



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 8S0N / pdb_00008s0n
Title : Crystal structure of the TMPRSS2 zymogen in complex with the nanobody A07
Authors : Duquerroy, S.; Fernandez, I.; Rey, F.
Deposited on : 2024-02-14
Resolution : 2.30 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

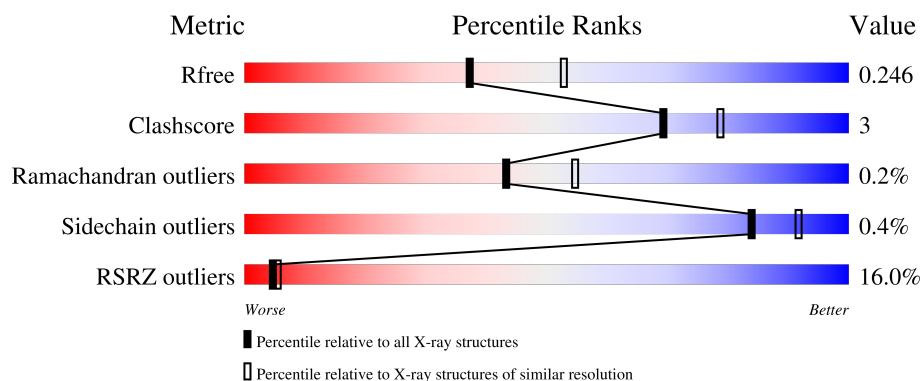
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	397	
1	C	397	
2	B	150	
2	D	150	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7251 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 Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2529	1606	437	463	23			
1	C	324	Total	C	N	O	S	0	1	0
			2535	1612	438	462	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ARG	-	expression tag	UNP O15393
A	106	SER	-	expression tag	UNP O15393
A	441	ALA	SER	engineered mutation	UNP O15393
A	493	GLY	-	expression tag	UNP O15393
A	494	PRO	-	expression tag	UNP O15393
A	495	PHE	-	expression tag	UNP O15393
A	496	GLU	-	expression tag	UNP O15393
A	497	ASP	-	expression tag	UNP O15393
A	498	ASP	-	expression tag	UNP O15393
A	499	ASP	-	expression tag	UNP O15393
A	500	ASP	-	expression tag	UNP O15393
A	501	LYS	-	expression tag	UNP O15393
C	105	ARG	-	expression tag	UNP O15393
C	106	SER	-	expression tag	UNP O15393
C	441	ALA	SER	engineered mutation	UNP O15393
C	493	GLY	-	expression tag	UNP O15393
C	494	PRO	-	expression tag	UNP O15393
C	495	PHE	-	expression tag	UNP O15393
C	496	GLU	-	expression tag	UNP O15393
C	497	ASP	-	expression tag	UNP O15393
C	498	ASP	-	expression tag	UNP O15393
C	499	ASP	-	expression tag	UNP O15393
C	500	ASP	-	expression tag	UNP O15393
C	501	LYS	-	expression tag	UNP O15393

- Molecule 2 is a protein called nanobody A07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			991	612	180	196	3			
2	D	129	Total	C	N	O	S	0	0	0
			987	610	179	195	3			

