</div> </div> </div>

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
3	CA	A	506	-	-	-	X
3	CA	C	505	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9280 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	414	Total	C	N	O	S	0	1	0
			3135	2018	514	595	8			
1	B	404	Total	C	N	O	S	0	1	0
			3111	1999	512	592	8			
1	C	393	Total	C	N	O	S	0	3	0
			3017	1943	491	575	8			

There are 105 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	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	?	-	GLN	deletion	UNP P42858
A	431	GLN	-	expression tag	UNP P42858
A	432	SER	-	expression tag	UNP P42858
A	433	TYR	-	expression tag	UNP P42858
A	434	GLN	-	expression tag	UNP P42858
A	435	ILE	-	expression tag	UNP P42858
A	436	THR	-	expression tag	UNP P42858
A	437	ALA	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP P42858
A	439	LYS	-	expression tag	UNP P42858
A	440	LEU	-	expression tag	UNP P42858
A	441	GLY	-	expression tag	UNP P42858
A	442	THR	-	expression tag	UNP P42858
A	443	GLY	-	expression tag	UNP P42858
A	444	ARG	-	expression tag	UNP P42858
A	445	ARG	-	expression tag	UNP P42858
A	446	PHE	-	expression tag	UNP P42858
A	447	THR	-	expression tag	UNP P42858
A	448	THR	-	expression tag	UNP P42858
A	449	SER	-	expression tag	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	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	?	-	GLN	deletion	UNP P42858
B	431	GLN	-	expression tag	UNP P42858
B	432	SER	-	expression tag	UNP P42858
B	433	TYR	-	expression tag	UNP P42858
B	434	GLN	-	expression tag	UNP P42858
B	435	ILE	-	expression tag	UNP P42858
B	436	THR	-	expression tag	UNP P42858
B	437	ALA	-	expression tag	UNP P42858
B	438	GLY	-	expression tag	UNP P42858
B	439	LYS	-	expression tag	UNP P42858
B	440	LEU	-	expression tag	UNP P42858
B	441	GLY	-	expression tag	UNP P42858
B	442	THR	-	expression tag	UNP P42858
B	443	GLY	-	expression tag	UNP P42858
B	444	ARG	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	ARG	-	expression tag	UNP P42858
B	446	PHE	-	expression tag	UNP P42858
B	447	THR	-	expression tag	UNP P42858
B	448	THR	-	expression tag	UNP P42858
B	449	SER	-	expression tag	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
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	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	?	-	GLN	deletion	UNP P42858
C	431	GLN	-	expression tag	UNP P42858
C	432	SER	-	expression tag	UNP P42858
C	433	TYR	-	expression tag	UNP P42858
C	434	GLN	-	expression tag	UNP P42858
C	435	ILE	-	expression tag	UNP P42858
C	436	THR	-	expression tag	UNP P42858
C	437	ALA	-	expression tag	UNP P42858
C	438	GLY	-	expression tag	UNP P42858
C	439	LYS	-	expression tag	UNP P42858
C	440	LEU	-	expression tag	UNP P42858
C	441	GLY	-	expression tag	UNP P42858
C	442	THR	-	expression tag	UNP P42858
C	443	GLY	-	expression tag	UNP P42858
C	444	ARG	-	expression tag	UNP P42858
C	445	ARG	-	expression tag	UNP P42858
C	446	PHE	-	expression tag	UNP P42858
C	447	THR	-	expression tag	UNP P42858
C	448	THR	-	expression tag	UNP P42858
C	449	SER	-	expression tag	UNP P42858

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	3	Total 3	Zn 3	0	0
2	C	2	Total 2	Zn 2	0	0

