



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2025 – 10:03 PM EDT

PDB ID : 9OLB / pdb\_00009olb  
Title : Identification of ligands for E3 ligases using fragment-based methods  
Authors : Phan, J.; Fesik, S.W.  
Deposited on : 2025-05-12  
Resolution : 2.62 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

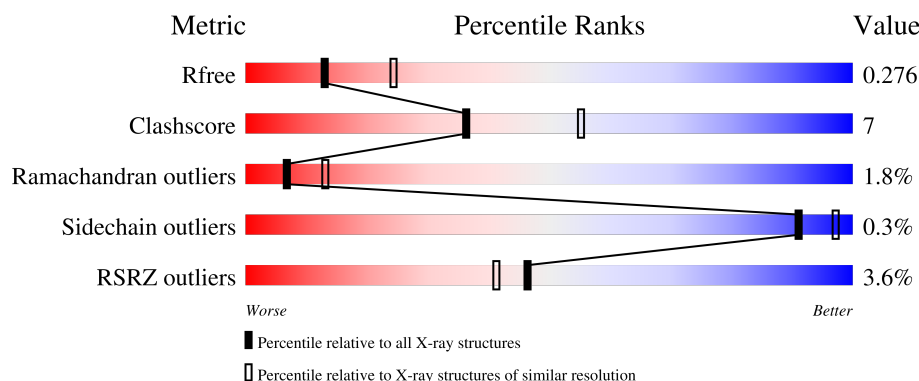
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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))
$R_{free}$	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	194	<div> <div>0%</div> <div>74%</div> <div>12%</div> <div>•</div> <div>13%</div> </div>
1	B	194	<div> <div>3%</div> <div>64%</div> <div>19%</div> <div>17%</div> </div>
1	C	194	<div> <div>3%</div> <div>71%</div> <div>12%</div> <div>•</div> <div>16%</div> </div>
2	D	10	<div> <div>40%</div> <div>50%</div> <div>40%</div> <div>10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3832 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 TNF receptor-associated factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1287	829	227	230	1			
1	B	161	Total	C	N	O	S	0	0	0
			1202	775	206	220	1			
1	C	162	Total	C	N	O	S	0	0	0
			1223	792	210	220	1			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	MET	-	initiating methionine	UNP Q9BUZ4
A	467	LEU	-	expression tag	UNP Q9BUZ4
A	468	GLU	-	expression tag	UNP Q9BUZ4
A	469	GLY	-	expression tag	UNP Q9BUZ4
A	470	LEU	-	expression tag	UNP Q9BUZ4
A	471	VAL	-	expression tag	UNP Q9BUZ4
A	472	PRO	-	expression tag	UNP Q9BUZ4
A	473	ARG	-	expression tag	UNP Q9BUZ4
A	474	GLY	-	expression tag	UNP Q9BUZ4
A	475	SER	-	expression tag	UNP Q9BUZ4
A	476	GLY	-	expression tag	UNP Q9BUZ4
A	477	SER	-	expression tag	UNP Q9BUZ4
A	478	SER	-	expression tag	UNP Q9BUZ4
A	479	HIS	-	expression tag	UNP Q9BUZ4
A	480	HIS	-	expression tag	UNP Q9BUZ4
A	481	HIS	-	expression tag	UNP Q9BUZ4
A	482	HIS	-	expression tag	UNP Q9BUZ4
A	483	HIS	-	expression tag	UNP Q9BUZ4
A	484	HIS	-	expression tag	UNP Q9BUZ4
B	291	MET	-	initiating methionine	UNP Q9BUZ4
B	467	LEU	-	expression tag	UNP Q9BUZ4
B	468	GLU	-	expression tag	UNP Q9BUZ4
B	469	GLY	-	expression tag	UNP Q9BUZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	LEU	-	expression tag	UNP Q9BUZ4
B	471	VAL	-	expression tag	UNP Q9BUZ4
B	472	PRO	-	expression tag	UNP Q9BUZ4
B	473	ARG	-	expression tag	UNP Q9BUZ4
B	474	GLY	-	expression tag	UNP Q9BUZ4
B	475	SER	-	expression tag	UNP Q9BUZ4
B	476	GLY	-	expression tag	UNP Q9BUZ4
B	477	SER	-	expression tag	UNP Q9BUZ4
B	478	SER	-	expression tag	UNP Q9BUZ4
B	479	HIS	-	expression tag	UNP Q9BUZ4
B	480	HIS	-	expression tag	UNP Q9BUZ4
B	481	HIS	-	expression tag	UNP Q9BUZ4
B	482	HIS	-	expression tag	UNP Q9BUZ4
B	483	HIS	-	expression tag	UNP Q9BUZ4
B	484	HIS	-	expression tag	UNP Q9BUZ4
C	291	MET	-	initiating methionine	UNP Q9BUZ4
C	467	LEU	-	expression tag	UNP Q9BUZ4
C	468	GLU	-	expression tag	UNP Q9BUZ4
C	469	GLY	-	expression tag	UNP Q9BUZ4
C	470	LEU	-	expression tag	UNP Q9BUZ4
C	471	VAL	-	expression tag	UNP Q9BUZ4
C	472	PRO	-	expression tag	UNP Q9BUZ4
C	473	ARG	-	expression tag	UNP Q9BUZ4
C	474	GLY	-	expression tag	UNP Q9BUZ4
C	475	SER	-	expression tag	UNP Q9BUZ4
C	476	GLY	-	expression tag	UNP Q9BUZ4
C	477	SER	-	expression tag	UNP Q9BUZ4
C	478	SER	-	expression tag	UNP Q9BUZ4
C	479	HIS	-	expression tag	UNP Q9BUZ4
C	480	HIS	-	expression tag	UNP Q9BUZ4
C	481	HIS	-	expression tag	UNP Q9BUZ4
C	482	HIS	-	expression tag	UNP Q9BUZ4
C	483	HIS	-	expression tag	UNP Q9BUZ4
C	484	HIS	-	expression tag	UNP Q9BUZ4

