



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:59 PM UTC

PDB ID : 7STG / pdb_00007stg
Title : Consequences of HLA single chain trimer mutations on peptide presentation and binding affinity
Authors : Finton, K.A.K.; Rupert, P.B.
Deposited on : 2021-11-12
Resolution : 2.70 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

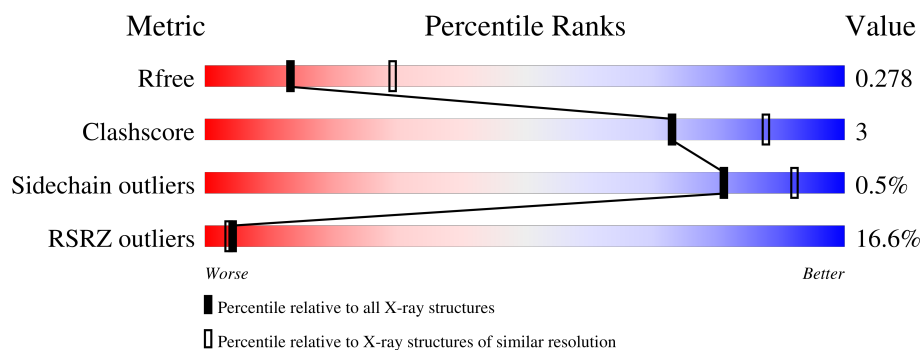
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	423	14% 83% • 13%
1	C	423	10% 82% • 15%
1	E	423	9% 82% • 14%
1	G	423	11% 84% • 12%
1	I	423	10% 84% • 13%
1	K	423	10% 85% • 12%

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Mol	Chain	Length	Quality of chain
1	M	423	
1	O	423	
1	Q	423	
1	S	423	
1	U	423	
1	W	423	
1	Y	423	
1	a	423	
1	c	423	
1	e	423	
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	
2	d	116	

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Mol	Chain	Length	Quality of chain
2	f	116	16% 91% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 107156 atoms, of which 50250 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 RPA-related protein RADX peptide,Beta-2-microglobulin,MH C class I antigen chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	H	N	O	S	0	0	0
			5205	1752	2426	496	518	13			
1	C	360	Total	C	H	N	O	S	0	0	0
			5207	1746	2444	493	511	13			
1	E	364	Total	C	H	N	O	S	0	0	0
			5290	1771	2487	496	523	13			
1	G	371	Total	C	H	N	O	S	0	0	0
			5277	1777	2463	501	524	12			
1	I	366	Total	C	H	N	O	S	0	0	0
			5248	1762	2459	497	517	13			
1	K	372	Total	C	H	N	O	S	0	0	0
			5291	1784	2466	503	525	13			
1	M	347	Total	C	H	N	O	S	0	0	0
			5018	1686	2355	470	494	13			
1	O	363	Total	C	H	N	O	S	0	0	0
			5201	1747	2437	491	513	13			
1	Q	371	Total	C	H	N	O	S	0	0	0
			5147	1744	2375	491	524	13			
1	S	340	Total	C	H	N	O	S	0	0	0
			4835	1634	2245	455	489	12			
1	U	343	Total	C	H	N	O	S	0	0	0
			4638	1585	2120	444	477	12			
1	W	341	Total	C	H	N	O	S	0	0	0
			4912	1652	2299	461	487	13			
1	Y	370	Total	C	H	N	O	S	0	0	0
			5124	1742	2361	489	519	13			
1	a	352	Total	C	H	N	O	S	0	0	0
			4938	1673	2288	470	495	12			
1	c	345	Total	C	H	N	O	S	0	0	0
			4732	1606	2177	451	486	12			
1	e	340	Total	C	H	N	O	S	0	0	0
			4905	1650	2300	457	486	12			

There are 688 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	linker	UNP Q6NSI4
A	11	GLY	-	linker	UNP Q6NSI4
A	12	GLY	-	linker	UNP Q6NSI4
A	13	GLY	-	linker	UNP Q6NSI4
A	14	SER	-	linker	UNP Q6NSI4
A	15	GLY	-	linker	UNP Q6NSI4
A	16	GLY	-	linker	UNP Q6NSI4
A	17	GLY	-	linker	UNP Q6NSI4
A	18	GLY	-	linker	UNP Q6NSI4
A	19	SER	-	linker	UNP Q6NSI4
A	20	GLY	-	linker	UNP Q6NSI4
A	21	GLY	-	linker	UNP Q6NSI4
A	22	GLY	-	linker	UNP Q6NSI4
A	23	GLY	-	linker	UNP Q6NSI4
A	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
C	11	GLY	-	linker	UNP Q6NSI4
C	12	GLY	-	linker	UNP Q6NSI4
C	13	GLY	-	linker	UNP Q6NSI4
C	14	SER	-	linker	UNP Q6NSI4
C	15	GLY	-	linker	UNP Q6NSI4
C	16	GLY	-	linker	UNP Q6NSI4
C	17	GLY	-	linker	UNP Q6NSI4
C	18	GLY	-	linker	UNP Q6NSI4
C	19	SER	-	linker	UNP Q6NSI4
C	20	GLY	-	linker	UNP Q6NSI4
C	21	GLY	-	linker	UNP Q6NSI4
C	22	GLY	-	linker	UNP Q6NSI4
C	23	GLY	-	linker	UNP Q6NSI4
C	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
E	11	GLY	-	linker	UNP Q6NSI4
E	12	GLY	-	linker	UNP Q6NSI4
E	13	GLY	-	linker	UNP Q6NSI4
E	14	SER	-	linker	UNP Q6NSI4
E	15	GLY	-	linker	UNP Q6NSI4
E	16	GLY	-	linker	UNP Q6NSI4
E	17	GLY	-	linker	UNP Q6NSI4
E	18	GLY	-	linker	UNP Q6NSI4
E	19	SER	-	linker	UNP Q6NSI4
E	20	GLY	-	linker	UNP Q6NSI4
E	21	GLY	-	linker	UNP Q6NSI4
E	22	GLY	-	linker	UNP Q6NSI4
E	23	GLY	-	linker	UNP Q6NSI4
E	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
G	11	GLY	-	linker	UNP Q6NSI4
G	12	GLY	-	linker	UNP Q6NSI4
G	13	GLY	-	linker	UNP Q6NSI4
G	14	SER	-	linker	UNP Q6NSI4
G	15	GLY	-	linker	UNP Q6NSI4
G	16	GLY	-	linker	UNP Q6NSI4
G	17	GLY	-	linker	UNP Q6NSI4
G	18	GLY	-	linker	UNP Q6NSI4
G	19	SER	-	linker	UNP Q6NSI4
G	20	GLY	-	linker	UNP Q6NSI4
G	21	GLY	-	linker	UNP Q6NSI4
G	22	GLY	-	linker	UNP Q6NSI4
G	23	GLY	-	linker	UNP Q6NSI4
G	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
I	11	GLY	-	linker	UNP Q6NSI4
I	12	GLY	-	linker	UNP Q6NSI4
I	13	GLY	-	linker	UNP Q6NSI4
I	14	SER	-	linker	UNP Q6NSI4
I	15	GLY	-	linker	UNP Q6NSI4
I	16	GLY	-	linker	UNP Q6NSI4
I	17	GLY	-	linker	UNP Q6NSI4
I	18	GLY	-	linker	UNP Q6NSI4
I	19	SER	-	linker	UNP Q6NSI4
I	20	GLY	-	linker	UNP Q6NSI4
I	21	GLY	-	linker	UNP Q6NSI4
I	22	GLY	-	linker	UNP Q6NSI4
I	23	GLY	-	linker	UNP Q6NSI4
I	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
K	11	GLY	-	linker	UNP Q6NSI4
K	12	GLY	-	linker	UNP Q6NSI4
K	13	GLY	-	linker	UNP Q6NSI4
K	14	SER	-	linker	UNP Q6NSI4
K	15	GLY	-	linker	UNP Q6NSI4
K	16	GLY	-	linker	UNP Q6NSI4
K	17	GLY	-	linker	UNP Q6NSI4
K	18	GLY	-	linker	UNP Q6NSI4
K	19	SER	-	linker	UNP Q6NSI4
K	20	GLY	-	linker	UNP Q6NSI4
K	21	GLY	-	linker	UNP Q6NSI4
K	22	GLY	-	linker	UNP Q6NSI4
K	23	GLY	-	linker	UNP Q6NSI4
K	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
M	11	GLY	-	linker	UNP Q6NSI4
M	12	GLY	-	linker	UNP Q6NSI4
M	13	GLY	-	linker	UNP Q6NSI4
M	14	SER	-	linker	UNP Q6NSI4
M	15	GLY	-	linker	UNP Q6NSI4
M	16	GLY	-	linker	UNP Q6NSI4
M	17	GLY	-	linker	UNP Q6NSI4
M	18	GLY	-	linker	UNP Q6NSI4
M	19	SER	-	linker	UNP Q6NSI4
M	20	GLY	-	linker	UNP Q6NSI4
M	21	GLY	-	linker	UNP Q6NSI4
M	22	GLY	-	linker	UNP Q6NSI4
M	23	GLY	-	linker	UNP Q6NSI4
M	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
O	11	GLY	-	linker	UNP Q6NSI4
O	12	GLY	-	linker	UNP Q6NSI4
O	13	GLY	-	linker	UNP Q6NSI4
O	14	SER	-	linker	UNP Q6NSI4
O	15	GLY	-	linker	UNP Q6NSI4
O	16	GLY	-	linker	UNP Q6NSI4
O	17	GLY	-	linker	UNP Q6NSI4
O	18	GLY	-	linker	UNP Q6NSI4
O	19	SER	-	linker	UNP Q6NSI4
O	20	GLY	-	linker	UNP Q6NSI4
O	21	GLY	-	linker	UNP Q6NSI4
O	22	GLY	-	linker	UNP Q6NSI4
O	23	GLY	-	linker	UNP Q6NSI4
O	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
Q	11	GLY	-	linker	UNP Q6NSI4
Q	12	GLY	-	linker	UNP Q6NSI4
Q	13	GLY	-	linker	UNP Q6NSI4
Q	14	SER	-	linker	UNP Q6NSI4
Q	15	GLY	-	linker	UNP Q6NSI4
Q	16	GLY	-	linker	UNP Q6NSI4
Q	17	GLY	-	linker	UNP Q6NSI4
Q	18	GLY	-	linker	UNP Q6NSI4
Q	19	SER	-	linker	UNP Q6NSI4
Q	20	GLY	-	linker	UNP Q6NSI4
Q	21	GLY	-	linker	UNP Q6NSI4
Q	22	GLY	-	linker	UNP Q6NSI4
Q	23	GLY	-	linker	UNP Q6NSI4
Q	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
S	11	GLY	-	linker	UNP Q6NSI4
S	12	GLY	-	linker	UNP Q6NSI4
S	13	GLY	-	linker	UNP Q6NSI4
S	14	SER	-	linker	UNP Q6NSI4
S	15	GLY	-	linker	UNP Q6NSI4
S	16	GLY	-	linker	UNP Q6NSI4
S	17	GLY	-	linker	UNP Q6NSI4
S	18	GLY	-	linker	UNP Q6NSI4
S	19	SER	-	linker	UNP Q6NSI4
S	20	GLY	-	linker	UNP Q6NSI4
S	21	GLY	-	linker	UNP Q6NSI4
S	22	GLY	-	linker	UNP Q6NSI4
S	23	GLY	-	linker	UNP Q6NSI4
S	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
U	11	GLY	-	linker	UNP Q6NSI4
U	12	GLY	-	linker	UNP Q6NSI4
U	13	GLY	-	linker	UNP Q6NSI4
U	14	SER	-	linker	UNP Q6NSI4
U	15	GLY	-	linker	UNP Q6NSI4
U	16	GLY	-	linker	UNP Q6NSI4
U	17	GLY	-	linker	UNP Q6NSI4
U	18	GLY	-	linker	UNP Q6NSI4
U	19	SER	-	linker	UNP Q6NSI4
U	20	GLY	-	linker	UNP Q6NSI4
U	21	GLY	-	linker	UNP Q6NSI4
U	22	GLY	-	linker	UNP Q6NSI4
U	23	GLY	-	linker	UNP Q6NSI4
U	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
W	11	GLY	-	linker	UNP Q6NSI4
W	12	GLY	-	linker	UNP Q6NSI4
W	13	GLY	-	linker	UNP Q6NSI4
W	14	SER	-	linker	UNP Q6NSI4
W	15	GLY	-	linker	UNP Q6NSI4
W	16	GLY	-	linker	UNP Q6NSI4
W	17	GLY	-	linker	UNP Q6NSI4
W	18	GLY	-	linker	UNP Q6NSI4
W	19	SER	-	linker	UNP Q6NSI4
W	20	GLY	-	linker	UNP Q6NSI4
W	21	GLY	-	linker	UNP Q6NSI4
W	22	GLY	-	linker	UNP Q6NSI4
W	23	GLY	-	linker	UNP Q6NSI4
W	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
Y	11	GLY	-	linker	UNP Q6NSI4
Y	12	GLY	-	linker	UNP Q6NSI4
Y	13	GLY	-	linker	UNP Q6NSI4
Y	14	SER	-	linker	UNP Q6NSI4
Y	15	GLY	-	linker	UNP Q6NSI4
Y	16	GLY	-	linker	UNP Q6NSI4
Y	17	GLY	-	linker	UNP Q6NSI4
Y	18	GLY	-	linker	UNP Q6NSI4
Y	19	SER	-	linker	UNP Q6NSI4
Y	20	GLY	-	linker	UNP Q6NSI4
Y	21	GLY	-	linker	UNP Q6NSI4
Y	22	GLY	-	linker	UNP Q6NSI4
Y	23	GLY	-	linker	UNP Q6NSI4
Y	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
a	11	GLY	-	linker	UNP Q6NSI4
a	12	GLY	-	linker	UNP Q6NSI4
a	13	GLY	-	linker	UNP Q6NSI4
a	14	SER	-	linker	UNP Q6NSI4
a	15	GLY	-	linker	UNP Q6NSI4
a	16	GLY	-	linker	UNP Q6NSI4
a	17	GLY	-	linker	UNP Q6NSI4
a	18	GLY	-	linker	UNP Q6NSI4
a	19	SER	-	linker	UNP Q6NSI4
a	20	GLY	-	linker	UNP Q6NSI4
a	21	GLY	-	linker	UNP Q6NSI4
a	22	GLY	-	linker	UNP Q6NSI4
a	23	GLY	-	linker	UNP Q6NSI4
a	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
c	11	GLY	-	linker	UNP Q6NSI4
c	12	GLY	-	linker	UNP Q6NSI4
c	13	GLY	-	linker	UNP Q6NSI4
c	14	SER	-	linker	UNP Q6NSI4
c	15	GLY	-	linker	UNP Q6NSI4
c	16	GLY	-	linker	UNP Q6NSI4
c	17	GLY	-	linker	UNP Q6NSI4
c	18	GLY	-	linker	UNP Q6NSI4
c	19	SER	-	linker	UNP Q6NSI4
c	20	GLY	-	linker	UNP Q6NSI4
c	21	GLY	-	linker	UNP Q6NSI4
c	22	GLY	-	linker	UNP Q6NSI4
c	23	GLY	-	linker	UNP Q6NSI4
c	24	SER	-	linker	UNP Q6NSI4
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	10	GLY	-	linker	UNP Q6NSI4
e	11	GLY	-	linker	UNP Q6NSI4
e	12	GLY	-	linker	UNP Q6NSI4
e	13	GLY	-	linker	UNP Q6NSI4
e	14	SER	-	linker	UNP Q6NSI4
e	15	GLY	-	linker	UNP Q6NSI4
e	16	GLY	-	linker	UNP Q6NSI4
e	17	GLY	-	linker	UNP Q6NSI4
e	18	GLY	-	linker	UNP Q6NSI4
e	19	SER	-	linker	UNP Q6NSI4
e	20	GLY	-	linker	UNP Q6NSI4
e	21	GLY	-	linker	UNP Q6NSI4
e	22	GLY	-	linker	UNP Q6NSI4
e	23	GLY	-	linker	UNP Q6NSI4
e	24	SER	-	linker	UNP Q6NSI4
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
			1642	524	792	147	175	4			
2	D	115	Total	C	H	N	O	S	0	0	0
			1621	521	779	145	172	4			
2	F	115	Total	C	H	N	O	S	0	0	0
			1616	520	774	145	173	4			
2	H	115	Total	C	H	N	O	S	0	0	0
			1638	524	790	146	174	4			
2	J	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	L	115	Total	C	H	N	O	S	0	0	0
			1637	523	790	146	174	4			
2	N	115	Total	C	H	N	O	S	0	0	0
			1635	523	788	146	174	4			
2	P	115	Total	C	H	N	O	S	0	0	0
			1648	529	795	146	174	4			
2	R	115	Total	C	H	N	O	S	0	0	0
			1622	521	779	145	173	4			
2	T	115	Total	C	H	N	O	S	0	0	0
			1642	524	793	146	175	4			
2	V	115	Total	C	H	N	O	S	0	0	0
			1611	518	770	145	174	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	115	Total	C	H	N	O	S	0	0	0
			1625	521	782	145	173	4			
2	Z	115	Total	C	H	N	O	S	0	0	0
			1626	521	781	146	174	4			
2	b	115	Total	C	H	N	O	S	0	0	0
			1633	526	784	145	174	4			
2	d	115	Total	C	H	N	O	S	0	0	0
			1626	521	781	146	174	4			
2	f	115	Total	C	H	N	O	S	0	0	0
			1631	526	785	144	172	4			