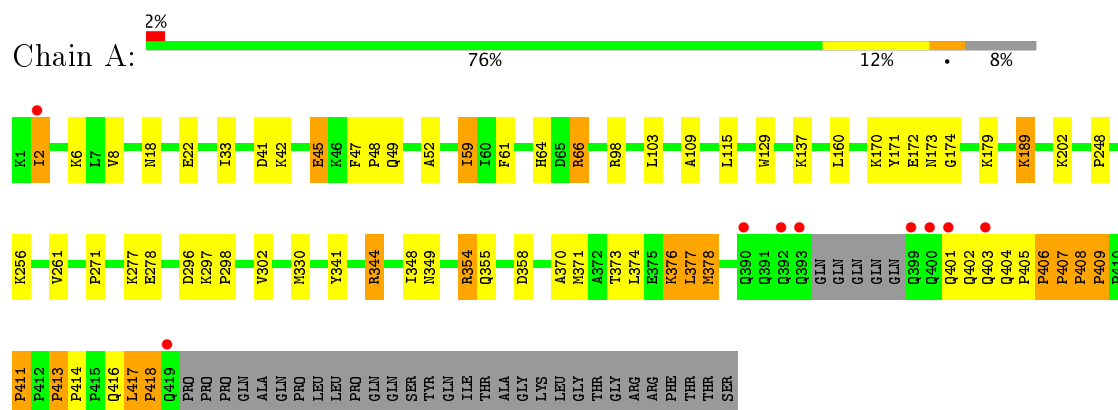
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	A	5	Total 5	Ca 5	0	0
3	C	4	Total 4	Ca 4	0	0

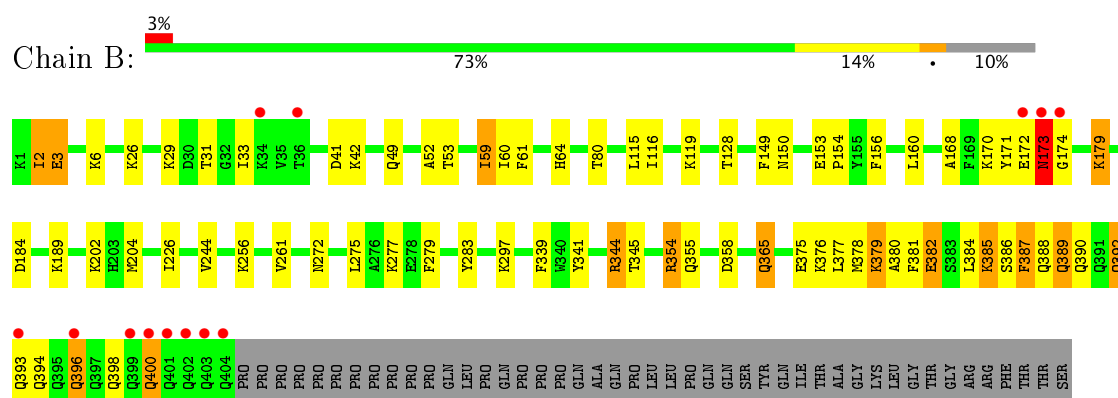
### 3 Residue-property plots

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

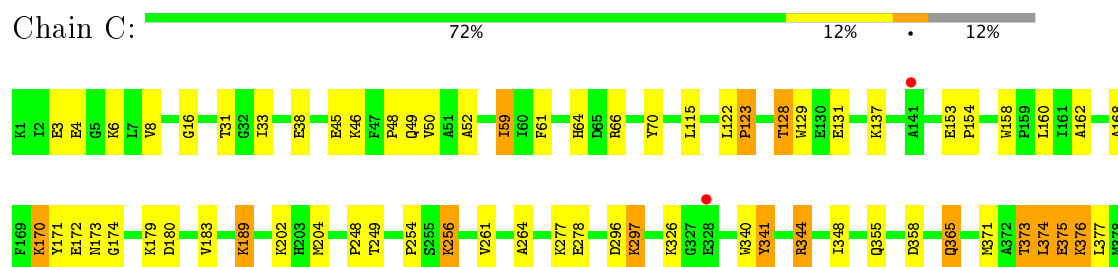
- Molecule 1: Maltose-binding periplasmic protein,Huntingtin



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin



- Molecule 1: Maltose-binding periplasmic protein,Huntingtin





[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.10Å 162.77Å 139.66Å 90.00° 98.85° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.25 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (40.00-3.50) 91.7 (39.25-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.243 , 0.281 0.251 , 0.290	Depositor DCC
$R_{free}$ test set	1316 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 14.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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	0.34	0/3218	0.49	0/4386
1	B	0.35	0/3186	0.48	0/4324
1	C	0.35	0/3097	0.50	0/4209
All	All	0.35	0/9501	0.49	0/12919

There are no bond length outliers.

