



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:57 PM UTC

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

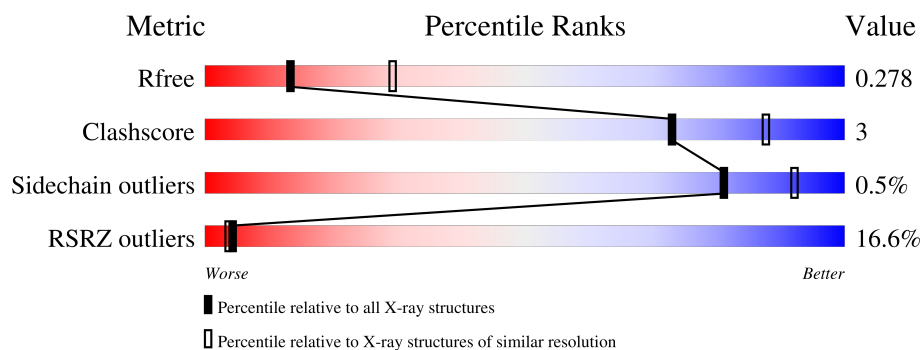
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	423	14% 83% 13%
1	C	423	10% 82% 15%
1	E	423	9% 82% 14%
1	G	423	11% 84% 12%
1	I	423	10% 84% 13%
1	K	423	10% 85% 12%

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Mol	Chain	Length	Quality of chain
1	M	423	
1	O	423	
1	Q	423	
1	S	423	
1	U	423	
1	W	423	
1	Y	423	
1	a	423	
1	c	423	
1	e	423	
2	B	116	
2	D	116	
2	F	116	
2	H	116	
2	J	116	
2	L	116	
2	N	116	
2	P	116	
2	R	116	
2	T	116	
2	V	116	
2	X	116	
2	Z	116	
2	b	116	
2	d	116	

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 107156 atoms, of which 50250 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RPA-related protein RADX peptide,Beta-2-microglobulin,MH C class I antigen chimera.

