



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 02:40 PM EDT

PDB ID : 7STG
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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

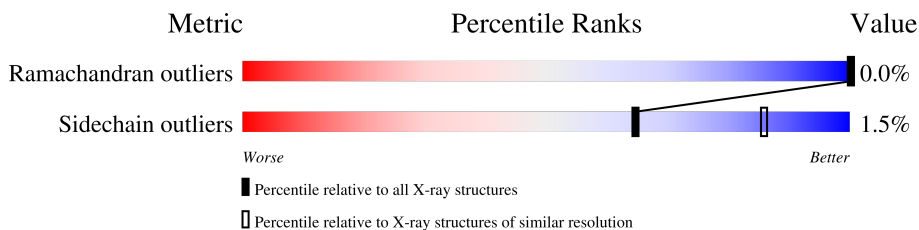
1 Overall quality at a glance i

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))
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)














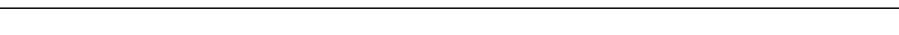

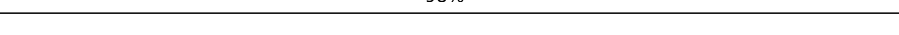
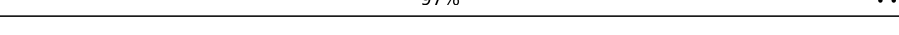
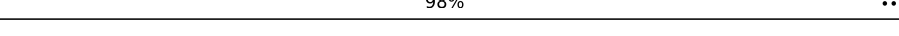
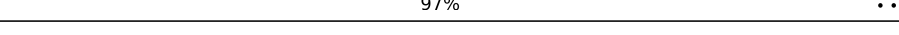
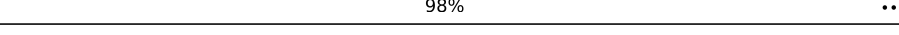
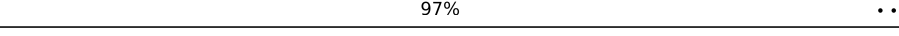
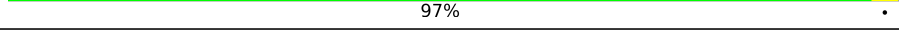
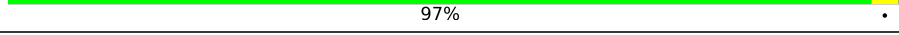
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	423	87% 13%
1	C	423	84% 15%
1	E	423	85% 14%
1	G	423	87% 12%
1	I	423	86% 13%
1	K	423	87% 12%
1	M	423	81% 18%
1	O	423	86% 14%
1	Q	423	87% 12%

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Mol	Chain	Length	Quality of chain
1	S	423	 79% 20%
1	U	423	 80% 19%
1	W	423	 80% 19%
1	Y	423	 87% 13%
1	a	423	 82% 17%
1	c	423	 81% 18%
1	e	423	 79% 20%
2	B	116	 98% ..
2	D	116	 97% ..
2	F	116	 97% ..
2	H	116	 99% .
2	J	116	 98% ..
2	L	116	 98% ..
2	N	116	 98% ..
2	P	116	 98% ..
2	R	116	 97% ..
2	T	116	 98% ..
2	V	116	 97% ..
2	X	116	 98% ..
2	Z	116	 97% ..
2	b	116	 97% ..
2	d	116	 97% ..
2	f	116	 98% ..

2 Entry composition [i](#)

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

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	
			Total	C	H	N	O				S
2	B	115	Total 1642	C 524	H 792	N 147	O 175	S 4	0	0	0
2	D	115	Total 1621	C 521	H 779	N 145	O 172	S 4	0	0	0
2	F	115	Total 1616	C 520	H 774	N 145	O 173	S 4	0	0	0
2	H	115	Total 1638	C 524	H 790	N 146	O 174	S 4	0	0	0
2	J	115	Total 1631	C 523	H 785	N 146	O 173	S 4	0	0	0
2	L	115	Total 1637	C 523	H 790	N 146	O 174	S 4	0	0	0
2	N	115	Total 1635	C 523	H 788	N 146	O 174	S 4	0	0	0
2	P	115	Total 1648	C 529	H 795	N 146	O 174	S 4	0	0	0
2	R	115	Total 1622	C 521	H 779	N 145	O 173	S 4	0	0	0
2	T	115	Total 1642	C 524	H 793	N 146	O 175	S 4	0	0	0
2	V	115	Total 1611	C 518	H 770	N 145	O 174	S 4	0	0	0

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

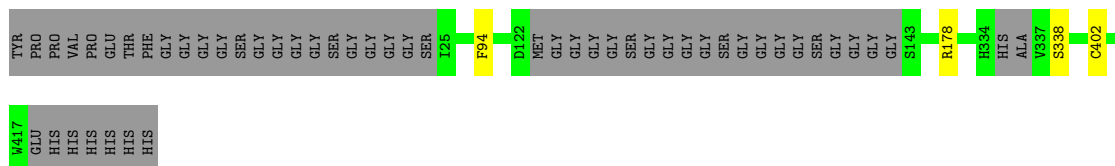
- Molecule 3 is water.

