



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2022 – 03:00 PM EST

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

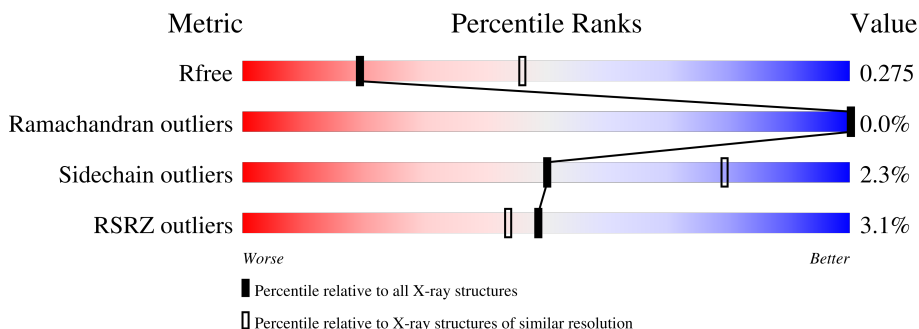
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4107 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	<div> <div>4%</div> <div>80%</div> <div>18%</div> </div>
1	C	429	<div> <div>2%</div> <div>82%</div> <div>16%</div> </div>
1	E	429	<div> <div>3%</div> <div>83%</div> <div>14%</div> </div>
1	G	429	<div> <div>3%</div> <div>84%</div> <div>15%</div> </div>
1	I	429	<div> <div>4%</div> <div>82%</div> <div>17%</div> </div>
1	K	429	<div> <div>5%</div> <div>86%</div> <div>12%</div> </div>

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

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Mol	Chain	Length	Quality of chain
2	f	116	<div><div></div><div>97%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 109155 atoms, of which 51318 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera.

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

There are 688 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 2 is a protein called VHH.

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

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

- Molecule 3 is water.

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

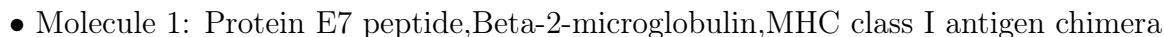
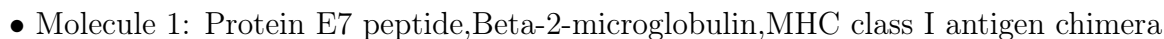
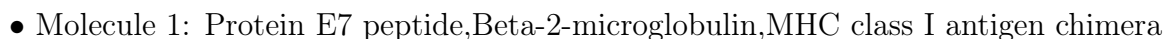
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	8	Total 8	O 8	0	0
3	P	6	Total 6	O 6	0	0
3	Q	11	Total 11	O 11	0	0
3	R	3	Total 3	O 3	0	0
3	S	8	Total 8	O 8	0	0
3	T	7	Total 7	O 7	0	0
3	U	5	Total 5	O 5	0	0
3	V	2	Total 2	O 2	0	0
3	W	4	Total 4	O 4	0	0
3	X	4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



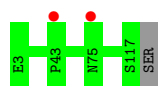
- Molecule 1: Protein E7 peptide, Beta-2-microglobulin, MHC class I antigen chimera





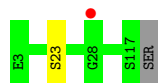
- [illegible]





- Molecule 2: VHH

Chain D: 98% ..



- Molecule 2: VHH

Chain F: 99% .



- Molecule 2: VHH

Chain H: 97% ..



- Molecule 2: VHH

Chain J: 97% ..



- Molecule 2: VHH

Chain L: 98% ..



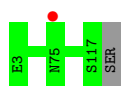
- Molecule 2: VHH

Chain N: 97% ..

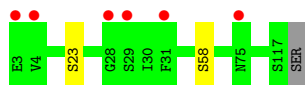


- Molecule 2: VHH

Chain P: 99% .



