



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 PM GMT

PDB ID : 4GQH  
Title : The Conformations and Interactions of the Four-Layer Aggregate Revealed by X-ray Crystallography Diffraction Implied the Importance of Peptides at Opposite Ends in Their Assemblies  
Authors : Li, X.Y.; Song, B.A.; Hu, D.Y.; Chen, X.; Wang, Z.C.; Zeng, M.J.; Yu, D.D.; Chen, Z.; Jin, L.H.; Yang, S.  
Deposited on : 2012-08-23  
Resolution : 3.06 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

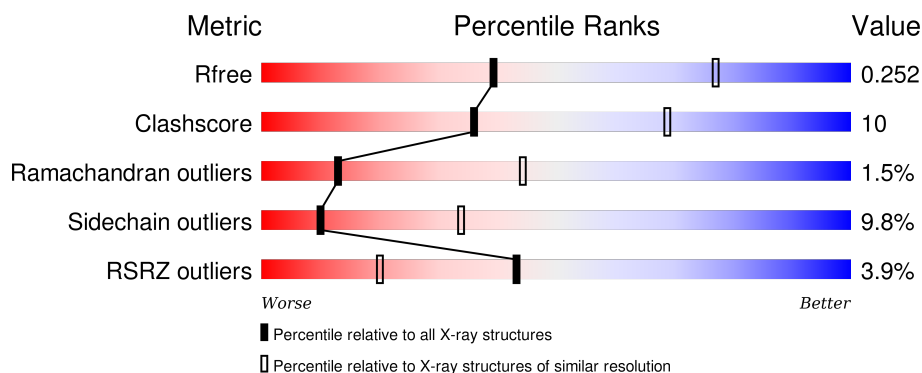
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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))
$R_{free}$	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	174	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>24%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	174	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	174	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>25%</div> <div>•</div> <div>17%</div> </div> </div>
1	D	174	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>28%</div> <div>•</div> <div>18%</div> </div> </div>
1	E	174	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>19%</div> <div>6%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	174	
1	G	174	
1	H	174	
1	I	174	
1	J	174	
1	K	174	
1	L	174	
1	M	174	
1	N	174	
1	O	174	
1	P	174	
1	Q	174	
1	R	174	
1	S	174	
1	T	174	
1	U	174	
1	V	174	
1	W	174	
1	X	174	
1	Y	174	
1	Z	174	
1	a	174	
1	b	174	
1	c	174	
1	d	174	

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Mol	Chain	Length	Quality of chain
1	e	174	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>71%</div><div>6%</div><div>23%</div></div>
1	f	174	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>70%</div><div>7%</div><div>23%</div></div>
1	h	174	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>68%</div><div>9%</div><div>23%</div></div>
1	i	174	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>70%</div><div>7%</div><div>23%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 36918 atoms, of which 0 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1115	703	195	216	1			
1	B	139	Total	C	N	O	S	0	0	0
			1096	691	192	212	1			
1	C	144	Total	C	N	O	S	0	0	0
			1132	713	197	221	1			
1	D	143	Total	C	N	O	S	0	0	0
			1126	709	199	217	1			
1	E	140	Total	C	N	O	S	0	0	0
			1100	693	193	213	1			
1	F	143	Total	C	N	O	S	0	0	0
			1131	712	199	219	1			
1	G	143	Total	C	N	O	S	0	0	0
			1131	715	199	216	1			
1	H	144	Total	C	N	O	S	0	0	0
			1135	714	200	220	1			
1	I	141	Total	C	N	O	S	0	0	0
			1111	701	194	215	1			
1	J	145	Total	C	N	O	S	0	0	0
			1143	719	201	222	1			
1	K	143	Total	C	N	O	S	0	0	0
			1131	712	199	219	1			
1	L	141	Total	C	N	O	S	0	0	0
			1111	701	194	215	1			
1	M	142	Total	C	N	O	S	0	0	0
			1122	707	198	216	1			
1	N	142	Total	C	N	O	S	0	0	0
			1122	707	198	216	1			
1	O	140	Total	C	N	O	S	0	0	0
			1100	693	193	213	1			
1	P	147	Total	C	N	O	S	0	0	0
			1157	728	203	225	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	146	Total	C	N	O	S	0	0	0
			1150	723	202	224	1			
1	R	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	S	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	T	132	Total	C	N	O	S	0	0	0
			1039	659	178	201	1			
1	U	133	Total	C	N	O	S	0	0	0
			1046	664	179	202	1			
1	V	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	W	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	X	131	Total	C	N	O	S	0	0	0
			1028	653	174	200	1			
1	Y	132	Total	C	N	O	S	0	0	0
			1035	658	175	201	1			
1	Z	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	a	131	Total	C	N	O	S	0	0	0
			1029	655	174	199	1			
1	b	132	Total	C	N	O	S	0	0	0
			1035	658	175	201	1			
1	c	136	Total	C	N	O	S	0	0	0
			1069	676	186	206	1			
1	d	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	e	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	f	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	h	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			
1	i	134	Total	C	N	O	S	0	0	0
			1054	668	181	204	1			