- Molecule 3 is water.

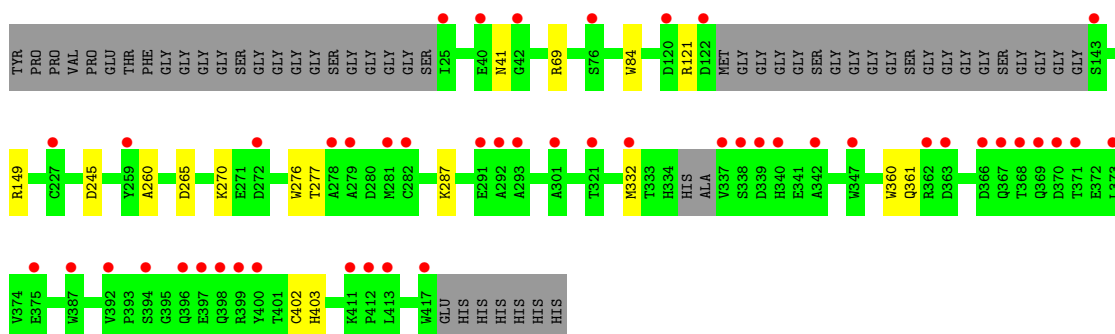
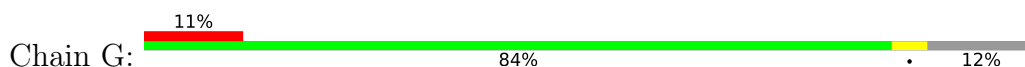
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	9	Total	O	0	0
			9	9		
3	C	10	Total	O	0	0
			10	10		
3	D	11	Total	O	0	0
			11	11		
3	E	10	Total	O	0	0
			10	10		
3	F	7	Total	O	0	0
			7	7		
3	G	1	Total	O	0	0
			1	1		
3	H	3	Total	O	0	0
			3	3		
3	I	1	Total	O	0	0
			1	1		
3	J	4	Total	O	0	0
			4	4		
3	K	1	Total	O	0	0
			1	1		
3	L	3	Total	O	0	0
			3	3		
3	N	2	Total	O	0	0
			2	2		
3	O	3	Total	O	0	0
			3	3		

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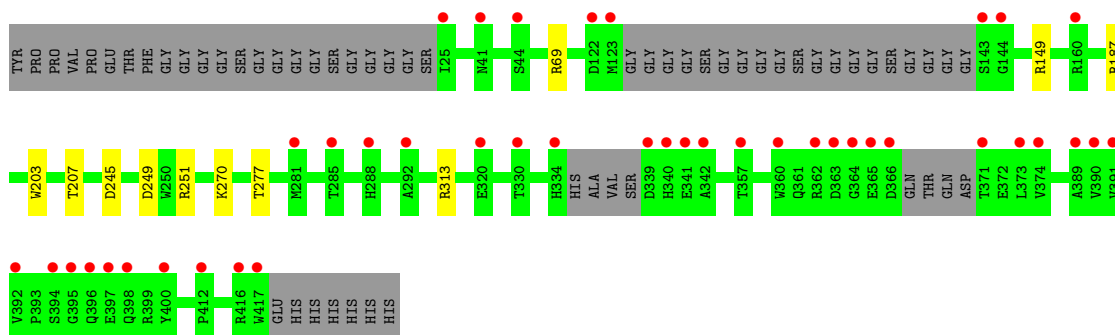
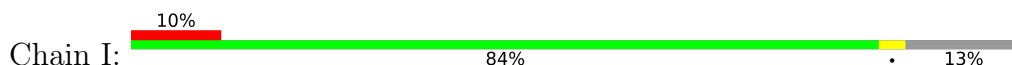
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	4	Total O 4 4	0	0
3	R	2	Total O 2 2	0	0
3	S	1	Total O 1 1	0	0
3	T	1	Total O 1 1	0	0
3	V	3	Total O 3 3	0	0
3	W	1	Total O 1 1	0	0
3	X	2	Total O 2 2	0	0
3	Z	1	Total O 1 1	0	0
3	b	1	Total O 1 1	0	0
3	d	2	Total O 2 2	0	0
3	e	3	Total O 3 3	0	0
3	f	2	Total O 2 2	0	0

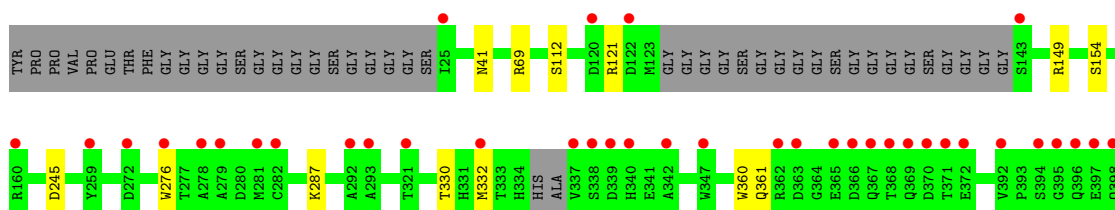
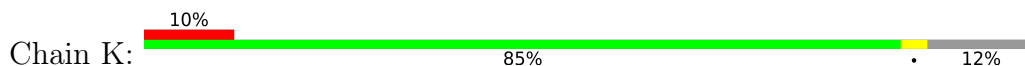
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

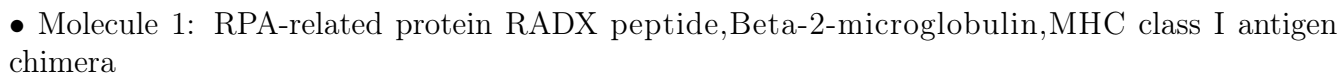


- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

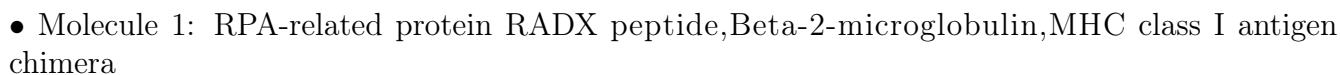


- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera



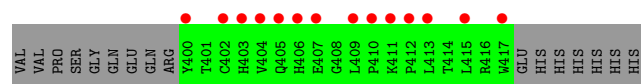


Response	Percentage
Good job	71%
Bad job	22%

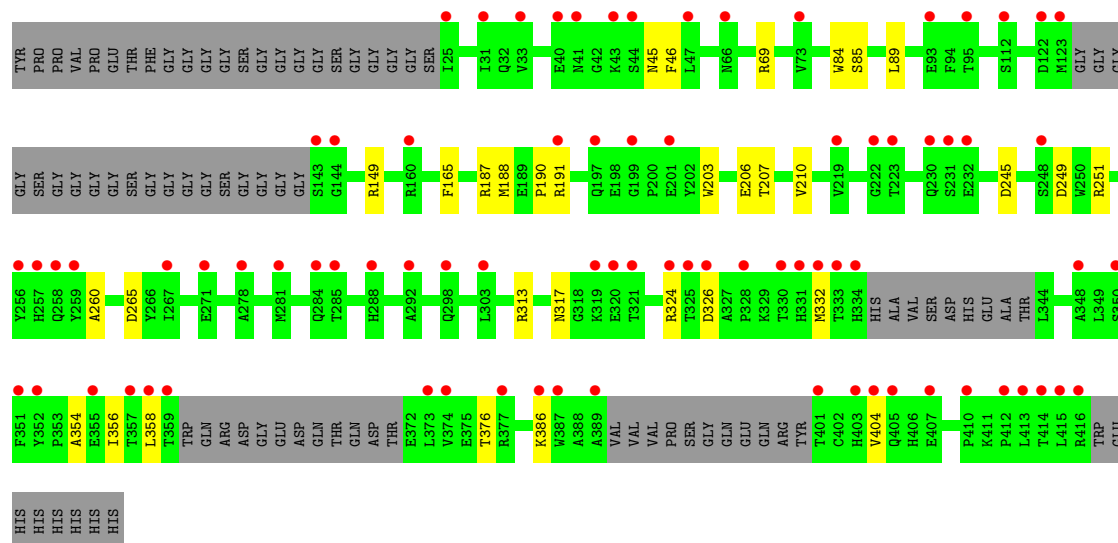
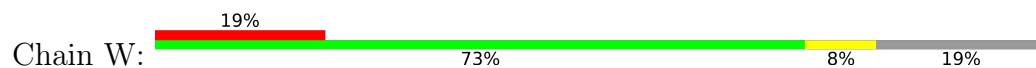


Response	Percentage
Yes	25%
No	75%
Don't know	6%
No answer	19%

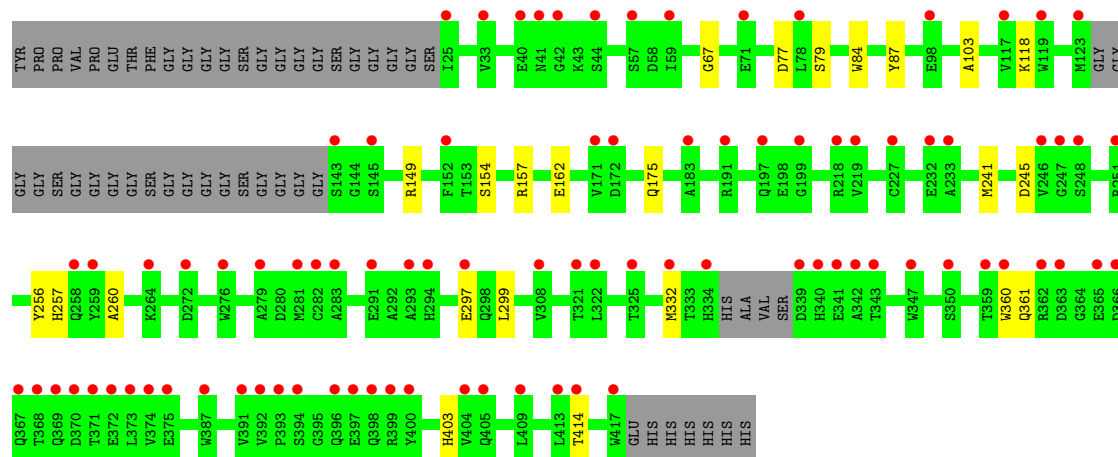
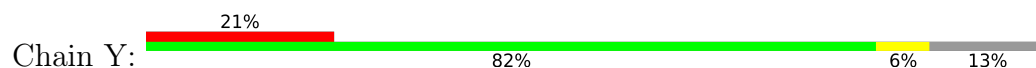




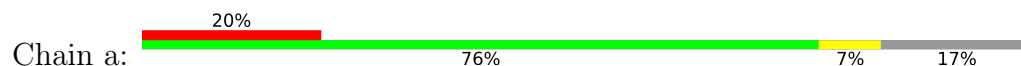
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

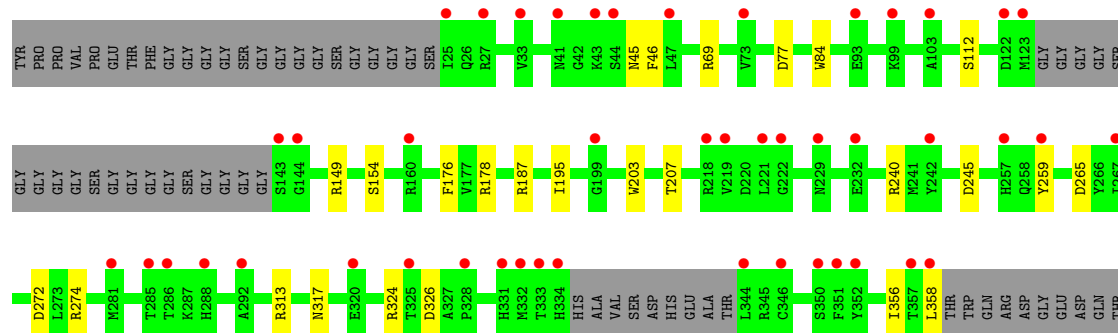


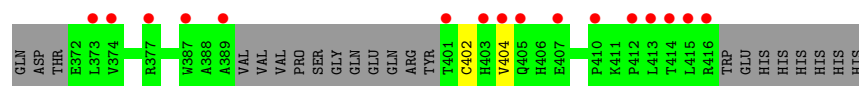
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera



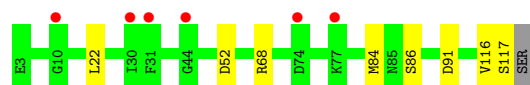
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera



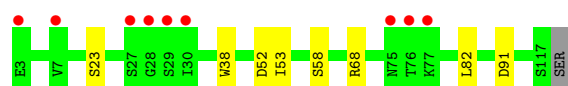




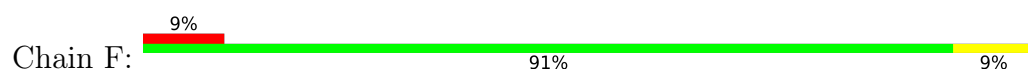
• Molecule 2: VHH



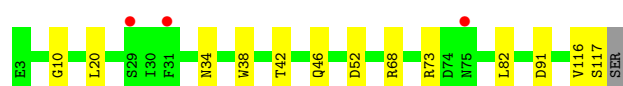
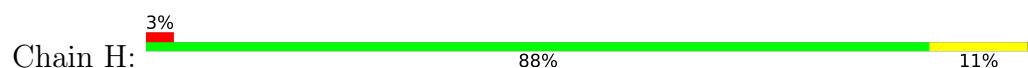
• Molecule 2: VHH



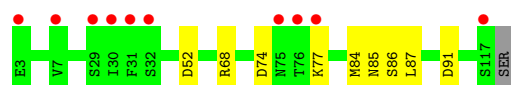
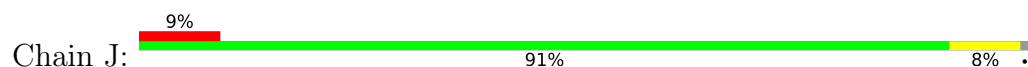
• Molecule 2: VHH



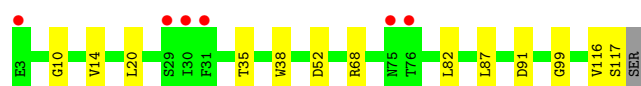
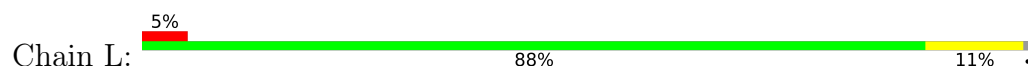
• Molecule 2: VHH



• Molecule 2: VHH



• Molecule 2: VHH

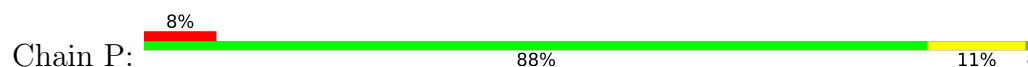


• Molecule 2: VHH

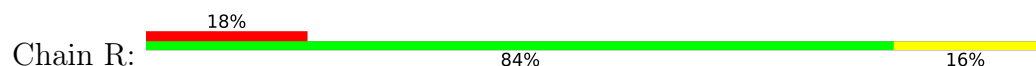




• Molecule 2: VHH



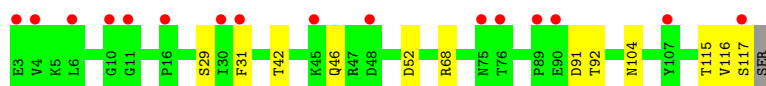
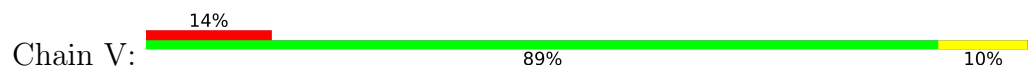
• Molecule 2: VHH



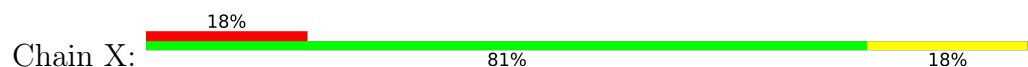
• Molecule 2: VHH



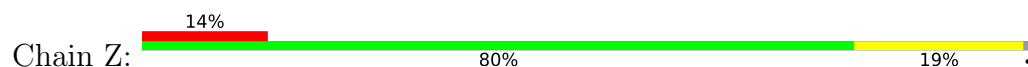
• Molecule 2: VHH



• Molecule 2: VHH

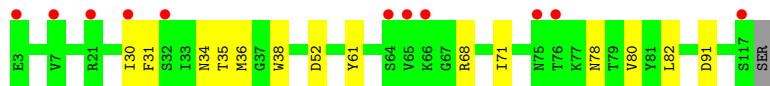


• Molecule 2: VHH



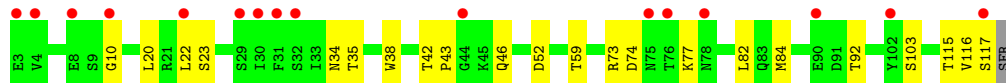
● Molecule 2: VHH

Chain b:  9% 87% 12%

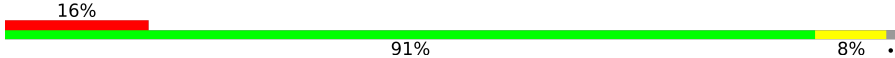


● Molecule 2: VHH

Chain d:  14% 80% 19%



● Molecule 2: VHH

Chain f:  16% 91% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.59Å 118.09Å 273.73Å 102.44° 102.41° 89.88°	Depositor
Resolution (Å)	48.86 – 2.70 48.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.86-2.70) 94.3 (48.86-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.242 , 0.276 (Not available) , 0.278	Depositor DCC
R_{free} test set	18559 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.347 for -k,h,k+l 0.347 for k,-h,h+l 0.368 for h,-k,-h-l 0.357 for -h,k,-k-l 0.437 for -k,-h,-l 0.296 for k,h,-h-k-l 0.300 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	107156	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8682e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.11	0/2856	0.27	0/3901
1	C	0.11	0/2842	0.26	0/3875
1	E	0.13	0/2882	0.29	0/3929
1	G	0.11	0/2894	0.27	0/3952
1	I	0.11	0/2868	0.27	0/3913
1	K	0.11	0/2906	0.28	0/3968
1	M	0.11	0/2738	0.28	0/3732
1	O	0.11	0/2842	0.28	0/3878
1	Q	0.12	0/2850	0.27	0/3895
1	S	0.13	0/2664	0.28	0/3636
1	U	0.10	0/2585	0.27	0/3533
1	W	0.11	0/2686	0.26	0/3661
1	Y	0.11	0/2842	0.27	0/3888
1	a	0.16	1/2725 (0.0%)	0.29	0/3721
1	c	0.10	0/2621	0.26	0/3576
1	e	0.13	0/2678	0.27	0/3651
2	B	0.12	0/865	0.30	0/1173
2	D	0.14	0/857	0.29	0/1163
2	F	0.12	0/857	0.29	0/1164
2	H	0.12	0/863	0.28	0/1171
2	J	0.12	0/861	0.29	0/1168
2	L	0.13	0/862	0.29	0/1169
2	N	0.13	0/862	0.30	0/1169
2	P	0.14	0/869	0.32	0/1178
2	R	0.10	0/858	0.30	0/1164
2	T	0.12	0/864	0.29	0/1172
2	V	0.12	0/856	0.29	0/1162
2	X	0.12	0/858	0.31	0/1164
2	Z	0.12	0/860	0.29	0/1166
2	b	0.10	0/865	0.26	0/1174
2	d	0.10	0/860	0.27	0/1166
2	f	0.11	0/862	0.29	0/1169
All	All	0.12	1/58258 (0.0%)	0.28	0/79401

