



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 2DVY / pdb_00002dvy
Title : Crystal structure of restriction endonucleases PabI
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Deposited on : 2006-08-01
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

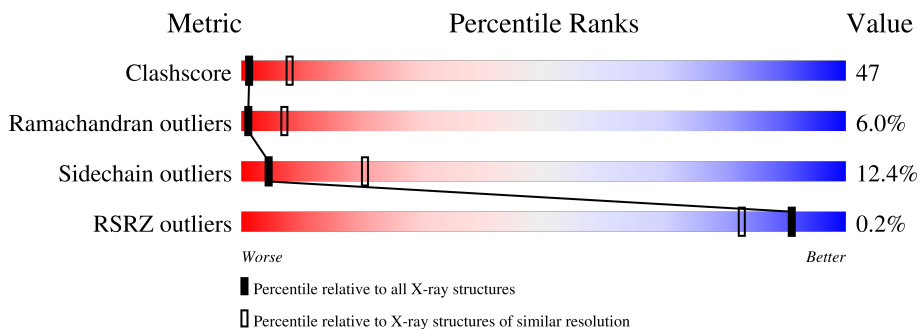
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	
1	F	226	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10623 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.

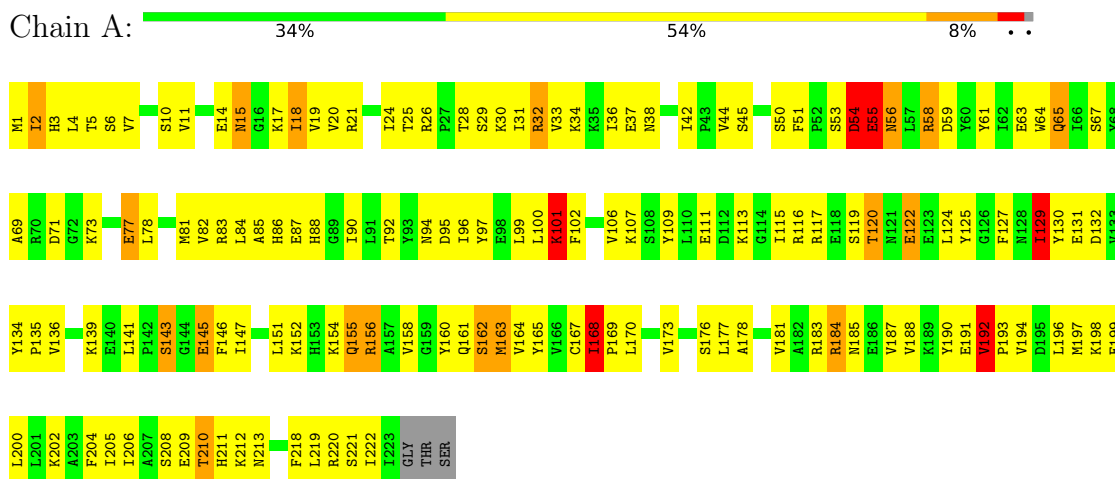
- Molecule 1 is a protein called Restriction endonuclease PabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1817	1167	310	335	5			
1	B	215	Total	C	N	O	S	0	0	0
			1747	1123	295	325	4			
1	C	218	Total	C	N	O	S	0	0	0
			1776	1142	300	329	5			
1	D	214	Total	C	N	O	S	0	0	0
			1747	1120	299	324	4			
1	E	223	Total	C	N	O	S	0	0	0
			1817	1167	310	335	5			
1	F	211	Total	C	N	O	S	0	0	0
			1719	1106	289	320	4			

