

Full wwPDB X-ray Structure Validation Report (i)

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:	4U1C
:	Crystal structure of the eIF3a/eIF3c PCI-domain heterodimer
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:	2014-07-15
:	3.50 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 https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 >=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 <=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	С	567	% 67%	27%	•••		
2	А	274	77%	22%	•		



4U1C

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6658 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 Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	С	544	Total 4442	C 2845	N 736	O 849	S 12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	246	MET	-	initiating methionine	UNP P32497

• Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	А	271	Total 2216	C 1429	N 356	0 427	$\frac{S}{4}$	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	222	SER	-	expression tag	UNP P38249
А	223	ASN	-	expression tag	UNP P38249
A	224	ALA	-	expression tag	UNP P38249



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 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: Eukaryotic translation initiation factor 3 subunit C





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	155.55\AA 155.55\AA 91.22\AA	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	44.90 - 3.50	Depositor
Resolution (A)	44.90 - 3.50	EDS
% Data completeness	$100.0 \ (44.90-3.50)$	Depositor
(in resolution range)	$100.0 \ (44.90-3.50)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.47 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1539)	Depositor
D D .	0.260 , 0.293	Depositor
Π, Π_{free}	0.270 , 0.296	DCC
R_{free} test set	1628 reflections $(9.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	179.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.28 , 122.8	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6658	wwPDB-VP
Average B, all atoms $(Å^2)$	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	0.33	0/4525	0.53	0/6120	
2	А	0.31	0/2264	0.50	0/3072	
All	All	0.32	0/6789	0.52	0/9192	

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	С	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	644	ARG	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	С	4442	0	4474	112	0
2	А	2216	0	2218	40	0
All	All	6658	0	6692	144	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 11.

All (144)) close	$\operatorname{contacts}$	within	the	same	$\operatorname{asymmetric}$	unit	are	listed	below,	sorted	$\mathbf{b}\mathbf{y}$	$ ext{their}$	clash
magnitu	de.													

