



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 PM UTC

PDB ID : 7SSH / pdb_00007ssh
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

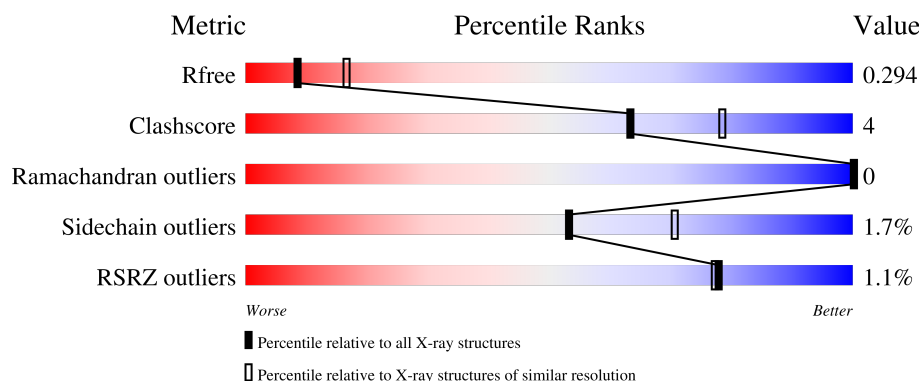
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	<div> <div>3%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
1	C	429	<div> <div>%</div> <div>80%</div> <div>5%</div> <div>15%</div> </div>
1	E	429	<div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
1	G	429	<div> <div>82%</div> <div>7%</div> <div>11%</div> </div>
1	I	429	<div> <div>78%</div> <div>6%</div> <div>16%</div> </div>

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

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Mol	Chain	Length	Quality of chain
2	d	116	<div><div><div>%</div><div><div></div><div>81%</div><div>16%</div><div></div></div><div></div></div></div>
2	f	116	<div><div><div>2%</div><div><div></div><div>83%</div><div>15%</div><div></div></div><div></div></div></div>

2 Entry composition

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 18 O	0	0
3	B	9	Total 9 O	0	0
3	C	9	Total 9 O	0	0

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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	0	0
			10	10		
3	Z	3	Total	O	0	0
			3	3		
3	a	8	Total	O	0	0
			8	8		
3	b	6	Total	O	0	0
			6	6		
3	c	11	Total	O	0	0
			11	11		
3	d	7	Total	O	0	0
			7	7		
3	e	5	Total	O	0	0
			5	5		
3	f	5	Total	O	0	0
			5	5		


Y1	T10	ASP	LEU	TTR	CYS	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	I95	T28	P29	Y94	N48	V51	D58	D62	L63	L64	E68	R69	I70	D77	L78	S79	Y87	F94	D120	ARG	ASP	MET	GLY	GLY	GLY	GLY	GLY	FER
----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: VHH

Chain F:  92% 7%




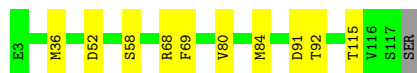
• Molecule 2: VHH

Chain H:  91% 9%



• Molecule 2: VHH

Chain J:  91% 9%



• Molecule 2: VHH

Chain L:  91% 8%




• Molecule 2: VHH

Chain N:  92% 7%




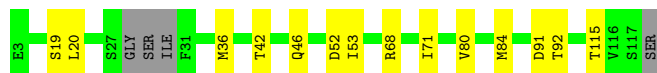
• Molecule 2: VHH

Chain P:  87% 12%




• Molecule 2: VHH

Chain R:  84% 12%

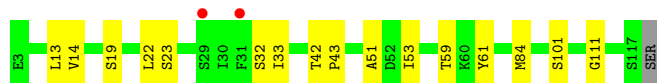
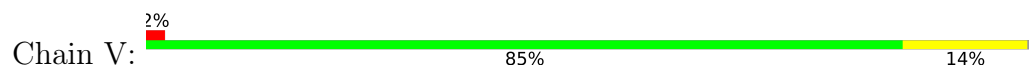


• Molecule 2: VHH

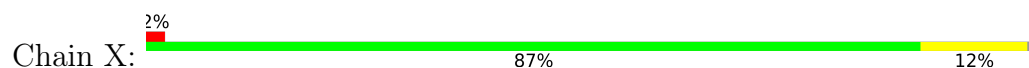
Chain T:  86% 12%



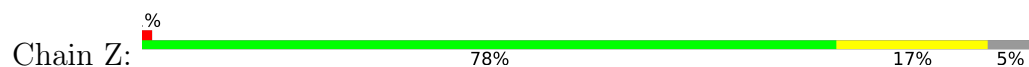
• Molecule 2: VHH



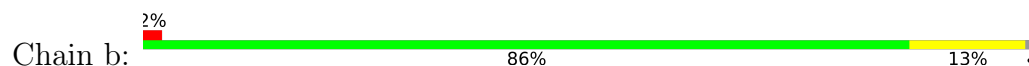
• Molecule 2: VHH



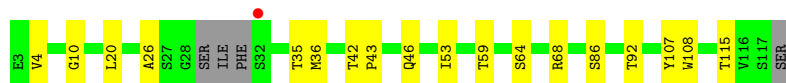
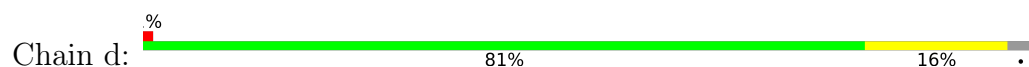
• Molecule 2: VHH