- Molecule 2 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	0	0	0
			64	38	11	15			

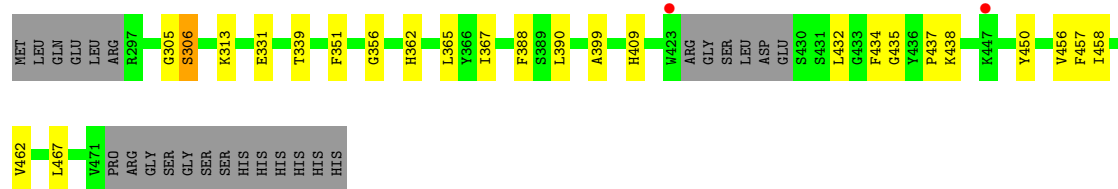
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	20	Total 20	O 20	0	0
3	C	18	Total 18	O 18	0	0

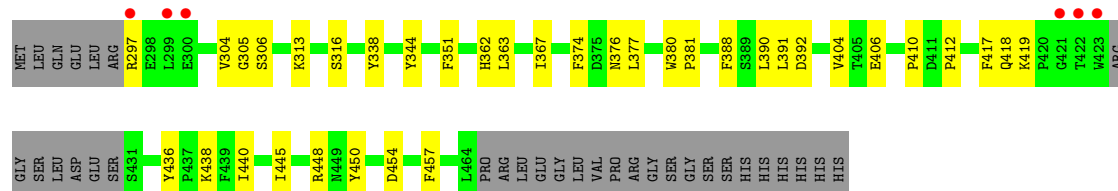
### 3 Residue-property plots [i](#)

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.

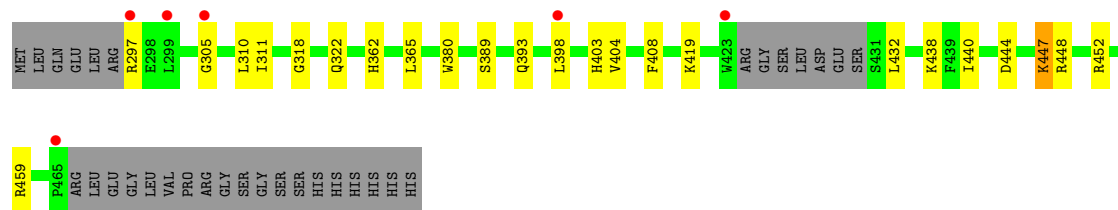
- Molecule 1: TNF receptor-associated factor 4