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	At0111-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:C:487:SER:HB2	1:C:506:ASN:HD21	1.26	0.98	
1:C:487:SER:HB2	1:C:506:ASN:ND2	2.03	0.73	
1:C:744:LEU:HD13	2:A:463:TRP:CG	2.24	0.72	
1:C:257:ARG:HH21	1:C:282:LEU:HD21	1.58	0.68	
1:C:582:GLN:HE22	1:C:612:ILE:H	1.42	0.67	
1:C:659:TYR:CG	1:C:676:LEU:HD21	2.31	0.66	
2:A:329:PHE:HE2	2:A:388:TYR:HB2	1.60	0.66	
1:C:443:LYS:NZ	1:C:451:MET:SD	2.64	0.66	
1:C:501:ARG:HG3	1:C:505:TYR:HE2	1.61	0.65	
1:C:681:SER:OG	1:C:686:ASN:O	2.15	0.64	
1:C:735:SER:HB2	2:A:484:HIS:H	1.62	0.64	
1:C:582:GLN:HB3	1:C:611:HIS:CE1	2.33	0.64	
1:C:595:ASN:HA	1:C:598:ALA:HB3	1.80	0.64	
1:C:637:TYR:OH	1:C:653:ARG:NH2	2.31	0.63	
1:C:380:PHE:O	1:C:383:SER:OG	2.15	0.63	
1:C:413:LEU:HD12	1:C:459:ILE:HD13	1.81	0.63	
2:A:386:GLU:HB3	2:A:407:LEU:HD21	1.81	0.62	
2:A:316:ALA:HB1	2:A:321:PHE:HE1	1.67	0.60	
1:C:523:LEU:HD11	1:C:550:LEU:HD22	1.84	0.58	
1:C:558:CYS:SG	1:C:712:SER:OG	2.59	0.58	
1:C:501:ARG:HG3	1:C:505:TYR:CE2	2.38	0.58	
2:A:390:ILE:HD12	2:A:403:GLN:HB3	1.85	0.58	
2:A:401:LYS:NZ	2:A:450:LYS:O	2.36	0.56	
1:C:684:LYS:HB3	2:A:467:LYS:NZ	2.22	0.55	
2:A:303:TRP:HE1	2:A:327:THR:HB	1.71	0.55	
1:C:304:PHE:HB3	1:C:375:ARG:HE	1.71	0.55	
2:A:329:PHE:CE2	2:A:388:TYR:HB2	2.42	0.55	
1:C:257:ARG:HE	1:C:282:LEU:HD11	1.72	0.54	
2:A:355:LEU:O	2:A:356:ASN:HB2	2.06	0.54	
1:C:335:THR:HG21	1:C:339:TYR:HB3	1.88	0.54	
1:C:351:ILE:O	1:C:355:PRO:HD2	2.08	0.54	
1:C:322:PHE:CE1	1:C:407:LEU:HG	2.42	0.54	
2:A:330:LEU:HD21	2:A:384:LEU:HD22	1.89	0.53	
1:C:346:ASP:N	1:C:347:PRO:HD2	2.24	0.52	
1:C:626:LEU:HD11	1:C:679:ALA:HB2	1.90	0.52	
2:A:443:VAL:HG11	2:A:448:LEU:HG	1.91	0.52	
1:C:668:PRO:HD3	1:C:677:PHE:CZ	2.44	0.52	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:305:LYS:NZ	2:A:355:LEU:O	2.42	0.52
1:C:531:ASN:O	1:C:535:PHE:HD1	1.92	0.51
1:C:304:PHE:CD1	1:C:375:ARG:HG2	2.45	0.51
1:C:343:GLU:OE2	1:C:420:LYS:HE3	2.11	0.51
1:C:546:VAL:O	1:C:550:LEU:HD23	2.11	0.51
1:C:640:ILE:HG13	1:C:730:LYS:HE3	1.94	0.50
1:C:653:ARG:HA	1:C:656:LEU:HD12	1.94	0.50
1:C:369:ILE:HA	1:C:372:PHE:HD2	1.77	0.50
1:C:304:PHE:CG	1:C:375:ARG:HG2	2.47	0.50
2:A:387:LEU:HD11	2:A:411:LEU:HD22	1.94	0.50
1:C:784:ILE:HA	1:C:787:LEU:HD12	1.93	0.49
2:A:389:ASP:O	2:A:393:VAL:HB	2.12	0.49
2:A:362:THR:O	2:A:365:GLU:N	2.46	0.49
1:C:671:LEU:HD12	1:C:672:ARG:N	2.28	0.49
1:C:642:VAL:HG21	1:C:763:LEU:HA	1.94	0.49
2:A:461:SER:O	2:A:465:ILE:HG13	2.13	0.48
1:C:577:ARG:HG2	1:C:582:GLN:O	2.13	0.48
1:C:737:SER:HB3	2:A:484:HIS:CD2	2.48	0.48
1:C:296:TYR:O	1:C:300:ILE:HG12	2.13	0.48
1:C:652:ILE:O	1:C:656:LEU:HG	2.14	0.48
1:C:452:GLU:OE1	1:C:478:TYR:OH	2.31	0.48
2:A:237:LEU:HA	2:A:266:LEU:HD13	1.96	0.48
1:C:370:PHE:CZ	1:C:431:ARG:HB3	2.48	0.48
1:C:377:ASP:O	1:C:380:PHE:HB3	2.13	0.48
1:C:555:PHE:HB2	1:C:563:CYS:SG	2.53	0.48
2:A:441:THR:HB	2:A:491:PHE:O	2.14	0.48
1:C:537:SER:O	1:C:541:ILE:HG12	2.14	0.48
1:C:516:PHE:CE1	1:C:554:ALA:HB2	2.49	0.48
2:A:337:LEU:HD21	2:A:427:VAL:HG13	1.95	0.48
1:C:349:ASP:O	1:C:352:GLU:N	2.39	0.47
1:C:656:LEU:HD23	1:C:676:LEU:HD12	1.96	0.47
1:C:349:ASP:N	1:C:349:ASP:OD1	2.47	0.47
1:C:395:LEU:O	1:C:399:ARG:HG2	2.14	0.47
1:C:416:GLU:HG2	1:C:464:LYS:HB2	1.97	0.47
1:C:684:LYS:HB3	2:A:467:LYS:HZ2	1.80	0.47
1:C:332:LEU:HB3	1:C:414:TYR:CE1	2.49	0.47
1:C:405:TYR:OH	1:C:440:ILE:HD11	2.15	0.47
1:C:744:LEU:HD13	2:A:463:TRP:CD1	2.49	0.47
1:C:536:ASP:OD1	1:C:537:SER:N	2.48	0.47
1:C:705:ASN:N	1:C:705:ASN:OD1	2.38	0.47
2:A:370:ILE:HG23	2:A:376:ILE:HG21	1.96	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:396:ILE:O	1:C:399:ARG:HB2	2.15	0.47
2:A:425:ARG:HB2	2:A:458:LEU:HD22	1.96	0.46
1:C:574:SER:HB3	1:C:650:LYS:NZ	2.29	0.46
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.62	0.46
2:A:352:TYR:CZ	2:A:360:LYS:HG2	2.51	0.46
1:C:500:LYS:HG2	1:C:528:VAL:HG11	1.97	0.46
1:C:528:VAL:O	1:C:529:GLN:NE2	2.48	0.46
1:C:767:ALA:HA	1:C:777:VAL:O	2.16	0.46
2:A:386:GLU:O	2:A:390:ILE:HG12	2.16	0.46
1:C:593:SER:HA	1:C:594:ASN:C	2.36	0.46
1:C:737:SER:OG	1:C:740:LYS:HD3	2.16	0.45
1:C:397:ARG:HA	1:C:397:ARG:HD2	1.55	0.45
1:C:632:ARG:HB3	1:C:644:ARG:HD3	1.96	0.45
1:C:283:LEU:HD11	1:C:299:LEU:HD22	1.98	0.45
1:C:487:SER:OG	1:C:488:THR:N	2.49	0.45
1:C:735:SER:HA	1:C:776:PHE:O	2.16	0.45
1:C:553:SER:HA	1:C:556:LYS:HD2	1.97	0.45
2:A:408:LEU:HD23	2:A:411:LEU:HD23	1.99	0.45
1:C:447:LEU:O	1:C:451:MET:HG3	2.17	0.45
2:A:270:SER:OG	2:A:272:ARG:O	2.35	0.44
1:C:301:PRO:HD3	1:C:372:PHE:CE1	2.52	0.44
1:C:300:ILE:HG22	1:C:304:PHE:CE2	2.52	0.44
1:C:744:LEU:HD13	2:A:463:TRP:CD2	2.52	0.44
1:C:384:LEU:HD21	1:C:397:ARG:HB3	1.99	0.44
1:C:426:GLU:O	1:C:430:THR:HG23	2.17	0.44
1:C:512:LEU:HA	1:C:512:LEU:HD23	1.73	0.44
2:A:449:TYR:O	2:A:453:THR:OG1	2.28	0.44
1:C:280:GLU:HA	1:C:283:LEU:HG	1.99	0.43
1:C:254:PHE:HE2	1:C:286:ALA:HB2	1.83	0.43
2:A:478:VAL:HG12	2:A:480:ILE:HG12	1.99	0.43
1:C:440:ILE:HG23	1:C:448:ILE:HG12	2.01	0.43
1:C:303:ARG:NH1	1:C:324:ASP:OD2	2.52	0.43
1:C:550:LEU:HD12	1:C:566:ILE:HD13	1.99	0.42
1:C:667:PRO:HG3	2:A:292:VAL:HB	2.01	0.42
1:C:254:PHE:CE2	1:C:286:ALA:HB2	2.54	0.42
1:C:734:SER:O	1:C:777:VAL:HA	2.19	0.42
1:C:497:ALA:O	1:C:501:ARG:HB2	2.19	0.42
1:C:441:TYR:CG	1:C:505:TYR:HD1	2.37	0.42
2:A:329:PHE:O	2:A:333:ILE:HG13	2.19	0.42
1:C:377:ASP:HA	1:C:404:ILE:HD13	2.01	0.42
1:C:627:LEU:HD21	1:C:717:VAL:HG22	2.01	0.42