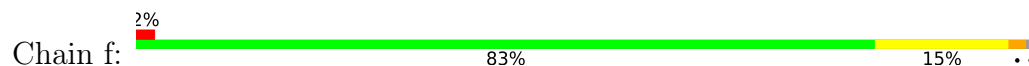
• Molecule 2: VHH



• Molecule 2: VHH



• Molecule 2: VHH



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.253 , 0.294 0.254 , 0.294	Depositor DCC
R_{free} test set	16950 reflections (4.51%)	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)	0.37 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/2851	0.28	0/3893
1	C	0.16	0/2847	0.27	0/3889
1	E	0.16	0/2865	0.27	0/3908
1	G	0.21	1/2971 (0.0%)	0.28	0/4059
1	I	0.16	0/2811	0.27	0/3836
1	K	0.18	0/2965	0.30	0/4052
1	M	0.17	0/2928	0.28	0/3999
1	O	0.16	0/2835	0.28	0/3868
1	Q	0.23	0/2928	0.33	0/4008
1	S	0.15	0/2695	0.27	0/3679
1	U	0.14	0/2542	0.27	0/3479
1	W	0.14	0/2657	0.28	0/3631
1	Y	0.21	0/2788	0.30	0/3814
1	a	0.17	0/2655	0.28	0/3624
1	c	0.16	0/2453	0.30	0/3352
1	e	0.16	0/2669	0.28	0/3648
2	B	0.18	0/854	0.28	0/1159
2	D	0.19	0/853	0.30	0/1158
2	F	0.22	0/861	0.29	0/1168
2	H	0.18	0/861	0.28	0/1168
2	J	0.17	0/857	0.29	0/1164
2	L	0.20	0/861	0.33	1/1168 (0.1%)
2	N	0.19	0/857	0.28	0/1164
2	P	0.33	1/857 (0.1%)	0.32	0/1164
2	R	0.14	0/834	0.28	0/1132
2	T	0.17	0/832	0.30	0/1132
2	V	0.15	0/859	0.29	0/1167
2	X	0.16	0/844	0.26	0/1148
2	Z	0.17	0/825	0.31	0/1119
2	b	0.16	0/841	0.27	0/1143
2	d	0.16	0/843	0.27	0/1143
2	f	0.61	1/853 (0.1%)	0.35	1/1159 (0.1%)
All	All	0.19	3/58052 (0.0%)	0.29	2/79195 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	36	MET	SD-CE	-17.10	1.36	1.79
2	P	43	PRO	N-CD	7.83	1.58	1.47
1	G	393	PRO	N-CD	-6.50	1.38	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	80	VAL	CG1-CB-CG2	5.47	122.84	110.80
2	L	50	VAL	N-CA-C	-5.09	106.70	111.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	2439	2439	19	0
1	C	2769	2419	2419	14	0
1	E	2787	2475	2475	13	0
1	G	2889	2530	2530	16	0
1	I	2734	2423	2423	14	0
1	K	2883	2516	2516	21	0
1	M	2849	2488	2488	14	0
1	O	2758	2435	2435	16	0
1	Q	2846	2437	2443	21	0
1	S	2618	2261	2261	25	0
1	U	2472	2100	2100	18	0
1	W	2587	2195	2195	16	0
1	Y	2711	2319	2319	23	0
1	a	2582	2226	2226	31	0
1	c	2388	2002	2002	32	0
1	e	2598	2198	2198	19	0
2	B	839	777	777	6	0
2	D	838	773	773	8	0
2	F	846	785	785	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	846	785	785	6	0
2	J	842	774	774	5	0
2	L	846	785	785	4	0
2	N	842	774	774	5	0
2	P	842	774	774	10	0
2	R	820	754	754	8	0
2	T	817	729	729	13	1
2	V	844	775	775	9	1
2	X	829	753	753	9	0
2	Z	811	748	748	15	0
2	b	826	745	745	9	0
2	d	829	768	768	11	0
2	f	838	766	766	16	0
3	A	18	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	8	0	0	0	0
3	E	23	0	0	0	0
3	F	5	0	0	0	0
3	G	25	0	0	1	0
3	H	7	0	0	0	0
3	I	9	0	0	0	0
3	J	5	0	0	0	0
3	K	15	0	0	0	0
3	L	8	0	0	0	0
3	M	13	0	0	0	0
3	N	2	0	0	0	0
3	O	7	0	0	0	0
3	P	6	0	0	0	0
3	Q	11	0	0	0	0
3	R	4	0	0	0	0
3	S	12	0	0	0	0
3	T	5	0	0	0	0
3	U	7	0	0	0	0
3	V	10	0	0	1	0
3	W	5	0	0	0	0
3	X	4	0	0	0	0
3	Y	10	0	0	0	0
3	Z	3	0	0	0	0
3	a	8	0	0	0	0
3	b	6	0	0	0	0
3	c	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	d	7	0	0	1	0
3	e	5	0	0	0	0
3	f	5	0	0	0	0
All	All	56883	49728	49734	424	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (424) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:10:THR:OG1	1:Y:220:ASP:OD2	1.90	0.87
1:e:118:LYS:NZ	2:f:105:ASP:OD1	2.10	0.84
1:a:67:GLY:O	2:b:35:THR:OG1	2.00	0.79
1:e:67:GLY:O	2:f:35:THR:OG1	2.01	0.79
1:C:69:ARG:NH2	2:D:52:ASP:OD2	2.17	0.78
2:d:108:TRP:O	3:d:201:HOH:O	2.01	0.78
1:a:245:ASP:OD2	1:a:256:TYR:OH	2.03	0.77
1:Y:10:THR:HG23	1:Y:286:THR:HG21	1.68	0.75
1:c:179:PHE:HB2	1:c:188:MET:HE2	1.68	0.74
1:K:330:THR:CG2	1:K:415:LEU:HD11	2.17	0.74
2:Z:42:THR:OG1	2:Z:46:GLN:O	2.03	0.74
1:U:179:PHE:HB2	1:U:188:MET:HE2	1.69	0.73
1:U:62:ASP:OD1	1:U:69:ARG:NH1	2.22	0.72
1:a:320:GLU:O	1:a:324:ARG:NH1	2.22	0.72
1:c:147:SER:OG	1:c:245:ASP:OD1	2.07	0.71
1:S:28:THR:HG22	1:S:110:THR:HB	1.74	0.70
2:T:65:VAL:HG21	2:T:69:PHE:CD2	2.26	0.69
1:c:2:MET:HE2	1:c:206:GLU:OE1	1.93	0.69
1:S:147:SER:OG	1:S:245:ASP:OD1	2.11	0.69
2:R:42:THR:OG1	2:R:46:GLN:O	2.11	0.68
1:Q:245:ASP:OD2	1:Q:256:TYR:OH	2.11	0.68
1:Y:241:MET:HE3	1:Y:258:GLN:HG3	1.76	0.67
1:c:105:ARG:HG3	1:c:116:ILE:HG12	1.77	0.67
1:W:89:LEU:HD22	1:W:378:PRO:HG2	1.76	0.67
1:c:69:ARG:HH11	1:c:69:ARG:HB2	1.59	0.66
2:f:65:VAL:HG23	2:f:68:ARG:HH21	1.60	0.66
1:c:188:MET:HG3	1:c:206:GLU:HB3	1.78	0.65
2:R:36:MET:HE2	2:R:80:VAL:HG22	1.78	0.65
1:A:37:HIS:H	1:A:45:ASN:HD21	1.44	0.65
1:A:179:PHE:HB2	1:A:188:MET:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASP:OD1	2:B:77:LYS:N	2.29	0.65
2:D:14:VAL:HG21	2:D:20:LEU:HG	1.79	0.65
1:Q:176:PHE:HD2	1:Q:195:ILE:HD13	1.62	0.65
1:E:2:MET:HE1	1:E:210:VAL:HB	1.78	0.64
2:X:22:LEU:HD22	2:X:84:MET:HE2	1.78	0.64
1:c:69:ARG:HB2	1:c:69:ARG:NH1	2.13	0.64
2:F:68:ARG:NH2	2:F:91:ASP:OD2	2.31	0.64
2:H:22:LEU:HG	2:H:84:MET:HE2	1.79	0.64
1:K:330:THR:HG22	1:K:415:LEU:HD11	1.79	0.63
2:P:34:ASN:OD1	2:P:55:SER:OG	2.15	0.63
2:f:53:ILE:HG13	2:f:59:THR:HG22	1.80	0.63
1:A:270:LYS:HE3	1:A:271:GLU:H	1.62	0.63
2:T:69:PHE:CD1	2:T:84:MET:HA	2.33	0.63
1:Q:176:PHE:CD2	1:Q:195:ILE:HD13	2.34	0.63
1:W:63:LEU:HB3	1:W:70:ILE:HD12	1.82	0.62
1:Y:148:MET:HE3	1:Y:150:TYR:CE2	2.34	0.62
2:b:53:ILE:HD12	2:b:59:THR:CG2	2.30	0.62
2:J:36:MET:HE3	2:J:80:VAL:HG13	1.81	0.62
1:I:69:ARG:NH2	2:J:52:ASP:OD2	2.33	0.61
1:c:2:MET:CE	1:c:206:GLU:OE1	2.49	0.61
1:G:245:ASP:OD2	1:G:256:TYR:OH	2.10	0.61
1:O:179:PHE:HB2	1:O:188:MET:HE2	1.82	0.61