There are 680 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P69687
A	-18	GLY	-	EXPRESSION TAG	UNP P69687
A	-17	SER	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	SER	-	EXPRESSION TAG	UNP P69687
A	-15	HIS	-	EXPRESSION TAG	UNP P69687
A	-14	HIS	-	EXPRESSION TAG	UNP P69687
A	-13	HIS	-	EXPRESSION TAG	UNP P69687
A	-12	HIS	-	EXPRESSION TAG	UNP P69687
A	-11	HIS	-	EXPRESSION TAG	UNP P69687
A	-10	HIS	-	EXPRESSION TAG	UNP P69687
A	-9	SER	-	EXPRESSION TAG	UNP P69687
A	-8	SER	-	EXPRESSION TAG	UNP P69687
A	-7	GLY	-	EXPRESSION TAG	UNP P69687
A	-6	LEU	-	EXPRESSION TAG	UNP P69687
A	-5	VAL	-	EXPRESSION TAG	UNP P69687
A	-4	PRO	-	EXPRESSION TAG	UNP P69687
A	-3	ARG	-	EXPRESSION TAG	UNP P69687
A	-2	GLY	-	EXPRESSION TAG	UNP P69687
A	-1	SER	-	EXPRESSION TAG	UNP P69687
A	0	HIS	-	EXPRESSION TAG	UNP P69687
B	-19	MET	-	EXPRESSION TAG	UNP P69687
B	-18	GLY	-	EXPRESSION TAG	UNP P69687
B	-17	SER	-	EXPRESSION TAG	UNP P69687
B	-16	SER	-	EXPRESSION TAG	UNP P69687
B	-15	HIS	-	EXPRESSION TAG	UNP P69687
B	-14	HIS	-	EXPRESSION TAG	UNP P69687
B	-13	HIS	-	EXPRESSION TAG	UNP P69687
B	-12	HIS	-	EXPRESSION TAG	UNP P69687
B	-11	HIS	-	EXPRESSION TAG	UNP P69687
B	-10	HIS	-	EXPRESSION TAG	UNP P69687
B	-9	SER	-	EXPRESSION TAG	UNP P69687
B	-8	SER	-	EXPRESSION TAG	UNP P69687
B	-7	GLY	-	EXPRESSION TAG	UNP P69687
B	-6	LEU	-	EXPRESSION TAG	UNP P69687
B	-5	VAL	-	EXPRESSION TAG	UNP P69687
B	-4	PRO	-	EXPRESSION TAG	UNP P69687
B	-3	ARG	-	EXPRESSION TAG	UNP P69687
B	-2	GLY	-	EXPRESSION TAG	UNP P69687
B	-1	SER	-	EXPRESSION TAG	UNP P69687
B	0	HIS	-	EXPRESSION TAG	UNP P69687
C	-19	MET	-	EXPRESSION TAG	UNP P69687
C	-18	GLY	-	EXPRESSION TAG	UNP P69687
C	-17	SER	-	EXPRESSION TAG	UNP P69687
C	-16	SER	-	EXPRESSION TAG	UNP P69687
C	-15	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP P69687
C	-13	HIS	-	EXPRESSION TAG	UNP P69687
C	-12	HIS	-	EXPRESSION TAG	UNP P69687
C	-11	HIS	-	EXPRESSION TAG	UNP P69687
C	-10	HIS	-	EXPRESSION TAG	UNP P69687
C	-9	SER	-	EXPRESSION TAG	UNP P69687
C	-8	SER	-	EXPRESSION TAG	UNP P69687
C	-7	GLY	-	EXPRESSION TAG	UNP P69687
C	-6	LEU	-	EXPRESSION TAG	UNP P69687
C	-5	VAL	-	EXPRESSION TAG	UNP P69687
C	-4	PRO	-	EXPRESSION TAG	UNP P69687
C	-3	ARG	-	EXPRESSION TAG	UNP P69687
C	-2	GLY	-	EXPRESSION TAG	UNP P69687
C	-1	SER	-	EXPRESSION TAG	UNP P69687
C	0	HIS	-	EXPRESSION TAG	UNP P69687
D	-19	MET	-	EXPRESSION TAG	UNP P69687
D	-18	GLY	-	EXPRESSION TAG	UNP P69687
D	-17	SER	-	EXPRESSION TAG	UNP P69687
D	-16	SER	-	EXPRESSION TAG	UNP P69687
D	-15	HIS	-	EXPRESSION TAG	UNP P69687
D	-14	HIS	-	EXPRESSION TAG	UNP P69687
D	-13	HIS	-	EXPRESSION TAG	UNP P69687
D	-12	HIS	-	EXPRESSION TAG	UNP P69687
D	-11	HIS	-	EXPRESSION TAG	UNP P69687
D	-10	HIS	-	EXPRESSION TAG	UNP P69687
D	-9	SER	-	EXPRESSION TAG	UNP P69687
D	-8	SER	-	EXPRESSION TAG	UNP P69687
D	-7	GLY	-	EXPRESSION TAG	UNP P69687
D	-6	LEU	-	EXPRESSION TAG	UNP P69687
D	-5	VAL	-	EXPRESSION TAG	UNP P69687
D	-4	PRO	-	EXPRESSION TAG	UNP P69687
D	-3	ARG	-	EXPRESSION TAG	UNP P69687
D	-2	GLY	-	EXPRESSION TAG	UNP P69687
D	-1	SER	-	EXPRESSION TAG	UNP P69687
D	0	HIS	-	EXPRESSION TAG	UNP P69687
E	-19	MET	-	EXPRESSION TAG	UNP P69687
E	-18	GLY	-	EXPRESSION TAG	UNP P69687
E	-17	SER	-	EXPRESSION TAG	UNP P69687
E	-16	SER	-	EXPRESSION TAG	UNP P69687
E	-15	HIS	-	EXPRESSION TAG	UNP P69687
E	-14	HIS	-	EXPRESSION TAG	UNP P69687
E	-13	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	EXPRESSION TAG	UNP P69687
E	-11	HIS	-	EXPRESSION TAG	UNP P69687
E	-10	HIS	-	EXPRESSION TAG	UNP P69687
E	-9	SER	-	EXPRESSION TAG	UNP P69687
E	-8	SER	-	EXPRESSION TAG	UNP P69687
E	-7	GLY	-	EXPRESSION TAG	UNP P69687
E	-6	LEU	-	EXPRESSION TAG	UNP P69687
E	-5	VAL	-	EXPRESSION TAG	UNP P69687
E	-4	PRO	-	EXPRESSION TAG	UNP P69687
E	-3	ARG	-	EXPRESSION TAG	UNP P69687
E	-2	GLY	-	EXPRESSION TAG	UNP P69687
E	-1	SER	-	EXPRESSION TAG	UNP P69687
E	0	HIS	-	EXPRESSION TAG	UNP P69687
F	-19	MET	-	EXPRESSION TAG	UNP P69687
F	-18	GLY	-	EXPRESSION TAG	UNP P69687
F	-17	SER	-	EXPRESSION TAG	UNP P69687
F	-16	SER	-	EXPRESSION TAG	UNP P69687
F	-15	HIS	-	EXPRESSION TAG	UNP P69687
F	-14	HIS	-	EXPRESSION TAG	UNP P69687
F	-13	HIS	-	EXPRESSION TAG	UNP P69687
F	-12	HIS	-	EXPRESSION TAG	UNP P69687
F	-11	HIS	-	EXPRESSION TAG	UNP P69687
F	-10	HIS	-	EXPRESSION TAG	UNP P69687
F	-9	SER	-	EXPRESSION TAG	UNP P69687
F	-8	SER	-	EXPRESSION TAG	UNP P69687
F	-7	GLY	-	EXPRESSION TAG	UNP P69687
F	-6	LEU	-	EXPRESSION TAG	UNP P69687
F	-5	VAL	-	EXPRESSION TAG	UNP P69687
F	-4	PRO	-	EXPRESSION TAG	UNP P69687
F	-3	ARG	-	EXPRESSION TAG	UNP P69687
F	-2	GLY	-	EXPRESSION TAG	UNP P69687
F	-1	SER	-	EXPRESSION TAG	UNP P69687
F	0	HIS	-	EXPRESSION TAG	UNP P69687
G	-19	MET	-	EXPRESSION TAG	UNP P69687
G	-18	GLY	-	EXPRESSION TAG	UNP P69687
G	-17	SER	-	EXPRESSION TAG	UNP P69687
G	-16	SER	-	EXPRESSION TAG	UNP P69687
G	-15	HIS	-	EXPRESSION TAG	UNP P69687
G	-14	HIS	-	EXPRESSION TAG	UNP P69687
G	-13	HIS	-	EXPRESSION TAG	UNP P69687
G	-12	HIS	-	EXPRESSION TAG	UNP P69687
G	-11	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	HIS	-	EXPRESSION TAG	UNP P69687
G	-9	SER	-	EXPRESSION TAG	UNP P69687
G	-8	SER	-	EXPRESSION TAG	UNP P69687
G	-7	GLY	-	EXPRESSION TAG	UNP P69687
G	-6	LEU	-	EXPRESSION TAG	UNP P69687
G	-5	VAL	-	EXPRESSION TAG	UNP P69687
G	-4	PRO	-	EXPRESSION TAG	UNP P69687
G	-3	ARG	-	EXPRESSION TAG	UNP P69687
G	-2	GLY	-	EXPRESSION TAG	UNP P69687
G	-1	SER	-	EXPRESSION TAG	UNP P69687
G	0	HIS	-	EXPRESSION TAG	UNP P69687
H	-19	MET	-	EXPRESSION TAG	UNP P69687
H	-18	GLY	-	EXPRESSION TAG	UNP P69687
H	-17	SER	-	EXPRESSION TAG	UNP P69687
H	-16	SER	-	EXPRESSION TAG	UNP P69687
H	-15	HIS	-	EXPRESSION TAG	UNP P69687
H	-14	HIS	-	EXPRESSION TAG	UNP P69687
H	-13	HIS	-	EXPRESSION TAG	UNP P69687
H	-12	HIS	-	EXPRESSION TAG	UNP P69687
H	-11	HIS	-	EXPRESSION TAG	UNP P69687
H	-10	HIS	-	EXPRESSION TAG	UNP P69687
H	-9	SER	-	EXPRESSION TAG	UNP P69687
H	-8	SER	-	EXPRESSION TAG	UNP P69687
H	-7	GLY	-	EXPRESSION TAG	UNP P69687
H	-6	LEU	-	EXPRESSION TAG	UNP P69687
H	-5	VAL	-	EXPRESSION TAG	UNP P69687
H	-4	PRO	-	EXPRESSION TAG	UNP P69687
H	-3	ARG	-	EXPRESSION TAG	UNP P69687
H	-2	GLY	-	EXPRESSION TAG	UNP P69687
H	-1	SER	-	EXPRESSION TAG	UNP P69687
H	0	HIS	-	EXPRESSION TAG	UNP P69687
I	-19	MET	-	EXPRESSION TAG	UNP P69687
I	-18	GLY	-	EXPRESSION TAG	UNP P69687
I	-17	SER	-	EXPRESSION TAG	UNP P69687
I	-16	SER	-	EXPRESSION TAG	UNP P69687
I	-15	HIS	-	EXPRESSION TAG	UNP P69687
I	-14	HIS	-	EXPRESSION TAG	UNP P69687
I	-13	HIS	-	EXPRESSION TAG	UNP P69687
I	-12	HIS	-	EXPRESSION TAG	UNP P69687
I	-11	HIS	-	EXPRESSION TAG	UNP P69687
I	-10	HIS	-	EXPRESSION TAG	UNP P69687
I	-9	SER	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	SER	-	EXPRESSION TAG	UNP P69687
I	-7	GLY	-	EXPRESSION TAG	UNP P69687
I	-6	LEU	-	EXPRESSION TAG	UNP P69687
I	-5	VAL	-	EXPRESSION TAG	UNP P69687
I	-4	PRO	-	EXPRESSION TAG	UNP P69687
I	-3	ARG	-	EXPRESSION TAG	UNP P69687
I	-2	GLY	-	EXPRESSION TAG	UNP P69687
I	-1	SER	-	EXPRESSION TAG	UNP P69687
I	0	HIS	-	EXPRESSION TAG	UNP P69687
J	-19	MET	-	EXPRESSION TAG	UNP P69687
J	-18	GLY	-	EXPRESSION TAG	UNP P69687
J	-17	SER	-	EXPRESSION TAG	UNP P69687
J	-16	SER	-	EXPRESSION TAG	UNP P69687
J	-15	HIS	-	EXPRESSION TAG	UNP P69687
J	-14	HIS	-	EXPRESSION TAG	UNP P69687
J	-13	HIS	-	EXPRESSION TAG	UNP P69687
J	-12	HIS	-	EXPRESSION TAG	UNP P69687
J	-11	HIS	-	EXPRESSION TAG	UNP P69687
J	-10	HIS	-	EXPRESSION TAG	UNP P69687
J	-9	SER	-	EXPRESSION TAG	UNP P69687
J	-8	SER	-	EXPRESSION TAG	UNP P69687
J	-7	GLY	-	EXPRESSION TAG	UNP P69687
J	-6	LEU	-	EXPRESSION TAG	UNP P69687
J	-5	VAL	-	EXPRESSION TAG	UNP P69687
J	-4	PRO	-	EXPRESSION TAG	UNP P69687
J	-3	ARG	-	EXPRESSION TAG	UNP P69687
J	-2	GLY	-	EXPRESSION TAG	UNP P69687
J	-1	SER	-	EXPRESSION TAG	UNP P69687
J	0	HIS	-	EXPRESSION TAG	UNP P69687
K	-19	MET	-	EXPRESSION TAG	UNP P69687
K	-18	GLY	-	EXPRESSION TAG	UNP P69687
K	-17	SER	-	EXPRESSION TAG	UNP P69687
K	-16	SER	-	EXPRESSION TAG	UNP P69687
K	-15	HIS	-	EXPRESSION TAG	UNP P69687
K	-14	HIS	-	EXPRESSION TAG	UNP P69687
K	-13	HIS	-	EXPRESSION TAG	UNP P69687
K	-12	HIS	-	EXPRESSION TAG	UNP P69687
K	-11	HIS	-	EXPRESSION TAG	UNP P69687
K	-10	HIS	-	EXPRESSION TAG	UNP P69687
K	-9	SER	-	EXPRESSION TAG	UNP P69687
