



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:01 AM UTC

PDB ID : 7PG8 / pdb_00007pg8
Title : NaV_Ae1/Sp1CTD_pore-ANT05 complex
Authors : Lolicato, M.; Arrigoni, C.
Deposited on : 2021-08-13
Resolution : 4.50 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

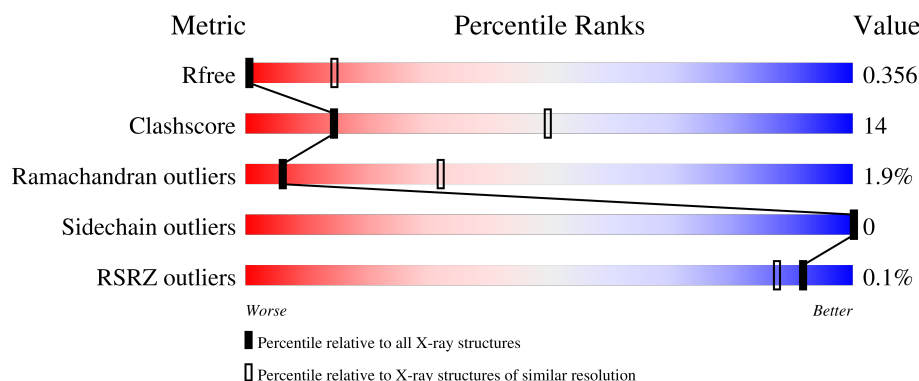
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.



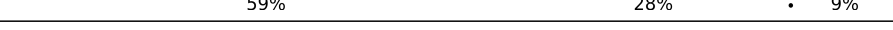
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	217	86% 13% .
1	D	217	86% 13% .
1	G	217	85% 14% .
1	J	217	85% 14% .
1	M	217	86% 13% .

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Mol	Chain	Length	Quality of chain
1	P	217	 84% 15% •
1	S	217	 85% 14% •
1	V	217	 84% 15% •
2	B	233	 77% 17% • 5%
2	F	233	 75% 19% • 5%
2	I	233	 78% 16% • 5%
2	L	233	 76% 18% • 5%
2	N	233	 78% 16% • 5%
2	R	233	 76% 18% • 5%
2	U	233	 78% 16% • 5%
2	X	233	 76% 18% • 5%
3	C	143	 61% 25% • 11%
3	E	143	 57% 31% • 10%
3	H	143	 59% 28% • 9%
3	K	143	 60% 25% 5% 10%
3	O	143	 63% 26% • 9%
3	Q	143	 57% 28% • 12%
3	T	143	 60% 29% • 9%
3	W	143	 60% 26% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22623 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 ANT05 H12 fab fragment, light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	M	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	V	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	S	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	G	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	D	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	J	215	Total	C	N	O	0	0	0
			1086	656	215	215			
1	A	215	Total	C	N	O	0	0	0
			1086	656	215	215			

- Molecule 2 is a protein called ANT05 H12 fab fragment, heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	F	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	I	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	L	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	N	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	R	221	Total	C	N	O	0	0	0
			1106	664	221	221			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	221	Total	C	N	O	0	0	0
			1106	664	221	221			
2	X	221	Total	C	N	O	0	0	0
			1106	664	221	221			

- Molecule 3 is a protein called Ion transport protein, Voltage-gated sodium channel.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	127	Total	C	N	O	0	0	0
			628	374	127	127			
3	E	128	Total	C	N	O	0	0	0
			633	377	128	128			
3	H	130	Total	C	N	O	0	0	0
			643	383	130	130			
3	K	129	Total	C	N	O	0	0	0
			638	380	129	129			
3	O	130	Total	C	N	O	0	0	0
			643	383	130	130			
3	Q	126	Total	C	N	O	0	0	0
			623	371	126	126			
3	T	130	Total	C	N	O	0	0	0
			641	381	130	130			
3	W	129	Total	C	N	O	0	0	0
			638	380	129	129			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
E	137	GLY	-	expression tag	UNP Q0ABW0
E	138	PRO	-	expression tag	UNP Q0ABW0
E	139	SER	-	expression tag	UNP Q0ABW0
E	140	SER	-	expression tag	UNP Q0ABW0
E	141	PRO	-	expression tag	UNP Q0ABW0
E	142	SER	-	expression tag	UNP Q0ABW0
H	137	GLY	-	expression tag	UNP Q0ABW0
H	138	PRO	-	expression tag	UNP Q0ABW0

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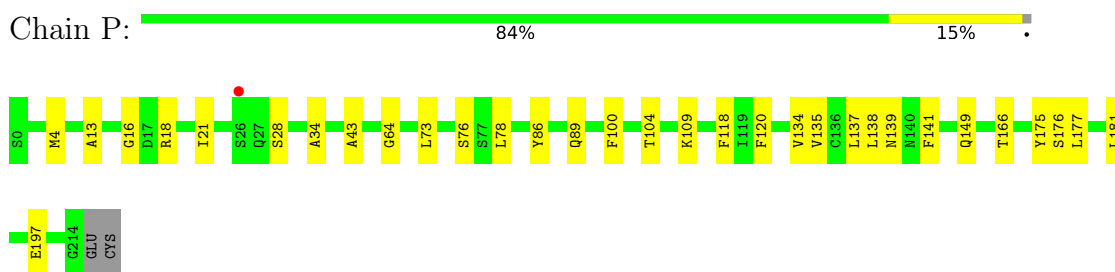
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Chain	Residue	Modelled	Actual	Comment	Reference
H	139	SER	-	expression tag	UNP Q0ABW0
H	140	SER	-	expression tag	UNP Q0ABW0
H	141	PRO	-	expression tag	UNP Q0ABW0
H	142	SER	-	expression tag	UNP Q0ABW0
K	137	GLY	-	expression tag	UNP Q0ABW0
K	138	PRO	-	expression tag	UNP Q0ABW0
K	139	SER	-	expression tag	UNP Q0ABW0
K	140	SER	-	expression tag	UNP Q0ABW0
K	141	PRO	-	expression tag	UNP Q0ABW0
K	142	SER	-	expression tag	UNP Q0ABW0
O	137	GLY	-	expression tag	UNP Q0ABW0
O	138	PRO	-	expression tag	UNP Q0ABW0
O	139	SER	-	expression tag	UNP Q0ABW0
O	140	SER	-	expression tag	UNP Q0ABW0
O	141	PRO	-	expression tag	UNP Q0ABW0
O	142	SER	-	expression tag	UNP Q0ABW0
Q	137	GLY	-	expression tag	UNP Q0ABW0
Q	138	PRO	-	expression tag	UNP Q0ABW0
Q	139	SER	-	expression tag	UNP Q0ABW0
Q	140	SER	-	expression tag	UNP Q0ABW0
Q	141	PRO	-	expression tag	UNP Q0ABW0
Q	142	SER	-	expression tag	UNP Q0ABW0
T	137	GLY	-	expression tag	UNP Q0ABW0
T	138	PRO	-	expression tag	UNP Q0ABW0
T	139	SER	-	expression tag	UNP Q0ABW0
T	140	SER	-	expression tag	UNP Q0ABW0
T	141	PRO	-	expression tag	UNP Q0ABW0
T	142	SER	-	expression tag	UNP Q0ABW0
W	137	GLY	-	expression tag	UNP Q0ABW0
W	138	PRO	-	expression tag	UNP Q0ABW0
W	139	SER	-	expression tag	UNP Q0ABW0
W	140	SER	-	expression tag	UNP Q0ABW0
W	141	PRO	-	expression tag	UNP Q0ABW0
W	142	SER	-	expression tag	UNP Q0ABW0

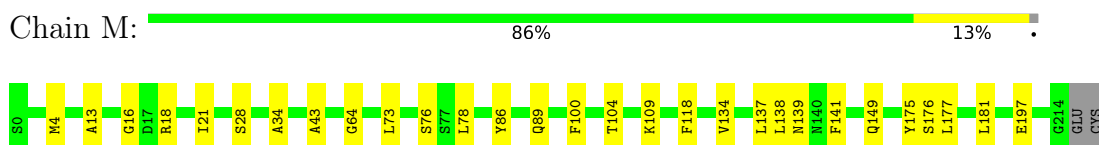
3 Residue-property plots

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.

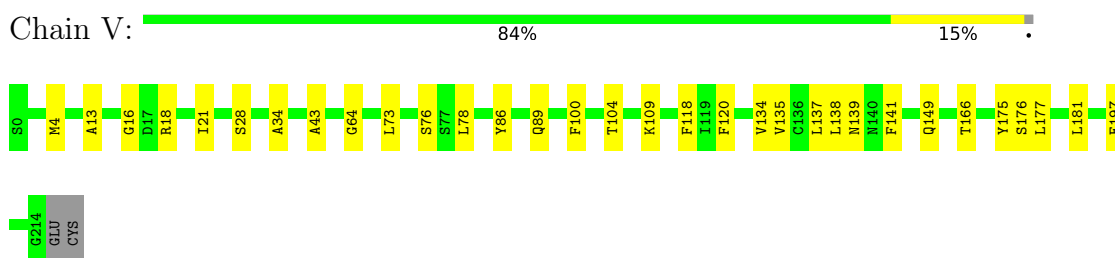
- Molecule 1: ANT05 H12 fab fragment, light chain



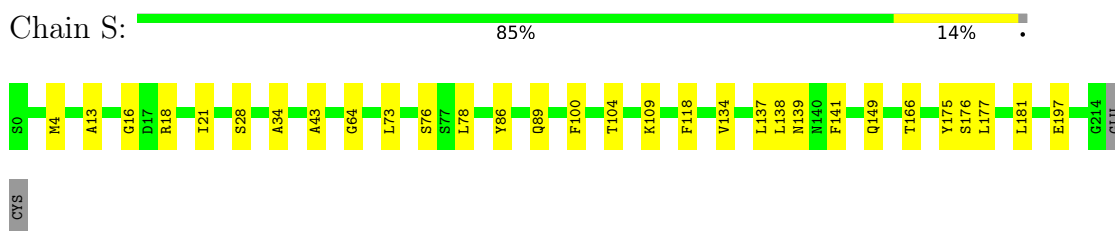
- Molecule 1: ANT05 H12 fab fragment, light chain



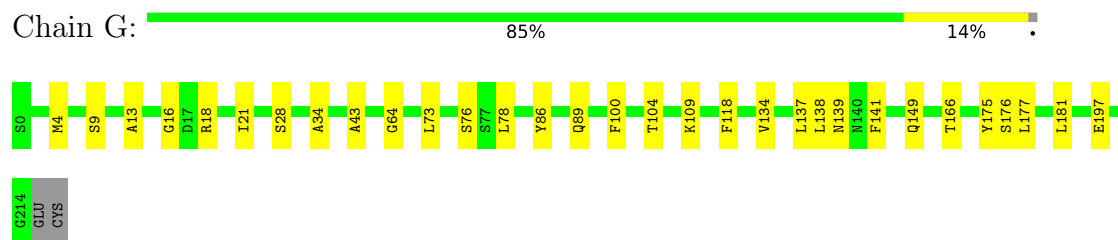
- Molecule 1: ANT05 H12 fab fragment, light chain