There are no bond angle outliers.

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	3135	0	3058	64	0
1	B	3111	0	3053	60	0
1	C	3017	0	2960	45	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
All	All	9280	0	9071	151	0

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 8.

The worst 5 of 151 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:376:LYS:CE	1:A:377:LEU:HD23	1.39	1.52
1:A:376:LYS:HE3	1:A:377:LEU:CD2	1.62	1.27
1:C:373:THR:CG2	1:C:376:LYS:HD2	1.67	1.24
1:A:378:MET:HA	1:A:378:MET:HE3	1.09	1.08
1:C:373:THR:HG23	1:C:376:LYS:HD2	1.30	1.08

There are no symmetry-related clashes.

## 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	411/449 (92%)	381 (93%)	18 (4%)	12 (3%)	5	38
1	B	403/449 (90%)	381 (94%)	19 (5%)	3 (1%)	25	68
1	C	394/449 (88%)	379 (96%)	10 (2%)	5 (1%)	14	55
All	All	1208/1347 (90%)	1141 (94%)	47 (4%)	20 (2%)	11	49

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	402	GLN
1	A	406	PRO
1	A	409	PRO
1	A	418	PRO

### 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	314/363 (86%)	290 (92%)	24 (8%)	15	51
1	B	313/363 (86%)	280 (90%)	33 (10%)	8	35
1	C	303/363 (84%)	269 (89%)	34 (11%)	7	32
All	All	930/1089 (85%)	839 (90%)	91 (10%)	10	38

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	LYS
1	B	387	PHE
1	C	374[A]	LEU
1	B	344	ARG
1	B	379	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	ASN
1	B	218	ASN
1	C	201	ASN
1	B	49	GLN
1	B	64	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 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	414/449 (92%)	-0.11	9 (2%) 62 53	78, 78, 97, 97	45 (10%)
1	B	404/449 (89%)	-0.05	13 (3%) 48 40	78, 78, 97, 97	33 (8%)
1	C	393/449 (87%)	-0.18	2 (0%) 90 86	78, 78, 96, 97	23 (5%)
All	All	1211/1347 (89%)	-0.11	24 (1%) 65 57	78, 78, 97, 97	101 (8%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	GLN	6.1
1	A	392	GLN	4.7
1	B	396	GLN	3.9
1	B	400	GLN	3.7
1	B	403	GLN	3.6

### 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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	C	505	1/1	0.88	0.46	7.52	78,78,78,78	0
3	CA	A	506	1/1	0.92	0.43	4.58	83,83,83,83	0
2	ZN	B	502	1/1	0.96	0.23	-	92,92,92,92	0
2	ZN	A	502	1/1	0.96	0.24	-	75,75,75,75	0
3	CA	A	505	1/1	0.86	0.72	-	73,73,73,73	1
2	ZN	A	503	1/1	0.94	0.28	-	103,103,103,103	0
3	CA	C	506	1/1	0.75	0.46	-	70,70,70,70	1
2	ZN	B	501	1/1	0.92	0.23	-	102,102,102,102	1
3	CA	A	508	1/1	0.89	0.22	-	105,105,105,105	0
3	CA	C	504	1/1	0.94	0.26	-	94,94,94,94	0
3	CA	C	503	1/1	0.86	0.28	-	94,94,94,94	0
3	CA	A	507	1/1	0.76	0.37	-	80,80,80,80	1
3	CA	B	503	1/1	0.89	0.24	-	86,86,86,86	0
2	ZN	C	501	1/1	0.96	0.27	-	73,73,73,73	0
2	ZN	A	501	1/1	0.81	0.27	-	108,108,108,108	0
3	CA	A	504	1/1	0.73	0.32	-	73,73,73,73	1
2	ZN	C	502	1/1	0.98	0.28	-	96,96,96,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.