K	-8	SER	-	EXPRESSION TAG	UNP P69687
K	-7	GLY	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	LEU	-	EXPRESSION TAG	UNP P69687
K	-5	VAL	-	EXPRESSION TAG	UNP P69687
K	-4	PRO	-	EXPRESSION TAG	UNP P69687
K	-3	ARG	-	EXPRESSION TAG	UNP P69687
K	-2	GLY	-	EXPRESSION TAG	UNP P69687
K	-1	SER	-	EXPRESSION TAG	UNP P69687
K	0	HIS	-	EXPRESSION TAG	UNP P69687
L	-19	MET	-	EXPRESSION TAG	UNP P69687
L	-18	GLY	-	EXPRESSION TAG	UNP P69687
L	-17	SER	-	EXPRESSION TAG	UNP P69687
L	-16	SER	-	EXPRESSION TAG	UNP P69687
L	-15	HIS	-	EXPRESSION TAG	UNP P69687
L	-14	HIS	-	EXPRESSION TAG	UNP P69687
L	-13	HIS	-	EXPRESSION TAG	UNP P69687
L	-12	HIS	-	EXPRESSION TAG	UNP P69687
L	-11	HIS	-	EXPRESSION TAG	UNP P69687
L	-10	HIS	-	EXPRESSION TAG	UNP P69687
L	-9	SER	-	EXPRESSION TAG	UNP P69687
L	-8	SER	-	EXPRESSION TAG	UNP P69687
L	-7	GLY	-	EXPRESSION TAG	UNP P69687
L	-6	LEU	-	EXPRESSION TAG	UNP P69687
L	-5	VAL	-	EXPRESSION TAG	UNP P69687
L	-4	PRO	-	EXPRESSION TAG	UNP P69687
L	-3	ARG	-	EXPRESSION TAG	UNP P69687
L	-2	GLY	-	EXPRESSION TAG	UNP P69687
L	-1	SER	-	EXPRESSION TAG	UNP P69687
L	0	HIS	-	EXPRESSION TAG	UNP P69687
M	-19	MET	-	EXPRESSION TAG	UNP P69687
M	-18	GLY	-	EXPRESSION TAG	UNP P69687
M	-17	SER	-	EXPRESSION TAG	UNP P69687
M	-16	SER	-	EXPRESSION TAG	UNP P69687
M	-15	HIS	-	EXPRESSION TAG	UNP P69687
M	-14	HIS	-	EXPRESSION TAG	UNP P69687
M	-13	HIS	-	EXPRESSION TAG	UNP P69687
M	-12	HIS	-	EXPRESSION TAG	UNP P69687
M	-11	HIS	-	EXPRESSION TAG	UNP P69687
M	-10	HIS	-	EXPRESSION TAG	UNP P69687
M	-9	SER	-	EXPRESSION TAG	UNP P69687
M	-8	SER	-	EXPRESSION TAG	UNP P69687
M	-7	GLY	-	EXPRESSION TAG	UNP P69687
M	-6	LEU	-	EXPRESSION TAG	UNP P69687
M	-5	VAL	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	PRO	-	EXPRESSION TAG	UNP P69687
M	-3	ARG	-	EXPRESSION TAG	UNP P69687
M	-2	GLY	-	EXPRESSION TAG	UNP P69687
M	-1	SER	-	EXPRESSION TAG	UNP P69687
M	0	HIS	-	EXPRESSION TAG	UNP P69687
N	-19	MET	-	EXPRESSION TAG	UNP P69687
N	-18	GLY	-	EXPRESSION TAG	UNP P69687
N	-17	SER	-	EXPRESSION TAG	UNP P69687
N	-16	SER	-	EXPRESSION TAG	UNP P69687
N	-15	HIS	-	EXPRESSION TAG	UNP P69687
N	-14	HIS	-	EXPRESSION TAG	UNP P69687
N	-13	HIS	-	EXPRESSION TAG	UNP P69687
N	-12	HIS	-	EXPRESSION TAG	UNP P69687
N	-11	HIS	-	EXPRESSION TAG	UNP P69687
N	-10	HIS	-	EXPRESSION TAG	UNP P69687
N	-9	SER	-	EXPRESSION TAG	UNP P69687
N	-8	SER	-	EXPRESSION TAG	UNP P69687
N	-7	GLY	-	EXPRESSION TAG	UNP P69687
N	-6	LEU	-	EXPRESSION TAG	UNP P69687
N	-5	VAL	-	EXPRESSION TAG	UNP P69687
N	-4	PRO	-	EXPRESSION TAG	UNP P69687
N	-3	ARG	-	EXPRESSION TAG	UNP P69687
N	-2	GLY	-	EXPRESSION TAG	UNP P69687
N	-1	SER	-	EXPRESSION TAG	UNP P69687
N	0	HIS	-	EXPRESSION TAG	UNP P69687
O	-19	MET	-	EXPRESSION TAG	UNP P69687
O	-18	GLY	-	EXPRESSION TAG	UNP P69687
O	-17	SER	-	EXPRESSION TAG	UNP P69687
O	-16	SER	-	EXPRESSION TAG	UNP P69687
O	-15	HIS	-	EXPRESSION TAG	UNP P69687
O	-14	HIS	-	EXPRESSION TAG	UNP P69687
O	-13	HIS	-	EXPRESSION TAG	UNP P69687
O	-12	HIS	-	EXPRESSION TAG	UNP P69687
O	-11	HIS	-	EXPRESSION TAG	UNP P69687
O	-10	HIS	-	EXPRESSION TAG	UNP P69687
O	-9	SER	-	EXPRESSION TAG	UNP P69687
O	-8	SER	-	EXPRESSION TAG	UNP P69687
O	-7	GLY	-	EXPRESSION TAG	UNP P69687
O	-6	LEU	-	EXPRESSION TAG	UNP P69687
O	-5	VAL	-	EXPRESSION TAG	UNP P69687
O	-4	PRO	-	EXPRESSION TAG	UNP P69687
O	-3	ARG	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	EXPRESSION TAG	UNP P69687
O	-1	SER	-	EXPRESSION TAG	UNP P69687
O	0	HIS	-	EXPRESSION TAG	UNP P69687
P	-19	MET	-	EXPRESSION TAG	UNP P69687
P	-18	GLY	-	EXPRESSION TAG	UNP P69687
P	-17	SER	-	EXPRESSION TAG	UNP P69687
P	-16	SER	-	EXPRESSION TAG	UNP P69687
P	-15	HIS	-	EXPRESSION TAG	UNP P69687
P	-14	HIS	-	EXPRESSION TAG	UNP P69687
P	-13	HIS	-	EXPRESSION TAG	UNP P69687
P	-12	HIS	-	EXPRESSION TAG	UNP P69687
P	-11	HIS	-	EXPRESSION TAG	UNP P69687
P	-10	HIS	-	EXPRESSION TAG	UNP P69687
P	-9	SER	-	EXPRESSION TAG	UNP P69687
P	-8	SER	-	EXPRESSION TAG	UNP P69687
P	-7	GLY	-	EXPRESSION TAG	UNP P69687
P	-6	LEU	-	EXPRESSION TAG	UNP P69687
P	-5	VAL	-	EXPRESSION TAG	UNP P69687
P	-4	PRO	-	EXPRESSION TAG	UNP P69687
P	-3	ARG	-	EXPRESSION TAG	UNP P69687
P	-2	GLY	-	EXPRESSION TAG	UNP P69687
P	-1	SER	-	EXPRESSION TAG	UNP P69687
P	0	HIS	-	EXPRESSION TAG	UNP P69687
Q	-19	MET	-	EXPRESSION TAG	UNP P69687
Q	-18	GLY	-	EXPRESSION TAG	UNP P69687
Q	-17	SER	-	EXPRESSION TAG	UNP P69687
Q	-16	SER	-	EXPRESSION TAG	UNP P69687
Q	-15	HIS	-	EXPRESSION TAG	UNP P69687
Q	-14	HIS	-	EXPRESSION TAG	UNP P69687
Q	-13	HIS	-	EXPRESSION TAG	UNP P69687
Q	-12	HIS	-	EXPRESSION TAG	UNP P69687
Q	-11	HIS	-	EXPRESSION TAG	UNP P69687
Q	-10	HIS	-	EXPRESSION TAG	UNP P69687
Q	-9	SER	-	EXPRESSION TAG	UNP P69687
Q	-8	SER	-	EXPRESSION TAG	UNP P69687
Q	-7	GLY	-	EXPRESSION TAG	UNP P69687
Q	-6	LEU	-	EXPRESSION TAG	UNP P69687
Q	-5	VAL	-	EXPRESSION TAG	UNP P69687
Q	-4	PRO	-	EXPRESSION TAG	UNP P69687
Q	-3	ARG	-	EXPRESSION TAG	UNP P69687
Q	-2	GLY	-	EXPRESSION TAG	UNP P69687
Q	-1	SER	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	HIS	-	EXPRESSION TAG	UNP P69687
R	-19	MET	-	EXPRESSION TAG	UNP P69687
R	-18	GLY	-	EXPRESSION TAG	UNP P69687
R	-17	SER	-	EXPRESSION TAG	UNP P69687
R	-16	SER	-	EXPRESSION TAG	UNP P69687
R	-15	HIS	-	EXPRESSION TAG	UNP P69687
R	-14	HIS	-	EXPRESSION TAG	UNP P69687
R	-13	HIS	-	EXPRESSION TAG	UNP P69687
R	-12	HIS	-	EXPRESSION TAG	UNP P69687
R	-11	HIS	-	EXPRESSION TAG	UNP P69687
R	-10	HIS	-	EXPRESSION TAG	UNP P69687
R	-9	SER	-	EXPRESSION TAG	UNP P69687
R	-8	SER	-	EXPRESSION TAG	UNP P69687
R	-7	GLY	-	EXPRESSION TAG	UNP P69687
R	-6	LEU	-	EXPRESSION TAG	UNP P69687
R	-5	VAL	-	EXPRESSION TAG	UNP P69687
R	-4	PRO	-	EXPRESSION TAG	UNP P69687
R	-3	ARG	-	EXPRESSION TAG	UNP P69687
R	-2	GLY	-	EXPRESSION TAG	UNP P69687
R	-1	SER	-	EXPRESSION TAG	UNP P69687
R	0	HIS	-	EXPRESSION TAG	UNP P69687
S	-19	MET	-	EXPRESSION TAG	UNP P69687
S	-18	GLY	-	EXPRESSION TAG	UNP P69687
S	-17	SER	-	EXPRESSION TAG	UNP P69687
S	-16	SER	-	EXPRESSION TAG	UNP P69687
S	-15	HIS	-	EXPRESSION TAG	UNP P69687
S	-14	HIS	-	EXPRESSION TAG	UNP P69687
S	-13	HIS	-	EXPRESSION TAG	UNP P69687
S	-12	HIS	-	EXPRESSION TAG	UNP P69687
S	-11	HIS	-	EXPRESSION TAG	UNP P69687
S	-10	HIS	-	EXPRESSION TAG	UNP P69687
S	-9	SER	-	EXPRESSION TAG	UNP P69687
S	-8	SER	-	EXPRESSION TAG	UNP P69687
S	-7	GLY	-	EXPRESSION TAG	UNP P69687
S	-6	LEU	-	EXPRESSION TAG	UNP P69687
S	-5	VAL	-	EXPRESSION TAG	UNP P69687
S	-4	PRO	-	EXPRESSION TAG	UNP P69687
S	-3	ARG	-	EXPRESSION TAG	UNP P69687
S	-2	GLY	-	EXPRESSION TAG	UNP P69687
S	-1	SER	-	EXPRESSION TAG	UNP P69687
S	0	HIS	-	EXPRESSION TAG	UNP P69687
T	-19	MET	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-18	GLY	-	EXPRESSION TAG	UNP P69687
T	-17	SER	-	EXPRESSION TAG	UNP P69687
T	-16	SER	-	EXPRESSION TAG	UNP P69687
T	-15	HIS	-	EXPRESSION TAG	UNP P69687
T	-14	HIS	-	EXPRESSION TAG	UNP P69687
T	-13	HIS	-	EXPRESSION TAG	UNP P69687
T	-12	HIS	-	EXPRESSION TAG	UNP P69687
T	-11	HIS	-	EXPRESSION TAG	UNP P69687
T	-10	HIS	-	EXPRESSION TAG	UNP P69687
T	-9	SER	-	EXPRESSION TAG	UNP P69687
T	-8	SER	-	EXPRESSION TAG	UNP P69687
T	-7	GLY	-	EXPRESSION TAG	UNP P69687
T	-6	LEU	-	EXPRESSION TAG	UNP P69687
T	-5	VAL	-	EXPRESSION TAG	UNP P69687
T	-4	PRO	-	EXPRESSION TAG	UNP P69687
T	-3	ARG	-	EXPRESSION TAG	UNP P69687
T	-2	GLY	-	EXPRESSION TAG	UNP P69687
T	-1	SER	-	EXPRESSION TAG	UNP P69687
T	0	HIS	-	EXPRESSION TAG	UNP P69687
U	-19	MET	-	EXPRESSION TAG	UNP P69687
U	-18	GLY	-	EXPRESSION TAG	UNP P69687
U	-17	SER	-	EXPRESSION TAG	UNP P69687
U	-16	SER	-	EXPRESSION TAG	UNP P69687
U	-15	HIS	-	EXPRESSION TAG	UNP P69687
U	-14	HIS	-	EXPRESSION TAG	UNP P69687
U	-13	HIS	-	EXPRESSION TAG	UNP P69687
U	-12	HIS	-	EXPRESSION TAG	UNP P69687
U	-11	HIS	-	EXPRESSION TAG	UNP P69687
U	-10	HIS	-	EXPRESSION TAG	UNP P69687
U	-9	SER	-	EXPRESSION TAG	UNP P69687
U	-8	SER	-	EXPRESSION TAG	UNP P69687
U	-7	GLY	-	EXPRESSION TAG	UNP P69687
U	-6	LEU	-	EXPRESSION TAG	UNP P69687
U	-5	VAL	-	EXPRESSION TAG	UNP P69687
U	-4	PRO	-	EXPRESSION TAG	UNP P69687
U	-3	ARG	-	EXPRESSION TAG	UNP P69687
U	-2	GLY	-	EXPRESSION TAG	UNP P69687
U	-1	SER	-	EXPRESSION TAG	UNP P69687
U	0	HIS	-	EXPRESSION TAG	UNP P69687
V	-19	MET	-	EXPRESSION TAG	UNP P69687
V	-18	GLY	-	EXPRESSION TAG	UNP P69687
