



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:49 PM UTC

PDB ID : 7ST3 / pdb_00007st3
Title : Consequences of HLA single chain trimer mutations on peptide presentation and binding affinity
Authors : Finton, K.A.K.; Rupert, P.B.
Deposited on : 2021-11-11
Resolution : 2.78 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

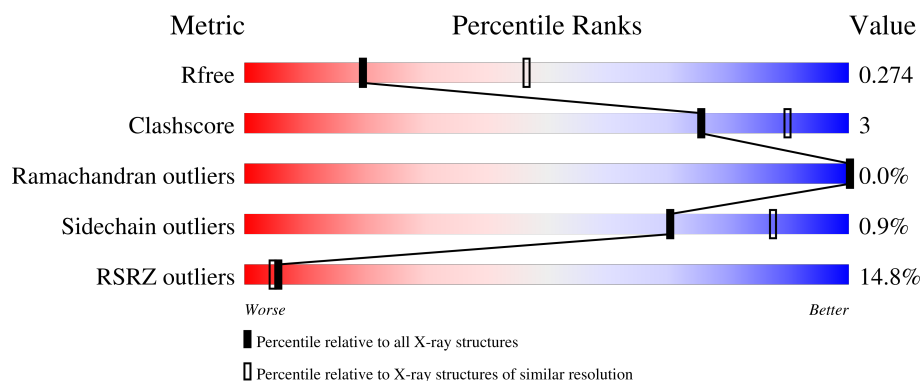
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	429	11% 79% 18%
1	C	429	10% 77% 16%
1	E	429	11% 79% 14%
1	G	429	11% 80% 15%
1	I	429	10% 79% 17%

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Mol	Chain	Length	Quality of chain
1	K	429	
1	M	429	
1	O	429	
1	Q	429	
1	S	429	
1	U	429	
1	W	429	
1	Y	429	
1	a	429	
1	c	429	
1	e	429	
2	B	116	
2	D	116	
2	F	116	
2	H	116	
2	J	116	
2	L	116	
2	N	116	
2	P	116	
2	R	116	
2	T	116	
2	V	116	
2	X	116	
2	Z	116	
2	b	116	

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Mol	Chain	Length	Quality of chain
2	d	116	 5% 91% 9% •
2	f	116	 9% 87% 12% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 109155 atoms, of which 51318 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 Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	352	Total	C	H	N	O	S	0	0	0
			5065	1700	2373	476	503	13			
1	C	361	Total	C	H	N	O	S	0	0	0
			5214	1757	2442	486	515	14			
1	E	368	Total	C	H	N	O	S	0	0	0
			5342	1789	2512	500	527	14			
1	G	366	Total	C	H	N	O	S	0	0	0
			5261	1773	2459	491	524	14			
1	I	358	Total	C	H	N	O	S	0	0	0
			5191	1742	2442	486	508	13			
1	K	376	Total	C	H	N	O	S	0	0	0
			5293	1788	2463	499	530	13			
1	M	372	Total	C	H	N	O	S	0	0	0
			5264	1775	2456	496	524	13			
1	O	361	Total	C	H	N	O	S	0	0	0
			5155	1737	2411	485	509	13			
1	Q	375	Total	C	H	N	O	S	0	0	0
			5378	1809	2517	502	537	13			
1	S	345	Total	C	H	N	O	S	0	0	0
			4977	1680	2324	464	497	12			
1	U	348	Total	C	H	N	O	S	0	0	0
			4873	1652	2261	455	493	12			
1	W	350	Total	C	H	N	O	S	0	0	0
			5042	1703	2356	469	501	13			
1	Y	376	Total	C	H	N	O	S	0	0	0
			5409	1819	2532	507	538	13			
1	a	357	Total	C	H	N	O	S	0	0	0
			5187	1742	2436	482	514	13			
1	c	352	Total	C	H	N	O	S	0	0	0
			5039	1702	2352	471	503	11			
1	e	354	Total	C	H	N	O	S	0	0	0
			5150	1730	2419	482	507	12			