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

There are 688 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	linker	UNP Q6NSI4
A	11	GLY	-	linker	UNP Q6NSI4
A	12	GLY	-	linker	UNP Q6NSI4
A	13	GLY	-	linker	UNP Q6NSI4
A	14	SER	-	linker	UNP Q6NSI4
A	15	GLY	-	linker	UNP Q6NSI4
A	16	GLY	-	linker	UNP Q6NSI4
A	17	GLY	-	linker	UNP Q6NSI4
A	18	GLY	-	linker	UNP Q6NSI4
A	19	SER	-	linker	UNP Q6NSI4
A	20	GLY	-	linker	UNP Q6NSI4
A	21	GLY	-	linker	UNP Q6NSI4
A	22	GLY	-	linker	UNP Q6NSI4
A	23	GLY	-	linker	UNP Q6NSI4
A	24	SER	-	linker	UNP Q6NSI4
A	124	GLY	-	linker	UNP P16213
A	125	GLY	-	linker	UNP P16213
A	126	GLY	-	linker	UNP P16213
A	127	GLY	-	linker	UNP P16213
A	128	SER	-	linker	UNP P16213
A	129	GLY	-	linker	UNP P16213
A	130	GLY	-	linker	UNP P16213
A	131	GLY	-	linker	UNP P16213
A	132	GLY	-	linker	UNP P16213
A	133	SER	-	linker	UNP P16213
A	134	GLY	-	linker	UNP P16213
A	135	GLY	-	linker	UNP P16213
A	136	GLY	-	linker	UNP P16213
A	137	GLY	-	linker	UNP P16213
A	138	SER	-	linker	UNP P16213
A	139	GLY	-	linker	UNP P16213
A	140	GLY	-	linker	UNP P16213
A	141	GLY	-	linker	UNP P16213
A	142	GLY	-	linker	UNP P16213
A	143	SER	-	linker	UNP P16213
A	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
A	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
A	419	HIS	-	expression tag	UNP A0A678ZGP6
A	420	HIS	-	expression tag	UNP A0A678ZGP6
A	421	HIS	-	expression tag	UNP A0A678ZGP6
A	422	HIS	-	expression tag	UNP A0A678ZGP6
A	423	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP A0A678ZGP6
C	10	GLY	-	linker	UNP Q6NSI4
C	11	GLY	-	linker	UNP Q6NSI4
C	12	GLY	-	linker	UNP Q6NSI4
C	13	GLY	-	linker	UNP Q6NSI4
C	14	SER	-	linker	UNP Q6NSI4
C	15	GLY	-	linker	UNP Q6NSI4
C	16	GLY	-	linker	UNP Q6NSI4
C	17	GLY	-	linker	UNP Q6NSI4
C	18	GLY	-	linker	UNP Q6NSI4
C	19	SER	-	linker	UNP Q6NSI4
C	20	GLY	-	linker	UNP Q6NSI4
C	21	GLY	-	linker	UNP Q6NSI4
C	22	GLY	-	linker	UNP Q6NSI4
C	23	GLY	-	linker	UNP Q6NSI4
C	24	SER	-	linker	UNP Q6NSI4
C	124	GLY	-	linker	UNP P16213
C	125	GLY	-	linker	UNP P16213
C	126	GLY	-	linker	UNP P16213
C	127	GLY	-	linker	UNP P16213
C	128	SER	-	linker	UNP P16213
C	129	GLY	-	linker	UNP P16213
C	130	GLY	-	linker	UNP P16213
C	131	GLY	-	linker	UNP P16213
C	132	GLY	-	linker	UNP P16213
C	133	SER	-	linker	UNP P16213
C	134	GLY	-	linker	UNP P16213
C	135	GLY	-	linker	UNP P16213
C	136	GLY	-	linker	UNP P16213
C	137	GLY	-	linker	UNP P16213
C	138	SER	-	linker	UNP P16213
C	139	GLY	-	linker	UNP P16213
C	140	GLY	-	linker	UNP P16213
C	141	GLY	-	linker	UNP P16213
C	142	GLY	-	linker	UNP P16213
C	143	SER	-	linker	UNP P16213
C	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
C	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
C	419	HIS	-	expression tag	UNP A0A678ZGP6
C	420	HIS	-	expression tag	UNP A0A678ZGP6
C	421	HIS	-	expression tag	UNP A0A678ZGP6
C	422	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	423	HIS	-	expression tag	UNP A0A678ZGP6
C	424	HIS	-	expression tag	UNP A0A678ZGP6
E	10	GLY	-	linker	UNP Q6NSI4
E	11	GLY	-	linker	UNP Q6NSI4
E	12	GLY	-	linker	UNP Q6NSI4
E	13	GLY	-	linker	UNP Q6NSI4
E	14	SER	-	linker	UNP Q6NSI4
E	15	GLY	-	linker	UNP Q6NSI4
E	16	GLY	-	linker	UNP Q6NSI4
E	17	GLY	-	linker	UNP Q6NSI4
E	18	GLY	-	linker	UNP Q6NSI4
E	19	SER	-	linker	UNP Q6NSI4
E	20	GLY	-	linker	UNP Q6NSI4
E	21	GLY	-	linker	UNP Q6NSI4
E	22	GLY	-	linker	UNP Q6NSI4
E	23	GLY	-	linker	UNP Q6NSI4
E	24	SER	-	linker	UNP Q6NSI4
E	124	GLY	-	linker	UNP P16213
E	125	GLY	-	linker	UNP P16213
E	126	GLY	-	linker	UNP P16213
E	127	GLY	-	linker	UNP P16213
E	128	SER	-	linker	UNP P16213
E	129	GLY	-	linker	UNP P16213
E	130	GLY	-	linker	UNP P16213
E	131	GLY	-	linker	UNP P16213
E	132	GLY	-	linker	UNP P16213
E	133	SER	-	linker	UNP P16213
E	134	GLY	-	linker	UNP P16213
E	135	GLY	-	linker	UNP P16213
E	136	GLY	-	linker	UNP P16213
E	137	GLY	-	linker	UNP P16213
E	138	SER	-	linker	UNP P16213
E	139	GLY	-	linker	UNP P16213
E	140	GLY	-	linker	UNP P16213
E	141	GLY	-	linker	UNP P16213
E	142	GLY	-	linker	UNP P16213
E	143	SER	-	linker	UNP P16213
E	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
E	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
E	419	HIS	-	expression tag	UNP A0A678ZGP6
E	420	HIS	-	expression tag	UNP A0A678ZGP6
E	421	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	422	HIS	-	expression tag	UNP A0A678ZGP6
E	423	HIS	-	expression tag	UNP A0A678ZGP6
E	424	HIS	-	expression tag	UNP A0A678ZGP6
G	10	GLY	-	linker	UNP Q6NSI4
G	11	GLY	-	linker	UNP Q6NSI4
G	12	GLY	-	linker	UNP Q6NSI4
G	13	GLY	-	linker	UNP Q6NSI4
G	14	SER	-	linker	UNP Q6NSI4
G	15	GLY	-	linker	UNP Q6NSI4
G	16	GLY	-	linker	UNP Q6NSI4
G	17	GLY	-	linker	UNP Q6NSI4
G	18	GLY	-	linker	UNP Q6NSI4
G	19	SER	-	linker	UNP Q6NSI4
G	20	GLY	-	linker	UNP Q6NSI4
G	21	GLY	-	linker	UNP Q6NSI4
G	22	GLY	-	linker	UNP Q6NSI4
G	23	GLY	-	linker	UNP Q6NSI4
G	24	SER	-	linker	UNP Q6NSI4
G	124	GLY	-	linker	UNP P16213
G	125	GLY	-	linker	UNP P16213
G	126	GLY	-	linker	UNP P16213
G	127	GLY	-	linker	UNP P16213
G	128	SER	-	linker	UNP P16213
G	129	GLY	-	linker	UNP P16213
G	130	GLY	-	linker	UNP P16213
G	131	GLY	-	linker	UNP P16213
G	132	GLY	-	linker	UNP P16213
G	133	SER	-	linker	UNP P16213
G	134	GLY	-	linker	UNP P16213
G	135	GLY	-	linker	UNP P16213
G	136	GLY	-	linker	UNP P16213
G	137	GLY	-	linker	UNP P16213
G	138	SER	-	linker	UNP P16213
G	139	GLY	-	linker	UNP P16213
G	140	GLY	-	linker	UNP P16213
G	141	GLY	-	linker	UNP P16213
G	142	GLY	-	linker	UNP P16213
G	143	SER	-	linker	UNP P16213
G	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
G	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
G	419	HIS	-	expression tag	UNP A0A678ZGP6
G	420	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	421	HIS	-	expression tag	UNP A0A678ZGP6
G	422	HIS	-	expression tag	UNP A0A678ZGP6
G	423	HIS	-	expression tag	UNP A0A678ZGP6
G	424	HIS	-	expression tag	UNP A0A678ZGP6
I	10	GLY	-	linker	UNP Q6NSI4
I	11	GLY	-	linker	UNP Q6NSI4
I	12	GLY	-	linker	UNP Q6NSI4
I	13	GLY	-	linker	UNP Q6NSI4
I	14	SER	-	linker	UNP Q6NSI4
I	15	GLY	-	linker	UNP Q6NSI4
I	16	GLY	-	linker	UNP Q6NSI4
I	17	GLY	-	linker	UNP Q6NSI4
I	18	GLY	-	linker	UNP Q6NSI4
I	19	SER	-	linker	UNP Q6NSI4
I	20	GLY	-	linker	UNP Q6NSI4
I	21	GLY	-	linker	UNP Q6NSI4
I	22	GLY	-	linker	UNP Q6NSI4
I	23	GLY	-	linker	UNP Q6NSI4
I	24	SER	-	linker	UNP Q6NSI4
I	124	GLY	-	linker	UNP P16213
I	125	GLY	-	linker	UNP P16213
I	126	GLY	-	linker	UNP P16213
I	127	GLY	-	linker	UNP P16213
I	128	SER	-	linker	UNP P16213
I	129	GLY	-	linker	UNP P16213
I	130	GLY	-	linker	UNP P16213
I	131	GLY	-	linker	UNP P16213
I	132	GLY	-	linker	UNP P16213
I	133	SER	-	linker	UNP P16213
I	134	GLY	-	linker	UNP P16213
I	135	GLY	-	linker	UNP P16213
I	136	GLY	-	linker	UNP P16213
I	137	GLY	-	linker	UNP P16213
I	138	SER	-	linker	UNP P16213
I	139	GLY	-	linker	UNP P16213
I	140	GLY	-	linker	UNP P16213
I	141	GLY	-	linker	UNP P16213
I	142	GLY	-	linker	UNP P16213
I	143	SER	-	linker	UNP P16213
I	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
I	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