1:Q:361:GLN:OE1	1:Q:403:HIS:NE2	2.35	0.60
2:F:90:GLU:H	2:F:90:GLU:CD	2.09	0.60
1:K:171:VAL:HG11	1:K:322:LEU:HD13	1.84	0.60
1:A:63:LEU:HB3	1:A:70:ILE:HD12	1.84	0.59
1:U:34:TYR:HE1	1:U:48:ASN:HD22	1.50	0.59
1:O:69:ARG:NH2	2:P:52:ASP:OD2	2.35	0.59
2:F:14:VAL:HG21	2:F:20:LEU:HG	1.84	0.59
2:P:84:MET:HE2	2:P:87:LEU:HD21	1.84	0.59
1:I:93:GLU:OE1	1:I:93:GLU:N	2.35	0.59
2:Z:53:ILE:HD12	2:Z:59:THR:CG2	2.31	0.59
2:b:53:ILE:HB	2:b:71:ILE:HD13	1.83	0.59
2:d:42:THR:HB	2:d:43:PRO:HD2	1.85	0.59
1:S:157:ARG:NH2	1:S:162:GLU:O	2.36	0.59
2:d:42:THR:OG1	2:d:46:GLN:O	2.21	0.59
1:G:206:GLU:OE2	1:G:209:LYS:NZ	2.36	0.59
1:K:149:ARG:HD3	1:K:241:MET:HE2	1.84	0.58
1:a:220:ASP:C	1:a:224:LEU:HD12	2.28	0.58
2:f:65:VAL:HG21	2:f:69:PHE:CD2	2.38	0.58
1:e:80:PHE:HE2	1:e:84:TRP:CZ3	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:65:VAL:HG21	2:T:69:PHE:CE2	2.39	0.58
1:a:220:ASP:OD2	1:a:259:TYR:OH	2.16	0.58
1:e:313:ARG:O	1:e:317:ASN:ND2	2.30	0.58
2:D:68:ARG:NH2	2:D:91:ASP:OD2	2.37	0.57
1:Y:290:TRP:CD1	1:Y:295:VAL:HG21	2.39	0.57
1:G:63:LEU:HB3	1:G:70:ILE:HD12	1.85	0.57
1:W:204:ASP:O	1:W:207:THR:OG1	2.23	0.57
1:Y:330:THR:HG21	1:Y:413:LEU:HD21	1.85	0.57
1:c:179:PHE:HB2	1:c:188:MET:CE	2.34	0.57
2:D:34:ASN:O	2:D:73:ARG:NH1	2.37	0.57
1:c:48:ASN:OD1	1:c:89:LEU:HD11	2.03	0.57
2:f:6:LEU:HD22	2:f:24:CYS:SG	2.44	0.57
2:L:74:ASP:OD2	2:L:77:LYS:N	2.36	0.57
1:S:28:THR:HG22	1:S:110:THR:CB	2.35	0.56
2:X:84:MET:HB3	2:X:87:LEU:HD21	1.87	0.56
1:a:69:ARG:NH2	2:b:52:ASP:OD2	2.38	0.56
1:I:149:ARG:NH2	1:I:245:ASP:OD1	2.38	0.56
2:P:68:ARG:NH2	2:P:91:ASP:OD2	2.38	0.56
1:a:320:GLU:HA	1:a:324:ARG:HH22	1.70	0.56
1:M:149:ARG:NH2	1:M:245:ASP:OD1	2.39	0.56
1:S:276:TRP:HZ2	1:S:295:VAL:HG23	1.69	0.56
1:E:270:LYS:HD3	1:E:277:THR:HG23	1.88	0.56
1:O:269:LEU:HD23	1:O:273:LEU:HD22	1.87	0.55
1:Y:358:LEU:HD12	1:Y:386:LYS:HD3	1.87	0.55
2:N:14:VAL:HG21	2:N:20:LEU:HG	1.89	0.55
2:H:92:THR:HG23	2:H:115:THR:HA	1.89	0.55
1:C:118:LYS:NZ	2:D:103:SER:O	2.39	0.55
1:M:266:TYR:HD1	1:M:267:ILE:HG22	1.71	0.55
1:A:179:PHE:HB2	1:A:188:MET:CE	2.36	0.55
1:G:238:VAL:HG11	1:G:259:TYR:OH	2.07	0.54
1:a:3:LEU:CD2	1:a:302:TYR:CD2	2.89	0.54
1:Y:179:PHE:HB2	1:Y:188:MET:HE2	1.88	0.54
2:Z:22:LEU:HD21	2:Z:84:MET:HE3	1.89	0.54
1:e:69:ARG:HH12	2:f:60:LYS:CB	2.21	0.54
1:I:245:ASP:HB2	1:I:254:ARG:HG2	1.88	0.54
2:R:68:ARG:NH2	2:R:91:ASP:OD2	2.39	0.54
1:I:171:VAL:HG11	1:I:322:LEU:HD13	1.90	0.54
2:V:111:GLY:O	3:V:201:HOH:O	2.19	0.54
1:A:188:MET:HE3	1:A:210:VAL:HG21	1.89	0.54
1:c:63:LEU:HB3	1:c:70:ILE:HD12	1.88	0.53
1:I:373:LEU:HD12	1:I:388:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:65:VAL:CG2	2:T:69:PHE:CD2	2.92	0.53
2:T:86:SER:O	2:T:86:SER:OG	2.26	0.53
2:V:13:LEU:HD12	2:V:14:VAL:H	1.73	0.53
1:S:108:HIS:ND1	1:S:110:THR:OG1	2.37	0.53
2:R:92:THR:HG23	2:R:115:THR:HA	1.90	0.53
1:K:346:CYS:SG	1:K:415:LEU:HD12	2.49	0.53
1:a:220:ASP:O	1:a:224:LEU:HD12	2.09	0.53
2:b:53:ILE:HD12	2:b:59:THR:HG22	1.91	0.53
1:G:373:LEU:HD12	1:G:388:ALA:HB2	1.90	0.53
1:U:147:SER:HB3	1:U:245:ASP:OD1	2.08	0.53
1:A:45:ASN:ND2	1:A:46:PHE:H	2.07	0.53
1:a:302:TYR:CD1	1:a:306:THR:HB	2.44	0.53
1:C:297:GLU:OE2	1:C:300:ARG:NH2	2.42	0.52
1:G:69:ARG:NH2	2:H:52:ASP:OD2	2.42	0.52
1:K:373:LEU:CD1	1:K:388:ALA:HB2	2.39	0.52
2:Z:53:ILE:HD12	2:Z:59:THR:HG22	1.89	0.52
2:V:42:THR:HB	2:V:43:PRO:HD2	1.91	0.52
1:S:69:ARG:CZ	2:T:60:LYS:HD3	2.39	0.52
1:S:332:MET:HE3	1:S:360:TRP:HH2	1.74	0.52
1:U:292:ALA:O	1:U:294:HIS:CE1	2.62	0.52
2:d:26:ALA:HB2	2:d:36:MET:HE1	1.91	0.52
2:Z:92:THR:HG23	2:Z:115:THR:HA	1.91	0.52
1:K:149:ARG:HD3	1:K:241:MET:CE	2.38	0.52
2:X:34:ASN:O	2:X:73:ARG:NH2	2.42	0.52
1:e:69:ARG:HH12	2:f:60:LYS:HB2	1.74	0.52
1:I:86:PHE:HE1	1:I:153:THR:HG21	1.75	0.52
2:X:84:MET:HE1	2:X:114:VAL:HG21	1.92	0.52
1:c:36:ARG:HG3	1:c:379:ALA:O	2.10	0.51
1:Q:63:LEU:HB3	1:Q:70:ILE:HD12	1.91	0.51
2:F:4:VAL:HG21	2:F:107:TYR:CE2	2.44	0.51
1:S:148:MET:HE1	1:S:150:TYR:CE2	2.46	0.51
2:V:22:LEU:HD13	2:V:84:MET:CE	2.40	0.51
1:M:220:ASP:O	1:M:224:LEU:HD12	2.11	0.51
1:O:2:MET:HE1	1:O:188:MET:HE3	1.91	0.51
1:c:1:TYR:HA	1:c:206:GLU:OE2	2.10	0.51
1:c:62:ASP:OD2	1:c:69:ARG:NE	2.44	0.51
1:G:171:VAL:HG11	1:G:322:LEU:HD13	1.92	0.50
2:L:84:MET:HE2	2:L:87:LEU:HD21	1.93	0.50
1:S:2:MET:HE1	1:S:210:VAL:HB	1.93	0.50
1:c:2:MET:HE1	1:c:210:VAL:HB	1.92	0.50
2:T:41:GLN:NE2	2:T:46:GLN:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:63:LEU:HB3	1:U:70:ILE:HD12	1.93	0.50
1:c:67:GLY:O	2:d:35:THR:OG1	2.23	0.50
1:C:198:GLU:OE1	1:C:198:GLU:HA	2.10	0.50
1:I:220:ASP:O	1:I:224:LEU:HD12	2.12	0.50
1:W:188:MET:H	1:W:207:THR:HG22	1.76	0.50
1:M:373:LEU:CD2	1:M:388:ALA:HB2	2.41	0.49
1:Y:355:GLU:OE1	1:Y:355:GLU:HA	2.12	0.49
1:A:69:ARG:NH2	2:B:52:ASP:OD2	2.44	0.49
2:d:26:ALA:HB2	2:d:36:MET:CE	2.42	0.49
1:M:217:HIS:CD2	1:M:240:ARG:HH21	2.31	0.49
1:M:250:TRP:O	1:M:312:ARG:NH2	2.41	0.49
1:Y:10:THR:CB	1:Y:220:ASP:OD2	2.59	0.49
1:C:179:PHE:HB2	1:C:188:MET:SD	2.52	0.49
2:Z:10:GLY:O	2:Z:20:LEU:HD22	2.13	0.49
2:d:64:SER:O	2:d:68:ARG:NH1	2.45	0.49
1:M:373:LEU:HD21	1:M:388:ALA:HB2	1.94	0.49
1:E:69:ARG:NH2	2:F:52:ASP:OD2	2.46	0.49
1:M:414:THR:C	1:M:415:LEU:HD23	2.38	0.49
1:U:77:ASP:OD2	1:U:175:GLN:NE2	2.46	0.49
1:S:276:TRP:CZ2	1:S:295:VAL:HG23	2.48	0.48
1:C:2:MET:HE2	1:C:188:MET:HE2	1.95	0.48
1:O:68:GLU:HB2	2:P:34:ASN:HD21	1.78	0.48
1:S:356:ILE:HD12	1:S:406:HIS:CD2	2.47	0.48