There are 688 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5J	GLY	-	linker	UNP P03129
A	5K	GLY	-	linker	UNP P03129
A	5L	GLY	-	linker	UNP P03129
A	5M	GLY	-	linker	UNP P03129
A	5N	SER	-	linker	UNP P03129
A	5O	GLY	-	linker	UNP P03129
A	5P	GLY	-	linker	UNP P03129
A	5Q	GLY	-	linker	UNP P03129
A	5R	GLY	-	linker	UNP P03129
A	5S	SER	-	linker	UNP P03129
A	5T	GLY	-	linker	UNP P03129
A	5U	GLY	-	linker	UNP P03129
A	5V	GLY	-	linker	UNP P03129
A	5W	GLY	-	linker	UNP P03129
A	5X	SER	-	linker	UNP P03129
A	124	GLY	-	linker	UNP P16213
A	125	GLY	-	linker	UNP P16213
A	126	GLY	-	linker	UNP P16213
A	127	GLY	-	linker	UNP P16213
A	128	SER	-	linker	UNP P16213
A	129	GLY	-	linker	UNP P16213
A	130	GLY	-	linker	UNP P16213
A	131	GLY	-	linker	UNP P16213
A	132	GLY	-	linker	UNP P16213
A	133	SER	-	linker	UNP P16213
A	134	GLY	-	linker	UNP P16213
A	135	GLY	-	linker	UNP P16213
A	136	GLY	-	linker	UNP P16213
A	137	GLY	-	linker	UNP P16213
A	138	SER	-	linker	UNP P16213
A	139	GLY	-	linker	UNP P16213
A	140	GLY	-	linker	UNP P16213
A	141	GLY	-	linker	UNP P16213
A	142	GLY	-	linker	UNP P16213
A	143	SER	-	linker	UNP P16213
A	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
A	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
A	419	HIS	-	expression tag	UNP A0A678ZGP6
A	420	HIS	-	expression tag	UNP A0A678ZGP6
A	421	HIS	-	expression tag	UNP A0A678ZGP6
A	422	HIS	-	expression tag	UNP A0A678ZGP6
A	423	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP A0A678ZGP6
C	5J	GLY	-	linker	UNP P03129
C	5K	GLY	-	linker	UNP P03129
C	5L	GLY	-	linker	UNP P03129
C	5M	GLY	-	linker	UNP P03129
C	5N	SER	-	linker	UNP P03129
C	5O	GLY	-	linker	UNP P03129
C	5P	GLY	-	linker	UNP P03129
C	5Q	GLY	-	linker	UNP P03129
C	5R	GLY	-	linker	UNP P03129
C	5S	SER	-	linker	UNP P03129
C	5T	GLY	-	linker	UNP P03129
C	5U	GLY	-	linker	UNP P03129
C	5V	GLY	-	linker	UNP P03129
C	5W	GLY	-	linker	UNP P03129
C	5X	SER	-	linker	UNP P03129
C	124	GLY	-	linker	UNP P16213
C	125	GLY	-	linker	UNP P16213
C	126	GLY	-	linker	UNP P16213
C	127	GLY	-	linker	UNP P16213
C	128	SER	-	linker	UNP P16213
C	129	GLY	-	linker	UNP P16213
C	130	GLY	-	linker	UNP P16213
C	131	GLY	-	linker	UNP P16213
C	132	GLY	-	linker	UNP P16213
C	133	SER	-	linker	UNP P16213
C	134	GLY	-	linker	UNP P16213
C	135	GLY	-	linker	UNP P16213
C	136	GLY	-	linker	UNP P16213
C	137	GLY	-	linker	UNP P16213
C	138	SER	-	linker	UNP P16213
C	139	GLY	-	linker	UNP P16213
C	140	GLY	-	linker	UNP P16213
C	141	GLY	-	linker	UNP P16213
C	142	GLY	-	linker	UNP P16213
C	143	SER	-	linker	UNP P16213
C	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
C	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
C	419	HIS	-	expression tag	UNP A0A678ZGP6
C	420	HIS	-	expression tag	UNP A0A678ZGP6
C	421	HIS	-	expression tag	UNP A0A678ZGP6
C	422	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	423	HIS	-	expression tag	UNP A0A678ZGP6
C	424	HIS	-	expression tag	UNP A0A678ZGP6
E	5J	GLY	-	linker	UNP P03129
E	5K	GLY	-	linker	UNP P03129
E	5L	GLY	-	linker	UNP P03129
E	5M	GLY	-	linker	UNP P03129
E	5N	SER	-	linker	UNP P03129
E	5O	GLY	-	linker	UNP P03129
E	5P	GLY	-	linker	UNP P03129
E	5Q	GLY	-	linker	UNP P03129
E	5R	GLY	-	linker	UNP P03129
E	5S	SER	-	linker	UNP P03129
E	5T	GLY	-	linker	UNP P03129
E	5U	GLY	-	linker	UNP P03129
E	5V	GLY	-	linker	UNP P03129
E	5W	GLY	-	linker	UNP P03129
E	5X	SER	-	linker	UNP P03129
E	124	GLY	-	linker	UNP P16213
E	125	GLY	-	linker	UNP P16213
E	126	GLY	-	linker	UNP P16213
E	127	GLY	-	linker	UNP P16213
E	128	SER	-	linker	UNP P16213
E	129	GLY	-	linker	UNP P16213
E	130	GLY	-	linker	UNP P16213
E	131	GLY	-	linker	UNP P16213
E	132	GLY	-	linker	UNP P16213
E	133	SER	-	linker	UNP P16213
E	134	GLY	-	linker	UNP P16213
E	135	GLY	-	linker	UNP P16213
E	136	GLY	-	linker	UNP P16213
E	137	GLY	-	linker	UNP P16213
E	138	SER	-	linker	UNP P16213
E	139	GLY	-	linker	UNP P16213
E	140	GLY	-	linker	UNP P16213
E	141	GLY	-	linker	UNP P16213
E	142	GLY	-	linker	UNP P16213
E	143	SER	-	linker	UNP P16213
E	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
E	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
E	419	HIS	-	expression tag	UNP A0A678ZGP6
E	420	HIS	-	expression tag	UNP A0A678ZGP6
E	421	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	422	HIS	-	expression tag	UNP A0A678ZGP6
E	423	HIS	-	expression tag	UNP A0A678ZGP6
E	424	HIS	-	expression tag	UNP A0A678ZGP6
G	5J	GLY	-	linker	UNP P03129
G	5K	GLY	-	linker	UNP P03129
G	5L	GLY	-	linker	UNP P03129
G	5M	GLY	-	linker	UNP P03129
G	5N	SER	-	linker	UNP P03129
G	5O	GLY	-	linker	UNP P03129
G	5P	GLY	-	linker	UNP P03129
G	5Q	GLY	-	linker	UNP P03129
G	5R	GLY	-	linker	UNP P03129
G	5S	SER	-	linker	UNP P03129
G	5T	GLY	-	linker	UNP P03129
G	5U	GLY	-	linker	UNP P03129
G	5V	GLY	-	linker	UNP P03129
G	5W	GLY	-	linker	UNP P03129
G	5X	SER	-	linker	UNP P03129
G	124	GLY	-	linker	UNP P16213
G	125	GLY	-	linker	UNP P16213
G	126	GLY	-	linker	UNP P16213
G	127	GLY	-	linker	UNP P16213
G	128	SER	-	linker	UNP P16213
G	129	GLY	-	linker	UNP P16213
G	130	GLY	-	linker	UNP P16213
G	131	GLY	-	linker	UNP P16213
G	132	GLY	-	linker	UNP P16213
G	133	SER	-	linker	UNP P16213
G	134	GLY	-	linker	UNP P16213
G	135	GLY	-	linker	UNP P16213
G	136	GLY	-	linker	UNP P16213
G	137	GLY	-	linker	UNP P16213
G	138	SER	-	linker	UNP P16213
G	139	GLY	-	linker	UNP P16213
G	140	GLY	-	linker	UNP P16213
G	141	GLY	-	linker	UNP P16213
G	142	GLY	-	linker	UNP P16213
G	143	SER	-	linker	UNP P16213
G	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
G	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
G	419	HIS	-	expression tag	UNP A0A678ZGP6
G	420	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	421	HIS	-	expression tag	UNP A0A678ZGP6
G	422	HIS	-	expression tag	UNP A0A678ZGP6
G	423	HIS	-	expression tag	UNP A0A678ZGP6
G	424	HIS	-	expression tag	UNP A0A678ZGP6
I	5J	GLY	-	linker	UNP P03129
I	5K	GLY	-	linker	UNP P03129
I	5L	GLY	-	linker	UNP P03129
I	5M	GLY	-	linker	UNP P03129
I	5N	SER	-	linker	UNP P03129
I	5O	GLY	-	linker	UNP P03129
I	5P	GLY	-	linker	UNP P03129
I	5Q	GLY	-	linker	UNP P03129
I	5R	GLY	-	linker	UNP P03129
I	5S	SER	-	linker	UNP P03129
I	5T	GLY	-	linker	UNP P03129
I	5U	GLY	-	linker	UNP P03129
I	5V	GLY	-	linker	UNP P03129
I	5W	GLY	-	linker	UNP P03129
I	5X	SER	-	linker	UNP P03129
I	124	GLY	-	linker	UNP P16213
I	125	GLY	-	linker	UNP P16213
I	126	GLY	-	linker	UNP P16213
I	127	GLY	-	linker	UNP P16213
I	128	SER	-	linker	UNP P16213
I	129	GLY	-	linker	UNP P16213
I	130	GLY	-	linker	UNP P16213
I	131	GLY	-	linker	UNP P16213
I	132	GLY	-	linker	UNP P16213
I	133	SER	-	linker	UNP P16213
I	134	GLY	-	linker	UNP P16213
I	135	GLY	-	linker	UNP P16213
I	136	GLY	-	linker	UNP P16213
I	137	GLY	-	linker	UNP P16213
I	138	SER	-	linker	UNP P16213
I	139	GLY	-	linker	UNP P16213
I	140	GLY	-	linker	UNP P16213
I	141	GLY	-	linker	UNP P16213
I	142	GLY	-	linker	UNP P16213
I	143	SER	-	linker	UNP P16213
I	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
I	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
I	419	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	420	HIS	-	expression tag	UNP A0A678ZGP6
I	421	HIS	-	expression tag	UNP A0A678ZGP6
I	422	HIS	-	expression tag	UNP A0A678ZGP6
I	423	HIS	-	expression tag	UNP A0A678ZGP6
I	424	HIS	-	expression tag	UNP A0A678ZGP6
K	5J	GLY	-	linker	UNP P03129
K	5K	GLY	-	linker	UNP P03129
K	5L	GLY	-	linker	UNP P03129
K	5M	GLY	-	linker	UNP P03129
K	5N	SER	-	linker	UNP P03129
K	5O	GLY	-	linker	UNP P03129
K	5P	GLY	-	linker	UNP P03129
K	5Q	GLY	-	linker	UNP P03129
K	5R	GLY	-	linker	UNP P03129
K	5S	SER	-	linker	UNP P03129
K	5T	GLY	-	linker	UNP P03129
K	5U	GLY	-	linker	UNP P03129
K	5V	GLY	-	linker	UNP P03129
K	5W	GLY	-	linker	UNP P03129
K	5X	SER	-	linker	UNP P03129
K	124	GLY	-	linker	UNP P16213
K	125	GLY	-	linker	UNP P16213
K	126	GLY	-	linker	UNP P16213
K	127	GLY	-	linker	UNP P16213
K	128	SER	-	linker	UNP P16213
K	129	GLY	-	linker	UNP P16213
K	130	GLY	-	linker	UNP P16213
K	131	GLY	-	linker	UNP P16213
K	132	GLY	-	linker	UNP P16213
K	133	SER	-	linker	UNP P16213
K	134	GLY	-	linker	UNP P16213
K	135	GLY	-	linker	UNP P16213
K	136	GLY	-	linker	UNP P16213
K	137	GLY	-	linker	UNP P16213
K	138	SER	-	linker	UNP P16213
K	139	GLY	-	linker	UNP P16213
K	140	GLY	-	linker	UNP P16213
K	141	GLY	-	linker	UNP P16213
K	142	GLY	-	linker	UNP P16213
K	143	SER	-	linker	UNP P16213
K	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
K	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	419	HIS	-	expression tag	UNP A0A678ZGP6
K	420	HIS	-	expression tag	UNP A0A678ZGP6
K	421	HIS	-	expression tag	UNP A0A678ZGP6
K	422	HIS	-	expression tag	UNP A0A678ZGP6
K	423	HIS	-	expression tag	UNP A0A678ZGP6
K	424	HIS	-	expression tag	UNP A0A678ZGP6
M	5J	GLY	-	linker	UNP P03129
M	5K	GLY	-	linker	UNP P03129
M	5L	GLY	-	linker	UNP P03129
M	5M	GLY	-	linker	UNP P03129
M	5N	SER	-	linker	UNP P03129
M	5O	GLY	-	linker	UNP P03129
M	5P	GLY	-	linker	UNP P03129
M	5Q	GLY	-	linker	UNP P03129
M	5R	GLY	-	linker	UNP P03129
M	5S	SER	-	linker	UNP P03129
M	5T	GLY	-	linker	UNP P03129
M	5U	GLY	-	linker	UNP P03129
M	5V	GLY	-	linker	UNP P03129
M	5W	GLY	-	linker	UNP P03129
M	5X	SER	-	linker	UNP P03129
M	124	GLY	-	linker	UNP P16213
M	125	GLY	-	linker	UNP P16213
M	126	GLY	-	linker	UNP P16213
M	127	GLY	-	linker	UNP P16213
M	128	SER	-	linker	UNP P16213
M	129	GLY	-	linker	UNP P16213
M	130	GLY	-	linker	UNP P16213
M	131	GLY	-	linker	UNP P16213
M	132	GLY	-	linker	UNP P16213
M	133	SER	-	linker	UNP P16213
M	134	GLY	-	linker	UNP P16213
M	135	GLY	-	linker	UNP P16213
M	136	GLY	-	linker	UNP P16213
M	137	GLY	-	linker	UNP P16213
M	138	SER	-	linker	UNP P16213
M	139	GLY	-	linker	UNP P16213
M	140	GLY	-	linker	UNP P16213
M	141	GLY	-	linker	UNP P16213
M	142	GLY	-	linker	UNP P16213
M	143	SER	-	linker	UNP P16213
M	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
M	419	HIS	-	expression tag	UNP A0A678ZGP6
M	420	HIS	-	expression tag	UNP A0A678ZGP6
M	421	HIS	-	expression tag	UNP A0A678ZGP6
M	422	HIS	-	expression tag	UNP A0A678ZGP6
M	423	HIS	-	expression tag	UNP A0A678ZGP6
M	424	HIS	-	expression tag	UNP A0A678ZGP6
O	5J	GLY	-	linker	UNP P03129
O	5K	GLY	-	linker	UNP P03129
O	5L	GLY	-	linker	UNP P03129
O	5M	GLY	-	linker	UNP P03129
O	5N	SER	-	linker	UNP P03129
O	5O	GLY	-	linker	UNP P03129
O	5P	GLY	-	linker	UNP P03129
O	5Q	GLY	-	linker	UNP P03129
O	5R	GLY	-	linker	UNP P03129
O	5S	SER	-	linker	UNP P03129
O	5T	GLY	-	linker	UNP P03129
O	5U	GLY	-	linker	UNP P03129
O	5V	GLY	-	linker	UNP P03129
O	5W	GLY	-	linker	UNP P03129
O	5X	SER	-	linker	UNP P03129
O	124	GLY	-	linker	UNP P16213
O	125	GLY	-	linker	UNP P16213
O	126	GLY	-	linker	UNP P16213
O	127	GLY	-	linker	UNP P16213
O	128	SER	-	linker	UNP P16213
O	129	GLY	-	linker	UNP P16213
O	130	GLY	-	linker	UNP P16213
O	131	GLY	-	linker	UNP P16213
O	132	GLY	-	linker	UNP P16213
O	133	SER	-	linker	UNP P16213
O	134	GLY	-	linker	UNP P16213
O	135	GLY	-	linker	UNP P16213
O	136	GLY	-	linker	UNP P16213
O	137	GLY	-	linker	UNP P16213
O	138	SER	-	linker	UNP P16213
O	139	GLY	-	linker	UNP P16213
O	140	GLY	-	linker	UNP P16213
O	141	GLY	-	linker	UNP P16213
O	142	GLY	-	linker	UNP P16213
O	143	SER	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
O	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
O	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
O	419	HIS	-	expression tag	UNP A0A678ZGP6
O	420	HIS	-	expression tag	UNP A0A678ZGP6
O	421	HIS	-	expression tag	UNP A0A678ZGP6
O	422	HIS	-	expression tag	UNP A0A678ZGP6
O	423	HIS	-	expression tag	UNP A0A678ZGP6
O	424	HIS	-	expression tag	UNP A0A678ZGP6
Q	5J	GLY	-	linker	UNP P03129
Q	5K	GLY	-	linker	UNP P03129
Q	5L	GLY	-	linker	UNP P03129
Q	5M	GLY	-	linker	UNP P03129
Q	5N	SER	-	linker	UNP P03129
Q	5O	GLY	-	linker	UNP P03129
Q	5P	GLY	-	linker	UNP P03129
Q	5Q	GLY	-	linker	UNP P03129
Q	5R	GLY	-	linker	UNP P03129
Q	5S	SER	-	linker	UNP P03129
Q	5T	GLY	-	linker	UNP P03129
Q	5U	GLY	-	linker	UNP P03129
Q	5V	GLY	-	linker	UNP P03129
Q	5W	GLY	-	linker	UNP P03129
Q	5X	SER	-	linker	UNP P03129
Q	124	GLY	-	linker	UNP P16213
Q	125	GLY	-	linker	UNP P16213
Q	126	GLY	-	linker	UNP P16213
Q	127	GLY	-	linker	UNP P16213
Q	128	SER	-	linker	UNP P16213
Q	129	GLY	-	linker	UNP P16213
Q	130	GLY	-	linker	UNP P16213
Q	131	GLY	-	linker	UNP P16213
Q	132	GLY	-	linker	UNP P16213
Q	133	SER	-	linker	UNP P16213
Q	134	GLY	-	linker	UNP P16213
Q	135	GLY	-	linker	UNP P16213
Q	136	GLY	-	linker	UNP P16213
Q	137	GLY	-	linker	UNP P16213
Q	138	SER	-	linker	UNP P16213
Q	139	GLY	-	linker	UNP P16213
Q	140	GLY	-	linker	UNP P16213
Q	141	GLY	-	linker	UNP P16213
Q	142	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	143	SER	-	linker	UNP P16213
Q	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
Q	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
Q	419	HIS	-	expression tag	UNP A0A678ZGP6
Q	420	HIS	-	expression tag	UNP A0A678ZGP6
Q	421	HIS	-	expression tag	UNP A0A678ZGP6
Q	422	HIS	-	expression tag	UNP A0A678ZGP6
Q	423	HIS	-	expression tag	UNP A0A678ZGP6
Q	424	HIS	-	expression tag	UNP A0A678ZGP6
S	5J	GLY	-	linker	UNP P03129
S	5K	GLY	-	linker	UNP P03129
S	5L	GLY	-	linker	UNP P03129
S	5M	GLY	-	linker	UNP P03129
S	5N	SER	-	linker	UNP P03129
S	5O	GLY	-	linker	UNP P03129
S	5P	GLY	-	linker	UNP P03129
S	5Q	GLY	-	linker	UNP P03129
S	5R	GLY	-	linker	UNP P03129
S	5S	SER	-	linker	UNP P03129
S	5T	GLY	-	linker	UNP P03129
S	5U	GLY	-	linker	UNP P03129
S	5V	GLY	-	linker	UNP P03129
S	5W	GLY	-	linker	UNP P03129
S	5X	SER	-	linker	UNP P03129
S	124	GLY	-	linker	UNP P16213
S	125	GLY	-	linker	UNP P16213
S	126	GLY	-	linker	UNP P16213
S	127	GLY	-	linker	UNP P16213
S	128	SER	-	linker	UNP P16213
S	129	GLY	-	linker	UNP P16213
S	130	GLY	-	linker	UNP P16213
S	131	GLY	-	linker	UNP P16213
S	132	GLY	-	linker	UNP P16213
S	133	SER	-	linker	UNP P16213
S	134	GLY	-	linker	UNP P16213
S	135	GLY	-	linker	UNP P16213
S	136	GLY	-	linker	UNP P16213
S	137	GLY	-	linker	UNP P16213
S	138	SER	-	linker	UNP P16213
S	139	GLY	-	linker	UNP P16213
S	140	GLY	-	linker	UNP P16213
S	141	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
S	142	GLY	-	linker	UNP P16213
S	143	SER	-	linker	UNP P16213
S	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
S	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
S	419	HIS	-	expression tag	UNP A0A678ZGP6
S	420	HIS	-	expression tag	UNP A0A678ZGP6
S	421	HIS	-	expression tag	UNP A0A678ZGP6
S	422	HIS	-	expression tag	UNP A0A678ZGP6
S	423	HIS	-	expression tag	UNP A0A678ZGP6
S	424	HIS	-	expression tag	UNP A0A678ZGP6
U	5J	GLY	-	linker	UNP P03129
U	5K	GLY	-	linker	UNP P03129
U	5L	GLY	-	linker	UNP P03129
U	5M	GLY	-	linker	UNP P03129
U	5N	SER	-	linker	UNP P03129
U	5O	GLY	-	linker	UNP P03129
U	5P	GLY	-	linker	UNP P03129
U	5Q	GLY	-	linker	UNP P03129
U	5R	GLY	-	linker	UNP P03129
U	5S	SER	-	linker	UNP P03129
U	5T	GLY	-	linker	UNP P03129
U	5U	GLY	-	linker	UNP P03129
U	5V	GLY	-	linker	UNP P03129
U	5W	GLY	-	linker	UNP P03129
U	5X	SER	-	linker	UNP P03129
U	124	GLY	-	linker	UNP P16213
U	125	GLY	-	linker	UNP P16213
U	126	GLY	-	linker	UNP P16213
U	127	GLY	-	linker	UNP P16213
U	128	SER	-	linker	UNP P16213
U	129	GLY	-	linker	UNP P16213
U	130	GLY	-	linker	UNP P16213
U	131	GLY	-	linker	UNP P16213
U	132	GLY	-	linker	UNP P16213
U	133	SER	-	linker	UNP P16213
U	134	GLY	-	linker	UNP P16213
U	135	GLY	-	linker	UNP P16213
U	136	GLY	-	linker	UNP P16213
U	137	GLY	-	linker	UNP P16213
U	138	SER	-	linker	UNP P16213
U	139	GLY	-	linker	UNP P16213
U	140	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
U	141	GLY	-	linker	UNP P16213
U	142	GLY	-	linker	UNP P16213
U	143	SER	-	linker	UNP P16213
U	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
U	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
U	419	HIS	-	expression tag	UNP A0A678ZGP6
U	420	HIS	-	expression tag	UNP A0A678ZGP6
U	421	HIS	-	expression tag	UNP A0A678ZGP6
U	422	HIS	-	expression tag	UNP A0A678ZGP6
U	423	HIS	-	expression tag	UNP A0A678ZGP6
U	424	HIS	-	expression tag	UNP A0A678ZGP6
W	5J	GLY	-	linker	UNP P03129
W	5K	GLY	-	linker	UNP P03129
W	5L	GLY	-	linker	UNP P03129
W	5M	GLY	-	linker	UNP P03129
W	5N	SER	-	linker	UNP P03129
W	5O	GLY	-	linker	UNP P03129
W	5P	GLY	-	linker	UNP P03129
W	5Q	GLY	-	linker	UNP P03129
W	5R	GLY	-	linker	UNP P03129
W	5S	SER	-	linker	UNP P03129
W	5T	GLY	-	linker	UNP P03129
W	5U	GLY	-	linker	UNP P03129
W	5V	GLY	-	linker	UNP P03129
W	5W	GLY	-	linker	UNP P03129
W	5X	SER	-	linker	UNP P03129
W	124	GLY	-	linker	UNP P16213
W	125	GLY	-	linker	UNP P16213
W	126	GLY	-	linker	UNP P16213
W	127	GLY	-	linker	UNP P16213
W	128	SER	-	linker	UNP P16213
W	129	GLY	-	linker	UNP P16213
W	130	GLY	-	linker	UNP P16213
W	131	GLY	-	linker	UNP P16213
W	132	GLY	-	linker	UNP P16213
W	133	SER	-	linker	UNP P16213
W	134	GLY	-	linker	UNP P16213
W	135	GLY	-	linker	UNP P16213
W	136	GLY	-	linker	UNP P16213
W	137	GLY	-	linker	UNP P16213
W	138	SER	-	linker	UNP P16213
W	139	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
W	140	GLY	-	linker	UNP P16213
W	141	GLY	-	linker	UNP P16213
W	142	GLY	-	linker	UNP P16213
W	143	SER	-	linker	UNP P16213
W	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
W	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
W	419	HIS	-	expression tag	UNP A0A678ZGP6
W	420	HIS	-	expression tag	UNP A0A678ZGP6
W	421	HIS	-	expression tag	UNP A0A678ZGP6
W	422	HIS	-	expression tag	UNP A0A678ZGP6
W	423	HIS	-	expression tag	UNP A0A678ZGP6
W	424	HIS	-	expression tag	UNP A0A678ZGP6
Y	5J	GLY	-	linker	UNP P03129
Y	5K	GLY	-	linker	UNP P03129
Y	5L	GLY	-	linker	UNP P03129
Y	5M	GLY	-	linker	UNP P03129
Y	5N	SER	-	linker	UNP P03129
Y	5O	GLY	-	linker	UNP P03129
Y	5P	GLY	-	linker	UNP P03129
Y	5Q	GLY	-	linker	UNP P03129
Y	5R	GLY	-	linker	UNP P03129
Y	5S	SER	-	linker	UNP P03129
Y	5T	GLY	-	linker	UNP P03129
Y	5U	GLY	-	linker	UNP P03129
Y	5V	GLY	-	linker	UNP P03129
Y	5W	GLY	-	linker	UNP P03129
Y	5X	SER	-	linker	UNP P03129
Y	124	GLY	-	linker	UNP P16213
Y	125	GLY	-	linker	UNP P16213
Y	126	GLY	-	linker	UNP P16213
Y	127	GLY	-	linker	UNP P16213
Y	128	SER	-	linker	UNP P16213
Y	129	GLY	-	linker	UNP P16213
Y	130	GLY	-	linker	UNP P16213
Y	131	GLY	-	linker	UNP P16213
Y	132	GLY	-	linker	UNP P16213
Y	133	SER	-	linker	UNP P16213
Y	134	GLY	-	linker	UNP P16213
Y	135	GLY	-	linker	UNP P16213
Y	136	GLY	-	linker	UNP P16213
Y	137	GLY	-	linker	UNP P16213
Y	138	SER	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	139	GLY	-	linker	UNP P16213
Y	140	GLY	-	linker	UNP P16213
Y	141	GLY	-	linker	UNP P16213
Y	142	GLY	-	linker	UNP P16213
Y	143	SER	-	linker	UNP P16213
Y	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
Y	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
Y	419	HIS	-	expression tag	UNP A0A678ZGP6
Y	420	HIS	-	expression tag	UNP A0A678ZGP6
Y	421	HIS	-	expression tag	UNP A0A678ZGP6
Y	422	HIS	-	expression tag	UNP A0A678ZGP6
Y	423	HIS	-	expression tag	UNP A0A678ZGP6
Y	424	HIS	-	expression tag	UNP A0A678ZGP6
a	5J	GLY	-	linker	UNP P03129
a	5K	GLY	-	linker	UNP P03129
a	5L	GLY	-	linker	UNP P03129
a	5M	GLY	-	linker	UNP P03129
a	5N	SER	-	linker	UNP P03129
a	5O	GLY	-	linker	UNP P03129
a	5P	GLY	-	linker	UNP P03129
a	5Q	GLY	-	linker	UNP P03129
a	5R	GLY	-	linker	UNP P03129
a	5S	SER	-	linker	UNP P03129
a	5T	GLY	-	linker	UNP P03129
a	5U	GLY	-	linker	UNP P03129
a	5V	GLY	-	linker	UNP P03129
a	5W	GLY	-	linker	UNP P03129
a	5X	SER	-	linker	UNP P03129
a	124	GLY	-	linker	UNP P16213
a	125	GLY	-	linker	UNP P16213
a	126	GLY	-	linker	UNP P16213
a	127	GLY	-	linker	UNP P16213
a	128	SER	-	linker	UNP P16213
a	129	GLY	-	linker	UNP P16213
a	130	GLY	-	linker	UNP P16213
a	131	GLY	-	linker	UNP P16213
a	132	GLY	-	linker	UNP P16213
a	133	SER	-	linker	UNP P16213
a	134	GLY	-	linker	UNP P16213
a	135	GLY	-	linker	UNP P16213
a	136	GLY	-	linker	UNP P16213
a	137	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
a	138	SER	-	linker	UNP P16213
a	139	GLY	-	linker	UNP P16213
a	140	GLY	-	linker	UNP P16213
a	141	GLY	-	linker	UNP P16213
a	142	GLY	-	linker	UNP P16213
a	143	SER	-	linker	UNP P16213
a	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
a	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
a	419	HIS	-	expression tag	UNP A0A678ZGP6
a	420	HIS	-	expression tag	UNP A0A678ZGP6
a	421	HIS	-	expression tag	UNP A0A678ZGP6
a	422	HIS	-	expression tag	UNP A0A678ZGP6
a	423	HIS	-	expression tag	UNP A0A678ZGP6
a	424	HIS	-	expression tag	UNP A0A678ZGP6
c	5J	GLY	-	linker	UNP P03129
c	5K	GLY	-	linker	UNP P03129
c	5L	GLY	-	linker	UNP P03129
c	5M	GLY	-	linker	UNP P03129
c	5N	SER	-	linker	UNP P03129
c	5O	GLY	-	linker	UNP P03129
c	5P	GLY	-	linker	UNP P03129
c	5Q	GLY	-	linker	UNP P03129
c	5R	GLY	-	linker	UNP P03129
c	5S	SER	-	linker	UNP P03129
c	5T	GLY	-	linker	UNP P03129
c	5U	GLY	-	linker	UNP P03129
c	5V	GLY	-	linker	UNP P03129
c	5W	GLY	-	linker	UNP P03129
c	5X	SER	-	linker	UNP P03129
c	124	GLY	-	linker	UNP P16213
c	125	GLY	-	linker	UNP P16213
c	126	GLY	-	linker	UNP P16213
c	127	GLY	-	linker	UNP P16213
c	128	SER	-	linker	UNP P16213
c	129	GLY	-	linker	UNP P16213
c	130	GLY	-	linker	UNP P16213
c	131	GLY	-	linker	UNP P16213
c	132	GLY	-	linker	UNP P16213
c	133	SER	-	linker	UNP P16213
c	134	GLY	-	linker	UNP P16213
c	135	GLY	-	linker	UNP P16213
c	136	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
c	137	GLY	-	linker	UNP P16213
c	138	SER	-	linker	UNP P16213
c	139	GLY	-	linker	UNP P16213
c	140	GLY	-	linker	UNP P16213
c	141	GLY	-	linker	UNP P16213
c	142	GLY	-	linker	UNP P16213
c	143	SER	-	linker	UNP P16213
c	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
c	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
c	419	HIS	-	expression tag	UNP A0A678ZGP6
c	420	HIS	-	expression tag	UNP A0A678ZGP6
c	421	HIS	-	expression tag	UNP A0A678ZGP6
c	422	HIS	-	expression tag	UNP A0A678ZGP6
c	423	HIS	-	expression tag	UNP A0A678ZGP6
c	424	HIS	-	expression tag	UNP A0A678ZGP6
e	5J	GLY	-	linker	UNP P03129
e	5K	GLY	-	linker	UNP P03129
e	5L	GLY	-	linker	UNP P03129
e	5M	GLY	-	linker	UNP P03129
e	5N	SER	-	linker	UNP P03129
e	5O	GLY	-	linker	UNP P03129
e	5P	GLY	-	linker	UNP P03129
e	5Q	GLY	-	linker	UNP P03129
e	5R	GLY	-	linker	UNP P03129
e	5S	SER	-	linker	UNP P03129
e	5T	GLY	-	linker	UNP P03129
e	5U	GLY	-	linker	UNP P03129
e	5V	GLY	-	linker	UNP P03129
e	5W	GLY	-	linker	UNP P03129
e	5X	SER	-	linker	UNP P03129
e	124	GLY	-	linker	UNP P16213
e	125	GLY	-	linker	UNP P16213
e	126	GLY	-	linker	UNP P16213
e	127	GLY	-	linker	UNP P16213
e	128	SER	-	linker	UNP P16213
e	129	GLY	-	linker	UNP P16213
e	130	GLY	-	linker	UNP P16213
e	131	GLY	-	linker	UNP P16213
e	132	GLY	-	linker	UNP P16213
e	133	SER	-	linker	UNP P16213
e	134	GLY	-	linker	UNP P16213
e	135	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
e	136	GLY	-	linker	UNP P16213
e	137	GLY	-	linker	UNP P16213
e	138	SER	-	linker	UNP P16213
e	139	GLY	-	linker	UNP P16213
e	140	GLY	-	linker	UNP P16213
e	141	GLY	-	linker	UNP P16213
e	142	GLY	-	linker	UNP P16213
e	143	SER	-	linker	UNP P16213
e	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
e	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
e	419	HIS	-	expression tag	UNP A0A678ZGP6
e	420	HIS	-	expression tag	UNP A0A678ZGP6
e	421	HIS	-	expression tag	UNP A0A678ZGP6
e	422	HIS	-	expression tag	UNP A0A678ZGP6
e	423	HIS	-	expression tag	UNP A0A678ZGP6
e	424	HIS	-	expression tag	UNP A0A678ZGP6