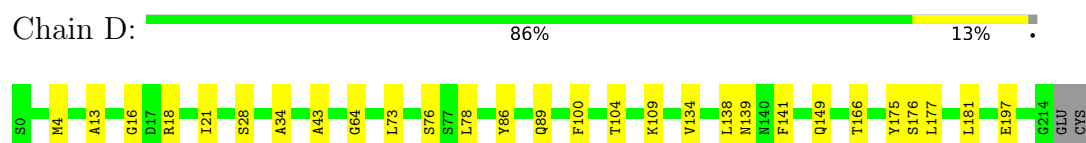
- Molecule 1: ANT05 H12 fab fragment, light chain



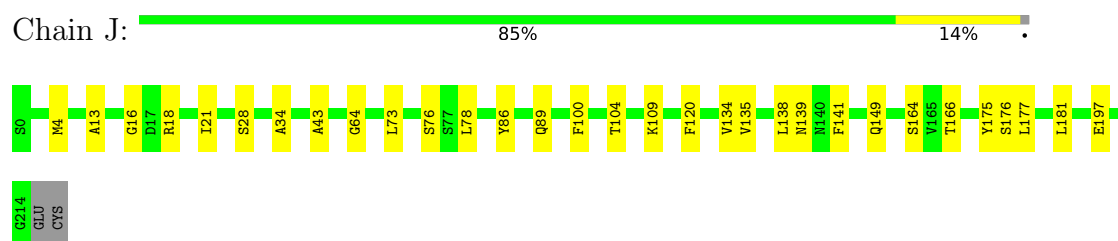
- Molecule 1: ANT05 H12 fab fragment, light chain



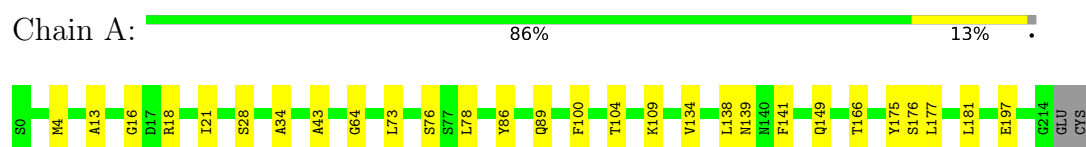
- Molecule 1: ANT05 H12 fab fragment, light chain



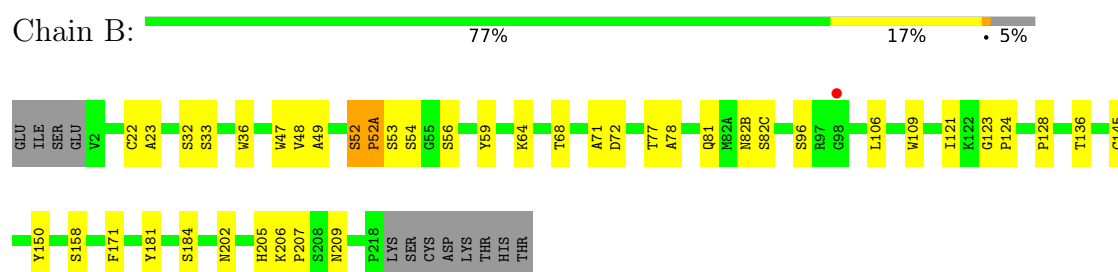
- Molecule 1: ANT05 H12 fab fragment, light chain



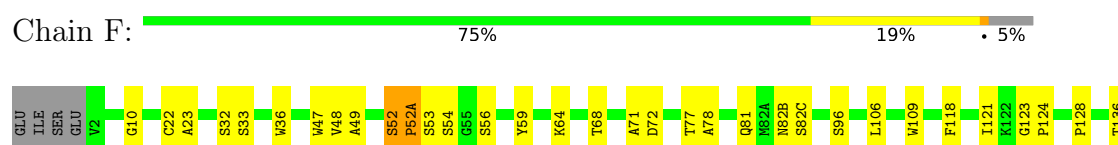
- Molecule 1: ANT05 H12 fab fragment, light chain



- Molecule 2: ANT05 H12 fab fragment, heavy chain



- Molecule 2: ANT05 H12 fab fragment, heavy chain





- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain I: 78% 16% • 5%



- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain L: 76% 18% • 5%



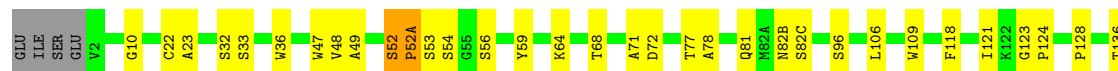
- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain N: 78% 16% • 5%



- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain R: 76% 18% • 5%



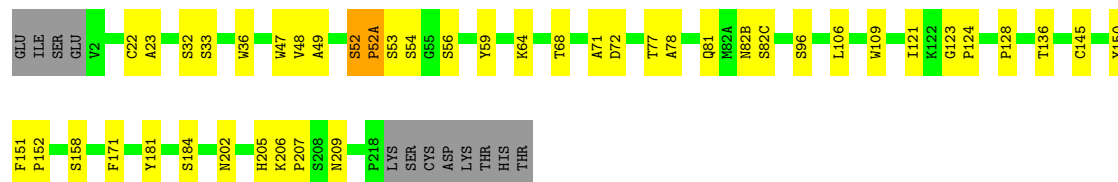
- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain U: 78% 16% • 5%



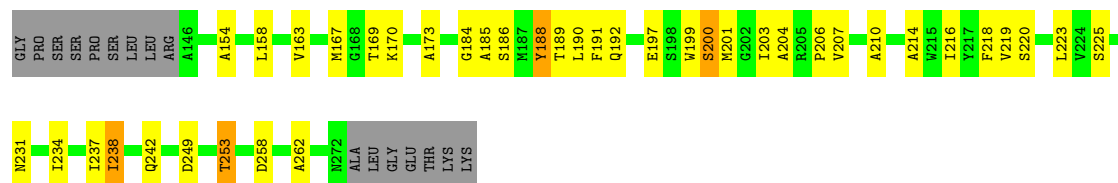
- Molecule 2: ANT05 H12 fab fragment, heavy chain

Chain X: 76% 18% 5%



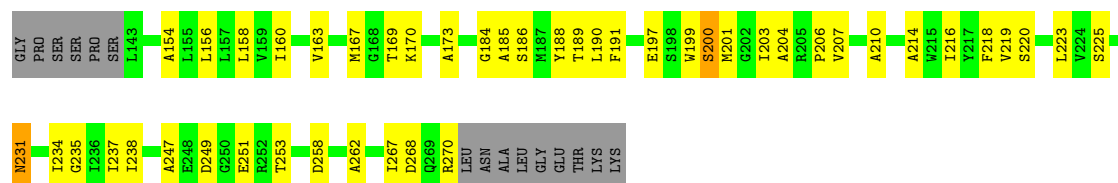
- Molecule 3: Ion transport protein, Voltage-gated sodium channel

Chain C: 61% 25% 11%



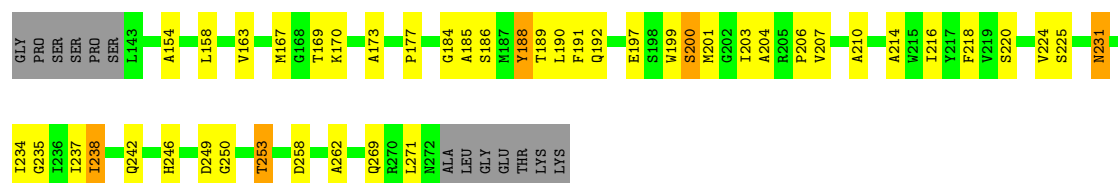
- Molecule 3: Ion transport protein, Voltage-gated sodium channel

Chain E: 57% 31% 10%



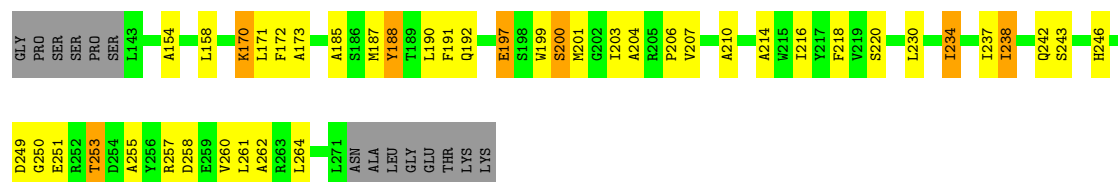
- Molecule 3: Ion transport protein, Voltage-gated sodium channel

Chain H: 59% 28% 9%

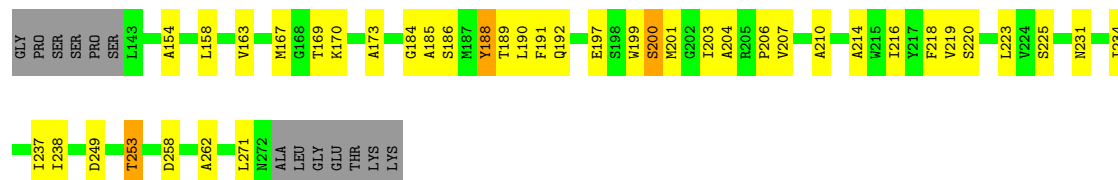


- Molecule 3: Ion transport protein, Voltage-gated sodium channel

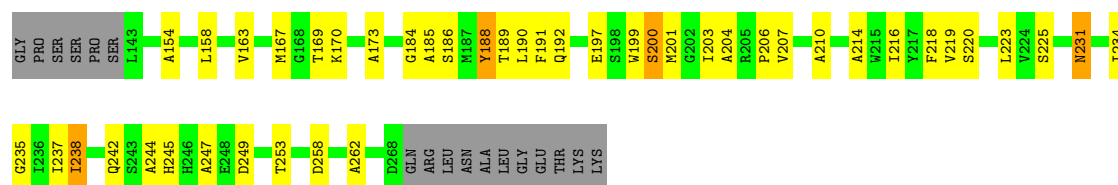
Chain K: 60% 25% 5% 10%



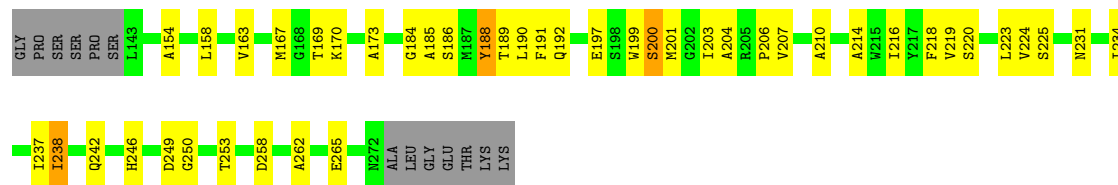
- Molecule 3: Ion transport protein, Voltage-gated sodium channel



