



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:11 PM UTC

PDB ID : 1FC3 / pdb_00001fc3
Title : THE CRYSTAL STRUCTURE OF TRANS-ACTIVATION DOMAIN OF
THE SPORULATION RESPONSE REGULATOR, SPO0A
Authors : Lewis, R.J.; Krzywda, S.; Wilkinson, A.J.
Deposited on : 2000-07-17
Resolution : 2.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	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

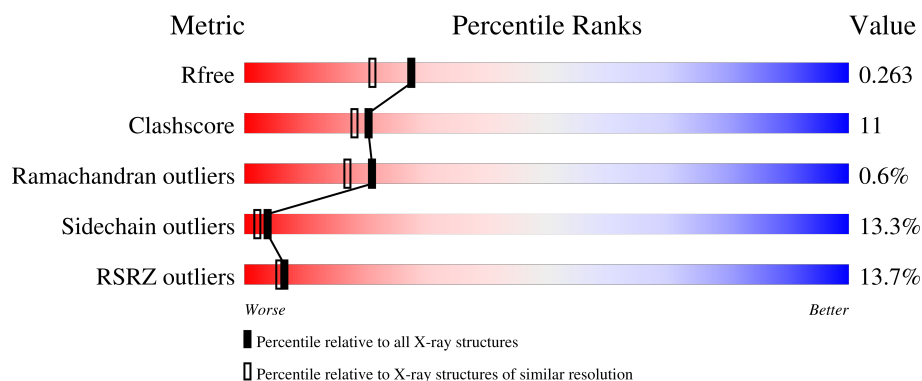
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 ≥ 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	120	12% 64% 29% 5% ..
1	B	120	8% 67% 15% • 16%
1	C	120	18% 66% 22% 7% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2983 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 SPO0A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	31	3	0
			940	602	163	173	2			
1	B	101	Total	C	N	O	S	29	2	0
			804	516	141	144	3			
1	C	116	Total	C	N	O	S	34	4	0
			920	587	157	174	2			

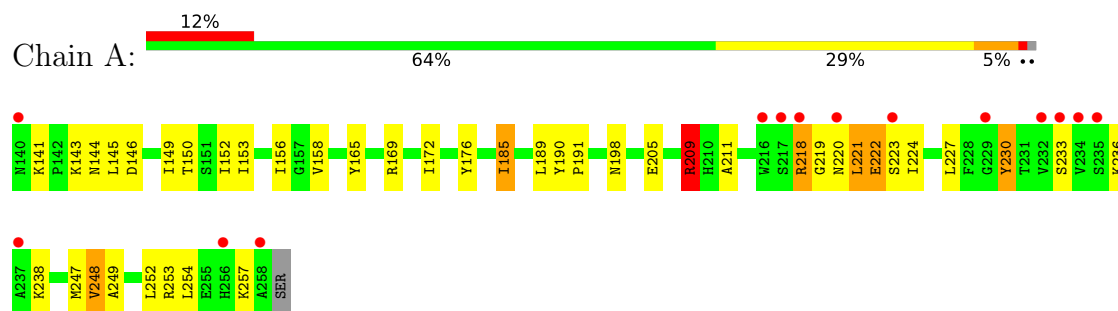
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total	O	0	0
			92	92		
2	B	95	Total	O	0	0
			95	95		
2	C	132	Total	O	0	0
			132	132		

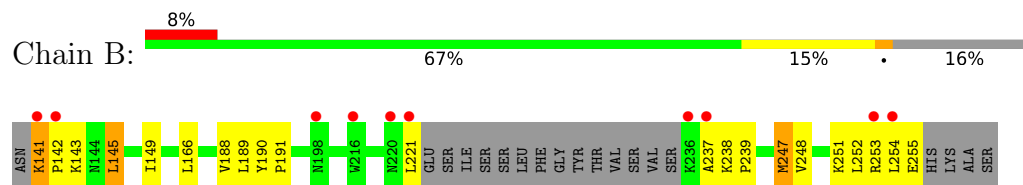
3 Residue-property plots [i](#)

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.

