wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 11:29 AM EDT

PDB ID	:	7SSH
Title	:	Single chain trimer HLA-A*02:01 (Y108A) with HPV.16 E7 peptide YMLDLQPETTDLYC
Authors	:	Finton, K.A.K.; Rupert, P.B.
Deposited on	:	2021-11-11
Resolution	:	2.73 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 (1)) were used in the production of this report:

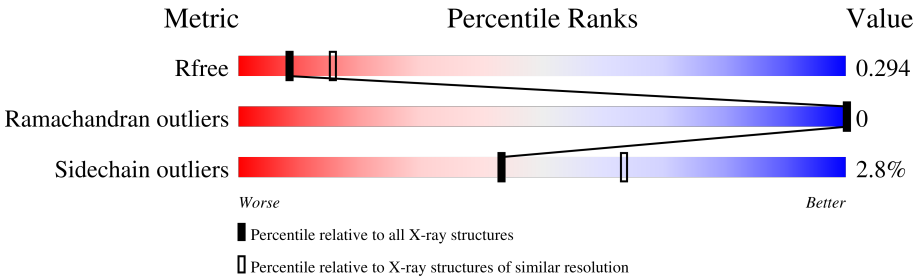
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.73 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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%

Mol	Chain	Length	Quality of chain
1	A	429	84% · 14%
1	C	429	84% · 15%
1	E	429	83% · 16%
1	G	429	87% · 11%
1	I	429	81% · 16%
1	K	429	88% · 11%
1	M	429	86% · 12%
1	O	429	82% · 16%

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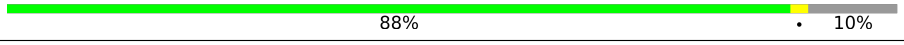
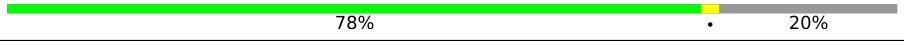
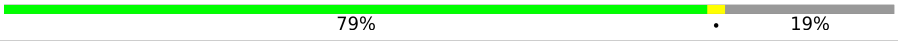
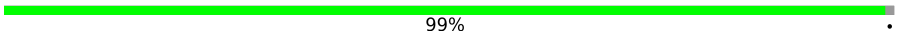
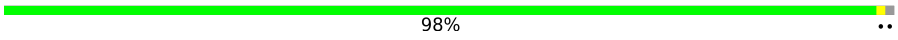
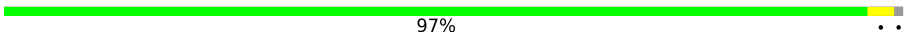
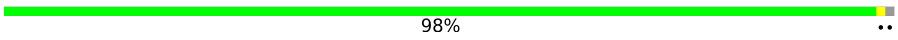
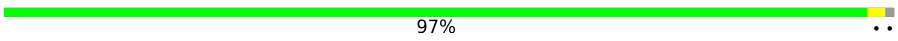
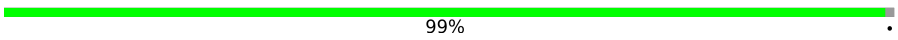
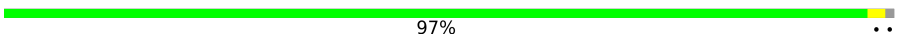
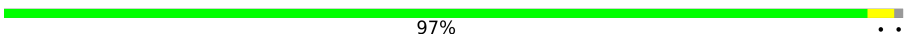
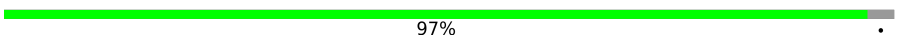
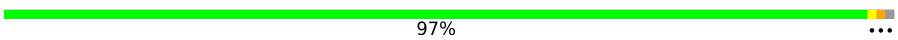
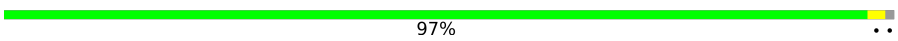
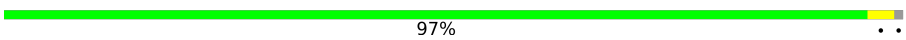
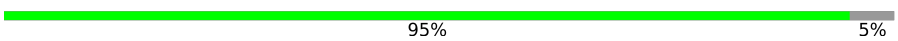
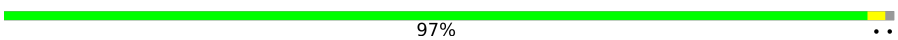
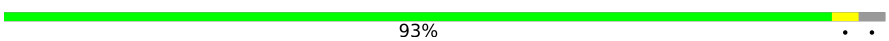
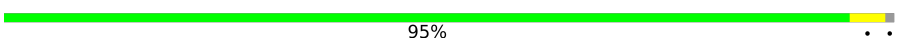
Mol	Chain	Length	Quality of chain
1	Q	429	
1	S	429	
1	U	429	
1	W	429	
1	Y	429	
1	a	429	
1	c	429	
1	e	429	
2	B	116	
2	D	116	
2	F	116	
2	H	116	
2	J	116	
2	L	116	
2	N	116	
2	P	116	
2	R	116	
2	T	116	
2	V	116	
2	X	116	
2	Z	116	
2	b	116	
2	d	116	
2	f	116	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 106611 atoms, of which 49728 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	S	0	0	0
			5214	1754	2439	492	518	11			
1	C	366	Total	C	H	N	O	S	0	0	0
			5188	1752	2419	489	518	10			
1	E	362	Total	C	H	N	O	S	0	0	0
			5262	1765	2475	492	520	10			
1	G	382	Total	C	H	N	O	S	0	0	0
			5419	1829	2530	512	537	11			
1	I	359	Total	C	H	N	O	S	0	0	0
			5157	1737	2423	484	502	11			
1	K	382	Total	C	H	N	O	S	0	0	0
			5399	1824	2516	512	536	11			
1	M	378	Total	C	H	N	O	S	0	0	0
			5337	1803	2488	505	530	11			
1	O	361	Total	C	H	N	O	S	0	0	0
			5193	1745	2435	492	510	11			
1	Q	384	Total	C	H	N	O	S	0	0	0
			5283	1801	2437	499	535	11			
1	S	344	Total	C	H	N	O	S	0	0	0
			4879	1657	2261	463	488	10			
1	U	333	Total	C	H	N	O	S	0	0	0
			4572	1574	2100	422	466	10			
1	W	347	Total	C	H	N	O	S	0	0	0
			4782	1634	2195	450	493	10			
1	Y	365	Total	C	H	N	O	S	0	0	0
			5030	1720	2319	470	510	11			
1	a	342	Total	C	H	N	O	S	0	0	0
			4808	1635	2226	450	487	10			
1	c	327	Total	C	H	N	O	S	0	0	0
			4390	1518	2002	410	450	10			
1	e	353	Total	C	H	N	O	S	0	0	0
			4796	1645	2198	452	491	10			