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

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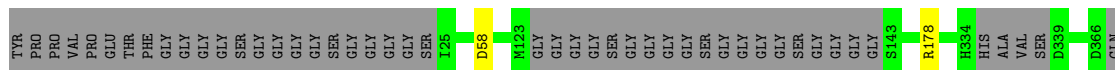
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	4	Total O 4 4	0	0
3	R	2	Total O 2 2	0	0
3	S	1	Total O 1 1	0	0
3	T	1	Total O 1 1	0	0
3	V	3	Total O 3 3	0	0
3	W	1	Total O 1 1	0	0
3	X	2	Total O 2 2	0	0
3	Z	1	Total O 1 1	0	0
3	b	1	Total O 1 1	0	0
3	d	2	Total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



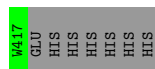
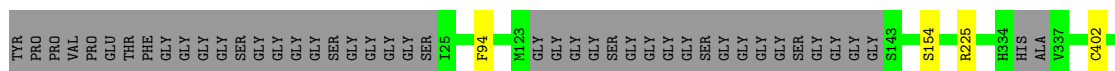
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

Chain I: 86% 13%



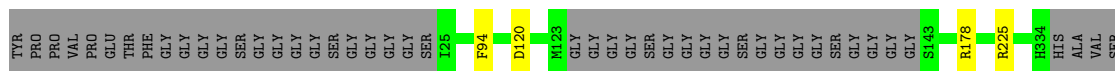
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

Chain K: 87% 12%



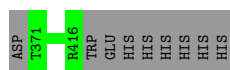
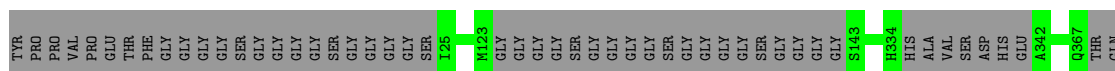
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

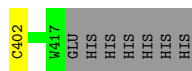
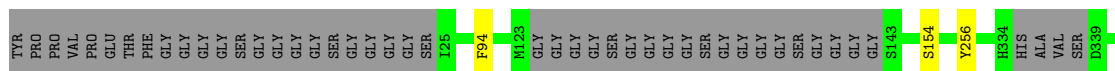
Chain M: 81% 18%



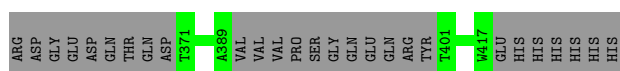
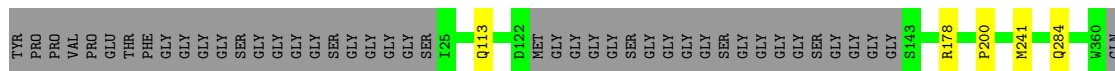
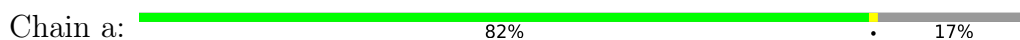
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

Chain O: 86% 14%

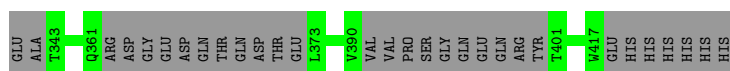
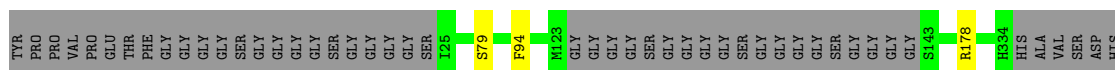
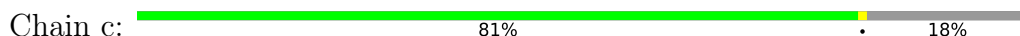




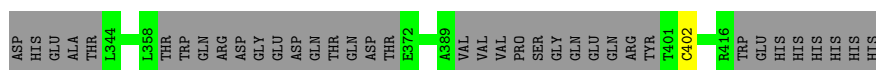
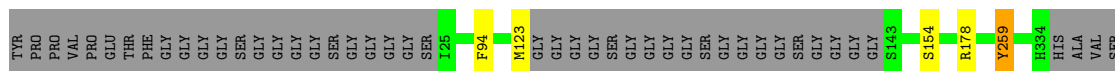
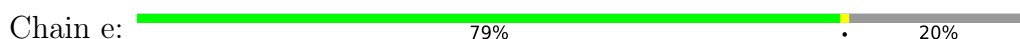
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera



- 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

Chain F:  97%



- Molecule 2: VHH

Chain H:  99%



- Molecule 2: VHH

Chain J:  98%



- Molecule 2: VHH

Chain L:  98%



- Molecule 2: VHH

Chain N:  98%



- Molecule 2: VHH

Chain P:  98%



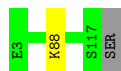
- Molecule 2: VHH

Chain R:  97%



- Molecule 2: VHH

Chain T: 98%



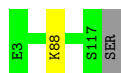
- Molecule 2: VHH

Chain V: 97%



- Molecule 2: VHH

Chain X: 98%



- Molecule 2: VHH

Chain Z: 97%



- Molecule 2: VHH

Chain b: 97%



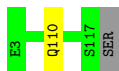
- Molecule 2: VHH

Chain d: 97%



- Molecule 2: VHH

Chain f: 98%



4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	94.3 (48.86-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.242 , 0.276	Depositor
Wilson B-factor (Å ²)	53.4	Xtrriage
Anisotropy	0.281	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.347 for -k,h,k+1 0.347 for k,-h,h+1 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+1	Xtrriage
Total number of atoms	107156	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

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	0.25	0/2856	0.50	0/3901
1	C	0.25	0/2842	0.49	0/3875
1	E	0.26	0/2882	0.51	0/3929
1	G	0.25	0/2894	0.50	0/3952
1	I	0.25	0/2868	0.50	0/3913
1	K	0.25	0/2906	0.50	0/3968
1	M	0.25	0/2738	0.50	0/3732
1	O	0.25	0/2842	0.50	0/3878
1	Q	0.26	0/2850	0.49	0/3895
1	S	0.27	0/2664	0.50	0/3636
1	U	0.25	0/2585	0.50	0/3533
1	W	0.25	0/2686	0.50	0/3661
1	Y	0.25	0/2842	0.49	0/3888
1	a	0.28	1/2725 (0.0%)	0.50	0/3721
1	c	0.25	0/2621	0.49	0/3576
1	e	0.29	1/2678 (0.0%)	0.50	0/3651
2	B	0.26	0/865	0.53	0/1173
2	D	0.27	0/857	0.53	0/1163
2	F	0.27	0/857	0.53	0/1164
2	H	0.27	0/863	0.52	0/1171
2	J	0.27	0/861	0.53	0/1168
2	L	0.27	0/862	0.52	0/1169
2	N	0.27	0/862	0.53	0/1169
2	P	0.27	0/869	0.53	0/1178
2	R	0.26	0/858	0.52	0/1164
2	T	0.26	0/864	0.53	0/1172
2	V	0.27	0/856	0.52	0/1162
2	X	0.27	0/858	0.53	0/1164
2	Z	0.27	0/860	0.52	0/1166
2	b	0.25	0/865	0.51	0/1174
2	d	0.26	0/860	0.52	0/1166
2	f	0.26	0/862	0.52	0/1169
All	All	0.26	2/58258 (0.0%)	0.51	0/79401