		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:C:254:PHE:CZ	1:C:291:GLU:HB3	2.55	0.42
1:C:383:SER:O	1:C:387:ILE:HG13	2.20	0.41
1:C:659:TYR:CD2	1:C:676:LEU:HD21	2.55	0.41
1:C:413:LEU:HD12	1:C:459:ILE:HG21	2.00	0.41
1:C:585:LEU:O	1:C:588:ILE:HG13	2.20	0.41
2:A:316:ALA:HB1	2:A:321:PHE:CE1	2.53	0.41
2:A:391:ILE:O	2:A:395:PHE:HB3	2.20	0.41
1:C:431:ARG:HD3	1:C:431:ARG:HA	1.94	0.41
1:C:572:SER:O	1:C:650:LYS:HD2	2.19	0.41
2:A:384:LEU:HD11	2:A:416:TYR:CE1	2.55	0.41
1:C:463:PHE:CZ	1:C:468:THR:HA	2.56	0.41
1:C:571:LEU:HD21	1:C:617:ILE:HG22	2.02	0.41
1:C:456:TRP:CZ2	1:C:469:SER:HB3	2.55	0.41
1:C:626:LEU:HD12	1:C:626:LEU:HA	1.77	0.41
2:A:376:ILE:O	2:A:380:VAL:HG23	2.20	0.41
1:C:350:PHE:HA	1:C:351:ILE:HA	1.66	0.41
1:C:387:ILE:HG22	1:C:388:ASP:N	2.35	0.41
1:C:337:ASP:HA	1:C:339:TYR:CE1	2.56	0.41
1:C:543:PHE:O	1:C:547:VAL:HG23	2.21	0.41
1:C:300:ILE:HD13	1:C:324:ASP:HB3	2.03	0.41
1:C:376:LEU:HA	1:C:376:LEU:HD23	1.92	0.40
2:A:257:TYR:HA	2:A:260:ILE:HD12	2.04	0.40
1:C:584:SER:OG	1:C:587:ARG:HD2	2.21	0.40
1:C:406:ASN:OD1	1:C:455:ALA:HA	2.21	0.40
1:C:747:LEU:HA	1:C:747:LEU:HD23	1.92	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	Perce	ntiles
1	С	542/567~(96%)	507 (94%)	35~(6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	А	$\fbox{269/274}\ (98\%)$	258~(96%)	11 (4%)	0	100 100
All	All	811/841 (96%)	765~(94%)	46 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	Perce	\mathbf{ntiles}
1	С	506/527~(96%)	487~(96%)	19 (4%)	33	65
2	А	250/252~(99%)	246~(98%)	4 (2%)	62	83
All	All	756/779~(97%)	733~(97%)	23 (3%)	41	71