● Molecule 2: VHH



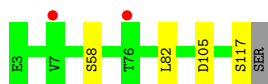
● Molecule 2: VHH



● Molecule 2: VHH



● Molecule 2: VHH



● Molecule 2: VHH



● Molecule 2: VHH



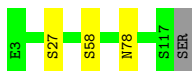
● Molecule 2: VHH





- Molecule 2: VHH

Chain f:  97% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.80Å 118.04Å 273.51Å 102.45° 102.45° 90.00°	Depositor
Resolution (Å)	50.48 – 2.78 50.48 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.48-2.78) 96.3 (50.48-2.78)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.238 , 0.275 0.238 , 0.275	Depositor DCC
$R_{free}$ test set	17167 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 8.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.357 for -k,h,k+l 0.357 for k,-h,h+l 0.409 for h,-k,-h-l 0.320 for -h,k,-k-l 0.398 for -k,-h,-l 0.366 for k,h,-h-k-l 0.336 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	109155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.27	0/2764	0.51	0/3766
1	C	0.27	0/2850	0.51	0/3887
1	E	0.27	0/2908	0.52	0/3964
1	G	0.27	0/2881	0.51	0/3932
1	I	0.27	0/2825	0.52	0/3850
1	K	0.27	0/2907	0.51	0/3969
1	M	0.27	0/2885	0.51	0/3938
1	O	0.27	0/2819	0.52	0/3846
1	Q	0.26	0/2941	0.51	0/4015
1	S	0.28	0/2729	0.52	0/3724
1	U	0.26	0/2682	0.51	0/3661
1	W	0.27	0/2763	0.51	0/3771
1	Y	0.27	0/2958	0.52	0/4039
1	a	0.27	0/2828	0.51	0/3855
1	c	0.26	0/2761	0.51	0/3765
1	e	0.27	0/2807	0.52	0/3826
2	B	0.28	0/858	0.53	0/1164
2	D	0.29	0/862	0.53	0/1169
2	F	0.28	0/862	0.53	0/1169
2	H	0.30	0/862	0.54	0/1169
2	J	0.29	0/868	0.54	0/1177
2	L	0.30	0/861	0.54	0/1168
2	N	0.33	0/858	0.57	0/1165
2	P	0.30	0/865	0.54	0/1174
2	R	0.27	0/851	0.53	0/1157
2	T	0.27	0/871	0.53	0/1181
2	V	0.28	0/865	0.52	0/1173
2	X	0.29	0/851	0.53	0/1157
2	Z	0.29	0/861	0.51	0/1168
2	b	0.28	0/869	0.54	0/1178
2	d	0.29	0/865	0.53	0/1173
2	f	0.29	0/870	0.54	0/1180
All	All	0.27	0/59107	0.52	0/80530

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [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	340/429 (79%)	323 (95%)	17 (5%)	0	100	100
1	C	349/429 (81%)	335 (96%)	14 (4%)	0	100	100
1	E	358/429 (83%)	342 (96%)	16 (4%)	0	100	100
1	G	356/429 (83%)	341 (96%)	15 (4%)	0	100	100
1	I	346/429 (81%)	332 (96%)	14 (4%)	0	100	100
1	K	368/429 (86%)	348 (95%)	20 (5%)	0	100	100
1	M	362/429 (84%)	347 (96%)	15 (4%)	0	100	100
1	O	349/429 (81%)	336 (96%)	13 (4%)	0	100	100
1	Q	367/429 (86%)	348 (95%)	19 (5%)	0	100	100
1	S	333/429 (78%)	316 (95%)	17 (5%)	0	100	100
1	U	336/429 (78%)	318 (95%)	18 (5%)	0	100	100
1	W	338/429 (79%)	325 (96%)	13 (4%)	0	100	100
1	Y	368/429 (86%)	356 (97%)	12 (3%)	0	100	100
1	a	345/429 (80%)	330 (96%)	15 (4%)	0	100	100
1	c	340/429 (79%)	323 (95%)	17 (5%)	0	100	100
1	e	342/429 (80%)	329 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	D	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	F	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	H	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	J	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	L	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	N	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	P	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	R	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	T	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	V	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	X	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	Z	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	b	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	d	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	f	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	17	44
All	All	7405/8720 (85%)	7085 (96%)	319 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	f	78	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/353 (72%)	249 (97%)	7 (3%)	44	75
1	C	263/353 (74%)	255 (97%)	8 (3%)	41	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	271/353 (77%)	260 (96%)	11 (4%)	30	61
1	G	266/353 (75%)	261 (98%)	5 (2%)	57	83
1	I	262/353 (74%)	256 (98%)	6 (2%)	50	79
1	K	261/353 (74%)	254 (97%)	7 (3%)	44	75
1	M	262/353 (74%)	254 (97%)	8 (3%)	40	71
1	O	257/353 (73%)	252 (98%)	5 (2%)	57	83
1	Q	271/353 (77%)	263 (97%)	8 (3%)	41	72
1	S	253/353 (72%)	242 (96%)	11 (4%)	29	59
1	U	242/353 (69%)	234 (97%)	8 (3%)	38	69
1	W	256/353 (72%)	249 (97%)	7 (3%)	44	75
1	Y	272/353 (77%)	268 (98%)	4 (2%)	65	87
1	a	264/353 (75%)	258 (98%)	6 (2%)	50	79
1	c	251/353 (71%)	247 (98%)	4 (2%)	62	86
1	e	261/353 (74%)	257 (98%)	4 (2%)	65	87
2	B	88/97 (91%)	88 (100%)	0	100	100
2	D	89/97 (92%)	88 (99%)	1 (1%)	73	90
2	F	89/97 (92%)	89 (100%)	0	100	100
2	H	89/97 (92%)	87 (98%)	2 (2%)	52	80
2	J	89/97 (92%)	87 (98%)	2 (2%)	52	80
2	L	88/97 (91%)	87 (99%)	1 (1%)	73	90
2	N	88/97 (91%)	86 (98%)	2 (2%)	50	79
2	P	89/97 (92%)	89 (100%)	0	100	100
2	R	85/97 (88%)	83 (98%)	2 (2%)	49	78
2	T	91/97 (94%)	90 (99%)	1 (1%)	73	90
2	V	90/97 (93%)	88 (98%)	2 (2%)	52	80
2	X	86/97 (89%)	82 (95%)	4 (5%)	26	56
2	Z	88/97 (91%)	87 (99%)	1 (1%)	73	90
2	b	90/97 (93%)	89 (99%)	1 (1%)	73	90
2	d	90/97 (93%)	90 (100%)	0	100	100
2	f	90/97 (93%)	88 (98%)	2 (2%)	52	80
All	All	5587/7200 (78%)	5457 (98%)	130 (2%)	50	79