V	-17	SER	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-16	SER	-	EXPRESSION TAG	UNP P69687
V	-15	HIS	-	EXPRESSION TAG	UNP P69687
V	-14	HIS	-	EXPRESSION TAG	UNP P69687
V	-13	HIS	-	EXPRESSION TAG	UNP P69687
V	-12	HIS	-	EXPRESSION TAG	UNP P69687
V	-11	HIS	-	EXPRESSION TAG	UNP P69687
V	-10	HIS	-	EXPRESSION TAG	UNP P69687
V	-9	SER	-	EXPRESSION TAG	UNP P69687
V	-8	SER	-	EXPRESSION TAG	UNP P69687
V	-7	GLY	-	EXPRESSION TAG	UNP P69687
V	-6	LEU	-	EXPRESSION TAG	UNP P69687
V	-5	VAL	-	EXPRESSION TAG	UNP P69687
V	-4	PRO	-	EXPRESSION TAG	UNP P69687
V	-3	ARG	-	EXPRESSION TAG	UNP P69687
V	-2	GLY	-	EXPRESSION TAG	UNP P69687
V	-1	SER	-	EXPRESSION TAG	UNP P69687
V	0	HIS	-	EXPRESSION TAG	UNP P69687
W	-19	MET	-	EXPRESSION TAG	UNP P69687
W	-18	GLY	-	EXPRESSION TAG	UNP P69687
W	-17	SER	-	EXPRESSION TAG	UNP P69687
W	-16	SER	-	EXPRESSION TAG	UNP P69687
W	-15	HIS	-	EXPRESSION TAG	UNP P69687
W	-14	HIS	-	EXPRESSION TAG	UNP P69687
W	-13	HIS	-	EXPRESSION TAG	UNP P69687
W	-12	HIS	-	EXPRESSION TAG	UNP P69687
W	-11	HIS	-	EXPRESSION TAG	UNP P69687
W	-10	HIS	-	EXPRESSION TAG	UNP P69687
W	-9	SER	-	EXPRESSION TAG	UNP P69687
W	-8	SER	-	EXPRESSION TAG	UNP P69687
W	-7	GLY	-	EXPRESSION TAG	UNP P69687
W	-6	LEU	-	EXPRESSION TAG	UNP P69687
W	-5	VAL	-	EXPRESSION TAG	UNP P69687
W	-4	PRO	-	EXPRESSION TAG	UNP P69687
W	-3	ARG	-	EXPRESSION TAG	UNP P69687
W	-2	GLY	-	EXPRESSION TAG	UNP P69687
W	-1	SER	-	EXPRESSION TAG	UNP P69687
W	0	HIS	-	EXPRESSION TAG	UNP P69687
X	-19	MET	-	EXPRESSION TAG	UNP P69687
X	-18	GLY	-	EXPRESSION TAG	UNP P69687
X	-17	SER	-	EXPRESSION TAG	UNP P69687
X	-16	SER	-	EXPRESSION TAG	UNP P69687
X	-15	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-14	HIS	-	EXPRESSION TAG	UNP P69687
X	-13	HIS	-	EXPRESSION TAG	UNP P69687
X	-12	HIS	-	EXPRESSION TAG	UNP P69687
X	-11	HIS	-	EXPRESSION TAG	UNP P69687
X	-10	HIS	-	EXPRESSION TAG	UNP P69687
X	-9	SER	-	EXPRESSION TAG	UNP P69687
X	-8	SER	-	EXPRESSION TAG	UNP P69687
X	-7	GLY	-	EXPRESSION TAG	UNP P69687
X	-6	LEU	-	EXPRESSION TAG	UNP P69687
X	-5	VAL	-	EXPRESSION TAG	UNP P69687
X	-4	PRO	-	EXPRESSION TAG	UNP P69687
X	-3	ARG	-	EXPRESSION TAG	UNP P69687
X	-2	GLY	-	EXPRESSION TAG	UNP P69687
X	-1	SER	-	EXPRESSION TAG	UNP P69687
X	0	HIS	-	EXPRESSION TAG	UNP P69687
Y	-19	MET	-	EXPRESSION TAG	UNP P69687
Y	-18	GLY	-	EXPRESSION TAG	UNP P69687
Y	-17	SER	-	EXPRESSION TAG	UNP P69687
Y	-16	SER	-	EXPRESSION TAG	UNP P69687
Y	-15	HIS	-	EXPRESSION TAG	UNP P69687
Y	-14	HIS	-	EXPRESSION TAG	UNP P69687
Y	-13	HIS	-	EXPRESSION TAG	UNP P69687
Y	-12	HIS	-	EXPRESSION TAG	UNP P69687
Y	-11	HIS	-	EXPRESSION TAG	UNP P69687
Y	-10	HIS	-	EXPRESSION TAG	UNP P69687
Y	-9	SER	-	EXPRESSION TAG	UNP P69687
Y	-8	SER	-	EXPRESSION TAG	UNP P69687
Y	-7	GLY	-	EXPRESSION TAG	UNP P69687
Y	-6	LEU	-	EXPRESSION TAG	UNP P69687
Y	-5	VAL	-	EXPRESSION TAG	UNP P69687
Y	-4	PRO	-	EXPRESSION TAG	UNP P69687
Y	-3	ARG	-	EXPRESSION TAG	UNP P69687
Y	-2	GLY	-	EXPRESSION TAG	UNP P69687
Y	-1	SER	-	EXPRESSION TAG	UNP P69687
Y	0	HIS	-	EXPRESSION TAG	UNP P69687
Z	-19	MET	-	EXPRESSION TAG	UNP P69687
Z	-18	GLY	-	EXPRESSION TAG	UNP P69687
Z	-17	SER	-	EXPRESSION TAG	UNP P69687
Z	-16	SER	-	EXPRESSION TAG	UNP P69687
Z	-15	HIS	-	EXPRESSION TAG	UNP P69687
Z	-14	HIS	-	EXPRESSION TAG	UNP P69687
Z	-13	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	-12	HIS	-	EXPRESSION TAG	UNP P69687
Z	-11	HIS	-	EXPRESSION TAG	UNP P69687
Z	-10	HIS	-	EXPRESSION TAG	UNP P69687
Z	-9	SER	-	EXPRESSION TAG	UNP P69687
Z	-8	SER	-	EXPRESSION TAG	UNP P69687
Z	-7	GLY	-	EXPRESSION TAG	UNP P69687
Z	-6	LEU	-	EXPRESSION TAG	UNP P69687
Z	-5	VAL	-	EXPRESSION TAG	UNP P69687
Z	-4	PRO	-	EXPRESSION TAG	UNP P69687
Z	-3	ARG	-	EXPRESSION TAG	UNP P69687
Z	-2	GLY	-	EXPRESSION TAG	UNP P69687
Z	-1	SER	-	EXPRESSION TAG	UNP P69687
Z	0	HIS	-	EXPRESSION TAG	UNP P69687
a	-19	MET	-	EXPRESSION TAG	UNP P69687
a	-18	GLY	-	EXPRESSION TAG	UNP P69687
a	-17	SER	-	EXPRESSION TAG	UNP P69687
a	-16	SER	-	EXPRESSION TAG	UNP P69687
a	-15	HIS	-	EXPRESSION TAG	UNP P69687
a	-14	HIS	-	EXPRESSION TAG	UNP P69687
a	-13	HIS	-	EXPRESSION TAG	UNP P69687
a	-12	HIS	-	EXPRESSION TAG	UNP P69687
a	-11	HIS	-	EXPRESSION TAG	UNP P69687
a	-10	HIS	-	EXPRESSION TAG	UNP P69687
a	-9	SER	-	EXPRESSION TAG	UNP P69687
a	-8	SER	-	EXPRESSION TAG	UNP P69687
a	-7	GLY	-	EXPRESSION TAG	UNP P69687
a	-6	LEU	-	EXPRESSION TAG	UNP P69687
a	-5	VAL	-	EXPRESSION TAG	UNP P69687
a	-4	PRO	-	EXPRESSION TAG	UNP P69687
a	-3	ARG	-	EXPRESSION TAG	UNP P69687
a	-2	GLY	-	EXPRESSION TAG	UNP P69687
a	-1	SER	-	EXPRESSION TAG	UNP P69687
a	0	HIS	-	EXPRESSION TAG	UNP P69687
b	-19	MET	-	EXPRESSION TAG	UNP P69687
b	-18	GLY	-	EXPRESSION TAG	UNP P69687
b	-17	SER	-	EXPRESSION TAG	UNP P69687
b	-16	SER	-	EXPRESSION TAG	UNP P69687
b	-15	HIS	-	EXPRESSION TAG	UNP P69687
b	-14	HIS	-	EXPRESSION TAG	UNP P69687
b	-13	HIS	-	EXPRESSION TAG	UNP P69687
b	-12	HIS	-	EXPRESSION TAG	UNP P69687
b	-11	HIS	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-10	HIS	-	EXPRESSION TAG	UNP P69687
b	-9	SER	-	EXPRESSION TAG	UNP P69687
b	-8	SER	-	EXPRESSION TAG	UNP P69687
b	-7	GLY	-	EXPRESSION TAG	UNP P69687
b	-6	LEU	-	EXPRESSION TAG	UNP P69687
b	-5	VAL	-	EXPRESSION TAG	UNP P69687
b	-4	PRO	-	EXPRESSION TAG	UNP P69687
b	-3	ARG	-	EXPRESSION TAG	UNP P69687
b	-2	GLY	-	EXPRESSION TAG	UNP P69687
b	-1	SER	-	EXPRESSION TAG	UNP P69687
b	0	HIS	-	EXPRESSION TAG	UNP P69687
c	-19	MET	-	EXPRESSION TAG	UNP P69687
c	-18	GLY	-	EXPRESSION TAG	UNP P69687
c	-17	SER	-	EXPRESSION TAG	UNP P69687
c	-16	SER	-	EXPRESSION TAG	UNP P69687
c	-15	HIS	-	EXPRESSION TAG	UNP P69687
c	-14	HIS	-	EXPRESSION TAG	UNP P69687
c	-13	HIS	-	EXPRESSION TAG	UNP P69687
c	-12	HIS	-	EXPRESSION TAG	UNP P69687
c	-11	HIS	-	EXPRESSION TAG	UNP P69687
c	-10	HIS	-	EXPRESSION TAG	UNP P69687
c	-9	SER	-	EXPRESSION TAG	UNP P69687
c	-8	SER	-	EXPRESSION TAG	UNP P69687
c	-7	GLY	-	EXPRESSION TAG	UNP P69687
c	-6	LEU	-	EXPRESSION TAG	UNP P69687
c	-5	VAL	-	EXPRESSION TAG	UNP P69687
c	-4	PRO	-	EXPRESSION TAG	UNP P69687
c	-3	ARG	-	EXPRESSION TAG	UNP P69687
c	-2	GLY	-	EXPRESSION TAG	UNP P69687
c	-1	SER	-	EXPRESSION TAG	UNP P69687
c	0	HIS	-	EXPRESSION TAG	UNP P69687
d	-19	MET	-	EXPRESSION TAG	UNP P69687
d	-18	GLY	-	EXPRESSION TAG	UNP P69687
d	-17	SER	-	EXPRESSION TAG	UNP P69687
d	-16	SER	-	EXPRESSION TAG	UNP P69687
d	-15	HIS	-	EXPRESSION TAG	UNP P69687
d	-14	HIS	-	EXPRESSION TAG	UNP P69687
d	-13	HIS	-	EXPRESSION TAG	UNP P69687
d	-12	HIS	-	EXPRESSION TAG	UNP P69687
d	-11	HIS	-	EXPRESSION TAG	UNP P69687
d	-10	HIS	-	EXPRESSION TAG	UNP P69687
d	-9	SER	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
d	-8	SER	-	EXPRESSION TAG	UNP P69687
d	-7	GLY	-	EXPRESSION TAG	UNP P69687
d	-6	LEU	-	EXPRESSION TAG	UNP P69687
d	-5	VAL	-	EXPRESSION TAG	UNP P69687
d	-4	PRO	-	EXPRESSION TAG	UNP P69687
d	-3	ARG	-	EXPRESSION TAG	UNP P69687
d	-2	GLY	-	EXPRESSION TAG	UNP P69687
d	-1	SER	-	EXPRESSION TAG	UNP P69687
d	0	HIS	-	EXPRESSION TAG	UNP P69687
e	-19	MET	-	EXPRESSION TAG	UNP P69687
e	-18	GLY	-	EXPRESSION TAG	UNP P69687
e	-17	SER	-	EXPRESSION TAG	UNP P69687
e	-16	SER	-	EXPRESSION TAG	UNP P69687
e	-15	HIS	-	EXPRESSION TAG	UNP P69687
e	-14	HIS	-	EXPRESSION TAG	UNP P69687
e	-13	HIS	-	EXPRESSION TAG	UNP P69687
e	-12	HIS	-	EXPRESSION TAG	UNP P69687
e	-11	HIS	-	EXPRESSION TAG	UNP P69687
e	-10	HIS	-	EXPRESSION TAG	UNP P69687
e	-9	SER	-	EXPRESSION TAG	UNP P69687
e	-8	SER	-	EXPRESSION TAG	UNP P69687
e	-7	GLY	-	EXPRESSION TAG	UNP P69687
e	-6	LEU	-	EXPRESSION TAG	UNP P69687
e	-5	VAL	-	EXPRESSION TAG	UNP P69687
e	-4	PRO	-	EXPRESSION TAG	UNP P69687
e	-3	ARG	-	EXPRESSION TAG	UNP P69687
e	-2	GLY	-	EXPRESSION TAG	UNP P69687
e	-1	SER	-	EXPRESSION TAG	UNP P69687
e	0	HIS	-	EXPRESSION TAG	UNP P69687
f	-19	MET	-	EXPRESSION TAG	UNP P69687
f	-18	GLY	-	EXPRESSION TAG	UNP P69687
f	-17	SER	-	EXPRESSION TAG	UNP P69687
f	-16	SER	-	EXPRESSION TAG	UNP P69687
f	-15	HIS	-	EXPRESSION TAG	UNP P69687
f	-14	HIS	-	EXPRESSION TAG	UNP P69687
f	-13	HIS	-	EXPRESSION TAG	UNP P69687
f	-12	HIS	-	EXPRESSION TAG	UNP P69687
f	-11	HIS	-	EXPRESSION TAG	UNP P69687
f	-10	HIS	-	EXPRESSION TAG	UNP P69687
f	-9	SER	-	EXPRESSION TAG	UNP P69687
f	-8	SER	-	EXPRESSION TAG	UNP P69687
f	-7	GLY	-	EXPRESSION TAG	UNP P69687