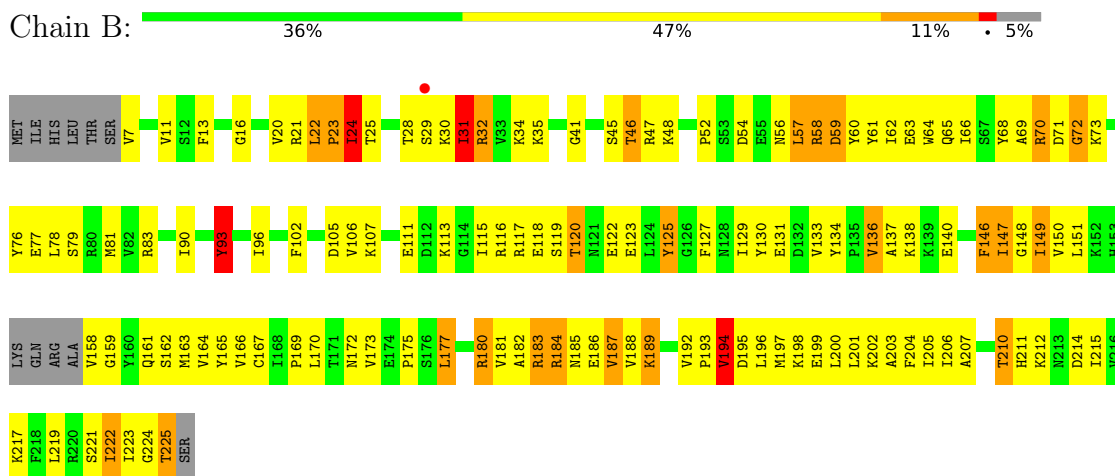
3 Residue-property plots

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: Restriction endonuclease PabI

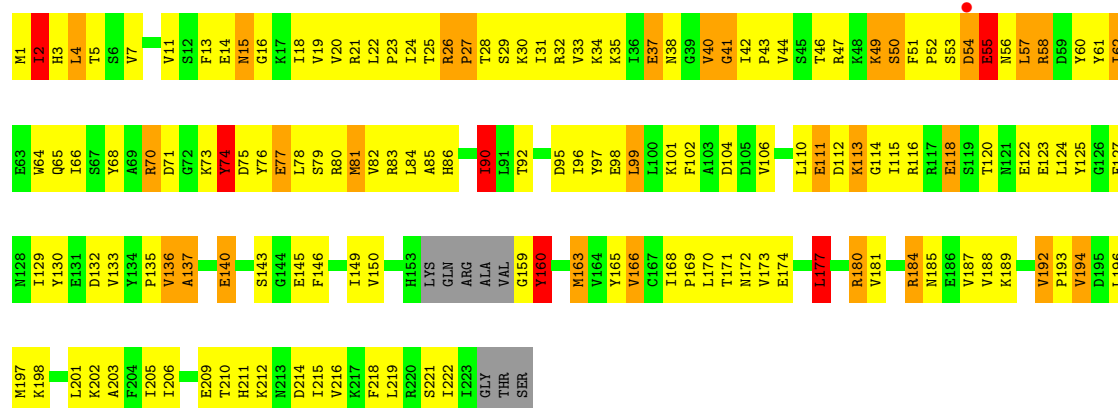


• Molecule 1: Restriction endonuclease PabI



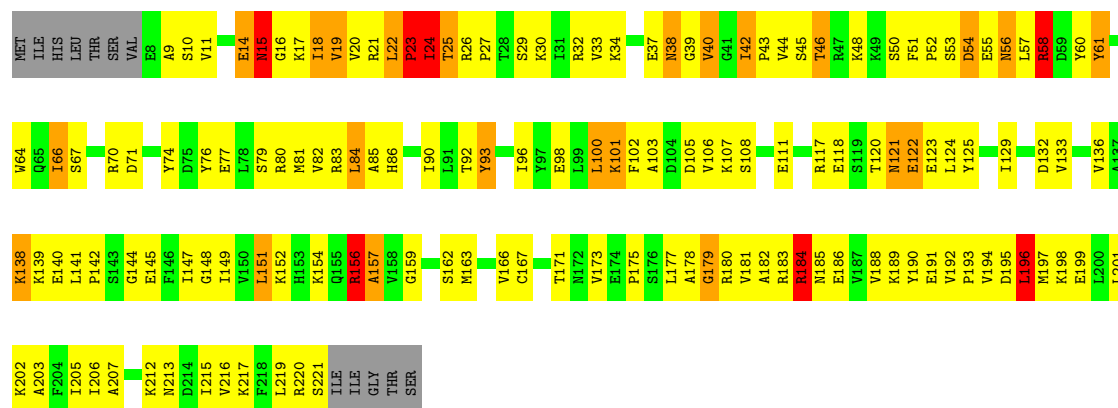
• Molecule 1: Restriction endonuclease PabI