I	419	HIS	-	expression tag	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	420	HIS	-	expression tag	UNP A0A678ZGP6
I	421	HIS	-	expression tag	UNP A0A678ZGP6
I	422	HIS	-	expression tag	UNP A0A678ZGP6
I	423	HIS	-	expression tag	UNP A0A678ZGP6
I	424	HIS	-	expression tag	UNP A0A678ZGP6
K	10	GLY	-	linker	UNP Q6NSI4
K	11	GLY	-	linker	UNP Q6NSI4
K	12	GLY	-	linker	UNP Q6NSI4
K	13	GLY	-	linker	UNP Q6NSI4
K	14	SER	-	linker	UNP Q6NSI4
K	15	GLY	-	linker	UNP Q6NSI4
K	16	GLY	-	linker	UNP Q6NSI4
K	17	GLY	-	linker	UNP Q6NSI4
K	18	GLY	-	linker	UNP Q6NSI4
K	19	SER	-	linker	UNP Q6NSI4
K	20	GLY	-	linker	UNP Q6NSI4
K	21	GLY	-	linker	UNP Q6NSI4
K	22	GLY	-	linker	UNP Q6NSI4
K	23	GLY	-	linker	UNP Q6NSI4
K	24	SER	-	linker	UNP Q6NSI4
K	124	GLY	-	linker	UNP P16213
K	125	GLY	-	linker	UNP P16213
K	126	GLY	-	linker	UNP P16213
K	127	GLY	-	linker	UNP P16213
K	128	SER	-	linker	UNP P16213
K	129	GLY	-	linker	UNP P16213
K	130	GLY	-	linker	UNP P16213
K	131	GLY	-	linker	UNP P16213
K	132	GLY	-	linker	UNP P16213
K	133	SER	-	linker	UNP P16213
K	134	GLY	-	linker	UNP P16213
K	135	GLY	-	linker	UNP P16213
K	136	GLY	-	linker	UNP P16213
K	137	GLY	-	linker	UNP P16213
K	138	SER	-	linker	UNP P16213
K	139	GLY	-	linker	UNP P16213
K	140	GLY	-	linker	UNP P16213
K	141	GLY	-	linker	UNP P16213
K	142	GLY	-	linker	UNP P16213
K	143	SER	-	linker	UNP P16213
K	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
K	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	419	HIS	-	expression tag	UNP A0A678ZGP6
K	420	HIS	-	expression tag	UNP A0A678ZGP6
K	421	HIS	-	expression tag	UNP A0A678ZGP6
K	422	HIS	-	expression tag	UNP A0A678ZGP6
K	423	HIS	-	expression tag	UNP A0A678ZGP6
K	424	HIS	-	expression tag	UNP A0A678ZGP6
M	10	GLY	-	linker	UNP Q6NSI4
M	11	GLY	-	linker	UNP Q6NSI4
M	12	GLY	-	linker	UNP Q6NSI4
M	13	GLY	-	linker	UNP Q6NSI4
M	14	SER	-	linker	UNP Q6NSI4
M	15	GLY	-	linker	UNP Q6NSI4
M	16	GLY	-	linker	UNP Q6NSI4
M	17	GLY	-	linker	UNP Q6NSI4
M	18	GLY	-	linker	UNP Q6NSI4
M	19	SER	-	linker	UNP Q6NSI4
M	20	GLY	-	linker	UNP Q6NSI4
M	21	GLY	-	linker	UNP Q6NSI4
M	22	GLY	-	linker	UNP Q6NSI4
M	23	GLY	-	linker	UNP Q6NSI4
M	24	SER	-	linker	UNP Q6NSI4
M	124	GLY	-	linker	UNP P16213
M	125	GLY	-	linker	UNP P16213
M	126	GLY	-	linker	UNP P16213
M	127	GLY	-	linker	UNP P16213
M	128	SER	-	linker	UNP P16213
M	129	GLY	-	linker	UNP P16213
M	130	GLY	-	linker	UNP P16213
M	131	GLY	-	linker	UNP P16213
M	132	GLY	-	linker	UNP P16213
M	133	SER	-	linker	UNP P16213
M	134	GLY	-	linker	UNP P16213
M	135	GLY	-	linker	UNP P16213
M	136	GLY	-	linker	UNP P16213
M	137	GLY	-	linker	UNP P16213
M	138	SER	-	linker	UNP P16213
M	139	GLY	-	linker	UNP P16213
M	140	GLY	-	linker	UNP P16213
M	141	GLY	-	linker	UNP P16213
M	142	GLY	-	linker	UNP P16213
M	143	SER	-	linker	UNP P16213
M	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
M	419	HIS	-	expression tag	UNP A0A678ZGP6
M	420	HIS	-	expression tag	UNP A0A678ZGP6
M	421	HIS	-	expression tag	UNP A0A678ZGP6
M	422	HIS	-	expression tag	UNP A0A678ZGP6
M	423	HIS	-	expression tag	UNP A0A678ZGP6
M	424	HIS	-	expression tag	UNP A0A678ZGP6
O	10	GLY	-	linker	UNP Q6NSI4
O	11	GLY	-	linker	UNP Q6NSI4
O	12	GLY	-	linker	UNP Q6NSI4
O	13	GLY	-	linker	UNP Q6NSI4
O	14	SER	-	linker	UNP Q6NSI4
O	15	GLY	-	linker	UNP Q6NSI4
O	16	GLY	-	linker	UNP Q6NSI4
O	17	GLY	-	linker	UNP Q6NSI4
O	18	GLY	-	linker	UNP Q6NSI4
O	19	SER	-	linker	UNP Q6NSI4
O	20	GLY	-	linker	UNP Q6NSI4
O	21	GLY	-	linker	UNP Q6NSI4
O	22	GLY	-	linker	UNP Q6NSI4
O	23	GLY	-	linker	UNP Q6NSI4
O	24	SER	-	linker	UNP Q6NSI4
O	124	GLY	-	linker	UNP P16213
O	125	GLY	-	linker	UNP P16213
O	126	GLY	-	linker	UNP P16213
O	127	GLY	-	linker	UNP P16213
O	128	SER	-	linker	UNP P16213
O	129	GLY	-	linker	UNP P16213
O	130	GLY	-	linker	UNP P16213
O	131	GLY	-	linker	UNP P16213
O	132	GLY	-	linker	UNP P16213
O	133	SER	-	linker	UNP P16213
O	134	GLY	-	linker	UNP P16213
O	135	GLY	-	linker	UNP P16213
O	136	GLY	-	linker	UNP P16213
O	137	GLY	-	linker	UNP P16213
O	138	SER	-	linker	UNP P16213
O	139	GLY	-	linker	UNP P16213
O	140	GLY	-	linker	UNP P16213
O	141	GLY	-	linker	UNP P16213
O	142	GLY	-	linker	UNP P16213
O	143	SER	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
O	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
O	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
O	419	HIS	-	expression tag	UNP A0A678ZGP6
O	420	HIS	-	expression tag	UNP A0A678ZGP6
O	421	HIS	-	expression tag	UNP A0A678ZGP6
O	422	HIS	-	expression tag	UNP A0A678ZGP6
O	423	HIS	-	expression tag	UNP A0A678ZGP6
O	424	HIS	-	expression tag	UNP A0A678ZGP6
Q	10	GLY	-	linker	UNP Q6NSI4
Q	11	GLY	-	linker	UNP Q6NSI4
Q	12	GLY	-	linker	UNP Q6NSI4
Q	13	GLY	-	linker	UNP Q6NSI4
Q	14	SER	-	linker	UNP Q6NSI4
Q	15	GLY	-	linker	UNP Q6NSI4
Q	16	GLY	-	linker	UNP Q6NSI4
Q	17	GLY	-	linker	UNP Q6NSI4
Q	18	GLY	-	linker	UNP Q6NSI4
Q	19	SER	-	linker	UNP Q6NSI4
Q	20	GLY	-	linker	UNP Q6NSI4
Q	21	GLY	-	linker	UNP Q6NSI4
Q	22	GLY	-	linker	UNP Q6NSI4
Q	23	GLY	-	linker	UNP Q6NSI4
Q	24	SER	-	linker	UNP Q6NSI4
Q	124	GLY	-	linker	UNP P16213
Q	125	GLY	-	linker	UNP P16213
Q	126	GLY	-	linker	UNP P16213
Q	127	GLY	-	linker	UNP P16213
Q	128	SER	-	linker	UNP P16213
Q	129	GLY	-	linker	UNP P16213
Q	130	GLY	-	linker	UNP P16213
Q	131	GLY	-	linker	UNP P16213
Q	132	GLY	-	linker	UNP P16213
Q	133	SER	-	linker	UNP P16213
Q	134	GLY	-	linker	UNP P16213
Q	135	GLY	-	linker	UNP P16213
Q	136	GLY	-	linker	UNP P16213
Q	137	GLY	-	linker	UNP P16213
Q	138	SER	-	linker	UNP P16213
Q	139	GLY	-	linker	UNP P16213
Q	140	GLY	-	linker	UNP P16213
Q	141	GLY	-	linker	UNP P16213
Q	142	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	143	SER	-	linker	UNP P16213
Q	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
Q	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
Q	419	HIS	-	expression tag	UNP A0A678ZGP6
Q	420	HIS	-	expression tag	UNP A0A678ZGP6
Q	421	HIS	-	expression tag	UNP A0A678ZGP6
Q	422	HIS	-	expression tag	UNP A0A678ZGP6
Q	423	HIS	-	expression tag	UNP A0A678ZGP6
Q	424	HIS	-	expression tag	UNP A0A678ZGP6
S	10	GLY	-	linker	UNP Q6NSI4
S	11	GLY	-	linker	UNP Q6NSI4
S	12	GLY	-	linker	UNP Q6NSI4
S	13	GLY	-	linker	UNP Q6NSI4
S	14	SER	-	linker	UNP Q6NSI4
S	15	GLY	-	linker	UNP Q6NSI4
S	16	GLY	-	linker	UNP Q6NSI4
S	17	GLY	-	linker	UNP Q6NSI4
S	18	GLY	-	linker	UNP Q6NSI4
S	19	SER	-	linker	UNP Q6NSI4
S	20	GLY	-	linker	UNP Q6NSI4
S	21	GLY	-	linker	UNP Q6NSI4
S	22	GLY	-	linker	UNP Q6NSI4
S	23	GLY	-	linker	UNP Q6NSI4
S	24	SER	-	linker	UNP Q6NSI4
S	124	GLY	-	linker	UNP P16213
S	125	GLY	-	linker	UNP P16213
S	126	GLY	-	linker	UNP P16213
S	127	GLY	-	linker	UNP P16213
S	128	SER	-	linker	UNP P16213
S	129	GLY	-	linker	UNP P16213
S	130	GLY	-	linker	UNP P16213
S	131	GLY	-	linker	UNP P16213
S	132	GLY	-	linker	UNP P16213
S	133	SER	-	linker	UNP P16213
S	134	GLY	-	linker	UNP P16213
S	135	GLY	-	linker	UNP P16213
S	136	GLY	-	linker	UNP P16213
S	137	GLY	-	linker	UNP P16213
S	138	SER	-	linker	UNP P16213
S	139	GLY	-	linker	UNP P16213
S	140	GLY	-	linker	UNP P16213
S	141	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
S	142	GLY	-	linker	UNP P16213
S	143	SER	-	linker	UNP P16213