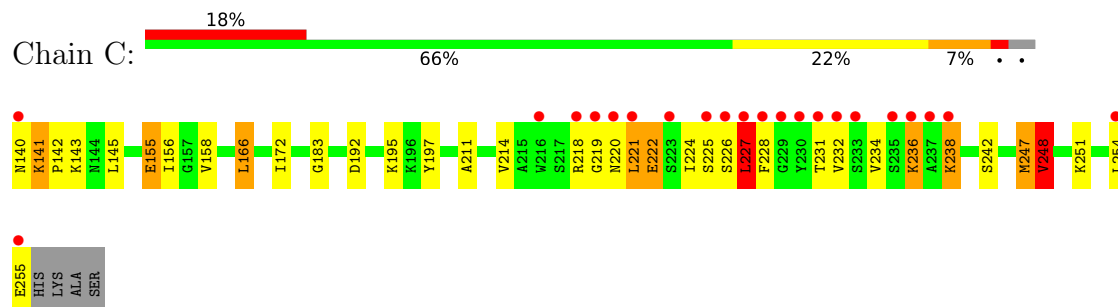
• Molecule 1: SPO0A



• Molecule 1: SPO0A



• Molecule 1: SPO0A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.12Å 53.41Å 53.72Å 90.82° 111.73° 111.32°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.6 (20.00-2.00) 87.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.25 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.258 0.215 , 0.263	Depositor DCC
R_{free} test set	1234 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2983	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	1.15	3/973 (0.3%)	1.34	12/1316 (0.9%)
1	B	1.03	1/828 (0.1%)	1.18	2/1117 (0.2%)
1	C	1.19	5/957 (0.5%)	1.26	8/1295 (0.6%)
All	All	1.13	9/2758 (0.3%)	1.27	22/3728 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	GLU	CA-CB	-12.29	1.33	1.53
1	C	232	VAL	CA-CB	8.87	1.66	1.54
1	C	195	LYS	CD-CE	8.77	1.78	1.52
1	A	236	LYS	CB-CG	7.68	1.75	1.52
1	B	255	GLU	CA-CB	6.08	1.65	1.53
1	C	247	MET	SD-CE	5.85	1.94	1.79
1	A	247	MET	CG-SD	5.64	1.94	1.80
1	C	255	GLU	CA-C	5.36	1.64	1.52
1	A	218	ARG	CA-C	5.17	1.59	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	GLU	N-CA-C	-9.17	101.86	113.23
1	B	237	ALA	N-CA-C	7.70	121.99	109.59
1	A	236	LYS	CA-CB-CG	-7.52	99.05	114.10
1	A	209	ARG	NE-CZ-NH2	-6.37	113.47	119.20
1	C	225	SER	N-CA-C	-6.33	105.69	113.41
1	C	222	GLU	N-CA-CB	-6.24	100.71	110.44
1	C	183	GLY	N-CA-C	6.21	121.94	113.99
1	C	248	VAL	CB-CA-C	6.03	120.28	112.14
1	A	141	LYS	N-CA-C	6.03	123.13	109.81
1	A	223	SER	N-CA-C	-6.00	105.96	113.28
1	A	218	ARG	CA-CB-CG	-5.95	102.19	114.10
1	C	222	GLU	CB-CA-C	5.95	121.62	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	GLY	N-CA-C	-5.94	99.11	113.18
1	A	219	GLY	O-C-N	5.92	131.89	122.36
1	A	218	ARG	CD-NE-CZ	-5.90	116.13	124.40
1	A	222	GLU	N-CA-C	-5.74	106.26	113.72
1	A	209	ARG	CG-CD-NE	-5.56	99.76	112.00
1	B	255	GLU	N-CA-CB	-5.39	101.33	110.50
1	A	185	ILE	N-CA-C	5.28	116.64	110.62
1	A	222	GLU	CB-CA-C	5.22	118.32	109.55
1	C	227	LEU	N-CA-C	-5.18	106.29	113.18
1	A	230	TYR	N-CA-C	5.17	116.61	111.07

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	940	0	975	28	0
1	B	804	0	841	9	1
1	C	920	0	945	22	1
2	A	92	0	0	1	0
2	B	95	0	0	0	0
2	C	132	0	0	1	0
All	All	2983	0	2761	58	1

