



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:15 PM UTC

PDB ID : 6TE4 / pdb_00006te4
Title : Structural insights into Pseudomonas aeruginosa Type six secretion system exported effector 8: Tse8 in complex with a peptide
Authors : Sainz-Polo, M.A.; Capuni, R.; Lucas, M.; Altuna, J.; Fucini, P.; Montanez, I.; Albesa-Jove, D.
Deposited on : 2019-11-11
Resolution : 2.29 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

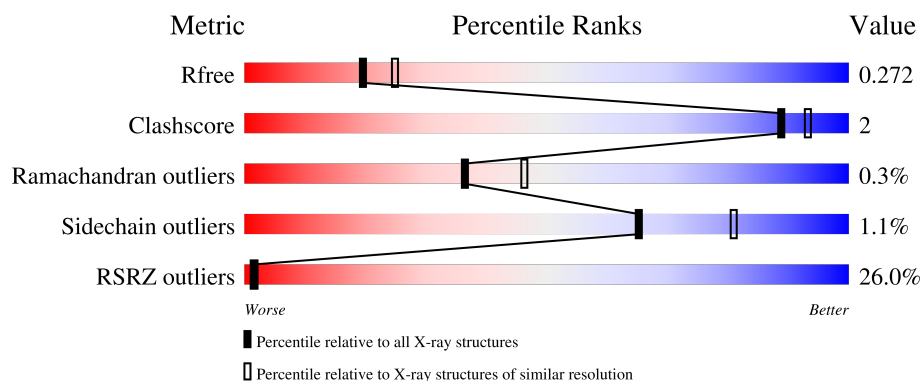
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	595	24% 89% 6% 5%
1	B	595	25% 92% • 5%
2	C	6	50% 17% 67% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8898 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 Tse8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4202	2640	748	798	16			
1	B	565	Total	C	N	O	S	0	0	0
			4153	2615	737	785	16			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP Q9HWL8
A	-24	MET	-	expression tag	UNP Q9HWL8
A	-23	GLY	-	expression tag	UNP Q9HWL8
A	-22	SER	-	expression tag	UNP Q9HWL8
A	-21	SER	-	expression tag	UNP Q9HWL8
A	-20	HIS	-	expression tag	UNP Q9HWL8
A	-19	HIS	-	expression tag	UNP Q9HWL8
A	-18	HIS	-	expression tag	UNP Q9HWL8
A	-17	HIS	-	expression tag	UNP Q9HWL8
A	-16	HIS	-	expression tag	UNP Q9HWL8
A	-15	HIS	-	expression tag	UNP Q9HWL8
A	-14	HIS	-	expression tag	UNP Q9HWL8
A	-13	HIS	-	expression tag	UNP Q9HWL8
A	-12	HIS	-	expression tag	UNP Q9HWL8
A	-11	SER	-	expression tag	UNP Q9HWL8
A	-10	SER	-	expression tag	UNP Q9HWL8
A	-9	GLY	-	expression tag	UNP Q9HWL8
A	-8	GLU	-	expression tag	UNP Q9HWL8
A	-7	ASN	-	expression tag	UNP Q9HWL8
A	-6	LEU	-	expression tag	UNP Q9HWL8
A	-5	TYR	-	expression tag	UNP Q9HWL8
A	-4	PHE	-	expression tag	UNP Q9HWL8
A	-3	GLN	-	expression tag	UNP Q9HWL8
A	-2	GLY	-	expression tag	UNP Q9HWL8
A	-1	GLY	-	expression tag	UNP Q9HWL8