There are 672 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10E	GLY	-	linker	UNP P03129
A	10F	GLY	-	linker	UNP P03129
A	10G	GLY	-	linker	UNP P03129
A	10H	GLY	-	linker	UNP P03129
A	10I	SER	-	linker	UNP P03129
A	10J	GLY	-	linker	UNP P03129
A	10K	GLY	-	linker	UNP P03129
A	10L	GLY	-	linker	UNP P03129
A	10M	GLY	-	linker	UNP P03129
A	10N	SER	-	linker	UNP P03129
A	10O	GLY	-	linker	UNP P03129
A	10P	GLY	-	linker	UNP P03129
A	10Q	GLY	-	linker	UNP P03129
A	10R	GLY	-	linker	UNP P03129
A	10S	SER	-	linker	UNP P03129
A	124	GLY	-	linker	UNP P16213
A	125	GLY	-	linker	UNP P16213
A	126	GLY	-	linker	UNP P16213
A	127	GLY	-	linker	UNP P16213
A	128	SER	-	linker	UNP P16213
A	129	GLY	-	linker	UNP P16213
A	130	GLY	-	linker	UNP P16213
A	131	GLY	-	linker	UNP P16213
A	132	GLY	-	linker	UNP P16213
A	133	SER	-	linker	UNP P16213
A	134	GLY	-	linker	UNP P16213
A	135	GLY	-	linker	UNP P16213
A	136	GLY	-	linker	UNP P16213
A	137	GLY	-	linker	UNP P16213
A	138	SER	-	linker	UNP P16213
A	139	GLY	-	linker	UNP P16213
A	140	GLY	-	linker	UNP P16213
A	141	GLY	-	linker	UNP P16213
A	142	GLY	-	linker	UNP P16213
A	143	SER	-	linker	UNP P16213
A	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12C	GLY	-	linker	UNP P03129
C	12D	GLY	-	linker	UNP P03129
C	12E	GLY	-	linker	UNP P03129
C	12F	GLY	-	linker	UNP P03129
C	12G	SER	-	linker	UNP P03129
C	12H	GLY	-	linker	UNP P03129
C	12I	GLY	-	linker	UNP P03129
C	12J	GLY	-	linker	UNP P03129
C	12K	GLY	-	linker	UNP P03129
C	12L	SER	-	linker	UNP P03129
C	12M	GLY	-	linker	UNP P03129
C	12N	GLY	-	linker	UNP P03129
C	12O	GLY	-	linker	UNP P03129
C	12P	GLY	-	linker	UNP P03129
C	12Q	SER	-	linker	UNP P03129
C	124	GLY	-	linker	UNP P16213
C	125	GLY	-	linker	UNP P16213
C	126	GLY	-	linker	UNP P16213
C	127	GLY	-	linker	UNP P16213
C	128	SER	-	linker	UNP P16213
C	129	GLY	-	linker	UNP P16213
C	130	GLY	-	linker	UNP P16213
C	131	GLY	-	linker	UNP P16213
C	132	GLY	-	linker	UNP P16213
C	133	SER	-	linker	UNP P16213
C	134	GLY	-	linker	UNP P16213
C	135	GLY	-	linker	UNP P16213
C	136	GLY	-	linker	UNP P16213
C	137	GLY	-	linker	UNP P16213
C	138	SER	-	linker	UNP P16213
C	139	GLY	-	linker	UNP P16213
C	140	GLY	-	linker	UNP P16213
C	141	GLY	-	linker	UNP P16213
C	142	GLY	-	linker	UNP P16213
C	143	SER	-	linker	UNP P16213
C	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	12C	GLY	-	linker	UNP P03129
E	12D	GLY	-	linker	UNP P03129
E	12E	GLY	-	linker	UNP P03129
E	12F	GLY	-	linker	UNP P03129
E	12G	SER	-	linker	UNP P03129
E	12H	GLY	-	linker	UNP P03129
E	12I	GLY	-	linker	UNP P03129
E	12J	GLY	-	linker	UNP P03129
E	12K	GLY	-	linker	UNP P03129
E	12L	SER	-	linker	UNP P03129
E	12M	GLY	-	linker	UNP P03129
E	12N	GLY	-	linker	UNP P03129
E	12O	GLY	-	linker	UNP P03129
E	12P	GLY	-	linker	UNP P03129
E	12Q	SER	-	linker	UNP P03129
E	124	GLY	-	linker	UNP P16213
E	125	GLY	-	linker	UNP P16213
E	126	GLY	-	linker	UNP P16213
E	127	GLY	-	linker	UNP P16213
E	128	SER	-	linker	UNP P16213
E	129	GLY	-	linker	UNP P16213
E	130	GLY	-	linker	UNP P16213
E	131	GLY	-	linker	UNP P16213
E	132	GLY	-	linker	UNP P16213
E	133	SER	-	linker	UNP P16213
E	134	GLY	-	linker	UNP P16213
E	135	GLY	-	linker	UNP P16213
E	136	GLY	-	linker	UNP P16213
E	137	GLY	-	linker	UNP P16213
E	138	SER	-	linker	UNP P16213
E	139	GLY	-	linker	UNP P16213
E	140	GLY	-	linker	UNP P16213
E	141	GLY	-	linker	UNP P16213
E	142	GLY	-	linker	UNP P16213
E	143	SER	-	linker	UNP P16213
E	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	12C	GLY	-	linker	UNP P03129
G	12D	GLY	-	linker	UNP P03129
G	12E	GLY	-	linker	UNP P03129
G	12F	GLY	-	linker	UNP P03129
G	12G	SER	-	linker	UNP P03129
G	12H	GLY	-	linker	UNP P03129
G	12I	GLY	-	linker	UNP P03129
G	12J	GLY	-	linker	UNP P03129
G	12K	GLY	-	linker	UNP P03129
G	12L	SER	-	linker	UNP P03129
G	12M	GLY	-	linker	UNP P03129
G	12N	GLY	-	linker	UNP P03129
G	12O	GLY	-	linker	UNP P03129
G	12P	GLY	-	linker	UNP P03129
G	12Q	SER	-	linker	UNP P03129
G	124	GLY	-	linker	UNP P16213
G	125	GLY	-	linker	UNP P16213
G	126	GLY	-	linker	UNP P16213
G	127	GLY	-	linker	UNP P16213
G	128	SER	-	linker	UNP P16213
G	129	GLY	-	linker	UNP P16213
G	130	GLY	-	linker	UNP P16213
G	131	GLY	-	linker	UNP P16213
G	132	GLY	-	linker	UNP P16213
G	133	SER	-	linker	UNP P16213
G	134	GLY	-	linker	UNP P16213
G	135	GLY	-	linker	UNP P16213
G	136	GLY	-	linker	UNP P16213
G	137	GLY	-	linker	UNP P16213
G	138	SER	-	linker	UNP P16213
G	139	GLY	-	linker	UNP P16213
G	140	GLY	-	linker	UNP P16213
G	141	GLY	-	linker	UNP P16213
G	142	GLY	-	linker	UNP P16213
G	143	SER	-	linker	UNP P16213
G	227	ALA	TYR	engineered mutation	UNP A0A678ZGP6
G	419	HIS	-	expression tag	UNP A0A678ZGP6
G	420	HIS	-	expression tag	UNP A0A678ZGP6
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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	12C	GLY	-	linker	UNP P03129
I	12D	GLY	-	linker	UNP P03129
I	12E	GLY	-	linker	UNP P03129
I	12F	GLY	-	linker	UNP P03129
I	12G	SER	-	linker	UNP P03129
I	12H	GLY	-	linker	UNP P03129
I	12I	GLY	-	linker	UNP P03129
I	12J	GLY	-	linker	UNP P03129
I	12K	GLY	-	linker	UNP P03129
I	12L	SER	-	linker	UNP P03129
I	12M	GLY	-	linker	UNP P03129
I	12N	GLY	-	linker	UNP P03129
I	12O	GLY	-	linker	UNP P03129
I	12P	GLY	-	linker	UNP P03129
I	12Q	SER	-	linker	UNP P03129
I	124	GLY	-	linker	UNP P16213
I	125	GLY	-	linker	UNP P16213
I	126	GLY	-	linker	UNP P16213
I	127	GLY	-	linker	UNP P16213
I	128	SER	-	linker	UNP P16213
I	129	GLY	-	linker	UNP P16213
I	130	GLY	-	linker	UNP P16213
I	131	GLY	-	linker	UNP P16213
I	132	GLY	-	linker	UNP P16213
I	133	SER	-	linker	UNP P16213
I	134	GLY	-	linker	UNP P16213
I	135	GLY	-	linker	UNP P16213
I	136	GLY	-	linker	UNP P16213
I	137	GLY	-	linker	UNP P16213
I	138	SER	-	linker	UNP P16213
I	139	GLY	-	linker	UNP P16213
I	140	GLY	-	linker	UNP P16213
I	141	GLY	-	linker	UNP P16213
I	142	GLY	-	linker	UNP P16213
I	143	SER	-	linker	UNP P16213
I	227	ALA	TYR	engineered mutation	UNP A0A678ZGP6
I	419	HIS	-	expression tag	UNP A0A678ZGP6
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