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 (58) 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:152[B]:ILE:HD11	1:A:227:LEU:HD22	1.52	0.92
1:A:176:TYR:HA	1:A:253:ARG:HH21	1.34	0.92
1:A:221:LEU:HD12	1:A:221:LEU:O	1.75	0.86
1:C:227:LEU:CD1	1:C:251:LYS:HE2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LEU:HD11	1:C:251:LYS:HE2	1.60	0.82
1:A:152[A]:ILE:HD12	1:A:252:LEU:HD21	1.63	0.80
1:A:152[A]:ILE:CD1	1:A:252:LEU:HD21	2.19	0.72
1:A:221:LEU:O	1:A:221:LEU:CD1	2.40	0.69
1:C:224:ILE:HG22	1:C:224:ILE:O	1.95	0.67
1:C:238:LYS:HD2	2:C:312:HOH:O	1.94	0.66
1:B:149:ILE:HG12	1:B:252:LEU:HD11	1.78	0.65
1:A:152[B]:ILE:CD1	1:A:227:LEU:HD22	2.25	0.61
1:C:156:ILE:HD11	1:C:228:PHE:HE2	1.66	0.60
1:A:221:LEU:O	1:A:221:LEU:CG	2.49	0.60
1:C:224:ILE:O	1:C:224:ILE:CG2	2.50	0.59
1:A:221:LEU:HD12	1:A:233:SER:OG	2.02	0.58
1:C:141:LYS:N	1:C:142:PRO:CD	2.67	0.58
1:A:205:GLU:OE1	1:A:209:ARG:HD3	2.04	0.57
1:A:257:LYS:HE3	2:A:281:HOH:O	2.03	0.57
1:A:176:TYR:HA	1:A:253:ARG:NH2	2.12	0.57
1:C:172:ILE:HG21	1:C:248:VAL:HG22	1.85	0.57
1:C:227:LEU:HD12	1:C:251:LYS:HE2	1.83	0.57
1:C:156:ILE:HD11	1:C:228:PHE:CE2	2.40	0.56
1:A:209:ARG:NH2	1:C:192:ASP:OD2	2.37	0.56
1:A:249:ALA:HB1	1:A:253:ARG:HH22	1.72	0.55
1:C:214:VAL:O	1:C:218:ARG:HG3	2.07	0.55
1:A:230:TYR:O	1:A:233:SER:HB3	2.10	0.52
1:C:141:LYS:N	1:C:142:PRO:HD3	2.25	0.51
1:A:249:ALA:HB1	1:A:253:ARG:NH2	2.25	0.51
1:C:166:LEU:HD11	1:C:197:TYR:CZ	2.45	0.51
1:A:150:THR:HG23	1:A:165:TYR:OH	2.11	0.50
1:A:189:LEU:C	1:A:189:LEU:HD23	2.36	0.50
1:C:221:LEU:HD12	1:C:221:LEU:O	2.12	0.50
1:A:146:ASP:OD2	1:A:169:ARG:NH2	2.31	0.49
1:A:149:ILE:O	1:A:152[B]:ILE:HG22	2.13	0.49
1:B:145:LEU:HD21	1:B:252:LEU:HD13	1.95	0.48
1:A:190:TYR:HB2	1:A:191:PRO:HD3	1.95	0.47
1:C:155[A]:GLU:HG2	1:C:227:LEU:CD2	2.45	0.47
1:C:227:LEU:HD12	1:C:251:LYS:CE	2.46	0.46
1:C:158:VAL:HG13	1:C:211:ALA:HB1	1.97	0.46
1:B:188:VAL:C	1:B:191:PRO:HD2	2.41	0.45
1:A:158:VAL:HG13	1:A:211:ALA:HB1	1.99	0.45
1:B:189:LEU:C	1:B:189:LEU:HD23	2.41	0.45
1:C:156:ILE:CD1	1:C:228:PHE:HE2	2.30	0.44
1:A:221:LEU:O	1:A:221:LEU:HG	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HG21	1:A:248:VAL:HG22	2.00	0.43
1:A:152[B]:ILE:HG23	1:A:153:ILE:N	2.34	0.43
1:C:238:LYS:O	1:C:238:LYS:HG2	2.18	0.43
1:C:166:LEU:HD11	1:C:197:TYR:CE2	2.53	0.42
1:C:141:LYS:H	1:C:142:PRO:HD3	1.84	0.42
1:B:141:LYS:O	1:B:142:PRO:C	2.63	0.42
1:A:144:ASN:HD22	1:A:144:ASN:HA	1.62	0.41
1:B:190:TYR:N	1:B:191:PRO:CD	2.83	0.41
1:A:185:ILE:HD13	1:A:185:ILE:HG21	1.85	0.40
1:B:190:TYR:HB2	1:B:191:PRO:HD3	2.02	0.40
1:B:238:LYS:HG3	1:B:239:PRO:HD2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:O	1:C:236:LYS:CB[1_766]	2.17	0.03