S	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
S	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
S	419	HIS	-	expression tag	UNP A0A678ZGP6
S	420	HIS	-	expression tag	UNP A0A678ZGP6
S	421	HIS	-	expression tag	UNP A0A678ZGP6
S	422	HIS	-	expression tag	UNP A0A678ZGP6
S	423	HIS	-	expression tag	UNP A0A678ZGP6
S	424	HIS	-	expression tag	UNP A0A678ZGP6
U	10	GLY	-	linker	UNP Q6NSI4
U	11	GLY	-	linker	UNP Q6NSI4
U	12	GLY	-	linker	UNP Q6NSI4
U	13	GLY	-	linker	UNP Q6NSI4
U	14	SER	-	linker	UNP Q6NSI4
U	15	GLY	-	linker	UNP Q6NSI4
U	16	GLY	-	linker	UNP Q6NSI4
U	17	GLY	-	linker	UNP Q6NSI4
U	18	GLY	-	linker	UNP Q6NSI4
U	19	SER	-	linker	UNP Q6NSI4
U	20	GLY	-	linker	UNP Q6NSI4
U	21	GLY	-	linker	UNP Q6NSI4
U	22	GLY	-	linker	UNP Q6NSI4
U	23	GLY	-	linker	UNP Q6NSI4
U	24	SER	-	linker	UNP Q6NSI4
U	124	GLY	-	linker	UNP P16213
U	125	GLY	-	linker	UNP P16213
U	126	GLY	-	linker	UNP P16213
U	127	GLY	-	linker	UNP P16213
U	128	SER	-	linker	UNP P16213
U	129	GLY	-	linker	UNP P16213
U	130	GLY	-	linker	UNP P16213
U	131	GLY	-	linker	UNP P16213
U	132	GLY	-	linker	UNP P16213
U	133	SER	-	linker	UNP P16213
U	134	GLY	-	linker	UNP P16213
U	135	GLY	-	linker	UNP P16213
U	136	GLY	-	linker	UNP P16213
U	137	GLY	-	linker	UNP P16213
U	138	SER	-	linker	UNP P16213
U	139	GLY	-	linker	UNP P16213
U	140	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
U	141	GLY	-	linker	UNP P16213
U	142	GLY	-	linker	UNP P16213
U	143	SER	-	linker	UNP P16213
U	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
U	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
U	419	HIS	-	expression tag	UNP A0A678ZGP6
U	420	HIS	-	expression tag	UNP A0A678ZGP6
U	421	HIS	-	expression tag	UNP A0A678ZGP6
U	422	HIS	-	expression tag	UNP A0A678ZGP6
U	423	HIS	-	expression tag	UNP A0A678ZGP6
U	424	HIS	-	expression tag	UNP A0A678ZGP6
W	10	GLY	-	linker	UNP Q6NSI4
W	11	GLY	-	linker	UNP Q6NSI4
W	12	GLY	-	linker	UNP Q6NSI4
W	13	GLY	-	linker	UNP Q6NSI4
W	14	SER	-	linker	UNP Q6NSI4
W	15	GLY	-	linker	UNP Q6NSI4
W	16	GLY	-	linker	UNP Q6NSI4
W	17	GLY	-	linker	UNP Q6NSI4
W	18	GLY	-	linker	UNP Q6NSI4
W	19	SER	-	linker	UNP Q6NSI4
W	20	GLY	-	linker	UNP Q6NSI4
W	21	GLY	-	linker	UNP Q6NSI4
W	22	GLY	-	linker	UNP Q6NSI4
W	23	GLY	-	linker	UNP Q6NSI4
W	24	SER	-	linker	UNP Q6NSI4
W	124	GLY	-	linker	UNP P16213
W	125	GLY	-	linker	UNP P16213
W	126	GLY	-	linker	UNP P16213
W	127	GLY	-	linker	UNP P16213
W	128	SER	-	linker	UNP P16213
W	129	GLY	-	linker	UNP P16213
W	130	GLY	-	linker	UNP P16213
W	131	GLY	-	linker	UNP P16213
W	132	GLY	-	linker	UNP P16213
W	133	SER	-	linker	UNP P16213
W	134	GLY	-	linker	UNP P16213
W	135	GLY	-	linker	UNP P16213
W	136	GLY	-	linker	UNP P16213
W	137	GLY	-	linker	UNP P16213
W	138	SER	-	linker	UNP P16213
W	139	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
W	140	GLY	-	linker	UNP P16213
W	141	GLY	-	linker	UNP P16213
W	142	GLY	-	linker	UNP P16213
W	143	SER	-	linker	UNP P16213
W	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
W	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
W	419	HIS	-	expression tag	UNP A0A678ZGP6
W	420	HIS	-	expression tag	UNP A0A678ZGP6
W	421	HIS	-	expression tag	UNP A0A678ZGP6
W	422	HIS	-	expression tag	UNP A0A678ZGP6
W	423	HIS	-	expression tag	UNP A0A678ZGP6
W	424	HIS	-	expression tag	UNP A0A678ZGP6
Y	10	GLY	-	linker	UNP Q6NSI4
Y	11	GLY	-	linker	UNP Q6NSI4
Y	12	GLY	-	linker	UNP Q6NSI4
Y	13	GLY	-	linker	UNP Q6NSI4
Y	14	SER	-	linker	UNP Q6NSI4
Y	15	GLY	-	linker	UNP Q6NSI4
Y	16	GLY	-	linker	UNP Q6NSI4
Y	17	GLY	-	linker	UNP Q6NSI4
Y	18	GLY	-	linker	UNP Q6NSI4
Y	19	SER	-	linker	UNP Q6NSI4
Y	20	GLY	-	linker	UNP Q6NSI4
Y	21	GLY	-	linker	UNP Q6NSI4
Y	22	GLY	-	linker	UNP Q6NSI4
Y	23	GLY	-	linker	UNP Q6NSI4
Y	24	SER	-	linker	UNP Q6NSI4
Y	124	GLY	-	linker	UNP P16213
Y	125	GLY	-	linker	UNP P16213
Y	126	GLY	-	linker	UNP P16213
Y	127	GLY	-	linker	UNP P16213
Y	128	SER	-	linker	UNP P16213
Y	129	GLY	-	linker	UNP P16213
Y	130	GLY	-	linker	UNP P16213
Y	131	GLY	-	linker	UNP P16213
Y	132	GLY	-	linker	UNP P16213
Y	133	SER	-	linker	UNP P16213
Y	134	GLY	-	linker	UNP P16213
Y	135	GLY	-	linker	UNP P16213
Y	136	GLY	-	linker	UNP P16213
Y	137	GLY	-	linker	UNP P16213
Y	138	SER	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	139	GLY	-	linker	UNP P16213
Y	140	GLY	-	linker	UNP P16213
Y	141	GLY	-	linker	UNP P16213
Y	142	GLY	-	linker	UNP P16213
Y	143	SER	-	linker	UNP P16213
Y	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
Y	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
Y	419	HIS	-	expression tag	UNP A0A678ZGP6
Y	420	HIS	-	expression tag	UNP A0A678ZGP6
Y	421	HIS	-	expression tag	UNP A0A678ZGP6
Y	422	HIS	-	expression tag	UNP A0A678ZGP6
Y	423	HIS	-	expression tag	UNP A0A678ZGP6
Y	424	HIS	-	expression tag	UNP A0A678ZGP6
a	10	GLY	-	linker	UNP Q6NSI4
a	11	GLY	-	linker	UNP Q6NSI4
a	12	GLY	-	linker	UNP Q6NSI4
a	13	GLY	-	linker	UNP Q6NSI4
a	14	SER	-	linker	UNP Q6NSI4
a	15	GLY	-	linker	UNP Q6NSI4
a	16	GLY	-	linker	UNP Q6NSI4
a	17	GLY	-	linker	UNP Q6NSI4
a	18	GLY	-	linker	UNP Q6NSI4
a	19	SER	-	linker	UNP Q6NSI4
a	20	GLY	-	linker	UNP Q6NSI4
a	21	GLY	-	linker	UNP Q6NSI4
a	22	GLY	-	linker	UNP Q6NSI4
a	23	GLY	-	linker	UNP Q6NSI4
a	24	SER	-	linker	UNP Q6NSI4
a	124	GLY	-	linker	UNP P16213
a	125	GLY	-	linker	UNP P16213
a	126	GLY	-	linker	UNP P16213
a	127	GLY	-	linker	UNP P16213
a	128	SER	-	linker	UNP P16213
a	129	GLY	-	linker	UNP P16213
a	130	GLY	-	linker	UNP P16213
a	131	GLY	-	linker	UNP P16213
a	132	GLY	-	linker	UNP P16213
a	133	SER	-	linker	UNP P16213
a	134	GLY	-	linker	UNP P16213
a	135	GLY	-	linker	UNP P16213
a	136	GLY	-	linker	UNP P16213
a	137	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
a	138	SER	-	linker	UNP P16213
a	139	GLY	-	linker	UNP P16213
a	140	GLY	-	linker	UNP P16213
a	141	GLY	-	linker	UNP P16213
a	142	GLY	-	linker	UNP P16213
a	143	SER	-	linker	UNP P16213
a	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
a	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
a	419	HIS	-	expression tag	UNP A0A678ZGP6
a	420	HIS	-	expression tag	UNP A0A678ZGP6
a	421	HIS	-	expression tag	UNP A0A678ZGP6
a	422	HIS	-	expression tag	UNP A0A678ZGP6
a	423	HIS	-	expression tag	UNP A0A678ZGP6
a	424	HIS	-	expression tag	UNP A0A678ZGP6
c	10	GLY	-	linker	UNP Q6NSI4
c	11	GLY	-	linker	UNP Q6NSI4
c	12	GLY	-	linker	UNP Q6NSI4
c	13	GLY	-	linker	UNP Q6NSI4
c	14	SER	-	linker	UNP Q6NSI4
c	15	GLY	-	linker	UNP Q6NSI4
c	16	GLY	-	linker	UNP Q6NSI4
c	17	GLY	-	linker	UNP Q6NSI4
c	18	GLY	-	linker	UNP Q6NSI4
c	19	SER	-	linker	UNP Q6NSI4
c	20	GLY	-	linker	UNP Q6NSI4
c	21	GLY	-	linker	UNP Q6NSI4
c	22	GLY	-	linker	UNP Q6NSI4
c	23	GLY	-	linker	UNP Q6NSI4
c	24	SER	-	linker	UNP Q6NSI4
c	124	GLY	-	linker	UNP P16213
c	125	GLY	-	linker	UNP P16213
c	126	GLY	-	linker	UNP P16213
c	127	GLY	-	linker	UNP P16213
c	128	SER	-	linker	UNP P16213
c	129	GLY	-	linker	UNP P16213
c	130	GLY	-	linker	UNP P16213
c	131	GLY	-	linker	UNP P16213
c	132	GLY	-	linker	UNP P16213
c	133	SER	-	linker	UNP P16213
c	134	GLY	-	linker	UNP P16213
c	135	GLY	-	linker	UNP P16213
c	136	GLY	-	linker	UNP P16213