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Chain	Residue	Modelled	Actual	Comment	Reference
K	12C	GLY	-	linker	UNP P03129
K	12D	GLY	-	linker	UNP P03129
K	12E	GLY	-	linker	UNP P03129
K	12F	GLY	-	linker	UNP P03129
K	12G	SER	-	linker	UNP P03129
K	12H	GLY	-	linker	UNP P03129
K	12I	GLY	-	linker	UNP P03129
K	12J	GLY	-	linker	UNP P03129
K	12K	GLY	-	linker	UNP P03129
K	12L	SER	-	linker	UNP P03129
K	12M	GLY	-	linker	UNP P03129
K	12N	GLY	-	linker	UNP P03129
K	12O	GLY	-	linker	UNP P03129
K	12P	GLY	-	linker	UNP P03129
K	12Q	SER	-	linker	UNP P03129
K	124	GLY	-	linker	UNP P16213
K	125	GLY	-	linker	UNP P16213
K	126	GLY	-	linker	UNP P16213
K	127	GLY	-	linker	UNP P16213
K	128	SER	-	linker	UNP P16213
K	129	GLY	-	linker	UNP P16213
K	130	GLY	-	linker	UNP P16213
K	131	GLY	-	linker	UNP P16213
K	132	GLY	-	linker	UNP P16213
K	133	SER	-	linker	UNP P16213
K	134	GLY	-	linker	UNP P16213
K	135	GLY	-	linker	UNP P16213
K	136	GLY	-	linker	UNP P16213
K	137	GLY	-	linker	UNP P16213
K	138	SER	-	linker	UNP P16213
K	139	GLY	-	linker	UNP P16213
K	140	GLY	-	linker	UNP P16213
K	141	GLY	-	linker	UNP P16213
K	142	GLY	-	linker	UNP P16213
K	143	SER	-	linker	UNP P16213
K	227	ALA	TYR	engineered mutation	UNP A0A678ZGP6
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

