



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2IBI / pdb\_00002ibi  
Title : Covalent Ubiquitin-USP2 Complex  
Authors : Walker, J.R.; Avvakumov, G.V.; Bernstein, G.; Xue, S.; Finerty Jr., P.J.; MacKenzie, F.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-09-11  
Resolution : 2.20 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (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

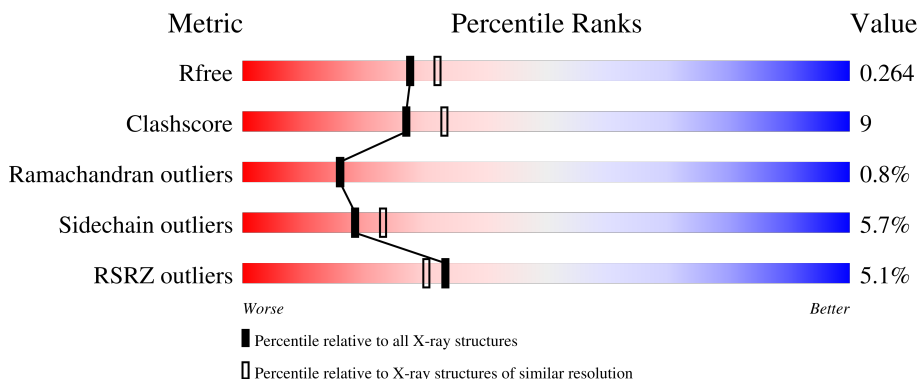
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	374	
2	B	75	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3422 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 Ubiquitin carboxyl-terminal hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2710	1699	487	504	20	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	MET	-	initiating methionine	UNP O75604
A	233	GLY	-	cloning artifact	UNP O75604
A	234	SER	-	cloning artifact	UNP O75604
A	235	SER	-	cloning artifact	UNP O75604
A	236	HIS	-	expression tag	UNP O75604
A	237	HIS	-	expression tag	UNP O75604
A	238	HIS	-	expression tag	UNP O75604
A	239	HIS	-	expression tag	UNP O75604
A	240	HIS	-	expression tag	UNP O75604
A	241	HIS	-	expression tag	UNP O75604
A	242	SER	-	cloning artifact	UNP O75604
A	243	SER	-	cloning artifact	UNP O75604
A	244	GLY	-	cloning artifact	UNP O75604
A	245	LEU	-	cloning artifact	UNP O75604
A	246	VAL	-	cloning artifact	UNP O75604
A	247	PRO	-	cloning artifact	UNP O75604
A	248	ARG	-	cloning artifact	UNP O75604
A	249	GLY	-	cloning artifact	UNP O75604
A	250	SER	-	cloning artifact	UNP O75604
A	472	ALA	GLU	engineered mutation	UNP O75604
A	473	ALA	LYS	engineered mutation	UNP O75604

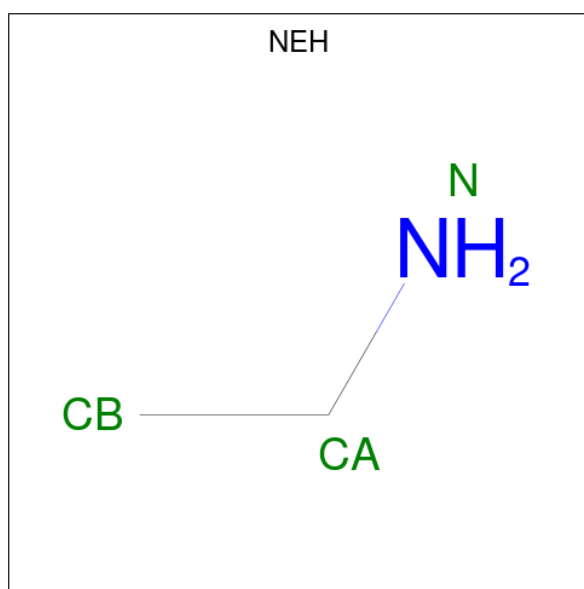
- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	75	608	382	108	117	1	0	1	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ETHANAMINE (CCD ID: NEH) (formula: C<sub>2</sub>H<sub>7</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	B	1	3	2	1	0	0