2:V:22:LEU:HD13	2:V:84:MET:HE2	1.96	0.48
2:P:33:ILE:HB	2:P:78:ASN:ND2	2.28	0.48
1:e:80:PHE:CE2	1:e:84:TRP:CZ3	3.01	0.48
2:f:84:MET:HB3	2:f:87:LEU:HD21	1.95	0.48
1:C:333:THR:CB	1:C:347:TRP:HZ3	2.27	0.48
2:D:113:GLN:HB2	1:E:313:ARG:HG3	1.95	0.48
2:f:34:ASN:O	2:f:73:ARG:NH1	2.39	0.48
1:G:4:ASP:HA	1:G:209:LYS:HD3	1.94	0.48
1:Q:69:ARG:NH2	2:R:52:ASP:OD2	2.46	0.48
1:S:148:MET:HE1	1:S:150:TYR:HE2	1.78	0.48
1:W:94:PHE:CE2	1:W:119:TRP:HZ3	2.32	0.48
1:c:69:ARG:HH11	1:c:69:ARG:CB	2.26	0.48
1:G:149:ARG:NH2	1:G:245:ASP:OD1	2.47	0.48
1:M:69:ARG:NH2	2:N:52:ASP:OD2	2.47	0.47
1:S:251:ARG:HH11	1:S:251:ARG:HB3	1.79	0.47
2:T:73:ARG:HG3	2:T:80:VAL:HG12	1.95	0.47
1:E:63:LEU:HB3	1:E:70:ILE:HD12	1.97	0.47
2:X:36:MET:HE3	2:X:80:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:48:ASN:OD1	1:c:91:TYR:HB3	2.13	0.47
2:d:53:ILE:HD12	2:d:59:THR:HG22	1.96	0.47
1:O:84:TRP:NE1	1:O:265:ASP:OD1	2.41	0.47
1:a:294:HIS:ND1	1:a:297:GLU:OE2	2.42	0.47
1:E:373:LEU:HD12	1:E:388:ALA:HB2	1.97	0.47
2:V:53:ILE:HG13	2:V:59:THR:HG22	1.96	0.47
2:B:63:ASP:HA	2:B:66:LYS:HE3	1.97	0.47
1:M:63:LEU:HB3	1:M:70:ILE:HD12	1.95	0.47
1:Q:330:THR:OG1	1:Q:415:LEU:HD11	2.14	0.47
1:U:34:TYR:CE1	1:U:48:ASN:HB2	2.49	0.47
2:d:10:GLY:O	2:d:20:LEU:HD22	2.15	0.47
1:G:297:GLU:N	1:G:297:GLU:OE1	2.47	0.47
1:I:84:TRP:NE1	1:I:265:ASP:OD1	2.38	0.47
1:Y:413:LEU:C	1:Y:413:LEU:HD12	2.39	0.47
1:a:220:ASP:O	1:a:223:THR:N	2.48	0.47
1:M:361:GLN:OE1	1:M:403:HIS:NE2	2.47	0.47
1:S:83:ASP:OD1	1:S:83:ASP:N	2.40	0.47
1:W:148:MET:HB2	1:W:311:LEU:HD13	1.97	0.47
1:e:84:TRP:CE2	1:e:260:ALA:HB2	2.50	0.47
2:B:64:SER:O	2:B:68:ARG:NH2	2.48	0.47
1:I:192:ALA:O	1:I:195:ILE:HG22	2.15	0.47
2:J:92:THR:HG23	2:J:115:THR:HA	1.97	0.47
2:L:22:LEU:HD12	2:L:82:LEU:HD23	1.97	0.47
1:Q:276:TRP:HZ2	1:Q:295:VAL:HG23	1.80	0.47
1:C:2:MET:CE	1:C:188:MET:HE2	2.45	0.46
2:H:84:MET:HB3	2:H:87:LEU:HD21	1.98	0.46
1:K:8:GLU:HG3	1:K:295:VAL:CG2	2.45	0.46
1:U:245:ASP:OD2	1:U:256:TYR:HE1	1.98	0.46
2:Z:22:LEU:HD11	2:Z:84:MET:HE2	1.97	0.46
1:c:28:THR:HG22	1:c:29:PRO:HD2	1.98	0.46
1:S:149:ARG:NH2	1:S:245:ASP:OD1	2.48	0.46
2:R:20:LEU:HB2	2:R:84:MET:HE3	1.97	0.46
1:W:75:HIS:HB3	1:W:90:TYR:CD2	2.51	0.46
1:K:8:GLU:HG3	1:K:295:VAL:HG21	1.97	0.46
1:S:148:MET:CE	1:S:150:TYR:CE2	2.99	0.46
1:E:178:ARG:C	1:E:188:MET:HE3	2.41	0.46
1:O:157:ARG:NH2	1:O:162:GLU:O	2.41	0.46
1:W:67:GLY:N	2:X:104:ASN:OD1	2.41	0.46
1:Y:84:TRP:CE2	1:Y:260:ALA:HB2	2.51	0.46
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.15	0.46
1:C:171:VAL:HG11	1:C:322:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:69:PHE:CE2	2:f:84:MET:HG2	2.50	0.46
2:J:68:ARG:NH2	2:J:91:ASP:OD2	2.47	0.46
1:K:374:VAL:HG11	1:K:387:TRP:CZ2	2.52	0.46
1:a:1:TYR:O	1:a:302:TYR:OH	2.27	0.46
1:c:198:GLU:OE2	1:c:198:GLU:HA	2.16	0.46
1:C:374:VAL:HG12	1:C:387:TRP:O	2.16	0.45
1:K:207:THR:HG22	1:K:211:LYS:HE3	1.98	0.45
1:Y:2:MET:HE3	1:Y:152:PHE:HZ	1.80	0.45
1:Y:118:LYS:NZ	2:Z:105:ASP:OD1	2.43	0.45
2:Z:68:ARG:NH2	2:Z:91:ASP:OD2	2.49	0.45
1:c:206:GLU:HA	1:c:209:LYS:HE2	1.98	0.45
1:W:94:PHE:HZ	1:W:119:TRP:CH2	2.34	0.45
1:c:178:ARG:NH2	1:c:189:GLU:OE1	2.49	0.45
2:F:90:GLU:N	2:F:90:GLU:OE1	2.48	0.45
1:K:272:ASP:OD1	1:K:272:ASP:N	2.45	0.45
1:Q:287:LYS:HB3	1:Q:287:LYS:HE3	1.69	0.45
1:S:84:TRP:NE1	1:S:265:ASP:OD1	2.42	0.45
1:a:346:CYS:O	1:a:387:TRP:HA	2.15	0.45
1:e:69:ARG:NH1	2:f:60:LYS:HB2	2.31	0.45
2:B:34:ASN:O	2:B:73:ARG:NH1	2.44	0.45
1:K:361:GLN:OE1	1:K:403:HIS:CD2	2.70	0.45
1:Q:206:GLU:O	1:Q:210:VAL:HG12	2.17	0.45
1:Q:354:ALA:HB2	1:Q:384:PHE:CD2	2.51	0.45
1:e:203:TRP:O	1:e:207:THR:OG1	2.32	0.45
1:c:311:LEU:O	1:c:315:LEU:HD23	2.17	0.45
1:e:241:MET:C	1:e:241:MET:HE3	2.41	0.45
1:C:178:ARG:HD3	1:C:191:ARG:CZ	2.46	0.45
1:E:220:ASP:OD2	1:E:259:TYR:OH	2.32	0.45
1:I:313:ARG:HG3	2:P:113:GLN:HB2	1.99	0.45
1:S:176:PHE:HD2	1:S:195:ILE:HD13	1.81	0.45
1:E:346:CYS:O	1:E:387:TRP:HA	2.17	0.45
1:M:4:ASP:HA	1:M:209:LYS:HD3	1.98	0.45
2:N:22:LEU:HG	2:N:84:MET:HE2	1.99	0.45
1:S:332:MET:CE	1:S:360:TRP:HH2	2.29	0.45
1:U:283:ALA:O	1:U:286:THR:OG1	2.29	0.45
1:c:247:GLY:N	1:c:253:LEU:HD12	2.31	0.45
1:G:373:LEU:CD1	1:G:388:ALA:HB2	2.47	0.45
2:J:69:PHE:CE2	2:J:84:MET:HG2	2.52	0.45
1:S:75:HIS:HB3	1:S:90:TYR:CD1	2.51	0.45
2:T:94:VAL:HG11	1:W:313:ARG:NH2	2.32	0.45
1:a:280:ASP:C	1:a:280:ASP:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:CB	1:A:70:ILE:HD12	2.46	0.44
1:I:220:ASP:C	1:I:224:LEU:HD12	2.42	0.44
1:U:1:TYR:N	1:U:150:TYR:OH	2.45	0.44
1:a:284:GLN:HG2	1:a:288:HIS:CE1	2.52	0.44
1:Q:373:LEU:HD12	1:Q:388:ALA:HB2	1.99	0.44
1:c:213:HIS:O	1:c:217:HIS:ND1	2.45	0.44
1:E:176:PHE:CD2	1:E:177:VAL:HG13	2.53	0.44
1:E:349:LEU:HD23	1:E:385:GLN:HG2	2.00	0.44
1:Y:252:PHE:HB2	1:Y:308:VAL:HG21	2.00	0.44
1:e:310:TRP:HA	1:e:313:ARG:HD3	2.00	0.44
1:Q:348:ALA:C	1:Q:349:LEU:HD23	2.42	0.44
2:Z:22:LEU:HD11	2:Z:84:MET:CE	2.47	0.44
2:X:6:LEU:HD22	2:X:24:CYS:SG	2.58	0.44
1:a:171:VAL:HG11	1:a:322:LEU:HD13	1.99	0.44
1:a:319:LYS:O	1:a:324:ARG:NH2	2.51	0.44
1:G:100:ASP:O	1:G:121:ARG:NH2	2.50	0.44
1:S:154:SER:HA	1:S:164:ARG:O	2.18	0.44
1:G:9:THR:HG22	1:G:10:THR:N	2.33	0.44
1:Q:79:SER:HB3	1:Q:87:TYR:CZ	2.53	0.44
2:T:63:ASP:C	2:T:65:VAL:H	2.26	0.44
1:a:238:VAL:HG11	1:a:259:TYR:OH	2.18	0.44
2:f:65:VAL:HG21	2:f:69:PHE:CG	2.53	0.44
1:O:415:LEU:N	1:O:415:LEU:HD22	2.33	0.43
2:f:36:MET:CE	2:f:80:VAL:HG13	2.49	0.43
2:Z:113:GLN:HB2	1:c:313:ARG:HG3	2.00	0.43
