Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:27 PM GMT

PDB ID	:	4OZR
Title	:	Crystal structure of the ligand binding domains of the Bovicola ovis ecdysone receptor EcR/USP heterodimer (methylene lactam crystal)
Authors	:	Ren, B.; Peat, T.S.; Streltsov, V.A.; Pollard, M.; Fernley, R.; Grusovin, J.; Seabrook, S.; Pilling, P.; Phan, T.; Lu, L.; Lovrecz, G.O.; Graham, L.D.; Hill, R.J.
Deposited on	:	2014-02-18
Resolution	:	2.70 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:

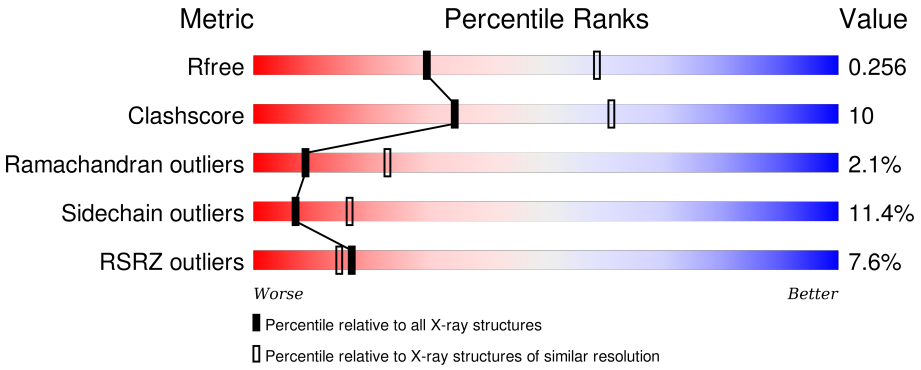
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	E	197	11% 63% 30% 6%
2	U	196	5% 77% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3214 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 Ecdysone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	197	Total	C	N	O	S	0	2	0
			1572	1011	261	291	9			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP E0VVT4
E	?	-	LYS	deletion	UNP E0VVT4
E	?	-	ARG	deletion	UNP E0VVT4
E	?	-	ILE	deletion	UNP E0VVT4
E	?	-	SER	deletion	UNP E0VVT4
E	?	-	ASN	deletion	UNP E0VVT4
E	?	-	ALA	deletion	UNP E0VVT4
E	?	-	PRO	deletion	UNP E0VVT4
E	?	-	SER	deletion	UNP E0VVT4
E	?	-	GLU	deletion	UNP E0VVT4
E	?	-	GLY	deletion	UNP E0VVT4
E	?	-	GLU	deletion	UNP E0VVT4
E	?	-	ASP	deletion	UNP E0VVT4
E	?	-	GLN	deletion	UNP E0VVT4
E	?	-	SER	deletion	UNP E0VVT4
E	?	-	ASP	deletion	UNP E0VVT4
E	?	-	LEU	deletion	UNP E0VVT4
E	?	-	ASN	deletion	UNP E0VVT4
E	?	-	PHE	deletion	UNP E0VVT4
E	?	-	ALA	deletion	UNP E0VVT4
E	?	-	ASN	deletion	UNP E0VVT4
E	?	-	ASN	deletion	UNP E0VVT4
E	?	-	GLN	deletion	UNP E0VVT4
E	?	-	PRO	deletion	UNP E0VVT4
E	?	-	TYR	deletion	UNP E0VVT4
E	?	-	THR	deletion	UNP E0VVT4
E	?	-	ARG	deletion	UNP E0VVT4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASP	deletion	UNP E0VVT4
E	?	-	SER	deletion	UNP E0VVT4
E	?	-	TYR	deletion	UNP E0VVT4
E	?	-	SER	deletion	UNP E0VVT4
E	?	-	LEU	deletion	UNP E0VVT4
E	?	-	ALA	deletion	UNP E0VVT4
E	?	-	GLY	deletion	UNP E0VVT4
E	?	-	MET	deletion	UNP E0VVT4
E	?	-	GLY	deletion	UNP E0VVT4
E	407	ALA	GLU	conflict	UNP E0VVT4

- Molecule 2 is a protein called Retinoid X receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	196	Total	C	N	O	S	0	2	0
			1551	992	279	274	6			

- Molecule 3 is water.