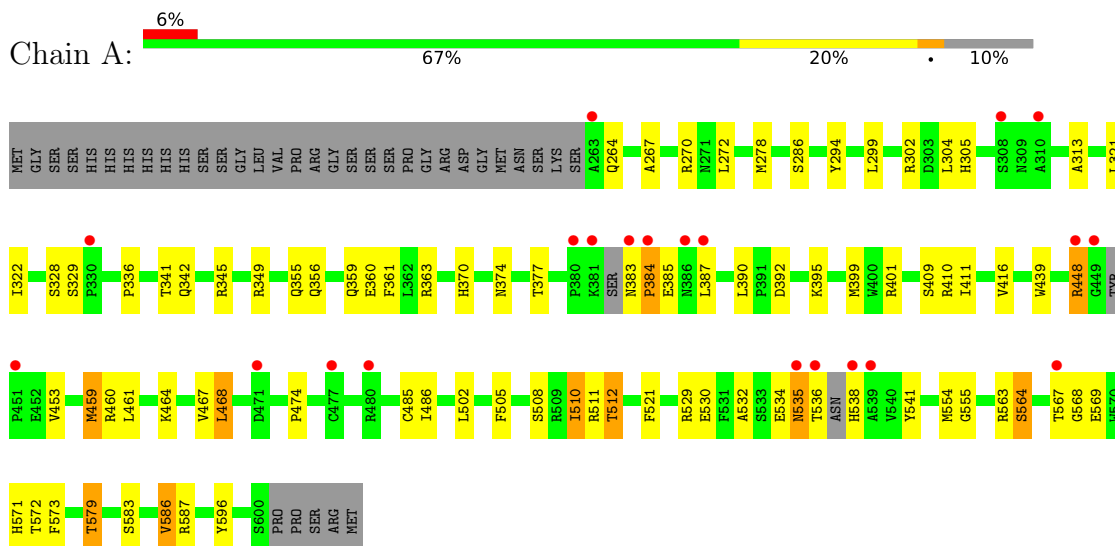
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	80	80	80	0	0
5	B	20	20	20	0	0

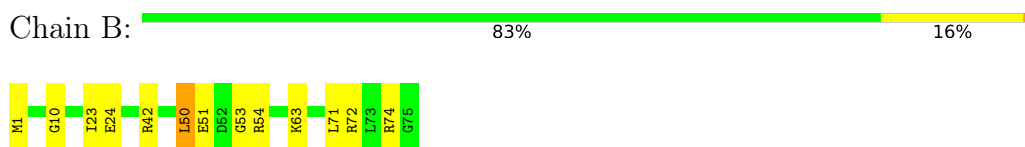
### 3 Residue-property plots [i](#)

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: Ubiquitin carboxyl-terminal hydrolase 2



- Molecule 2: Ubiquitin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.84Å 54.40Å 75.02Å 90.00° 107.66° 90.00°	Depositor
Resolution (Å)	28.01 – 2.20 28.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.01-2.20) 96.2 (28.01-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.259 0.193 , 0.264	Depositor DCC
$R_{free}$ test set	1002 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: NEH, 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	0.78	0/2768	0.92	3/3736 (0.1%)
2	B	0.77	0/614	0.95	0/825
All	All	0.77	0/3382	0.93	3/4561 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	SER	CA-C-N	6.12	127.50	119.84
1	A	329	SER	C-N-CA	6.12	127.50	119.84
1	A	535	ASN	N-CA-C	5.00	116.57	110.41

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	2710	0	2642	48	0
2	B	608	0	638	16	0
3	A	1	0	0	0	0
4	B	3	0	4	0	0
5	A	80	0	0	4	0
5	B	20	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3422	0	3284	61	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 9.