1:a:48:ASN:HB3	1:a:89:LEU:HD11	1.99	0.43
1:C:333:THR:CB	1:C:347:TRP:CZ3	3.00	0.43
1:O:346:CYS:O	1:O:387:TRP:HA	2.18	0.43
1:a:63:LEU:O	1:a:70:ILE:HG22	2.18	0.43
1:a:220:ASP:O	1:a:221:LEU:C	2.62	0.43
2:D:22:LEU:HD11	2:D:84:MET:CE	2.49	0.43
1:E:84:TRP:CE2	1:E:260:ALA:HB2	2.53	0.43
2:R:53:ILE:HG22	2:R:71:ILE:HD13	1.99	0.43
2:b:36:MET:HB2	2:b:80:VAL:HG11	2.01	0.43
1:A:381:ASP:OD1	1:A:383:THR:OG1	2.34	0.43
2:D:64:SER:O	2:D:68:ARG:NH1	2.52	0.43
1:e:50:TYR:CE1	1:e:378:PRO:CD	3.01	0.43
1:E:345:ARG:CB	1:E:347:TRP:CZ3	3.02	0.43
1:G:217:HIS:HE2	1:G:240:ARG:HH11	1.67	0.43
2:N:22:LEU:HD12	2:N:82:LEU:HD23	2.00	0.43
1:O:68:GLU:HB2	2:P:34:ASN:ND2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:147:SER:OG	1:a:245:ASP:OD1	2.35	0.43
2:d:4:VAL:HB	2:d:107:TYR:CD1	2.53	0.43
1:A:269:LEU:HG	1:A:273:LEU:HA	2.00	0.43
1:K:325:THR:HG21	1:K:407:GLU:OE1	2.18	0.43
1:U:346:CYS:O	1:U:387:TRP:HA	2.18	0.43
1:a:285:THR:HG22	1:a:286:THR:N	2.34	0.43
1:c:28:THR:HG22	1:c:29:PRO:CD	2.48	0.43
1:U:79:SER:HB3	1:U:87:TYR:CZ	2.54	0.43
2:T:68:ARG:NH2	2:T:86:SER:O	2.52	0.42
1:U:28:THR:OG1	1:U:29:PRO:HD2	2.19	0.42
1:W:94:PHE:CZ	1:W:119:TRP:CH2	3.07	0.42
1:c:32:GLN:OE1	1:c:377:ARG:NH1	2.47	0.42
1:C:95:THR:HG22	1:C:95:THR:O	2.18	0.42
1:Q:406:HIS:HB3	1:Q:409:LEU:HD12	2.01	0.42
1:e:80:PHE:N	1:e:80:PHE:CD1	2.87	0.42
1:G:386:LYS:NZ	3:G:503:HOH:O	2.47	0.42
2:H:20:LEU:HB2	2:H:84:MET:HE3	2.01	0.42
1:K:346:CYS:C	1:K:347:TRP:HD1	2.27	0.42
2:N:84:MET:HE1	2:N:114:VAL:HG21	2.02	0.42
1:a:164:ARG:CD	1:a:182:ASP:OD1	2.67	0.42
1:M:105:ARG:HE	1:M:114:PRO:HB2	1.84	0.42
1:S:374:VAL:O	1:S:386:LYS:HE3	2.18	0.42
1:U:387:TRP:CE3	1:U:387:TRP:C	2.97	0.42
1:W:84:TRP:CE2	1:W:260:ALA:HB2	2.54	0.42
2:Z:82:LEU:HD23	2:Z:84:MET:HE2	2.02	0.42
1:a:84:TRP:NE1	1:a:265:ASP:OD1	2.49	0.42
1:Q:350:SER:HA	1:Q:383:THR:HB	2.00	0.42
1:U:34:TYR:CE2	1:U:377:ARG:HD2	2.55	0.42
1:Y:9:THR:OG1	1:Y:10:THR:N	2.52	0.42
1:a:374:VAL:O	1:a:386:LYS:HE3	2.18	0.42
2:b:84:MET:HE2	2:b:87:LEU:HD21	2.01	0.42
1:c:280:ASP:O	1:c:284:GLN:OE1	2.38	0.42
1:A:171:VAL:HG11	1:A:322:LEU:HD13	2.01	0.42
1:K:147:SER:HB3	1:K:245:ASP:OD1	2.19	0.42
1:Y:79:SER:HB3	1:Y:87:TYR:CZ	2.54	0.42
1:c:281:MET:HA	1:c:284:GLN:OE1	2.19	0.42
1:e:50:TYR:CD1	1:e:378:PRO:HD2	2.55	0.42
1:A:4:ASP:HA	1:A:209:LYS:HD3	2.00	0.42
1:Y:217:HIS:NE2	1:Y:259:TYR:HE1	2.17	0.42
1:e:75:HIS:HB3	1:e:90:TYR:CD2	2.55	0.42
2:H:40:ARG:HD3	2:H:50:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:62:GLY:O	2:T:65:VAL:HG12	2.19	0.42
1:W:94:PHE:CE2	1:W:119:TRP:CZ3	3.08	0.42
1:a:63:LEU:HB2	1:a:70:ILE:CG2	2.49	0.42
1:a:148:MET:HE3	1:a:150:TYR:HE1	1.84	0.42
1:e:45:ASN:OD1	1:e:46:PHE:N	2.46	0.42
2:d:92:THR:HG23	2:d:115:THR:HA	2.01	0.41
1:A:62:ASP:OD2	1:A:69:ARG:NH1	2.53	0.41
1:O:252:PHE:HB2	1:O:308:VAL:HG21	2.02	0.41
2:P:87:LEU:HB3	2:P:116:VAL:HG21	2.02	0.41
1:S:3:LEU:HD23	1:S:302:TYR:CG	2.55	0.41
2:V:51:ALA:HB2	2:V:61:TYR:HD1	1.85	0.41
1:W:149:ARG:NH1	1:W:245:ASP:OD1	2.53	0.41
2:Z:84:MET:HB3	2:Z:87:LEU:HD21	2.02	0.41
1:K:403:HIS:CD2	1:K:414:THR:HG23	2.55	0.41
2:L:68:ARG:NH2	2:L:91:ASP:OD2	2.47	0.41
1:Y:194:TRP:CZ2	1:Y:322:LEU:HD21	2.55	0.41
1:C:297:GLU:OE2	1:C:300:ARG:NH1	2.52	0.41
1:O:3:LEU:HD23	1:O:302:TYR:CG	2.55	0.41
2:T:38:TRP:CH2	2:T:80:VAL:HG23	2.55	0.41
1:U:294:HIS:ND1	1:U:294:HIS:N	2.68	0.41
1:W:94:PHE:HZ	1:W:119:TRP:HH2	1.66	0.41
2:Z:34:ASN:O	2:Z:73:ARG:NH1	2.47	0.41
2:b:92:THR:HG23	2:b:115:THR:HA	2.02	0.41
1:e:202:TYR:O	1:e:206:GLU:HG2	2.21	0.41
1:O:179:PHE:CB	1:O:188:MET:HE2	2.51	0.41
2:R:19:SER:N	2:X:19:SER:OG	2.48	0.41
1:S:206:GLU:O	1:S:210:VAL:HG12	2.20	0.41
1:a:70:ILE:HD12	1:a:71:GLU:H	1.86	0.41
2:V:32:SER:O	2:V:33:ILE:HD13	2.19	0.41
2:b:6:LEU:HD23	2:b:26:ALA:HA	2.03	0.41
1:Q:270:LYS:CD	1:Q:271:GLU:H	2.33	0.41
1:Q:414:THR:O	1:Q:415:LEU:HD23	2.19	0.41
1:W:192:ALA:O	1:W:195:ILE:HG22	2.21	0.41
1:a:242:TYR:CD1	1:a:242:TYR:C	2.98	0.41
1:I:77:ASP:OD2	1:I:175:GLN:NE2	2.52	0.41
1:K:9:THR:HG22	1:K:10:THR:N	2.35	0.41
2:P:97:CYS:SG	2:P:98:TYR:N	2.93	0.41
2:f:65:VAL:CG2	2:f:69:PHE:CG	3.04	0.41
1:G:79:SER:HB3	1:G:87:TYR:CZ	2.56	0.41
1:K:162:GLU:CB	1:K:218:ARG:NH1	2.84	0.41
1:Q:80:PHE:CE1	1:Q:151:PHE:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:276:TRP:CZ2	1:Q:295:VAL:HG23	2.56	0.41
1:U:64:LEU:HA	1:U:68:GLU:O	2.21	0.41
2:V:22:LEU:CD1	2:V:84:MET:CE	2.99	0.41
1:c:37:HIS:CB	1:c:38:PRO:CD	2.98	0.41
2:f:92:THR:HG23	2:f:115:THR:HA	2.03	0.41
1:I:51:VAL:HG11	1:I:59:ILE:CD1	2.51	0.40
1:Y:355:GLU:OE1	1:Y:355:GLU:CA	2.69	0.40
1:Y:37:HIS:HB3	1:Y:38:PRO:HD2	2.03	0.40
1:e:95:THR:O	1:e:95:THR:OG1	2.35	0.40
1:A:270:LYS:HD2	1:A:270:LYS:HA	1.91	0.40
1:K:216:THR:O	1:K:220:ASP:OD1	2.39	0.40
1:O:402:CYS:SG	1:O:415:LEU:HD23	2.61	0.40
1:Q:373:LEU:CD1	1:Q:388:ALA:HB2	2.51	0.40
1:Y:188:MET:HE3	1:Y:210:VAL:HB	2.03	0.40
1:c:324:ARG:NH1	1:c:326:ASP:OD2	2.52	0.40
1:A:302:TYR:CD1	1:A:302:TYR:C	3.00	0.40
1:A:332:MET:CE	1:A:360:TRP:HH2	2.35	0.40
1:M:387:TRP:CE3	1:M:387:TRP:C	3.00	0.40
2:X:22:LEU:CD2	2:X:84:MET:HE2	2.50	0.40
1:Y:67:GLY:O	2:Z:35:THR:OG1	2.28	0.40
1:A:79:SER:HB3	1:A:87:TYR:CZ	2.56	0.40
2:B:38:TRP:CH2	2:B:80:VAL:HG23	2.56	0.40
1:K:79:SER:HB3	1:K:87:TYR:CZ	2.56	0.40
1:O:149:ARG:HH11	1:O:149:ARG:CG	2.35	0.40
1:O:328:PRO:HB3	1:O:351:PHE:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:86:SER:H	2:V:19:SER:HG[1_545]	1.25	0.35