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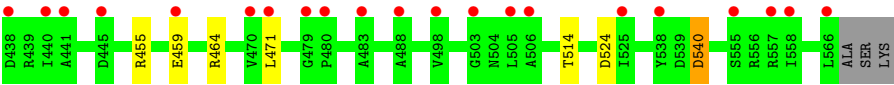
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9HWL8
B	-25	MET	-	initiating methionine	UNP Q9HWL8
B	-24	MET	-	expression tag	UNP Q9HWL8
B	-23	GLY	-	expression tag	UNP Q9HWL8
B	-22	SER	-	expression tag	UNP Q9HWL8
B	-21	SER	-	expression tag	UNP Q9HWL8
B	-20	HIS	-	expression tag	UNP Q9HWL8
B	-19	HIS	-	expression tag	UNP Q9HWL8
B	-18	HIS	-	expression tag	UNP Q9HWL8
B	-17	HIS	-	expression tag	UNP Q9HWL8
B	-16	HIS	-	expression tag	UNP Q9HWL8
B	-15	HIS	-	expression tag	UNP Q9HWL8
B	-14	HIS	-	expression tag	UNP Q9HWL8
B	-13	HIS	-	expression tag	UNP Q9HWL8
B	-12	HIS	-	expression tag	UNP Q9HWL8
B	-11	SER	-	expression tag	UNP Q9HWL8
B	-10	SER	-	expression tag	UNP Q9HWL8
B	-9	GLY	-	expression tag	UNP Q9HWL8
B	-8	GLU	-	expression tag	UNP Q9HWL8
B	-7	ASN	-	expression tag	UNP Q9HWL8
B	-6	LEU	-	expression tag	UNP Q9HWL8
B	-5	TYR	-	expression tag	UNP Q9HWL8
B	-4	PHE	-	expression tag	UNP Q9HWL8
B	-3	GLN	-	expression tag	UNP Q9HWL8
B	-2	GLY	-	expression tag	UNP Q9HWL8
B	-1	GLY	-	expression tag	UNP Q9HWL8
B	0	SER	-	expression tag	UNP Q9HWL8

- Molecule 2 is a protein called Pro-Pro-Leu-Ala-Ser-Lys.

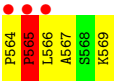
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			43	28	7	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total	O	0	0
			232	232		
3	B	268	Total	O	0	0
			268	268		



● Molecule 2: Pro-Pro-Leu-Ala-Ser-Lys



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.44Å 73.61Å 77.67Å 97.97° 114.95° 104.51°	Depositor
Resolution (Å)	56.63 – 2.29 56.63 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.8 (56.63-2.29) 94.8 (56.63-2.29)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.246 , 0.273 0.246 , 0.272	Depositor DCC
R_{free} test set	1980 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8898	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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	0.14	0/4303	0.28	0/5880
1	B	0.12	0/4254	0.26	0/5820
2	C	1.23	1/44 (2.3%)	1.63	0/57
All	All	0.16	1/8601 (0.0%)	0.29	0/11757

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	565	PRO	C-O	-5.49	1.16	1.24

There are no bond angle outliers.

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	4202	0	4113	17	0
1	B	4153	0	4033	11	0
2	C	43	0	48	6	0
3	A	232	0	0	1	0
3	B	268	0	0	2	0
All	All	8898	0	8194	32	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 2.