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	200	PRO	N-CD	-5.29	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2779	2426	2426	11	0
1	C	2763	2444	2449	7	0
1	E	2803	2487	2487	16	0
1	G	2814	2463	2463	12	0
1	I	2789	2459	2459	7	0
1	K	2825	2466	2466	9	0
1	M	2663	2355	2352	4	0
1	O	2764	2437	2437	9	0
1	Q	2772	2375	2374	27	0
1	S	2590	2245	2249	28	0
1	U	2518	2120	2120	14	0
1	W	2613	2299	2297	20	0
1	Y	2763	2361	2361	15	0
1	a	2650	2288	2291	21	0
1	c	2555	2177	2175	11	0
1	e	2605	2300	2298	25	0
2	B	850	792	792	5	0
2	D	842	779	779	4	0
2	F	842	774	774	6	0
2	H	848	790	790	7	0
2	J	846	785	785	5	0
2	L	847	790	788	7	0
2	N	847	788	788	7	0
2	P	853	795	795	9	0
2	R	843	779	779	9	0
2	T	849	793	793	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	841	770	770	8	0
2	X	843	782	782	14	0
2	Z	845	781	781	14	0
2	b	849	784	784	10	0
2	d	845	781	781	14	0
2	f	846	785	785	9	0
3	A	16	0	0	1	0
3	B	9	0	0	0	0
3	C	10	0	0	0	0
3	D	11	0	0	0	0
3	E	10	0	0	1	0
3	F	7	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
3	I	1	0	0	0	0
3	J	4	0	0	0	0
3	K	1	0	0	0	0
3	L	3	0	0	0	0
3	N	2	0	0	0	0
3	O	3	0	0	0	0
3	P	4	0	0	0	0
3	R	2	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	V	3	0	0	0	0
3	W	1	0	0	0	0
3	X	2	0	0	0	0
3	Z	1	0	0	0	0
3	b	1	0	0	0	0
3	d	2	0	0	0	0
3	e	3	0	0	0	0
3	f	2	0	0	0	0
All	All	56906	50250	50250	339	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 (339) 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:e:240:ARG:NH2	1:e:259:TYR:OH	1.83	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:240:ARG:CZ	1:e:259:TYR:OH	2.22	0.87
1:G:276:TRP:O	1:G:287:LYS:NZ	2.13	0.81
1:e:240:ARG:HE	1:e:259:TYR:HE1	1.24	0.81
1:Q:276:TRP:HB2	1:Q:287:LYS:HE2	1.64	0.80
1:W:190:PRO:O	1:W:191:ARG:NH1	2.15	0.80
1:e:272:ASP:OD1	1:e:274:ARG:N	2.16	0.79
2:J:74:ASP:OD2	2:J:77:LYS:N	2.16	0.79
1:I:149:ARG:NH2	1:I:245:ASP:OD1	2.17	0.78
1:W:149:ARG:NH2	1:W:245:ASP:OD1	2.17	0.77
1:S:240:ARG:CZ	1:S:259:TYR:HE1	1.95	0.77
2:d:92:THR:HG23	2:d:115:THR:HA	1.66	0.76
1:e:240:ARG:NE	1:e:259:TYR:CE1	2.54	0.75
1:a:324:ARG:NH1	1:a:326:ASP:OD2	2.19	0.75
2:X:22:LEU:HG	2:X:84:MET:HE2	1.69	0.74
1:U:69:ARG:NH2	2:V:52:ASP:OD2	2.22	0.73
2:X:36:MET:HE3	2:X:80:VAL:HG13	1.71	0.72
1:e:240:ARG:NH2	1:e:259:TYR:HH	1.85	0.72
1:a:249:ASP:OD2	1:a:251:ARG:NH1	2.21	0.72
2:R:8:GLU:OE1	2:R:111:GLY:N	2.19	0.70
1:e:240:ARG:NH2	1:e:259:TYR:CZ	2.60	0.70
1:a:200:PRO:HD2	1:a:201:GLU:H	1.56	0.69
1:c:69:ARG:NH2	2:d:52:ASP:OD2	2.26	0.69
1:W:249:ASP:OD2	1:W:251:ARG:NH1	2.26	0.68
1:E:332:MET:HE2	1:E:360:TRP:HH2	1.57	0.68
1:S:313:ARG:O	1:S:317:ASN:ND2	2.27	0.68
1:S:178:ARG:NH1	1:S:189:GLU:OE2	2.27	0.67
1:C:100:ASP:O	1:C:121:ARG:NH2	2.28	0.67
2:Z:92:THR:HG23	2:Z:115:THR:HA	1.76	0.66
1:C:69:ARG:NH2	2:D:52:ASP:OD2	2.30	0.65
1:E:69:ARG:NH2	2:F:52:ASP:OD2	2.29	0.65
2:P:22:LEU:HD13	2:P:84:MET:HE3	1.78	0.64
1:G:121:ARG:NH2	2:V:29:SER:OG	2.30	0.64
1:K:276:TRP:HB2	1:K:287:LYS:HE3	1.80	0.64
1:I:249:ASP:OD2	1:I:251:ARG:NH1	2.30	0.64
2:V:42:THR:OG1	2:V:46:GLN:O	2.15	0.63
1:S:328:PRO:HD3	1:S:406:HIS:CD2	2.33	0.63
1:W:203:TRP:O	1:W:207:THR:OG1	2.15	0.63
1:W:313:ARG:O	1:W:317:ASN:OD1	2.17	0.63
2:d:42:THR:OG1	2:d:46:GLN:O	2.17	0.63
1:a:69:ARG:NH2	2:b:52:ASP:OD2	2.32	0.62
1:Y:297:GLU:OE1	1:Y:297:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:92:THR:HG23	2:V:115:THR:HA	1.81	0.62
1:M:69:ARG:NH2	2:N:52:ASP:OD2	2.34	0.61
1:e:324:ARG:NH2	1:e:326:ASP:OD1	2.33	0.60
1:Q:118:LYS:NZ	2:R:105:ASP:OD1	2.35	0.60
2:b:68:ARG:NH2	2:b:91:ASP:OD2	2.33	0.60
2:X:84:MET:HB3	2:X:87:LEU:HD21	1.83	0.60
1:e:240:ARG:NE	1:e:259:TYR:HE1	1.93	0.60
1:e:203:TRP:O	1:e:207:THR:OG1	2.17	0.59
1:Q:48:ASN:OD1	1:Q:89:LEU:HD11	2.03	0.59
1:S:358:LEU:CD1	1:S:404:VAL:HG22	2.33	0.59
2:L:68:ARG:NH2	2:L:91:ASP:OD2	2.34	0.59
1:S:401:THR:O	1:S:401:THR:OG1	2.17	0.59
2:X:68:ARG:NH2	2:X:91:ASP:OD2	2.33	0.59
1:Y:332:MET:HE3	1:Y:360:TRP:HH2	1.67	0.59
1:A:69:ARG:NH2	2:B:52:ASP:OD2	2.35	0.59
1:Q:361:GLN:OE1	1:Q:403:HIS:NE2	2.35	0.59
2:T:53:ILE:HG13	2:T:59:THR:HG22	1.85	0.59
1:U:203:TRP:O	1:U:207:THR:OG1	2.20	0.58
1:A:179:PHE:HB2	1:A:188:MET:SD	2.44	0.58
1:E:332:MET:CE	1:E:360:TRP:HH2	2.16	0.58
1:Y:361:GLN:OE1	1:Y:403:HIS:NE2	2.34	0.58
2:P:22:LEU:HD22	2:P:84:MET:CE	2.33	0.58
1:E:321:THR:O	1:E:324:ARG:NH1	2.34	0.57
2:N:22:LEU:HD13	2:N:84:MET:HE3	1.86	0.57
1:M:328:PRO:HD3	1:M:406:HIS:ND1	2.18	0.57
1:Y:245:ASP:OD2	1:Y:256:TYR:OH	2.21	0.57
1:e:240:ARG:NH2	1:e:259:TYR:CE1	2.73	0.57
1:O:69:ARG:NH2	2:P:52:ASP:OD2	2.38	0.56
2:B:68:ARG:NH2	2:B:91:ASP:OD2	2.38	0.56
1:Q:330:THR:HG21	1:Q:415:LEU:HD11	1.88	0.56
2:F:74:ASP:OD2	2:F:77:LYS:N	2.38	0.56
1:G:69:ARG:NH2	2:H:52:ASP:OD2	2.39	0.56
1:a:149:ARG:NH2	1:a:245:ASP:OD1	2.39	0.56
2:f:36:MET:HE3	2:f:80:VAL:HG13	1.88	0.56
1:Y:103:ALA:HB3	2:Z:104:ASN:HD22	1.71	0.55
1:K:276:TRP:HB2	1:K:287:LYS:CE	2.36	0.55
1:S:406:HIS:CD2	1:S:408:GLY:H	2.24	0.55
1:e:69:ARG:NH2	2:f:52:ASP:OD2	2.40	0.55
2:Z:40:ARG:HD3	2:Z:50:VAL:HG22	1.88	0.55
2:B:22:LEU:HG	2:B:84:MET:HE2	1.87	0.55
1:e:77:ASP:OD1	1:e:178:ARG:NH1	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:352:TYR:CD2	1:S:353:PRO:HA	2.42	0.54
1:Y:118:LYS:NZ	2:Z:105:ASP:OD1	2.40	0.54
2:d:42:THR:HB	2:d:43:PRO:HD2	1.89	0.54
1:Q:41:ASN:OD1	2:b:31:PHE:HE1	1.89	0.54
2:Z:32:SER:O	2:Z:33:ILE:HD13	2.08	0.54
2:f:22:LEU:HD22	2:f:84:MET:HE2	1.89	0.54
1:G:270:LYS:HD3	1:G:277:THR:OG1	2.07	0.54
1:K:361:GLN:OE1	1:O:270:LYS:NZ	2.41	0.54
2:P:68:ARG:NH2	2:P:91:ASP:OD2	2.41	0.53
1:S:272:ASP:OD1	1:S:274:ARG:N	2.37	0.53
2:D:68:ARG:NH2	2:D:91:ASP:OD2	2.40	0.53
1:W:69:ARG:NH2	2:X:52:ASP:OD2	2.42	0.53
2:X:61:TYR:HB2	2:X:66:LYS:HE3	1.90	0.53
2:J:68:ARG:NH2	2:J:91:ASP:OD2	2.39	0.52
1:U:179:PHE:HB2	1:U:188:MET:SD	2.49	0.52
1:K:332:MET:HE3	1:K:360:TRP:HH2	1.75	0.52
2:N:68:ARG:NH2	2:N:91:ASP:OD2	2.43	0.52
1:Q:41:ASN:OD1	2:b:31:PHE:CE1	2.62	0.52
2:P:34:ASN:ND2	2:P:102:TYR:CE1	2.78	0.52
2:Z:53:ILE:HD12	2:Z:59:THR:HG22	1.92	0.52
1:M:276:TRP:HB2	1:M:287:LYS:HD2	1.92	0.52
2:R:42:THR:HB	2:R:43:PRO:HD2	1.92	0.52
1:a:96:PRO:HB2	1:a:121:ARG:NH2	2.25	0.52
2:b:36:MET:HB2	2:b:80:VAL:HG11	1.90	0.52
2:d:22:LEU:HG	2:d:84:MET:CE	2.40	0.52
1:e:240:ARG:CZ	1:e:259:TYR:CZ	2.94	0.51
2:X:38:TRP:CZ3	2:X:82:LEU:HB2	2.45	0.51
2:V:68:ARG:NH2	2:V:91:ASP:OD2	2.41	0.51
1:a:328:PRO:HD3	1:a:406:HIS:CD2	2.45	0.51
1:A:269:LEU:HD12	1:A:276:TRP:CZ3	2.46	0.51
1:I:69:ARG:NH2	2:J:52:ASP:OD2	2.43	0.51
2:d:22:LEU:HG	2:d:84:MET:HE2	1.92	0.51
1:E:187:ARG:HA	1:E:207:THR:HG23	1.92	0.51
1:C:270:LYS:NZ	1:G:361:GLN:OE1	2.44	0.50
1:S:178:ARG:HD3	1:S:191:ARG:CZ	2.42	0.50
1:W:324:ARG:NH2	1:W:326:ASP:OD1	2.43	0.50
1:G:41:ASN:ND2	2:V:31:PHE:CB	2.74	0.50
1:G:332:MET:CE	1:G:360:TRP:HH2	2.25	0.50
1:O:123:MET:HG3	1:O:347:TRP:CZ2	2.46	0.50
2:X:38:TRP:CH2	2:X:80:VAL:HG23	2.46	0.50
1:W:356:ILE:HG12	1:W:358:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:272:ASP:OD1	1:a:274:ARG:N	2.39	0.50
1:C:249:ASP:OD2	1:C:251:ARG:NH1	2.45	0.50
1:U:148:MET:HB2	1:U:311:LEU:HG	1.93	0.50
2:d:34:ASN:O	2:d:73:ARG:NH2	2.44	0.50
1:Y:157:ARG:NE	1:Y:162:GLU:O	2.41	0.50
1:a:188:MET:CE	1:a:210:VAL:HG21	2.42	0.50
1:c:149:ARG:NH2	1:c:245:ASP:OD1	2.44	0.50
2:R:84:MET:HB3	2:R:87:LEU:HD21	1.94	0.50
1:a:96:PRO:HB2	1:a:121:ARG:HH22	1.77	0.50
1:S:171:VAL:HG13	1:S:322:LEU:HD21	1.94	0.49
1:U:148:MET:C	1:U:149:ARG:HD2	2.37	0.49
1:A:269:LEU:CD1	1:A:276:TRP:CZ3	2.96	0.49
1:K:149:ARG:NH2	1:K:245:ASP:OD1	2.44	0.49
1:Q:330:THR:HG22	1:Q:415:LEU:HD21	1.94	0.49
1:c:179:PHE:HB2	1:c:188:MET:CE	2.42	0.49
2:H:42:THR:OG1	2:H:46:GLN:O	2.27	0.49
1:S:177:VAL:HB	1:S:188:MET:SD	2.52	0.49
1:S:69:ARG:NH2	2:T:52:ASP:OD2	2.46	0.49
1:S:187:ARG:HD3	1:S:207:THR:HG21	1.94	0.49
1:e:240:ARG:CZ	1:e:259:TYR:CE1	2.95	0.49
2:f:38:TRP:CZ3	2:f:82:LEU:HB2	2.49	0.48
1:E:190:PRO:O	1:E:191:ARG:NH1	2.47	0.48
1:Q:245:ASP:OD2	1:Q:256:TYR:OH	2.31	0.48
2:Z:42:THR:HB	2:Z:43:PRO:HD2	1.95	0.48
1:O:66:ASN:O	2:P:34:ASN:ND2	2.46	0.48
1:O:249:ASP:OD2	1:O:251:ARG:NH1	2.46	0.48
1:e:272:ASP:OD1	1:e:272:ASP:C	2.56	0.48
1:E:332:MET:CE	1:E:360:TRP:CH2	2.97	0.48
1:S:176:PHE:CD2	1:S:195:ILE:HD13	2.48	0.48
2:Z:8:GLU:OE2	2:Z:111:GLY:N	2.37	0.48
2:Z:89:PRO:O	2:Z:92:THR:OG1	2.19	0.48
1:c:108:HIS:N	1:c:111:LEU:HD12	2.29	0.48
1:W:188:MET:CE	1:W:210:VAL:HG21	2.44	0.47
1:E:297:GLU:CD	1:E:297:GLU:H	2.22	0.47
1:Q:84:TRP:NE1	1:Q:265:ASP:OD1	2.45	0.47
1:a:66:ASN:O	2:b:34:ASN:ND2	2.46	0.47
1:c:149:ARG:HD2	1:c:241:MET:HE2	1.94	0.47
2:f:36:MET:CE	2:f:80:VAL:HG13	2.45	0.47
1:G:361:GLN:NE2	1:G:403:HIS:NE2	2.62	0.47
2:H:34:ASN:O	2:H:73:ARG:NH2	2.45	0.47
2:f:22:LEU:HD13	2:f:84:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:TRP:O	1:E:207:THR:OG1	2.26	0.47
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.48	0.47
2:P:38:TRP:CZ3	2:P:82:LEU:HB2	2.50	0.47
1:S:352:TYR:CD2	1:S:353:PRO:CA	2.97	0.47
1:U:97:THR:O	1:U:121:ARG:NH1	2.47	0.47
2:R:92:THR:HG23	2:R:115:THR:HA	1.97	0.47
1:Y:403:HIS:CE1	1:Y:414:THR:HG22	2.50	0.47
1:A:269:LEU:HD12	1:A:276:TRP:CE3	2.50	0.47
1:I:187:ARG:HA	1:I:207:THR:HG23	1.97	0.47
1:Q:267:ILE:HA	1:Q:277:THR:O	2.15	0.47
1:S:269:LEU:HD21	1:S:273:LEU:HA	1.97	0.47
1:U:59:ILE:HG13	1:U:108:HIS:HD2	1.79	0.47
1:a:148:MET:HE2	1:a:314:TYR:CD2	2.49	0.47
2:b:30:ILE:O	2:b:78:ASN:ND2	2.43	0.47
1:S:187:ARG:NH2	1:S:204:ASP:OD1	2.48	0.47
1:S:240:ARG:NH1	1:S:259:TYR:HE1	2.13	0.47
1:W:206:GLU:O	1:W:210:VAL:HG23	2.15	0.47
2:Z:84:MET:HB3	2:Z:87:LEU:HD21	1.96	0.47
1:Y:77:ASP:OD2	1:Y:175:GLN:NE2	2.40	0.46
1:a:245:ASP:OD2	1:a:256:TYR:OH	2.30	0.46
1:a:149:ARG:HD3	1:a:241:MET:HE3	1.97	0.46
1:A:149:ARG:HD2	1:A:241:MET:HE2	1.97	0.46
1:U:176:PHE:CD2	1:U:177:VAL:HG13	2.50	0.46
2:X:53:ILE:HD12	2:X:59:THR:HG22	1.96	0.46
1:e:358:LEU:HD13	1:e:404:VAL:HG12	1.97	0.46
2:B:116:VAL:O	2:B:117:SER:C	2.58	0.46
1:K:41:ASN:OD1	1:K:121:ARG:NH2	2.48	0.46
1:S:272:ASP:OD1	1:S:272:ASP:C	2.58	0.46
1:Y:257:HIS:CD2	1:Y:299:LEU:HD21	2.51	0.46
1:I:203:TRP:O	1:I:207:THR:OG1	2.29	0.46
2:X:6:LEU:HD13	2:X:24:CYS:SG	2.55	0.46
2:X:6:LEU:HD23	2:X:26:ALA:HA	1.96	0.46
1:C:65:LYS:HG3	1:C:102:TYR:CE2	2.51	0.46
1:G:41:ASN:OD1	1:G:121:ARG:NH1	2.49	0.46
2:R:116:VAL:O	2:R:117:SER:C	2.59	0.46
1:U:308:VAL:HG12	1:U:312:ARG:HE	1.80	0.46
1:U:79:SER:HB3	1:U:87:TYR:CZ	2.51	0.46
1:Q:238:VAL:HG12	1:Q:261:TYR:HD1	1.80	0.46
1:A:332:MET:HE1	1:A:360:TRP:CH2	2.51	0.46
1:Y:149:ARG:HD2	1:Y:241:MET:HE2	1.98	0.46
2:L:10:GLY:O	2:L:20:LEU:HD22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:22:LEU:HD22	2:N:84:MET:HE2	1.97	0.45
1:I:313:ARG:HG3	2:P:113:GLN:HB2	1.98	0.45
2:T:53:ILE:HD12	2:T:71:ILE:HG23	1.99	0.45
2:D:38:TRP:CZ3	2:D:82:LEU:HB2	2.51	0.45
1:Q:330:THR:CG2	1:Q:415:LEU:HD21	2.46	0.45
1:S:247:GLY:N	1:S:253:LEU:HD21	2.31	0.45
2:d:38:TRP:CZ3	2:d:82:LEU:HB2	2.51	0.45
1:e:404:VAL:HG23	1:e:404:VAL:O	2.15	0.45
1:c:350:SER:HA	1:c:383:THR:HB	1.97	0.45
2:R:34:ASN:O	2:R:73:ARG:NH2	2.48	0.45
1:W:187:ARG:HA	1:W:207:THR:HG23	1.98	0.45
2:b:38:TRP:CZ3	2:b:82:LEU:HB2	2.52	0.45
1:e:313:ARG:O	1:e:317:ASN:OD1	2.34	0.45
2:J:85:ASN:O	2:J:86:SER:C	2.60	0.45
1:K:330:THR:HG22	1:K:415:LEU:HD21	1.99	0.45
2:T:53:ILE:CD1	2:T:59:THR:HG22	2.47	0.45
2:d:10:GLY:O	2:d:20:LEU:HD22	2.16	0.45
1:E:149:ARG:NH2	1:E:245:ASP:OD1	2.49	0.44
1:E:251:ARG:HG3	1:E:251:ARG:HH11	1.81	0.44
1:U:32:GLN:NE2	1:U:374:VAL:HG22	2.32	0.44
2:H:38:TRP:CZ3	2:H:82:LEU:HB2	2.52	0.44
1:K:69:ARG:NH2	2:L:52:ASP:OD2	2.50	0.44
1:Q:268:ALA:O	1:Q:277:THR:N	2.50	0.44
2:N:35:THR:O	2:N:99:GLY:HA2	2.17	0.44
1:S:78:LEU:HB3	1:S:166:ILE:HG21	2.00	0.44
1:S:148:MET:HE2	1:S:314:TYR:CD2	2.52	0.44
2:V:116:VAL:O	2:V:117:SER:C	2.59	0.44
2:b:38:TRP:CH2	2:b:80:VAL:HG23	2.52	0.44
2:d:34:ASN:O	2:d:73:ARG:NH1	2.50	0.44
1:Q:316:GLU:O	1:Q:319:LYS:HG2	2.17	0.44
1:G:149:ARG:NH2	1:G:245:ASP:OD1	2.49	0.44
1:O:149:ARG:NH2	1:O:245:ASP:OD1	2.49	0.44
1:c:67:GLY:O	2:d:35:THR:OG1	2.30	0.44
1:e:187:ARG:HA	1:e:207:THR:HG23	1.99	0.44
2:Z:34:ASN:O	2:Z:73:ARG:NH1	2.44	0.44
2:d:116:VAL:O	2:d:117:SER:C	2.61	0.44
1:A:340:HIS:O	1:A:394:SER:N	2.44	0.44
1:G:84:TRP:CE2	1:G:260:ALA:HB2	2.53	0.44
1:c:118:LYS:NZ	2:d:103:SER:O	2.47	0.44
2:H:10:GLY:O	2:H:20:LEU:HD22	2.17	0.44
2:L:38:TRP:CZ3	2:L:82:LEU:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:116:VAL:O	2:Z:117:SER:C	2.61	0.44
2:f:6:LEU:HD22	2:f:24:CYS:SG	2.57	0.44
2:F:68:ARG:NH2	2:F:91:ASP:OD2	2.41	0.43
2:L:116:VAL:O	2:L:117:SER:C	2.60	0.43
1:W:358:LEU:HD13	1:W:404:VAL:HG22	1.99	0.43
1:A:361:GLN:HG3	1:A:366:ASP:HA	1.99	0.43
1:K:332:MET:CE	1:K:360:TRP:HH2	2.31	0.43
1:e:45:ASN:OD1	1:e:46:PHE:N	2.46	0.43
1:a:272:ASP:OD1	1:a:272:ASP:C	2.61	0.43
2:f:22:LEU:HD13	2:f:84:MET:HE3	1.99	0.43
1:M:84:TRP:CE2	1:M:260:ALA:HB2	2.53	0.43
1:Q:403:HIS:CE1	1:Q:414:THR:HG23	2.53	0.43
2:L:35:THR:O	2:L:99:GLY:HA2	2.19	0.43
1:Q:79:SER:HB3	1:Q:87:TYR:CZ	2.53	0.43
1:Q:383:THR:C	1:Q:384:PHE:HD2	2.27	0.43
1:W:84:TRP:CE2	1:W:260:ALA:HB2	2.54	0.43
2:f:38:TRP:CH2	2:f:80:VAL:HG23	2.53	0.43
2:H:116:VAL:O	2:H:117:SER:C	2.62	0.43
2:F:38:TRP:CZ3	2:F:82:LEU:HB2	2.54	0.42
1:I:270:LYS:HE2	1:I:277:THR:OG1	2.19	0.42
1:S:78:LEU:HD11	1:S:86:PHE:CD1	2.54	0.42
1:E:109:VAL:N	3:E:501:HOH:O	2.43	0.42
1:O:360:TRP:CZ3	1:O:402:CYS:HB2	2.54	0.42
1:a:200:PRO:CD	1:a:201:GLU:H	2.27	0.42
2:P:53:ILE:HA	2:P:58:SER:O	2.19	0.42
1:Q:350:SER:HA	1:Q:383:THR:HB	2.00	0.42
1:e:176:PHE:CD2	1:e:195:ILE:HD13	2.54	0.42
2:Z:40:ARG:HD3	2:Z:50:VAL:CG2	2.49	0.42
1:C:249:ASP:OD1	1:C:249:ASP:N	2.52	0.42
1:Q:276:TRP:CZ2	1:Q:295:VAL:HG23	2.54	0.42
1:S:240:ARG:NH1	1:S:259:TYR:CE1	2.88	0.42
2:X:6:LEU:HD13	2:X:97:CYS:SG	2.59	0.42
2:X:14:VAL:HG11	2:X:87:LEU:HD12	2.01	0.42
1:e:149:ARG:NH1	1:e:245:ASP:OD1	2.52	0.42
1:Q:149:ARG:NH2	1:Q:245:ASP:OD1	2.52	0.42
1:a:179:PHE:CD2	1:a:179:PHE:C	2.97	0.42
2:N:38:TRP:CZ3	2:N:82:LEU:HB2	2.54	0.42
1:c:97:THR:O	1:c:121:ARG:NH1	2.44	0.42
2:F:53:ILE:HG13	2:F:59:THR:HG22	2.01	0.42
2:N:10:GLY:O	2:N:20:LEU:HD22	2.20	0.42
1:Q:165:PHE:CD2	1:Q:214:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:61:TYR:CE1	2:b:71:ILE:HG22	2.55	0.42
1:c:179:PHE:HB2	1:c:188:MET:HE2	2.01	0.42
1:A:178:ARG:NH1	1:A:191:ARG:HH21	2.18	0.41
1:Q:149:ARG:HG2	1:Q:241:MET:HE2	2.02	0.41
2:d:74:ASP:OD2	2:d:77:LYS:N	2.53	0.41
1:O:156:SER:HG	1:O:236:HIS:H	1.68	0.41
1:A:287:LYS:NZ	3:A:503:HOH:O	2.53	0.41
1:Q:75:HIS:HA	1:Q:89:LEU:O	2.21	0.41
1:Q:151:PHE:HB2	1:Q:168:VAL:HG23	2.01	0.41
1:S:45:ASN:OD1	1:S:46:PHE:N	2.48	0.41
1:Y:79:SER:HB3	1:Y:87:TYR:CZ	2.56	0.41
2:J:84:MET:HB3	2:J:87:LEU:HD21	2.01	0.41
1:O:224:LEU:HD13	1:O:261:TYR:CD1	2.56	0.41
2:T:35:THR:OG1	2:T:100:LEU:HB2	2.20	0.41
1:U:311:LEU:HD22	1:U:315:LEU:HD11	2.02	0.41
1:a:276:TRP:HB2	1:a:287:LYS:HG3	2.03	0.41
1:e:356:ILE:HG12	1:e:358:LEU:CD2	2.50	0.41
2:B:86:SER:H	2:F:85:ASN:ND2	2.19	0.41
1:E:84:TRP:CE2	1:E:260:ALA:HB2	2.55	0.41
1:Q:276:TRP:HZ2	1:Q:295:VAL:HG23	1.85	0.41
2:R:32:SER:O	2:R:33:ILE:HD13	2.21	0.41
2:T:69:PHE:CE2	2:T:84:MET:HE3	2.55	0.41
1:C:325:THR:HG21	1:C:408:GLY:HA2	2.01	0.41
2:L:14:VAL:HG11	2:L:87:LEU:HD13	2.02	0.41
2:R:38:TRP:CZ3	2:R:82:LEU:HB2	2.56	0.41
1:W:45:ASN:OD1	1:W:46:PHE:N	2.47	0.41
1:W:165:PHE:HE2	1:W:210:VAL:HG12	1.85	0.41
1:W:84:TRP:NE1	1:W:265:ASP:OD1	2.48	0.41
1:E:297:GLU:CD	1:E:297:GLU:N	2.78	0.41
1:S:78:LEU:HD11	1:S:86:PHE:HB3	2.03	0.41
2:X:69:PHE:CE1	2:X:84:MET:HB3	2.56	0.41
2:D:53:ILE:HA	2:D:58:SER:O	2.21	0.40
1:W:317:ASN:OD1	1:W:317:ASN:N	2.54	0.40
1:W:332:MET:HE3	1:W:332:MET:HB3	1.96	0.40
1:a:105:ARG:HG3	1:a:116:ILE:HG12	2.03	0.40
1:Q:221:LEU:CD2	1:Q:238:VAL:HG13	2.51	0.40
1:S:157:ARG:NH2	1:S:162:GLU:O	2.53	0.40
1:e:84:TRP:NE1	1:e:265:ASP:OD1	2.48	0.40
1:E:251:ARG:HG3	1:E:251:ARG:NH1	2.36	0.40
1:E:321:THR:O	1:E:324:ARG:HG2	2.22	0.40
1:U:67:GLY:N	2:V:104:ASN:OD1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:207:THR:HA	1:U:210:VAL:HG12	2.03	0.40
1:Y:157:ARG:NH2	1:Y:162:GLU:O	2.49	0.40
1:c:149:ARG:HG3	1:c:149:ARG:HH11	1.86	0.40
1:W:354:ALA:O	1:W:356:ILE:HG22	2.21	0.40
1:Y:84:TRP:CE2	1:Y:260:ALA:HB2	2.57	0.40
1:G:84:TRP:NE1	1:G:265:ASP:OD1	2.46	0.40
1:W:376:THR:OG1	1:W:386:LYS:HD2	2.22	0.40
1:Y:67:GLY:N	2:Z:104:ASN:OD1	2.43	0.40
1:a:61:VAL:HG22	1:a:106:VAL:HG22	2.04	0.40
1:a:345:ARG:CB	1:a:347:TRP:HZ3	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	258/347 (74%)	257 (100%)	1 (0%)	84	93
1	C	263/347 (76%)	261 (99%)	2 (1%)	73	88
1	E	269/347 (78%)	268 (100%)	1 (0%)	84	93
1	G	263/347 (76%)	262 (100%)	1 (0%)	84	93
1	I	263/347 (76%)	263 (100%)	0	100	100
1	K	263/347 (76%)	261 (99%)	2 (1%)	73	88
1	M	253/347 (73%)	252 (100%)	1 (0%)	84	93
1	O	261/347 (75%)	260 (100%)	1 (0%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	254/347 (73%)	252 (99%)	2 (1%)	73	88
1	S	245/347 (71%)	244 (100%)	1 (0%)	84	93
1	U	224/347 (65%)	221 (99%)	3 (1%)	61	83
1	W	248/347 (72%)	246 (99%)	2 (1%)	73	88
1	Y	251/347 (72%)	250 (100%)	1 (0%)	84	93
1	a	244/347 (70%)	244 (100%)	0	100	100
1	c	231/347 (67%)	231 (100%)	0	100	100
1	e	248/347 (72%)	245 (99%)	3 (1%)	63	84
2	B	90/97 (93%)	90 (100%)	0	100	100
2	D	87/97 (90%)	86 (99%)	1 (1%)	65	85
2	F	87/97 (90%)	87 (100%)	0	100	100
2	H	89/97 (92%)	89 (100%)	0	100	100
2	J	88/97 (91%)	88 (100%)	0	100	100
2	L	89/97 (92%)	89 (100%)	0	100	100
2	N	89/97 (92%)	89 (100%)	0	100	100
2	P	90/97 (93%)	89 (99%)	1 (1%)	65	85
2	R	87/97 (90%)	86 (99%)	1 (1%)	65	85
2	T	90/97 (93%)	90 (100%)	0	100	100
2	V	87/97 (90%)	87 (100%)	0	100	100
2	X	88/97 (91%)	87 (99%)	1 (1%)	65	85
2	Z	88/97 (91%)	87 (99%)	1 (1%)	65	85
2	b	89/97 (92%)	88 (99%)	1 (1%)	65	85
2	d	88/97 (91%)	86 (98%)	2 (2%)	44	73
2	f	88/97 (91%)	88 (100%)	0	100	100
All	All	5452/7104 (77%)	5423 (100%)	29 (0%)	81	92