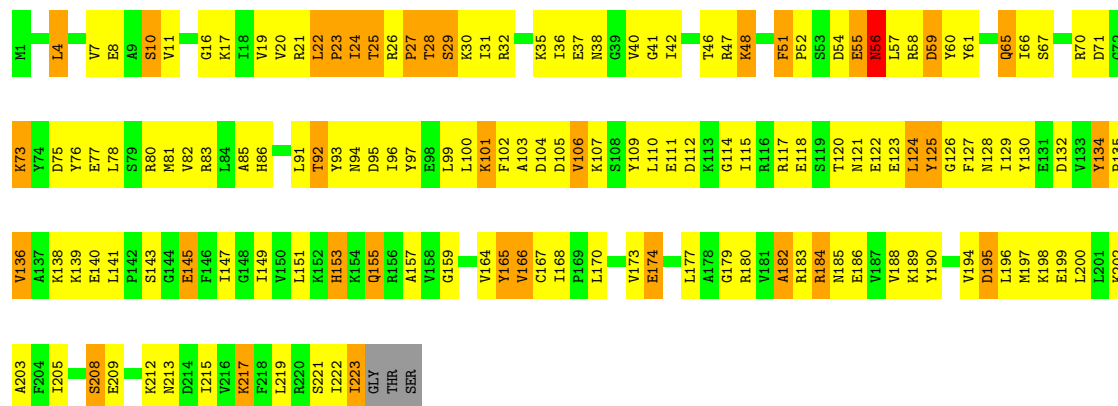
• Molecule 1: Restriction endonuclease PabI

Chain D: 31% 50% 10% 5%



• Molecule 1: Restriction endonuclease PabI

Chain E: 33% 50% 15% 2%



• Molecule 1: Restriction endonuclease PabI

Chain F: 17% 60% 15% 7%

K189	Y125	E63	MET
Y190	G126	W64	ILE
E191	F127	Q65	HIS
V192	N128	I66	LEU
P193	I129	S67	THR
V194	Y130	Y68	SER
D195		A69	VAL
L196	V133	R70	E8
M197	Y134	D71	A9
K198	P135	G72	S10
E199	V136	K73	V11
L200	A137	Y74	S12
L201	K138	D75	F13
K202	K138	Y76	E14
A203	E140	E77	N15
F204	L141	L78	G16
I205	P142	S79	K17
I206	S143	R80	I18
A207	G144	M81	V19
S208	E145	V82	V20
E209	F146	R83	R21
T210	I147	L84	L22
H211	G148	A85	P23
K212	I149	H86	I24
N213	V150	E87	T25
D214	L151	H88	S26
I215	K152	G89	P27
V216	HIS	I90	T28
K217	LYS	L91	S29
F218	GLN	T92	K30
L219	ARG	Y93	I31
R220	ALA	N94	R32
S221	V158	D95	V33
T222	G159	I96	K34
I223	Y160	Y97	K35
GLY		E98	I36
THR	M163	L99	E37
SER		L100	N38
		K101	
	V166	F102	I42
	C167	A103	P43
		D104	V44
	L170	D105	S45
	T171	V106	T46
	M172		R47
	V173		K48
	E174	Y109	K49
	P175	L110	S50
	S176	E111	F51
	L177	D112	
	A178	K113	S52
	G179	G114	S53
	R180	I115	D54
	V181	R116	E55
	A182	R117	N56
	R183		L57
	R184	T120	R58
	N185	N121	D59
	E186	E122	Y60
	V187	E123	Y61
	V188	L124	I62