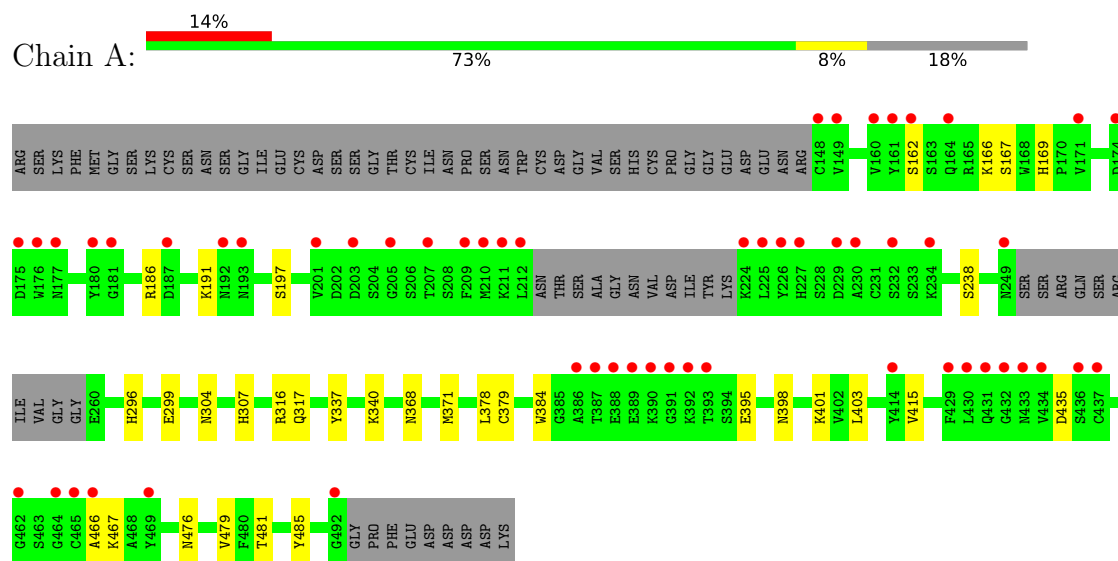
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	57	Total	O	0	0
			57	57		
3	D	19	Total	O	0	0
			19	19		
3	C	46	Total	O	0	0
			46	46		

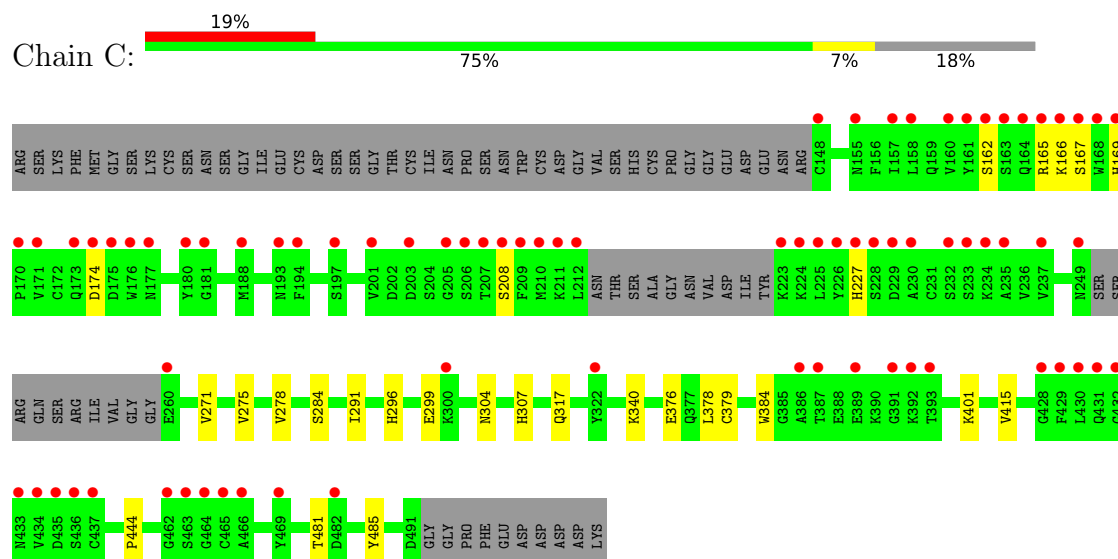
3 Residue-property plots

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.

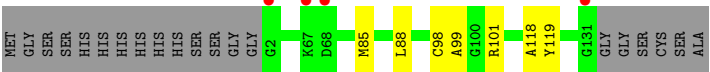
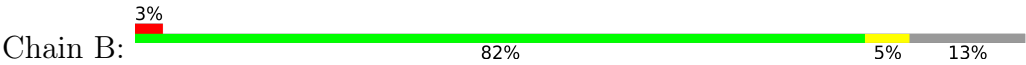
• Molecule 1: Transmembrane protease serine 2