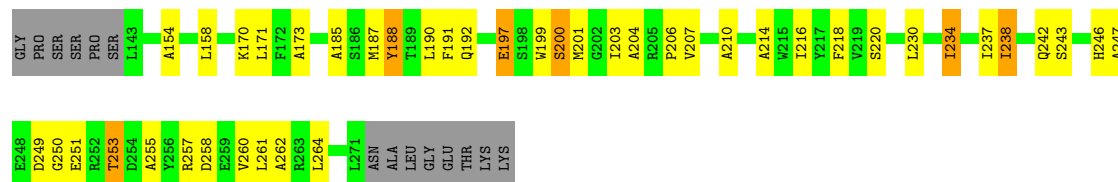
- Molecule 3: Ion transport protein, Voltage-gated sodium channel



- Molecule 3: Ion transport protein, Voltage-gated sodium channel



- Molecule 3: Ion transport protein, Voltage-gated sodium channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	127.17Å 127.17Å 445.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 4.50 15.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-4.50) 98.7 (15.00-4.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 4.54Å)	Xtriage
Refinement program	REFMAC 5.8.0	Depositor
R, R_{free}	0.303 , 0.352 0.317 , 0.356	Depositor DCC
R_{free} test set	2144 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	254.6	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 468.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.349 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22623	wwPDB-VP
Average B, all atoms (Å ²)	251.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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	1.30	0/1096	1.56	0/1535
1	D	1.30	0/1096	1.55	0/1535
1	G	1.30	0/1096	1.55	0/1535
1	J	1.30	0/1096	1.55	0/1535
1	M	1.30	0/1096	1.56	0/1535
1	P	1.30	0/1096	1.55	0/1535
1	S	1.30	0/1096	1.56	0/1535
1	V	1.30	0/1096	1.55	0/1535
2	B	1.28	0/1111	1.60	0/1540
2	F	1.28	0/1111	1.60	1/1540 (0.1%)
2	I	1.27	0/1111	1.59	0/1540
2	L	1.27	0/1111	1.60	0/1540
2	N	1.27	0/1111	1.60	0/1540
2	R	1.28	0/1111	1.60	1/1540 (0.1%)
2	U	1.27	0/1111	1.60	0/1540
2	X	1.27	0/1111	1.60	0/1540
3	C	1.31	5/627 (0.8%)	1.94	13/872 (1.5%)
3	E	1.30	5/632 (0.8%)	1.92	12/879 (1.4%)
3	H	1.31	6/642 (0.9%)	1.96	14/893 (1.6%)
3	K	1.35	6/637 (0.9%)	2.04	15/886 (1.7%)
3	O	1.32	5/642 (0.8%)	1.92	14/893 (1.6%)
3	Q	1.30	5/621 (0.8%)	1.94	13/862 (1.5%)
3	T	1.31	5/640 (0.8%)	1.93	14/889 (1.6%)
3	W	1.35	6/637 (0.9%)	2.04	13/886 (1.5%)
All	All	1.29	43/22734 (0.2%)	1.67	110/31660 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	I	0	1
2	L	0	1
2	N	0	1
2	R	0	1
2	U	0	1
2	X	0	1
3	C	0	1
3	E	0	2
3	H	0	1
3	K	0	1
3	O	0	1
3	Q	0	1
3	T	0	1
3	W	0	1
All	All	0	17

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	187	MET	C-O	-8.06	1.14	1.24
3	K	187	MET	C-O	-8.04	1.14	1.24
3	C	186	SER	C-O	6.58	1.31	1.24
3	O	186	SER	C-O	6.57	1.31	1.24
3	T	186	SER	C-O	6.53	1.31	1.24
3	H	186	SER	C-O	6.53	1.31	1.24
3	Q	186	SER	C-O	6.44	1.31	1.24
3	E	186	SER	C-O	6.44	1.31	1.24
3	W	188	TYR	C-O	-6.38	1.16	1.24
3	K	188	TYR	C-O	-6.36	1.16	1.24
3	H	200	SER	C-O	-6.09	1.16	1.24
3	T	200	SER	C-O	-6.06	1.16	1.24
3	W	264	LEU	C-O	-6.04	1.16	1.24
3	C	200	SER	C-O	-6.02	1.16	1.24
3	Q	200	SER	C-O	-6.02	1.16	1.24
3	O	200	SER	C-O	-6.01	1.16	1.24
3	E	200	SER	C-O	-6.00	1.16	1.24
3	K	200	SER	C-O	-5.96	1.16	1.24
3	W	200	SER	C-O	-5.87	1.16	1.24
3	K	264	LEU	C-O	-5.86	1.16	1.24
3	C	238	ILE	C-O	5.60	1.30	1.24
3	O	238	ILE	C-O	5.50	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	188	TYR	C-O	-5.49	1.17	1.24
3	T	238	ILE	C-O	5.46	1.30	1.24
3	H	188	TYR	C-O	-5.45	1.17	1.24
3	Q	188	TYR	C-O	-5.43	1.17	1.24
3	C	188	TYR	C-O	-5.43	1.17	1.24
3	O	188	TYR	C-O	-5.41	1.17	1.24
3	H	238	ILE	C-O	5.40	1.30	1.24
3	E	188	TYR	C-O	-5.39	1.17	1.24
3	H	225	SER	C-O	5.33	1.30	1.24
3	K	238	ILE	C-O	5.31	1.30	1.24
3	W	238	ILE	C-O	5.30	1.30	1.24
3	T	225	SER	C-O	5.27	1.30	1.24
3	E	225	SER	C-O	5.18	1.30	1.24
3	W	171	LEU	C-O	-5.16	1.17	1.24
3	Q	225	SER	C-O	5.15	1.30	1.24
3	E	238	ILE	C-O	5.13	1.29	1.24
3	Q	238	ILE	C-O	5.13	1.29	1.24
3	K	171	LEU	C-O	-5.11	1.17	1.24
3	C	225	SER	C-O	5.10	1.29	1.24
3	H	177	PRO	C-O	-5.09	1.17	1.24
3	O	225	SER	C-O	5.02	1.29	1.24

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	253	THR	CA-C-O	-7.25	113.23	120.70
3	O	234	ILE	O-C-N	7.03	128.80	121.91
3	C	234	ILE	O-C-N	6.98	128.75	121.91
3	E	201	MET	N-CA-C	-6.96	103.62	111.07
3	K	201	MET	N-CA-C	-6.96	103.62	111.07
3	Q	201	MET	N-CA-C	-6.95	103.63	111.07
3	W	201	MET	N-CA-C	-6.95	103.63	111.07
3	T	234	ILE	O-C-N	6.90	128.68	121.91
3	T	201	MET	N-CA-C	-6.90	103.69	111.07
3	H	234	ILE	O-C-N	6.90	128.67	121.91
3	H	201	MET	N-CA-C	-6.89	103.70	111.07
3	K	191	PHE	N-CA-C	-6.89	103.77	111.28
3	O	201	MET	N-CA-C	-6.88	103.71	111.07
3	C	201	MET	N-CA-C	-6.88	103.71	111.07
3	W	191	PHE	N-CA-C	-6.82	103.85	111.28
3	W	234	ILE	O-C-N	6.67	128.61	121.94
3	W	170	LYS	N-CA-C	-6.66	103.95	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	234	ILE	O-C-N	6.63	128.41	121.91
3	K	170	LYS	N-CA-C	-6.62	103.99	111.14
3	K	234	ILE	O-C-N	6.61	128.55	121.94
3	Q	234	ILE	O-C-N	6.61	128.38	121.91
3	H	169	THR	O-C-N	6.55	129.06	122.12
3	T	191	PHE	N-CA-C	-6.46	104.24	111.28
3	Q	191	PHE	N-CA-C	-6.45	104.25	111.28
3	C	191	PHE	N-CA-C	-6.44	104.26	111.28
3	E	191	PHE	N-CA-C	-6.43	104.27	111.28
3	O	191	PHE	N-CA-C	-6.43	104.27	111.28
3	H	191	PHE	N-CA-C	-6.39	104.31	111.28
3	T	169	THR	O-C-N	6.38	128.89	122.12
3	C	169	THR	O-C-N	6.29	128.79	122.12
3	O	169	THR	O-C-N	6.22	128.72	122.12
3	E	169	THR	O-C-N	6.03	128.51	122.12
3	Q	169	THR	O-C-N	6.02	128.50	122.12
3	C	231	ASN	N-CA-C	-5.56	105.30	111.36
3	O	231	ASN	N-CA-C	-5.55	105.31	111.36
3	H	231	ASN	N-CA-C	-5.55	105.31	111.36
3	T	231	ASN	N-CA-C	-5.53	105.34	111.36
3	E	231	ASN	N-CA-C	-5.47	105.40	111.36
3	Q	231	ASN	N-CA-C	-5.43	105.44	111.36
3	W	260	VAL	O-C-N	5.38	127.33	121.90
2	F	10	GLY	CA-C-O	-5.37	118.58	122.45
3	Q	237	ILE	CA-C-N	5.37	127.43	120.56
3	Q	237	ILE	C-N-CA	5.37	127.43	120.56
3	K	260	VAL	O-C-N	5.36	127.32	121.90
3	W	190	LEU	O-C-N	5.30	127.60	122.09
2	R	10	GLY	CA-C-O	-5.30	118.63	122.45
3	E	184	GLY	CA-C-N	5.30	128.37	120.31
3	E	184	GLY	C-N-CA	5.30	128.37	120.31
3	Q	184	GLY	CA-C-N	5.29	128.36	120.31
3	Q	184	GLY	C-N-CA	5.29	128.36	120.31
3	K	243	SER	CA-C-N	5.29	128.35	120.31
3	K	243	SER	C-N-CA	5.29	128.35	120.31
3	K	190	LEU	O-C-N	5.29	127.59	122.09
3	E	237	ILE	CA-C-N	5.29	127.33	120.56
3	E	237	ILE	C-N-CA	5.29	127.33	120.56
3	C	184	GLY	CA-C-N	5.28	128.34	120.31
3	C	184	GLY	C-N-CA	5.28	128.34	120.31
3	H	184	GLY	CA-C-N	5.28	128.33	120.31
3	H	184	GLY	C-N-CA	5.28	128.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	184	GLY	CA-C-N	5.27	128.32	120.31
3	O	184	GLY	C-N-CA	5.27	128.32	120.31
3	T	184	GLY	CA-C-N	5.27	128.31	120.31
3	T	184	GLY	C-N-CA	5.27	128.31	120.31
3	C	199	TRP	N-CA-C	-5.26	107.52	114.04
3	O	199	TRP	N-CA-C	-5.24	107.54	114.04
3	H	170	LYS	N-CA-C	-5.23	105.49	111.14
3	H	199	TRP	N-CA-C	-5.23	107.56	114.04
3	O	253	THR	CA-C-O	-5.21	115.35	120.82
3	W	253	THR	N-CA-C	-5.21	106.43	112.89
3	H	190	LEU	O-C-N	5.20	127.50	122.09
3	K	253	THR	N-CA-C	-5.19	106.45	112.89
3	T	199	TRP	N-CA-C	-5.19	107.60	114.04
3	H	224	VAL	CA-C-O	-5.18	115.68	121.17
3	E	190	LEU	O-C-N	5.17	127.47	122.09
3	E	199	TRP	N-CA-C	-5.16	107.64	114.04
3	H	237	ILE	CA-C-N	5.16	127.17	120.56
3	H	237	ILE	C-N-CA	5.16	127.17	120.56
3	T	237	ILE	CA-C-N	5.16	127.17	120.56
3	T	237	ILE	C-N-CA	5.16	127.17	120.56
3	T	190	LEU	O-C-N	5.16	127.45	122.09
3	O	190	LEU	O-C-N	5.15	127.44	122.09
3	Q	190	LEU	O-C-N	5.15	127.44	122.09
3	Q	199	TRP	N-CA-C	-5.14	107.66	114.04
3	O	237	ILE	CA-C-N	5.14	127.14	120.56
3	O	237	ILE	C-N-CA	5.14	127.14	120.56
3	W	237	ILE	O-C-N	5.14	126.93	121.89
3	C	237	ILE	CA-C-N	5.13	127.13	120.56
3	C	237	ILE	C-N-CA	5.13	127.13	120.56
3	K	190	LEU	CA-C-N	5.12	127.14	120.28
3	K	190	LEU	C-N-CA	5.12	127.14	120.28
3	C	190	LEU	O-C-N	5.12	127.41	122.09
3	O	271	LEU	N-CA-C	-5.11	105.90	111.82
3	K	199	TRP	N-CA-C	-5.10	107.72	114.04
3	T	170	LYS	N-CA-C	-5.09	105.62	111.07
3	W	190	LEU	CA-C-N	5.09	127.11	120.28
3	W	190	LEU	C-N-CA	5.09	127.11	120.28
3	T	265	GLU	N-CA-C	-5.09	107.07	113.28
3	W	199	TRP	N-CA-C	-5.09	107.72	114.04
3	O	170	LYS	N-CA-C	-5.09	105.64	111.14
3	T	224	VAL	CA-C-O	-5.09	115.78	121.17
3	Q	170	LYS	N-CA-C	-5.08	105.65	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	253	THR	CA-C-O	-5.08	115.49	120.82
3	C	170	LYS	N-CA-C	-5.04	105.69	111.14
3	W	243	SER	CA-C-N	5.04	127.97	120.31
3	W	243	SER	C-N-CA	5.04	127.97	120.31
3	E	170	LYS	N-CA-C	-5.03	105.69	111.07
3	Q	245	HIS	O-C-N	5.03	127.52	122.09
3	K	237	ILE	O-C-N	5.01	126.80	121.89
3	K	237	ILE	CA-C-N	5.00	126.97	120.56
3	K	237	ILE	C-N-CA	5.00	126.97	120.56