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Chain	Residue	Modelled	Actual	Comment	Reference
M	13B	GLY	-	linker	UNP P03129
M	13C	GLY	-	linker	UNP P03129
M	13D	GLY	-	linker	UNP P03129
M	13E	GLY	-	linker	UNP P03129
M	13F	SER	-	linker	UNP P03129
M	13G	GLY	-	linker	UNP P03129
M	13H	GLY	-	linker	UNP P03129
M	13I	GLY	-	linker	UNP P03129
M	13J	GLY	-	linker	UNP P03129
M	13K	SER	-	linker	UNP P03129
M	13L	GLY	-	linker	UNP P03129
M	13M	GLY	-	linker	UNP P03129
M	13N	GLY	-	linker	UNP P03129
M	13O	GLY	-	linker	UNP P03129
M	13P	SER	-	linker	UNP P03129
M	124	GLY	-	linker	UNP P16213
M	125	GLY	-	linker	UNP P16213
M	126	GLY	-	linker	UNP P16213
M	127	GLY	-	linker	UNP P16213
M	128	SER	-	linker	UNP P16213
M	129	GLY	-	linker	UNP P16213
M	130	GLY	-	linker	UNP P16213
M	131	GLY	-	linker	UNP P16213
M	132	GLY	-	linker	UNP P16213
M	133	SER	-	linker	UNP P16213
M	134	GLY	-	linker	UNP P16213
M	135	GLY	-	linker	UNP P16213
M	136	GLY	-	linker	UNP P16213
M	137	GLY	-	linker	UNP P16213
M	138	SER	-	linker	UNP P16213
M	139	GLY	-	linker	UNP P16213
M	140	GLY	-	linker	UNP P16213
M	141	GLY	-	linker	UNP P16213
M	142	GLY	-	linker	UNP P16213
M	143	SER	-	linker	UNP P16213
M	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
O	12C	GLY	-	linker	UNP P03129
O	12D	GLY	-	linker	UNP P03129
O	12E	GLY	-	linker	UNP P03129
O	12F	GLY	-	linker	UNP P03129
O	12G	SER	-	linker	UNP P03129
O	12H	GLY	-	linker	UNP P03129
O	12I	GLY	-	linker	UNP P03129
O	12J	GLY	-	linker	UNP P03129
O	12K	GLY	-	linker	UNP P03129
O	12L	SER	-	linker	UNP P03129
O	12M	GLY	-	linker	UNP P03129
O	12N	GLY	-	linker	UNP P03129
O	12O	GLY	-	linker	UNP P03129
O	12P	GLY	-	linker	UNP P03129
O	12Q	SER	-	linker	UNP P03129
O	124	GLY	-	linker	UNP P16213
O	125	GLY	-	linker	UNP P16213
O	126	GLY	-	linker	UNP P16213
O	127	GLY	-	linker	UNP P16213
O	128	SER	-	linker	UNP P16213
O	129	GLY	-	linker	UNP P16213
O	130	GLY	-	linker	UNP P16213
O	131	GLY	-	linker	UNP P16213
O	132	GLY	-	linker	UNP P16213
O	133	SER	-	linker	UNP P16213
O	134	GLY	-	linker	UNP P16213
O	135	GLY	-	linker	UNP P16213
O	136	GLY	-	linker	UNP P16213
O	137	GLY	-	linker	UNP P16213
O	138	SER	-	linker	UNP P16213
O	139	GLY	-	linker	UNP P16213
O	140	GLY	-	linker	UNP P16213
O	141	GLY	-	linker	UNP P16213
O	142	GLY	-	linker	UNP P16213
O	143	SER	-	linker	UNP P16213
O	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	12C	GLY	-	linker	UNP P03129
Q	12D	GLY	-	linker	UNP P03129
Q	12E	GLY	-	linker	UNP P03129
Q	12F	GLY	-	linker	UNP P03129
Q	12G	SER	-	linker	UNP P03129
Q	12H	GLY	-	linker	UNP P03129
Q	12I	GLY	-	linker	UNP P03129
Q	12J	GLY	-	linker	UNP P03129
Q	12K	GLY	-	linker	UNP P03129
Q	12L	SER	-	linker	UNP P03129
Q	12M	GLY	-	linker	UNP P03129
Q	12N	GLY	-	linker	UNP P03129
Q	12O	GLY	-	linker	UNP P03129
Q	12P	GLY	-	linker	UNP P03129
Q	12Q	SER	-	linker	UNP P03129
Q	124	GLY	-	linker	UNP P16213
Q	125	GLY	-	linker	UNP P16213
Q	126	GLY	-	linker	UNP P16213
Q	127	GLY	-	linker	UNP P16213
Q	128	SER	-	linker	UNP P16213
Q	129	GLY	-	linker	UNP P16213
Q	130	GLY	-	linker	UNP P16213
Q	131	GLY	-	linker	UNP P16213
Q	132	GLY	-	linker	UNP P16213
Q	133	SER	-	linker	UNP P16213
Q	134	GLY	-	linker	UNP P16213
Q	135	GLY	-	linker	UNP P16213
Q	136	GLY	-	linker	UNP P16213
Q	137	GLY	-	linker	UNP P16213
Q	138	SER	-	linker	UNP P16213
Q	139	GLY	-	linker	UNP P16213
Q	140	GLY	-	linker	UNP P16213
Q	141	GLY	-	linker	UNP P16213
Q	142	GLY	-	linker	UNP P16213
Q	143	SER	-	linker	UNP P16213
Q	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
S	12C	GLY	-	linker	UNP P03129
S	12D	GLY	-	linker	UNP P03129
S	12E	GLY	-	linker	UNP P03129
S	12F	GLY	-	linker	UNP P03129
S	12G	SER	-	linker	UNP P03129
S	12H	GLY	-	linker	UNP P03129
S	12I	GLY	-	linker	UNP P03129
S	12J	GLY	-	linker	UNP P03129
S	12K	GLY	-	linker	UNP P03129
S	12L	SER	-	linker	UNP P03129
S	12M	GLY	-	linker	UNP P03129
S	12N	GLY	-	linker	UNP P03129
S	12O	GLY	-	linker	UNP P03129
S	12P	GLY	-	linker	UNP P03129
S	12Q	SER	-	linker	UNP P03129
S	124	GLY	-	linker	UNP P16213
S	125	GLY	-	linker	UNP P16213
S	126	GLY	-	linker	UNP P16213
S	127	GLY	-	linker	UNP P16213
S	128	SER	-	linker	UNP P16213
S	129	GLY	-	linker	UNP P16213
S	130	GLY	-	linker	UNP P16213
S	131	GLY	-	linker	UNP P16213
S	132	GLY	-	linker	UNP P16213
S	133	SER	-	linker	UNP P16213
S	134	GLY	-	linker	UNP P16213
S	135	GLY	-	linker	UNP P16213
S	136	GLY	-	linker	UNP P16213
S	137	GLY	-	linker	UNP P16213
S	138	SER	-	linker	UNP P16213
S	139	GLY	-	linker	UNP P16213
S	140	GLY	-	linker	UNP P16213
S	141	GLY	-	linker	UNP P16213
S	142	GLY	-	linker	UNP P16213
S	143	SER	-	linker	UNP P16213
S	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
U	10E	GLY	-	linker	UNP P03129
U	10F	GLY	-	linker	UNP P03129
U	10G	GLY	-	linker	UNP P03129
U	10H	GLY	-	linker	UNP P03129
U	10I	SER	-	linker	UNP P03129
U	10J	GLY	-	linker	UNP P03129
U	10K	GLY	-	linker	UNP P03129
U	10L	GLY	-	linker	UNP P03129
U	10M	GLY	-	linker	UNP P03129
U	10N	SER	-	linker	UNP P03129
U	10O	GLY	-	linker	UNP P03129
U	10P	GLY	-	linker	UNP P03129
U	10Q	GLY	-	linker	UNP P03129
U	10R	GLY	-	linker	UNP P03129
U	10S	SER	-	linker	UNP P03129
U	124	GLY	-	linker	UNP P16213
U	125	GLY	-	linker	UNP P16213
U	126	GLY	-	linker	UNP P16213
U	127	GLY	-	linker	UNP P16213
U	128	SER	-	linker	UNP P16213
U	129	GLY	-	linker	UNP P16213
U	130	GLY	-	linker	UNP P16213
U	131	GLY	-	linker	UNP P16213
U	132	GLY	-	linker	UNP P16213
U	133	SER	-	linker	UNP P16213
U	134	GLY	-	linker	UNP P16213
U	135	GLY	-	linker	UNP P16213
U	136	GLY	-	linker	UNP P16213
U	137	GLY	-	linker	UNP P16213
U	138	SER	-	linker	UNP P16213
U	139	GLY	-	linker	UNP P16213
U	140	GLY	-	linker	UNP P16213
U	141	GLY	-	linker	UNP P16213
U	142	GLY	-	linker	UNP P16213
U	143	SER	-	linker	UNP P16213
U	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
W	12C	GLY	-	linker	UNP P03129
W	12D	GLY	-	linker	UNP P03129
W	12E	GLY	-	linker	UNP P03129
W	12F	GLY	-	linker	UNP P03129
W	12G	SER	-	linker	UNP P03129
W	12H	GLY	-	linker	UNP P03129
W	12I	GLY	-	linker	UNP P03129
W	12J	GLY	-	linker	UNP P03129
W	12K	GLY	-	linker	UNP P03129
W	12L	SER	-	linker	UNP P03129
W	12M	GLY	-	linker	UNP P03129
W	12N	GLY	-	linker	UNP P03129
W	12O	GLY	-	linker	UNP P03129
W	12P	GLY	-	linker	UNP P03129
W	12Q	SER	-	linker	UNP P03129
W	124	GLY	-	linker	UNP P16213
W	125	GLY	-	linker	UNP P16213
W	126	GLY	-	linker	UNP P16213
W	127	GLY	-	linker	UNP P16213
W	128	SER	-	linker	UNP P16213
W	129	GLY	-	linker	UNP P16213
W	130	GLY	-	linker	UNP P16213
W	131	GLY	-	linker	UNP P16213
W	132	GLY	-	linker	UNP P16213
W	133	SER	-	linker	UNP P16213
W	134	GLY	-	linker	UNP P16213
W	135	GLY	-	linker	UNP P16213
W	136	GLY	-	linker	UNP P16213
W	137	GLY	-	linker	UNP P16213
W	138	SER	-	linker	UNP P16213
W	139	GLY	-	linker	UNP P16213
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	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	10E	GLY	-	linker	UNP P03129
Y	10F	GLY	-	linker	UNP P03129
Y	10G	GLY	-	linker	UNP P03129
Y	10H	GLY	-	linker	UNP P03129
Y	10I	SER	-	linker	UNP P03129
Y	10J	GLY	-	linker	UNP P03129
Y	10K	GLY	-	linker	UNP P03129
Y	10L	GLY	-	linker	UNP P03129
Y	10M	GLY	-	linker	UNP P03129
Y	10N	SER	-	linker	UNP P03129
Y	10O	GLY	-	linker	UNP P03129
Y	10P	GLY	-	linker	UNP P03129
Y	10Q	GLY	-	linker	UNP P03129
Y	10R	GLY	-	linker	UNP P03129
Y	10S	SER	-	linker	UNP P03129
Y	124	GLY	-	linker	UNP P16213
Y	125	GLY	-	linker	UNP P16213
Y	126	GLY	-	linker	UNP P16213
Y	127	GLY	-	linker	UNP P16213
Y	128	SER	-	linker	UNP P16213
Y	129	GLY	-	linker	UNP P16213
Y	130	GLY	-	linker	UNP P16213
Y	131	GLY	-	linker	UNP P16213
Y	132	GLY	-	linker	UNP P16213
Y	133	SER	-	linker	UNP P16213
Y	134	GLY	-	linker	UNP P16213
Y	135	GLY	-	linker	UNP P16213
Y	136	GLY	-	linker	UNP P16213
Y	137	GLY	-	linker	UNP P16213
Y	138	SER	-	linker	UNP P16213
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	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
a	12C	GLY	-	linker	UNP P03129
a	12D	GLY	-	linker	UNP P03129
a	12E	GLY	-	linker	UNP P03129
a	12F	GLY	-	linker	UNP P03129
a	12G	SER	-	linker	UNP P03129
a	12H	GLY	-	linker	UNP P03129
a	12I	GLY	-	linker	UNP P03129
a	12J	GLY	-	linker	UNP P03129
a	12K	GLY	-	linker	UNP P03129
a	12L	SER	-	linker	UNP P03129
a	12M	GLY	-	linker	UNP P03129
a	12N	GLY	-	linker	UNP P03129
a	12O	GLY	-	linker	UNP P03129
a	12P	GLY	-	linker	UNP P03129
a	12Q	SER	-	linker	UNP P03129
a	124	GLY	-	linker	UNP P16213
a	125	GLY	-	linker	UNP P16213
a	126	GLY	-	linker	UNP P16213
a	127	GLY	-	linker	UNP P16213
a	128	SER	-	linker	UNP P16213
a	129	GLY	-	linker	UNP P16213
a	130	GLY	-	linker	UNP P16213
a	131	GLY	-	linker	UNP P16213
a	132	GLY	-	linker	UNP P16213
a	133	SER	-	linker	UNP P16213
a	134	GLY	-	linker	UNP P16213
a	135	GLY	-	linker	UNP P16213
a	136	GLY	-	linker	UNP P16213
a	137	GLY	-	linker	UNP P16213
a	138	SER	-	linker	UNP P16213
a	139	GLY	-	linker	UNP P16213
a	140	GLY	-	linker	UNP P16213
a	141	GLY	-	linker	UNP P16213
a	142	GLY	-	linker	UNP P16213
a	143	SER	-	linker	UNP P16213
a	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
c	10E	GLY	-	linker	UNP P03129
c	10F	GLY	-	linker	UNP P03129
c	10G	GLY	-	linker	UNP P03129
c	10H	GLY	-	linker	UNP P03129
c	10I	SER	-	linker	UNP P03129
c	10J	GLY	-	linker	UNP P03129
c	10K	GLY	-	linker	UNP P03129
c	10L	GLY	-	linker	UNP P03129
c	10M	GLY	-	linker	UNP P03129
c	10N	SER	-	linker	UNP P03129
c	10O	GLY	-	linker	UNP P03129
c	10P	GLY	-	linker	UNP P03129
c	10Q	GLY	-	linker	UNP P03129
c	10R	GLY	-	linker	UNP P03129
c	10S	SER	-	linker	UNP P03129
c	124	GLY	-	linker	UNP P16213
c	125	GLY	-	linker	UNP P16213
c	126	GLY	-	linker	UNP P16213
c	127	GLY	-	linker	UNP P16213
c	128	SER	-	linker	UNP P16213
c	129	GLY	-	linker	UNP P16213
c	130	GLY	-	linker	UNP P16213
c	131	GLY	-	linker	UNP P16213
c	132	GLY	-	linker	UNP P16213
c	133	SER	-	linker	UNP P16213
c	134	GLY	-	linker	UNP P16213
c	135	GLY	-	linker	UNP P16213
c	136	GLY	-	linker	UNP P16213
c	137	GLY	-	linker	UNP P16213
c	138	SER	-	linker	UNP P16213
c	139	GLY	-	linker	UNP P16213
c	140	GLY	-	linker	UNP P16213
c	141	GLY	-	linker	UNP P16213
c	142	GLY	-	linker	UNP P16213
c	143	SER	-	linker	UNP P16213
c	227	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
e	12C	GLY	-	linker	UNP P03129
e	12D	GLY	-	linker	UNP P03129
e	12E	GLY	-	linker	UNP P03129
e	12F	GLY	-	linker	UNP P03129
e	12G	SER	-	linker	UNP P03129
e	12H	GLY	-	linker	UNP P03129
e	12I	GLY	-	linker	UNP P03129
e	12J	GLY	-	linker	UNP P03129
e	12K	GLY	-	linker	UNP P03129
e	12L	SER	-	linker	UNP P03129
e	12M	GLY	-	linker	UNP P03129
e	12N	GLY	-	linker	UNP P03129
e	12O	GLY	-	linker	UNP P03129
e	12P	GLY	-	linker	UNP P03129
e	12Q	SER	-	linker	UNP P03129
e	124	GLY	-	linker	UNP P16213
e	125	GLY	-	linker	UNP P16213
e	126	GLY	-	linker	UNP P16213
e	127	GLY	-	linker	UNP P16213
e	128	SER	-	linker	UNP P16213
e	129	GLY	-	linker	UNP P16213
e	130	GLY	-	linker	UNP P16213
e	131	GLY	-	linker	UNP P16213
e	132	GLY	-	linker	UNP P16213
e	133	SER	-	linker	UNP P16213
e	134	GLY	-	linker	UNP P16213
e	135	GLY	-	linker	UNP P16213
e	136	GLY	-	linker	UNP P16213
e	137	GLY	-	linker	UNP P16213
e	138	SER	-	linker	UNP P16213
e	139	GLY	-	linker	UNP P16213
e	140	GLY	-	linker	UNP P16213
e	141	GLY	-	linker	UNP P16213
e	142	GLY	-	linker	UNP P16213
e	143	SER	-	linker	UNP P16213
e	227	ALA	TYR	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
			1616	520	777	145	170	4			
2	D	115	Total	C	H	N	O	S	0	0	0
			1611	519	773	144	171	4			
2	F	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	H	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	J	115	Total	C	H	N	O	S	0	0	0
			1616	520	774	145	173	4			
2	L	115	Total	C	H	N	O	S	0	0	0
			1631	523	785	146	173	4			
2	N	115	Total	C	H	N	O	S	0	0	0
			1616	520	774	145	173	4			
2	P	115	Total	C	H	N	O	S	0	0	0
			1616	520	774	145	173	4			
2	R	112	Total	C	H	N	O	S	0	0	0
			1574	508	754	140	168	4			
2	T	115	Total	C	H	N	O	S	0	0	0
			1546	506	729	139	168	4			
2	V	115	Total	C	H	N	O	S	0	0	0
			1619	521	775	146	173	4			
2	X	115	Total	C	H	N	O	S	0	0	0
			1582	514	753	140	171	4			
2	Z	110	Total	C	H	N	O	S	0	0	0
			1559	502	748	140	165	4			
2	b	115	Total	C	H	N	O	S	0	0	0
			1571	512	745	143	167	4			
2	d	112	Total	C	H	N	O	S	0	0	0
			1597	512	768	143	170	4			
2	f	115	Total	C	H	N	O	S	0	0	0
			1604	517	766	144	173	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	9	Total	O	0	0
			9	9		
3	C	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	8	Total O 8 8	0	0
3	E	23	Total O 23 23	0	0
3	F	5	Total O 5 5	0	0
3	G	25	Total O 25 25	0	0
3	H	7	Total O 7 7	0	0
3	I	9	Total O 9 9	0	0
3	J	5	Total O 5 5	0	0
3	K	15	Total O 15 15	0	0
3	L	8	Total O 8 8	0	0
3	M	13	Total O 13 13	0	0
3	N	2	Total O 2 2	0	0
3	O	7	Total O 7 7	0	0
3	P	6	Total O 6 6	0	0
3	Q	11	Total O 11 11	0	0
3	R	4	Total O 4 4	0	0
3	S	12	Total O 12 12	0	0
3	T	5	Total O 5 5	0	0
3	U	7	Total O 7 7	0	0
3	V	10	Total O 10 10	0	0
3	W	5	Total O 5 5	0	0
3	X	4	Total O 4 4	0	0