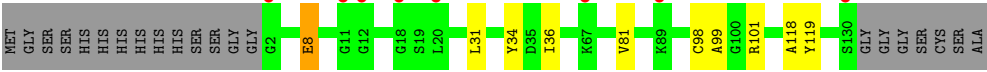
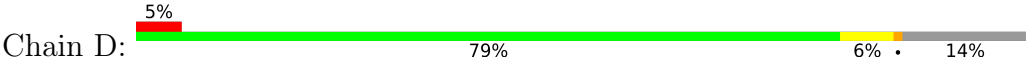
• Molecule 1: Transmembrane protease serine 2



• Molecule 2: nanobody A07



● Molecule 2: nanobody A07



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.87Å 54.46Å 165.82Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	24.42 – 2.30 24.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	82.6 (24.42-2.30) 73.4 (24.42-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.211 , 0.246 0.211 , 0.246	Depositor DCC
R_{free} test set	2556 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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	0.18	0/2598	0.53	0/3534
1	C	0.18	0/2607	0.55	0/3548
2	B	0.19	0/1012	0.48	0/1373
2	D	0.16	0/1008	0.43	0/1368
All	All	0.18	0/7225	0.52	0/9823

There are no bond length outliers.

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	2529	0	2422	23	0
1	C	2535	0	2434	20	0
2	B	991	0	945	5	0
2	D	987	0	942	8	0
3	A	87	0	0	4	0
3	B	57	0	0	1	0
3	C	46	0	0	0	0
3	D	19	0	0	0	0
All	All	7251	0	6743	48	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 3.

All (48) 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:C:167:SER:OG	1:C:169:HIS:NE2	2.20	0.73
1:A:304:ASN:HB3	1:A:307:HIS:CD2	2.26	0.70
1:C:304:ASN:HB3	1:C:307:HIS:CD2	2.28	0.68
1:A:296:HIS:HA	1:A:299:GLU:HG3	1.77	0.66
1:C:296:HIS:HA	1:C:299:GLU:HG3	1.77	0.66
1:A:167:SER:OG	1:A:169:HIS:NE2	2.28	0.65
1:A:401:LYS:NZ	1:C:376:GLU:OE1	2.28	0.65
1:A:435:ASP:HA	1:A:466:ALA:HB2	1.80	0.64
2:D:31:LEU:HD13	2:D:81:VAL:HG23	1.84	0.60
1:A:186:ARG:HG2	1:A:191:LYS:O	2.04	0.58
1:A:485:TYR:OH	3:A:601:HOH:O	2.15	0.57
1:C:165:ARG:HG3	1:C:227:HIS:CE1	2.41	0.56
1:A:316:ARG:NH1	3:A:602:HOH:O	2.38	0.56
2:D:118:ALA:C	1:C:340:LYS:HE3	2.31	0.55
1:A:162:SER:O	1:A:166:LYS:N	2.41	0.54