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	52	SER	Peptide
3	C	173	ALA	Peptide
3	E	173	ALA	Peptide
3	E	268	ASP	Peptide
2	F	52	SER	Peptide
3	H	173	ALA	Peptide
2	I	52	SER	Peptide
3	K	173	ALA	Peptide
2	L	52	SER	Peptide
2	N	52	SER	Peptide
3	O	173	ALA	Peptide
3	Q	173	ALA	Peptide
2	R	52	SER	Peptide
3	T	173	ALA	Peptide
2	U	52	SER	Peptide
3	W	173	ALA	Peptide
2	X	52	SER	Peptide

5.2 Too-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 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	1086	0	540	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1086	0	540	16	0
1	G	1086	0	540	17	0
1	J	1086	0	540	18	0
1	M	1086	0	540	16	0
1	P	1086	0	540	18	0
1	S	1086	0	540	17	0
1	V	1086	0	540	18	0
2	B	1106	0	563	27	0
2	F	1106	0	563	26	0
2	I	1106	0	563	26	0
2	L	1106	0	563	27	0
2	N	1106	0	563	26	0
2	R	1106	0	563	26	0
2	U	1106	0	563	25	0
2	X	1106	0	563	28	0
3	C	628	0	295	15	0
3	E	633	0	297	17	0
3	H	643	0	301	17	0
3	K	638	0	299	19	0
3	O	643	0	301	14	0
3	Q	623	0	292	17	0
3	T	641	0	296	16	0
3	W	638	0	299	19	0
All	All	22623	0	11204	472	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 14.