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Chain	Residue	Modelled	Actual	Comment	Reference
f	-6	LEU	-	EXPRESSION TAG	UNP P69687
f	-5	VAL	-	EXPRESSION TAG	UNP P69687
f	-4	PRO	-	EXPRESSION TAG	UNP P69687
f	-3	ARG	-	EXPRESSION TAG	UNP P69687
f	-2	GLY	-	EXPRESSION TAG	UNP P69687
f	-1	SER	-	EXPRESSION TAG	UNP P69687
f	0	HIS	-	EXPRESSION TAG	UNP P69687
h	-19	MET	-	EXPRESSION TAG	UNP P69687
h	-18	GLY	-	EXPRESSION TAG	UNP P69687
h	-17	SER	-	EXPRESSION TAG	UNP P69687
h	-16	SER	-	EXPRESSION TAG	UNP P69687
h	-15	HIS	-	EXPRESSION TAG	UNP P69687
h	-14	HIS	-	EXPRESSION TAG	UNP P69687
h	-13	HIS	-	EXPRESSION TAG	UNP P69687
h	-12	HIS	-	EXPRESSION TAG	UNP P69687
h	-11	HIS	-	EXPRESSION TAG	UNP P69687
h	-10	HIS	-	EXPRESSION TAG	UNP P69687
h	-9	SER	-	EXPRESSION TAG	UNP P69687
h	-8	SER	-	EXPRESSION TAG	UNP P69687
h	-7	GLY	-	EXPRESSION TAG	UNP P69687
h	-6	LEU	-	EXPRESSION TAG	UNP P69687
h	-5	VAL	-	EXPRESSION TAG	UNP P69687
h	-4	PRO	-	EXPRESSION TAG	UNP P69687
h	-3	ARG	-	EXPRESSION TAG	UNP P69687
h	-2	GLY	-	EXPRESSION TAG	UNP P69687
h	-1	SER	-	EXPRESSION TAG	UNP P69687
h	0	HIS	-	EXPRESSION TAG	UNP P69687
i	-19	MET	-	EXPRESSION TAG	UNP P69687
i	-18	GLY	-	EXPRESSION TAG	UNP P69687
i	-17	SER	-	EXPRESSION TAG	UNP P69687
i	-16	SER	-	EXPRESSION TAG	UNP P69687
i	-15	HIS	-	EXPRESSION TAG	UNP P69687
i	-14	HIS	-	EXPRESSION TAG	UNP P69687
i	-13	HIS	-	EXPRESSION TAG	UNP P69687
i	-12	HIS	-	EXPRESSION TAG	UNP P69687
i	-11	HIS	-	EXPRESSION TAG	UNP P69687
i	-10	HIS	-	EXPRESSION TAG	UNP P69687
i	-9	SER	-	EXPRESSION TAG	UNP P69687
i	-8	SER	-	EXPRESSION TAG	UNP P69687
i	-7	GLY	-	EXPRESSION TAG	UNP P69687
i	-6	LEU	-	EXPRESSION TAG	UNP P69687
i	-5	VAL	-	EXPRESSION TAG	UNP P69687