1:A:299:GLU:OE2	1:A:337:TYR:OH	2.18	0.53
1:C:162:SER:O	1:C:166:LYS:N	2.42	0.53
2:D:8:GLU:N	2:D:8:GLU:OE1	2.44	0.51
1:A:403:LEU:HD13	1:C:378:LEU:HD22	1.91	0.50
1:A:317:GLN:HE21	1:A:384:TRP:CG	2.30	0.50
1:C:275:VAL:O	1:C:278:VAL:HG22	2.12	0.49
1:C:271:VAL:HG21	1:C:291:ILE:HD13	1.94	0.49
1:A:340:LYS:HE3	2:B:118:ALA:C	2.38	0.48
2:D:99:ALA:HA	2:D:119:TYR:O	2.14	0.48
1:C:317:GLN:HE21	1:C:384:TRP:CG	2.32	0.47
1:C:284:SER:OG	1:C:444:PRO:HB3	2.14	0.47
1:A:395:GLU:OE2	3:A:602:HOH:O	2.21	0.47
1:A:378:LEU:HD12	1:A:379:CYS:N	2.30	0.46
2:B:85:MET:HB3	2:B:88:LEU:HD21	1.98	0.45
1:A:398:ASN:HB2	3:A:635:HOH:O	2.16	0.45
2:D:119:TYR:CE1	1:C:340:LYS:HE2	2.51	0.44
1:C:378:LEU:HD12	1:C:379:CYS:N	2.33	0.44
2:D:36:ILE:HG13	2:D:81:VAL:HG21	2.00	0.44
1:A:368:ASN:O	1:A:371:MET:HG2	2.18	0.44
1:A:476:ASN:O	1:A:479:VAL:HG22	2.18	0.44
1:A:340:LYS:HE2	2:B:119:TYR:CE1	2.54	0.43
1:A:378:LEU:HD23	1:C:376:GLU:HB2	2.00	0.43
2:B:99:ALA:HA	2:B:119:TYR:O	2.19	0.42
1:A:467:LYS:HD3	1:A:467:LYS:HA	1.82	0.42
2:D:119:TYR:CD1	1:C:340:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:THR:HG22	1:C:485:TYR:CE2	2.54	0.42
1:A:481:THR:HG22	1:A:485:TYR:CE2	2.55	0.42
1:A:197:SER:HA	1:A:238:SER:O	2.20	0.41
2:D:34:TYR:HA	2:D:101:ARG:O	2.21	0.41
1:C:174:ASP:N	1:C:174:ASP:OD1	2.53	0.40
1:C:169:HIS:ND1	1:C:208:SER:O	2.54	0.40
2:B:101:ARG:HD2	3:B:239:HOH:O	2.22	0.40
1:C:378:LEU:HD21	1:C:401:LYS:HE2	2.03	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	Percentiles	
1	A	318/397 (80%)	307 (96%)	10 (3%)	1 (0%)	36	46
1	C	319/397 (80%)	309 (97%)	9 (3%)	1 (0%)	36	46
2	B	128/150 (85%)	124 (97%)	4 (3%)	0	100	100
2	D	127/150 (85%)	123 (97%)	4 (3%)	0	100	100
All	All	892/1094 (82%)	863 (97%)	27 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	VAL
1	C	415	VAL