All (472) 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)
2:F:52(A):PRO:HG3	2:F:56:SER:CB	2.16	0.76
2:I:52(A):PRO:HG3	2:I:56:SER:CB	2.17	0.75
2:X:52(A):PRO:HG3	2:X:56:SER:CB	2.17	0.75
2:R:52(A):PRO:HG3	2:R:56:SER:CB	2.16	0.74
2:U:52(A):PRO:HG3	2:U:56:SER:CB	2.17	0.74
2:N:52(A):PRO:HG3	2:N:56:SER:CB	2.17	0.74
2:B:52(A):PRO:HG3	2:B:56:SER:CB	2.17	0.74
2:L:52(A):PRO:HG3	2:L:56:SER:CB	2.17	0.73
1:V:43:ALA:HB1	2:X:109:TRP:CB	2.18	0.73
3:H:246:HIS:O	3:H:250:GLY:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:246:HIS:O	3:T:250:GLY:N	2.24	0.68
1:S:43:ALA:HB1	2:U:109:TRP:CB	2.26	0.66
3:T:200:SER:O	3:T:204:ALA:N	2.29	0.65
3:H:200:SER:O	3:H:204:ALA:N	2.29	0.65
1:M:43:ALA:HB1	2:N:109:TRP:CB	2.27	0.65
3:E:216:ILE:O	3:E:220:SER:N	2.30	0.65
2:I:52(A):PRO:CG	2:I:56:SER:CB	2.75	0.64
2:X:52(A):PRO:CG	2:X:56:SER:CB	2.75	0.64
2:F:52(A):PRO:CG	2:F:56:SER:CB	2.76	0.64
2:N:52(A):PRO:CG	2:N:56:SER:CB	2.75	0.64
2:B:52(A):PRO:CG	2:B:56:SER:CB	2.75	0.64
3:W:216:ILE:O	3:W:220:SER:N	2.30	0.64
3:Q:200:SER:O	3:Q:204:ALA:N	2.29	0.64
3:O:200:SER:O	3:O:204:ALA:N	2.29	0.64
2:R:52(A):PRO:CG	2:R:56:SER:CB	2.76	0.64
2:U:52(A):PRO:CG	2:U:56:SER:CB	2.75	0.64
3:C:154:ALA:O	3:C:158:LEU:N	2.30	0.63
3:K:200:SER:O	3:K:204:ALA:N	2.29	0.63
3:Q:216:ILE:O	3:Q:220:SER:N	2.30	0.63
2:L:52(A):PRO:CG	2:L:56:SER:CB	2.76	0.63
3:C:216:ILE:O	3:C:220:SER:N	2.30	0.63
3:E:154:ALA:O	3:E:158:LEU:N	2.30	0.63
1:J:141:PHE:N	1:J:175:TYR:O	2.32	0.63
3:C:200:SER:O	3:C:204:ALA:N	2.29	0.62
3:W:200:SER:O	3:W:204:ALA:N	2.29	0.62
1:A:141:PHE:N	1:A:175:TYR:O	2.32	0.62
3:W:154:ALA:O	3:W:158:LEU:N	2.29	0.62
1:G:141:PHE:N	1:G:175:TYR:O	2.32	0.62
3:E:200:SER:O	3:E:204:ALA:N	2.29	0.62
3:K:154:ALA:O	3:K:158:LEU:N	2.29	0.62
3:T:216:ILE:O	3:T:220:SER:N	2.29	0.62
1:V:141:PHE:N	1:V:175:TYR:O	2.32	0.61
3:K:216:ILE:O	3:K:220:SER:N	2.30	0.61
3:Q:154:ALA:O	3:Q:158:LEU:N	2.30	0.61
3:T:154:ALA:O	3:T:158:LEU:N	2.30	0.60
2:L:71:ALA:HA	2:L:78:ALA:HA	1.84	0.60
3:H:216:ILE:O	3:H:220:SER:N	2.29	0.60
3:W:246:HIS:O	3:W:250:GLY:N	2.33	0.60
2:X:71:ALA:HA	2:X:78:ALA:HA	1.84	0.60
2:F:150:TYR:O	2:F:181:TYR:N	2.35	0.60
2:L:150:TYR:O	2:L:181:TYR:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:150:TYR:O	2:N:181:TYR:N	2.35	0.60
1:A:43:ALA:HB1	2:B:109:TRP:CB	2.32	0.59
2:X:150:TYR:O	2:X:181:TYR:N	2.35	0.59
1:S:86:TYR:O	1:S:104:THR:N	2.35	0.59
2:R:150:TYR:O	2:R:181:TYR:N	2.35	0.59
1:G:86:TYR:O	1:G:104:THR:N	2.35	0.59
2:B:150:TYR:O	2:B:181:TYR:N	2.35	0.59
2:U:71:ALA:HA	2:U:78:ALA:HA	1.84	0.59
1:S:141:PHE:N	1:S:175:TYR:O	2.32	0.59
2:N:71:ALA:HA	2:N:78:ALA:HA	1.84	0.59
1:P:34:ALA:O	1:P:89:GLN:N	2.36	0.59
2:I:150:TYR:O	2:I:181:TYR:N	2.35	0.59
1:M:141:PHE:N	1:M:175:TYR:O	2.32	0.59
1:G:34:ALA:O	1:G:89:GLN:N	2.36	0.59
1:D:86:TYR:O	1:D:104:THR:N	2.36	0.59
3:K:246:HIS:O	3:K:250:GLY:N	2.33	0.59
3:O:216:ILE:O	3:O:220:SER:N	2.30	0.59
1:V:86:TYR:O	1:V:104:THR:N	2.36	0.59
2:R:71:ALA:HA	2:R:78:ALA:HA	1.84	0.59
2:U:150:TYR:O	2:U:181:TYR:N	2.35	0.59
1:D:16:GLY:H	1:D:78:LEU:CB	2.16	0.59
1:A:34:ALA:O	1:A:89:GLN:N	2.36	0.59
2:F:71:ALA:HA	2:F:78:ALA:HA	1.83	0.59
1:S:16:GLY:H	1:S:78:LEU:CB	2.17	0.58
1:D:141:PHE:N	1:D:175:TYR:O	2.32	0.58
1:A:86:TYR:O	1:A:104:THR:N	2.36	0.58
3:H:154:ALA:O	3:H:158:LEU:N	2.30	0.58
1:J:34:ALA:O	1:J:89:GLN:N	2.36	0.58
1:J:86:TYR:O	1:J:104:THR:N	2.36	0.58
1:S:34:ALA:O	1:S:89:GLN:N	2.36	0.58
2:I:68:THR:N	2:I:81:GLN:O	2.34	0.58
1:M:16:GLY:H	1:M:78:LEU:CB	2.16	0.58
2:I:71:ALA:HA	2:I:78:ALA:HA	1.85	0.58
1:P:86:TYR:O	1:P:104:THR:N	2.36	0.58
3:E:267:ILE:O	3:E:270:ARG:N	2.34	0.58
1:G:16:GLY:H	1:G:78:LEU:CB	2.17	0.58
1:P:141:PHE:N	1:P:175:TYR:O	2.32	0.58
1:D:34:ALA:O	1:D:89:GLN:N	2.36	0.58
2:B:71:ALA:HA	2:B:78:ALA:HA	1.84	0.58
2:F:68:THR:N	2:F:81:GLN:O	2.34	0.58
2:L:68:THR:N	2:L:81:GLN:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:34:ALA:O	1:V:89:GLN:N	2.36	0.57
1:A:16:GLY:H	1:A:78:LEU:CB	2.17	0.57
3:C:203:ILE:O	3:C:207:VAL:N	2.37	0.57
3:H:203:ILE:O	3:H:207:VAL:N	2.37	0.57
3:O:154:ALA:O	3:O:158:LEU:N	2.30	0.57
1:J:16:GLY:H	1:J:78:LEU:CB	2.16	0.57
1:M:34:ALA:O	1:M:89:GLN:N	2.36	0.57
1:V:16:GLY:H	1:V:78:LEU:CB	2.17	0.57
1:P:16:GLY:H	1:P:78:LEU:CB	2.16	0.57
1:M:86:TYR:O	1:M:104:THR:N	2.36	0.57
3:W:203:ILE:O	3:W:207:VAL:N	2.37	0.57
3:E:203:ILE:O	3:E:207:VAL:N	2.37	0.57
3:K:249:ASP:O	3:K:253:THR:N	2.37	0.57
3:T:203:ILE:O	3:T:207:VAL:N	2.37	0.56
2:R:68:THR:N	2:R:81:GLN:O	2.34	0.56
3:O:249:ASP:O	3:O:253:THR:N	2.38	0.56
2:B:68:THR:N	2:B:81:GLN:O	2.34	0.56
3:O:203:ILE:O	3:O:207:VAL:N	2.37	0.56
3:Q:203:ILE:O	3:Q:207:VAL:N	2.37	0.56
3:Q:249:ASP:O	3:Q:253:THR:N	2.39	0.56
3:T:249:ASP:O	3:T:253:THR:N	2.39	0.56
1:D:43:ALA:HB1	2:F:109:TRP:CB	2.36	0.56
3:C:249:ASP:O	3:C:253:THR:N	2.39	0.55
1:M:134:VAL:O	1:M:181:LEU:N	2.40	0.55
2:R:52:SER:C	2:R:53:SER:N	2.65	0.55
2:X:52:SER:C	2:X:53:SER:N	2.65	0.55
1:G:134:VAL:O	1:G:181:LEU:N	2.40	0.55
3:E:249:ASP:O	3:E:253:THR:N	2.39	0.55
2:L:52:SER:C	2:L:53:SER:N	2.65	0.55
1:A:134:VAL:O	1:A:181:LEU:N	2.40	0.55
3:W:185:ALA:O	3:W:188:TYR:CB	2.55	0.55
3:W:251:GLU:O	3:W:255:ALA:N	2.40	0.55
2:I:52:SER:C	2:I:53:SER:N	2.65	0.55
3:K:203:ILE:O	3:K:207:VAL:N	2.37	0.55
3:H:249:ASP:O	3:H:253:THR:N	2.40	0.54
2:B:52:SER:C	2:B:53:SER:N	2.65	0.54
2:X:68:THR:N	2:X:81:GLN:O	2.34	0.54
1:J:134:VAL:O	1:J:181:LEU:N	2.40	0.54
2:U:52(A):PRO:HD2	2:U:56:SER:H	1.72	0.54
1:V:134:VAL:N	1:V:181:LEU:O	2.39	0.54
2:N:52:SER:C	2:N:53:SER:N	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:52:SER:C	2:U:53:SER:N	2.65	0.54
2:F:52:SER:C	2:F:53:SER:N	2.65	0.54
2:U:23:ALA:HA	2:U:77:THR:HA	1.90	0.54
3:K:251:GLU:O	3:K:255:ALA:N	2.39	0.54
3:W:214:ALA:O	3:W:218:PHE:N	2.41	0.54
1:P:134:VAL:O	1:P:181:LEU:N	2.40	0.54
1:V:134:VAL:O	1:V:181:LEU:N	2.40	0.54
1:S:134:VAL:O	1:S:181:LEU:N	2.40	0.54
3:K:214:ALA:O	3:K:218:PHE:N	2.41	0.54
1:D:134:VAL:O	1:D:181:LEU:N	2.40	0.54
3:K:185:ALA:O	3:K:188:TYR:CB	2.55	0.54
2:U:68:THR:N	2:U:81:GLN:O	2.34	0.54
3:C:214:ALA:O	3:C:218:PHE:N	2.41	0.54
3:Q:206:PRO:O	3:Q:210:ALA:HB3	2.08	0.54
2:I:52(A):PRO:HD2	2:I:56:SER:H	1.72	0.53
3:E:206:PRO:O	3:E:210:ALA:HB3	2.08	0.53
3:O:214:ALA:O	3:O:218:PHE:N	2.41	0.53
3:W:249:ASP:O	3:W:253:THR:N	2.37	0.53
1:D:134:VAL:N	1:D:181:LEU:O	2.39	0.53
2:B:52(A):PRO:HD2	2:B:56:SER:H	1.73	0.53
1:P:64:GLY:HA2	1:P:73:LEU:HA	1.91	0.53
1:A:134:VAL:N	1:A:181:LEU:O	2.39	0.53
3:H:214:ALA:O	3:H:218:PHE:N	2.41	0.53
3:T:214:ALA:O	3:T:218:PHE:N	2.41	0.53
2:B:23:ALA:HA	2:B:77:THR:HA	1.90	0.53
3:O:206:PRO:O	3:O:210:ALA:HB3	2.09	0.53
3:K:206:PRO:O	3:K:210:ALA:HB3	2.09	0.53
2:X:52(A):PRO:HD2	2:X:56:SER:H	1.73	0.53
3:T:206:PRO:O	3:T:210:ALA:HB3	2.09	0.53
1:M:134:VAL:N	1:M:181:LEU:O	2.39	0.53
1:D:64:GLY:HA2	1:D:73:LEU:HA	1.91	0.53
2:F:22:CYS:O	2:F:78:ALA:N	2.39	0.53
2:N:23:ALA:HA	2:N:77:THR:HA	1.90	0.53
2:N:82(B):ASN:O	2:N:82(C):SER:N	2.42	0.53
2:X:23:ALA:HA	2:X:77:THR:HA	1.90	0.53
3:Q:214:ALA:O	3:Q:218:PHE:N	2.42	0.53
1:A:64:GLY:HA2	1:A:73:LEU:HA	1.91	0.53
1:V:64:GLY:HA2	1:V:73:LEU:HA	1.91	0.53
2:N:68:THR:N	2:N:81:GLN:O	2.34	0.53
2:U:22:CYS:O	2:U:78:ALA:N	2.39	0.53
2:L:52(A):PRO:HD2	2:L:56:SER:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:82(B):ASN:O	2:U:82(C):SER:N	2.42	0.52
2:B:82(B):ASN:O	2:B:82(C):SER:N	2.42	0.52
2:I:82(B):ASN:O	2:I:82(C):SER:N	2.43	0.52
2:L:23:ALA:HA	2:L:77:THR:HA	1.90	0.52
3:H:206:PRO:O	3:H:210:ALA:HB3	2.09	0.52
1:J:64:GLY:HA2	1:J:73:LEU:HA	1.91	0.52
2:L:82(B):ASN:O	2:L:82(C):SER:N	2.42	0.52
2:F:23:ALA:HA	2:F:77:THR:HA	1.90	0.52
2:R:82(B):ASN:O	2:R:82(C):SER:N	2.43	0.52
2:X:82(B):ASN:O	2:X:82(C):SER:N	2.42	0.52
3:E:214:ALA:O	3:E:218:PHE:N	2.42	0.52
2:F:82(B):ASN:O	2:F:82(C):SER:N	2.42	0.52
2:R:23:ALA:HA	2:R:77:THR:HA	1.91	0.52
2:R:52(A):PRO:HD2	2:R:56:SER:H	1.74	0.52
2:I:36:TRP:O	2:I:48:VAL:N	2.43	0.52
1:M:64:GLY:HA2	1:M:73:LEU:HA	1.91	0.52
1:G:64:GLY:HA2	1:G:73:LEU:HA	1.92	0.52
2:I:23:ALA:HA	2:I:77:THR:HA	1.90	0.52
2:X:36:TRP:O	2:X:48:VAL:N	2.43	0.52
3:C:206:PRO:O	3:C:210:ALA:HB3	2.09	0.52
3:W:206:PRO:O	3:W:210:ALA:HB3	2.09	0.52
2:N:52(A):PRO:HD2	2:N:56:SER:H	1.73	0.52
2:R:22:CYS:O	2:R:78:ALA:N	2.39	0.52
2:N:36:TRP:O	2:N:48:VAL:N	2.43	0.52
2:F:52(A):PRO:HD2	2:F:56:SER:H	1.74	0.51
2:U:36:TRP:O	2:U:48:VAL:N	2.43	0.51
1:G:134:VAL:N	1:G:181:LEU:O	2.39	0.51
1:S:64:GLY:HA2	1:S:73:LEU:HA	1.92	0.51
2:R:36:TRP:O	2:R:48:VAL:N	2.43	0.51
2:L:36:TRP:O	2:L:48:VAL:N	2.43	0.51
1:P:43:ALA:HB1	2:R:109:TRP:CB	2.40	0.51
1:P:134:VAL:N	1:P:181:LEU:O	2.39	0.51
2:N:22:CYS:O	2:N:78:ALA:N	2.39	0.50
1:P:138:LEU:O	1:P:177:LEU:N	2.32	0.50
2:B:72:ASP:N	2:B:77:THR:O	2.41	0.50
3:W:188:TYR:O	3:W:192:GLN:N	2.33	0.50
1:D:138:LEU:O	1:D:177:LEU:N	2.32	0.50
2:B:22:CYS:O	2:B:78:ALA:N	2.39	0.50
1:P:18:ARG:HA	1:P:76:SER:HA	1.95	0.49
1:M:18:ARG:HA	1:M:76:SER:HA	1.95	0.49
1:J:134:VAL:N	1:J:181:LEU:O	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:CYS:O	2:L:78:ALA:N	2.39	0.49
2:U:158:SER:O	2:U:202:ASN:N	2.46	0.49
3:C:185:ALA:O	3:C:189:THR:N	2.41	0.49
1:S:13:ALA:O	1:S:109:LYS:N	2.43	0.49
1:G:18:ARG:HA	1:G:76:SER:HA	1.94	0.49
1:A:18:ARG:HA	1:A:76:SER:HA	1.95	0.49
2:R:33:SER:H	2:R:96:SER:CB	2.26	0.49
2:B:36:TRP:O	2:B:48:VAL:N	2.43	0.49
2:U:49:ALA:HA	2:U:59:TYR:HA	1.95	0.49
3:T:185:ALA:O	3:T:189:THR:N	2.40	0.49
2:B:33:SER:H	2:B:96:SER:CB	2.26	0.49
2:B:158:SER:O	2:B:202:ASN:N	2.46	0.49
2:X:49:ALA:HA	2:X:59:TYR:HA	1.95	0.49
2:X:158:SER:O	2:X:202:ASN:N	2.45	0.49
2:I:49:ALA:HA	2:I:59:TYR:HA	1.95	0.49
2:L:49:ALA:HA	2:L:59:TYR:HA	1.95	0.49
2:N:33:SER:H	2:N:96:SER:CB	2.26	0.49
1:J:89:GLN:HA	1:J:100:PHE:HA	1.95	0.48
1:G:13:ALA:O	1:G:109:LYS:N	2.43	0.48
2:F:158:SER:O	2:F:202:ASN:N	2.46	0.48
3:H:163:VAL:O	3:H:167:MET:N	2.44	0.48
1:P:13:ALA:O	1:P:109:LYS:N	2.43	0.48
1:J:13:ALA:O	1:J:109:LYS:N	2.43	0.48
2:B:128:PRO:HA	2:B:145:CYS:HA	1.95	0.48
2:F:49:ALA:HA	2:F:59:TYR:HA	1.95	0.48
3:O:163:VAL:O	3:O:167:MET:N	2.44	0.48
1:V:18:ARG:HA	1:V:76:SER:HA	1.94	0.48
1:S:18:ARG:HA	1:S:76:SER:HA	1.95	0.48
1:D:18:ARG:HA	1:D:76:SER:HA	1.95	0.48
2:R:49:ALA:HA	2:R:59:TYR:HA	1.95	0.48
2:U:72:ASP:N	2:U:77:THR:O	2.41	0.48
3:Q:244:ALA:HA	3:Q:247:ALA:HB3	1.95	0.48
1:G:43:ALA:HB1	2:I:109:TRP:CB	2.44	0.48
2:F:36:TRP:O	2:F:48:VAL:N	2.43	0.48
2:I:158:SER:O	2:I:202:ASN:N	2.45	0.48
2:N:158:SER:O	2:N:202:ASN:N	2.45	0.48
2:R:128:PRO:HA	2:R:145:CYS:HA	1.95	0.48
2:R:158:SER:O	2:R:202:ASN:N	2.46	0.48