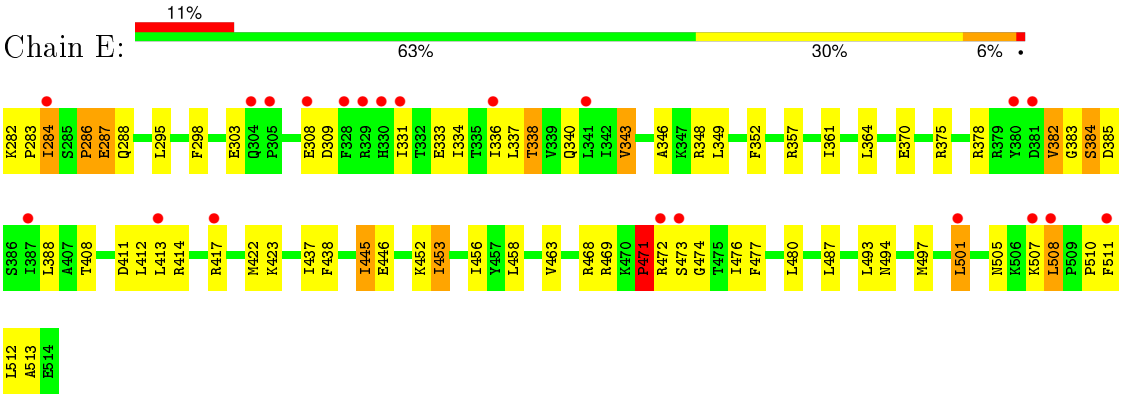
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	28	Total	O	0	0
			28	28		
3	U	63	Total	O	0	0
			63	63		

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.

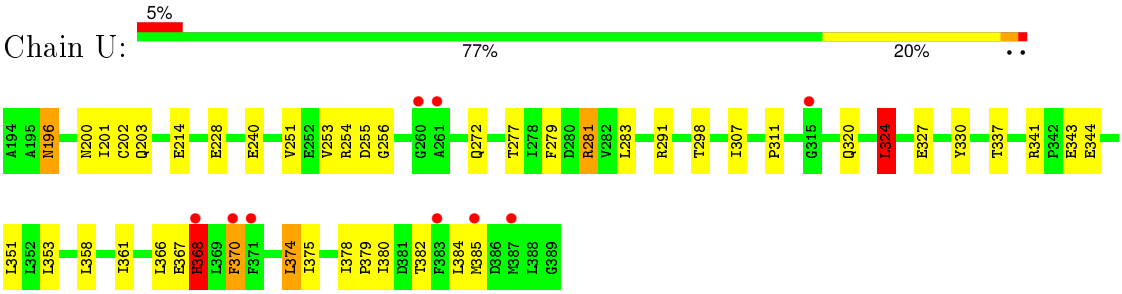
- Molecule 1: Ecdysone receptor

Chain E:



- Molecule 2: Retinoid X receptor

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	153.67Å 42.43Å 86.67Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	68.03 – 2.70 69.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (68.03-2.70) 88.0 (69.37-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.224 , 0.259 0.219 , 0.256	Depositor DCC
R_{free} test set	623 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 72.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 13309 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3214	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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

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	E	0.27	0/1601	0.55	0/2161
2	U	0.24	0/1586	0.56	2/2147 (0.1%)
All	All	0.26	0/3187	0.55	2/4308 (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	E	0	1
2	U	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	367	GLU	N-CA-C	-6.16	94.38	111.00
2	U	324	LEU	CA-CB-CG	5.85	128.75	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	471	PRO	Peptide
2	U	384	LEU	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	E	1572	0	1597	40	0
2	U	1551	0	1582	24	0
3	E	28	0	0	4	1
3	U	63	0	0	8	3
All	All	3214	0	3179	63	3

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 10.