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	259	TYR	CD1-CE1	-6.13	1.30	1.39
1	a	200	PRO	N-CD	-5.39	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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/423 (86%)	348 (96%)	15 (4%)	0	100	100
1	C	352/423 (83%)	343 (97%)	9 (3%)	0	100	100
1	E	356/423 (84%)	344 (97%)	12 (3%)	0	100	100
1	G	365/423 (86%)	345 (94%)	19 (5%)	1 (0%)	41	66
1	I	358/423 (85%)	341 (95%)	17 (5%)	0	100	100
1	K	366/423 (86%)	349 (95%)	17 (5%)	0	100	100
1	M	337/423 (80%)	328 (97%)	8 (2%)	1 (0%)	41	66
1	O	355/423 (84%)	340 (96%)	15 (4%)	0	100	100
1	Q	365/423 (86%)	346 (95%)	19 (5%)	0	100	100
1	S	330/423 (78%)	318 (96%)	12 (4%)	0	100	100
1	U	333/423 (79%)	319 (96%)	14 (4%)	0	100	100
1	W	331/423 (78%)	321 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	364/423 (86%)	345 (95%)	19 (5%)	0	100	100
1	a	344/423 (81%)	329 (96%)	15 (4%)	0	100	100
1	c	335/423 (79%)	323 (96%)	12 (4%)	0	100	100
1	e	330/423 (78%)	322 (98%)	8 (2%)	0	100	100
2	B	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
2	D	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	F	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	H	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	J	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	L	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	N	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	P	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	R	113/116 (97%)	108 (96%)	4 (4%)	1 (1%)	17	40
2	T	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	V	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	X	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	Z	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	b	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	d	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	f	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
All	All	7392/8624 (86%)	7092 (96%)	297 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	78	ASN
1	G	338	SER
1	M	120	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/347 (74%)	255 (99%)	3 (1%)	71	88
1	C	263/347 (76%)	259 (98%)	4 (2%)	65	86
1	E	269/347 (78%)	265 (98%)	4 (2%)	65	86
1	G	263/347 (76%)	260 (99%)	3 (1%)	73	90
1	I	263/347 (76%)	261 (99%)	2 (1%)	81	93
1	K	263/347 (76%)	259 (98%)	4 (2%)	65	86
1	M	253/347 (73%)	249 (98%)	4 (2%)	62	85
1	O	261/347 (75%)	261 (100%)	0	100	100
1	Q	254/347 (73%)	251 (99%)	3 (1%)	71	88
1	S	245/347 (71%)	240 (98%)	5 (2%)	55	81
1	U	224/347 (65%)	220 (98%)	4 (2%)	59	83
1	W	248/347 (72%)	244 (98%)	4 (2%)	62	85
1	Y	251/347 (72%)	247 (98%)	4 (2%)	62	85
1	a	244/347 (70%)	240 (98%)	4 (2%)	62	85
1	c	231/347 (67%)	228 (99%)	3 (1%)	69	87
1	e	248/347 (72%)	242 (98%)	6 (2%)	49	77
2	B	90/97 (93%)	89 (99%)	1 (1%)	73	90
2	D	87/97 (90%)	85 (98%)	2 (2%)	50	78
2	F	87/97 (90%)	85 (98%)	2 (2%)	50	78
2	H	89/97 (92%)	89 (100%)	0	100	100
2	J	88/97 (91%)	87 (99%)	1 (1%)	73	90
2	L	89/97 (92%)	88 (99%)	1 (1%)	73	90
2	N	89/97 (92%)	88 (99%)	1 (1%)	73	90
2	P	90/97 (93%)	89 (99%)	1 (1%)	73	90
2	R	87/97 (90%)	86 (99%)	1 (1%)	73	90
2	T	90/97 (93%)	89 (99%)	1 (1%)	73	90
2	V	87/97 (90%)	85 (98%)	2 (2%)	50	78
2	X	88/97 (91%)	87 (99%)	1 (1%)	73	90
2	Z	88/97 (91%)	86 (98%)	2 (2%)	50	78
2	b	89/97 (92%)	86 (97%)	3 (3%)	37	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	88/97 (91%)	85 (97%)	3 (3%)	37	66
2	f	88/97 (91%)	87 (99%)	1 (1%)	73	90
All	All	5452/7104 (77%)	5372 (98%)	80 (2%)	65	86

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	94	PHE
1	A	361	GLN
2	B	110	GLN
1	C	94	PHE
1	C	178	ARG
1	C	332	MET
1	C	402	CYS
2	D	23	SER
2	D	66	LYS
1	E	58	ASP
1	E	94	PHE
1	E	178	ARG
1	E	402	CYS
2	F	23	SER
2	F	88	LYS
1	G	94	PHE
1	G	178	ARG
1	G	402	CYS
1	I	58	ASP
1	I	178	ARG
2	J	23	SER
1	K	94	PHE
1	K	154	SER
1	K	225	ARG
1	K	402	CYS
2	L	23	SER
1	M	94	PHE
1	M	178	ARG
1	M	225	ARG
1	M	402	CYS
2	N	64	SER
2	P	23	SER
1	Q	94	PHE

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Mol	Chain	Res	Type
1	Q	256	TYR
1	Q	402	CYS
2	R	23	SER
1	S	121	ARG
1	S	259	TYR
1	S	352	TYR
1	S	355	GLU
1	S	402	CYS
2	T	88	LYS
1	U	94	PHE
1	U	149	ARG
1	U	248	SER
1	U	346	CYS
2	V	63	ASP
2	V	103	SER
1	W	58	ASP
1	W	85	SER
1	W	94	PHE
1	W	317	ASN
2	X	88	LYS
1	Y	94	PHE
1	Y	154	SER
1	Y	256	TYR
1	Y	402	CYS
2	Z	64	SER
2	Z	103	SER
1	a	113	GLN
1	a	178	ARG
1	a	241	MET
1	a	284	GLN
2	b	35	THR
2	b	43	PRO
2	b	63	ASP
1	c	79	SER
1	c	94	PHE
1	c	178	ARG
2	d	23	SER
2	d	29	SER
2	d	59	THR
1	e	94	PHE
1	e	123	MET
1	e	154	SER

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Mol	Chain	Res	Type
1	e	178	ARG
1	e	259	TYR
1	e	402	CYS
2	f	110	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	197	GLN
2	F	78	ASN
1	S	406	HIS
1	U	48	ASN
2	f	110	GLN

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 monosaccharides 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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.