- Molecule 2 is a protein called VHH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	115	Total	C	H	N	O	S	0	0	0
			1625	521	782	145	173	4			
2	D	115	Total	C	H	N	O	S	0	0	0
			1635	523	788	146	174	4			
2	F	115	Total	C	H	N	O	S	0	0	0
			1635	523	788	146	174	4			
2	H	115	Total	C	H	N	O	S	0	0	0
			1635	523	788	146	174	4			
2	J	115	Total	C	H	N	O	S	0	0	0
			1644	529	792	146	173	4			
2	L	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	N	115	Total	C	H	N	O	S	0	0	0
			1620	520	777	145	174	4			
2	P	115	Total	C	H	N	O	S	0	0	0
			1633	526	784	145	174	4			
2	R	115	Total	C	H	N	O	S	0	0	0
			1594	516	758	144	172	4			
2	T	115	Total	C	H	N	O	S	0	0	0
			1655	530	800	146	175	4			
2	V	115	Total	C	H	N	O	S	0	0	0
			1639	524	789	147	175	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	115	Total	C	H	N	O	S	0	0	0
			1599	517	763	142	173	4			
2	Z	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	b	115	Total	C	H	N	O	S	0	0	0
			1648	529	795	146	174	4			
2	d	115	Total	C	H	N	O	S	0	0	0
			1642	524	792	147	175	4			
2	f	115	Total	C	H	N	O	S	0	0	0
			1651	530	797	146	174	4			

- Molecule 3 is water.

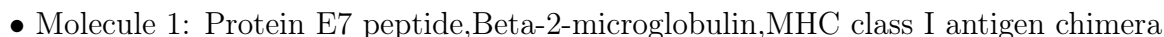
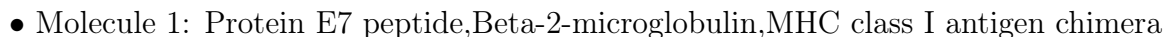
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			6	6		
3	B	2	Total	O	0	0
			2	2		
3	C	8	Total	O	0	0
			8	8		
3	D	3	Total	O	0	0
			3	3		
3	E	6	Total	O	0	0
			6	6		
3	F	6	Total	O	0	0
			6	6		
3	G	11	Total	O	0	0
			11	11		
3	H	4	Total	O	0	0
			4	4		
3	I	7	Total	O	0	0
			7	7		
3	J	4	Total	O	0	0
			4	4		
3	K	8	Total	O	0	0
			8	8		
3	L	7	Total	O	0	0
			7	7		
3	M	8	Total	O	0	0
			8	8		
3	N	6	Total	O	0	0
			6	6		

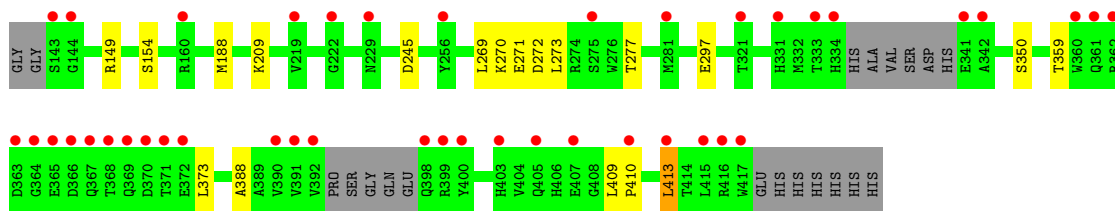
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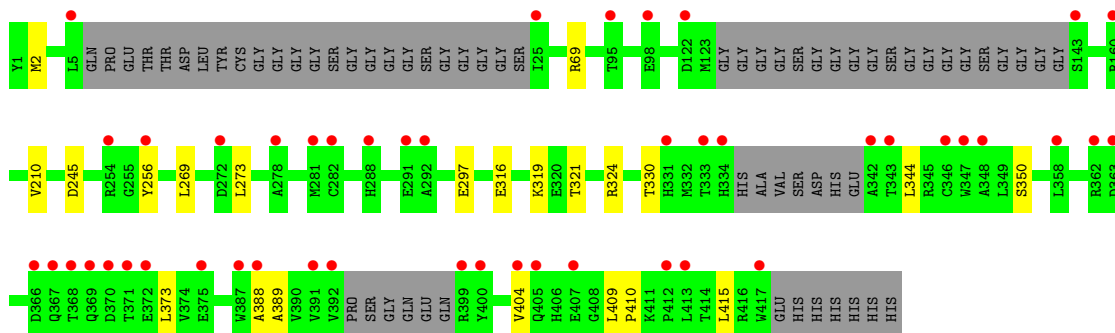
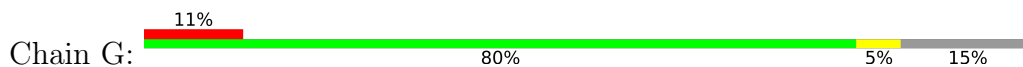
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	8	Total O 8 8	0	0
3	P	6	Total O 6 6	0	0
3	Q	11	Total O 11 11	0	0
3	R	3	Total O 3 3	0	0
3	S	8	Total O 8 8	0	0
3	T	7	Total O 7 7	0	0
3	U	5	Total O 5 5	0	0
3	V	2	Total O 2 2	0	0
3	W	4	Total O 4 4	0	0
3	X	4	Total O 4 4	0	0
3	Y	9	Total O 9 9	0	0
3	Z	3	Total O 3 3	0	0
3	a	11	Total O 11 11	0	0
3	b	7	Total O 7 7	0	0
3	c	10	Total O 10 10	0	0
3	d	4	Total O 4 4	0	0
3	e	7	Total O 7 7	0	0
3	f	3	Total O 3 3	0	0

- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

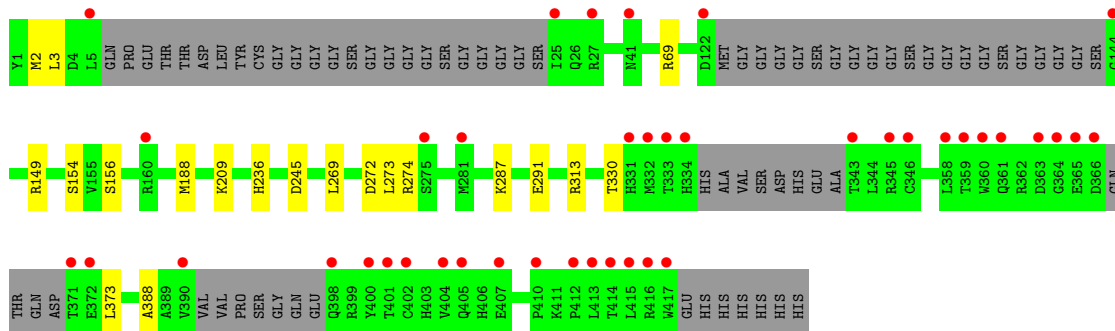
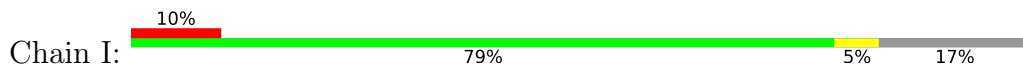




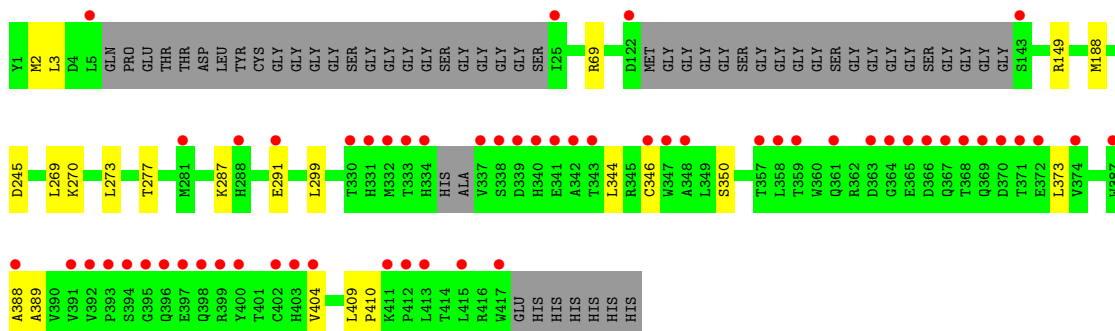
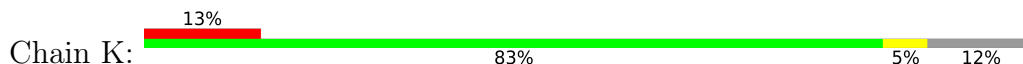
- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

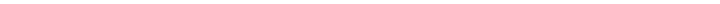


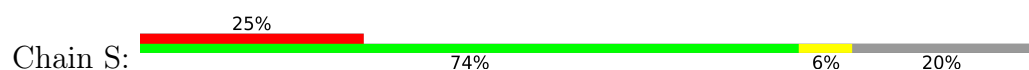
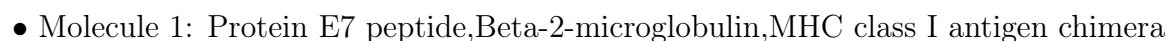
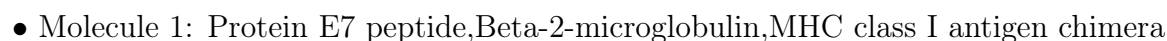
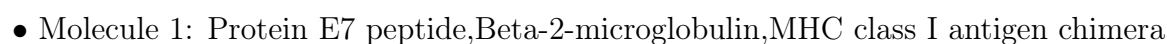
- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

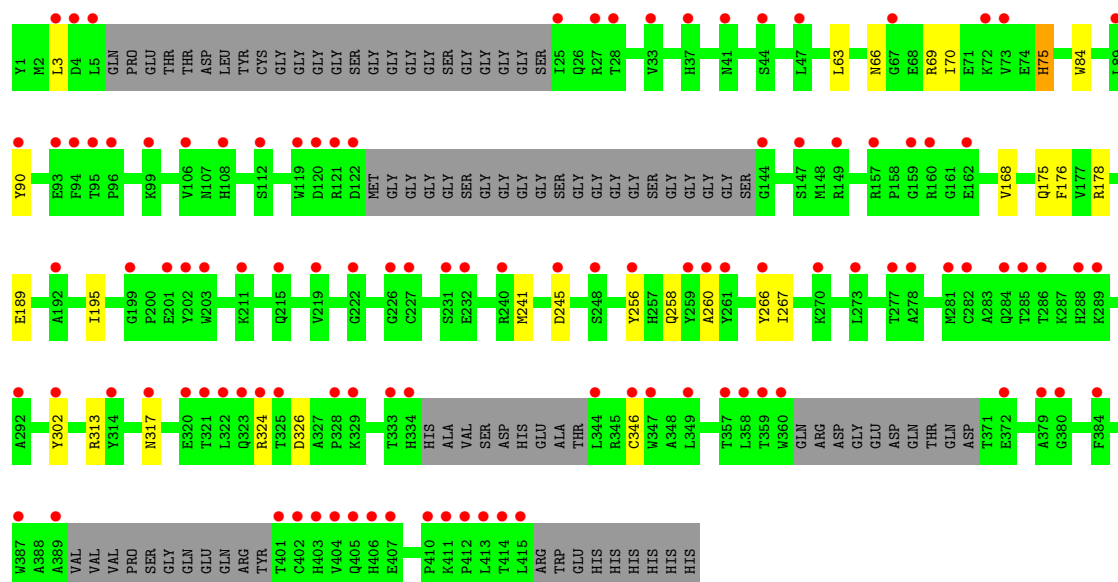


- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

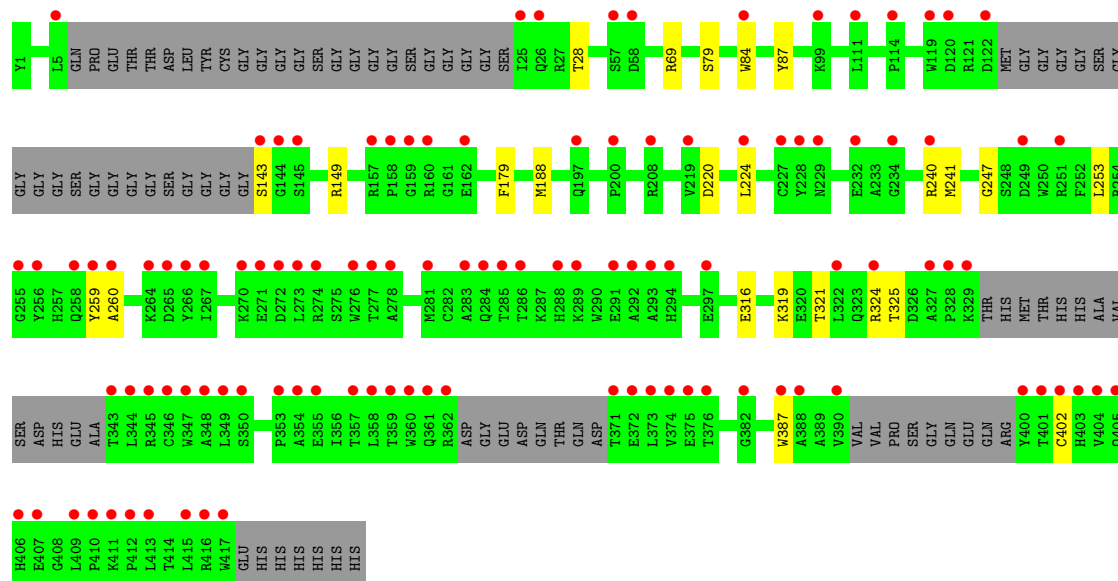
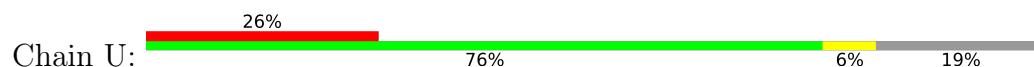


- Chain M: 

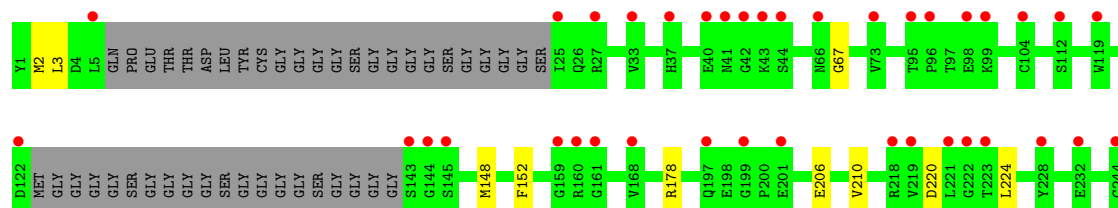
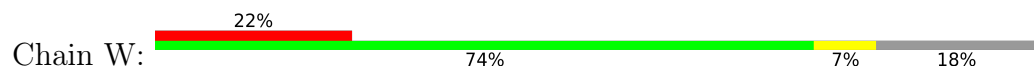


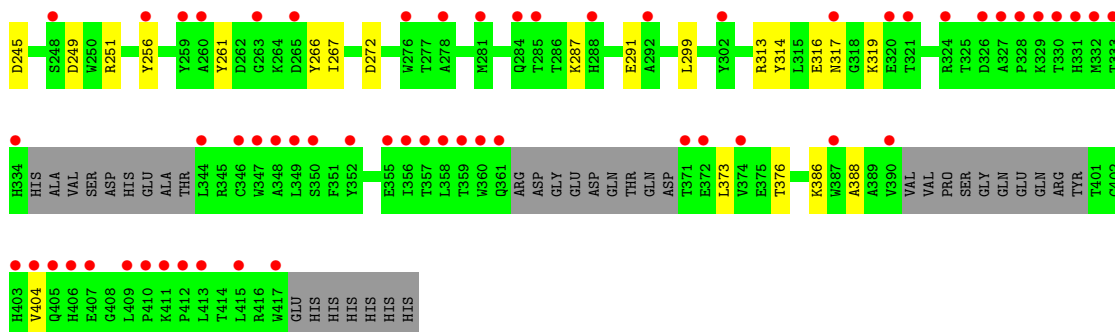


- Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

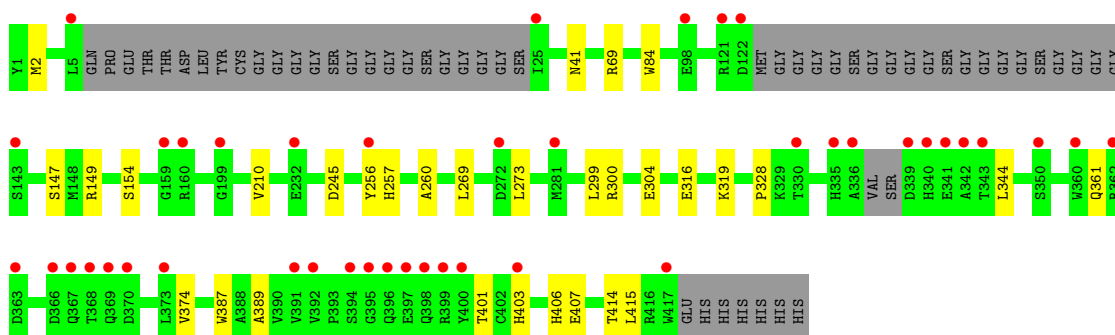
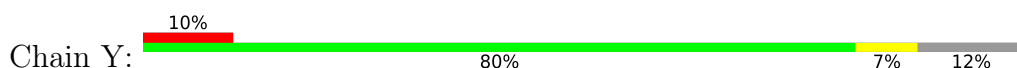


- Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

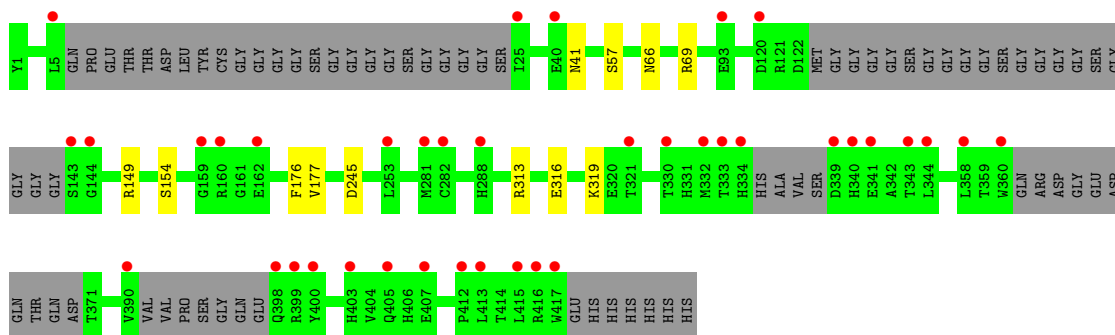
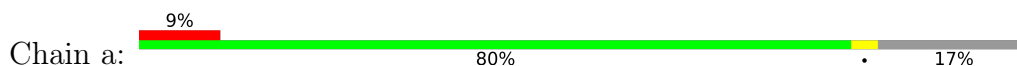




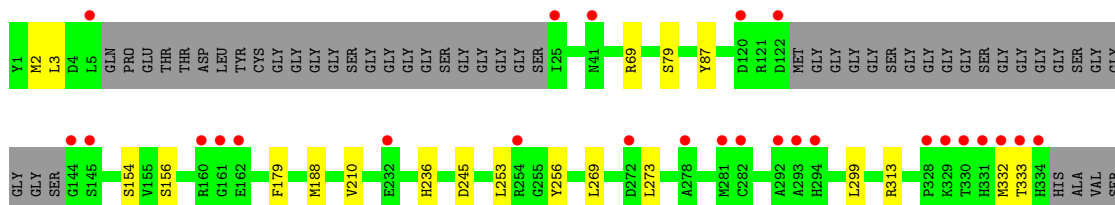
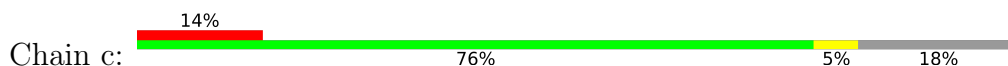
- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

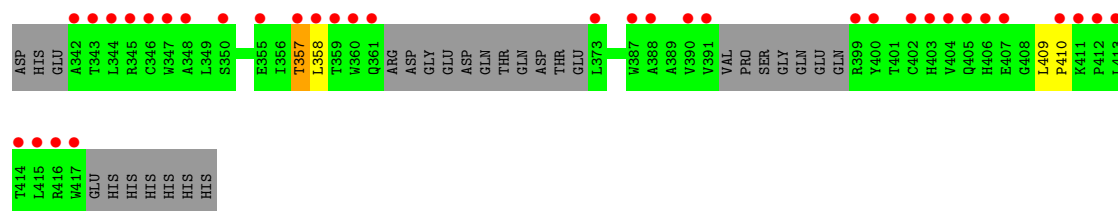


- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

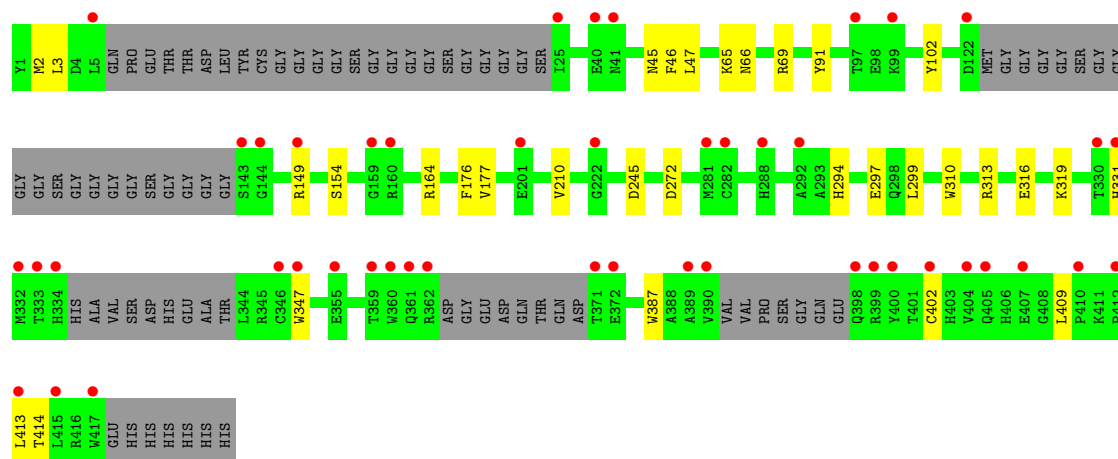
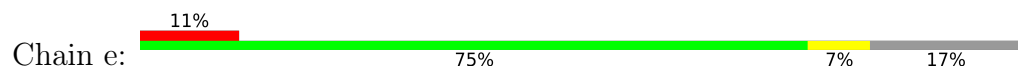


- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera

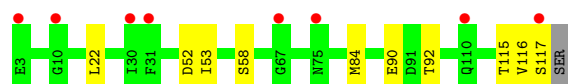
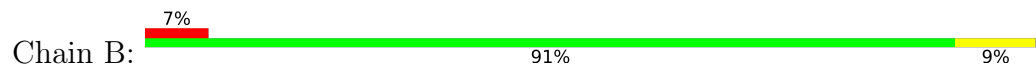




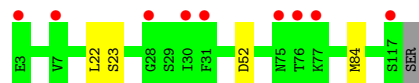
- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera



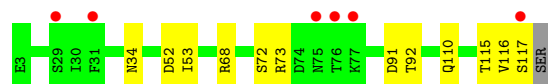
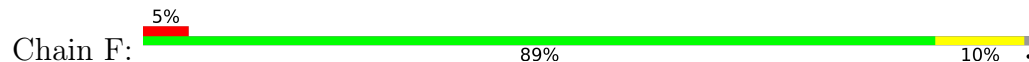
- Molecule 2: VHH



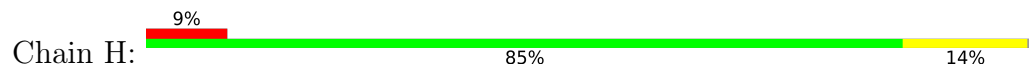
- Molecule 2: VHH

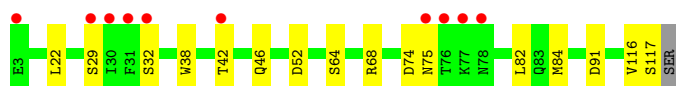


- Molecule 2: VHH

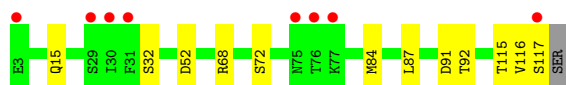
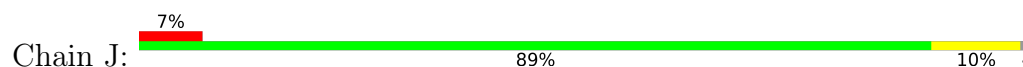


- Molecule 2: VHH

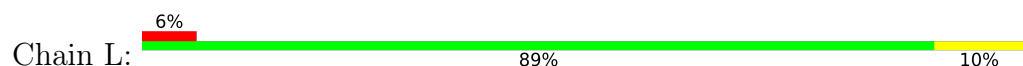




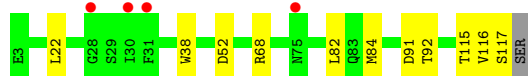
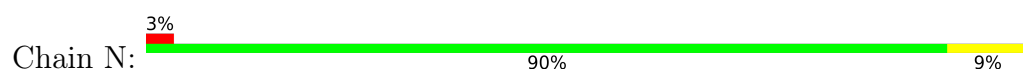
• Molecule 2: VHH



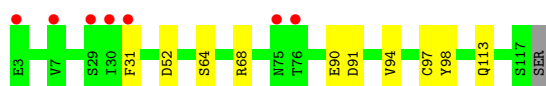
• Molecule 2: VHH



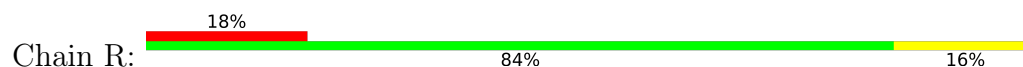
• Molecule 2: VHH



• Molecule 2: VHH



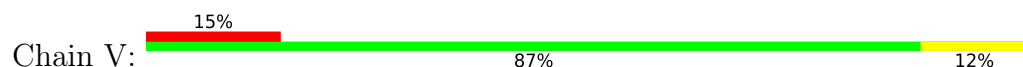
• Molecule 2: VHH



• Molecule 2: VHH

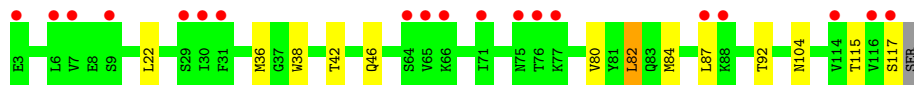
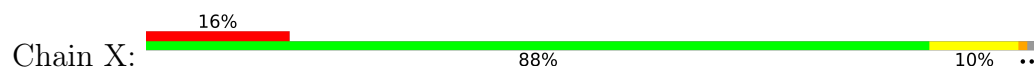


• Molecule 2: VHH

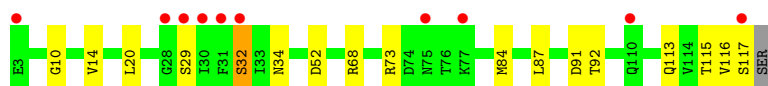
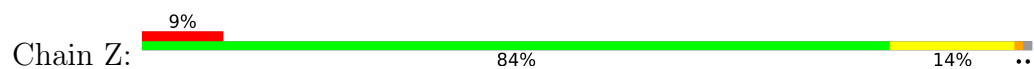




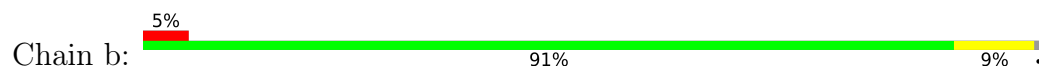
● Molecule 2: VHH



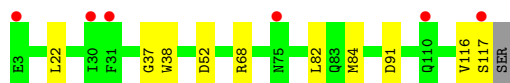
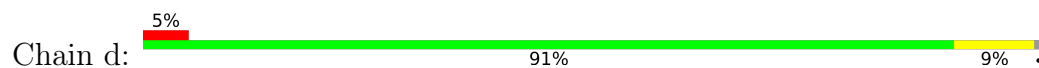
● Molecule 2: VHH



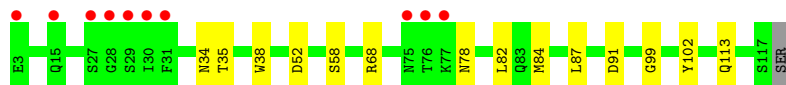
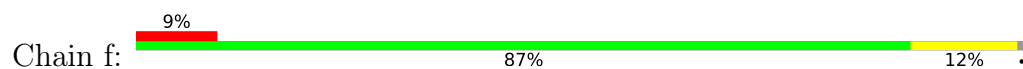
● Molecule 2: VHH



● Molecule 2: VHH



● Molecule 2: VHH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.80Å 118.04Å 273.51Å 102.45° 102.45° 90.00°	Depositor
Resolution (Å)	50.48 – 2.78 50.48 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.48-2.78) 96.7 (50.48-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.238 , 0.275 0.238 , 0.274	Depositor DCC
R_{free} test set	17173 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.357 for -k,h,k+l 0.357 for k,-h,h+l 0.409 for h,-k,-h-l 0.320 for -h,k,-k-l 0.398 for -k,-h,-l 0.366 for k,h,-h-k-l 0.336 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	109155	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.42% 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	0/2764	0.30	0/3766
1	C	0.14	0/2850	0.31	0/3887
1	E	0.15	0/2908	0.32	0/3964
1	G	0.15	0/2881	0.30	0/3932
1	I	0.15	0/2825	0.31	0/3850
1	K	0.15	0/2907	0.30	0/3969
1	M	0.16	0/2885	0.33	0/3938
1	O	0.15	0/2819	0.30	0/3846
1	Q	0.14	0/2941	0.31	0/4015
1	S	0.18	0/2729	0.31	0/3724
1	U	0.13	0/2682	0.31	0/3661
1	W	0.14	0/2763	0.31	0/3771
1	Y	0.15	0/2958	0.32	0/4039
1	a	0.14	0/2828	0.30	0/3855
1	c	0.14	0/2761	0.30	0/3765
1	e	0.15	0/2807	0.31	0/3826
2	B	0.15	0/858	0.33	0/1164
2	D	0.17	0/862	0.34	0/1169
2	F	0.15	0/862	0.32	0/1169
2	H	0.18	0/862	0.34	0/1169
2	J	0.15	0/868	0.33	0/1177
2	L	0.17	0/861	0.35	0/1168
2	N	0.24	0/858	0.38	0/1165
2	P	0.16	0/865	0.34	0/1174
2	R	0.13	0/851	0.33	0/1157
2	T	0.14	0/871	0.31	0/1181
2	V	0.14	0/865	0.31	0/1173
2	X	0.15	0/851	0.34	0/1157
2	Z	0.15	0/861	0.32	0/1168
2	b	0.15	0/869	0.33	0/1178
2	d	0.18	0/865	0.32	0/1173
2	f	0.16	0/870	0.35	0/1180
All	All	0.15	0/59107	0.31	0/80530