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	254 (98%)	4 (2%)	55	72
1	C	256/351 (73%)	252 (98%)	4 (2%)	55	72
1	E	266/351 (76%)	260 (98%)	6 (2%)	44	65
1	G	267/351 (76%)	262 (98%)	5 (2%)	50	68
1	I	256/351 (73%)	254 (99%)	2 (1%)	73	83
1	K	265/351 (76%)	261 (98%)	4 (2%)	57	73
1	M	262/351 (75%)	258 (98%)	4 (2%)	57	73
1	O	259/351 (74%)	254 (98%)	5 (2%)	50	68
1	Q	256/351 (73%)	253 (99%)	3 (1%)	63	77
1	S	241/351 (69%)	237 (98%)	4 (2%)	53	71
1	U	221/351 (63%)	215 (97%)	6 (3%)	39	61
1	W	234/351 (67%)	228 (97%)	6 (3%)	40	62
1	Y	245/351 (70%)	239 (98%)	6 (2%)	43	63
1	a	238/351 (68%)	232 (98%)	6 (2%)	42	63
1	c	207/351 (59%)	203 (98%)	4 (2%)	50	68
1	e	229/351 (65%)	225 (98%)	4 (2%)	53	71
2	B	86/97 (89%)	82 (95%)	4 (5%)	23	43
2	D	86/97 (89%)	86 (100%)	0	100	100
2	F	88/97 (91%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	88/97 (91%)	87 (99%)	1 (1%)	65	79
2	J	87/97 (90%)	86 (99%)	1 (1%)	65	79
2	L	88/97 (91%)	88 (100%)	0	100	100
2	N	87/97 (90%)	86 (99%)	1 (1%)	65	79
2	P	87/97 (90%)	87 (100%)	0	100	100
2	R	85/97 (88%)	85 (100%)	0	100	100
2	T	80/97 (82%)	78 (98%)	2 (2%)	42	63
2	V	87/97 (90%)	85 (98%)	2 (2%)	44	65
2	X	84/97 (87%)	82 (98%)	2 (2%)	43	63
2	Z	84/97 (87%)	83 (99%)	1 (1%)	63	77
2	b	81/97 (84%)	79 (98%)	2 (2%)	42	63
2	d	87/97 (90%)	86 (99%)	1 (1%)	65	79
2	f	86/97 (89%)	85 (99%)	1 (1%)	63	77
All	All	5331/7168 (74%)	5240 (98%)	91 (2%)	53	71