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	120/120 (100%)	114 (95%)	5 (4%)	1 (1%)	16	11
1	B	99/120 (82%)	95 (96%)	4 (4%)	0	100	100
1	C	118/120 (98%)	110 (93%)	7 (6%)	1 (1%)	16	11
All	All	337/360 (94%)	319 (95%)	16 (5%)	2 (1%)	21	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	LEU

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Mol	Chain	Res	Type
1	A	220	ASN

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	104/102 (102%)	93 (89%)	11 (11%)	6	4
1	B	87/102 (85%)	77 (88%)	10 (12%)	5	3
1	C	103/102 (101%)	83 (81%)	20 (19%)	1	1
All	All	294/306 (96%)	253 (86%)	41 (14%)	4	2

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LYS
1	A	145	LEU
1	A	198	ASN
1	A	209	ARG
1	A	218	ARG
1	A	221	LEU
1	A	222	GLU
1	A	224	ILE
1	A	238	LYS
1	A	248	VAL
1	A	254	LEU
1	B	141	LYS
1	B	143	LYS
1	B	145	LEU
1	B	166	LEU
1	B	221	LEU
1	B	247[A]	MET
1	B	247[B]	MET
1	B	248	VAL
1	B	251	LYS
1	B	253	ARG

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Mol	Chain	Res	Type
1	C	140	ASN
1	C	141	LYS
1	C	143	LYS
1	C	145	LEU
1	C	155[A]	GLU
1	C	155[B]	GLU
1	C	166	LEU
1	C	220	ASN
1	C	221	LEU
1	C	222	GLU
1	C	226	SER
1	C	227	LEU
1	C	231	THR
1	C	234	VAL
1	C	236	LYS
1	C	238	LYS
1	C	242[A]	SER
1	C	242[B]	SER
1	C	247	MET
1	C	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	144	ASN

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 oligosaccharides 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	118/120 (98%)	0.64	14 (11%) 9 8	11, 28, 41, 60	9 (7%)
1	B	101/120 (84%)	0.43	10 (9%) 13 11	17, 27, 39, 49	9 (8%)
1	C	116/120 (96%)	0.75	22 (18%) 3 3	17, 27, 51, 53	14 (12%)
All	All	335/360 (93%)	0.61	46 (13%) 6 6	11, 27, 47, 60	32 (9%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	TYR	6.6
1	C	232	VAL	5.2
1	A	217	SER	5.2
1	A	223	SER	4.8
1	C	140	ASN	4.7
1	C	229	GLY	4.7
1	C	219	GLY	4.5
1	C	233	SER	4.5
1	B	142	PRO	4.4
1	C	237	ALA	4.3
1	B	220	ASN	4.2
1	C	225	SER	4.1
1	A	220	ASN	4.0
1	C	220	ASN	4.0
1	C	235	SER	3.9
1	A	235	SER	3.7
1	C	228	PHE	3.7
1	C	231	THR	3.6
1	A	233	SER	3.4
1	B	221	LEU	3.4
1	A	237	ALA	3.3
1	A	234	VAL	3.2
1	C	236	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	236	LYS	3.1
1	A	216	TRP	3.0
1	A	140	ASN	2.9
1	C	221	LEU	2.9
1	A	256	HIS	2.7
1	C	218	ARG	2.7
1	C	255	GLU	2.7
1	A	232	VAL	2.7
1	A	218	ARG	2.6
1	A	258	ALA	2.6
1	C	254	LEU	2.6
1	B	198	ASN	2.3
1	B	253	ARG	2.3
1	C	223	SER	2.3
1	C	227	LEU	2.3
1	B	254	LEU	2.3
1	A	229	GLY	2.2
1	B	216	TRP	2.2
1	C	216	TRP	2.2
1	C	226	SER	2.1
1	B	237	ALA	2.1
1	B	141	LYS	2.0
1	C	238	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.