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

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	2692	2373	2373	7	0
1	C	2772	2442	2442	16	0
1	E	2830	2512	2512	21	0
1	G	2802	2459	2459	11	0
1	I	2749	2442	2442	12	0
1	K	2830	2463	2463	10	0
1	M	2808	2456	2456	17	0
1	O	2744	2411	2411	11	0
1	Q	2861	2517	2517	20	0
1	S	2653	2324	2324	21	0
1	U	2612	2261	2261	16	0
1	W	2686	2356	2355	19	0
1	Y	2877	2532	2532	17	0
1	a	2751	2436	2436	7	0
1	c	2687	2352	2352	13	0
1	e	2731	2419	2419	20	0
2	B	843	782	782	8	0
2	D	847	788	788	2	0
2	F	847	788	788	6	0
2	H	847	788	788	10	0
2	J	852	792	792	6	0
2	L	846	785	785	6	0
2	N	843	777	777	6	0
2	P	849	784	784	7	0
2	R	836	758	758	12	0
2	T	855	800	800	6	0
2	V	850	789	792	7	0
2	X	836	763	763	8	0
2	Z	846	785	785	10	0
2	b	853	795	795	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	850	792	792	7	0
2	f	854	797	797	8	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
3	C	8	0	0	0	0
3	D	3	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	11	0	0	0	0
3	H	4	0	0	0	0
3	I	7	0	0	0	0
3	J	4	0	0	0	0
3	K	8	0	0	0	0
3	L	7	0	0	0	0
3	M	8	0	0	0	0
3	N	6	0	0	0	0
3	O	8	0	0	0	0
3	P	6	0	0	0	0
3	Q	11	0	0	0	0
3	R	3	0	0	0	0
3	S	8	0	0	1	0
3	T	7	0	0	0	0
3	U	5	0	0	0	0
3	V	2	0	0	0	0
3	W	4	0	0	0	0
3	X	4	0	0	0	0
3	Y	9	0	0	0	0
3	Z	3	0	0	0	0
3	a	11	0	0	0	0
3	b	7	0	0	0	0
3	c	10	0	0	0	0
3	d	4	0	0	0	0
3	e	7	0	0	0	0
3	f	3	0	0	0	0
All	All	57837	51318	51320	327	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 (327) 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:S:313:ARG:O	1:S:317:ASN:OD1	1.85	0.94
1:U:316:GLU:OE2	1:U:319:LYS:NZ	2.01	0.92
1:E:269:LEU:HD23	1:E:273:LEU:HD12	1.59	0.83
1:c:245:ASP:OD2	1:c:256:TYR:OH	1.98	0.81
1:Q:361:GLN:OE1	1:Q:403:HIS:NE2	2.16	0.78
2:L:68:ARG:NH2	2:L:91:ASP:OD2	2.19	0.74
1:W:245:ASP:OD2	1:W:256:TYR:OH	2.05	0.74
1:K:269:LEU:HD23	1:K:273:LEU:HD12	1.72	0.72
1:C:149:ARG:NH2	1:C:172:ASP:O	2.26	0.69
1:S:245:ASP:OD2	1:S:256:TYR:OH	2.11	0.68
1:Y:361:GLN:OE1	1:Y:403:HIS:NE2	2.27	0.67
1:M:149:ARG:HG2	1:M:149:ARG:HH11	1.61	0.66
1:O:149:ARG:NH2	1:O:245:ASP:OD1	2.28	0.66
2:R:92:THR:HG23	2:R:115:THR:HA	1.77	0.66
1:G:245:ASP:OD2	1:G:256:TYR:OH	2.14	0.65
2:P:68:ARG:NH2	2:P:91:ASP:OD2	2.30	0.64
1:Q:178:ARG:HD3	1:Q:191:ARG:CZ	2.28	0.63
1:M:361:GLN:HE22	1:M:403:HIS:CD2	2.17	0.63
2:F:53:ILE:HD13	2:F:73:ARG:HB2	1.81	0.63
1:e:294:HIS:HB3	1:e:297:GLU:OE1	1.99	0.62
1:Q:69:ARG:NH2	2:R:52:ASP:OD2	2.33	0.61
1:M:330:THR:CG2	1:M:415:LEU:HD21	2.30	0.61
1:c:69:ARG:NH2	2:d:52:ASP:OD2	2.34	0.61
2:V:68:ARG:NH2	2:V:91:ASP:OD2	2.34	0.60
1:Y:69:ARG:NH2	2:Z:52:ASP:OD2	2.34	0.60
1:e:149:ARG:NH2	1:e:245:ASP:OD1	2.35	0.60
1:U:316:GLU:O	1:U:319:LYS:HG2	2.01	0.60
1:Q:245:ASP:OD2	1:Q:256:TYR:OH	2.20	0.60
2:X:42:THR:OG1	2:X:46:GLN:O	2.20	0.60
1:a:149:ARG:NH2	1:a:245:ASP:OD1	2.34	0.60
1:c:3:LEU:HD11	1:c:299:LEU:HD22	1.85	0.59
1:M:69:ARG:NH2	2:N:52:ASP:OD2	2.36	0.59
1:C:2:MET:HE1	1:C:210:VAL:HB	1.85	0.59
1:K:149:ARG:NH2	1:K:245:ASP:OD1	2.36	0.59
1:I:149:ARG:NH2	1:I:245:ASP:OD1	2.34	0.58
2:J:15:GLN:OE1	2:J:117:SER:OG	2.16	0.58
1:K:69:ARG:NH2	2:L:52:ASP:OD2	2.35	0.58
1:a:69:ARG:NH2	2:b:52:ASP:OD2	2.35	0.58
1:e:347:TRP:HD1	1:e:387:TRP:HB3	1.69	0.58
1:C:316:GLU:OE2	1:C:319:LYS:NZ	2.37	0.58
1:Y:245:ASP:OD2	1:Y:256:TYR:OH	2.22	0.58
1:c:179:PHE:HB2	1:c:188:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:HD23	1:E:273:LEU:CD1	2.32	0.57
2:J:68:ARG:NH2	2:J:91:ASP:OD2	2.37	0.57
1:G:330:THR:CG2	1:G:415:LEU:HD11	2.35	0.57
1:S:176:PHE:CD2	1:S:195:ILE:HD13	2.40	0.57
1:c:2:MET:HE1	1:c:210:VAL:HB	1.87	0.57
2:Z:68:ARG:NH2	2:Z:91:ASP:OD2	2.37	0.57
1:A:2:MET:HE1	1:A:210:VAL:HB	1.86	0.57
2:b:68:ARG:NH2	2:b:91:ASP:OD2	2.39	0.56
1:E:120:ASP:HB3	1:E:123:MET:HG3	1.87	0.56
2:R:38:TRP:CZ3	2:R:82:LEU:HB2	2.40	0.56
2:d:68:ARG:NH2	2:d:91:ASP:OD2	2.38	0.56
1:A:69:ARG:NH2	2:B:52:ASP:OD2	2.39	0.56
1:Y:414:THR:C	1:Y:415:LEU:HD23	2.30	0.56
2:T:68:ARG:NH2	2:T:91:ASP:OD1	2.38	0.56
2:B:22:LEU:HD22	2:B:84:MET:HE2	1.87	0.55
1:S:324:ARG:NH1	1:S:326:ASP:OD2	2.40	0.55
1:Y:2:MET:HE1	1:Y:210:VAL:HB	1.88	0.55
1:G:69:ARG:NH2	2:H:52:ASP:OD2	2.40	0.54
1:S:69:ARG:NH2	2:T:52:ASP:OD2	2.40	0.54
1:Y:300:ARG:HG2	1:Y:304:GLU:OE1	2.07	0.54
2:V:92:THR:HG23	2:V:115:THR:HA	1.90	0.54
1:c:245:ASP:CG	1:c:256:TYR:HH	2.14	0.54
1:W:313:ARG:O	1:W:317:ASN:OD1	2.25	0.54
1:Y:361:GLN:OE1	1:Y:403:HIS:CD2	2.61	0.54
1:E:69:ARG:NH2	2:F:52:ASP:OD2	2.41	0.53
2:R:22:LEU:HD23	2:R:84:MET:SD	2.48	0.53
1:E:409:LEU:HD13	1:E:413:LEU:HD12	1.89	0.53
2:F:68:ARG:NH2	2:F:91:ASP:OD2	2.42	0.53
1:O:3:LEU:HD11	1:O:299:LEU:HD22	1.90	0.53
1:M:361:GLN:NE2	1:M:403:HIS:CD2	2.77	0.53
1:O:316:GLU:OE2	1:O:319:LYS:NZ	2.40	0.53
1:U:69:ARG:NH2	2:V:52:ASP:OD2	2.41	0.53
2:f:68:ARG:NH2	2:f:91:ASP:OD2	2.42	0.53
1:U:149:ARG:HD2	1:U:241:MET:CE	2.40	0.52
2:X:38:TRP:CD2	2:X:82:LEU:HD12	2.45	0.52
1:Y:361:GLN:OE1	1:Y:401:THR:CG2	2.58	0.52
1:A:178:ARG:HD3	1:A:191:ARG:CZ	2.40	0.52
1:E:2:MET:HE1	1:E:188:MET:SD	2.49	0.52
1:S:245:ASP:CG	1:S:256:TYR:HH	2.17	0.52
2:N:68:ARG:NH2	2:N:91:ASP:OD2	2.43	0.52
1:I:272:ASP:OD1	1:I:272:ASP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:401:THR:OG1	1:Q:414:THR:HG23	2.10	0.52
2:B:22:LEU:HD13	2:B:84:MET:CE	2.39	0.52
1:Q:148:MET:HE3	1:Q:307:CYS:SG	2.50	0.52
2:X:84:MET:HB3	2:X:87:LEU:HD21	1.92	0.52
1:M:2:MET:HE1	1:M:188:MET:SD	2.50	0.52
2:V:10:GLY:O	2:V:20:LEU:HD22	2.10	0.52
1:G:316:GLU:O	1:G:319:LYS:HD3	2.10	0.51
1:S:3:LEU:HD23	1:S:302:TYR:CG	2.45	0.51
1:S:176:PHE:HD2	1:S:195:ILE:HD13	1.76	0.51
1:U:84:TRP:CZ3	1:U:260:ALA:HB3	2.46	0.51
1:W:148:MET:HE2	1:W:314:TYR:CE2	2.46	0.51
1:W:376:THR:HA	1:W:386:LYS:HG3	1.93	0.51
1:I:313:ARG:NH1	2:P:94:VAL:HG11	2.26	0.51
1:W:287:LYS:O	1:W:291:GLU:HG3	2.11	0.51
1:K:270:LYS:HD3	1:K:277:THR:OG1	2.09	0.50
2:R:84:MET:HB3	2:R:87:LEU:HD21	1.92	0.50
1:E:272:ASP:OD1	1:E:272:ASP:C	2.55	0.50
1:G:2:MET:HE1	1:G:210:VAL:HB	1.94	0.50
1:O:272:ASP:C	1:O:272:ASP:OD1	2.54	0.50
1:Y:374:VAL:HG11	1:Y:387:TRP:CZ2	2.47	0.50
1:O:100:ASP:O	1:O:121:ARG:NH2	2.34	0.49
1:U:321:THR:O	1:U:324:ARG:HG2	2.12	0.49
2:Z:116:VAL:O	2:Z:117:SER:C	2.55	0.49
1:I:272:ASP:OD1	1:I:274:ARG:N	2.36	0.49
2:B:116:VAL:O	2:B:117:SER:C	2.55	0.49
1:E:271:GLU:O	1:E:273:LEU:HD22	2.11	0.49
2:R:116:VAL:O	2:R:117:SER:C	2.56	0.49
1:S:66:ASN:O	2:T:34:ASN:ND2	2.43	0.49
2:Z:34:ASN:O	2:Z:73:ARG:NH1	2.43	0.49
1:G:269:LEU:HD23	1:G:273:LEU:HD12	1.94	0.49
1:Q:1:TYR:CD2	1:Q:310:TRP:CE2	3.01	0.49
2:Z:84:MET:HB3	2:Z:87:LEU:HD21	1.93	0.49
1:E:25:ILE:N	1:E:25:ILE:HD12	2.28	0.48
1:e:65:LYS:HG3	1:e:102:TYR:CE2	2.48	0.48
1:U:179:PHE:HB2	1:U:188:MET:SD	2.54	0.48
2:J:84:MET:HB3	2:J:87:LEU:HD21	1.95	0.48
1:e:69:ARG:NH2	2:f:52:ASP:OD2	2.46	0.48
1:I:69:ARG:NH2	2:J:52:ASP:OD2	2.46	0.48
2:R:68:ARG:NH2	2:R:91:ASP:OD2	2.47	0.48
1:e:66:ASN:O	2:f:34:ASN:ND2	2.47	0.48
1:C:120:ASP:O	1:C:123:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:258:GLN:OE1	3:S:501:HOH:O	2.20	0.48
1:M:328:PRO:HD3	1:M:406:HIS:ND1	2.28	0.48
1:G:297:GLU:N	1:G:297:GLU:OE1	2.47	0.48
2:J:92:THR:HG23	2:J:115:THR:HA	1.95	0.48
1:W:3:LEU:HD11	1:W:299:LEU:HD22	1.96	0.48
1:e:2:MET:HE1	1:e:210:VAL:HB	1.96	0.48
2:X:36:MET:HB2	2:X:80:VAL:HG11	1.96	0.48
1:C:69:ARG:NH2	2:D:52:ASP:OD2	2.47	0.47
2:H:64:SER:O	2:H:68:ARG:NH1	2.47	0.47
1:W:373:LEU:HD12	1:W:388:ALA:HB2	1.95	0.47
1:W:148:MET:HE2	1:W:314:TYR:CD2	2.50	0.47
1:W:206:GLU:O	1:W:210:VAL:HG12	2.13	0.47
1:U:84:TRP:CZ3	1:U:260:ALA:CB	2.98	0.47
1:e:272:ASP:C	1:e:272:ASP:OD1	2.57	0.47
1:W:272:ASP:C	1:W:272:ASP:OD1	2.57	0.47
1:c:332:MET:HG3	1:c:333:THR:N	2.29	0.47
1:C:65:LYS:HG3	1:C:102:TYR:CE2	2.50	0.47
1:S:168:VAL:CG1	1:S:175:GLN:HG3	2.45	0.47
1:E:3:LEU:O	1:E:209:LYS:HD2	2.14	0.47
2:L:92:THR:HG23	2:L:115:THR:HA	1.97	0.47
1:C:302:TYR:CD2	1:C:303:LEU:HD23	2.50	0.47
1:Q:190:PRO:O	1:Q:191:ARG:HD3	2.15	0.47
1:S:241:MET:HE3	1:S:241:MET:C	2.40	0.47
2:H:42:THR:OG1	2:H:46:GLN:O	2.30	0.47
1:I:269:LEU:HG	1:I:273:LEU:HA	1.97	0.47
1:U:220:ASP:O	1:U:224:LEU:HD23	2.15	0.47
2:X:22:LEU:HG	2:X:84:MET:SD	2.55	0.47
1:W:266:TYR:HD2	1:W:267:ILE:HG22	1.78	0.46
1:C:269:LEU:HD23	1:C:273:LEU:HD22	1.97	0.46
2:H:29:SER:O	2:H:32:SER:OG	2.32	0.46
2:N:116:VAL:O	2:N:117:SER:C	2.57	0.46
1:e:45:ASN:OD1	1:e:46:PHE:N	2.44	0.46
2:H:74:ASP:OD1	2:H:75:ASN:N	2.49	0.46
1:M:178:ARG:HD3	1:M:191:ARG:CZ	2.45	0.46
2:d:22:LEU:HG	2:d:84:MET:HE2	1.98	0.46
1:O:69:ARG:NH2	2:P:52:ASP:OD2	2.48	0.46
1:S:245:ASP:CG	1:S:256:TYR:OH	2.59	0.46
1:e:331:HIS:O	1:e:347:TRP:HB2	2.16	0.46
1:e:294:HIS:CB	1:e:297:GLU:OE1	2.64	0.46
1:K:2:MET:HE1	1:K:188:MET:SD	2.56	0.46
1:e:154:SER:HA	1:e:164:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:316:GLU:O	1:e:319:LYS:HG2	2.17	0.45
2:D:22:LEU:HG	2:D:84:MET:CE	2.46	0.45
1:M:321:THR:O	1:M:324:ARG:HG2	2.16	0.45
2:L:22:LEU:CD1	2:L:84:MET:HE2	2.46	0.45
1:W:220:ASP:O	1:W:224:LEU:HG	2.16	0.45
2:H:22:LEU:HD11	2:H:84:MET:CE	2.47	0.45
1:E:100:ASP:O	1:E:121:ARG:NH1	2.46	0.45
1:a:316:GLU:O	1:a:319:LYS:HG2	2.16	0.45
2:f:84:MET:HB3	2:f:87:LEU:HD21	1.98	0.45
2:B:22:LEU:HD13	2:B:84:MET:HE2	1.98	0.45
2:d:116:VAL:O	2:d:117:SER:C	2.60	0.45
1:e:3:LEU:HD11	1:e:299:LEU:HD22	1.99	0.45
1:S:178:ARG:NH1	1:S:189:GLU:OE2	2.50	0.45
1:Y:147:SER:HB2	1:Y:149:ARG:NH1	2.32	0.45
2:d:22:LEU:HG	2:d:84:MET:CE	2.47	0.45
1:e:409:LEU:HD13	1:e:413:LEU:HG	1.98	0.45
2:f:35:THR:O	2:f:99:GLY:HA2	2.17	0.45
2:F:92:THR:HG23	2:F:115:THR:HA	1.98	0.44
1:W:249:ASP:OD2	1:W:251:ARG:NE	2.50	0.44
2:Z:10:GLY:O	2:Z:20:LEU:HD22	2.18	0.44
1:C:156:SER:HG	1:C:236:HIS:H	1.63	0.44
1:O:272:ASP:OD1	1:O:274:ARG:N	2.41	0.44
1:Q:179:PHE:HB2	1:Q:188:MET:SD	2.57	0.44
1:E:270:LYS:HE3	1:E:277:THR:OG1	2.17	0.44
2:V:72:SER:O	2:V:80:VAL:HG23	2.17	0.44
2:V:116:VAL:O	2:V:117:SER:C	2.60	0.44
1:Y:316:GLU:O	1:Y:319:LYS:HG2	2.16	0.44
1:E:273:LEU:HD22	1:E:273:LEU:N	2.33	0.44
2:H:22:LEU:CD1	2:H:84:MET:HE2	2.48	0.44
1:C:37:HIS:HB3	1:C:38:PRO:HD2	1.98	0.44
1:G:344:LEU:O	1:G:389:ALA:HA	2.17	0.44
2:H:116:VAL:O	2:H:117:SER:C	2.59	0.44
2:P:97:CYS:SG	2:P:98:TYR:N	2.90	0.44
1:M:361:GLN:HE22	1:M:403:HIS:CE1	2.35	0.44
1:Q:28:THR:HG23	1:Q:29:PRO:HD2	2.00	0.44
1:W:313:ARG:O	1:W:316:GLU:N	2.50	0.44
1:c:357:THR:O	1:c:358:LEU:HD23	2.18	0.44
1:E:122:ASP:O	1:E:123:MET:HG2	2.18	0.44
2:V:38:TRP:CZ3	2:V:82:LEU:HB2	2.53	0.44
1:W:67:GLY:N	2:X:104:ASN:OD1	2.42	0.44
2:Z:92:THR:HG23	2:Z:115:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:374:VAL:HG11	1:Q:387:TRP:CZ2	2.53	0.43
1:U:247:GLY:N	1:U:253:LEU:HD12	2.33	0.43
1:K:344:LEU:O	1:K:389:ALA:HA	2.18	0.43
1:M:387:TRP:CE3	1:M:387:TRP:C	2.96	0.43
1:M:178:ARG:CD	1:M:191:ARG:CZ	2.96	0.43
2:P:64:SER:O	2:P:68:ARG:NH1	2.51	0.43
1:S:84:TRP:CE2	1:S:260:ALA:HB2	2.53	0.43
1:U:143:SER:CB	1:U:325:THR:HG21	2.48	0.43
1:A:387:TRP:CD1	1:A:387:TRP:C	2.97	0.43
1:S:245:ASP:OD2	1:S:256:TYR:CE2	2.72	0.43
1:U:84:TRP:CH2	1:U:260:ALA:HB2	2.53	0.43
1:C:272:ASP:OD1	1:C:272:ASP:C	2.60	0.43
1:G:373:LEU:HD13	1:G:388:ALA:HB2	2.00	0.43
1:C:121:ARG:HD3	2:P:31:PHE:CD1	2.54	0.43
1:Q:1:TYR:CE1	1:Q:209:LYS:NZ	2.87	0.43
1:Q:344:LEU:O	1:Q:389:ALA:HA	2.18	0.43
2:Z:14:VAL:HG11	2:Z:87:LEU:HD12	2.01	0.43
1:C:347:TRP:CZ3	1:C:387:TRP:CD1	3.07	0.43
1:K:3:LEU:HD11	1:K:299:LEU:HD22	2.01	0.43
1:Q:276:TRP:HB2	1:Q:287:LYS:HG3	2.00	0.43
1:c:156:SER:HG	1:c:236:HIS:H	1.65	0.43
1:e:310:TRP:HA	1:e:313:ARG:HD3	2.01	0.43
1:G:409:LEU:O	1:G:410:PRO:C	2.62	0.43
2:R:34:ASN:O	2:R:73:ARG:NH1	2.46	0.43
1:U:387:TRP:CD1	1:U:387:TRP:C	2.97	0.43
2:X:38:TRP:CE3	2:X:82:LEU:HD12	2.54	0.43
1:I:156:SER:HG	1:I:236:HIS:H	1.67	0.43
2:T:65:VAL:HG21	2:T:69:PHE:CD2	2.53	0.43
2:B:53:ILE:HA	2:B:58:SER:O	2.19	0.42
1:K:373:LEU:HD13	1:K:388:ALA:HB2	2.01	0.42
1:K:409:LEU:O	1:K:410:PRO:C	2.62	0.42
1:S:75:HIS:HB3	1:S:90:TYR:CD2	2.54	0.42
2:f:34:ASN:ND2	2:f:102:TYR:CE1	2.87	0.42
1:A:344:LEU:O	1:A:389:ALA:HA	2.19	0.42
1:E:373:LEU:HD12	1:E:388:ALA:HB2	2.01	0.42
1:A:346:CYS:O	1:A:387:TRP:HA	2.19	0.42
1:C:47:LEU:O	1:C:91:TYR:HA	2.19	0.42
1:E:66:ASN:O	2:F:34:ASN:ND2	2.46	0.42
1:E:409:LEU:HD22	1:E:413:LEU:HD11	2.01	0.42
1:E:297:GLU:OE1	1:E:297:GLU:N	2.51	0.42
2:L:116:VAL:O	2:L:117:SER:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:241:MET:HE3	1:S:241:MET:O	2.20	0.42
2:N:22:LEU:HG	2:N:84:MET:HE2	2.02	0.42
1:W:224:LEU:HD12	1:W:261:TYR:CD1	2.54	0.42
1:W:316:GLU:O	1:W:319:LYS:HG2	2.19	0.42
2:R:36:MET:HB2	2:R:80:VAL:HG11	2.01	0.42
1:c:269:LEU:HD23	1:c:273:LEU:HD23	2.01	0.42
1:c:409:LEU:O	1:c:410:PRO:C	2.63	0.42
1:M:257:HIS:HB3	1:M:269:LEU:HD12	2.02	0.42
1:Q:332:MET:HE1	1:Q:416:ARG:C	2.44	0.42
2:Z:29:SER:O	2:Z:32:SER:OG	2.37	0.42
1:A:37:HIS:HB3	1:A:38:PRO:HD2	2.02	0.42
1:E:149:ARG:NH2	1:E:245:ASP:OD1	2.53	0.42
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.53	0.42
1:I:313:ARG:HG2	2:P:113:GLN:HB2	2.01	0.42
1:Q:79:SER:HB3	1:Q:87:TYR:CZ	2.55	0.42
2:L:38:TRP:CZ3	2:L:82:LEU:HB2	2.55	0.42
1:a:176:PHE:CD2	1:a:177:VAL:HG13	2.55	0.42
2:B:92:THR:HG23	2:B:115:THR:HA	2.02	0.42
1:I:2:MET:HE1	1:I:188:MET:CE	2.50	0.42
1:Q:46:PHE:CZ	1:Q:93:GLU:HG3	2.55	0.42
1:U:79:SER:HB3	1:U:87:TYR:CZ	2.55	0.41
1:W:404:VAL:O	1:W:404:VAL:HG12	2.20	0.41
2:X:92:THR:HG23	2:X:115:THR:HA	2.01	0.41
1:E:409:LEU:O	1:E:410:PRO:C	2.64	0.41
1:U:84:TRP:HH2	1:U:259:TYR:C	2.28	0.41
2:b:38:TRP:CZ3	2:b:82:LEU:HB2	2.55	0.41
2:b:61:TYR:HB2	2:b:66:LYS:HD2	2.02	0.41
1:I:3:LEU:O	1:I:209:LYS:HD2	2.21	0.41
1:M:149:ARG:HG2	1:M:149:ARG:NH1	2.31	0.41
1:Y:269:LEU:HD13	1:Y:273:LEU:HD12	2.01	0.41
1:C:355:GLU:OE1	1:C:355:GLU:HA	2.20	0.41
2:J:116:VAL:O	2:J:117:SER:C	2.62	0.41
1:S:241:MET:HE1	1:S:256:TYR:HB2	2.03	0.41
1:Y:344:LEU:O	1:Y:389:ALA:HA	2.20	0.41
1:I:287:LYS:O	1:I:291:GLU:HG3	2.21	0.41
1:O:269:LEU:HG	1:O:273:LEU:HA	2.01	0.41
1:Q:188:MET:SD	1:Q:210:VAL:HG11	2.61	0.41
1:Y:328:PRO:HD3	1:Y:406:HIS:ND1	2.36	0.41
1:a:66:ASN:O	2:b:34:ASN:ND2	2.50	0.41
1:c:79:SER:HB3	1:c:87:TYR:CZ	2.55	0.41
1:M:344:LEU:O	1:M:389:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:TRP:CZ3	2:H:82:LEU:HB2	2.56	0.41
1:Q:269:LEU:HD23	1:Q:273:LEU:HD12	2.02	0.41
1:S:266:TYR:HD2	1:S:267:ILE:HG22	1.85	0.41
2:f:38:TRP:CZ3	2:f:82:LEU:HB2	2.56	0.41
1:K:287:LYS:O	1:K:291:GLU:HG3	2.20	0.41
2:N:92:THR:HG23	2:N:115:THR:HA	2.03	0.41
2:Z:113:GLN:HB2	1:c:313:ARG:HG2	2.02	0.41
2:d:38:TRP:CZ3	2:d:82:LEU:HB2	2.56	0.41
1:e:47:LEU:O	1:e:91:TYR:HA	2.21	0.41
1:e:149:ARG:CG	1:e:149:ARG:HH11	2.34	0.41
1:E:2:MET:HE2	1:E:188:MET:HE2	2.03	0.41
1:Y:84:TRP:CE2	1:Y:260:ALA:HB2	2.55	0.41
1:Y:149:ARG:NH1	1:Y:256:TYR:HE2	2.19	0.41
1:M:152:PHE:HB2	1:M:240:ARG:HB3	2.03	0.40
1:e:402:CYS:O	1:e:414:THR:HA	2.21	0.40
2:B:90:GLU:OE2	2:B:90:GLU:N	2.54	0.40
1:C:45:ASN:OD1	1:C:46:PHE:N	2.49	0.40
1:I:373:LEU:HD12	1:I:388:ALA:HB2	2.02	0.40
2:N:38:TRP:CZ3	2:N:82:LEU:HB2	2.56	0.40
1:O:178:ARG:HH21	1:O:180:ASP:HB2	1.86	0.40
2:T:42:THR:HG23	2:T:44:GLY:N	2.36	0.40
1:Y:257:HIS:CD2	1:Y:299:LEU:HD21	2.57	0.40
2:b:84:MET:HB3	2:b:87:LEU:HD21	2.02	0.40
1:O:176:PHE:CD2	1:O:177:VAL:HG13	2.56	0.40
2:T:42:THR:HG22	2:T:46:GLN:O	2.22	0.40
1:U:240:ARG:HG3	1:U:259:TYR:HD1	1.87	0.40
2:F:116:VAL:O	2:F:117:SER:C	2.65	0.40
1:G:321:THR:O	1:G:324:ARG:HG2	2.21	0.40
1:M:331:HIS:CD2	1:M:332:MET:H	2.40	0.40
2:R:31:PHE:CB	1:a:41:ASN:CB	2.99	0.40
1:W:2:MET:HE3	1:W:152:PHE:CE2	2.57	0.40
2:d:37:GLY:HA3	2:d:52:ASP:HA	2.04	0.40
1:O:47:LEU:O	1:O:91:TYR:HA	2.21	0.40
1:Q:224:LEU:HD13	1:Q:261:TYR:CD1	2.57	0.40
2:R:22:LEU:CD2	2:R:84:MET:SD	3.09	0.40
2:R:73:ARG:HG3	2:R:80:VAL:HG12	2.04	0.40
1:S:63:LEU:O	1:S:70:ILE:HG13	2.21	0.40
1:a:313:ARG:HG3	2:f:113:GLN:HB2	2.03	0.40
1:e:176:PHE:CD2	1:e:177:VAL:HG13	2.56	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	340/429 (79%)	323 (95%)	17 (5%)	0	100	100
1	C	349/429 (81%)	335 (96%)	14 (4%)	0	100	100
1	E	358/429 (83%)	342 (96%)	16 (4%)	0	100	100
1	G	356/429 (83%)	341 (96%)	15 (4%)	0	100	100
1	I	346/429 (81%)	332 (96%)	14 (4%)	0	100	100
1	K	368/429 (86%)	348 (95%)	20 (5%)	0	100	100
1	M	362/429 (84%)	347 (96%)	15 (4%)	0	100	100
1	O	349/429 (81%)	336 (96%)	13 (4%)	0	100	100
1	Q	367/429 (86%)	348 (95%)	19 (5%)	0	100	100
1	S	333/429 (78%)	316 (95%)	17 (5%)	0	100	100
1	U	336/429 (78%)	318 (95%)	18 (5%)	0	100	100
1	W	338/429 (79%)	325 (96%)	13 (4%)	0	100	100
1	Y	368/429 (86%)	356 (97%)	12 (3%)	0	100	100
1	a	345/429 (80%)	330 (96%)	15 (4%)	0	100	100
1	c	340/429 (79%)	323 (95%)	17 (5%)	0	100	100
1	e	342/429 (80%)	329 (96%)	13 (4%)	0	100	100
2	B	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	D	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	F	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	H	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	J	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	L	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	N	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	P	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	R	113/116 (97%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	V	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	X	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	Z	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	b	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	d	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	f	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	14	37
All	All	7405/8720 (85%)	7085 (96%)	319 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	f	78	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/353 (72%)	253 (99%)	3 (1%)	63	84
1	C	263/353 (74%)	260 (99%)	3 (1%)	65	85
1	E	271/353 (77%)	266 (98%)	5 (2%)	51	79
1	G	266/353 (75%)	264 (99%)	2 (1%)	73	89
1	I	262/353 (74%)	260 (99%)	2 (1%)	73	89
1	K	261/353 (74%)	258 (99%)	3 (1%)	65	85
1	M	262/353 (74%)	258 (98%)	4 (2%)	57	81
1	O	257/353 (73%)	255 (99%)	2 (1%)	73	89
1	Q	271/353 (77%)	270 (100%)	1 (0%)	84	93
1	S	253/353 (72%)	251 (99%)	2 (1%)	73	89
1	U	242/353 (69%)	240 (99%)	2 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	256/353 (72%)	255 (100%)	1 (0%)	84	93
1	Y	272/353 (77%)	269 (99%)	3 (1%)	65	85
1	a	264/353 (75%)	262 (99%)	2 (1%)	73	89
1	c	251/353 (71%)	248 (99%)	3 (1%)	63	84
1	e	261/353 (74%)	261 (100%)	0	100	100
2	B	88/97 (91%)	88 (100%)	0	100	100
2	D	89/97 (92%)	88 (99%)	1 (1%)	65	85
2	F	89/97 (92%)	87 (98%)	2 (2%)	45	75
2	H	89/97 (92%)	89 (100%)	0	100	100
2	J	89/97 (92%)	87 (98%)	2 (2%)	45	75
2	L	88/97 (91%)	87 (99%)	1 (1%)	65	85
2	N	88/97 (91%)	88 (100%)	0	100	100
2	P	89/97 (92%)	88 (99%)	1 (1%)	65	85
2	R	85/97 (88%)	84 (99%)	1 (1%)	63	84
2	T	91/97 (94%)	91 (100%)	0	100	100
2	V	90/97 (93%)	89 (99%)	1 (1%)	65	85
2	X	86/97 (89%)	84 (98%)	2 (2%)	44	75
2	Z	88/97 (91%)	87 (99%)	1 (1%)	65	85
2	b	90/97 (93%)	90 (100%)	0	100	100
2	d	90/97 (93%)	90 (100%)	0	100	100
2	f	90/97 (93%)	89 (99%)	1 (1%)	65	85
All	All	5587/7200 (78%)	5536 (99%)	51 (1%)	70	87