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	Percentiles	
1	A	273/337 (81%)	273 (100%)	0	100	100
1	C	274/337 (81%)	274 (100%)	0	100	100
2	B	106/120 (88%)	105 (99%)	1 (1%)	70	84
2	D	106/120 (88%)	104 (98%)	2 (2%)	50	69
All	All	759/914 (83%)	756 (100%)	3 (0%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	98	CYS
2	D	8	GLU
2	D	98	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	HIS
1	A	336	ASN
1	A	418	ASN
2	B	33	HIS
2	D	59	HIS
1	C	164	GLN
1	C	307	HIS
1	C	336	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 [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	324/397 (81%)	0.71	56 (17%) 4 4	26, 48, 115, 157	0
1	C	324/397 (81%)	1.19	77 (23%) 2 2	33, 63, 138, 176	1 (0%)
2	B	130/150 (86%)	0.21	4 (3%) 51 53	32, 46, 72, 109	0
2	D	129/150 (86%)	0.82	8 (6%) 26 28	48, 64, 91, 111	0
All	All	907/1094 (82%)	0.82	145 (15%) 5 5	26, 57, 123, 176	1 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	ALA	6.4
1	A	225	LEU	6.2
1	C	387	THR	6.2
1	A	387	THR	5.9
1	A	224	LYS	5.5
1	A	175	ASP	5.5
1	C	223	LYS	5.3
1	C	201	VAL	5.2
1	A	389	GLU	5.1
1	A	162	SER	4.9
1	C	386	ALA	4.8
1	C	148	CYS	4.8
1	A	212	LEU	4.7
1	C	212	LEU	4.7
1	C	205	GLY	4.5
1	C	226	TYR	4.4
1	C	432	GLY	4.4
1	A	465	CYS	4.3
1	A	386	ALA	4.3
1	C	232	SER	4.2
1	C	176	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	230	ALA	4.2
1	C	162	SER	4.2
1	A	176	TRP	4.2
1	C	167	SER	4.1
1	C	225	LEU	4.1
1	C	229	ASP	4.1
1	C	434	VAL	4.0
1	C	228	SER	3.9
1	A	201	VAL	3.9
1	A	431	GLN	3.9
2	B	131	GLY	3.9
1	A	229	ASP	3.9
1	C	249	ASN	3.9
1	A	392	LYS	3.9
1	C	224	LYS	3.9
1	C	465	CYS	3.8
1	C	164	GLN	3.8
1	C	389	GLU	3.8
1	A	434	VAL	3.8
2	B	2	GLY	3.8
1	A	466	ALA	3.7
1	A	433	ASN	3.6
1	C	161	TYR	3.6
1	A	432	GLY	3.6
1	C	163	SER	3.6
2	D	2	GLY	3.6
1	C	464	GLY	3.5
1	A	226	TYR	3.5
1	A	148	CYS	3.5
1	C	160	VAL	3.4
1	C	234	LYS	3.4
1	A	205	GLY	3.4
1	C	431	GLN	3.4
1	C	169	HIS	3.4
1	C	168	TRP	3.4
1	C	207	THR	3.4
1	C	166	LYS	3.4
1	C	181	GLY	3.4
1	A	492	GLY	3.3
1	C	429	PHE	3.3
1	A	249	ASN	3.3
1	C	203	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	3.3
1	C	209	PHE	3.2
1	A	232	SER	3.2
1	C	233	SER	3.2
1	C	171	VAL	3.2
1	C	170	PRO	3.2
2	D	20	LEU	3.2
1	C	260	GLU	3.1
1	A	160	VAL	3.1
1	A	164	GLN	3.1
1	C	165	ARG	3.1
1	C	463	SER	3.1
1	C	433	ASN	3.1
1	A	211	LYS	3.0
1	A	390	LYS	3.0
2	B	67	LYS	3.0
1	A	430	LEU	2.9
1	A	174	ASP	2.9
1	C	175	ASP	2.9
1	A	436	SER	2.9
1	C	180	TYR	2.9
1	C	237	VAL	2.9
1	C	393	THR	2.9
1	C	227	HIS	2.8
1	A	210	MET	2.8
1	C	210	MET	2.8
1	C	392	LYS	2.8
1	A	209	PHE	2.8
1	A	437	CYS	2.7
1	A	181	GLY	2.7
1	C	157	ILE	2.7
1	C	174	ASP	2.6
1	A	462	GLY	2.6
1	C	208	SER	2.6
1	C	155	ASN	2.6
2	D	67	LYS	2.6
1	C	177	ASN	2.5
1	A	180	TYR	2.5
1	C	188	MET	2.5
2	D	11	GLY	2.5
1	C	211	LYS	2.5
1	A	393	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	428	GLY	2.4
1	A	388	GLU	2.4
1	C	391	GLY	2.4
1	C	194	PHE	2.4
1	A	161	TYR	2.4
2	D	130	SER	2.3
1	C	466	ALA	2.3
1	A	429	PHE	2.3
1	C	435	ASP	2.3
2	D	12	GLY	2.3
1	A	230	ALA	2.3
1	A	171	VAL	2.3
1	A	193	ASN	2.2
1	C	193	ASN	2.2
1	A	414	TYR	2.2
1	C	462	GLY	2.2
1	C	469	TYR	2.2
1	A	192	ASN	2.2
1	A	234	LYS	2.2
1	C	437	CYS	2.2
1	C	197	SER	2.2
1	A	203	ASP	2.1
1	C	206	SER	2.1
1	C	430	LEU	2.1
2	D	89	LYS	2.1
1	A	227	HIS	2.1
1	C	173	GLN	2.1
1	A	391	GLY	2.1
1	C	436	SER	2.1
1	A	149	VAL	2.1
1	A	187	ASP	2.1
2	B	68	ASP	2.1
1	A	469	TYR	2.1
1	C	322	TYR	2.1
1	C	300	LYS	2.0
1	A	207	THR	2.0
1	A	464	GLY	2.0
2	D	18	GLY	2.0
1	A	177	ASN	2.0
1	C	482	ASP	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.