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	154	SER
2	b	21	ARG
1	K	407	GLU
1	K	402	CYS
1	c	154	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	331	HIS
1	M	361	GLN
1	Y	284	GLN
1	S	317	ASN
1	K	284	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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	352/429 (82%)	-0.09	17 (4%) 30 24	27, 48, 100, 122	0
1	C	361/429 (84%)	-0.15	9 (2%) 57 52	31, 50, 106, 150	0
1	E	368/429 (85%)	-0.07	11 (2%) 50 45	31, 51, 107, 150	0
1	G	366/429 (85%)	-0.14	11 (3%) 50 45	27, 49, 102, 148	0
1	I	358/429 (83%)	-0.08	17 (4%) 31 25	27, 46, 100, 136	0
1	K	376/429 (87%)	-0.03	23 (6%) 21 16	20, 44, 112, 142	0
1	M	372/429 (86%)	-0.03	24 (6%) 18 14	21, 44, 109, 136	0
1	O	361/429 (84%)	-0.14	12 (3%) 46 41	26, 47, 99, 144	0
1	Q	375/429 (87%)	0.07	6 (1%) 72 69	42, 66, 108, 139	0
1	S	345/429 (80%)	0.09	14 (4%) 37 32	49, 71, 106, 141	0
1	U	348/429 (81%)	0.34	30 (8%) 10 7	44, 68, 117, 150	0
1	W	350/429 (81%)	0.10	14 (4%) 38 33	49, 70, 113, 143	0
1	Y	376/429 (87%)	-0.12	5 (1%) 77 75	28, 48, 101, 128	0
1	a	357/429 (83%)	-0.14	6 (1%) 70 67	33, 50, 100, 129	0
1	c	352/429 (82%)	0.04	15 (4%) 35 30	27, 51, 106, 137	0
1	e	354/429 (82%)	-0.12	8 (2%) 60 55	33, 51, 99, 133	0
2	B	115/116 (99%)	-0.22	2 (1%) 70 67	27, 37, 72, 93	0
2	D	115/116 (99%)	-0.27	1 (0%) 84 82	30, 42, 81, 99	0
2	F	115/116 (99%)	-0.35	0 100 100	29, 42, 75, 98	0
2	H	115/116 (99%)	-0.29	0 100 100	27, 38, 80, 135	0
2	J	115/116 (99%)	-0.24	2 (1%) 70 67	26, 40, 81, 110	0
2	L	115/116 (99%)	-0.31	0 100 100	23, 33, 72, 97	0
2	N	115/116 (99%)	-0.29	0 100 100	23, 35, 69, 86	0
2	P	115/116 (99%)	-0.32	1 (0%) 84 82	26, 38, 80, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	R	115/116 (99%)	0.11	6 (5%) 27 22	44, 59, 102, 150	0
2	T	115/116 (99%)	-0.06	0 100 100	41, 56, 80, 109	0
2	V	115/116 (99%)	-0.02	2 (1%) 70 67	42, 55, 91, 120	0
2	X	115/116 (99%)	0.01	2 (1%) 70 67	46, 63, 101, 131	0
2	Z	115/116 (99%)	-0.09	1 (0%) 84 82	29, 42, 86, 136	0
2	b	115/116 (99%)	-0.20	0 100 100	28, 41, 67, 104	0
2	d	115/116 (99%)	-0.22	0 100 100	27, 37, 70, 108	0
2	f	115/116 (99%)	-0.22	0 100 100	32, 43, 88, 116	0
All	All	7611/8720 (87%)	-0.07	239 (3%) 49 44	20, 52, 103, 150	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	413	LEU	6.9
1	A	391	VAL	6.6
1	M	397	GLU	6.3
1	e	371	THR	6.1
1	U	278	ALA	5.9

## 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 monosaccharides 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.