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	300	ILE
1	С	309	ASN
1	С	326	SER
1	С	348	ILE
1	С	407	LEU
1	С	441	TYR
1	С	473	LEU
1	С	483	ILE
1	С	529	GLN
1	С	550	LEU
1	С	571	LEU
1	С	582	GLN
1	С	589	SER
1	С	648	SER
1	С	652	ILE
1	С	738	VAL
1	С	771	ASP
1	С	778	VAL



Continued from previous page...

Mol	Chain	Res	Type
1	С	782	ASP
2	А	229	ASP
2	А	250	LEU
2	А	399	THR
2	А	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	495	ASN
1	С	529	GLN
1	С	564	HIS
1	С	582	GLN
1	С	611	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)

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 (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^{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	$ $ $<$ $\mathbf{RSRZ}>$	# RSRZ > 2		>2	$OWAB(Å^2)$	Q<0.9
1	С	544/567~(95%)	-0.26	4 (0%)	87	83	94, 165, 214, 231	0
2	А	271/274 (98%)	-0.32	1 (0%)	92	90	141, 181, 202, 216	0
All	All	815/841~(96%)	-0.28	5(0%)	89	86	94, 169, 209, 231	0

All (5) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	781	GLY	2.9
1	С	726	PHE	2.4
1	С	594	ASN	2.2
2	А	495	PRO	2.1
1	С	593	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.

