wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 02:40 PM EDT

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

This is a 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 (i) 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 (i)) were used in the production of this report:

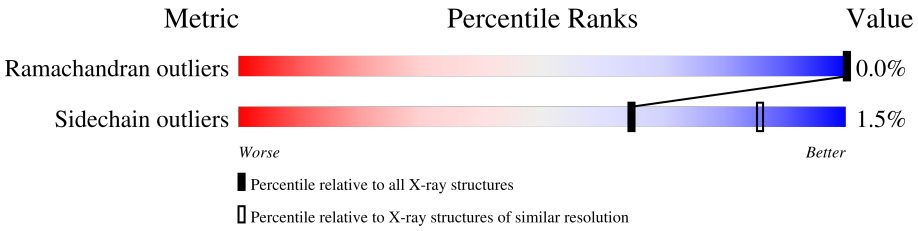
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

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

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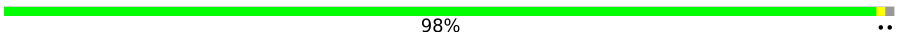
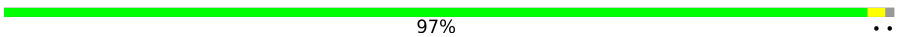
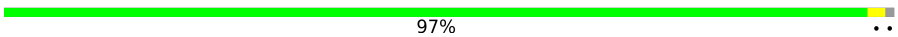
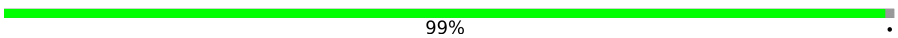
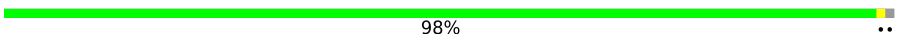
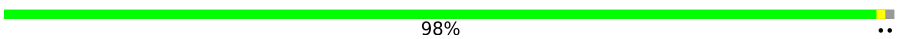
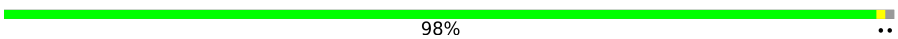
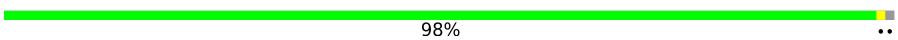
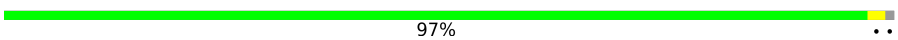
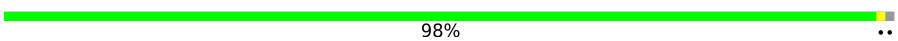
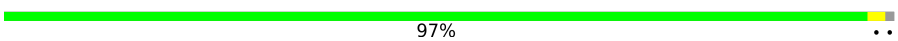
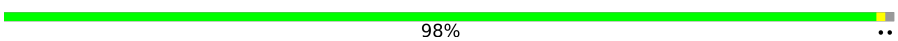
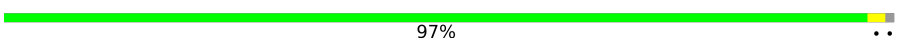
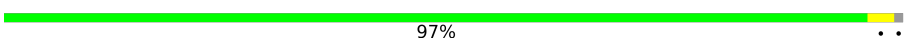
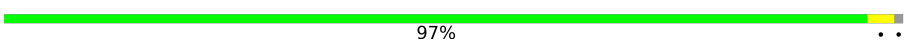
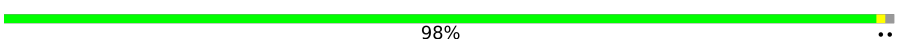
Mol	Chain	Length	Quality of chain
1	S	423	
1	U	423	
1	W	423	
1	Y	423	
1	a	423	
1	c	423	
1	e	423	
2	B	116	
2	D	116	
2	F	116	
2	H	116	
2	J	116	
2	L	116	
2	N	116	
2	P	116	
2	R	116	
2	T	116	
2	V	116	
2	X	116	
2	Z	116	
2	b	116	
2	d	116	
2	f	116	

2 Entry composition (i)

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

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

- Molecule 1 is a protein called RPA-related protein RADX peptide,Beta-2-microglobulin,MHC 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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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	4	Total O 4 4	0	0
3	R	2	Total O 2 2	0	0
3	S	1	Total O 1 1	0	0
3	T	1	Total O 1 1	0	0
3	V	3	Total O 3 3	0	0
3	W	1	Total O 1 1	0	0
3	X	2	Total O 2 2	0	0
3	Z	1	Total O 1 1	0	0
3	b	1	Total O 1 1	0	0
3	d	2	Total O 2 2	0	0
3	e	3	Total O 3 3	0	0
3	f	2	Total O 2 2	0	0