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	94	PHE
1	A	346	CYS
1	A	402	CYS
2	B	23	SER
2	B	70	THR
2	B	90	GLU
2	B	117	SER
1	C	154	SER
1	C	330	THR
1	C	346	CYS
1	C	402	CYS
1	E	154	SER
1	E	277	THR
1	E	287	LYS
1	E	346	CYS
1	E	350	SER
1	E	402	CYS
1	G	94	PHE

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Mol	Chain	Res	Type
1	G	306	THR
1	G	332	MET
1	G	346	CYS
1	G	402	CYS
2	H	66	LYS
1	I	349	LEU
1	I	402	CYS
2	J	58	SER
1	K	94	PHE
1	K	154	SER
1	K	272	ASP
1	K	402	CYS
1	M	224	LEU
1	M	331	HIS
1	M	346	CYS
1	M	402	CYS
2	N	23	SER
1	O	210	VAL
1	O	346	CYS
1	O	349	LEU
1	O	350	SER
1	O	402	CYS
1	Q	57	SER
1	Q	346	CYS
1	Q	402	CYS
1	S	112	SER
1	S	346	CYS
1	S	350	SER
1	S	402	CYS
2	T	86	SER
2	T	117	SER
1	U	51	VAL
1	U	58	ASP
1	U	94	PHE
1	U	145	SER
1	U	154	SER
1	U	346	CYS
2	V	23	SER
2	V	101	SER
1	W	35	SER
1	W	75	HIS
1	W	154	SER