All (32) 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:134:ASN:OD1	2:C:565:PRO:HB2	1.90	0.71
1:A:373:LEU:HB3	2:C:567:ALA:HB3	1.77	0.66
1:B:464:ARG:NH1	3:B:609:HOH:O	2.32	0.58
2:C:564:PRO:CB	2:C:565:PRO:HD3	2.41	0.50
1:B:236:ASP:OD1	1:B:265:ARG:NH2	2.42	0.48
2:C:564:PRO:HB2	2:C:565:PRO:HD3	1.97	0.47
1:B:200:THR:HG1	1:B:514:THR:HG1	1.63	0.47
1:A:38:ASP:OD1	1:A:48:ALA:N	2.35	0.46
2:C:564:PRO:N	2:C:565:PRO:HD3	2.31	0.45
1:B:540:ASP:N	1:B:540:ASP:OD1	2.48	0.45
1:A:201:PRO:HB2	1:A:205:VAL:HB	1.98	0.45
1:A:524:ASP:OD1	1:A:524:ASP:N	2.49	0.45
1:B:201:PRO:HB2	1:B:205:VAL:HB	1.97	0.45
1:B:524:ASP:OD1	1:B:524:ASP:N	2.47	0.45
1:A:540:ASP:OD1	1:A:540:ASP:N	2.49	0.45
1:B:85:ASP:HA	1:B:126:LYS:HE2	1.99	0.44
1:B:368:PHE:O	1:B:372:GLU:N	2.47	0.44
1:A:287:PRO:HB3	1:A:342:PHE:HB2	2.00	0.44
1:A:368:PHE:O	1:A:372:GLU:N	2.50	0.43
1:A:284:PHE:HB3	1:A:471:LEU:HD13	2.00	0.43
1:A:430:ALA:HA	1:A:434:ILE:HG13	2.01	0.43
1:A:236:ASP:OD1	1:A:265:ARG:NH2	2.49	0.43
1:B:182:GLU:HA	1:B:186:SER:HB2	2.01	0.42
2:C:564:PRO:N	2:C:565:PRO:CD	2.80	0.42
1:A:436:PRO:HD2	1:A:439:ARG:NE	2.34	0.42
1:A:85:ASP:HA	1:A:126:LYS:HE2	2.01	0.42
1:A:132:MET:HE1	1:A:212:TRP:CZ3	2.55	0.41
1:A:371:ASP:HA	1:A:375:GLU:OE1	2.21	0.41
1:A:207:SER:OG	1:A:251:ARG:NH2	2.53	0.41
1:B:455:ARG:HA	1:B:459:GLU:HB3	2.01	0.41
1:A:3:GLU:OE1	3:A:602:HOH:O	2.22	0.40
1:B:146:GLU:OE2	3:B:601:HOH:O	2.22	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	562/595 (94%)	544 (97%)	17 (3%)	1 (0%)	43	55
1	B	563/595 (95%)	546 (97%)	16 (3%)	1 (0%)	43	55
2	C	4/6 (67%)	2 (50%)	1 (25%)	1 (25%)	0	0
All	All	1129/1196 (94%)	1092 (97%)	34 (3%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	565	PRO
1	B	136	GLY
1	A	136	GLY

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	424/455 (93%)	419 (99%)	5 (1%)	63	79
1	B	411/455 (90%)	409 (100%)	2 (0%)	81	90
2	C	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	840/915 (92%)	831 (99%)	9 (1%)	65	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	96	SER
1	A	231	LEU
1	A	376	LEU
1	A	540	ASP
1	B	471	LEU
1	B	540	ASP
2	C	566	LEU
2	C	569	LYS