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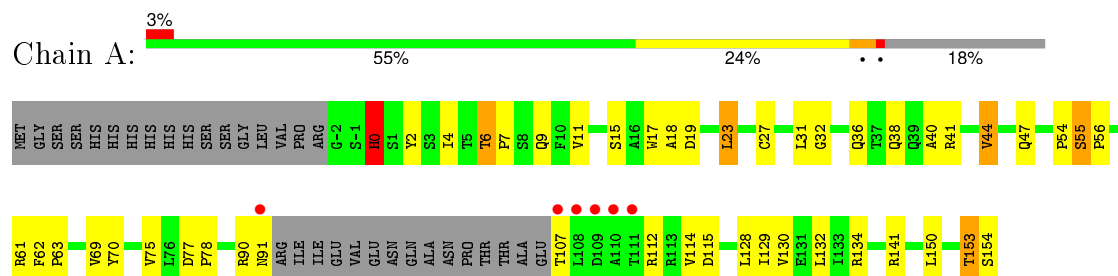
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Chain	Residue	Modelled	Actual	Comment	Reference
i	-4	PRO	-	EXPRESSION TAG	UNP P69687
i	-3	ARG	-	EXPRESSION TAG	UNP P69687
i	-2	GLY	-	EXPRESSION TAG	UNP P69687
i	-1	SER	-	EXPRESSION TAG	UNP P69687
i	0	HIS	-	EXPRESSION TAG	UNP P69687

