



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:01 PM GMT

PDB ID : 2DX1
Title : Crystal structure of RhoGEF protein Asef
Authors : Murayama, K.; Kato-Murayama, M.; Terada, T.; Shirouzu, M.; Yokoyama, S.;
RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-08-22
Resolution : 2.36 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

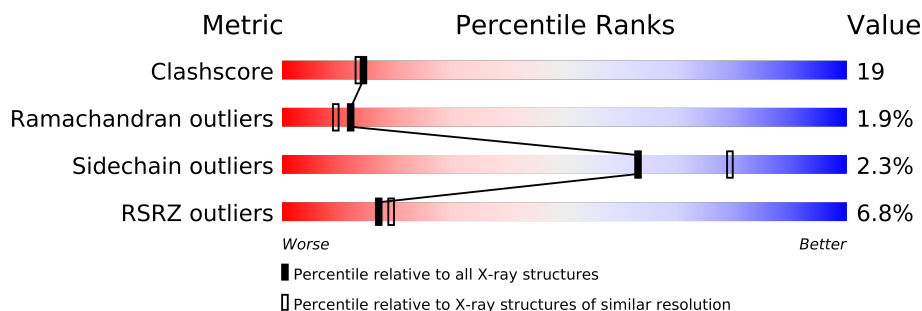
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.36 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))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	482	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3266 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Rho guanine nucleotide exchange factor 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	Se	0	0	0
			3202	2024	575	584	11	8			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLY	-	EXPRESSION TAG	UNP Q9NR80
A	60	SER	-	EXPRESSION TAG	UNP Q9NR80
A	61	SER	-	EXPRESSION TAG	UNP Q9NR80
A	62	GLY	-	EXPRESSION TAG	UNP Q9NR80
A	63	SER	-	EXPRESSION TAG	UNP Q9NR80
A	64	SER	-	EXPRESSION TAG	UNP Q9NR80
A	65	GLY	-	EXPRESSION TAG	UNP Q9NR80

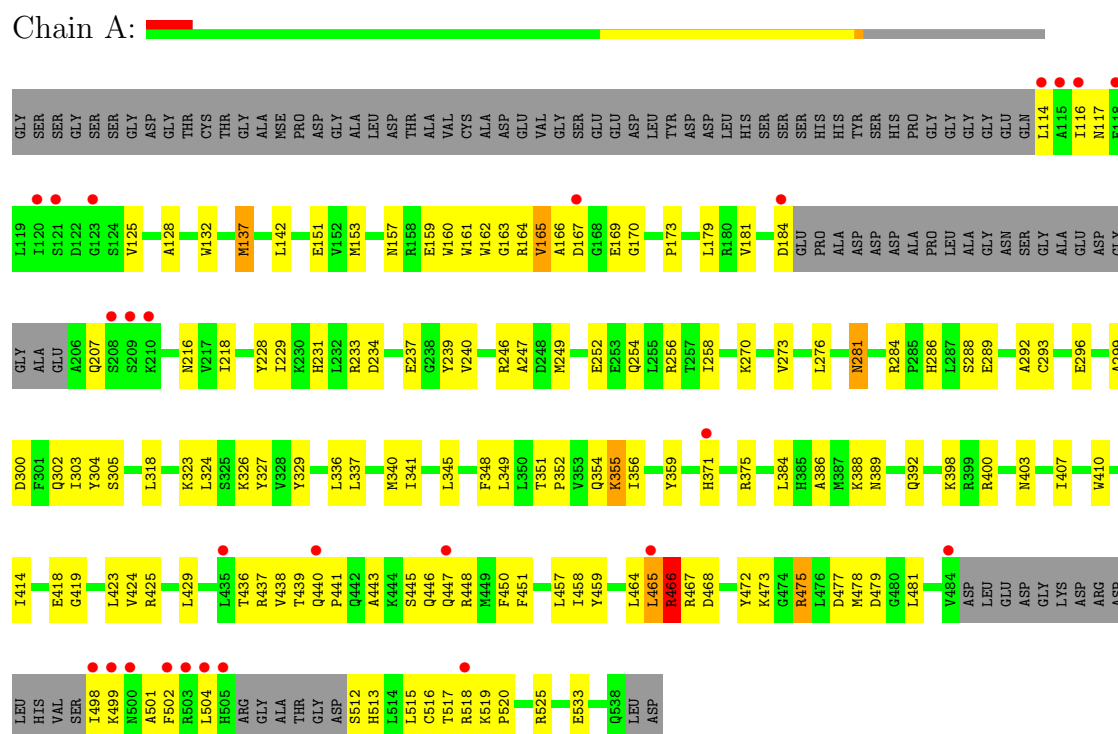
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		