All (61) 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:521:PHE:O	1:A:587:ARG:HD3	1.74	0.88
1:A:579:THR:HG22	5:A:33:HOH:O	1.77	0.85
2:B:42:ARG:HD2	2:B:72:ARG:CG	2.16	0.75
2:B:42:ARG:HD2	2:B:72:ARG:HG3	1.69	0.73
1:A:572:THR:HB	1:A:579:THR:HG23	1.76	0.67
1:A:387:LEU:HD12	1:A:399:MET:CE	2.25	0.66
2:B:72:ARG:NH2	5:B:95:HOH:O	2.29	0.59
1:A:341:THR:O	1:A:345:ARG:HD3	2.03	0.58
1:A:294:TYR:CD1	1:A:410:ARG:HG2	2.39	0.58
1:A:554[A]:MET:HA	2:B:74[A]:ARG:HD2	1.86	0.57
1:A:387:LEU:HB3	1:A:390:LEU:HD12	1.89	0.55
2:B:42:ARG:HD3	2:B:71:LEU:O	2.07	0.55
1:A:360:GLU:OE1	2:B:72:ARG:HD3	2.06	0.55
1:A:510:ILE:HG22	1:A:511:ARG:HB2	1.89	0.55
2:B:10:GLY:CA	5:B:86:HOH:O	2.55	0.54
2:B:23:ILE:HG12	2:B:50:LEU:HB3	1.90	0.53
1:A:532:ALA:CB	1:A:535:ASN:HB2	2.39	0.53
1:A:541:TYR:HB3	1:A:596:TYR:HB3	1.89	0.53
1:A:363:ARG:NH1	5:A:75:HOH:O	2.40	0.52
1:A:270:ARG:HD2	1:A:272:LEU:HD23	1.92	0.52
1:A:305:HIS:HE1	1:A:374:ASN:O	1.92	0.51
1:A:286:SER:HA	1:A:322:ILE:HD12	1.92	0.51
1:A:349:ARG:HD2	5:A:40:HOH:O	2.10	0.51
1:A:416:VAL:HG22	1:A:439:TRP:CE2	2.45	0.51
1:A:563:ARG:HD2	1:A:568:GLY:HA2	1.92	0.51
1:A:567:THR:HG22	1:A:569:GLU:OE2	2.12	0.49
2:B:23:ILE:HD12	2:B:54:ARG:O	2.12	0.49
1:A:341:THR:O	1:A:345:ARG:CD	2.61	0.49
1:A:355:GLN:OE1	1:A:555:GLY:HA2	2.14	0.48
1:A:532:ALA:HB1	1:A:535:ASN:HB2	1.96	0.48
1:A:564:SER:HB3	1:A:567:THR:HB	1.96	0.47
1:A:321:LEU:HD11	1:A:336:PRO:HB3	1.96	0.47
2:B:1:MET:HE2	2:B:63:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASN:ND2	1:A:536:THR:H	2.13	0.46
1:A:583:SER:HA	1:A:586:VAL:HG13	1.96	0.46
1:A:278:MET:HG3	1:A:361:PHE:CZ	2.51	0.46
1:A:459:MET:HE2	1:A:459:MET:HB2	1.51	0.46
1:A:512:THR:HB	5:A:101:HOH:O	2.15	0.46
1:A:461:LEU:HD12	1:A:464:LYS:HD2	1.98	0.45
1:A:313:ALA:HB3	1:A:342:GLN:OE1	2.15	0.45
1:A:474:PRO:HG2	1:A:485:CYS:SG	2.56	0.45
1:A:267:ALA:HB2	1:A:328:SER:OG	2.17	0.45
1:A:467:VAL:HG22	1:A:486:ILE:HD12	1.99	0.45
1:A:460:ARG:HD3	1:A:530:GLU:OE2	2.16	0.45
1:A:359:GLN:OE1	2:B:42:ARG:NH2	2.42	0.45
1:A:535:ASN:CG	1:A:536:THR:H	2.25	0.44
1:A:468:LEU:HB3	1:A:474:PRO:HD3	2.00	0.44
2:B:24:GLU:OE2	2:B:53:GLY:N	2.51	0.44
1:A:383:ASN:HA	1:A:384:PRO:HD3	1.87	0.43
2:B:42:ARG:HD2	2:B:72:ARG:HG2	1.96	0.43
1:A:374:ASN:HA	1:A:409:SER:HB3	2.00	0.43
2:B:51:GLU:O	2:B:54:ARG:HG2	2.19	0.42
1:A:387:LEU:CD1	1:A:399:MET:CE	2.97	0.41
1:A:387:LEU:HD12	1:A:399:MET:HE3	2.00	0.41
2:B:10:GLY:N	5:B:86:HOH:O	2.53	0.41
1:A:571:HIS:HB2	1:A:573:PHE:CE2	2.56	0.41
2:B:1:MET:HE2	2:B:63:LYS:H	1.86	0.41
1:A:583:SER:HA	1:A:586:VAL:CG1	2.51	0.41
1:A:370:HIS:HA	1:A:411:ILE:HG13	2.02	0.40
1:A:392:ASP:HA	1:A:395:LYS:HG2	2.02	0.40
1:A:299:LEU:HD23	1:A:302:ARG:HE	1.86	0.40