1:S:89:GLN:HA	1:S:100:PHE:HA	1.95	0.48
1:D:89:GLN:HA	1:D:100:PHE:HA	1.95	0.48
2:F:128:PRO:HA	2:F:145:CYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:89:GLN:HA	1:P:100:PHE:HA	1.95	0.48
2:B:49:ALA:HA	2:B:59:TYR:HA	1.95	0.48
2:L:158:SER:O	2:L:202:ASN:N	2.45	0.48
1:S:134:VAL:N	1:S:181:LEU:O	2.39	0.48
2:F:33:SER:H	2:F:96:SER:CB	2.26	0.48
2:L:128:PRO:HA	2:L:145:CYS:HA	1.96	0.48
2:N:128:PRO:HA	2:N:145:CYS:HA	1.96	0.48
2:U:33:SER:H	2:U:96:SER:CB	2.27	0.48
3:E:185:ALA:O	3:E:189:THR:N	2.41	0.48
1:A:89:GLN:HA	1:A:100:PHE:HA	1.95	0.48
2:X:128:PRO:HA	2:X:145:CYS:HA	1.95	0.48
1:M:149:GLN:O	1:M:197:GLU:N	2.41	0.47
1:V:89:GLN:HA	1:V:100:PHE:HA	1.95	0.47
3:C:206:PRO:O	3:C:210:ALA:N	2.48	0.47
2:N:49:ALA:HA	2:N:59:TYR:HA	1.95	0.47
2:X:33:SER:H	2:X:96:SER:CB	2.27	0.47
1:M:89:GLN:HA	1:M:100:PHE:HA	1.95	0.47
1:G:89:GLN:HA	1:G:100:PHE:HA	1.95	0.47
1:J:18:ARG:HA	1:J:76:SER:HA	1.94	0.47
2:I:128:PRO:HA	2:I:145:CYS:HA	1.96	0.47
2:X:123:GLY:N	2:X:124:PRO:HD3	2.30	0.47
1:J:43:ALA:HB1	2:L:109:TRP:CB	2.44	0.47
1:J:138:LEU:O	1:J:177:LEU:N	2.32	0.47
2:I:33:SER:H	2:I:96:SER:CB	2.27	0.47
3:Q:206:PRO:O	3:Q:210:ALA:N	2.48	0.47
3:T:206:PRO:O	3:T:210:ALA:N	2.47	0.47
3:W:206:PRO:O	3:W:210:ALA:N	2.48	0.47
2:I:22:CYS:O	2:I:78:ALA:N	2.39	0.47
3:Q:185:ALA:O	3:Q:189:THR:N	2.41	0.47
1:A:138:LEU:O	1:A:177:LEU:N	2.32	0.47
3:E:206:PRO:O	3:E:210:ALA:N	2.48	0.47
3:H:206:PRO:O	3:H:210:ALA:N	2.48	0.47
2:I:72:ASP:N	2:I:77:THR:O	2.41	0.47
2:N:72:ASP:N	2:N:77:THR:O	2.41	0.47
2:U:128:PRO:HA	2:U:145:CYS:HA	1.96	0.47
3:W:230:LEU:O	3:W:234:ILE:N	2.40	0.47
2:I:123:GLY:N	2:I:124:PRO:HD3	2.30	0.47
3:K:206:PRO:O	3:K:210:ALA:N	2.48	0.47
1:P:21:ILE:N	1:P:73:LEU:O	2.48	0.47
3:H:185:ALA:O	3:H:189:THR:N	2.40	0.47
3:O:188:TYR:O	3:O:192:GLN:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:206:PRO:O	3:O:210:ALA:N	2.48	0.47
1:V:139:ASN:HA	1:V:176:SER:HA	1.98	0.46
1:S:138:LEU:O	1:S:177:LEU:N	2.32	0.46
1:A:13:ALA:O	1:A:109:LYS:N	2.43	0.46
1:A:149:GLN:O	1:A:197:GLU:N	2.41	0.46
1:J:139:ASN:HA	1:J:176:SER:HA	1.98	0.46
2:X:22:CYS:O	2:X:78:ALA:N	2.39	0.46
2:U:123:GLY:N	2:U:124:PRO:HD3	2.30	0.46
3:O:185:ALA:O	3:O:189:THR:N	2.40	0.46
1:M:21:ILE:N	1:M:73:LEU:O	2.47	0.46
1:G:138:LEU:O	1:G:177:LEU:N	2.32	0.46
1:S:139:ASN:HA	1:S:176:SER:HA	1.98	0.46
2:B:123:GLY:N	2:B:124:PRO:HD3	2.31	0.46
2:L:33:SER:H	2:L:96:SER:CB	2.27	0.46
2:N:123:GLY:N	2:N:124:PRO:HD3	2.31	0.46
3:T:258:ASP:O	3:T:262:ALA:N	2.49	0.46
2:F:72:ASP:N	2:F:77:THR:O	2.41	0.46
2:L:123:GLY:N	2:L:124:PRO:HD3	2.30	0.46
3:Q:163:VAL:O	3:Q:167:MET:N	2.44	0.46
2:F:123:GLY:N	2:F:124:PRO:HD3	2.31	0.46
3:H:188:TYR:O	3:H:192:GLN:N	2.34	0.46
3:K:192:GLN:O	3:K:197:GLU:N	2.49	0.46
2:R:123:GLY:N	2:R:124:PRO:HD3	2.31	0.45
1:G:139:ASN:HA	1:G:176:SER:HA	1.98	0.45
3:Q:238:ILE:O	3:Q:242:GLN:N	2.48	0.45
1:M:138:LEU:O	1:M:177:LEU:N	2.32	0.45
1:J:166:THR:N	1:J:176:SER:O	2.44	0.45
1:D:13:ALA:O	1:D:109:LYS:N	2.43	0.45
1:A:139:ASN:HA	1:A:176:SER:HA	1.97	0.45
1:P:139:ASN:HA	1:P:176:SER:HA	1.98	0.45
3:Q:258:ASP:O	3:Q:262:ALA:N	2.50	0.45
3:W:192:GLN:O	3:W:197:GLU:N	2.49	0.45
1:M:139:ASN:HA	1:M:176:SER:HA	1.98	0.45
1:S:21:ILE:N	1:S:73:LEU:O	2.47	0.45
1:V:21:ILE:N	1:V:73:LEU:O	2.47	0.45
1:D:21:ILE:N	1:D:73:LEU:O	2.48	0.45
2:L:72:ASP:N	2:L:77:THR:O	2.41	0.45
3:K:206:PRO:O	3:K:210:ALA:CB	2.65	0.45
1:J:149:GLN:O	1:J:197:GLU:N	2.41	0.45
1:P:166:THR:N	1:P:176:SER:O	2.44	0.44
2:B:52(A):PRO:HG2	2:B:56:SER:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:206:PRO:O	3:E:210:ALA:CB	2.65	0.44
3:W:247:ALA:O	3:W:251:GLU:N	2.45	0.44
1:M:13:ALA:O	1:M:109:LYS:N	2.43	0.44
2:N:52(A):PRO:CG	2:N:56:SER:H	2.31	0.44
3:O:258:ASP:O	3:O:262:ALA:N	2.50	0.44
3:Q:219:VAL:O	3:Q:223:LEU:N	2.46	0.44
1:V:118:PHE:O	1:V:137:LEU:N	2.48	0.44
1:D:139:ASN:HA	1:D:176:SER:HA	1.97	0.44
1:D:166:THR:N	1:D:176:SER:O	2.44	0.44
2:B:52(A):PRO:CG	2:B:56:SER:H	2.31	0.44
1:V:138:LEU:O	1:V:177:LEU:N	2.32	0.44
3:W:206:PRO:O	3:W:210:ALA:CB	2.65	0.44
1:V:13:ALA:O	1:V:109:LYS:N	2.43	0.44
2:B:158:SER:N	2:B:202:ASN:O	2.51	0.44
2:X:72:ASP:N	2:X:77:THR:O	2.41	0.44
2:U:206:LYS:N	2:U:207:PRO:CD	2.81	0.44
1:G:21:ILE:N	1:G:73:LEU:O	2.47	0.44
2:F:52(A):PRO:CG	2:F:56:SER:H	2.31	0.44
2:F:52(A):PRO:C	2:F:54:SER:H	2.26	0.44
2:R:52(A):PRO:CG	2:R:56:SER:H	2.31	0.44
3:K:258:ASP:O	3:K:262:ALA:N	2.51	0.44
1:S:166:THR:N	1:S:176:SER:O	2.44	0.43
1:A:21:ILE:N	1:A:73:LEU:O	2.47	0.43
2:B:206:LYS:N	2:B:207:PRO:CD	2.81	0.43
2:N:52(A):PRO:C	2:N:54:SER:H	2.26	0.43
2:N:158:SER:N	2:N:202:ASN:O	2.51	0.43
2:R:52(A):PRO:C	2:R:54:SER:H	2.26	0.43
3:C:206:PRO:O	3:C:210:ALA:CB	2.66	0.43
3:E:258:ASP:O	3:E:262:ALA:N	2.50	0.43
3:Q:206:PRO:O	3:Q:210:ALA:CB	2.65	0.43
2:B:52(A):PRO:C	2:B:54:SER:H	2.26	0.43
2:I:52(A):PRO:CG	2:I:56:SER:H	2.31	0.43
2:I:206:LYS:N	2:I:207:PRO:CD	2.81	0.43
2:N:205:HIS:O	2:N:209:ASN:N	2.51	0.43
2:N:206:LYS:N	2:N:207:PRO:CD	2.81	0.43
3:H:269:GLN:C	3:H:271:LEU:H	2.26	0.43
2:L:52(A):PRO:CG	2:L:56:SER:H	2.31	0.43
2:X:52(A):PRO:CG	2:X:56:SER:H	2.31	0.43
3:C:258:ASP:O	3:C:262:ALA:N	2.50	0.43
3:T:163:VAL:O	3:T:167:MET:N	2.44	0.43
3:W:258:ASP:O	3:W:262:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52(A):PRO:HD2	2:I:56:SER:N	2.34	0.43
2:L:205:HIS:O	2:L:209:ASN:N	2.52	0.43
2:R:206:LYS:N	2:R:207:PRO:CD	2.81	0.43
3:W:238:ILE:O	3:W:242:GLN:N	2.50	0.43
2:F:205:HIS:O	2:F:209:ASN:N	2.52	0.43
2:F:206:LYS:N	2:F:207:PRO:CD	2.81	0.43
2:X:52(A):PRO:HD2	2:X:56:SER:N	2.34	0.43
1:G:118:PHE:O	1:G:137:LEU:N	2.48	0.43
1:G:166:THR:N	1:G:176:SER:O	2.44	0.43
2:B:205:HIS:O	2:B:209:ASN:N	2.51	0.43
2:R:158:SER:N	2:R:202:ASN:O	2.51	0.43
2:U:52(A):PRO:CG	2:U:56:SER:H	2.31	0.43
2:U:52(A):PRO:C	2:U:54:SER:H	2.27	0.43
2:X:171:PHE:N	2:X:184:SER:O	2.49	0.43
3:K:230:LEU:O	3:K:234:ILE:N	2.40	0.43
3:T:219:VAL:O	3:T:223:LEU:N	2.47	0.43
2:L:206:LYS:N	2:L:207:PRO:CD	2.81	0.43
2:U:52(A):PRO:HD2	2:U:56:SER:N	2.33	0.43
2:X:52(A):PRO:C	2:X:54:SER:H	2.26	0.43
3:H:206:PRO:O	3:H:210:ALA:CB	2.66	0.43
3:O:206:PRO:O	3:O:210:ALA:CB	2.66	0.43
2:F:171:PHE:N	2:F:184:SER:O	2.49	0.43
2:L:52(A):PRO:C	2:L:54:SER:H	2.26	0.43
2:R:72:ASP:N	2:R:77:THR:O	2.41	0.43
2:X:158:SER:N	2:X:202:ASN:O	2.51	0.43
3:H:258:ASP:O	3:H:262:ALA:N	2.49	0.43
2:B:52(A):PRO:HD2	2:B:56:SER:N	2.34	0.43
2:L:158:SER:N	2:L:202:ASN:O	2.51	0.43
1:V:166:THR:N	1:V:176:SER:O	2.44	0.42
1:S:149:GLN:O	1:S:197:GLU:N	2.41	0.42
2:F:52(A):PRO:HD2	2:F:56:SER:N	2.34	0.42
2:I:52(A):PRO:C	2:I:54:SER:H	2.27	0.42
2:X:206:LYS:N	2:X:207:PRO:CD	2.81	0.42
1:J:21:ILE:N	1:J:73:LEU:O	2.47	0.42
2:I:158:SER:N	2:I:202:ASN:O	2.51	0.42
2:L:52(A):PRO:HD2	2:L:56:SER:N	2.34	0.42
3:C:163:VAL:O	3:C:167:MET:N	2.44	0.42
2:I:52(A):PRO:HG2	2:I:56:SER:CB	2.49	0.42
2:I:205:HIS:O	2:I:209:ASN:N	2.51	0.42
2:R:52(A):PRO:HD2	2:R:56:SER:N	2.34	0.42
2:U:205:HIS:O	2:U:209:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:205:HIS:O	2:X:209:ASN:N	2.52	0.42
3:C:238:ILE:O	3:C:242:GLN:N	2.49	0.42
3:H:238:ILE:O	3:H:242:GLN:N	2.49	0.42
1:M:118:PHE:O	1:M:137:LEU:N	2.47	0.42
2:I:52(A):PRO:CD	2:I:56:SER:H	2.32	0.42
2:L:52(A):PRO:HG2	2:L:56:SER:CB	2.48	0.42
2:R:205:HIS:O	2:R:209:ASN:N	2.52	0.42
3:Q:231:ASN:O	3:Q:235:GLY:N	2.43	0.42
3:T:206:PRO:O	3:T:210:ALA:CB	2.66	0.42
1:A:166:THR:N	1:A:176:SER:O	2.44	0.42
2:R:52(A):PRO:HG2	2:R:56:SER:CB	2.50	0.42
3:T:238:ILE:O	3:T:242:GLN:N	2.49	0.42
2:N:52(A):PRO:HG2	2:N:56:SER:CB	2.48	0.42
2:X:52(A):PRO:CD	2:X:56:SER:H	2.33	0.42
3:T:188:TYR:O	3:T:192:GLN:N	2.34	0.42
1:G:149:GLN:O	1:G:197:GLU:N	2.41	0.42
2:N:52(A):PRO:HD2	2:N:56:SER:N	2.34	0.42
3:K:188:TYR:O	3:K:192:GLN:N	2.32	0.42
3:H:231:ASN:O	3:H:235:GLY:N	2.45	0.42
2:L:171:PHE:N	2:L:184:SER:O	2.50	0.42
2:X:151:PHE:HA	2:X:152:PRO:HA	1.90	0.41
3:K:257:ARG:O	3:K:261:LEU:N	2.53	0.41
3:E:219:VAL:O	3:E:223:LEU:N	2.46	0.41
1:J:120:PHE:N	1:J:135:VAL:O	2.51	0.41
2:X:52(A):PRO:HG2	2:X:56:SER:CB	2.49	0.41
3:Q:188:TYR:O	3:Q:192:GLN:N	2.34	0.41
1:V:120:PHE:N	1:V:135:VAL:O	2.51	0.41
1:P:118:PHE:O	1:P:137:LEU:N	2.47	0.41
3:C:188:TYR:O	3:C:192:GLN:N	2.34	0.41
3:K:170:LYS:O	3:K:172:PHE:N	2.54	0.41
3:K:238:ILE:O	3:K:242:GLN:N	2.50	0.41
3:W:257:ARG:O	3:W:261:LEU:N	2.53	0.41
1:D:149:GLN:O	1:D:197:GLU:N	2.41	0.41
2:F:52(A):PRO:CD	2:F:56:SER:H	2.34	0.41
2:R:141:ALA:O	2:R:189:VAL:N	2.47	0.41
2:U:158:SER:N	2:U:202:ASN:O	2.51	0.41
3:C:219:VAL:O	3:C:223:LEU:N	2.47	0.41
3:E:156:LEU:O	3:E:160:ILE:N	2.54	0.41
3:E:163:VAL:O	3:E:167:MET:N	2.44	0.41
2:N:52(A):PRO:CD	2:N:56:SER:H	2.33	0.41
2:U:52(A):PRO:HG2	2:U:56:SER:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:151:PHE:HA	2:F:152:PRO:HA	1.88	0.40
3:O:219:VAL:O	3:O:223:LEU:N	2.47	0.40
1:P:120:PHE:N	1:P:135:VAL:O	2.52	0.40
1:P:149:GLN:O	1:P:197:GLU:N	2.41	0.40
1:S:118:PHE:O	1:S:137:LEU:N	2.47	0.40
2:B:52(A):PRO:CD	2:B:56:SER:H	2.33	0.40
2:B:171:PHE:N	2:B:184:SER:O	2.49	0.40
3:E:231:ASN:O	3:E:235:GLY:N	2.43	0.40
1:V:149:GLN:O	1:V:197:GLU:N	2.41	0.40
3:E:247:ALA:O	3:E:251:GLU:N	2.46	0.40
1:J:164:SER:CB	2:L:172:PRO:HD2	2.52	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	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	14	49
1	D	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	14	49
1	G	213/217 (98%)	186 (87%)	24 (11%)	3 (1%)	9	39
1	J	213/217 (98%)	187 (88%)	24 (11%)	2 (1%)	14	49
1	M	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	14	49
1	P	213/217 (98%)	188 (88%)	23 (11%)	2 (1%)	14	49
1	S	213/217 (98%)	186 (87%)	25 (12%)	2 (1%)	14	49
1	V	213/217 (98%)	187 (88%)	24 (11%)	2 (1%)	14	49
2	B	211/233 (91%)	179 (85%)	25 (12%)	7 (3%)	3	21
2	F	211/233 (91%)	179 (85%)	24 (11%)	8 (4%)	2	19
2	I	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	3	21
2	N	211/233 (91%)	179 (85%)	25 (12%)	7 (3%)	3	21
2	R	211/233 (91%)	180 (85%)	23 (11%)	8 (4%)	2	19
2	U	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	3	21
2	X	211/233 (91%)	180 (85%)	24 (11%)	7 (3%)	3	21
3	C	125/143 (87%)	117 (94%)	7 (6%)	1 (1%)	16	53
3	E	126/143 (88%)	116 (92%)	9 (7%)	1 (1%)	16	53
3	H	128/143 (90%)	117 (91%)	10 (8%)	1 (1%)	16	53
3	K	127/143 (89%)	116 (91%)	10 (8%)	1 (1%)	16	53
3	O	128/143 (90%)	120 (94%)	7 (6%)	1 (1%)	16	53
3	Q	122/143 (85%)	113 (93%)	8 (7%)	1 (1%)	16	53
3	T	128/143 (90%)	118 (92%)	9 (7%)	1 (1%)	16	53
3	W	127/143 (89%)	116 (91%)	10 (8%)	1 (1%)	16	53
All	All	4403/4744 (93%)	3868 (88%)	452 (10%)	83 (2%)	6	32