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 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: Rho guanine nucleotide exchange factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.93Å 79.82Å 68.00Å 90.00° 123.25° 90.00°	Depositor
Resolution (Å)	34.61 – 2.36 34.61 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.61-2.36) 99.8 (34.61-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.299 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 18697 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3266	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	A	0.50	0/3256	0.64	0/4367

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3161	124	0
2	A	64	0	0	4	0
All	All	3266	0	3161	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:ASP:OD2	1:A:525:ARG:HG3	1.64	0.95
1:A:116:ILE:H	1:A:116:ILE:HD12	1.38	0.86
1:A:292:ALA:O	1:A:296:GLU:HG3	1.77	0.85
1:A:229:ILE:HD11	1:A:270:LYS:HA	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:ARG:HH11	1:A:468:ASP:HB2	1.41	0.83
1:A:300:ASP:O	1:A:303:ILE:HG12	1.81	0.81
1:A:457:LEU:CB	1:A:478:MSE:HE3	2.12	0.80
1:A:289:GLU:OE2	1:A:375:ARG:HD3	1.82	0.79
1:A:246:ARG:NH2	1:A:249:MSE:HE2	1.99	0.78
1:A:234:ASP:HB3	1:A:340:MSE:HE3	1.66	0.78
1:A:457:LEU:HB2	1:A:478:MSE:HE3	1.69	0.74
1:A:116:ILE:HD12	1:A:116:ILE:N	2.05	0.72
1:A:498:ILE:HD11	1:A:520:PRO:HG3	1.71	0.71
1:A:340:MSE:HE2	1:A:348:PHE:CE1	2.26	0.71
1:A:439:THR:HG23	1:A:441:PRO:HD2	1.72	0.71
1:A:466:ARG:NH1	1:A:468:ASP:HB2	2.06	0.70
1:A:128:ALA:HB2	1:A:179:LEU:HD23	1.75	0.68
1:A:518:ARG:HG3	1:A:519:LYS:HG3	1.75	0.68
1:A:137:MSE:HE3	1:A:410:TRP:HB2	1.76	0.67
1:A:498:ILE:CD1	1:A:520:PRO:HG3	2.25	0.66
1:A:116:ILE:CD1	1:A:116:ILE:H	2.06	0.66
1:A:418:GLU:HB2	1:A:472:TYR:CE2	2.31	0.66
1:A:165:VAL:HG12	1:A:166:ALA:H	1.62	0.65
1:A:457:LEU:HB3	1:A:478:MSE:HE3	1.79	0.64
1:A:371:HIS:H	1:A:371:HIS:CD2	2.15	0.63
1:A:165:VAL:HG12	1:A:166:ALA:N	2.14	0.63
1:A:477:ASP:OD1	1:A:479:ASP:HB2	1.98	0.63
1:A:340:MSE:HE2	1:A:348:PHE:CZ	2.33	0.63
1:A:239:TYR:CE1	1:A:340:MSE:HE1	2.34	0.62
1:A:410:TRP:CZ2	1:A:414:ILE:HD11	2.34	0.62
1:A:137:MSE:HG3	1:A:429:LEU:HD22	1.81	0.62
1:A:386:ALA:HA	1:A:389:ASN:HD22	1.64	0.62
1:A:472:TYR:OH	1:A:475:ARG:HD2	2.01	0.61
1:A:384:LEU:O	1:A:388:LYS:HG3	2.02	0.60
1:A:132:TRP:CD2	1:A:398:LYS:HE2	2.37	0.59
1:A:218:ILE:HD13	1:A:288:SER:HB2	1.84	0.59
1:A:351:THR:HA	1:A:354:GLN:HE21	1.68	0.59
1:A:439:THR:CG2	1:A:441:PRO:HD2	2.31	0.59
1:A:436:THR:HG22	1:A:447:GLN:CB	2.33	0.59
1:A:464:LEU:O	1:A:465:LEU:HB2	2.02	0.58
1:A:229:ILE:HD12	1:A:273:VAL:HG21	1.85	0.58
1:A:438:VAL:HG13	1:A:445:SER:HB3	1.87	0.57
1:A:481:LEU:HD23	1:A:504:LEU:HB2	1.88	0.55
1:A:436:THR:HG22	1:A:447:GLN:HB3	1.88	0.55
1:A:345:LEU:HD12	1:A:345:LEU:O	2.08	0.54
1:A:386:ALA:HA	1:A:389:ASN:ND2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:GLU:OE1	1:A:173:PRO:HB3	2.07	0.53
1:A:281:ASN:C	1:A:281:ASN:HD22	2.10	0.53
1:A:137:MSE:HE3	1:A:410:TRP:CG	2.43	0.53
1:A:354:GLN:NE2	2:A:575:HOH:O	2.42	0.52
1:A:424:VAL:HG12	1:A:425:ARG:HG3	1.91	0.52
1:A:326:LYS:HE3	1:A:327:TYR:HE1	1.74	0.52
1:A:410:TRP:CE2	1:A:414:ILE:HD11	2.44	0.52
1:A:371:HIS:CD2	1:A:371:HIS:N	2.77	0.52
1:A:304:TYR:CD2	1:A:356:ILE:HB	2.45	0.52