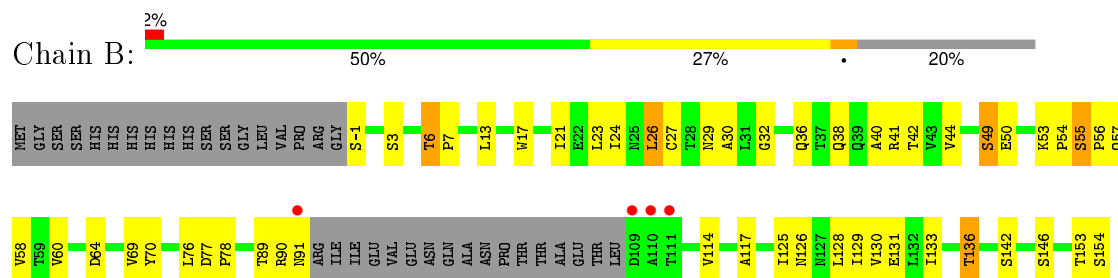
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

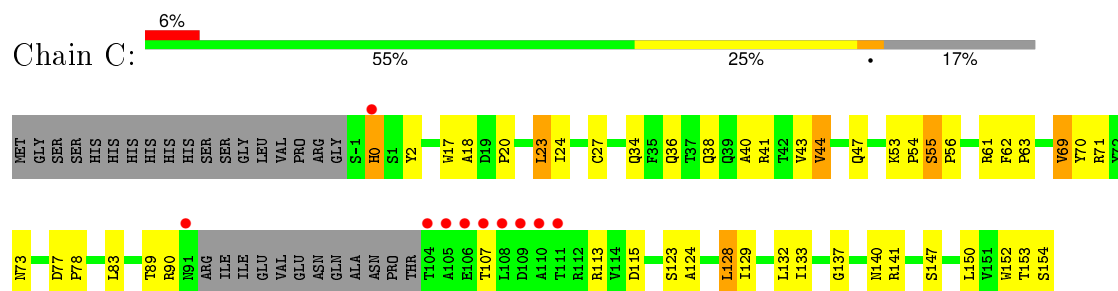
#### • Molecule 1: Capsid protein



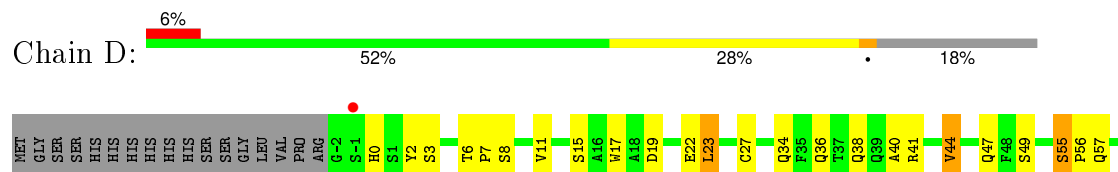
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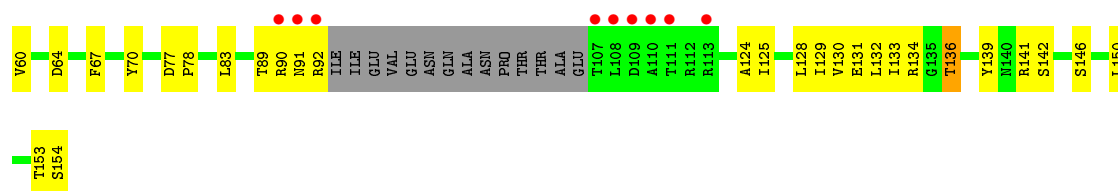
#### • Molecule 1: Capsid protein



#### • Molecule 1: Capsid protein



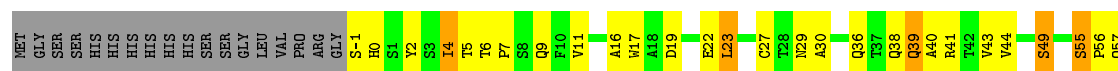




• Molecule 1: Capsid protein



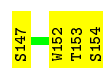
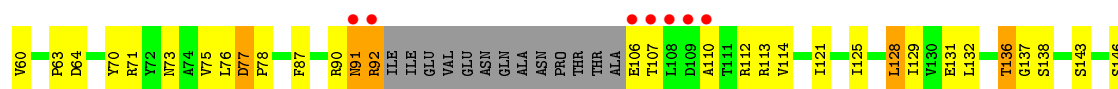
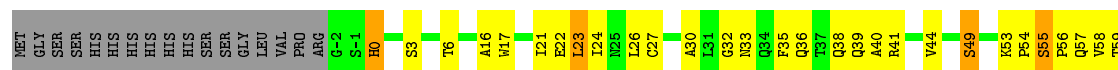
• Molecule 1: Capsid protein