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Chain	Residue	Modelled	Actual	Comment	Reference
c	137	GLY	-	linker	UNP P16213
c	138	SER	-	linker	UNP P16213
c	139	GLY	-	linker	UNP P16213
c	140	GLY	-	linker	UNP P16213
c	141	GLY	-	linker	UNP P16213
c	142	GLY	-	linker	UNP P16213
c	143	SER	-	linker	UNP P16213
c	227	CYS	TYR	engineered mutation	UNP A0A678ZGP6
c	282	CYS	ALA	engineered mutation	UNP A0A678ZGP6
c	419	HIS	-	expression tag	UNP A0A678ZGP6
c	420	HIS	-	expression tag	UNP A0A678ZGP6
c	421	HIS	-	expression tag	UNP A0A678ZGP6
c	422	HIS	-	expression tag	UNP A0A678ZGP6
c	423	HIS	-	expression tag	UNP A0A678ZGP6
c	424	HIS	-	expression tag	UNP A0A678ZGP6
e	10	GLY	-	linker	UNP Q6NSI4
e	11	GLY	-	linker	UNP Q6NSI4
e	12	GLY	-	linker	UNP Q6NSI4
e	13	GLY	-	linker	UNP Q6NSI4
e	14	SER	-	linker	UNP Q6NSI4
e	15	GLY	-	linker	UNP Q6NSI4
e	16	GLY	-	linker	UNP Q6NSI4
e	17	GLY	-	linker	UNP Q6NSI4
e	18	GLY	-	linker	UNP Q6NSI4
e	19	SER	-	linker	UNP Q6NSI4
e	20	GLY	-	linker	UNP Q6NSI4
e	21	GLY	-	linker	UNP Q6NSI4
e	22	GLY	-	linker	UNP Q6NSI4
e	23	GLY	-	linker	UNP Q6NSI4
e	24	SER	-	linker	UNP Q6NSI4
e	124	GLY	-	linker	UNP P16213
e	125	GLY	-	linker	UNP P16213
e	126	GLY	-	linker	UNP P16213
e	127	GLY	-	linker	UNP P16213
e	128	SER	-	linker	UNP P16213
e	129	GLY	-	linker	UNP P16213
e	130	GLY	-	linker	UNP P16213
e	131	GLY	-	linker	UNP P16213
e	132	GLY	-	linker	UNP P16213
e	133	SER	-	linker	UNP P16213
e	134	GLY	-	linker	UNP P16213
e	135	GLY	-	linker	UNP P16213