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	154	SER
1	A	346	CYS
1	C	154	SER
1	C	330	THR
1	C	350	SER
2	D	23	SER
1	E	3	LEU
1	E	154	SER

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Mol	Chain	Res	Type
1	E	350	SER
1	E	359	THR
1	E	413	LEU
2	F	72	SER
2	F	110	GLN
1	G	350	SER
1	G	404	VAL
1	I	154	SER
1	I	330	THR
2	J	32	SER
2	J	72	SER
1	K	346	CYS
1	K	350	SER
1	K	404	VAL
2	L	58	SER
1	M	154	SER
1	M	346	CYS
1	M	350	SER
1	M	359	THR
1	O	154	SER
1	O	350	SER
2	P	90	GLU
1	Q	57	SER
2	R	9	SER
1	S	75	HIS
1	S	346	CYS
1	U	28	THR
1	U	402	CYS
2	V	59	THR
1	W	178	ARG
2	X	82	LEU
2	X	117	SER
1	Y	41	ASN
1	Y	154	SER
1	Y	407	GLU
2	Z	32	SER
1	a	57	SER
1	a	154	SER
1	c	154	SER
1	c	253	LEU
1	c	357	THR
2	f	58	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
2	B	113	GLN
1	C	37	HIS
1	C	75	HIS
1	C	258	GLN
1	C	331	HIS
2	F	46	GLN
1	G	75	HIS
1	G	331	HIS
1	I	37	HIS
2	J	113	GLN
1	K	37	HIS
1	K	284	GLN
1	M	37	HIS
1	M	331	HIS
1	M	361	GLN
2	N	83	GLN
2	N	113	GLN
1	O	37	HIS
1	O	75	HIS
1	O	175	GLN
1	Q	37	HIS
1	Q	113	GLN
1	Q	175	GLN
2	R	113	GLN
1	S	239	GLN
1	S	284	GLN
1	U	37	HIS
1	W	37	HIS
1	W	175	GLN
1	W	197	GLN
1	W	229	ASN
2	X	85	ASN
2	X	113	GLN
1	Y	37	HIS
1	Y	75	HIS
1	Y	284	GLN
1	Y	288	HIS
2	b	113	GLN
1	c	37	HIS
2	d	113	GLN

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Mol	Chain	Res	Type
1	e	37	HIS
1	e	75	HIS

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	352/429 (82%)	0.73	49 (13%) 6 5	30, 52, 108, 134	0
1	C	361/429 (84%)	0.71	44 (12%) 8 7	33, 55, 114, 159	0
1	E	368/429 (85%)	0.71	47 (12%) 7 6	32, 56, 114, 158	0
1	G	366/429 (85%)	0.68	47 (12%) 7 6	30, 53, 109, 155	0
1	I	358/429 (83%)	0.54	41 (11%) 9 7	29, 51, 110, 144	0
1	K	376/429 (87%)	0.71	57 (15%) 5 4	24, 48, 120, 155	0
1	M	372/429 (86%)	0.67	59 (15%) 5 4	24, 48, 115, 151	0
1	O	361/429 (84%)	0.58	43 (11%) 9 7	27, 51, 106, 151	0
1	Q	375/429 (87%)	1.31	80 (21%) 2 2	47, 72, 117, 147	0
1	S	345/429 (80%)	1.71	108 (31%) 1 1	54, 78, 114, 152	0
1	U	348/429 (81%)	1.68	110 (31%) 1 1	48, 74, 126, 159	0
1	W	350/429 (81%)	1.60	96 (27%) 1 1	51, 76, 123, 156	0
1	Y	376/429 (87%)	0.60	42 (11%) 10 8	31, 52, 109, 135	0
1	a	357/429 (83%)	0.68	38 (10%) 11 9	34, 55, 107, 138	0
1	c	352/429 (82%)	0.87	61 (17%) 4 3	30, 55, 115, 150	0
1	e	354/429 (82%)	0.72	46 (12%) 7 6	35, 55, 106, 145	0
2	B	115/116 (99%)	0.26	8 (6%) 22 18	30, 40, 77, 100	0
2	D	115/116 (99%)	0.26	9 (7%) 19 15	32, 45, 86, 106	0
2	F	115/116 (99%)	0.15	6 (5%) 33 27	31, 47, 82, 109	0
2	H	115/116 (99%)	0.24	10 (8%) 16 13	29, 42, 84, 150	0
2	J	115/116 (99%)	0.21	8 (6%) 22 18	27, 44, 89, 116	0
2	L	115/116 (99%)	0.08	7 (6%) 27 22	24, 37, 82, 104	0
2	N	115/116 (99%)	0.08	4 (3%) 47 40	25, 38, 75, 94	0
2	P	115/116 (99%)	0.14	7 (6%) 27 22	28, 41, 85, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	R	115/116 (99%)	1.30	21 (18%) 3 2	49, 64, 112, 159	0
2	T	115/116 (99%)	1.09	13 (11%) 10 8	44, 62, 88, 121	0
2	V	115/116 (99%)	1.04	17 (14%) 5 5	46, 60, 96, 127	0
2	X	115/116 (99%)	1.38	19 (16%) 4 3	50, 69, 111, 139	0
2	Z	115/116 (99%)	0.43	10 (8%) 16 13	32, 46, 93, 145	0
2	b	115/116 (99%)	0.21	6 (5%) 33 27	29, 45, 76, 114	0
2	d	115/116 (99%)	0.18	6 (5%) 33 27	29, 40, 75, 120	0
2	f	115/116 (99%)	0.34	10 (8%) 16 13	34, 47, 95, 127	0
All	All	7611/8720 (87%)	0.79	1129 (14%) 5 5	24, 57, 112, 159	0