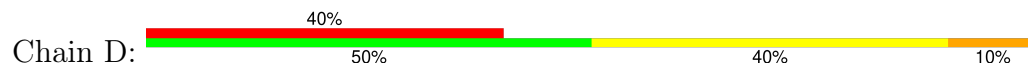
- Molecule 1: TNF receptor-associated factor 4

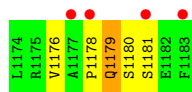


- Molecule 1: TNF receptor-associated factor 4



- Molecule 2: Epidermal growth factor receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.55Å 84.96Å 68.02Å 90.00° 113.64° 90.00°	Depositor
Resolution (Å)	29.25 – 2.62 29.25 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.25-2.62) 99.3 (29.25-2.62)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.202 , 0.276 0.204 , 0.276	Depositor DCC
$R_{free}$ test set	803 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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](#)

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	0.40	0/1325	0.61	0/1805
1	B	0.37	0/1239	0.56	0/1691
1	C	0.37	0/1261	0.58	0/1721
2	D	0.90	0/64	2.19	2/87 (2.3%)
All	All	0.39	0/3889	0.64	2/5304 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1179	GLN	N-CA-CB	-12.80	90.46	111.20
2	D	1179	GLN	N-CA-C	-9.94	94.14	109.85

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	1287	0	1186	18	0
1	B	1202	0	1063	21	0
1	C	1223	0	1105	12	0
2	D	64	0	50	7	0
3	A	18	0	0	0	0
3	B	20	0	0	1	0
3	C	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3832	0	3404	51	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 7.