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Mol	Chain	Res	Type
1	W	178	ARG
1	W	313	ARG
1	W	346	CYS
2	X	58	SER
2	X	117	SER
1	Y	28	THR
1	Y	109	VAL
1	Y	154	SER
1	Y	275	SER
1	Y	344	LEU
1	Y	402	CYS
2	Z	117	SER
1	a	154	SER
1	a	214	SER
1	a	285	THR
1	a	324	ARG
1	a	346	CYS
1	a	402	CYS
2	b	55	SER
2	b	117	SER
1	c	94	PHE
1	c	154	SER
1	c	346	CYS
1	c	402	CYS
2	d	86	SER
1	e	275	SER
1	e	277	THR
1	e	313	ARG
1	e	402	CYS
2	f	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	45	ASN
1	A	323	GLN
1	A	403	HIS
1	C	37	HIS
1	E	37	HIS
1	E	361	GLN
1	E	403	HIS

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Mol	Chain	Res	Type
1	G	37	HIS
1	G	197	GLN
1	G	403	HIS
1	I	37	HIS
1	I	146	HIS
2	J	113	GLN
1	K	37	HIS
1	M	32	GLN
2	N	113	GLN
1	O	284	GLN
2	P	113	GLN
1	Q	6	GLN
1	Q	75	HIS
1	Q	236	HIS
2	R	110	GLN
2	R	113	GLN
1	S	175	GLN
1	S	236	HIS
2	T	41	GLN
1	U	37	HIS
1	U	146	HIS
1	W	37	HIS
2	X	85	ASN
2	X	113	GLN
1	a	37	HIS
1	a	236	HIS
2	b	41	GLN
2	d	113	GLN
2	f	46	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/429 (85%)	-0.53	11 (2%) 52 50	27, 53, 106, 139	0
1	C	366/429 (85%)	-0.65	5 (1%) 73 72	30, 52, 93, 127	0
1	E	362/429 (84%)	-0.71	2 (0%) 85 85	31, 52, 90, 114	0
1	G	382/429 (89%)	-0.72	1 (0%) 90 91	23, 51, 105, 121	0
1	I	359/429 (83%)	-0.72	1 (0%) 90 91	24, 52, 89, 122	0
1	K	382/429 (89%)	-0.69	1 (0%) 90 91	23, 52, 98, 122	0
1	M	378/429 (88%)	-0.42	12 (3%) 50 48	30, 55, 119, 144	0
1	O	361/429 (84%)	-0.71	3 (0%) 82 82	29, 51, 87, 119	0
1	Q	384/429 (89%)	-0.49	0 100 100	43, 68, 100, 120	0
1	S	344/429 (80%)	-0.36	3 (0%) 81 81	48, 69, 96, 113	0
1	U	333/429 (77%)	-0.37	3 (0%) 81 81	43, 67, 102, 114	0
1	W	347/429 (80%)	-0.19	7 (2%) 65 62	51, 72, 98, 111	0
1	Y	365/429 (85%)	-0.31	4 (1%) 78 77	47, 67, 102, 134	0
1	a	342/429 (79%)	-0.31	2 (0%) 85 85	41, 69, 100, 114	0
1	c	327/429 (76%)	-0.17	9 (2%) 55 52	47, 71, 103, 114	0
1	e	353/429 (82%)	-0.15	7 (1%) 65 62	49, 72, 104, 139	0
2	B	115/116 (99%)	-0.97	1 (0%) 81 81	27, 41, 77, 84	0
2	D	115/116 (99%)	-0.85	0 100 100	28, 45, 80, 90	0
2	F	115/116 (99%)	-0.94	0 100 100	27, 44, 76, 85	0
2	H	115/116 (99%)	-0.96	0 100 100	29, 41, 72, 84	0
2	J	115/116 (99%)	-0.99	0 100 100	29, 43, 81, 100	0
2	L	115/116 (99%)	-0.96	0 100 100	27, 41, 75, 87	0
2	N	115/116 (99%)	-0.96	0 100 100	26, 40, 74, 99	0
2	P	115/116 (99%)	-0.88	0 100 100	29, 45, 83, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	R	112/116 (96%)	-0.62	0 100 100	47, 61, 90, 109	0
2	T	115/116 (99%)	-0.58	0 100 100	46, 58, 90, 96	0
2	V	115/116 (99%)	-0.46	2 (1%) 69 66	41, 61, 87, 99	0
2	X	115/116 (99%)	-0.38	2 (1%) 69 66	53, 66, 91, 108	0
2	Z	110/116 (94%)	-0.59	1 (0%) 81 81	45, 61, 85, 116	0
2	b	115/116 (99%)	-0.47	2 (1%) 69 66	44, 58, 87, 116	0
2	d	112/116 (96%)	-0.57	1 (0%) 81 81	45, 58, 85, 105	0
2	f	115/116 (99%)	-0.50	2 (1%) 69 66	45, 61, 88, 106	0
All	All	7582/8720 (86%)	-0.54	82 (1%) 78 77	23, 61, 98, 144	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	HIS	4.9
1	M	417	TRP	4.5
1	c	405	GLN	4.3
2	b	29	SER	4.3
1	c	279	ALA	3.9
1	Y	339	ASP	3.8
1	c	347	TRP	3.7
1	a	333	THR	3.7
1	S	144	GLY	3.5
1	M	394	SER	3.4
1	U	279	ALA	3.3
1	c	343	THR	3.2
1	Y	342	ALA	3.2
1	M	412	PRO	3.1
1	M	362	ARG	3.1
1	M	339	ASP	3.0
1	M	392	VAL	3.0
1	A	414	THR	3.0
1	A	143	SER	3.0
1	W	412	PRO	2.9
1	M	393	PRO	2.9
1	I	417	TRP	2.9
1	A	396	GLN	2.9
1	M	396	GLN	2.9
1	e	144	GLY	2.9
1	C	358	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	2.8
1	A	398	GLN	2.8
1	S	401	THR	2.8
2	X	28	GLY	2.8
1	c	389	ALA	2.8
1	e	390	VAL	2.8
1	A	399	ARG	2.8
2	V	29	SER	2.7
1	M	398	GLN	2.6
1	W	416	ARG	2.6
1	W	348	ALA	2.6
1	a	144	GLY	2.5
2	f	28	GLY	2.5
1	c	10	THR	2.4
1	e	414	THR	2.4
1	G	394	SER	2.4
1	W	100	ASP	2.4
1	Y	397	GLU	2.4
1	e	399	ARG	2.4
1	C	391	VAL	2.4
1	M	340	HIS	2.3
1	W	44	SER	2.3
1	W	122	ASP	2.3
2	b	31	PHE	2.3
1	W	415	LEU	2.3
1	A	397	GLU	2.3
1	M	397	GLU	2.3
1	e	44	SER	2.3
1	E	331	HIS	2.2
1	C	399	ARG	2.2
2	f	75	ASN	2.2
1	C	398	GLN	2.2
1	O	122	ASP	2.2
2	V	31	PHE	2.2
1	M	338	SER	2.1
1	c	348	ALA	2.1
1	O	343	THR	2.1
1	U	390	VAL	2.1
1	Y	363	ASP	2.1
1	C	410	PRO	2.1
1	E	328	PRO	2.1
1	A	394	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	397	GLU	2.1
1	c	388	ALA	2.1
2	B	3	GLU	2.1
1	A	387	TRP	2.1
1	S	360	TRP	2.1
2	Z	76	THR	2.1
1	e	344	LEU	2.1
2	X	30	ILE	2.1
1	e	358	LEU	2.0
1	c	234	GLY	2.0
1	K	122	ASP	2.0
2	d	32	SER	2.0
1	U	360	TRP	2.0
1	A	392	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.