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.57Å 113.96Å 89.17Å 90.00° 116.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.00) 94.6 (20.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.318 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10623	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 [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	0.65	0/1853	1.12	13/2501 (0.5%)
1	B	0.60	0/1781	1.06	8/2404 (0.3%)
1	C	0.68	0/1811	1.15	11/2444 (0.5%)
1	D	0.57	1/1782 (0.1%)	1.03	10/2404 (0.4%)
1	E	0.54	0/1853	1.04	10/2501 (0.4%)
1	F	0.50	0/1752	1.02	10/2364 (0.4%)
All	All	0.59	1/10832 (0.0%)	1.07	62/14618 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	ARG	CZ-NH2	5.32	1.40	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TYR	N-CA-C	10.76	126.76	112.88
1	A	120	THR	N-CA-C	-10.32	96.10	110.35
1	D	101	LYS	N-CA-C	-8.87	101.19	111.03
1	C	192	VAL	N-CA-C	8.32	116.16	107.76
1	F	22	LEU	CA-C-N	8.20	130.09	119.84

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	1817	0	1859	152	0
1	B	1747	0	1776	138	0
1	C	1776	0	1810	186	0
1	D	1747	0	1775	181	0
1	E	1817	0	1859	195	0
1	F	1719	0	1750	247	0
All	All	10623	0	10829	1012	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 47.

The worst 5 of 1012 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:D:124:LEU:HB2	1:D:129:ILE:HD11	1.16	1.16
1:F:13:PHE:HB2	1:F:84:LEU:HD21	1.33	1.09
1:A:61:TYR:CD2	1:A:167:CYS:HB3	1.94	1.01
1:E:132:ASP:HB2	1:F:134:TYR:HB2	1.38	1.00
1:F:50:SER:HA	1:F:181:VAL:HB	1.42	0.99

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	221/226 (98%)	178 (80%)	33 (15%)	10 (4%)	2	12
1	B	211/226 (93%)	165 (78%)	37 (18%)	9 (4%)	2	12
1	C	214/226 (95%)	173 (81%)	30 (14%)	11 (5%)	1	10
1	D	212/226 (94%)	150 (71%)	46 (22%)	16 (8%)	1	4
1	E	221/226 (98%)	171 (77%)	35 (16%)	15 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	207/226 (92%)	141 (68%)	50 (24%)	16 (8%)	1	4
All	All	1286/1356 (95%)	978 (76%)	231 (18%)	77 (6%)	1	7

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	56	ASN
1	A	184	ARG
1	B	57	LEU
1	C	49	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	202/204 (99%)	178 (88%)	24 (12%)	5	22
1	B	194/204 (95%)	170 (88%)	24 (12%)	4	20
1	C	198/204 (97%)	168 (85%)	30 (15%)	3	14
1	D	193/204 (95%)	171 (89%)	22 (11%)	5	24
1	E	202/204 (99%)	177 (88%)	25 (12%)	4	20
1	F	191/204 (94%)	170 (89%)	21 (11%)	6	25
All	All	1180/1224 (96%)	1034 (88%)	146 (12%)	4	20

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	143	SER
1	F	196	LEU
1	E	166	VAL
1	F	52	PRO
1	C	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	211	HIS
1	F	65	GLN
1	F	213	ASN
1	C	65	GLN
1	C	38	ASN

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 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 [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, 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	223/226 (98%)	-0.31	0 100 100	31, 52, 76, 91	0
1	B	215/226 (95%)	-0.18	1 (0%) 87 72	29, 59, 87, 94	0
1	C	218/226 (96%)	-0.32	1 (0%) 87 72	22, 48, 78, 95	0
1	D	214/226 (94%)	0.12	0 100 100	25, 80, 113, 119	0
1	E	223/226 (98%)	-0.04	0 100 100	39, 70, 101, 110	0
1	F	211/226 (93%)	0.28	1 (0%) 87 72	45, 80, 118, 134	0
All	All	1304/1356 (96%)	-0.08	3 (0%) 91 83	22, 65, 104, 134	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	SER	2.7
1	F	51	PHE	2.7
1	C	54	ASP	2.2

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.