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

- Molecule 2 is a protein called VHH.

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

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

- Molecule 3 is water.

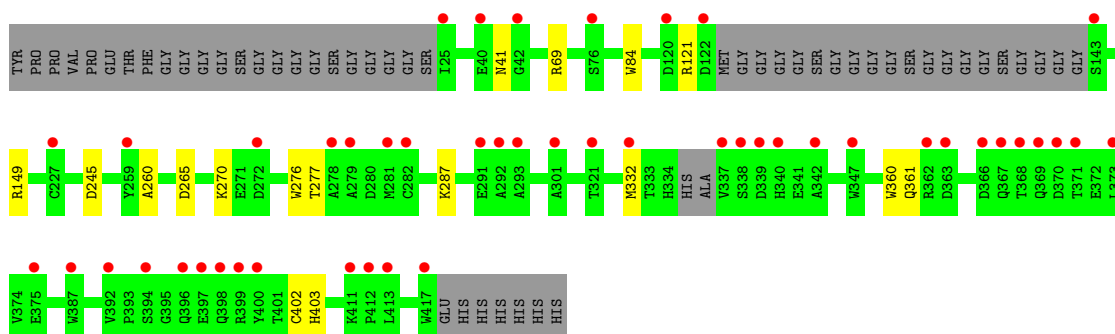
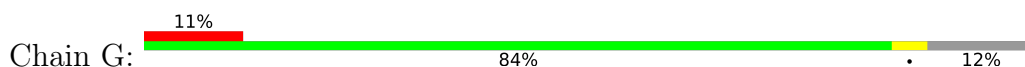
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	9	Total	O	0	0
			9	9		
3	C	10	Total	O	0	0
			10	10		
3	D	11	Total	O	0	0
			11	11		
3	E	10	Total	O	0	0
			10	10		
3	F	7	Total	O	0	0
			7	7		
3	G	1	Total	O	0	0
			1	1		
3	H	3	Total	O	0	0
			3	3		
3	I	1	Total	O	0	0
			1	1		
3	J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

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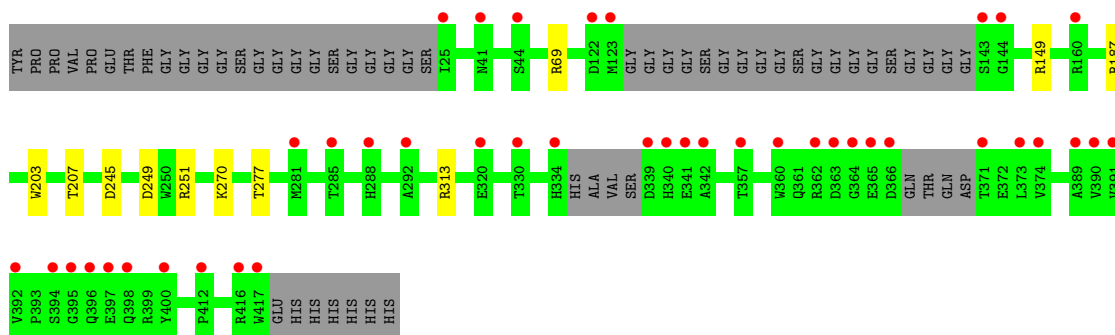
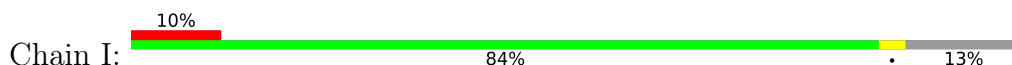
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	4	Total 4	O 4	0	0
3	R	2	Total 2	O 2	0	0
3	S	1	Total 1	O 1	0	0
3	T	1	Total 1	O 1	0	0
3	V	3	Total 3	O 3	0	0
3	W	1	Total 1	O 1	0	0
3	X	2	Total 2	O 2	0	0
3	Z	1	Total 1	O 1	0	0
3	b	1	Total 1	O 1	0	0
3	d	2	Total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

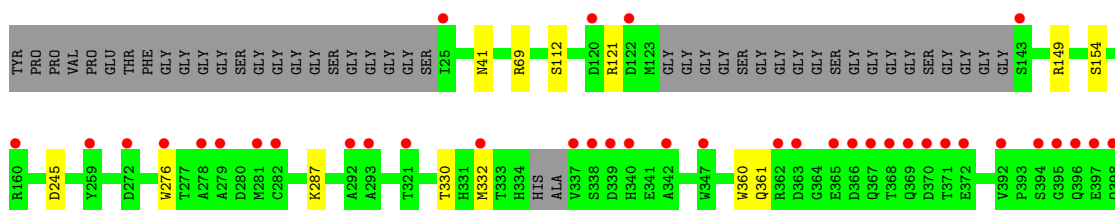
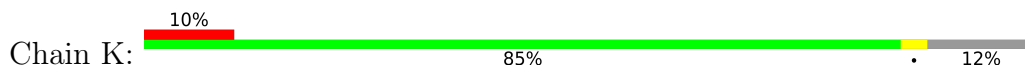
- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

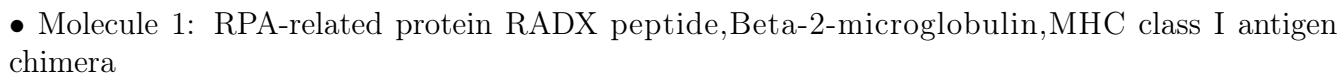


- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera

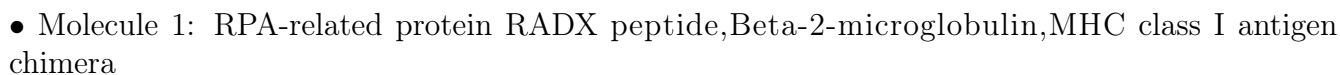


- Molecule 1: RPA-related protein RADX peptide, Beta-2-microglobulin, MHC class I antigen chimera



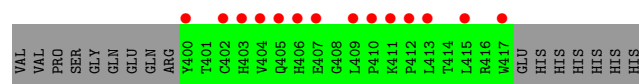


Frequency	Percentage
Daily	22%
Often	71%
Sometimes	9%
Never	20%

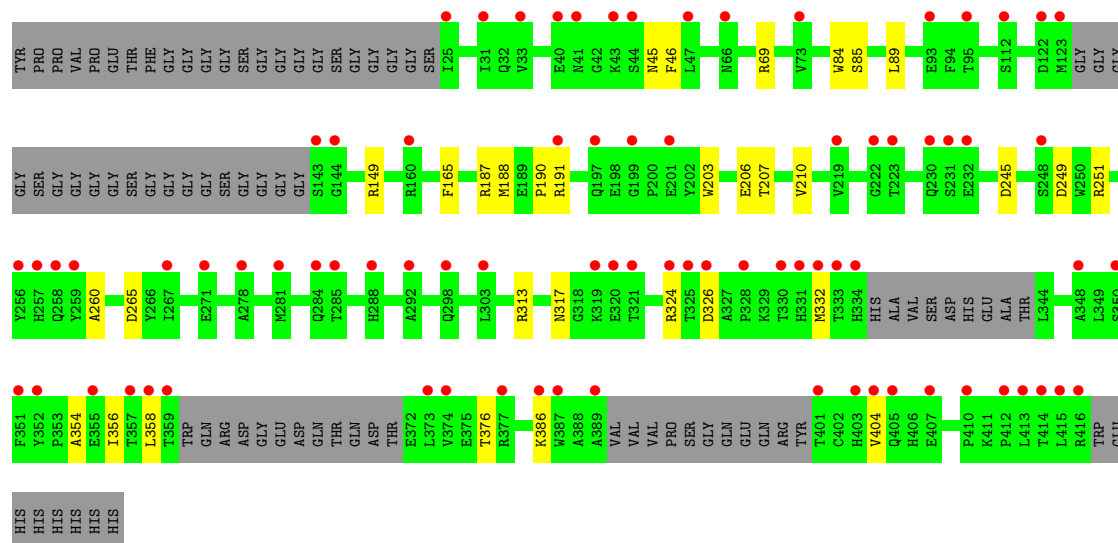
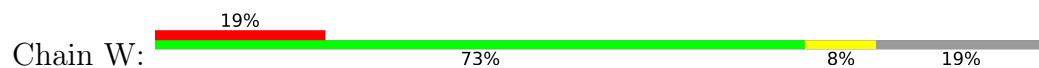