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	C	248	SER
1	C	414	THR
2	D	23	SER
1	E	402	CYS

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Mol	Chain	Res	Type
1	G	402	CYS
1	K	112	SER
1	K	154	SER
1	M	402	CYS
1	O	414	THR
2	P	23	SER
1	Q	51	VAL
1	Q	321	THR
2	R	86	SER
1	S	401	THR
1	U	156	SER
1	U	175	GLN
1	U	248	SER
1	W	85	SER
1	W	89	LEU
2	X	58	SER
1	Y	154	SER
2	Z	64	SER
2	b	35	THR
2	d	23	SER
2	d	59	THR
1	e	112	SER
1	e	154	SER
1	e	402	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
2	B	15	GLN
2	B	75	ASN
2	B	113	GLN
1	C	37	HIS
1	E	37	HIS
1	E	41	ASN
1	E	197	GLN
1	E	403	HIS
2	F	78	ASN
1	G	37	HIS
1	I	37	HIS
2	J	85	ASN
2	J	113	GLN

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Mol	Chain	Res	Type
1	K	37	HIS
2	L	83	GLN
1	M	37	HIS
2	N	113	GLN
1	O	37	HIS
1	Q	37	HIS
1	Q	230	GLN
1	Q	294	HIS
2	R	113	GLN
1	S	406	HIS
1	U	48	ASN
1	W	37	HIS
1	W	113	GLN
2	X	85	ASN
2	X	113	GLN
1	Y	37	HIS
1	Y	41	ASN
1	Y	323	GLN
1	a	288	HIS
1	a	406	HIS
2	b	113	GLN
1	c	37	HIS
1	e	37	HIS
1	e	113	GLN
1	e	258	GLN
2	f	83	GLN
2	f	110	GLN