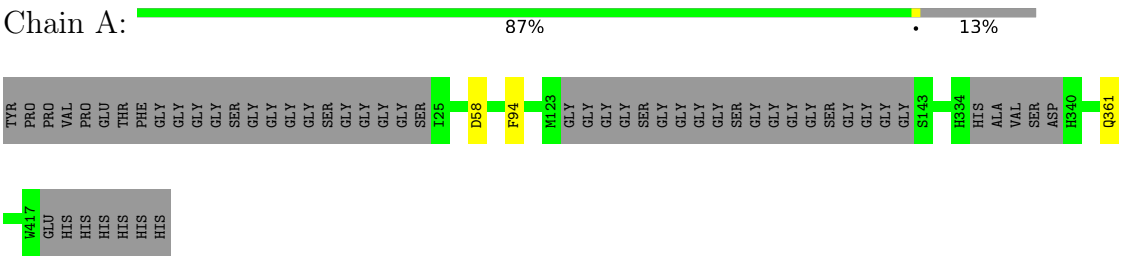
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

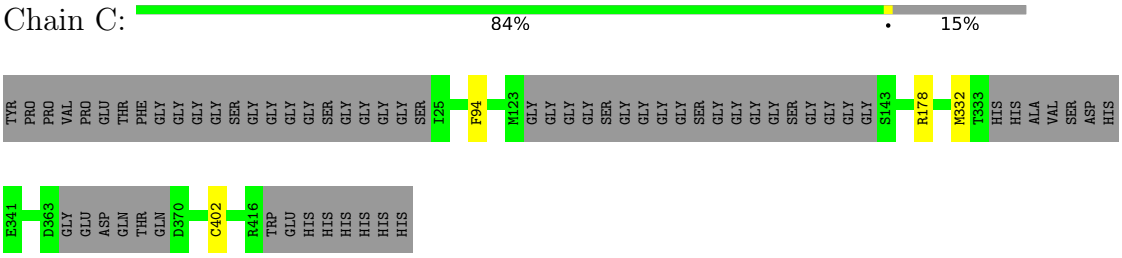
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain A:



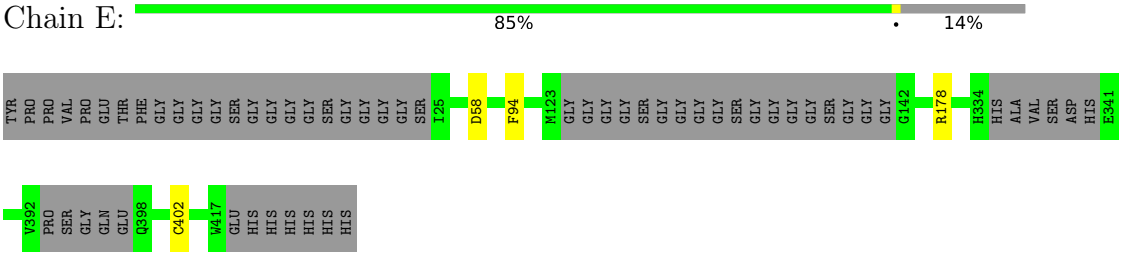
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain C:



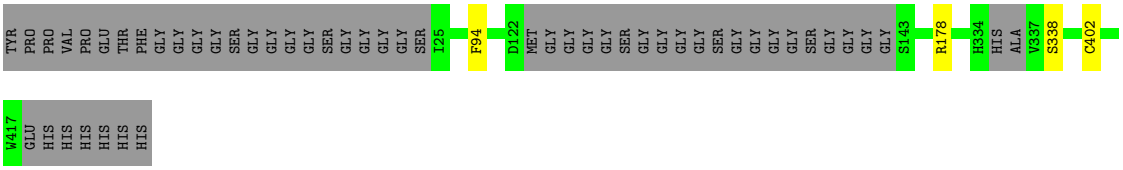
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain E:



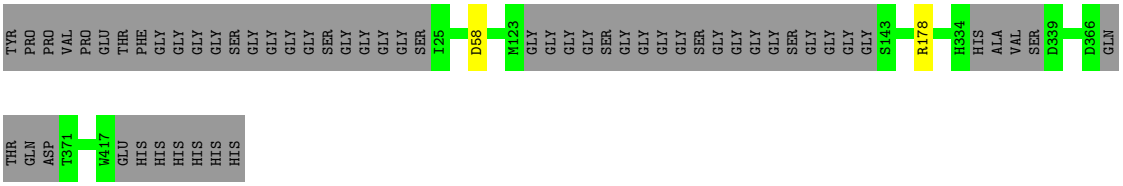
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain G:



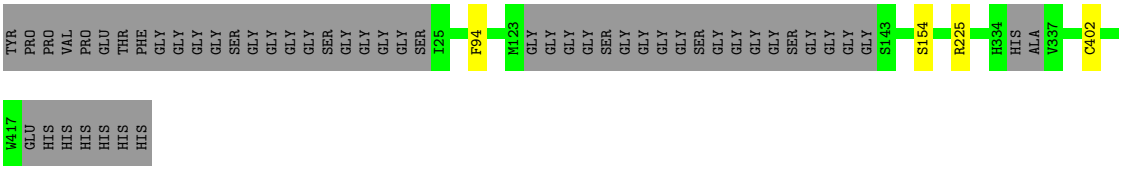
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain I:



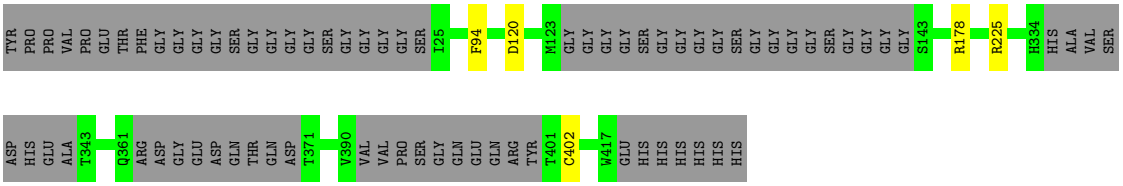
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain K:



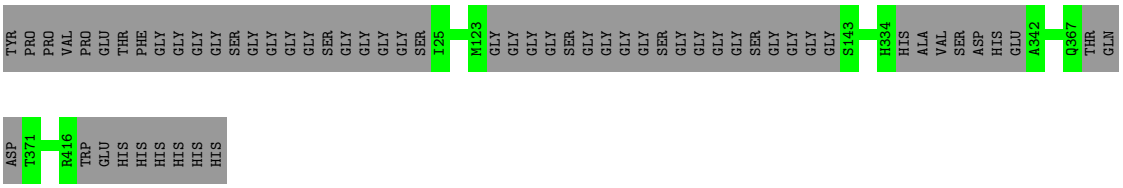
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain M:



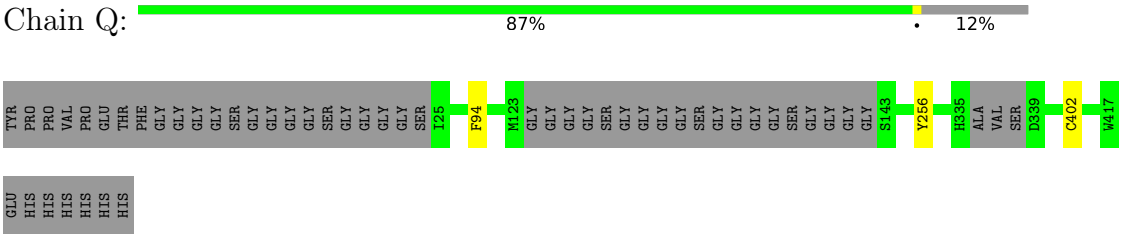
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain O:



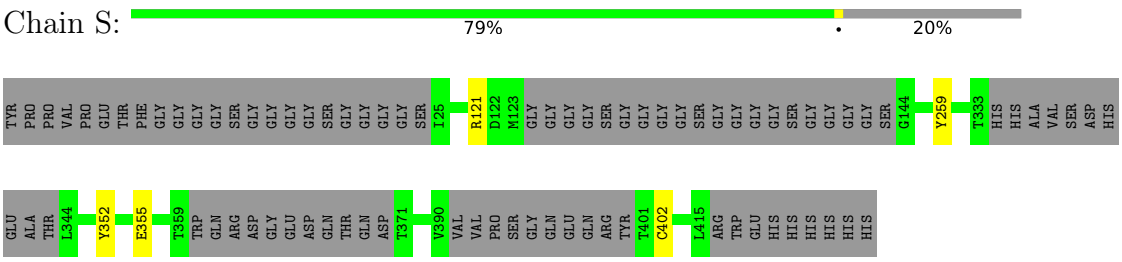
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain Q:



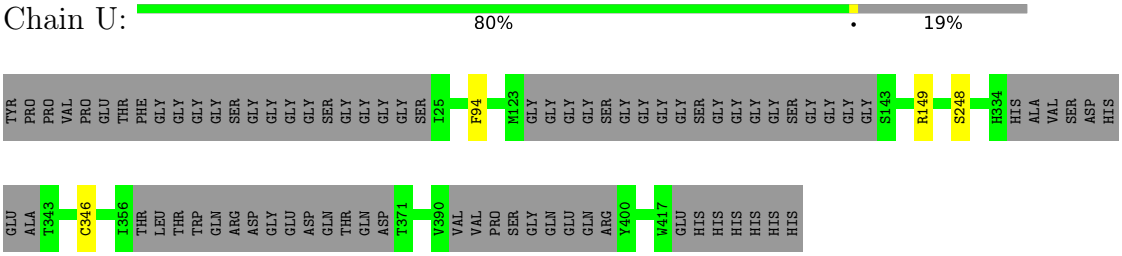
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain S:



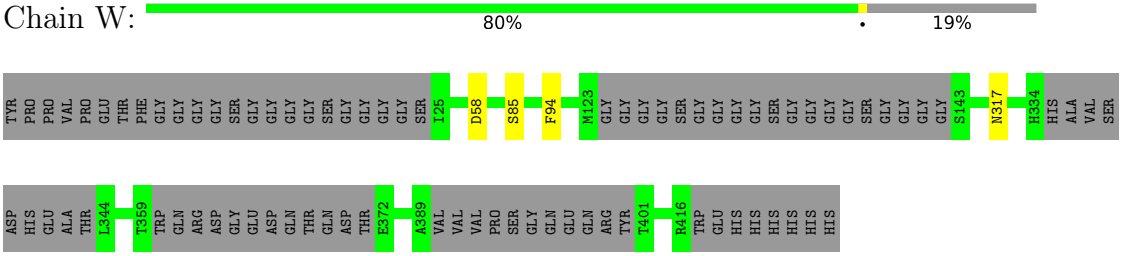
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain U:



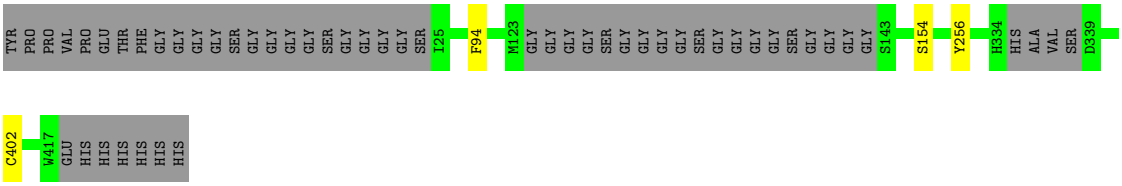
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain W:



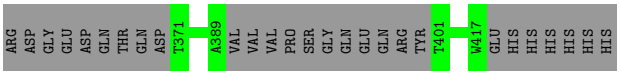
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain Y:



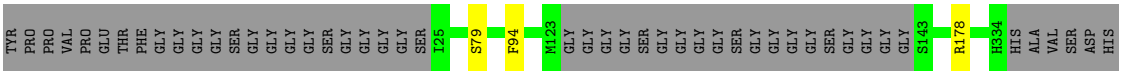
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

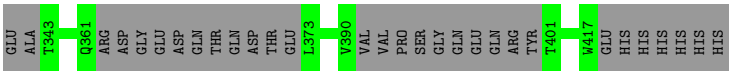
Chain a:



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

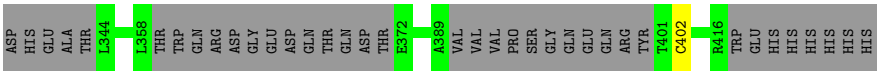
Chain c:





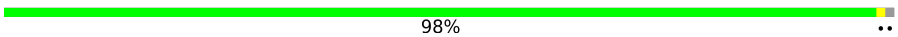
• Molecule 1: RPA-related protein RADX peptide,Beta-2-microglobulin,MHC class I antigen chimera

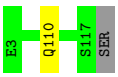
Chain e:



• Molecule 2: VHH

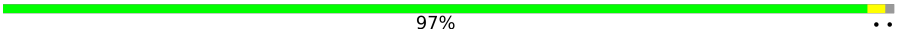
Chain B:



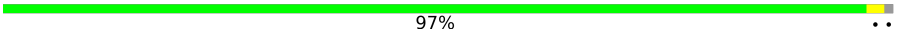


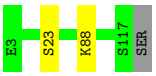
• Molecule 2: VHH

Chain D:

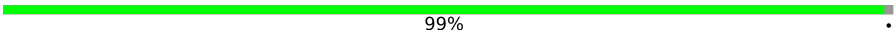


• Molecule 2: VHH

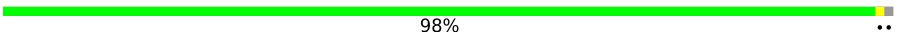
Chain F: 

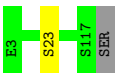


• Molecule 2: VHH

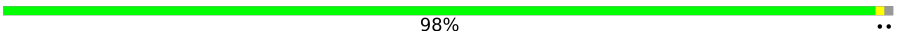
Chain H: 

• Molecule 2: VHH

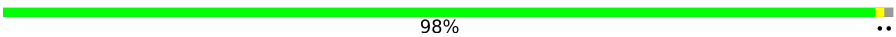
Chain J: 

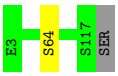


• Molecule 2: VHH

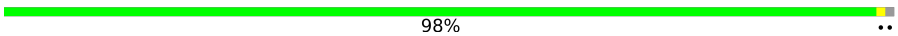
Chain L: 

• Molecule 2: VHH

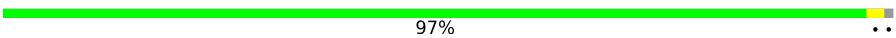
Chain N: 



• Molecule 2: VHH

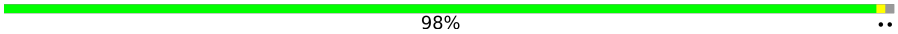
Chain P: 

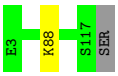
• Molecule 2: VHH

Chain R: 

• Molecule 2: VHH

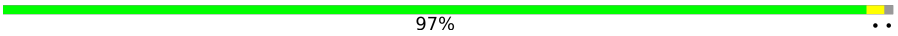
Chain T:

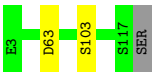




• Molecule 2: VHH

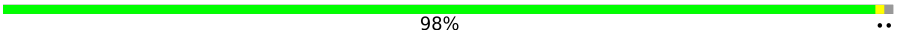
Chain V:

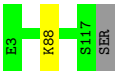




• Molecule 2: VHH

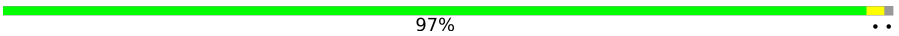
Chain X:

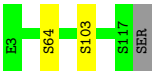




• Molecule 2: VHH

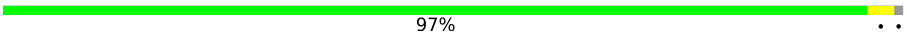
Chain Z:

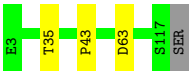




• Molecule 2: VHH

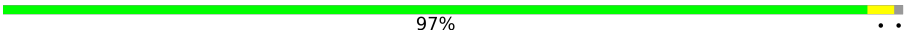
Chain b:

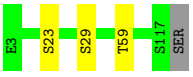




• Molecule 2: VHH

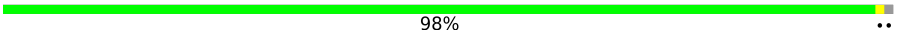
Chain d:

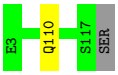




• Molecule 2: VHH

Chain f:




E3
Q110
S117
SER

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	117.59Å 118.09Å 273.73Å 102.44° 102.41° 89.88°	Depositor
Resolution (Å)	48.86 – 2.70	Depositor
% Data completeness (in resolution range)	94.3 (48.86-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.242 , 0.276	Depositor
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.281	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	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
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.*

[1] Intensities estimated from amplitudes.

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	259	TYR	CD1-CE1	-6.13	1.30	1.39
1	a	200	PRO	N-CD	-5.39	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

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

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

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	402	CYS
2	d	29	SER
2	Z	103	SER
2	b	43	PRO
1	e	154	SER

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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