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

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

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	564/595 (94%)	1.57	144 (25%)  	13, 24, 35, 54	0
1	B	565/595 (94%)	1.57	148 (26%)  	12, 23, 36, 62	0
2	C	6/6 (100%)	2.85	3 (50%)  	26, 28, 33, 35	0
All	All	1135/1196 (94%)	1.58	295 (25%)  	12, 23, 36, 62	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	ASP	9.6
1	B	421	ALA	7.6
1	A	70	GLY	7.3
1	A	125	GLY	6.7
1	A	419	LEU	6.6
2	C	565	PRO	5.7
1	B	416	GLU	5.4
1	B	422	GLY	5.2
1	A	418	ASP	5.1
1	A	72	PRO	5.1
1	B	247	GLY	5.1
1	B	430	ALA	4.8
1	A	421	ALA	4.7
1	B	70	GLY	4.7
1	A	416	GLU	4.6
1	A	68	ALA	4.4
1	A	338	ILE	4.4
1	A	255	TRP	4.3
2	C	564	PRO	4.2
1	B	419	LEU	4.2
1	B	91	GLY	4.0
1	A	471	LEU	4.0
1	A	344	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	438	ASP	3.9
1	A	422	GLY	3.8
1	A	491	ASP	3.8
1	B	396	LEU	3.8
1	B	434	ILE	3.7
1	B	414	ASN	3.7
1	A	208	VAL	3.7
1	B	433	GLY	3.6
1	A	396	LEU	3.6
1	B	423	MET	3.6
1	B	440	ILE	3.6
1	B	483	ALA	3.6
1	B	19	GLY	3.5
1	A	378	ALA	3.5
1	B	506	ALA	3.5
1	A	14	ASP	3.5
1	B	110	ALA	3.5
1	A	417	GLY	3.5
1	B	373	LEU	3.5
1	A	56	ALA	3.4
1	B	425	GLU	3.4
1	A	414	ASN	3.4
1	A	267	ALA	3.4
1	B	366	LYS	3.3
1	B	505	LEU	3.3
1	A	393	LEU	3.3
1	A	305	ILE	3.3
1	A	434	ILE	3.3
1	A	445	ASP	3.3
1	B	415	ARG	3.3
1	A	243	PRO	3.3
1	A	263	GLU	3.3
1	A	12	LEU	3.2
1	B	431	GLU	3.2
1	A	238	VAL	3.2
1	A	433	GLY	3.2
1	B	90	LYS	3.2
1	A	465	LEU	3.1
1	B	413	PRO	3.1
1	B	436	PRO	3.1
1	A	443	LEU	3.1
1	B	555	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	3.1
1	A	65	ALA	3.1
1	A	493	ALA	3.1
2	C	566	LEU	3.1
1	B	17	GLU	3.1
1	A	426	TYR	3.0
1	B	398	ASP	3.0
1	B	175	ALA	3.0
1	B	407	HIS	3.0
1	A	64	ASP	3.0
1	A	273	ALA	3.0
1	B	538	TYR	3.0
1	B	112	THR	3.0
1	A	19	GLY	3.0
1	B	503	GLY	3.0
1	B	435	LYS	3.0
1	A	249	LEU	2.9
1	B	21	THR	2.9
1	B	406	PRO	2.9
1	B	409	PRO	2.9
1	B	274	ALA	2.9
1	B	355	ALA	2.9
1	B	208	VAL	2.9
1	A	324	GLU	2.9
1	B	470	VAL	2.9
1	A	397	ALA	2.9
1	B	205	VAL	2.9
1	B	417	GLY	2.8
1	B	420	ALA	2.8
1	A	109	ASP	2.8
1	B	78	GLY	2.8
1	B	391	PRO	2.8
1	B	15	ALA	2.8
1	B	441	ALA	2.8
1	A	395	ARG	2.8
1	B	285	GLY	2.8
1	A	337	VAL	2.8
1	A	427	VAL	2.8
1	B	404	ILE	2.8
1	A	438	ASP	2.8
1	B	459	GLU	2.8
1	B	26	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	240	ALA	2.8
1	A	69	ARG	2.8
1	A	404	ILE	2.7
1	A	31	LEU	2.7
1	A	124	LEU	2.7
1	A	423	MET	2.7
1	B	408	ASP	2.7
1	B	362	GLY	2.7
1	B	480	PRO	2.7
1	A	492	ILE	2.7
1	B	291	ILE	2.7
1	B	437	TRP	2.7
1	A	286	VAL	2.7
1	A	400	ASP	2.7
1	B	2	ILE	2.7
1	A	280	ALA	2.6
1	A	224	TYR	2.6
1	A	375	GLU	2.6
1	A	517	VAL	2.6
1	A	555	SER	2.6
1	B	376	LEU	2.6
1	A	71	GLU	2.6
1	A	274	ALA	2.6
1	B	424	ASP	2.6
1	A	336	GLU	2.6
1	A	278	ALA	2.6
1	B	215	THR	2.6
1	B	354	GLY	2.6
1	B	381	PHE	2.6