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

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	369/423 (87%)	0.87	60 (16%) 4 4	38, 64, 128, 165	0
1	C	360/423 (85%)	0.59	41 (11%) 10 8	34, 57, 120, 151	0
1	E	364/423 (86%)	0.56	38 (10%) 11 10	37, 58, 109, 147	0
1	G	371/423 (87%)	0.72	48 (12%) 7 6	32, 61, 112, 145	0
1	I	366/423 (86%)	0.51	42 (11%) 9 8	37, 57, 114, 165	0
1	K	372/423 (87%)	0.65	44 (11%) 9 7	31, 60, 114, 146	0
1	M	347/423 (82%)	0.72	44 (12%) 8 7	36, 58, 112, 137	0
1	O	363/423 (85%)	0.54	41 (11%) 10 8	37, 56, 117, 170	0
1	Q	371/423 (87%)	1.52	90 (24%) 2 1	58, 87, 131, 157	0
1	S	340/423 (80%)	1.51	95 (27%) 1 1	60, 86, 130, 155	0
1	U	343/423 (81%)	1.72	107 (31%) 1 1	57, 90, 137, 172	0
1	W	341/423 (80%)	1.43	80 (23%) 2 1	57, 82, 125, 171	0
1	Y	370/423 (87%)	1.37	89 (24%) 2 1	54, 81, 125, 165	0
1	a	352/423 (83%)	1.38	83 (23%) 2 1	55, 82, 130, 154	0
1	c	345/423 (81%)	1.60	94 (27%) 1 1	53, 85, 134, 170	0
1	e	340/423 (80%)	1.24	62 (18%) 3 3	52, 78, 120, 147	0
2	B	115/116 (99%)	0.13	6 (5%) 33 29	33, 47, 91, 123	0
2	D	115/116 (99%)	0.23	9 (7%) 19 16	33, 49, 99, 122	0
2	F	115/116 (99%)	0.21	10 (8%) 16 13	33, 50, 93, 143	0
2	H	115/116 (99%)	0.14	3 (2%) 57 54	36, 48, 93, 135	0
2	J	115/116 (99%)	0.24	10 (8%) 16 13	35, 48, 89, 134	0
2	L	115/116 (99%)	0.15	6 (5%) 33 29	34, 47, 94, 126	0
2	N	115/116 (99%)	0.17	8 (6%) 22 19	32, 46, 94, 111	0
2	P	115/116 (99%)	0.20	9 (7%) 19 16	31, 48, 96, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	R	115/116 (99%)	1.26	21 (18%) 3 3	59, 78, 126, 171	0
2	T	115/116 (99%)	1.14	15 (13%) 7 6	56, 71, 103, 149	0
2	V	115/116 (99%)	1.20	16 (13%) 6 5	52, 70, 109, 144	0
2	X	115/116 (99%)	1.29	21 (18%) 3 3	57, 80, 129, 176	0
2	Z	115/116 (99%)	1.24	16 (13%) 6 5	55, 73, 121, 208	0
2	b	115/116 (99%)	0.95	11 (9%) 13 11	52, 66, 107, 139	0
2	d	115/116 (99%)	1.02	16 (13%) 6 5	49, 66, 109, 156	0
2	f	115/116 (99%)	1.15	19 (16%) 4 4	55, 74, 119, 166	0
All	All	7554/8624 (87%)	0.96	1254 (16%) 4 4	31, 72, 123, 208	0

All (1254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	143	SER	11.1
1	M	143	SER	9.5
1	U	347	TRP	9.3
1	Y	143	SER	9.1
1	C	143	SER	8.7
1	W	334	HIS	8.3
1	A	143	SER	8.3
1	O	371	THR	8.0
1	G	143	SER	7.9
1	S	25	ILE	7.8
2	Z	30	ILE	7.8
1	K	143	SER	7.7
1	Q	143	SER	7.7
1	e	143	SER	7.7
1	M	25	ILE	7.7
1	Y	339	ASP	7.6
1	e	334	HIS	7.5
1	c	347	TRP	7.5
2	R	31	PHE	7.5
1	C	363	ASP	7.5
1	S	144	GLY	7.4
2	T	31	PHE	7.4
2	d	75	ASN	7.3
1	A	340	HIS	7.2
1	I	143	SER	7.2
1	e	25	ILE	7.1