All (1129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	SER	10.8
1	W	143	SER	9.8
1	C	143	SER	9.6
1	Y	143	SER	9.5
1	M	143	SER	9.4
2	R	31	PHE	9.1
1	W	122	ASP	9.0
1	U	407	GLU	8.9
1	E	122	ASP	8.5
1	K	143	SER	8.3
1	G	143	SER	8.2
1	U	404	VAL	8.1
2	J	75	ASN	8.1
2	X	29	SER	8.0
1	S	5	LEU	7.9
1	M	339	ASP	7.8
1	a	5	LEU	7.7
1	M	413	LEU	7.6
1	C	370	ASP	7.4
1	c	404	VAL	7.4
2	P	75	ASN	7.3
1	K	339	ASP	7.3
1	U	122	ASP	7.3
1	Y	5	LEU	7.3
1	Q	363	ASP	7.3
1	U	143	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	363	ASP	7.2
2	R	29	SER	7.1
1	U	413	LEU	7.0
1	I	334	HIS	6.9
1	U	405	GLN	6.9
1	U	360	TRP	6.8
1	a	334	HIS	6.8
1	c	413	LEU	6.7
1	U	5	LEU	6.7
1	A	413	LEU	6.7
1	e	5	LEU	6.7
1	c	144	GLY	6.6
1	W	407	GLU	6.6
1	E	392	VAL	6.6
2	Z	31	PHE	6.6
1	c	331	HIS	6.6
1	A	347	TRP	6.5
1	K	347	TRP	6.5
1	K	417	TRP	6.5
1	W	334	HIS	6.5
1	W	417	TRP	6.5
1	G	407	GLU	6.4
1	W	25	ILE	6.4
1	S	222	GLY	6.3
1	A	5	LEU	6.3
1	a	143	SER	6.3
1	e	122	ASP	6.3
1	c	5	LEU	6.3
1	W	144	GLY	6.2
1	c	399	ARG	6.2
1	A	407	GLU	6.2
1	E	407	GLU	6.2
1	K	342	ALA	6.2
1	C	391	VAL	6.2
1	C	361	GLN	6.1
1	Q	144	GLY	6.1
1	c	417	TRP	6.1
1	e	417	TRP	6.1
1	M	347	TRP	6.1
1	W	5	LEU	6.1
1	S	122	ASP	6.1
1	E	5	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	G	122	ASP	6.1
1	Q	5	LEU	6.1
1	c	403	HIS	6.0
1	e	143	SER	6.0
1	a	339	ASP	6.0
1	A	359	THR	6.0
1	I	5	LEU	6.0
1	K	413	LEU	6.0
2	T	75	ASN	6.0
1	A	331	HIS	5.9
2	H	75	ASN	5.9
1	U	412	PRO	5.9
1	S	144	GLY	5.9
1	S	334	HIS	5.9
1	Y	122	ASP	5.9
1	c	400	TYR	5.9
1	A	343	THR	5.9
2	f	29	SER	5.8
1	I	144	GLY	5.8
1	E	363	ASP	5.8
1	W	41	ASN	5.8
2	J	29	SER	5.7
1	a	417	TRP	5.7
2	X	76	THR	5.7
1	Q	417	TRP	5.7
1	c	407	GLU	5.6
1	e	334	HIS	5.6
1	A	417	TRP	5.6
1	K	366	ASP	5.6
1	O	143	SER	5.6
1	Q	338	SER	5.6
1	O	363	ASP	5.6
1	K	122	ASP	5.5
1	U	387	TRP	5.5
1	M	342	ALA	5.5
1	C	412	PRO	5.5
2	B	31	PHE	5.5
2	Z	29	SER	5.5
1	U	417	TRP	5.5
1	c	122	ASP	5.5
1	E	400	TYR	5.5
1	K	5	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
2	F	75	ASN	5.5
1	E	143	SER	5.4
1	W	347	TRP	5.4
1	A	414	THR	5.4
1	E	334	HIS	5.4
1	W	160	ARG	5.3
1	W	281	MET	5.3
1	U	229	ASN	5.3
1	c	412	PRO	5.2
1	C	407	GLU	5.2
1	S	160	ARG	5.2
1	S	414	THR	5.2
1	c	342	ALA	5.2
1	C	25	ILE	5.2
1	G	417	TRP	5.2
1	U	329	LYS	5.1
1	A	403	HIS	5.1
1	S	159	GLY	5.1
1	a	407	GLU	5.1
1	U	371	THR	5.1
1	c	333	THR	5.1
1	M	398	GLN	5.1
1	G	5	LEU	5.1
1	U	256	TYR	5.1
1	c	25	ILE	5.1
1	S	320	GLU	5.1
1	S	407	GLU	5.1
1	K	370	ASP	5.1
1	I	366	ASP	5.0
1	e	371	THR	5.0
2	R	3	GLU	5.0
1	G	366	ASP	5.0
2	b	3	GLU	5.0
1	K	367	GLN	5.0
1	M	403	HIS	5.0
1	O	417	TRP	5.0
1	C	144	GLY	4.9
1	M	367	GLN	4.9
1	G	392	VAL	4.9
1	A	399	ARG	4.9
1	O	400	TYR	4.9
1	a	281	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	e	25	ILE	4.9
2	R	75	ASN	4.9
1	Y	367	GLN	4.8
1	U	343	THR	4.8
1	C	417	TRP	4.8
1	c	347	TRP	4.8
1	G	367	GLN	4.8
1	S	358	LEU	4.8
1	A	122	ASP	4.8
2	L	75	ASN	4.8
1	O	412	PRO	4.8
2	V	31	PHE	4.8
1	e	362	ARG	4.8
1	M	369	GLN	4.8
1	S	372	GLU	4.7
2	R	30	ILE	4.7
2	X	31	PHE	4.7
1	M	417	TRP	4.7
1	c	405	GLN	4.7
2	X	3	GLU	4.7
1	c	346	CYS	4.7
1	E	370	ASP	4.7
2	D	3	GLU	4.7
1	G	342	ALA	4.7
1	Q	122	ASP	4.7
1	e	398	GLN	4.7
1	W	222	GLY	4.7
1	K	346	CYS	4.7
1	O	5	LEU	4.7
1	M	392	VAL	4.7
1	a	160	ARG	4.6
1	M	370	ASP	4.6
1	Y	339	ASP	4.6
1	M	394	SER	4.6
1	U	362	ARG	4.6
1	A	404	VAL	4.6
1	A	401	THR	4.6
1	G	281	MET	4.6
2	J	3	GLU	4.6
1	a	340	HIS	4.6
1	c	343	THR	4.6
1	G	370	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
2	X	75	ASN	4.6
1	U	346	CYS	4.5
1	O	342	ALA	4.5
1	W	410	PRO	4.5
1	E	366	ASP	4.5
1	O	367	GLN	4.5
1	M	399	ARG	4.5
1	K	397	GLU	4.5
1	O	361	GLN	4.5
1	c	332	MET	4.5
1	I	416	ARG	4.5
1	O	399	ARG	4.5
1	O	366	ASP	4.5
1	E	365	GLU	4.5
1	Q	335	HIS	4.5
1	S	232	GLU	4.5
1	C	5	LEU	4.4
1	U	388	ALA	4.4
1	K	412	PRO	4.4
1	M	407	GLU	4.4
1	U	120	ASP	4.4
2	D	75	ASN	4.4
1	W	199	GLY	4.4
1	W	412	PRO	4.4
1	c	361	GLN	4.4
1	U	372	GLU	4.4
1	W	346	CYS	4.4
1	W	360	TRP	4.4
1	Q	366	ASP	4.4
1	K	394	SER	4.4
1	M	5	LEU	4.4
1	O	334	HIS	4.4
1	Q	160	ARG	4.4
1	I	400	TYR	4.4
1	Q	396	GLN	4.4
1	O	407	GLU	4.4
1	Y	370	ASP	4.3
1	M	395	GLY	4.3
2	J	31	PHE	4.3
2	f	31	PHE	4.3
1	I	25	ILE	4.3
2	b	75	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	362	ARG	4.3
2	B	75	ASN	4.3
1	M	331	HIS	4.3
1	S	415	LEU	4.3
1	Q	339	ASP	4.3
1	U	348	ALA	4.3
1	Y	396	GLN	4.3
2	R	28	GLY	4.3
1	Y	417	TRP	4.2
1	I	363	ASP	4.2
1	O	122	ASP	4.2
1	I	41	ASN	4.2
1	Q	25	ILE	4.2
1	S	25	ILE	4.2
1	W	330	THR	4.2
1	K	363	ASP	4.2
1	K	398	GLN	4.2
1	W	405	GLN	4.2
1	U	406	HIS	4.2
1	E	368	THR	4.2
1	K	391	VAL	4.2
2	P	31	PHE	4.2
1	I	401	THR	4.2
1	S	344	LEU	4.2
1	E	391	VAL	4.1
1	e	347	TRP	4.1
1	Q	232	GLU	4.1
1	U	144	GLY	4.1
2	Z	30	ILE	4.1
1	C	333	THR	4.1
1	W	329	LYS	4.1
1	M	400	TYR	4.1
1	a	360	TRP	4.1
1	E	403	HIS	4.1
2	L	31	PHE	4.1
1	e	412	PRO	4.0
1	U	347	TRP	4.0
1	U	402	CYS	4.0
1	W	372	GLU	4.0
1	E	360	TRP	4.0
1	Q	370	ASP	4.0
1	O	391	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	281	MET	4.0
1	Q	367	GLN	4.0
1	Q	98	GLU	4.0
1	A	345	ARG	4.0
1	U	400	TYR	4.0
1	S	162	GLU	4.0
1	A	400	TYR	4.0
1	K	368	THR	3.9
1	Q	294	HIS	3.9
1	W	415	LEU	3.9
1	Y	363	ASP	3.9
1	a	400	TYR	3.9
1	A	391	VAL	3.9
1	K	338	SER	3.9
1	M	160	ARG	3.9
2	Z	3	GLU	3.9
1	I	346	CYS	3.9
1	K	25	ILE	3.9
2	R	44	GLY	3.9
1	c	414	THR	3.9
1	A	160	ARG	3.9
1	G	362	ARG	3.9
1	K	396	GLN	3.9
1	U	232	GLU	3.9
1	S	413	LEU	3.9
1	U	354	ALA	3.9
1	A	346	CYS	3.9
1	U	276	TRP	3.9
1	e	330	THR	3.9
1	E	44	SER	3.9
1	C	358	LEU	3.9
1	K	395	GLY	3.9
1	e	407	GLU	3.8
1	I	122	ASP	3.8
1	K	369	GLN	3.8
1	Q	368	THR	3.8
1	S	93	GLU	3.8
1	G	413	LEU	3.8
1	U	403	HIS	3.8
1	M	281	MET	3.8
1	S	219	VAL	3.8
1	K	400	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	415	LEU	3.8
1	Q	281	MET	3.8
1	S	281	MET	3.8
1	Y	394	SER	3.8
2	Z	28	GLY	3.8
2	F	31	PHE	3.8
1	e	160	ARG	3.8
1	U	410	PRO	3.8
1	E	367	GLN	3.8
1	E	417	TRP	3.8
1	Y	397	GLU	3.8
1	a	162	GLU	3.8
1	K	340	HIS	3.8
1	G	368	THR	3.7
1	M	334	HIS	3.7
2	N	75	ASN	3.7
2	Z	75	ASN	3.7
2	d	30	ILE	3.7
1	e	144	GLY	3.7
1	W	359	THR	3.7
1	Y	340	HIS	3.7
2	B	30	ILE	3.7
1	S	149	ARG	3.7
1	U	274	ARG	3.7
1	U	278	ALA	3.7
1	c	345	ARG	3.7
2	R	45	LYS	3.7
2	H	31	PHE	3.7
1	S	273	LEU	3.7
1	A	371	THR	3.7
1	Y	391	VAL	3.7
1	I	361	GLN	3.7
1	S	95	THR	3.6
2	P	30	ILE	3.6
1	A	387	TRP	3.6
1	C	342	ALA	3.6
1	G	348	ALA	3.6
1	K	348	ALA	3.6
1	Q	394	SER	3.6
1	S	44	SER	3.6
1	K	281	MET	3.6
1	I	407	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	e	405	GLN	3.6
1	e	413	LEU	3.6
2	f	30	ILE	3.6
1	S	41	ASN	3.6
1	C	399	ARG	3.6
1	S	121	ARG	3.6
1	G	347	TRP	3.6
1	U	281	MET	3.6
1	I	365	GLU	3.6
1	I	398	GLN	3.6
2	V	3	GLU	3.6
2	J	30	ILE	3.6
1	U	416	ARG	3.6
1	S	360	TRP	3.6
1	c	281	MET	3.6
1	W	40	GLU	3.6
2	T	3	GLU	3.6
2	J	77	LYS	3.6
1	A	25	ILE	3.6
1	K	371	THR	3.6
1	U	260	ALA	3.6
1	M	393	PRO	3.6
1	S	404	VAL	3.6
1	S	405	GLN	3.6
2	N	30	ILE	3.5
1	M	343	THR	3.5
1	C	122	ASP	3.5
1	W	201	GLU	3.5
1	U	411	LYS	3.5
2	T	7	VAL	3.5
1	K	331	HIS	3.5
2	V	29	SER	3.5
1	a	25	ILE	3.5
1	C	359	THR	3.5
1	Q	343	THR	3.5
1	U	376	THR	3.5
1	W	357	THR	3.5
1	C	341	GLU	3.5
1	K	372	GLU	3.5
1	c	360	TRP	3.5
1	O	390	VAL	3.5
1	c	390	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	Q	231	SER	3.5
1	Q	407	GLU	3.5
1	e	361	GLN	3.5
1	Q	391	VAL	3.5
1	S	288	HIS	3.5
1	W	331	HIS	3.5
1	U	350	SER	3.5
2	J	76	THR	3.5
1	W	99	LYS	3.5
1	A	412	PRO	3.5
1	O	358	LEU	3.5
1	Q	413	LEU	3.5
1	a	390	VAL	3.5
1	Q	362	ARG	3.5
1	K	361	GLN	3.4
2	T	31	PHE	3.4
1	Y	160	ARG	3.4
1	E	333	THR	3.4
1	Q	397	GLU	3.4
1	c	388	ALA	3.4
2	L	67	GLY	3.4
1	S	245	ASP	3.4
1	W	413	LEU	3.4
1	Y	369	GLN	3.4
2	R	4	VAL	3.4
1	E	25	ILE	3.4
1	M	346	CYS	3.4
1	U	344	LEU	3.4
1	G	363	ASP	3.4
1	K	392	VAL	3.4
1	A	332	MET	3.4
1	W	328	PRO	3.4
1	I	364	GLY	3.4
1	U	288	HIS	3.4
1	M	122	ASP	3.4
1	W	219	VAL	3.4
1	U	25	ILE	3.3
2	F	77	LYS	3.3
1	Q	228	TYR	3.3
1	O	343	THR	3.3
1	U	357	THR	3.3
1	Y	98	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	P	3	GLU	3.3
1	e	281	MET	3.3
1	U	264	LYS	3.3
2	X	117	SER	3.3
1	I	333	THR	3.3
1	S	410	PRO	3.3
1	C	160	ARG	3.3
1	G	160	ARG	3.3
1	Q	149	ARG	3.3
1	W	44	SER	3.3
1	e	399	ARG	3.3
1	U	328	PRO	3.3
1	E	123	MET	3.3
1	E	364	GLY	3.3
2	X	30	ILE	3.3
2	L	29	SER	3.3
1	G	400	TYR	3.3
1	U	292	ALA	3.3
1	G	371	THR	3.2
1	I	414	THR	3.2
2	R	42	THR	3.2
1	Q	364	GLY	3.2
1	E	342	ALA	3.2
1	E	362	ARG	3.2
1	M	412	PRO	3.2
2	H	29	SER	3.2
2	P	29	SER	3.2
2	R	32	SER	3.2
1	S	302	TYR	3.2
1	c	348	ALA	3.2
1	U	390	VAL	3.2
1	W	374	VAL	3.2
1	Y	25	ILE	3.2
2	d	31	PHE	3.2
1	Q	272	ASP	3.2
1	C	413	LEU	3.2
2	R	8	GLU	3.2
1	U	158	PRO	3.2
1	K	359	THR	3.2
2	f	76	THR	3.2
1	O	25	ILE	3.2
1	O	281	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	c	411	LYS	3.2
1	U	297	GLU	3.2
1	a	405	GLN	3.2
1	S	333	THR	3.2
1	a	333	THR	3.2
1	a	343	THR	3.2
1	E	144	GLY	3.2
1	E	275	SER	3.2
1	Y	336	ALA	3.2
2	V	30	ILE	3.2
1	c	329	LYS	3.1
1	M	341	GLU	3.1
1	Q	71	GLU	3.1
1	M	340	HIS	3.1
1	e	331	HIS	3.1
1	A	405	GLN	3.1
1	W	285	THR	3.1
1	I	360	TRP	3.1
1	A	348	ALA	3.1
1	Q	342	ALA	3.1
1	S	112	SER	3.1
1	G	391	VAL	3.1
1	W	73	VAL	3.1
1	Q	256	TYR	3.1
1	U	289	LYS	3.1
1	O	405	GLN	3.1
1	Q	369	GLN	3.1
1	U	286	THR	3.1
2	D	28	GLY	3.1
1	S	73	VAL	3.1
1	W	112	SER	3.1
1	W	390	VAL	3.1
2	T	117	SER	3.1
1	K	399	ARG	3.1
1	U	273	LEU	3.1
1	G	291	GLU	3.1
1	U	355	GLU	3.1
1	G	412	PRO	3.1
1	G	369	GLN	3.1
1	A	333	THR	3.1
1	G	278	ALA	3.1
1	M	388	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	c	402	CYS	3.1
1	U	240	ARG	3.1
1	W	27	ARG	3.1
1	U	409	LEU	3.1
2	T	87	LEU	3.1
2	X	87	LEU	3.1
1	Y	366	ASP	3.1
1	W	361	GLN	3.1
1	Q	371	THR	3.1
1	S	199	GLY	3.1
1	a	144	GLY	3.1
2	P	76	THR	3.1
1	S	94	PHE	3.1
1	O	413	LEU	3.0
1	Q	269	LEU	3.0
1	c	334	HIS	3.0
1	S	328	PRO	3.0
1	S	412	PRO	3.0
1	E	398	GLN	3.0
1	K	343	THR	3.0
1	S	99	LYS	3.0
1	C	360	TRP	3.0
1	U	224	LEU	3.0
1	W	349	LEU	3.0
1	M	396	GLN	3.0
1	W	159	GLY	3.0
1	c	330	THR	3.0
1	W	348	ALA	3.0
1	Q	224	LEU	3.0
1	W	221	LEU	3.0
1	M	397	GLU	3.0
1	Y	398	GLN	3.0
1	G	25	ILE	3.0
1	I	160	ARG	3.0
1	Q	347	TRP	3.0
1	e	360	TRP	3.0