Response	Percentage
Yes	25%
No	75%
Don't know	6%
No answer	19%

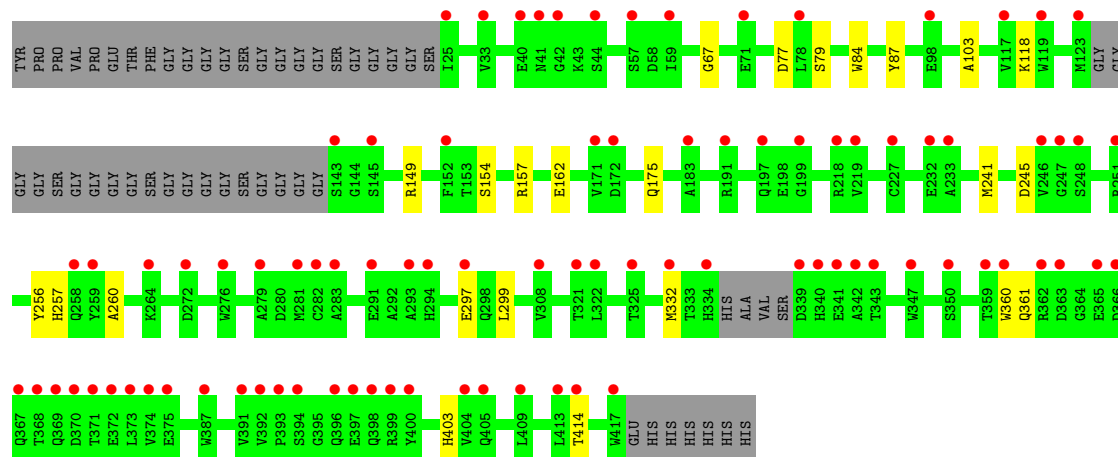
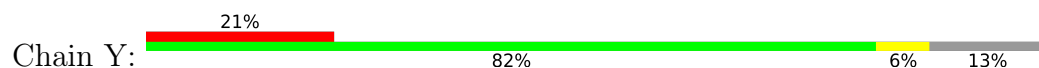




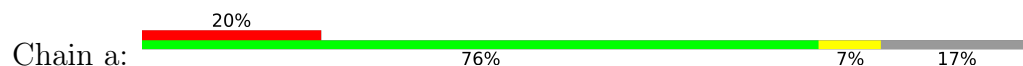
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

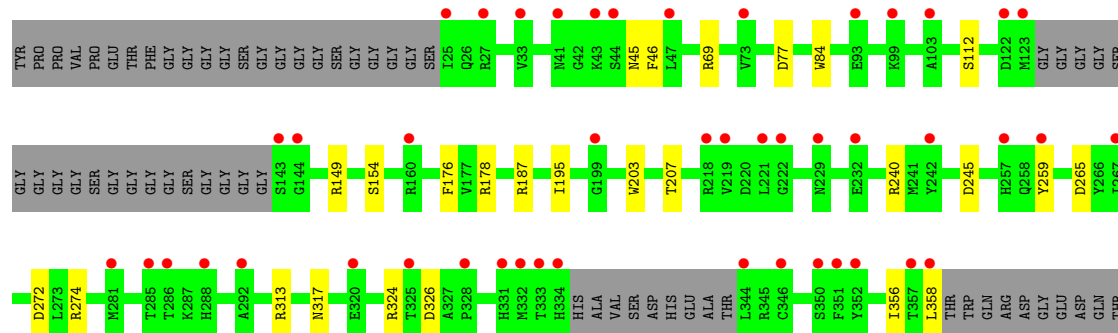


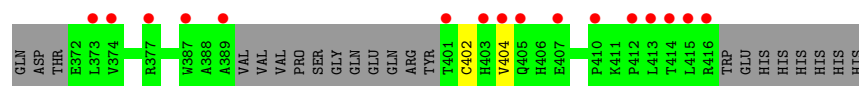
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera



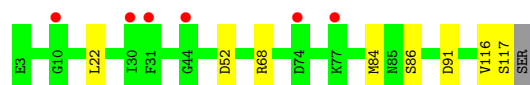
- Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera



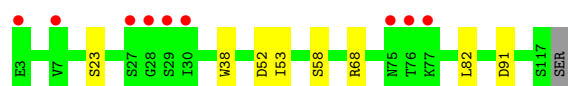




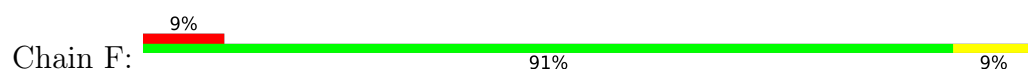
• Molecule 2: VHH



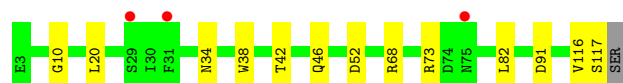
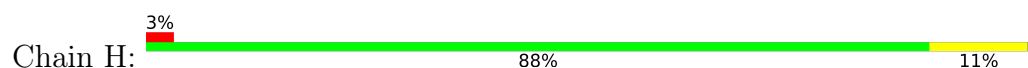
• Molecule 2: VHH



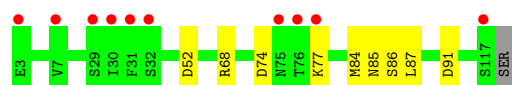
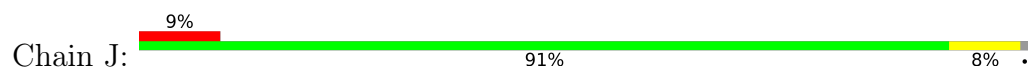
• Molecule 2: VHH



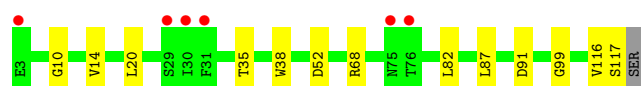
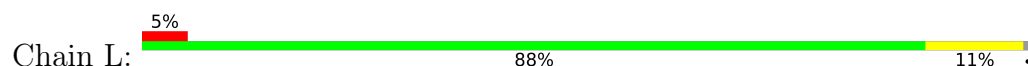
• Molecule 2: VHH



• Molecule 2: VHH



• Molecule 2: VHH

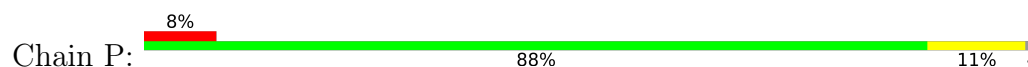


• Molecule 2: VHH

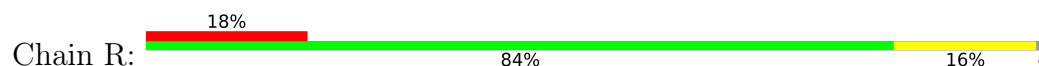




• Molecule 2: VHH



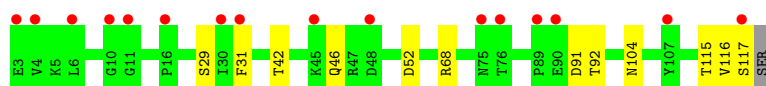
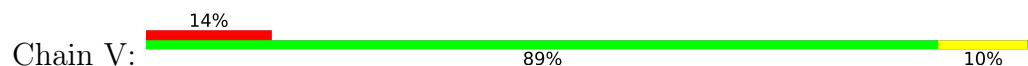
• Molecule 2: VHH