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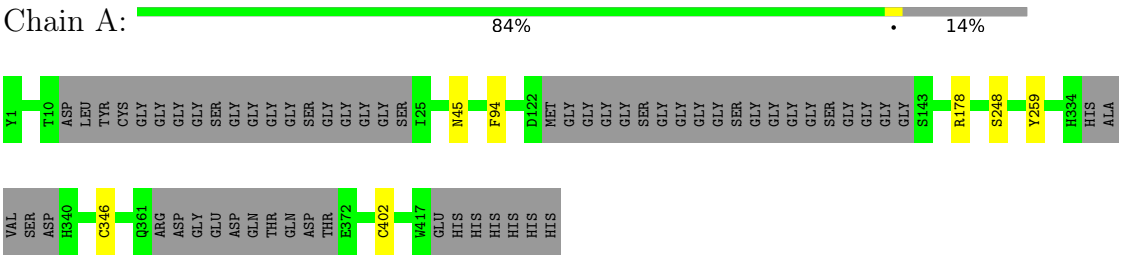
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Y	10	Total O 10 10	0	0
3	Z	3	Total O 3 3	0	0
3	a	8	Total O 8 8	0	0
3	b	6	Total O 6 6	0	0
3	c	11	Total O 11 11	0	0
3	d	7	Total O 7 7	0	0
3	e	5	Total O 5 5	0	0
3	f	5	Total O 5 5	0	0

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.