1	c	406	HIS	3.0
1	Y	281	MET	3.0
2	V	10	GLY	3.0
1	K	388	ALA	3.0
1	W	278	ALA	3.0
1	W	404	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	Y	392	VAL	3.0
1	A	409	LEU	2.9
1	W	358	LEU	2.9
1	K	288	HIS	2.9
1	Q	340	HIS	2.9
1	S	227	CYS	2.9
1	W	284	GLN	2.9
1	E	281	MET	2.9
1	S	260	ALA	2.9
1	M	391	VAL	2.9
1	S	349	LEU	2.9
2	f	77	LYS	2.9
1	O	410	PRO	2.9
1	W	350	SER	2.9
2	Z	32	SER	2.9
1	U	197	GLN	2.9
1	U	284	GLN	2.9
2	B	110	GLN	2.9
1	S	285	THR	2.9
1	c	357	THR	2.9
1	K	358	LEU	2.9
1	a	413	LEU	2.9
1	A	406	HIS	2.9
1	W	43	LYS	2.9
1	a	332	MET	2.9
1	M	416	ARG	2.9
1	A	402	CYS	2.9
1	Q	395	GLY	2.9
1	M	371	THR	2.9
1	Q	393	PRO	2.9
1	U	353	PRO	2.9
1	W	197	GLN	2.9
1	S	286	THR	2.9
1	W	371	THR	2.9
2	D	76	THR	2.9
1	U	327	ALA	2.9
1	E	372	GLU	2.8
1	O	371	THR	2.8
1	I	390	VAL	2.8
1	Q	254	ARG	2.8
1	A	144	GLY	2.8
1	Q	159	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	389	ALA	2.8
1	G	388	ALA	2.8
1	M	414	THR	2.8
1	U	228	TYR	2.8
1	K	393	PRO	2.8
2	d	110	GLN	2.8
1	M	411	LYS	2.8
1	e	41	ASN	2.8
1	I	413	LEU	2.8
1	S	67	GLY	2.8
1	a	415	LEU	2.8
2	R	10	GLY	2.8
1	S	4	ASP	2.8
2	D	7	VAL	2.8
2	d	3	GLU	2.8
1	S	323	GLN	2.8
1	S	203	TRP	2.8
2	T	29	SER	2.8
2	Z	117	SER	2.8
2	V	11	GLY	2.8
1	K	332	MET	2.8
1	M	332	MET	2.8
1	e	390	VAL	2.8
1	Q	400	TYR	2.8
1	U	345	ARG	2.8
1	U	119	TRP	2.7
1	W	344	LEU	2.7
1	Y	373	LEU	2.7
1	c	415	LEU	2.7
1	C	222	GLY	2.7
2	N	28	GLY	2.7
2	f	75	ASN	2.7
1	S	37	HIS	2.7
1	O	401	THR	2.7
1	c	328	PRO	2.7
1	S	282	CYS	2.7
1	A	329	LYS	2.7
2	H	30	ILE	2.7
1	U	111	LEU	2.7
1	c	358	LEU	2.7
1	Q	288	HIS	2.7
1	G	98	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	341	GLU	2.7
1	W	98	GLU	2.7
1	U	285	THR	2.7
1	c	292	ALA	2.7
2	b	7	VAL	2.7
1	c	373	LEU	2.7
1	M	144	GLY	2.7
2	F	29	SER	2.7
1	K	291	GLU	2.7
1	I	359	THR	2.7
1	S	33	VAL	2.7
1	Q	58	ASP	2.7
1	S	325	THR	2.7
1	U	359	THR	2.7
1	I	412	PRO	2.7
1	M	410	PRO	2.7
1	S	329	LYS	2.7
2	T	77	LYS	2.7
2	X	77	LYS	2.7
1	G	405	GLN	2.7
1	G	358	LEU	2.7
1	Q	334	HIS	2.7
1	U	160	ARG	2.7
1	U	255	GLY	2.7
1	c	416	ARG	2.7
2	f	28	GLY	2.7
1	O	44	SER	2.7
1	O	365	GLU	2.7
1	O	360	TRP	2.7
2	b	117	SER	2.7
1	W	292	ALA	2.7
2	T	116	VAL	2.7
2	X	65	VAL	2.7
1	W	333	THR	2.7
1	a	321	THR	2.7
2	V	43	PRO	2.7
1	S	215	GLN	2.6
1	U	157	ARG	2.6
1	U	234	GLY	2.6
1	c	41	ASN	2.6
1	M	404	VAL	2.6
2	D	31	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	76	THR	2.6
2	N	31	PHE	2.6
1	G	272	ASP	2.6
1	S	47	LEU	2.6
1	E	399	ARG	2.6
1	W	403	HIS	2.6
1	S	289	LYS	2.6
1	U	145	SER	2.6
1	U	277	THR	2.6
1	c	120	ASP	2.6
1	e	332	MET	2.6
2	L	30	ILE	2.6
1	U	208	ARG	2.6
1	E	341	GLU	2.6
1	Q	297	GLU	2.6
1	Y	395	GLY	2.6
1	O	41	ASN	2.6
1	c	278	ALA	2.6
1	e	410	PRO	2.6
2	P	7	VAL	2.6
1	E	369	GLN	2.6
1	I	371	THR	2.6
1	Q	119	TRP	2.6
1	U	361	GLN	2.6
1	W	387	TRP	2.6
1	Y	368	THR	2.6
1	M	256	TYR	2.6
1	S	259	TYR	2.6
1	O	411	LYS	2.6
1	E	222	GLY	2.6
1	M	402	CYS	2.6
1	Q	227	CYS	2.6
1	Q	246	VAL	2.6
2	X	7	VAL	2.6
1	C	343	THR	2.5
1	Q	330	THR	2.5
1	U	258	GLN	2.6
1	W	321	THR	2.5
1	S	119	TRP	2.5
1	S	347	TRP	2.5
1	U	267	ILE	2.5
1	a	253	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	e	415	LEU	2.5
1	E	410	PRO	2.5
1	A	388	ALA	2.5
1	A	357	THR	2.5
1	G	343	THR	2.5
1	W	223	THR	2.5
1	I	417	TRP	2.5
1	S	387	TRP	2.5
1	A	344	LEU	2.5
1	Q	289	LYS	2.5
1	c	344	LEU	2.5
2	X	66	LYS	2.5
1	K	365	GLU	2.5
1	S	266	TYR	2.5
1	W	232	GLU	2.5
1	W	256	TYR	2.5
1	K	364	GLY	2.5
1	S	226	GLY	2.5
1	Y	159	GLY	2.5
1	e	222	GLY	2.5
1	U	200	PRO	2.5
1	E	361	GLN	2.5
1	W	260	ALA	2.5
1	I	343	THR	2.5
1	K	402	CYS	2.5
2	L	76	THR	2.5
2	J	117	SER	2.5
1	M	387	TRP	2.5
2	H	77	LYS	2.5
1	C	149	ARG	2.5
1	S	89	LEU	2.5
1	a	344	LEU	2.5
1	S	201	GLU	2.5
1	G	256	TYR	2.5
1	U	259	TYR	2.5
1	W	161	GLY	2.5
1	C	410	PRO	2.5
1	U	26	GLN	2.5
1	W	332	MET	2.5
1	C	41	ASN	2.5
1	O	414	THR	2.5
1	U	358	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	373	LEU	2.5
1	Y	399	ARG	2.5
1	a	399	ARG	2.5
1	K	387	TRP	2.5
2	V	22	LEU	2.5
1	A	334	HIS	2.5
1	G	288	HIS	2.5
1	e	355	GLU	2.5
1	C	400	TYR	2.5
2	R	11	GLY	2.5
1	e	404	VAL	2.5
1	S	72	LYS	2.4
1	Q	286	THR	2.4
2	b	76	THR	2.4
2	X	6	LEU	2.4
1	S	402	CYS	2.4
1	e	282	CYS	2.4
1	e	346	CYS	2.4
2	b	29	SER	2.4
1	C	347	TRP	2.4
1	U	272	ASP	2.4
1	a	120	ASP	2.4
1	e	288	HIS	2.4
1	A	372	GLU	2.4
1	O	232	GLU	2.4
1	c	410	PRO	2.4
2	B	10	GLY	2.4
1	e	400	TYR	2.4
1	S	384	PHE	2.4
2	Z	77	LYS	2.4
1	M	368	THR	2.4
1	S	277	THR	2.4
1	W	145	SER	2.4
1	W	406	HIS	2.4
2	X	9	SER	2.4
1	O	346	CYS	2.4
1	S	120	ASP	2.4
1	c	387	TRP	2.4
1	e	402	CYS	2.4
2	L	3	GLU	2.4
1	O	159	GLY	2.4
1	A	411	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	e	99	LYS	2.4
1	Q	298	GLN	2.4
1	S	202	TYR	2.4
1	U	374	VAL	2.4
1	G	95	THR	2.4
1	K	330	THR	2.4
1	S	321	THR	2.4
2	V	78	ASN	2.4
1	W	37	HIS	2.4
1	a	403	HIS	2.4
1	c	145	SER	2.4
1	G	387	TRP	2.4
2	V	66	LYS	2.4
1	S	106	VAL	2.4
1	Q	399	ARG	2.4
1	S	278	ALA	2.4
1	U	266	TYR	2.4
1	Q	253	LEU	2.4
2	D	30	ILE	2.4
1	G	334	HIS	2.4
1	S	403	HIS	2.4
1	C	397	GLU	2.4
1	S	231	SER	2.4
1	c	162	GLU	2.4
2	X	64	SER	2.4
1	Q	120	ASP	2.4
1	U	249	ASP	2.4
1	C	282	CYS	2.4
1	G	346	CYS	2.4
1	I	410	PRO	2.4
1	E	405	GLN	2.4
1	Q	197	GLN	2.4
1	K	404	VAL	2.4
1	a	416	ARG	2.4
1	S	292	ALA	2.4
1	A	256	TYR	2.3
2	V	102	TYR	2.3
1	e	333	THR	2.3
1	M	288	HIS	2.3
1	Y	335	HIS	2.3
1	S	317	ASN	2.3
1	U	162	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	U	291	GLU	2.3
1	C	346	CYS	2.3
1	I	358	LEU	2.3
1	S	192	ALA	2.3
2	R	107	TYR	2.3
1	G	331	HIS	2.3
1	c	294	HIS	2.3
1	U	271	GLU	2.3
2	B	3	GLU	2.3
1	S	147	SER	2.3
1	U	57	SER	2.3
1	c	272	ASP	2.3
1	O	144	GLY	2.3
2	f	15	GLN	2.3
1	E	415	LEU	2.3
1	I	415	LEU	2.3
1	M	389	ALA	2.3
1	Q	3	LEU	2.3
1	U	293	ALA	2.3
1	W	356	ILE	2.3
1	O	288	HIS	2.3
1	K	357	THR	2.3
1	U	401	THR	2.3
1	Y	256	TYR	2.3
1	Y	400	TYR	2.3
1	A	232	GLU	2.3
1	I	372	GLU	2.3
1	M	162	GLU	2.3
1	Q	271	GLU	2.3
1	S	211	LYS	2.3
1	a	93	GLU	2.3
2	H	3	GLU	2.3
1	S	324	ARG	2.3
1	I	405	GLN	2.3
1	Y	199	GLY	2.3
1	K	374	VAL	2.3
1	A	358	LEU	2.3
1	Q	346	CYS	2.3
1	U	227	CYS	2.3
2	X	114	VAL	2.3
1	U	322	LEU	2.3
1	M	25	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	e	292	ALA	2.3
1	A	330	THR	2.3
1	S	357	THR	2.3
1	S	401	THR	2.3
1	C	256	TYR	2.3
1	S	256	TYR	2.3
1	Y	232	GLU	2.3
1	E	160	ARG	2.3
1	Y	350	SER	2.3
1	C	159	GLY	2.3
1	Y	360	TRP	2.3
2	R	111	GLY	2.3
1	W	33	VAL	2.3
1	Q	292	ALA	2.2
1	S	346	CYS	2.2
1	U	283	ALA	2.2
1	W	104	CYS	2.2
1	W	244	CYS	2.2
1	c	282	CYS	2.2
1	I	281	MET	2.2
1	I	332	MET	2.2
1	O	333	THR	2.2
1	S	28	THR	2.2
1	e	359	THR	2.2
1	c	355	GLU	2.2
2	f	3	GLU	2.2
1	C	405	GLN	2.2
1	W	326	ASP	2.2
1	a	398	GLN	2.2
1	U	159	GLY	2.2
1	U	382	GLY	2.2
1	E	219	VAL	2.2
1	E	413	LEU	2.2
1	K	337	VAL	2.2
1	S	389	ALA	2.2
1	S	406	HIS	2.2
1	U	294	HIS	2.2
2	D	77	LYS	2.2
1	Q	282	CYS	2.2
1	a	282	CYS	2.2
1	G	372	GLU	2.2
1	G	375	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	40	GLU	2.2
1	U	375	GLU	2.2
1	M	41	ASN	2.2
1	Q	121	ARG	2.2
1	U	251	ARG	2.2
1	Y	362	ARG	2.2
1	c	160	ARG	2.2
2	d	75	ASN	2.2
1	S	248	SER	2.2
1	W	42	GLY	2.2
2	T	64	SER	2.2
2	d	117	SER	2.2
1	Q	171	VAL	2.2
1	W	119	TRP	2.2
1	K	334	HIS	2.2
1	Y	342	ALA	2.2
1	E	371	THR	2.2
1	G	282	CYS	2.2
1	W	320	GLU	2.2
1	Y	341	GLU	2.2
1	c	359	THR	2.2
1	Y	121	ARG	2.2
1	S	261	TYR	2.2
1	S	314	TYR	2.2
1	C	99	LYS	2.2
1	O	364	GLY	2.2
1	Q	234	GLY	2.2
1	Q	44	SER	2.2
1	Q	373	LEU	2.2
1	A	390	VAL	2.2
1	I	331	HIS	2.2
1	W	288	HIS	2.2
1	a	288	HIS	2.2
1	K	333	THR	2.2
1	Q	321	THR	2.2
1	Y	343	THR	2.2
1	A	416	ARG	2.2
1	E	416	ARG	2.2
1	I	27	ARG	2.2
1	I	402	CYS	2.2
1	M	282	CYS	2.2
1	S	27	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	324	ARG	2.2
1	e	149	ARG	2.2
1	E	256	TYR	2.2
1	W	317	ASN	2.2
1	S	270	LYS	2.2
1	S	380	GLY	2.2
1	W	265	ASP	2.2
1	c	350	SER	2.2
1	c	391	VAL	2.2
2	T	9	SER	2.2
1	K	403	HIS	2.2
1	S	108	HIS	2.2
2	V	4	VAL	2.2
2	V	80	VAL	2.2
1	S	379	ALA	2.1
1	c	293	ALA	2.1
1	e	389	ALA	2.1
1	C	320	GLU	2.1
1	a	341	GLU	2.1
1	G	399	ARG	2.1
1	S	359	THR	2.1
1	W	95	THR	2.1
1	Y	330	THR	2.1
1	C	284	GLN	2.1
1	M	229	ASN	2.1
1	Q	1	TYR	2.1
1	S	411	LYS	2.1
1	C	332	MET	2.1
1	M	415	LEU	2.1
1	c	161	GLY	2.1
1	e	159	GLY	2.1
1	E	390	VAL	2.1
1	W	168	VAL	2.1
1	W	248	SER	2.1
2	V	117	SER	2.1
2	X	116	VAL	2.1
1	A	389	ALA	2.1
1	M	348	ALA	2.1
1	Q	278	ALA	2.1
1	C	98	GLU	2.1
1	W	355	GLU	2.1
1	e	372	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	157	ARG	2.1
1	S	240	ARG	2.1
1	U	324	ARG	2.1
1	G	333	THR	2.1
1	K	411	LYS	2.1
1	Q	158	PRO	2.1
1	W	411	LYS	2.1
1	a	412	PRO	2.1
2	T	15	GLN	2.1
1	O	415	LEU	2.1
1	U	415	LEU	2.1
2	V	75	ASN	2.1
1	C	331	HIS	2.1
1	U	58	ASP	2.1
1	Y	272	ASP	2.1
2	R	105	ASP	2.1
2	B	117	SER	2.1
1	Q	341	GLU	2.1
1	S	96	PRO	2.1
2	Z	110	GLN	2.1
1	M	358	LEU	2.1
1	Q	322	LEU	2.1
1	S	322	LEU	2.1
1	a	358	LEU	2.1
2	V	82	LEU	2.1
1	A	294	HIS	2.1
1	W	228	TYR	2.1
1	W	259	TYR	2.1
1	W	263	GLY	2.1
1	W	352	TYR	2.1
1	Y	403	HIS	2.1
1	Q	219	VAL	2.1
1	U	219	VAL	2.1
2	D	117	SER	2.1
2	f	27	SER	2.1
1	O	345	ARG	2.1
1	a	40	GLU	2.1
1	e	40	GLU	2.1
1	e	201	GLU	2.1
1	O	347	TRP	2.1
1	U	84	TRP	2.1
1	W	276	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	99	LYS	2.1
2	H	76	THR	2.1
1	Q	398	GLN	2.1
1	S	284	GLN	2.1
2	T	6	LEU	2.1
1	E	229	ASN	2.1
2	H	78	ASN	2.1
1	C	402	CYS	2.1
1	E	331	HIS	2.1
1	a	159	GLY	2.1
2	R	109	GLY	2.1
1	I	404	VAL	2.1
2	V	50	VAL	2.1
1	Q	27	ARG	2.0
1	G	292	ALA	2.0
1	W	327	ALA	2.0
1	c	232	GLU	2.0
2	F	117	SER	2.0
2	H	32	SER	2.0
2	R	117	SER	2.0
1	U	270	LYS	2.0
2	X	88	LYS	2.0
2	R	38	TRP	2.0
2	H	42	THR	2.0
1	M	409	LEU	2.0
1	U	349	LEU	2.0
2	R	41	GLN	2.0
2	B	67	GLY	2.0
2	X	71	ILE	2.0
1	O	362	ARG	2.0
1	W	218	ARG	2.0
1	c	254	ARG	2.0
1	Q	348	ALA	2.0
1	U	265	ASP	2.0
1	C	44	SER	2.0
1	I	275	SER	2.0
1	C	95	THR	2.0
1	E	321	THR	2.0
1	M	97	THR	2.0
1	U	114	PRO	2.0
1	W	96	PRO	2.0
1	a	330	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	e	97	THR	2.0
1	A	373	LEU	2.0
1	S	3	LEU	2.0
1	W	409	LEU	2.0
1	W	66	ASN	2.0
1	G	254	ARG	2.0
1	G	404	VAL	2.0
1	I	345	ARG	2.0
1	M	337	VAL	2.0
1	S	90	TYR	2.0
1	W	302	TYR	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.