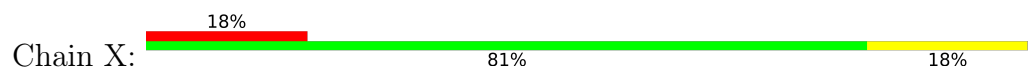
• Molecule 2: VHH



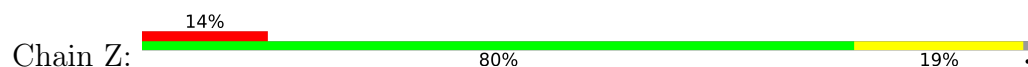
• Molecule 2: VHH



• Molecule 2: VHH

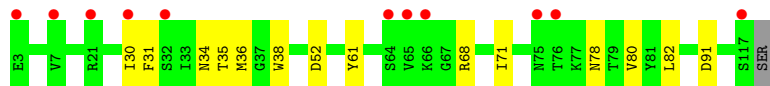


• Molecule 2: VHH



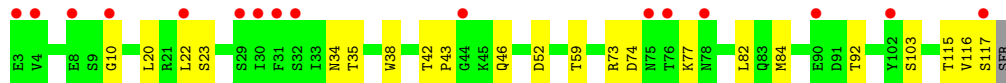
- Molecule 2: VHH

Chain b:  9% 87% 12%

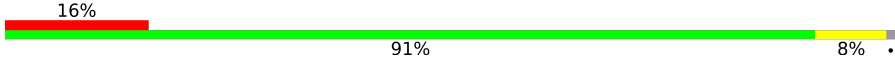


- Molecule 2: VHH

Chain d:  14% 80% 19%



- Molecule 2: VHH

Chain f:  16% 91% 8%



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/2856	0.27	0/3901
1	C	0.11	0/2842	0.26	0/3875
1	E	0.13	0/2882	0.29	0/3929
1	G	0.11	0/2894	0.27	0/3952
1	I	0.11	0/2868	0.27	0/3913
1	K	0.11	0/2906	0.28	0/3968
1	M	0.11	0/2738	0.28	0/3732
1	O	0.11	0/2842	0.28	0/3878
1	Q	0.12	0/2850	0.27	0/3895
1	S	0.13	0/2664	0.28	0/3636
1	U	0.10	0/2585	0.27	0/3533
1	W	0.11	0/2686	0.26	0/3661
1	Y	0.11	0/2842	0.27	0/3888
1	a	0.16	1/2725 (0.0%)	0.29	0/3721
1	c	0.10	0/2621	0.26	0/3576
1	e	0.13	0/2678	0.27	0/3651
2	B	0.12	0/865	0.30	0/1173
2	D	0.14	0/857	0.29	0/1163
2	F	0.12	0/857	0.29	0/1164
2	H	0.12	0/863	0.28	0/1171
2	J	0.12	0/861	0.29	0/1168
2	L	0.13	0/862	0.29	0/1169
2	N	0.13	0/862	0.30	0/1169
2	P	0.14	0/869	0.32	0/1178
2	R	0.10	0/858	0.30	0/1164
2	T	0.12	0/864	0.29	0/1172
2	V	0.12	0/856	0.29	0/1162
2	X	0.12	0/858	0.31	0/1164
2	Z	0.12	0/860	0.29	0/1166
2	b	0.10	0/865	0.26	0/1174
2	d	0.10	0/860	0.27	0/1166
2	f	0.11	0/862	0.29	0/1169
All	All	0.12	1/58258 (0.0%)	0.28	0/79401

All (1) bond length outliers are listed below:

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

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 339 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:240:ARG:NH2	1:e:259:TYR:OH	1.83	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:240:ARG:CZ	1:e:259:TYR:OH	2.22	0.87
1:G:276:TRP:O	1:G:287:LYS:NZ	2.13	0.81
1:e:240:ARG:HE	1:e:259:TYR:HE1	1.24	0.81
1:Q:276:TRP:HB2	1:Q:287:LYS:HE2	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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%)	257 (100%)	1 (0%)	84	93
1	C	263/347 (76%)	261 (99%)	2 (1%)	73	88
1	E	269/347 (78%)	268 (100%)	1 (0%)	84	93
1	G	263/347 (76%)	262 (100%)	1 (0%)	84	93
1	I	263/347 (76%)	263 (100%)	0	100	100
1	K	263/347 (76%)	261 (99%)	2 (1%)	73	88
1	M	253/347 (73%)	252 (100%)	1 (0%)	84	93
1	O	261/347 (75%)	260 (100%)	1 (0%)	84	93
1	Q	254/347 (73%)	252 (99%)	2 (1%)	73	88
1	S	245/347 (71%)	244 (100%)	1 (0%)	84	93
1	U	224/347 (65%)	221 (99%)	3 (1%)	61	83
1	W	248/347 (72%)	246 (99%)	2 (1%)	73	88
1	Y	251/347 (72%)	250 (100%)	1 (0%)	84	93

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

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	401	THR
1	e	154	SER
1	U	248	SER
2	d	23	SER
1	U	175	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	113	GLN

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Mol	Chain	Res	Type
1	c	37	HIS
1	Y	37	HIS
1	a	288	HIS
1	e	113	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/423 (87%)	0.87	60 (16%) 4 4	38, 64, 128, 165	0
1	C	360/423 (85%)	0.59	41 (11%) 10 8	34, 57, 120, 151	0
1	E	364/423 (86%)	0.56	38 (10%) 11 10	37, 58, 109, 147	0
1	G	371/423 (87%)	0.72	48 (12%) 7 6	32, 61, 112, 145	0
1	I	366/423 (86%)	0.51	42 (11%) 9 8	37, 57, 114, 165	0
1	K	372/423 (87%)	0.65	44 (11%) 9 7	31, 60, 114, 146	0
1	M	347/423 (82%)	0.72	44 (12%) 8 7	36, 58, 112, 137	0
1	O	363/423 (85%)	0.54	41 (11%) 10 8	37, 56, 117, 170	0
1	Q	371/423 (87%)	1.52	90 (24%) 2 1	58, 87, 131, 157	0
1	S	340/423 (80%)	1.51	95 (27%) 1 1	60, 86, 130, 155	0
1	U	343/423 (81%)	1.72	107 (31%) 1 1	57, 90, 137, 172	0
1	W	341/423 (80%)	1.43	80 (23%) 2 1	57, 82, 125, 171	0
1	Y	370/423 (87%)	1.37	89 (24%) 2 1	54, 81, 125, 165	0
1	a	352/423 (83%)	1.38	83 (23%) 2 1	55, 82, 130, 154	0
1	c	345/423 (81%)	1.60	94 (27%) 1 1	53, 85, 134, 170	0
1	e	340/423 (80%)	1.24	62 (18%) 3 3	52, 78, 120, 147	0
2	B	115/116 (99%)	0.13	6 (5%) 33 29	33, 47, 91, 123	0
2	D	115/116 (99%)	0.23	9 (7%) 19 16	33, 49, 99, 122	0
2	F	115/116 (99%)	0.21	10 (8%) 16 13	33, 50, 93, 143	0
2	H	115/116 (99%)	0.14	3 (2%) 57 54	36, 48, 93, 135	0
2	J	115/116 (99%)	0.24	10 (8%) 16 13	35, 48, 89, 134	0
2	L	115/116 (99%)	0.15	6 (5%) 33 29	34, 47, 94, 126	0
2	N	115/116 (99%)	0.17	8 (6%) 22 19	32, 46, 94, 111	0
2	P	115/116 (99%)	0.20	9 (7%) 19 16	31, 48, 96, 127	0

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

The worst 5 of 1254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	143	SER	11.1
1	M	143	SER	9.5
1	U	347	TRP	9.3
1	Y	143	SER	9.1
1	C	143	SER	8.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.