All (51) 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:432:LEU:HD22	2:D:1179:GLN:HG2	1.74	0.69
1:B:297:ARG:N	3:B:501:HOH:O	2.26	0.69
1:C:297:ARG:N	3:C:501:HOH:O	2.29	0.65
1:A:356:GLY:H	2:D:1176:VAL:HG21	1.64	0.63
1:A:339:THR:HG22	1:A:462:VAL:HG21	1.82	0.62
1:A:331:GLU:HB3	1:A:351:PHE:CE2	2.37	0.59
1:B:390:LEU:HD21	1:B:450:TYR:HB3	1.83	0.58
1:A:437:PRO:HD3	2:D:1181:SER:HB3	1.84	0.58
1:B:406:GLU:HB3	1:B:436:TYR:CZ	2.39	0.57
1:C:404:VAL:HG21	1:C:440:ILE:HD12	1.87	0.57
1:C:311:ILE:HG12	1:C:459:ARG:HG3	1.87	0.56
1:C:362:HIS:CD2	1:C:438:LYS:HB3	2.42	0.55
1:B:392:ASP:OD1	1:B:448:ARG:NH1	2.39	0.55
1:B:374:PHE:HB3	1:B:377:LEU:HD12	1.88	0.54
1:C:444:ASP:O	1:C:447:LYS:HB2	2.07	0.54
1:A:434:PHE:CE2	2:D:1180:SER:HB3	2.42	0.54
1:A:435:GLY:O	2:D:1181:SER:HA	2.07	0.54
1:A:313:LYS:HE3	1:A:457:PHE:CZ	2.43	0.53
1:B:338:TYR:HA	1:B:344:TYR:O	2.09	0.53
1:A:365:LEU:HD21	1:A:458:ILE:HD12	1.91	0.52
1:A:390:LEU:HD11	1:A:456:VAL:HG13	1.91	0.52
1:B:306:SER:O	1:B:306:SER:OG	2.23	0.50
1:B:380:TRP:CG	1:B:419:LYS:HB3	2.45	0.50
1:A:367:ILE:HB	1:A:388:PHE:CZ	2.47	0.50
1:B:367:ILE:HB	1:B:388:PHE:HZ	1.75	0.50
1:A:467:LEU:HD21	1:C:408:PHE:HB2	1.92	0.49
1:A:390:LEU:HD21	1:A:450:TYR:HB3	1.94	0.49
1:B:313:LYS:HD2	1:B:457:PHE:CZ	2.46	0.49
2:D:1176:VAL:HG13	2:D:1178:PRO:HG3	1.93	0.49
1:A:362:HIS:CE1	1:A:438:LYS:HG2	2.48	0.48
1:B:380:TRP:HA	1:B:381:PRO:C	2.39	0.48
1:B:391:LEU:HD12	1:B:457:PHE:HB3	1.96	0.46
1:B:362:HIS:CE1	1:B:438:LYS:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:GLY:O	1:C:322:GLN:HG3	2.14	0.46
1:C:389:SER:HB2	1:C:459:ARG:HB3	1.99	0.45
1:B:410:PRO:HB3	1:B:417:PHE:CE2	2.51	0.45
1:A:367:ILE:HB	1:A:388:PHE:HZ	1.82	0.44
1:C:380:TRP:CG	1:C:419:LYS:HB2	2.52	0.44
1:B:376:ASN:OD1	1:B:419:LYS:NZ	2.50	0.44
1:B:412:PRO:O	1:B:418:GLN:NE2	2.50	0.44
1:C:365:LEU:HD23	1:C:365:LEU:HA	1.67	0.44
2:D:1176:VAL:CG1	2:D:1178:PRO:HG3	2.47	0.44
1:A:305:GLY:O	1:A:306:SER:HB3	2.19	0.43
1:A:409:HIS:NE2	1:C:403:HIS:O	2.49	0.42
1:B:351:PHE:O	1:B:363:LEU:HD12	2.19	0.42
1:B:404:VAL:HG21	1:B:440:ILE:HD12	2.02	0.41
1:B:367:ILE:HB	1:B:388:PHE:CZ	2.56	0.41
1:C:393:GLN:O	1:C:452:ARG:NH1	2.54	0.41
1:B:316:SER:HA	1:B:454:ASP:OD2	2.20	0.41
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.85	0.40
1:B:445:ILE:HA	1:B:445:ILE:HD12	1.73	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	165/194 (85%)	153 (93%)	10 (6%)	2 (1%)	11	22
1	B	157/194 (81%)	151 (96%)	4 (2%)	2 (1%)	10	20
1	C	158/194 (81%)	139 (88%)	14 (9%)	5 (3%)	3	5
2	D	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
All	All	488/592 (82%)	449 (92%)	30 (6%)	9 (2%)	7	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	VAL
1	C	432	LEU
1	A	306	SER
1	B	305	GLY
1	C	305	GLY
1	C	448	ARG
1	A	399	ALA
1	C	398	LEU
1	C	447	LYS

### 5.3.2 Protein sidechains ⓘ

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	124/166 (75%)	124 (100%)	0	100	100
1	B	111/166 (67%)	111 (100%)	0	100	100
1	C	115/166 (69%)	114 (99%)	1 (1%)	75	89
2	D	6/9 (67%)	6 (100%)	0	100	100
All	All	356/507 (70%)	355 (100%)	1 (0%)	91	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN

### 5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

## 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	169/194 (87%)	-0.18	2 (1%) 76 73	28, 40, 64, 72	0
1	B	161/194 (82%)	-0.10	6 (3%) 45 40	28, 39, 67, 93	0
1	C	162/194 (83%)	-0.16	6 (3%) 45 40	30, 39, 66, 84	0
2	D	10/10 (100%)	1.49	4 (40%) 1 1	50, 60, 65, 68	0
All	All	502/592 (84%)	-0.12	18 (3%) 46 41	28, 40, 66, 93	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	TRP	4.9
1	C	423	TRP	3.6
1	B	422	THR	3.6
1	B	421	GLY	3.0
1	C	299	LEU	3.0
2	D	1183	PHE	2.9
1	C	305	GLY	2.9
1	B	297	ARG	2.8
2	D	1177	ALA	2.7
2	D	1178	PRO	2.6
2	D	1181	SER	2.5
1	B	300	GLU	2.4
1	C	465	PRO	2.3
1	A	423	TRP	2.3
1	A	447	LYS	2.2
1	B	299	LEU	2.2
1	C	297	ARG	2.1
1	C	398	LEU	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.