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Mol	Chain	Res	Type	RSRZ
2	R	29	SER	7.1
1	c	25	ILE	7.1
1	U	332	MET	7.1
1	U	376	THR	7.1
1	a	25	ILE	7.0
1	M	361	GLN	6.9
1	O	367	GLN	6.9
1	E	363	ASP	6.8
1	c	143	SER	6.7
2	f	76	THR	6.7
1	c	413	LEU	6.7
1	E	122	ASP	6.6
1	a	417	TRP	6.6
1	U	413	LEU	6.6
1	a	360	TRP	6.6
1	C	370	ASP	6.6
1	A	417	TRP	6.5
1	c	361	GLN	6.5
1	c	332	MET	6.5
1	U	412	PRO	6.5
1	U	346	CYS	6.5
1	M	347	TRP	6.5
1	e	41	ASN	6.5
2	V	75	ASN	6.4
1	a	401	THR	6.4
1	I	366	ASP	6.4
2	F	75	ASN	6.3
1	I	339	ASP	6.3
1	G	366	ASP	6.3
1	G	394	SER	6.2
1	G	122	ASP	6.2
1	W	25	ILE	6.2
2	Z	31	PHE	6.2
1	E	334	HIS	6.2
2	J	75	ASN	6.1
1	S	333	THR	6.1
2	D	29	SER	6.1
1	Y	417	TRP	6.0
1	c	412	PRO	6.0
1	a	143	SER	6.0
1	Y	363	ASP	6.0
1	U	25	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	Q	335	HIS	5.9
1	I	365	GLU	5.9
1	c	281	MET	5.9
1	I	122	ASP	5.9
1	K	122	ASP	5.9
1	E	143	SER	5.8
1	M	417	TRP	5.8
2	Z	3	GLU	5.8
2	f	3	GLU	5.8
1	c	404	VAL	5.8
2	P	3	GLU	5.8
1	O	400	TYR	5.8
1	c	122	ASP	5.7
2	R	30	ILE	5.7
1	G	363	ASP	5.7
1	a	339	ASP	5.7
1	Y	281	MET	5.7
2	H	75	ASN	5.6
1	Y	340	HIS	5.6
2	b	75	ASN	5.6
1	a	41	ASN	5.6
1	c	376	THR	5.6
1	e	122	ASP	5.6
1	S	44	SER	5.6
1	U	143	SER	5.6
1	c	346	CYS	5.5
2	d	10	GLY	5.5
1	M	343	THR	5.5
1	Q	25	ILE	5.4
2	H	29	SER	5.4
1	K	339	ASP	5.4
1	M	122	ASP	5.4
1	Q	400	TYR	5.4
1	a	371	THR	5.4
1	I	25	ILE	5.4
1	K	366	ASP	5.3
1	K	417	TRP	5.3
2	X	75	ASN	5.3
2	b	7	VAL	5.3
1	E	142	GLY	5.3
1	G	417	TRP	5.3
1	W	41	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
2	Z	4	VAL	5.3
1	c	144	GLY	5.2
1	E	417	TRP	5.2
1	Q	363	ASP	5.2
2	V	3	GLU	5.2
1	I	334	HIS	5.2
2	X	29	SER	5.2
1	U	403	HIS	5.2
1	A	363	ASP	5.2
1	c	390	VAL	5.2
1	E	398	GLN	5.1
2	R	3	GLU	5.1
1	U	281	MET	5.1
1	e	415	LEU	5.1
1	O	412	PRO	5.1
1	U	331	HIS	5.1
1	Y	25	ILE	5.1
1	c	407	GLU	5.1
1	O	394	SER	5.0
2	J	29	SER	5.0
1	E	392	VAL	5.0
1	U	328	PRO	5.0
1	a	278	ALA	5.0
1	M	371	THR	5.0
2	D	75	ASN	5.0
2	N	31	PHE	5.0
2	Z	29	SER	4.9
1	A	122	ASP	4.9
1	Q	366	ASP	4.9
1	M	401	THR	4.9
1	M	331	HIS	4.9
2	F	29	SER	4.9
1	A	366	ASP	4.9
1	W	95	THR	4.9
1	c	417	TRP	4.9
1	c	328	PRO	4.9
1	Q	339	ASP	4.9
1	W	401	THR	4.9
1	U	387	TRP	4.9
1	W	328	PRO	4.9
1	A	367	GLN	4.9
1	W	281	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	S	95	THR	4.9
1	W	407	GLU	4.9
2	D	3	GLU	4.9
1	W	144	GLY	4.9
1	A	369	GLN	4.8
1	Q	413	LEU	4.8
1	A	370	ASP	4.8
1	U	122	ASP	4.8
1	K	25	ILE	4.8
1	a	95	THR	4.8
1	c	387	TRP	4.8
1	e	328	PRO	4.8
1	E	365	GLU	4.8
1	S	41	ASN	4.8
2	Z	75	ASN	4.8
1	E	412	PRO	4.8
1	S	415	LEU	4.8
1	U	259	TYR	4.8
1	W	259	TYR	4.8
1	A	347	TRP	4.8
1	e	222	GLY	4.7
2	R	75	ASN	4.7
1	Q	281	MET	4.7
1	S	123	MET	4.7
1	U	405	GLN	4.7
1	E	371	THR	4.6
1	C	122	ASP	4.6
1	M	281	MET	4.6
1	U	279	ALA	4.6
1	S	357	THR	4.6
1	K	394	SER	4.6
1	S	390	VAL	4.6
1	a	281	MET	4.6
2	D	76	THR	4.6
1	G	339	ASP	4.6
1	I	363	ASP	4.6
1	K	370	ASP	4.6
1	Y	370	ASP	4.6
1	c	120	ASP	4.6
1	A	331	HIS	4.6
1	O	334	HIS	4.6
1	U	144	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	c	264	LYS	4.6
2	P	76	THR	4.6
1	G	367	GLN	4.6
1	Q	369	GLN	4.6
1	Q	279	ALA	4.5
1	Q	360	TRP	4.5
1	U	406	HIS	4.5
1	e	401	THR	4.5
2	X	76	THR	4.5
1	A	412	PRO	4.5
2	J	31	PHE	4.5
1	A	25	ILE	4.5
1	G	25	ILE	4.5
1	C	333	THR	4.5
1	e	44	SER	4.5
1	M	334	HIS	4.5
1	U	417	TRP	4.5
1	c	359	THR	4.5
1	Y	394	SER	4.5
1	W	405	GLN	4.5
1	A	392	VAL	4.5
1	c	374	VAL	4.5
1	a	232	GLU	4.5
1	c	406	HIS	4.4
1	c	360	TRP	4.4
1	A	404	VAL	4.4
1	C	391	VAL	4.4
1	c	331	HIS	4.4
1	E	25	ILE	4.4
1	A	394	SER	4.4
1	e	229	ASN	4.4
1	G	362	ARG	4.4
1	U	330	THR	4.4
1	c	329	LYS	4.4
1	Q	98	GLU	4.4
1	Q	394	SER	4.4
2	P	75	ASN	4.4
1	M	413	LEU	4.4
1	a	120	ASP	4.3
1	Q	342	ALA	4.3
1	Y	369	GLN	4.3
2	X	3	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	Q	340	HIS	4.3
1	A	399	ARG	4.3
1	e	407	GLU	4.3
1	Y	413	LEU	4.3
1	a	122	ASP	4.3
1	O	365	GLU	4.3
1	A	360	TRP	4.3
1	G	281	MET	4.3
1	E	367	GLN	4.3
1	G	396	GLN	4.3
1	O	25	ILE	4.3
1	Q	371	THR	4.3
1	M	404	VAL	4.3
1	Q	370	ASP	4.2
1	Q	259	TYR	4.2
1	O	122	ASP	4.2
1	U	41	ASN	4.2
2	N	75	ASN	4.2
1	U	350	SER	4.2
1	W	359	THR	4.2
1	c	411	LYS	4.2
1	K	342	ALA	4.2
1	c	402	CYS	4.2
2	T	75	ASN	4.2
1	I	394	SER	4.2
1	a	407	GLU	4.2
1	e	414	THR	4.2
1	U	160	ARG	4.2
1	I	400	TYR	4.2
2	F	30	ILE	4.2
1	E	370	ASP	4.1
1	W	44	SER	4.1
1	M	415	LEU	4.1
1	W	122	ASP	4.1
1	C	396	GLN	4.1
1	e	387	TRP	4.1
1	c	324	ARG	4.1
1	O	143	SER	4.1
1	c	172	ASP	4.1
1	C	416	ARG	4.1
1	A	374	VAL	4.1
1	O	391	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	U	386	LYS	4.0
1	e	281	MET	4.0
2	d	30	ILE	4.0
1	Q	373	LEU	4.0
1	a	329	LYS	4.0
1	W	222	GLY	4.0
1	Y	400	TYR	4.0
1	Y	366	ASP	4.0
1	a	335	HIS	4.0
2	d	4	VAL	4.0
1	G	371	THR	4.0
1	U	329	LYS	4.0
1	c	330	THR	4.0
1	M	332	MET	4.0
1	A	397	GLU	4.0
1	C	341	GLU	4.0
1	a	336	ALA	4.0
1	A	413	LEU	4.0
1	M	390	VAL	4.0
1	W	325	THR	4.0
1	S	405	GLN	4.0
1	Y	197	GLN	4.0
1	S	160	ARG	3.9
2	V	4	VAL	3.9
1	a	328	PRO	3.9
1	G	399	ARG	3.9
1	U	334	HIS	3.9
1	c	415	LEU	3.9
1	C	400	TYR	3.9
1	K	363	ASP	3.9
1	S	120	ASP	3.9
2	T	7	VAL	3.9
2	f	75	ASN	3.9
2	b	3	GLU	3.9
1	A	334	HIS	3.9
1	I	292	ALA	3.9
1	a	273	LEU	3.9
1	G	370	ASP	3.9
1	Q	417	TRP	3.9
1	C	371	THR	3.9
1	E	368	THR	3.9
1	U	343	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	U	407	GLU	3.9
2	J	3	GLU	3.9
1	U	409	LEU	3.9
2	b	76	THR	3.8
2	T	3	GLU	3.8
1	S	344	LEU	3.8
1	a	349	LEU	3.8
1	e	358	LEU	3.8
1	K	399	ARG	3.8
1	c	272	ASP	3.8
1	a	340	HIS	3.8
2	T	6	LEU	3.8
1	O	342	ALA	3.8
1	G	400	TYR	3.8
1	U	197	GLN	3.8
1	Q	44	SER	3.8
2	J	30	ILE	3.8
1	A	362	ARG	3.8
1	W	33	VAL	3.8
1	a	160	ARG	3.8
1	O	366	ASP	3.8
2	R	78	ASN	3.8
1	c	221	LEU	3.8
1	c	403	HIS	3.8
1	Y	42	GLY	3.8
2	R	11	GLY	3.8
1	M	272	ASP	3.7
1	U	297	GLU	3.7
1	U	400	TYR	3.7
1	C	394	SER	3.7
2	B	31	PHE	3.7
1	M	407	GLU	3.7
1	U	323	GLN	3.7
1	O	363	ASP	3.7
1	G	413	LEU	3.7
1	Y	360	TRP	3.7
1	A	342	ALA	3.7
2	f	77	LYS	3.7
1	E	366	ASP	3.7
1	S	122	ASP	3.7
2	L	31	PHE	3.7
1	C	412	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	285	THR	3.7
1	U	277	THR	3.7
1	A	387	TRP	3.7
1	Q	362	ARG	3.7
2	R	32	SER	3.7
1	S	33	VAL	3.7
1	S	281	MET	3.7
1	K	367	GLN	3.7
1	O	361	GLN	3.7
1	U	221	LEU	3.6
1	U	273	LEU	3.6
1	U	286	THR	3.6
1	W	285	THR	3.6
1	Y	347	TRP	3.6
1	U	278	ALA	3.6
1	U	348	ALA	3.6
1	c	279	ALA	3.6
1	e	259	TYR	3.6
1	a	200	PRO	3.6
1	Q	398	GLN	3.6
2	f	87	LEU	3.6
1	S	401	THR	3.6
1	W	199	GLY	3.6
1	a	259	TYR	3.6
1	U	402	CYS	3.6
1	Q	391	VAL	3.6
1	S	73	VAL	3.6
1	S	232	GLU	3.6
1	U	374	VAL	3.6
2	N	3	GLU	3.6
1	Q	409	LEU	3.6
1	S	273	LEU	3.6
1	K	371	THR	3.6
1	K	272	ASP	3.6
1	a	389	ALA	3.6
1	W	351	PHE	3.6
1	A	391	VAL	3.6
1	U	404	VAL	3.6
1	Y	396	GLN	3.6
1	U	43	LYS	3.6
1	W	288	HIS	3.6
1	G	368	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	S	278	ALA	3.6
1	Q	367	GLN	3.6
1	K	413	LEU	3.6
1	M	346	CYS	3.6
2	b	117	SER	3.6
2	V	30	ILE	3.5
1	M	414	THR	3.5
1	Y	371	THR	3.5
1	I	412	PRO	3.5
1	a	73	VAL	3.5
2	J	7	VAL	3.5
2	X	7	VAL	3.5
2	X	77	LYS	3.5
1	W	257	HIS	3.5
2	F	117	SER	3.5
2	X	117	SER	3.5
1	U	327	ALA	3.5
1	Y	387	TRP	3.5
2	V	45	LYS	3.5
2	H	31	PHE	3.5
1	C	415	LEU	3.5
1	e	288	HIS	3.5
2	D	30	ILE	3.5
1	E	281	MET	3.5
1	E	341	GLU	3.5
1	A	405	GLN	3.5
1	S	219	VAL	3.5
1	U	246	VAL	3.5
1	c	350	SER	3.5
2	f	30	ILE	3.5
1	W	357	THR	3.5
1	Q	293	ALA	3.5
1	M	412	PRO	3.5
1	S	328	PRO	3.5
1	Q	278	ALA	3.4
2	L	75	ASN	3.4
1	W	412	PRO	3.4
1	c	358	LEU	3.4
2	F	31	PHE	3.4
1	M	160	ARG	3.4
1	U	266	TYR	3.4
1	S	407	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	369	GLN	3.4
1	Y	33	VAL	3.4
2	f	7	VAL	3.4
1	Q	387	TRP	3.4
1	G	259	TYR	3.4
2	d	117	SER	3.4
2	f	117	SER	3.4
1	e	357	THR	3.4
1	G	342	ALA	3.4
1	O	373	LEU	3.4
1	G	392	VAL	3.4
1	Q	219	VAL	3.4
1	W	223	THR	3.4
1	c	401	THR	3.4
1	K	412	PRO	3.4
1	M	232	GLU	3.4
1	a	93	GLU	3.4
1	c	297	GLU	3.4
1	W	389	ALA	3.4
1	S	288	HIS	3.4
1	Q	272	ASP	3.4
1	a	338	SER	3.3
2	Z	32	SER	3.3
1	A	160	ARG	3.3
1	e	412	PRO	3.3
1	G	279	ALA	3.3
1	O	144	GLY	3.3
1	Q	374	VAL	3.3
2	d	31	PHE	3.3
1	S	325	THR	3.3
1	c	232	GLU	3.3
1	c	388	ALA	3.3
2	f	67	GLY	3.3
1	I	41	ASN	3.3
1	a	326	ASP	3.3
2	B	30	ILE	3.3
1	c	373	LEU	3.3
1	c	334	HIS	3.3
2	d	44	GLY	3.3
1	K	279	ALA	3.3
1	I	417	TRP	3.3
1	W	415	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	Y	71	GLU	3.3
2	N	76	THR	3.3
1	G	398	GLN	3.3
1	S	259	TYR	3.3
1	U	380	GLY	3.3
1	U	411	LYS	3.3
1	E	292	ALA	3.3
1	c	41	ASN	3.3
1	U	324	ARG	3.2
1	A	368	THR	3.2
1	C	343	THR	3.2
1	S	332	MET	3.2
1	a	412	PRO	3.2
2	V	90	GLU	3.2
1	Y	398	GLN	3.2
1	O	390	VAL	3.2
1	U	33	VAL	3.2
1	O	320	GLU	3.2
1	a	372	GLU	3.2
1	e	413	LEU	3.2
1	S	285	THR	3.2
1	Y	334	HIS	3.2
1	A	395	GLY	3.2
1	W	350	SER	3.2
1	U	293	ALA	3.2
1	O	413	LEU	3.2
1	W	413	LEU	3.2
1	c	160	ARG	3.2
1	C	123	MET	3.2
1	C	292	ALA	3.2
2	X	19	SER	3.2
2	X	30	ILE	3.2
2	D	7	VAL	3.2
1	Y	399	ARG	3.1
1	a	162	GLU	3.1
1	Q	393	PRO	3.1
1	W	331	HIS	3.1
2	Z	76	THR	3.1
1	W	387	TRP	3.1
1	S	292	ALA	3.1
1	G	337	VAL	3.1
1	I	391	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	Q	33	VAL	3.1
1	S	93	GLU	3.1
1	C	398	GLN	3.1
1	U	371	THR	3.1
1	a	414	THR	3.1
1	S	222	GLY	3.1
1	C	360	TRP	3.1
1	G	347	TRP	3.1
1	W	292	ALA	3.1
1	Y	44	SER	3.1
1	Y	145	SER	3.1
2	X	116	VAL	3.1
1	e	416	ARG	3.1
1	A	407	GLU	3.1
1	M	330	THR	3.1
2	R	10	GLY	3.1
2	R	12	GLY	3.1
1	A	346	CYS	3.1
1	E	389	ALA	3.1
1	U	292	ALA	3.1
1	U	296	ALA	3.1
1	Q	160	ARG	3.1
1	U	149	ARG	3.1
2	F	7	VAL	3.1
1	Q	123	MET	3.1
1	e	123	MET	3.1
2	Z	23	SER	3.1
1	A	365	GLU	3.1
1	a	341	GLU	3.1
1	M	405	GLN	3.1
1	K	347	TRP	3.1
1	c	123	MET	3.1
1	S	355	GLU	3.0
1	Y	98	GLU	3.0
1	Y	232	GLU	3.0
1	U	29	PRO	3.0
1	S	284	GLN	3.0
1	O	343	THR	3.0
1	S	408	GLY	3.0
1	U	28	THR	3.0
2	J	77	LYS	3.0
2	P	77	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	281	MET	3.0
1	K	362	ARG	3.0
1	U	240	ARG	3.0
1	e	389	ALA	3.0
1	M	387	TRP	3.0
1	Q	404	VAL	3.0
1	W	358	LEU	3.0
2	d	3	GLU	3.0
2	f	78	ASN	3.0
1	a	410	PRO	3.0
1	S	82	LYS	3.0
1	I	371	THR	3.0
1	Q	399	ARG	3.0
1	e	325	THR	3.0
1	c	348	ALA	3.0
1	a	288	HIS	3.0
2	F	3	GLU	3.0
1	A	400	TYR	3.0
1	A	272	ASP	3.0
1	c	405	GLN	3.0
1	W	123	MET	3.0
1	Y	368	THR	3.0
2	d	76	THR	3.0
1	S	233	ALA	3.0
1	e	219	VAL	3.0
2	f	31	PHE	3.0
1	c	409	LEU	3.0
1	M	403	HIS	3.0
2	D	27	SER	3.0
1	a	149	ARG	3.0
1	e	160	ARG	3.0
1	A	343	THR	3.0
1	C	401	THR	3.0
1	a	285	THR	3.0
1	K	293	ALA	3.0
1	U	354	ALA	3.0
1	c	278	ALA	3.0
1	Y	171	VAL	3.0
2	X	87	LEU	2.9
2	f	19	SER	2.9
1	E	369	GLN	2.9
2	N	30	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	333	THR	2.9
1	U	333	THR	2.9
1	S	320	GLU	2.9
1	U	264	LYS	2.9
1	A	123	MET	2.9
1	a	332	MET	2.9
1	U	265	ASP	2.9
1	W	256	TYR	2.9
1	c	216	THR	2.9
1	I	342	ALA	2.9
1	I	389	ALA	2.9
1	S	106	VAL	2.9
1	Y	391	VAL	2.9
1	a	219	VAL	2.9
1	e	73	VAL	2.9
1	Y	409	LEU	2.9
1	c	269	LEU	2.9
1	G	397	GLU	2.9
1	Q	396	GLN	2.9
1	c	416	ARG	2.9
1	A	259	TYR	2.9
1	G	120	ASP	2.9
1	Y	259	TYR	2.9
1	W	330	THR	2.9
1	a	357	THR	2.9
1	S	351	PHE	2.9
1	U	257	HIS	2.9