All (63) 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)
2:U:256:GLY:O	3:U:437:HOH:O	1.85	0.93
1:E:422:MET:O	1:E:469:ARG:NH2	2.13	0.79
1:E:468:ARG:NH1	3:E:601:HOH:O	2.19	0.76
2:U:214:GLU:OE2	3:U:401:HOH:O	2.03	0.75
2:U:337:THR:O	3:U:439:HOH:O	2.09	0.71
1:E:303:GLU:O	1:E:375:ARG:NH1	2.21	0.67
2:U:375:ILE:O	2:U:379:PRO:HD2	1.94	0.67
2:U:343:GLU:OE1	3:U:402:HOH:O	2.14	0.66
2:U:196:ASN:ND2	3:U:434:HOH:O	2.29	0.66
1:E:282:LYS:HG3	1:E:283:PRO:HD3	1.81	0.62
2:U:240:GLU:OE2	3:U:426:HOH:O	2.16	0.61
1:E:445:ILE:HG12	1:E:446:GLU:HG3	1.81	0.61
1:E:414:ARG:HA	1:E:417:ARG:HE	1.65	0.60
1:E:333:GLU:O	1:E:336:ILE:HG13	2.02	0.60
2:U:254:ARG:NE	3:U:403:HOH:O	2.17	0.59
1:E:473:SER:N	1:E:474:GLY:HA2	2.19	0.58
1:E:458:LEU:HD11	2:U:353:LEU:HD11	1.86	0.58
1:E:411:ASP:OD1	1:E:414:ARG:NH1	2.39	0.55
1:E:438:PHE:CE1	1:E:453:ILE:HD11	2.41	0.55
1:E:348:ARG:NE	3:E:602:HOH:O	2.38	0.55
1:E:337:LEU:O	1:E:340:GLN:HG2	2.07	0.55
1:E:303:GLU:OE1	1:E:378:ARG:NH1	2.32	0.53
1:E:512:LEU:HD23	1:E:512:LEU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:ARG:HG3	3:E:625:HOH:O	2.08	0.52
1:E:286:PRO:HD2	1:E:288:GLN:OE1	2.10	0.51
1:E:357:ARG:O	1:E:361:ILE:HG12	2.11	0.50
2:U:272[A]:GLN:NE2	3:U:404:HOH:O	2.18	0.50
1:E:370:GLU:HB3	1:E:487:LEU:HD13	1.95	0.48
1:E:508:LEU:HD21	1:E:513:ALA:HB2	1.95	0.48
2:U:368[A]:HIS:ND1	2:U:370:PHE:HB3	2.28	0.48
1:E:288:GLN:OE1	1:E:463:VAL:HG21	2.13	0.48
2:U:251:VAL:O	2:U:291:ARG:NH1	2.47	0.48
2:U:251:VAL:HG13	2:U:291:ARG:HB2	1.96	0.48
1:E:477:PHE:HB3	3:E:611:HOH:O	2.14	0.47
2:U:255:ASP:HA	2:U:283:LEU:HD21	1.97	0.47
2:U:378:ILE:O	2:U:382:THR:HG22	2.15	0.47
1:E:383:GLY:HA2	1:E:384:SER:HA	1.67	0.46
2:U:202:CYS:SG	2:U:203:GLN:N	2.88	0.46
1:E:308:GLU:N	1:E:308:GLU:OE1	2.49	0.45
1:E:469:ARG:O	1:E:471:PRO:HD3	2.17	0.45
2:U:200:ASN:OD1	2:U:201:ILE:N	2.50	0.45
1:E:352:PHE:HD1	1:E:438:PHE:CE1	2.36	0.44
1:E:343:VAL:HB	1:E:364:LEU:HD13	1.98	0.44
2:U:320:GLN:O	2:U:324:LEU:HD13	2.17	0.44
2:U:341:ARG:NH1	2:U:344:GLU:OE2	2.51	0.44
2:U:254:ARG:HA	2:U:254:ARG:HD3	1.80	0.43
1:E:340:GLN:HA	1:E:343:VAL:HG13	1.99	0.43
1:E:472:ARG:HA	1:E:473:SER:HA	1.81	0.43
2:U:327:GLU:O	2:U:330:TYR:HB2	2.19	0.43
2:U:307:ILE:HD11	2:U:358:LEU:HD13	2.01	0.43
1:E:286:PRO:HB2	1:E:287[B]:GLU:OE1	2.19	0.42
1:E:382:VAL:HA	1:E:383:GLY:HA3	1.76	0.42
1:E:298:PHE:CD1	1:E:348:ARG:HG3	2.55	0.42
1:E:284:ILE:HA	1:E:284:ILE:HD12	1.89	0.42
1:E:331:ILE:O	1:E:331:ILE:HG22	2.20	0.41
1:E:507:LYS:O	1:E:508:LEU:HD13	2.20	0.41
1:E:501:LEU:HA	1:E:501:LEU:HD22	1.91	0.41
1:E:423:LYS:HD3	1:E:423:LYS:HA	1.90	0.41
1:E:346:ALA:HB2	1:E:437:ILE:HD13	2.03	0.41
2:U:281:ARG:HG2	2:U:361:ILE:HG12	2.03	0.41
1:E:334:ILE:O	1:E:338:THR:HG23	2.21	0.41
2:U:256:GLY:HA2	2:U:279:PHE:HZ	1.85	0.40
1:E:452:LYS:HD3	1:E:452:LYS:HA	1.91	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:412:HOH:O	3:U:412:HOH:O[2_556]	1.47	0.73
3:E:626:HOH:O	3:U:425:HOH:O[2_556]	2.14	0.06
3:U:418:HOH:O	3:U:419:HOH:O[4_556]	2.16	0.04