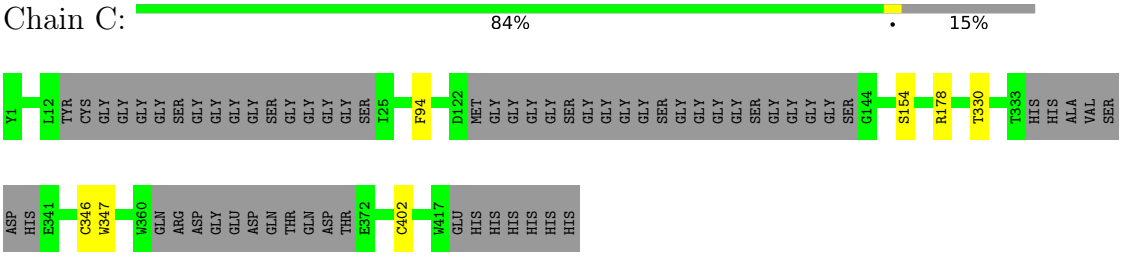
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain A:



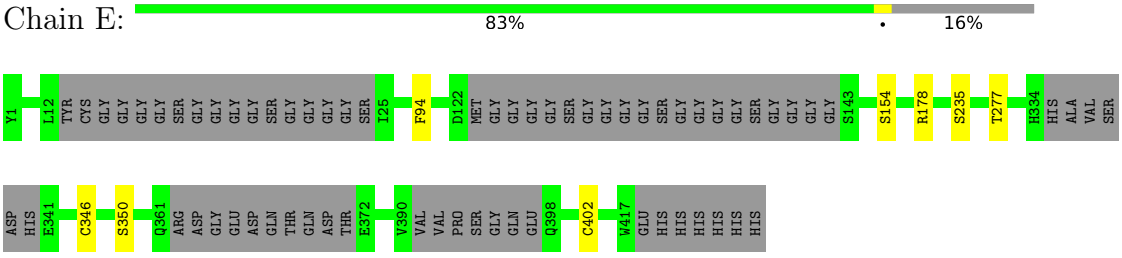
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain C:



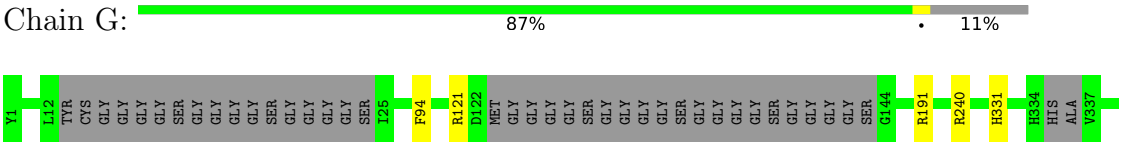
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

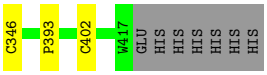
Chain E:



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

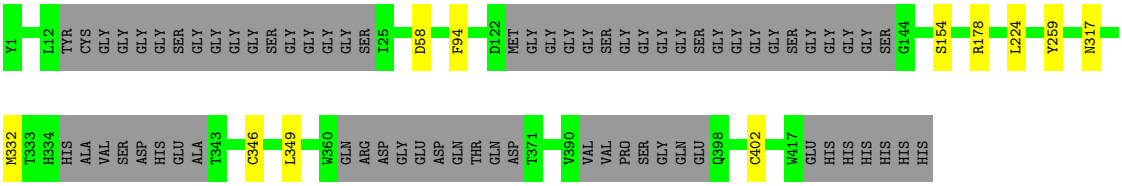
Chain G:





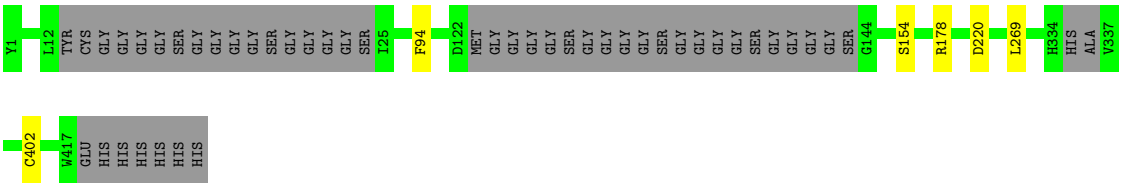
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain I:



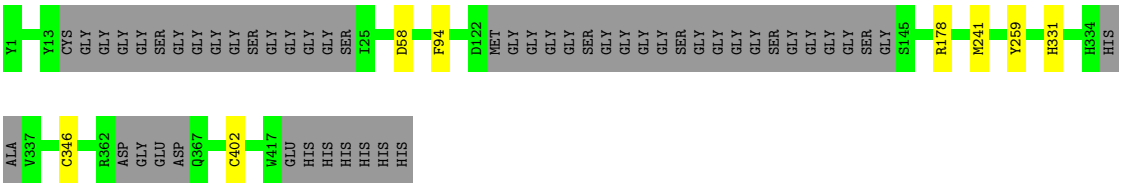
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain K:



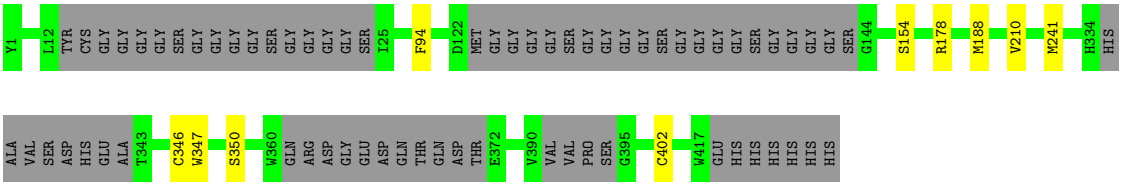
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain M:



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

Chain O:

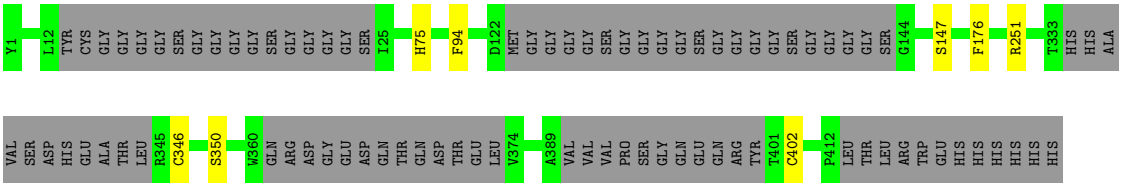


• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain Q:

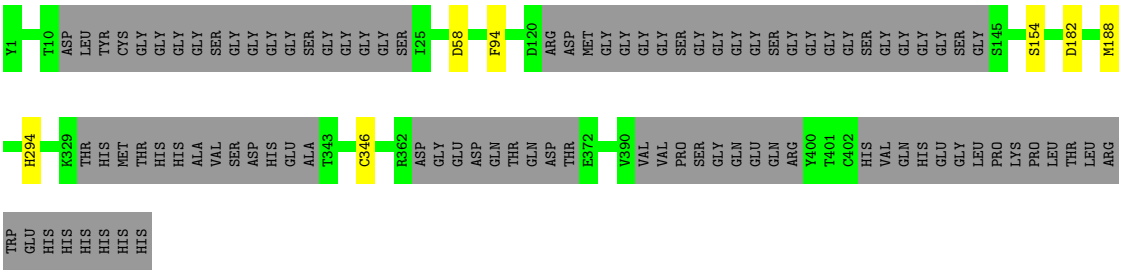
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain S:



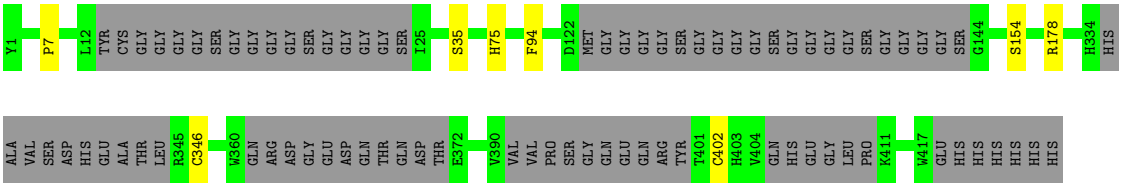
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain U:



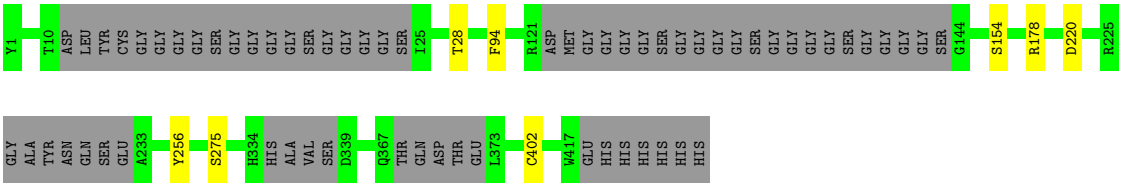
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain W:



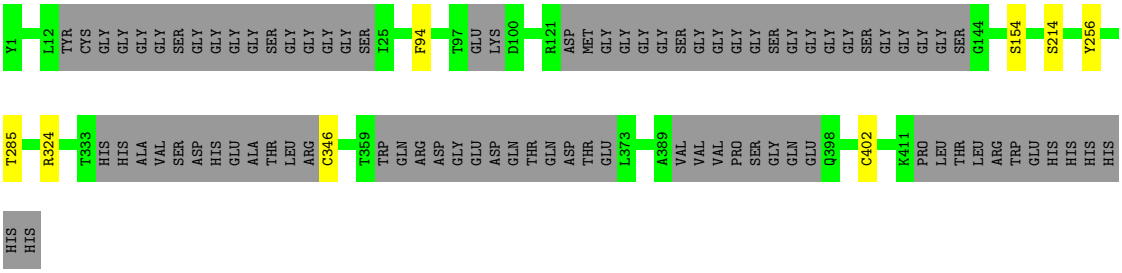
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain Y:



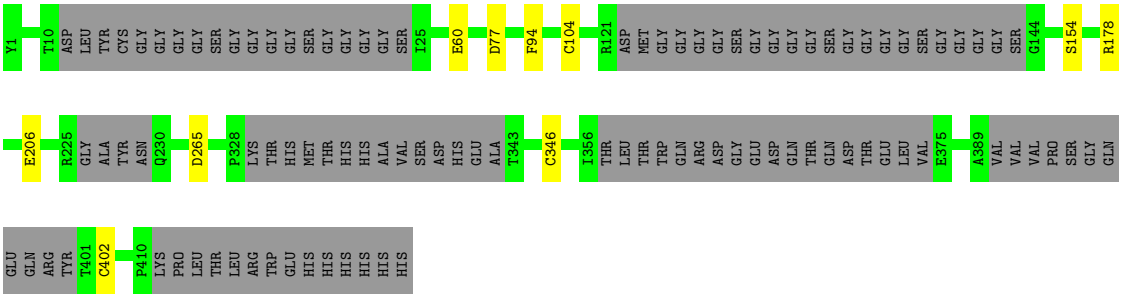
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain a:



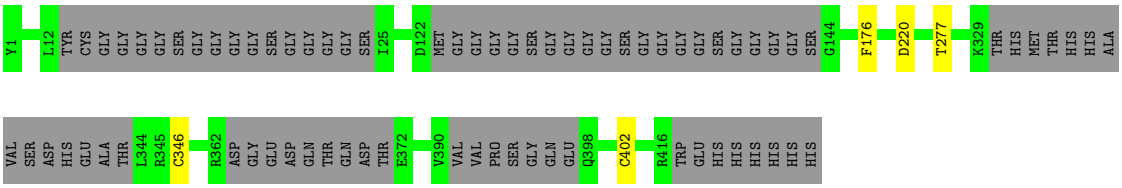
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain c:



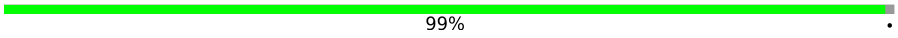
• Molecule 1: Protein E7 peptide,Beta-2-microglobulin,MHC class I antigen chimera

Chain e:



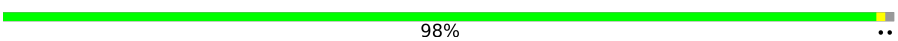
• Molecule 2: VHH

Chain B:



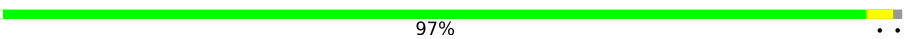
• Molecule 2: VHH

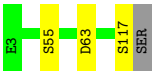
Chain D:



• Molecule 2: VHH

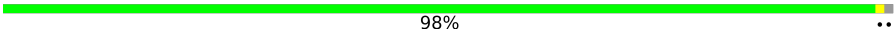
Chain F:

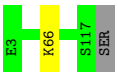




• Molecule 2: VHH

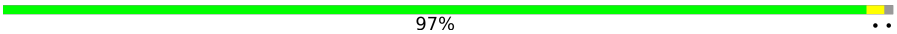
Chain H:

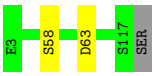




• Molecule 2: VHH

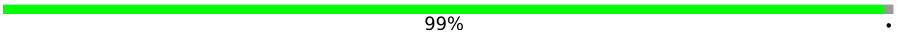
Chain J:





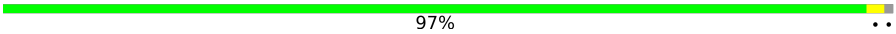
• Molecule 2: VHH

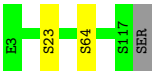
Chain L:



• Molecule 2: VHH

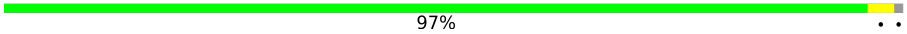
Chain N:

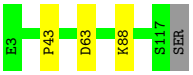




• Molecule 2: VHH

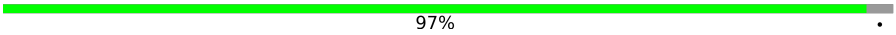
Chain P:





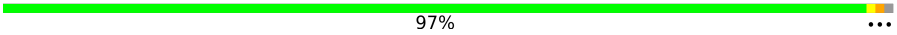
• Molecule 2: VHH

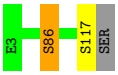
Chain R:



• Molecule 2: VHH

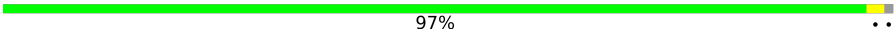
Chain T:

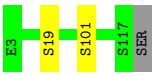




• Molecule 2: VHH

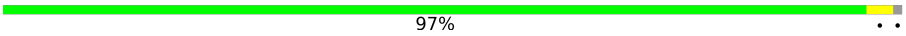
Chain V:





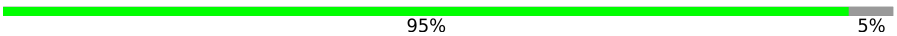
• Molecule 2: VHH

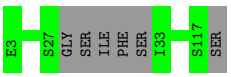
Chain X:



• Molecule 2: VHH

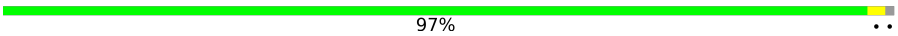
Chain Z:





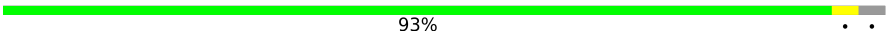
• Molecule 2: VHH

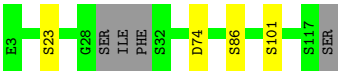
Chain b:



• Molecule 2: VHH

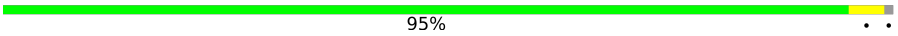
Chain d:

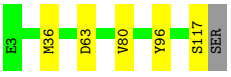




• Molecule 2: VHH

Chain f:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	117.68Å 118.92Å 274.99Å 77.60° 77.60° 89.95°	Depositor
Resolution (Å)	49.19 – 2.73 49.19 – 2.73	Depositor EDS
% Data completeness (in resolution range)	88.3 (49.19-2.73) 88.1 (49.19-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.253 , 0.294 0.252 , 0.294	Depositor DCC
R_{free} test set	16938 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 17.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.347 for -k,h,-k+l 0.347 for k,-h,-h+l 0.389 for h,-k,h-l 0.397 for -h,k,k-l 0.359 for -k,-h,-l 0.346 for k,h,h+k-l 0.348 for -h,-k,-h-k+l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	106611	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/2851	0.50	0/3893
1	C	0.28	0/2847	0.49	0/3889
1	E	0.27	0/2865	0.49	0/3908
1	G	0.30	1/2971 (0.0%)	0.49	0/4059
1	I	0.28	0/2811	0.50	0/3836
1	K	0.29	0/2965	0.51	0/4052
1	M	0.28	0/2928	0.49	0/3999
1	O	0.28	0/2835	0.51	0/3868
1	Q	0.29	0/2928	0.50	0/4008
1	S	0.27	0/2695	0.49	0/3679
1	U	0.27	0/2542	0.48	0/3479
1	W	0.27	0/2657	0.48	0/3631
1	Y	0.30	0/2788	0.50	1/3814 (0.0%)
1	a	0.28	0/2655	0.50	0/3624
1	c	0.29	0/2453	0.50	1/3352 (0.0%)
1	e	0.27	0/2669	0.48	0/3648
2	B	0.30	0/854	0.51	0/1159
2	D	0.30	0/853	0.53	0/1158
2	F	0.31	0/861	0.52	0/1168
2	H	0.30	0/861	0.52	0/1168
2	J	0.30	0/857	0.53	0/1164
2	L	0.30	0/861	0.51	0/1168
2	N	0.30	0/857	0.51	0/1164
2	P	0.40	1/857 (0.1%)	0.53	0/1164
2	R	0.27	0/834	0.52	0/1132
2	T	0.29	0/832	0.53	0/1132
2	V	0.28	0/859	0.51	0/1167
2	X	0.29	0/844	0.50	0/1148
2	Z	0.29	0/825	0.53	0/1119
2	b	0.28	0/841	0.51	0/1143
2	d	0.28	0/843	0.50	0/1143
2	f	0.40	1/853 (0.1%)	0.58	1/1159 (0.1%)
All	All	0.29	3/58052 (0.0%)	0.50	3/79195 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	43	PRO	N-CD	7.76	1.58	1.47
2	f	36	MET	SD-CE	-7.33	1.36	1.77
1	G	393	PRO	N-CD	-6.57	1.38	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	f	80	VAL	CG1-CB-CG2	7.46	122.84	110.90
1	Y	220	ASP	CB-CG-OD1	7.29	124.86	118.30
1	c	206	GLU	OE1-CD-OE2	-5.43	116.78	123.30

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	358/429 (83%)	348 (97%)	10 (3%)	0	100	100
1	C	356/429 (83%)	349 (98%)	7 (2%)	0	100	100
1	E	350/429 (82%)	340 (97%)	10 (3%)	0	100	100
1	G	374/429 (87%)	357 (96%)	17 (4%)	0	100	100
1	I	347/429 (81%)	337 (97%)	10 (3%)	0	100	100
1	K	374/429 (87%)	363 (97%)	11 (3%)	0	100	100
1	M	368/429 (86%)	353 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	349/429 (81%)	340 (97%)	9 (3%)	0	100	100
1	Q	378/429 (88%)	363 (96%)	15 (4%)	0	100	100
1	S	332/429 (77%)	320 (96%)	12 (4%)	0	100	100
1	U	321/429 (75%)	310 (97%)	11 (3%)	0	100	100
1	W	333/429 (78%)	324 (97%)	9 (3%)	0	100	100
1	Y	353/429 (82%)	343 (97%)	10 (3%)	0	100	100
1	a	328/429 (76%)	314 (96%)	14 (4%)	0	100	100
1	c	313/429 (73%)	301 (96%)	12 (4%)	0	100	100
1	e	341/429 (80%)	332 (97%)	9 (3%)	0	100	100
2	B	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	D	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	F	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	H	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
2	J	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	L	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
2	N	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	P	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	R	108/116 (93%)	105 (97%)	3 (3%)	0	100	100
2	T	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
2	V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	X	113/116 (97%)	105 (93%)	8 (7%)	0	100	100
2	Z	106/116 (91%)	102 (96%)	4 (4%)	0	100	100
2	b	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
2	d	108/116 (93%)	104 (96%)	4 (4%)	0	100	100
2	f	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
All	All	7366/8720 (84%)	7116 (97%)	250 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	258/351 (74%)	251 (97%)	7 (3%)	44	65
1	C	256/351 (73%)	249 (97%)	7 (3%)	44	65
1	E	266/351 (76%)	258 (97%)	8 (3%)	41	61
1	G	267/351 (76%)	260 (97%)	7 (3%)	46	66
1	I	256/351 (73%)	245 (96%)	11 (4%)	29	48
1	K	265/351 (76%)	259 (98%)	6 (2%)	50	70
1	M	262/351 (75%)	254 (97%)	8 (3%)	40	60
1	O	259/351 (74%)	249 (96%)	10 (4%)	32	53
1	Q	256/351 (73%)	249 (97%)	7 (3%)	44	65
1	S	241/351 (69%)	233 (97%)	8 (3%)	38	59
1	U	221/351 (63%)	214 (97%)	7 (3%)	39	59
1	W	234/351 (67%)	226 (97%)	8 (3%)	37	58
1	Y	245/351 (70%)	238 (97%)	7 (3%)	42	62
1	a	238/351 (68%)	230 (97%)	8 (3%)	37	58
1	c	207/351 (59%)	198 (96%)	9 (4%)	29	48
1	e	229/351 (65%)	224 (98%)	5 (2%)	52	71
2	B	86/97 (89%)	86 (100%)	0	100	100
2	D	86/97 (89%)	85 (99%)	1 (1%)	71	83
2	F	88/97 (91%)	85 (97%)	3 (3%)	37	58
2	H	88/97 (91%)	87 (99%)	1 (1%)	73	84
2	J	87/97 (90%)	85 (98%)	2 (2%)	50	70
2	L	88/97 (91%)	88 (100%)	0	100	100
2	N	87/97 (90%)	85 (98%)	2 (2%)	50	70
2	P	87/97 (90%)	85 (98%)	2 (2%)	50	70
2	R	85/97 (88%)	85 (100%)	0	100	100
2	T	80/97 (82%)	78 (98%)	2 (2%)	47	67
2	V	87/97 (90%)	86 (99%)	1 (1%)	73	84
2	X	84/97 (87%)	81 (96%)	3 (4%)	35	55
2	Z	84/97 (87%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	b	81/97 (84%)	79 (98%)	2 (2%)	47 67
2	d	87/97 (90%)	83 (95%)	4 (5%)	27 46
2	f	86/97 (89%)	83 (96%)	3 (4%)	36 57
All	All	5331/7168 (74%)	5182 (97%)	149 (3%)	43 63

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	256	TYR
1	e	277	THR
1	a	154	SER
1	c	94	PHE
1	K	154	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	41	GLN
1	S	175	GLN
1	O	284	GLN
1	M	32	GLN
1	Q	6	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.