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ILE
2	F	121	ILE
2	I	121	ILE
2	L	121	ILE
2	N	121	ILE
2	R	121	ILE
2	U	121	ILE
2	X	121	ILE
1	P	4	MET
1	P	28	SER
1	M	4	MET
1	M	28	SER
1	V	4	MET
1	V	28	SER
1	S	4	MET
1	S	28	SER
1	G	4	MET
1	G	28	SER
1	D	4	MET

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Mol	Chain	Res	Type
1	D	28	SER
1	J	4	MET
1	J	28	SER
1	A	4	MET
1	A	28	SER
2	B	47	TRP
2	B	52(A)	PRO
2	F	47	TRP
2	F	52(A)	PRO
2	F	136	THR
2	I	47	TRP
2	I	52(A)	PRO
2	I	136	THR
2	L	47	TRP
2	L	52(A)	PRO
2	L	136	THR
2	N	47	TRP
2	N	52(A)	PRO
2	R	47	TRP
2	R	52(A)	PRO
2	R	136	THR
2	U	47	TRP
2	U	52(A)	PRO
2	U	136	THR
2	X	47	TRP
2	X	52(A)	PRO
2	X	136	THR
3	K	197	GLU
3	W	197	GLU
2	B	32	SER
2	B	136	THR
2	F	32	SER
2	I	32	SER
2	L	32	SER
2	N	32	SER
2	N	136	THR
2	R	32	SER
2	U	32	SER
2	X	32	SER
3	C	197	GLU
3	E	197	GLU
3	H	197	GLU