1:A:153:MSE:CE	1:A:164:ARG:HB2	2.40	0.52
1:A:440:GLN:N	1:A:441:PRO:CD	2.73	0.51
1:A:502:PHE:O	1:A:512:SER:HA	2.10	0.51
1:A:276:LEU:HD23	1:A:293:CYS:SG	2.50	0.51
1:A:336:LEU:O	1:A:337:LEU:HD23	2.10	0.51
1:A:153:MSE:HE3	1:A:162:TRP:CD1	2.46	0.51
1:A:326:LYS:HE3	1:A:327:TYR:CE1	2.46	0.50
1:A:284:ARG:HB3	1:A:286:HIS:CE1	2.47	0.50
1:A:437:ARG:HA	1:A:515:LEU:HD23	1.94	0.50
1:A:137:MSE:HE1	2:A:588:HOH:O	2.11	0.49
1:A:418:GLU:HB2	1:A:472:TYR:HE2	1.75	0.49
1:A:114:LEU:O	1:A:117:ASN:ND2	2.44	0.49
1:A:137:MSE:HE3	1:A:410:TRP:CB	2.42	0.49
1:A:137:MSE:HE3	1:A:410:TRP:CD1	2.47	0.49
1:A:437:ARG:HD2	1:A:450:PHE:HZ	1.78	0.49
1:A:323:LYS:O	1:A:324:LEU:HD23	2.14	0.48
1:A:247:ALA:HA	2:A:559:HOH:O	2.13	0.48
1:A:400:ARG:HB3	1:A:400:ARG:HH11	1.79	0.48
1:A:162:TRP:CH2	1:A:170:GLY:HA2	2.49	0.48
1:A:410:TRP:CH2	1:A:414:ILE:HD11	2.49	0.48
1:A:499:LYS:HB3	1:A:516:CYS:HB3	1.96	0.48
1:A:355:LYS:HE2	1:A:359:TYR:CE2	2.49	0.47
1:A:351:THR:OG1	1:A:352:PRO:HD3	2.14	0.47
1:A:437:ARG:HH11	1:A:446:GLN:NE2	2.13	0.47
1:A:498:ILE:O	1:A:516:CYS:HB2	2.15	0.46
1:A:114:LEU:HD12	1:A:114:LEU:N	2.31	0.46
1:A:132:TRP:CH2	1:A:354:GLN:HG2	2.50	0.46
1:A:464:LEU:O	1:A:465:LEU:CB	2.64	0.46
1:A:233:ARG:HG3	1:A:237:GLU:OE2	2.16	0.46
1:A:425:ARG:NH1	1:A:477:ASP:OD2	2.49	0.46
1:A:388:LYS:O	1:A:392:GLN:HG3	2.16	0.46
1:A:450:PHE:C	1:A:451:PHE:CD1	2.89	0.45
1:A:498:ILE:HD12	1:A:520:PRO:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:MSE:HE3	1:A:162:TRP:HD1	1.80	0.45
1:A:400:ARG:HB3	1:A:400:ARG:NH1	2.32	0.45
1:A:403:ASN:O	1:A:407:ILE:HG13	2.16	0.45
1:A:229:ILE:HD12	1:A:273:VAL:CG2	2.47	0.44
1:A:254:GLN:O	1:A:258:ILE:HG13	2.17	0.44
1:A:207:GLN:OE1	1:A:207:GLN:HA	2.17	0.44
1:A:116:ILE:HG12	1:A:179:LEU:HD11	2.00	0.44
1:A:142:LEU:HD21	1:A:165:VAL:HG23	1.98	0.44
1:A:252:GLU:O	1:A:256:ARG:HG3	2.18	0.43
1:A:299:ALA:O	1:A:302:GLN:HB2	2.17	0.43
1:A:318:LEU:HD11	1:A:349:LEU:HD12	1.99	0.43
1:A:329:TYR:N	1:A:329:TYR:CD2	2.86	0.43
1:A:125:VAL:O	1:A:125:VAL:HG12	2.19	0.42
1:A:181:VAL:CG1	1:A:216:ASN:HB3	2.49	0.42
1:A:137:MSE:CE	1:A:410:TRP:HB2	2.45	0.42
1:A:437:ARG:HB3	1:A:515:LEU:CD2	2.49	0.42
1:A:458:ILE:HG22	1:A:459:TYR:N	2.33	0.42
1:A:498:ILE:HD13	1:A:498:ILE:N	2.35	0.42
1:A:153:MSE:HE2	1:A:164:ARG:HB2	2.01	0.42
1:A:231:HIS:HD2	2:A:579:HOH:O	2.02	0.41
1:A:157:ASN:O	1:A:161:TRP:NE1	2.52	0.41
1:A:157:ASN:HB2	1:A:160:TRP:O	2.20	0.41
1:A:423:LEU:HA	1:A:423:LEU:HD23	1.83	0.41
1:A:501:ALA:HA	1:A:513:HIS:O	2.20	0.41
1:A:498:ILE:CG2	1:A:517:THR:OG1	2.68	0.41
1:A:318:LEU:HA	1:A:318:LEU:HD23	1.84	0.41
1:A:151:GLU:OE1	1:A:164:ARG:NH2	2.41	0.41
1:A:448:ARG:HH21	1:A:473:LYS:HE2	1.86	0.41
1:A:440:GLN:O	1:A:441:PRO:C	2.59	0.40
1:A:498:ILE:HD12	1:A:520:PRO:CA	2.51	0.40
1:A:318:LEU:HD11	1:A:349:LEU:CD1	2.51	0.40
1:A:163:GLY:O	1:A:169:GLU:CB	2.69	0.40
1:A:231:HIS:CE1	1:A:341:ILE:HD13	2.56	0.40
1:A:351:THR:N	1:A:352:PRO:CD	2.85	0.40
1:A:437:ARG:HD2	1:A:450:PHE:CZ	2.56	0.40
1:A:228:TYR:CE1	1:A:355:LYS:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	377/482 (78%)	340 (90%)	30 (8%)	7 (2%)	12 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ARG
1	A	443	ALA
1	A	465	LEU
1	A	467	ARG
1	A	165	VAL
1	A	419	GLY
1	A	240	VAL