1	A	364	VAL	2.6
1	B	305	ILE	2.6
1	A	370	HIS	2.6
1	B	12	LEU	2.5
1	A	420	ALA	2.5
1	A	449	GLY	2.5
1	A	63	SER	2.5
1	B	262	SER	2.5
1	B	264	VAL	2.5
1	A	234	ILE	2.5
1	A	258	ILE	2.5
1	A	230	ASP	2.5
1	B	121	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	2.5
1	A	362	GLY	2.5
1	B	393	LEU	2.5
1	A	261	ALA	2.5
1	B	230	ASP	2.5
1	B	317	PRO	2.5
1	B	93	THR	2.5
1	A	7	VAL	2.5
1	A	557	ARG	2.5
1	B	87	TYR	2.5
1	B	231	LEU	2.5
1	A	95	ALA	2.5
1	A	523	ALA	2.5
1	A	413	PRO	2.5
1	B	54	PRO	2.5
1	B	61	GLN	2.5
1	B	254	PRO	2.5
1	A	514	THR	2.4
1	B	301	GLU	2.4
1	A	27	VAL	2.4
1	B	525	ILE	2.4
1	B	325	GLN	2.4
1	B	41	GLY	2.4
1	B	69	ARG	2.4
1	A	51	VAL	2.4
1	A	440	ILE	2.4
1	A	437	TRP	2.4
1	B	71	GLU	2.4
1	A	23	ALA	2.4
1	B	397	ALA	2.4
1	A	453	THR	2.4
1	A	384	PHE	2.4
1	A	475	VAL	2.4
1	A	20	ARG	2.4
1	B	164	ASN	2.4
1	B	68	ALA	2.4
1	B	365	SER	2.4
1	A	376	LEU	2.4
1	B	53	ASN	2.3
1	B	142	TYR	2.3
1	A	554	GLY	2.3
1	A	15	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	268	SER	2.3
1	B	222	VAL	2.3
1	B	557	ARG	2.3
1	B	196	LEU	2.3
1	A	3	GLU	2.3
1	B	14	ASP	2.3
1	B	261	ALA	2.3
1	B	558	ILE	2.3
1	B	111	PHE	2.3
1	B	113	VAL	2.3
1	A	57	LEU	2.3
1	A	123	CYS	2.3
1	B	566	LEU	2.3
1	A	242	ASP	2.3
1	B	201	PRO	2.3
1	A	350	GLY	2.3
1	B	39	ALA	2.3
1	B	62	ALA	2.3
1	B	271	ALA	2.3
1	B	238	VAL	2.3
1	B	427	VAL	2.3
1	A	564	PRO	2.3
1	B	479	GLY	2.3
1	A	379	TRP	2.3
1	A	300	SER	2.3
1	A	11	GLU	2.3
1	B	364	VAL	2.3
1	B	109	ASP	2.2
1	B	176	ALA	2.2
1	B	181	GLU	2.2
1	A	13	ARG	2.2
1	B	303	PRO	2.2
1	A	459	GLU	2.2
1	A	365	SER	2.2
1	B	18	SER	2.2
1	B	426	TYR	2.2
1	B	250	TRP	2.2
1	A	412	LEU	2.2
1	A	559	VAL	2.2
1	B	340	VAL	2.2
1	A	457	ASP	2.2
1	B	389	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	2.2
1	B	56	ALA	2.2
1	B	302	SER	2.2
1	A	269	TYR	2.2
1	A	385	LEU	2.2
1	B	211	ASN	2.2
1	A	120	GLY	2.2
1	A	122	ILE	2.1
1	A	250	TRP	2.1
1	B	471	LEU	2.1
1	A	236	ASP	2.1
1	B	400	ASP	2.1
1	A	266	PRO	2.1
1	A	372	GLU	2.1
1	A	526	GLY	2.1
1	B	210	GLY	2.1
1	A	231	LEU	2.1
1	A	507	ILE	2.1
1	A	256	VAL	2.1
1	B	256	VAL	2.1
1	B	314	HIS	2.1
1	B	275	GLY	2.1
1	A	93	THR	2.1
1	A	439	ARG	2.1
1	A	180	ALA	2.1
1	B	488	ALA	2.1
1	A	102	LYS	2.1
1	A	85	ASP	2.1
1	A	241	ASP	2.1
1	B	74	GLY	2.1
1	A	415	ARG	2.1
1	A	22	THR	2.1
1	B	268	SER	2.1
1	A	435	LYS	2.1
1	A	469	ALA	2.1
1	A	92	LEU	2.1
1	A	314	HIS	2.1
1	B	30	TYR	2.1
1	B	334	GLY	2.1
1	A	245	THR	2.0
1	B	299	THR	2.0
1	A	110	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	2.0
1	A	394	ASN	2.0
1	A	408	ASP	2.0
1	B	16	LEU	2.0
1	B	85	ASP	2.0
1	B	88	LEU	2.0
1	A	558	ILE	2.0
1	B	40	PRO	2.0
1	A	239	VAL	2.0
1	B	498	VAL	2.0
1	B	374	TRP	2.0
1	A	159	ALA	2.0
1	B	48	ALA	2.0
1	B	65	ALA	2.0
1	B	335	ALA	2.0
1	B	64	ASP	2.0
1	B	383	ASP	2.0
1	B	445	ASP	2.0
1	A	518	PRO	2.0
1	B	79	ILE	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.