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Mol	Chain	Res	Type
3	O	197	GLU
3	Q	197	GLU
3	T	197	GLU
2	B	106	LEU
2	F	106	LEU
2	I	106	LEU
2	L	64	LYS
2	L	106	LEU
2	N	106	LEU
2	U	106	LEU
2	X	64	LYS
2	X	106	LEU
2	B	64	LYS
2	F	64	LYS
2	F	118	PHE
2	I	64	LYS
2	N	64	LYS
2	R	64	LYS
2	R	106	LEU
2	R	118	PHE
2	U	64	LYS
1	G	9	SER

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	11/192 (6%)	11 (100%)	0	100	100
1	D	11/192 (6%)	11 (100%)	0	100	100
1	G	11/192 (6%)	11 (100%)	0	100	100
1	J	11/192 (6%)	11 (100%)	0	100	100
1	M	11/192 (6%)	11 (100%)	0	100	100
1	P	11/192 (6%)	11 (100%)	0	100	100
1	S	11/192 (6%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	11/192 (6%)	11 (100%)	0	100	100
2	B	12/195 (6%)	12 (100%)	0	100	100
2	F	12/195 (6%)	12 (100%)	0	100	100
2	I	12/195 (6%)	12 (100%)	0	100	100
2	L	12/195 (6%)	12 (100%)	0	100	100
2	N	12/195 (6%)	12 (100%)	0	100	100
2	R	12/195 (6%)	12 (100%)	0	100	100
2	U	12/195 (6%)	12 (100%)	0	100	100
2	X	12/195 (6%)	12 (100%)	0	100	100
All	All	184/3096 (6%)	184 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	6
2	B	6
2	F	6
2	I	6
2	N	6
2	R	6
2	U	6
2	X	6
3	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	51:ILE	C	52:SER	N	4.00
1	B	51:ILE	C	52:SER	N	3.99
1	F	51:ILE	C	52:SER	N	3.99
1	I	51:ILE	C	52:SER	N	3.99
1	N	51:ILE	C	52:SER	N	3.99
1	R	51:ILE	C	52:SER	N	3.99
1	U	51:ILE	C	52:SER	N	3.99
1	X	51:ILE	C	52:SER	N	3.99
1	N	82(C):SER	C	82(D):LEU	N	3.73
1	X	82(C):SER	C	82(D):LEU	N	3.73
1	B	82(C):SER	C	82(D):LEU	N	3.72
1	F	82(C):SER	C	82(D):LEU	N	3.72
1	I	82(C):SER	C	82(D):LEU	N	3.72
1	L	82(C):SER	C	82(D):LEU	N	3.72
1	R	82(C):SER	C	82(D):LEU	N	3.72
1	U	82(C):SER	C	82(D):LEU	N	3.72
1	B	81:GLN	C	82(A):MET	N	3.60
1	F	81:GLN	C	82(A):MET	N	3.60
1	I	81:GLN	C	82(A):MET	N	3.60
1	L	81:GLN	C	82(A):MET	N	3.60
1	N	81:GLN	C	82(A):MET	N	3.60
1	R	81:GLN	C	82(A):MET	N	3.60
1	U	81:GLN	C	82(A):MET	N	3.60
1	X	81:GLN	C	82(A):MET	N	3.60
1	B	82(B):ASN	C	82(C):SER	N	3.45
1	F	82(B):ASN	C	82(C):SER	N	3.45
1	I	82(B):ASN	C	82(C):SER	N	3.45

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	82(B):ASN	C	82(C):SER	N	3.45
1	N	82(B):ASN	C	82(C):SER	N	3.45
1	R	82(B):ASN	C	82(C):SER	N	3.45
1	U	82(B):ASN	C	82(C):SER	N	3.45
1	X	82(B):ASN	C	82(C):SER	N	3.45
1	X	82(D):LEU	C	83:ARG	N	3.44
1	B	82(D):LEU	C	83:ARG	N	3.43
1	F	82(D):LEU	C	83:ARG	N	3.43
1	I	82(D):LEU	C	83:ARG	N	3.43
1	L	82(D):LEU	C	83:ARG	N	3.43
1	N	82(D):LEU	C	83:ARG	N	3.43
1	R	82(D):LEU	C	83:ARG	N	3.43
1	U	82(D):LEU	C	83:ARG	N	3.43
1	B	82(A):MET	C	82(B):ASN	N	3.42
1	F	82(A):MET	C	82(B):ASN	N	3.42
1	I	82(A):MET	C	82(B):ASN	N	3.42
1	L	82(A):MET	C	82(B):ASN	N	3.42
1	N	82(A):MET	C	82(B):ASN	N	3.42
1	R	82(A):MET	C	82(B):ASN	N	3.42
1	U	82(A):MET	C	82(B):ASN	N	3.42
1	X	82(A):MET	C	82(B):ASN	N	3.42
1	Q	246:HIS	C	247:ALA	N	3.39

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	215/217 (99%)	-0.83	0 100 100	147, 298, 423, 525	0
1	D	215/217 (99%)	-0.97	0 100 100	148, 269, 366, 492	0
1	G	215/217 (99%)	-0.91	0 100 100	117, 234, 324, 439	0
1	J	215/217 (99%)	-0.96	0 100 100	129, 232, 297, 349	0
1	M	215/217 (99%)	-0.88	0 100 100	139, 303, 434, 496	0
1	P	215/217 (99%)	-0.92	1 (0%) 87 75	145, 264, 363, 524	0
1	S	215/217 (99%)	-0.94	0 100 100	128, 229, 331, 409	0
1	V	215/217 (99%)	-0.94	0 100 100	143, 244, 309, 329	0
2	B	221/233 (94%)	-0.93	1 (0%) 87 75	127, 258, 436, 544	0
2	F	221/233 (94%)	-0.96	0 100 100	113, 230, 360, 430	0
2	I	221/233 (94%)	-0.95	0 100 100	103, 216, 320, 638	0
2	L	221/233 (94%)	-0.92	1 (0%) 87 75	109, 223, 347, 541	0
2	N	221/233 (94%)	-0.87	0 100 100	138, 255, 448, 599	0
2	R	221/233 (94%)	-0.93	0 100 100	109, 225, 386, 472	0
2	U	221/233 (94%)	-0.93	0 100 100	116, 218, 347, 613	0
2	X	221/233 (94%)	-0.93	0 100 100	111, 223, 343, 534	0
3	C	127/143 (88%)	-1.04	0 100 100	168, 262, 456, 528	0
3	E	128/143 (89%)	-1.04	0 100 100	177, 263, 374, 428	0
3	H	130/143 (90%)	-1.04	0 100 100	139, 223, 322, 342	0
3	K	129/143 (90%)	-1.17	0 100 100	113, 218, 310, 382	0
3	O	130/143 (90%)	-1.10	0 100 100	149, 260, 364, 455	0
3	Q	126/143 (88%)	-0.99	0 100 100	177, 252, 339, 423	0
3	T	130/143 (90%)	-1.06	0 100 100	147, 229, 326, 362	0
3	W	129/143 (90%)	-1.16	0 100 100	120, 228, 319, 365	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4517/4744 (95%)	-0.96	3 (0%) 92 87	103, 243, 373, 638	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	26	SER	2.8
2	L	99	TRP	2.5
2	B	98	GLY	2.3

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.