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	346/406 (85%)	338 (98%)	8 (2%)	63 79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	MSE
1	A	184	ASP
1	A	281	ASN
1	A	305	SER
1	A	355	LYS
1	A	466	ARG
1	A	475	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	231	HIS
1	A	278	GLN
1	A	281	ASN
1	A	354	GLN
1	A	371	HIS
1	A	385	HIS
1	A	389	ASN
1	A	392	GLN
1	A	446	GLN
1	A	505	HIS
1	A	513	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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

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, 95th 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	A	385/482 (79%)	0.28	26 (6%) 17 19	25, 49, 90, 106	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	PHE	7.3
1	A	115	ALA	7.0
1	A	484	VAL	5.7
1	A	184	ASP	4.3
1	A	118	GLU	3.8
1	A	504	LEU	3.4
1	A	503	ARG	3.2
1	A	123	GLY	3.2
1	A	167	ASP	3.1
1	A	120	ILE	3.1
1	A	465	LEU	3.0
1	A	435	LEU	2.9
1	A	121	SER	2.9
1	A	518	ARG	2.7
1	A	116	ILE	2.6
1	A	440	GLN	2.6
1	A	447	GLN	2.5
1	A	371	HIS	2.4
1	A	114	LEU	2.4
1	A	208	SER	2.4
1	A	209	SER	2.3
1	A	498	ILE	2.3
1	A	500	ASN	2.3
1	A	210	LYS	2.3
1	A	505	HIS	2.2
1	A	499	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.