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	328/374 (88%)	312 (95%)	13 (4%)	3 (1%)	14	14
2	B	74/75 (99%)	71 (96%)	3 (4%)	0	100	100
All	All	402/449 (90%)	383 (95%)	16 (4%)	3 (1%)	16	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	SER
1	A	448	ARG
1	A	384	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	302/335 (90%)	282 (93%)	20 (7%)	15	18
2	B	69/68 (102%)	68 (99%)	1 (1%)	59	75
All	All	371/403 (92%)	350 (94%)	21 (6%)	18	23

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	304	LEU
1	A	356	GLN
1	A	377	THR
1	A	385	GLU
1	A	401	ARG
1	A	448	ARG
1	A	453	VAL
1	A	459	MET
1	A	468	LEU
1	A	502	LEU
1	A	505	PHE
1	A	510	ILE

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Mol	Chain	Res	Type
1	A	512	THR
1	A	529	ARG
1	A	534	GLU
1	A	538	HIS
1	A	564	SER
1	A	579	THR
1	A	586	VAL
2	B	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	305	HIS
1	A	309	ASN
1	A	371	ASN
1	A	383	ASN
1	A	535	ASN
1	A	548	ASN
2	B	31	GLN
2	B	60	ASN

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NEH	B	76	1,2	2,2,2	0.41	0	0,1,1	-	-

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	335/374 (89%)	0.20	21 (6%) 26 23	19, 43, 74, 111	1 (0%)
2	B	75/75 (100%)	-0.07	0 100 100	17, 42, 56, 61	1 (1%)
All	All	410/449 (91%)	0.15	21 (5%) 33 30	17, 43, 68, 111	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	538	HIS	4.5
1	A	449	GLY	3.9
1	A	477	CYS	3.5
1	A	536	THR	3.4
1	A	448	ARG	3.3
1	A	263	ALA	2.8
1	A	451	PRO	2.8
1	A	383	ASN	2.6
1	A	387	LEU	2.5
1	A	386	ASN	2.5
1	A	310	ALA	2.4
1	A	535	ASN	2.3
1	A	308	SER	2.3
1	A	539	ALA	2.3
1	A	480	ARG	2.3
1	A	471	ASP	2.3
1	A	384	PRO	2.3
1	A	330	PRO	2.2
1	A	381	LYS	2.2
1	A	380	PRO	2.1
1	A	567	THR	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
4	NEH	B	76	3/3	0.94	0.09	35,35,36,37	0
3	ZN	A	1	1/1	1.00	0.03	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.