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	E	193/197 (98%)	178 (92%)	9 (5%)	6 (3%)	5 12
2	U	196/196 (100%)	183 (93%)	9 (5%)	4 (2%)	9 24
All	All	389/393 (99%)	361 (93%)	18 (5%)	10 (3%)	9 16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	368[A]	HIS
2	U	368[B]	HIS
1	E	511	PHE
2	U	374	LEU
1	E	286	PRO
1	E	471	PRO
2	U	366	LEU
1	E	287[A]	GLU
1	E	287[B]	GLU
1	E	510	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	E	172/180 (96%)	148 (86%)	24 (14%)	4 10
2	U	164/166 (99%)	149 (91%)	15 (9%)	12 26
All	All	336/346 (97%)	297 (88%)	39 (12%)	7 16

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	284	ILE
1	E	295	LEU
1	E	309	ASP
1	E	338	THR
1	E	343	VAL
1	E	349	LEU
1	E	382	VAL
1	E	384	SER
1	E	385	ASP
1	E	388	LEU
1	E	408	THR
1	E	412	LEU
1	E	413	LEU
1	E	445	ILE
1	E	453	ILE
1	E	456	ILE
1	E	476	ILE
1	E	480	LEU
1	E	493	LEU
1	E	494	ASN
1	E	497	MET
1	E	501	LEU
1	E	505	ASN
1	E	508	LEU
2	U	196	ASN
2	U	228	GLU
2	U	253	VAL
2	U	277	THR
2	U	281	ARG
2	U	298	THR
2	U	311	PRO
2	U	324	LEU
2	U	351	LEU

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Mol	Chain	Res	Type
2	U	368[A]	HIS
2	U	368[B]	HIS
2	U	370	PHE
2	U	374	LEU
2	U	380	ILE
2	U	385	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	309:ASP	C	328:PHE	N	17.51
1	E	388:LEU	C	407:ALA	N	14.10

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	E	197/197 (100%)	0.53	21 (10%) 8 6	27, 55, 118, 142	0
2	U	196/196 (100%)	0.22	9 (4%) 36 35	21, 44, 96, 129	0
All	All	393/393 (100%)	0.38	30 (7%) 17 15	21, 48, 110, 142	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	380	TYR	3.8
1	E	330	HIS	3.6
2	U	387	MET	3.5
2	U	260	GLY	3.5
1	E	413	LEU	3.5
1	E	381	ASP	3.3
1	E	329	ARG	3.0
1	E	501	LEU	3.0
2	U	371	PHE	3.0
2	U	368[A]	HIS	2.8
2	U	383	PHE	2.8
1	E	417	ARG	2.8
1	E	308	GLU	2.8
2	U	261	ALA	2.7
1	E	511	PHE	2.6
1	E	387	ILE	2.6
1	E	472	ARG	2.6
1	E	341	LEU	2.5
1	E	336	ILE	2.4
1	E	305	PRO	2.4
1	E	508	LEU	2.3
1	E	331	ILE	2.3
1	E	507	LYS	2.3
1	E	304	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	U	370	PHE	2.2
1	E	328	PHE	2.2
2	U	385	MET	2.2
2	U	315	GLY	2.1
1	E	284	ILE	2.0
1	E	473	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.