1	K	396	GLN	2.9
1	e	332	MET	2.9
2	d	29	SER	2.9
1	E	144	GLY	2.9
1	K	259	TYR	2.9
2	V	11	GLY	2.9
1	c	162	GLU	2.8
1	e	93	GLU	2.8
2	L	3	GLU	2.8
1	Y	405	GLN	2.8
1	e	267	ILE	2.8
2	b	30	ILE	2.8
2	N	44	GLY	2.8
1	A	371	THR	2.8
1	a	292	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	a	358	LEU	2.8
1	G	340	HIS	2.8
1	Q	162	GLU	2.8
1	G	369	GLN	2.8
1	Q	235	SER	2.8
2	d	32	SER	2.8
1	M	289	LYS	2.8
2	V	10	GLY	2.8
1	C	359	THR	2.8
1	Q	233	ALA	2.8
1	Q	343	THR	2.8
1	Y	233	ALA	2.8
1	K	340	HIS	2.8
1	W	73	VAL	2.8
1	Y	375	GLU	2.8
1	O	123	MET	2.8
1	C	25	ILE	2.8
1	U	119	TRP	2.8
2	N	77	LYS	2.8
2	V	117	SER	2.8
2	f	29	SER	2.8
1	Q	122	ASP	2.8
1	C	389	ALA	2.8
1	E	285	THR	2.8
1	c	343	THR	2.8
1	e	285	THR	2.8
1	K	397	GLU	2.8
1	S	34	TYR	2.8
1	a	404	VAL	2.8
1	S	412	PRO	2.8
1	a	377	ARG	2.8
1	I	398	GLN	2.8
1	c	197	GLN	2.8
1	Q	276	TRP	2.8
1	U	229	ASN	2.8
1	A	358	LEU	2.8
1	S	373	LEU	2.8
1	S	409	LEU	2.8
1	W	326	ASP	2.8
1	A	281	MET	2.8
1	O	333	THR	2.8
1	U	390	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	Y	414	THR	2.8
1	e	351	PHE	2.8
1	c	259	TYR	2.8
1	A	398	GLN	2.7
1	I	396	GLN	2.7
1	Q	197	GLN	2.7
1	C	44	SER	2.7
1	a	221	LEU	2.7
1	a	144	GLY	2.7
1	E	372	GLU	2.7
1	Q	232	GLU	2.7
1	Q	271	GLU	2.7
1	Q	359	THR	2.7
1	E	362	ARG	2.7
1	E	391	VAL	2.7
1	O	120	ASP	2.7
1	Y	374	VAL	2.7
2	R	4	VAL	2.7
1	Y	282	CYS	2.7
1	U	415	LEU	2.7
2	d	22	LEU	2.7
1	A	332	MET	2.7
1	I	144	GLY	2.7
1	W	112	SER	2.7
1	Y	276	TRP	2.7
1	c	145	SER	2.7
1	S	331	HIS	2.7
1	W	160	ARG	2.7
1	Y	397	GLU	2.7
1	Q	388	ALA	2.7
1	S	389	ALA	2.7
2	P	7	VAL	2.7
1	Q	50	TYR	2.7
1	E	123	MET	2.7
1	I	373	LEU	2.7
1	W	332	MET	2.7
1	C	144	GLY	2.7
1	C	288	HIS	2.7
2	X	9	SER	2.7
1	S	372	GLU	2.7
1	K	392	VAL	2.7
1	W	219	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	374	VAL	2.7
1	U	172	ASP	2.7
1	G	412	PRO	2.7
1	a	72	LYS	2.7
1	e	405	GLN	2.7
1	M	259	TYR	2.7
1	S	346	CYS	2.7
1	M	358	LEU	2.7
1	a	415	LEU	2.7
1	U	313	ARG	2.7
1	C	372	GLU	2.7
1	I	360	TRP	2.7
1	S	317	ASN	2.7
1	e	232	GLU	2.7
1	U	276	TRP	2.7
1	C	374	VAL	2.7
1	C	411	LYS	2.7
1	O	292	ALA	2.7
1	U	171	VAL	2.7
1	a	348	ALA	2.7
1	Q	120	ASP	2.7
1	S	267	ILE	2.6
1	G	332	MET	2.6
1	S	149	ARG	2.6
1	e	320	GLU	2.6
1	C	342	ALA	2.6
1	I	285	THR	2.6
1	I	330	THR	2.6
1	Q	384	PHE	2.6
1	W	404	VAL	2.6
1	a	330	THR	2.6
1	e	410	PRO	2.6
1	E	415	LEU	2.6
1	W	303	LEU	2.6
1	Y	251	ARG	2.6
1	a	346	CYS	2.6
1	e	403	HIS	2.6
1	O	411	LYS	2.6
1	S	329	LYS	2.6
2	R	111	GLY	2.6
2	T	66	LYS	2.6
1	C	390	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	c	147	SER	2.6
2	P	29	SER	2.6
1	O	285	THR	2.6
2	D	77	LYS	2.6
1	c	380	GLY	2.6
2	X	28	GLY	2.6
1	Q	117	VAL	2.6
1	c	292	ALA	2.6
1	e	33	VAL	2.6
2	f	25	ALA	2.6
2	f	43	PRO	2.6
1	W	248	SER	2.6
1	W	333	THR	2.6
1	a	235	SER	2.6
1	c	276	TRP	2.6
2	F	32	SER	2.6
2	J	117	SER	2.6
2	L	29	SER	2.6
2	b	64	SER	2.6
1	Y	332	MET	2.6
1	W	267	ILE	2.6
1	S	47	LEU	2.6
1	W	47	LEU	2.6
1	a	324	ARG	2.6
1	I	288	HIS	2.6
1	Y	341	GLU	2.6
1	U	282	CYS	2.6
1	A	279	ALA	2.6
1	O	392	VAL	2.6
1	O	398	GLN	2.6
1	I	44	SER	2.5
1	U	223	THR	2.5
1	c	267	ILE	2.5
1	S	324	ARG	2.5
1	e	218	ARG	2.5
1	K	400	TYR	2.5
1	Q	171	VAL	2.5
1	U	410	PRO	2.5
1	Y	117	VAL	2.5
1	M	278	ALA	2.5
1	O	405	GLN	2.5
1	Q	183	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	V	31	PHE	2.5
1	Y	123	MET	2.5
1	a	231	SER	2.5
2	P	117	SER	2.5
2	T	117	SER	2.5
1	U	356	ILE	2.5
2	P	30	ILE	2.5
1	S	27	ARG	2.5
1	S	72	LYS	2.5
2	B	77	LYS	2.5
1	U	288	HIS	2.5
1	S	348	ALA	2.5
1	W	278	ALA	2.5
1	a	405	GLN	2.5
1	M	123	MET	2.5
1	I	357	THR	2.5
1	O	414	THR	2.5
2	T	76	THR	2.5
1	S	195	ILE	2.5
1	S	326	ASP	2.5
1	U	27	ARG	2.5
2	f	91	ASP	2.5
1	W	403	HIS	2.5
1	a	334	HIS	2.5
1	Q	71	GLU	2.5
1	S	98	GLU	2.5
1	U	247	GLY	2.5
1	a	222	GLY	2.5
1	c	33	VAL	2.5
1	e	292	ALA	2.5
1	e	333	THR	2.5
2	F	76	THR	2.5
2	F	77	LYS	2.5
2	d	78	ASN	2.5
2	L	30	ILE	2.5
2	X	23	SER	2.5
1	U	120	ASP	2.5
1	U	272	ASP	2.5
1	Y	272	ASP	2.5
1	e	257	HIS	2.5
1	a	159	GLY	2.5
1	Q	29	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	R	89	PRO	2.5
1	S	404	VAL	2.5
1	U	284	GLN	2.5
1	W	284	GLN	2.5
1	Y	392	VAL	2.5
2	b	65	VAL	2.5
2	T	9	SER	2.4
2	X	64	SER	2.4
1	M	406	HIS	2.4
1	Q	347	TRP	2.4
2	V	48	ASP	2.4
1	G	40	GLU	2.4
1	W	40	GLU	2.4
1	W	355	GLU	2.4
1	a	40	GLU	2.4
1	c	247	GLY	2.4
2	V	89	PRO	2.4
1	A	396	GLN	2.4
1	S	99	LYS	2.4
1	e	374	VAL	2.4
1	Q	167	ALA	2.4
1	Q	283	ALA	2.4
1	W	321	THR	2.4
1	W	416	ARG	2.4
2	R	112	THR	2.4
1	M	373	LEU	2.4
1	W	373	LEU	2.4
1	a	409	LEU	2.4
2	T	30	ILE	2.4
2	Z	117	SER	2.4
1	E	360	TRP	2.4
1	K	120	ASP	2.4
1	A	162	GLU	2.4
1	c	355	GLU	2.4
1	K	332	MET	2.4
1	A	410	PRO	2.4
1	S	42	GLY	2.4
1	c	353	PRO	2.4
1	Q	264	LYS	2.4
1	W	319	LYS	2.4
1	C	361	GLN	2.4
1	Y	404	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	33	VAL	2.4
1	Y	152	PHE	2.4
1	O	359	THR	2.4
1	Q	286	THR	2.4
1	a	333	THR	2.4
1	G	338	SER	2.4
1	A	372	GLU	2.4
1	I	341	GLU	2.4
1	M	360	TRP	2.4
1	Q	282	CYS	2.4
1	Q	402	CYS	2.4
1	S	119	TRP	2.4
1	c	282	CYS	2.4
1	Q	247	GLY	2.4
1	a	408	GLY	2.4
2	D	28	GLY	2.4
2	X	67	GLY	2.4
1	a	337	VAL	2.4
1	Q	157	ARG	2.4
1	S	283	ALA	2.4
1	G	373	LEU	2.4
1	W	414	THR	2.4
1	c	116	ILE	2.4
1	e	344	LEU	2.4
1	O	401	THR	2.4
1	U	375	GLU	2.4
1	Y	40	GLU	2.4
2	d	90	GLU	2.4
1	Y	227	CYS	2.4
1	M	328	PRO	2.4
1	Q	144	GLY	2.4
1	K	398	GLN	2.4
1	O	396	GLN	2.4
1	Q	26	GLN	2.4
1	S	197	GLN	2.4
1	I	160	ARG	2.4
1	K	337	VAL	2.4
1	W	324	ARG	2.4
1	U	388	ALA	2.4
1	S	299	LEU	2.3
1	U	111	LEU	2.3
1	c	344	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	V	6	LEU	2.3
1	a	343	THR	2.3
1	c	333	THR	2.3
1	c	357	THR	2.3
1	C	229	ASN	2.3
1	I	281	MET	2.3
1	S	172	ASP	2.3
1	S	350	SER	2.3
1	e	99	LYS	2.3
1	M	282	CYS	2.3
1	W	230	GLN	2.3
2	Z	10	GLY	2.3
1	Y	362	ARG	2.3
1	I	374	VAL	2.3
1	I	390	VAL	2.3
1	A	273	LEU	2.3
1	A	409	LEU	2.3
1	K	292	ALA	2.3
1	W	348	ALA	2.3
1	Q	368	THR	2.3
1	c	217	HIS	2.3
1	I	123	MET	2.3
1	W	231	SER	2.3
2	B	74	ASP	2.3
1	S	298	GLN	2.3
1	Y	199	GLY	2.3
1	e	27	ARG	2.3
1	e	199	GLY	2.3
1	C	392	VAL	2.3
1	M	374	VAL	2.3
1	A	348	ALA	2.3
1	E	233	ALA	2.3
1	O	389	ALA	2.3
1	a	279	ALA	2.3
1	e	47	LEU	2.3
2	R	6	LEU	2.3
1	S	321	THR	2.3
1	a	266	TYR	2.3
1	c	286	THR	2.3
1	C	40	GLU	2.3
1	W	232	GLU	2.3
1	Y	297	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	c	43	LYS	2.3
2	d	8	GLU	2.3
1	G	76	SER	2.3
1	S	235	SER	2.3
2	f	64	SER	2.3
1	Q	328	PRO	2.3
1	W	410	PRO	2.3
1	K	276	TRP	2.3
1	I	395	GLY	2.3
1	W	197	GLN	2.3
2	R	44	GLY	2.3
1	Y	308	VAL	2.3
1	Y	322	LEU	2.3
1	c	273	LEU	2.3
1	G	278	ALA	2.3
1	Y	294	HIS	2.3
1	I	320	GLU	2.3
1	c	98	GLU	2.3
1	K	160	ARG	2.3
2	R	9	SER	2.3
1	A	234	GLY	2.3
1	c	119	TRP	2.3
1	A	373	LEU	2.3
1	S	117	VAL	2.3
1	S	221	LEU	2.3
1	S	253	LEU	2.3
1	c	171	VAL	2.3
1	Q	176	PHE	2.3
1	c	212	ALA	2.2
1	Q	294	HIS	2.2
1	S	406	HIS	2.2
1	W	386	LYS	2.2
1	Q	330	THR	2.2
1	Y	321	THR	2.2
1	Q	397	GLU	2.2
1	Y	365	GLU	2.2
1	C	149	ARG	2.2
2	b	21	ARG	2.2
2	X	43	PRO	2.2
1	E	120	ASP	2.2
1	S	249	ASP	2.2
1	W	258	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	57	SER	2.2
1	Y	367	GLN	2.2
1	a	248	SER	2.2
2	T	32	SER	2.2
1	G	387	TRP	2.2
1	Y	119	TRP	2.2
1	e	373	LEU	2.2
1	K	278	ALA	2.2
1	Y	264	LYS	2.2
1	Y	293	ALA	2.2
1	c	354	ALA	2.2
2	Z	33	ILE	2.2
1	O	332	MET	2.2
1	S	359	THR	2.2
1	c	237	THR	2.2
1	c	321	THR	2.2
2	V	76	THR	2.2
1	c	228	TYR	2.2
1	a	121	ARG	2.2
1	c	240	ARG	2.2
1	G	42	GLY	2.2
1	K	395	GLY	2.2
1	S	248	SER	2.2
1	Y	248	SER	2.2
2	B	44	GLY	2.2
2	X	27	SER	2.2
1	U	224	LEU	2.2
1	Y	78	LEU	2.2
1	Y	373	LEU	2.2
1	G	411	LYS	2.2
1	O	360	TRP	2.2
1	Q	289	LYS	2.2
1	U	287	LYS	2.2
1	Y	246	VAL	2.2
1	Q	332	MET	2.2
1	W	31	ILE	2.2
2	P	31	PHE	2.2
2	X	31	PHE	2.2
1	Y	183	ALA	2.2
1	E	227	CYS	2.2
1	E	343	THR	2.2
1	G	282	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	237	THR	2.2
1	Y	291	GLU	2.2
2	L	76	THR	2.2
1	E	259	TYR	2.2
1	Q	158	PRO	2.2
1	Y	393	PRO	2.2
1	A	329	LYS	2.2
1	U	270	LYS	2.2
1	W	43	LYS	2.2
2	B	10	GLY	2.2
1	e	350	SER	2.2
2	b	66	LYS	2.2
1	U	116	ILE	2.2
1	U	217	HIS	2.2
1	Y	59	ILE	2.2
1	U	233	ALA	2.2
1	a	268	ALA	2.2
1	A	297	GLU	2.2
1	U	232	GLU	2.2
1	W	201	GLU	2.2
1	M	333	THR	2.2
1	Y	343	THR	2.2
1	O	416	ARG	2.2
1	S	227	CYS	2.2
1	U	274	ARG	2.2
1	c	312	ARG	2.2
1	M	41	ASN	2.2
1	O	259	TYR	2.2
1	e	352	TYR	2.2
2	V	16	PRO	2.2
1	Q	405	GLN	2.2
1	Q	270	LYS	2.2
1	U	82	LYS	2.2
1	c	289	LYS	2.2
1	C	159	GLY	2.2
1	Q	111	LEU	2.2
1	S	413	LEU	2.2
1	a	47	LEU	2.2
2	T	11	GLY	2.2
1	O	281	MET	2.2
1	O	350	SER	2.2
1	Y	219	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	e	404	VAL	2.2
1	S	290	TRP	2.1
1	Y	342	ALA	2.1
1	c	293	ALA	2.1
1	K	365	GLU	2.1
1	Q	365	GLU	2.1
1	U	372	GLU	2.1
1	K	368	THR	2.1
1	S	223	THR	2.1
1	S	330	THR	2.1
1	a	286	THR	2.1
1	e	286	THR	2.1
2	R	92	THR	2.1
2	X	115	THR	2.1
1	e	346	CYS	2.1
1	A	289	LYS	2.1
1	S	242	TYR	2.1
2	R	77	LYS	2.1
2	d	102	TYR	2.1
1	S	64	LEU	2.1
2	T	13	LEU	2.1
1	C	403	HIS	2.1
1	Q	392	VAL	2.1
1	c	257	HIS	2.1
1	e	331	HIS	2.1
1	U	248	SER	2.1
1	a	327	ALA	2.1
1	K	372	GLU	2.1
1	Q	375	GLU	2.1
1	C	27	ARG	2.1
1	K	416	ARG	2.1
1	W	377	ARG	2.1
1	G	321	THR	2.1
1	Q	306	THR	2.1
1	S	414	THR	2.1
1	a	321	THR	2.1
1	c	414	THR	2.1
1	S	96	PRO	2.1
2	Z	77	LYS	2.1
1	U	230	GLN	2.1
1	Y	350	SER	2.1
1	A	292	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	292	ALA	2.1
1	G	301	ALA	2.1
1	M	297	GLU	2.1
1	U	304	GLU	2.1
1	a	320	GLU	2.1
1	S	121	ARG	2.1
1	U	208	ARG	2.1
1	S	286	THR	2.1
2	Z	35	THR	2.1
1	a	411	LYS	2.1
1	e	43	LYS	2.1
1	U	353	PRO	2.1
1	C	281	MET	2.1
2	R	41	GLN	2.1
1	E	403	HIS	2.1
1	a	42	GLY	2.1
1	e	144	GLY	2.1
1	E	390	VAL	2.1
1	U	117	VAL	2.1
2	f	116	VAL	2.1
1	G	272	ASP	2.1
1	Y	172	ASP	2.1
1	A	350	SER	2.1
1	G	293	ALA	2.1
1	W	93	GLU	2.1
1	Y	191	ARG	2.1
1	Y	279	ALA	2.1
2	b	32	SER	2.1
1	G	375	GLU	2.1
1	I	397	GLU	2.1
1	U	157	ARG	2.1
1	Q	401	THR	2.1
1	S	371	THR	2.1
1	a	325	THR	2.1
2	J	76	THR	2.1
2	X	36	MET	2.1
1	W	298	GLN	2.1
1	Y	258	GLN	2.1
1	M	344	LEU	2.1
2	Z	49	LEU	2.1
1	G	227	CYS	2.1
1	I	340	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	402	CYS	2.1
1	Y	247	GLY	2.1
1	c	382	GLY	2.1
1	U	352	TYR	2.1
2	V	107	TYR	2.1
1	G	291	GLU	2.0
1	W	191	ARG	2.0
1	Y	218	ARG	2.0
1	K	338	SER	2.0
1	Q	292	ALA	2.0
1	Y	283	ALA	2.0
2	J	32	SER	2.0
1	a	82	LYS	2.0
2	R	45	LYS	2.0
1	A	276	TRP	2.0
1	K	321	THR	2.0
1	Y	359	THR	2.0
1	U	349	LEU	2.0
1	c	111	LEU	2.0
1	c	349	LEU	2.0
1	e	221	LEU	2.0
1	Y	41	ASN	2.0
1	a	403	HIS	2.0
2	N	10	GLY	2.0
1	E	400	TYR	2.0
1	I	392	VAL	2.0
1	K	282	CYS	2.0
1	S	266	TYR	2.0
1	W	352	TYR	2.0
2	Z	107	TYR	2.0
1	I	362	ARG	2.0
1	A	278	ALA	2.0
1	Q	249	ASP	2.0
1	U	98	GLU	2.0
1	U	162	GLU	2.0
1	W	271	GLU	2.0
1	W	320	GLU	2.0
1	Y	372	GLU	2.0
1	Q	354	ALA	2.0
1	S	268	ALA	2.0
1	e	103	ALA	2.0
2	T	64	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	Y	325	THR	2.0
2	T	70	THR	2.0
2	f	36	MET	2.0
1	S	403	HIS	2.0
1	I	364	GLY	2.0
1	W	66	ASN	2.0
1	I	416	ARG	2.0
1	a	27	ARG	2.0
1	e	377	ARG	2.0
1	e	242	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.