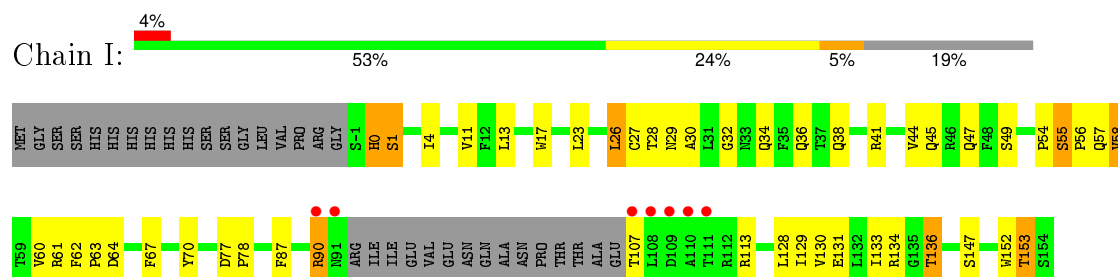
• Molecule 1: Capsid protein



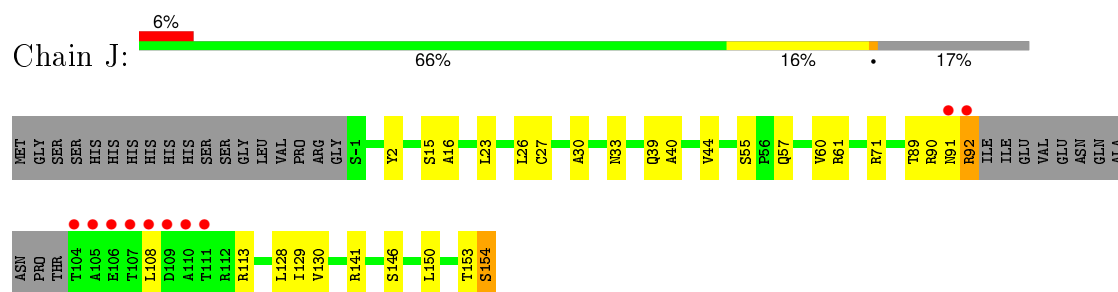
• Molecule 1: Capsid protein



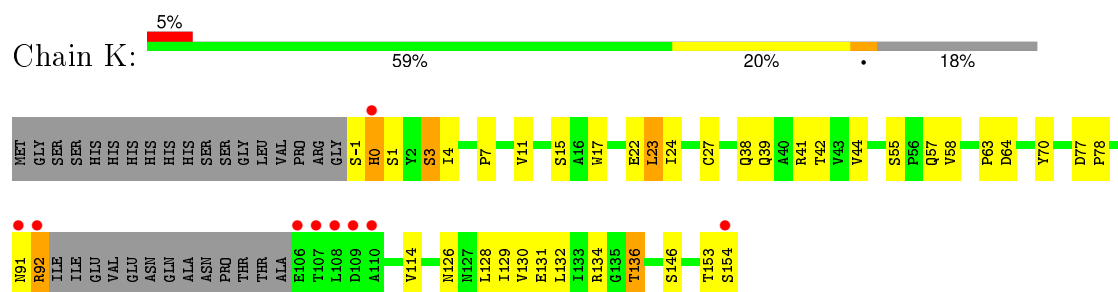
- Molecule 1: Capsid protein



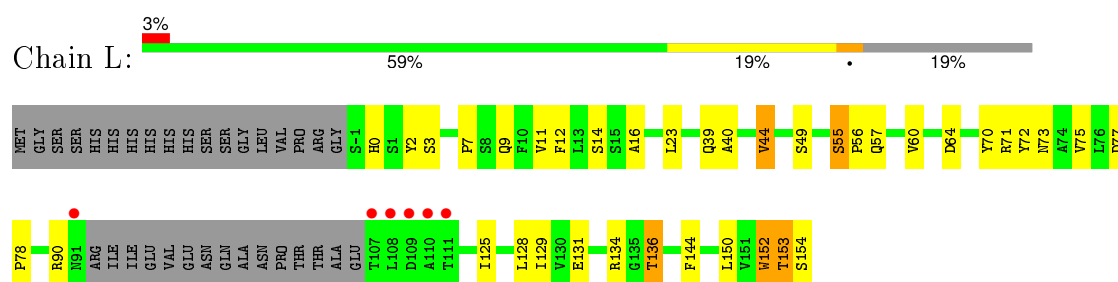
- Molecule 1: Capsid protein



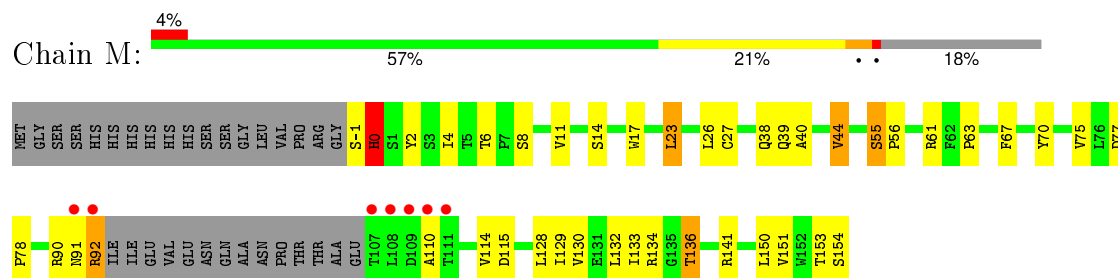
- Molecule 1: Capsid protein



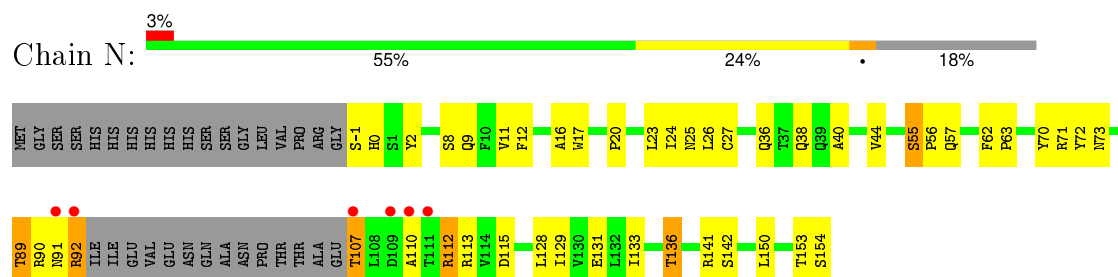
- Molecule 1: Capsid protein



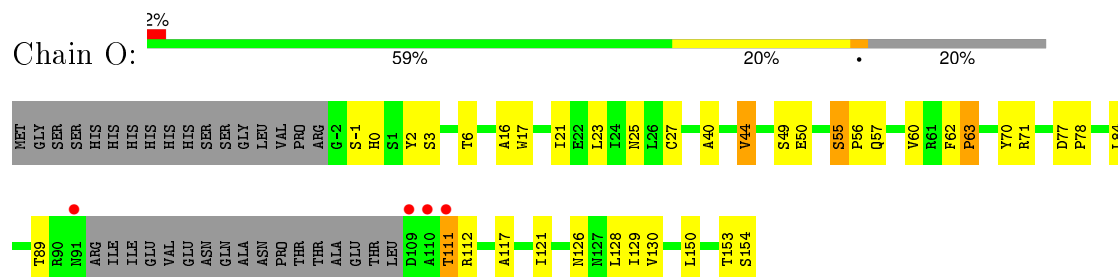
- Molecule 1: Capsid protein



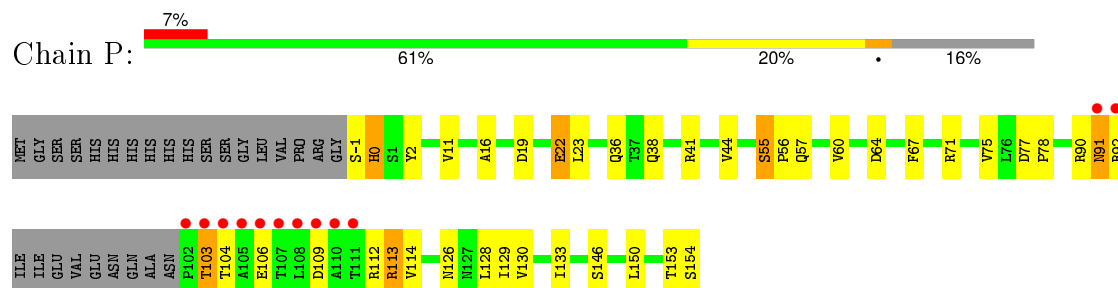
- Molecule 1: Capsid protein



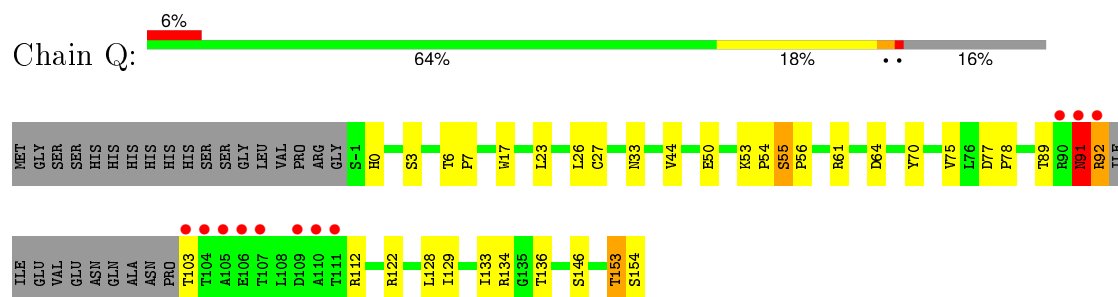
- Molecule 1: Capsid protein



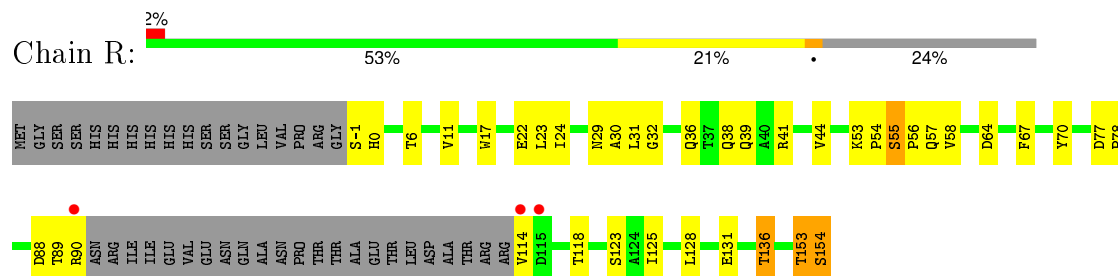
- Molecule 1: Capsid protein



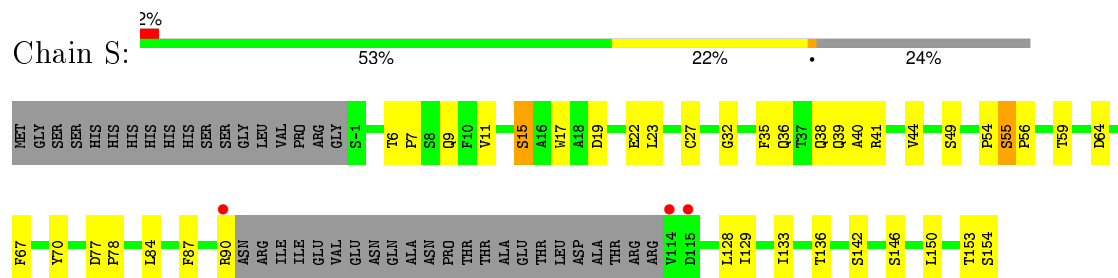
- Molecule 1: Capsid protein



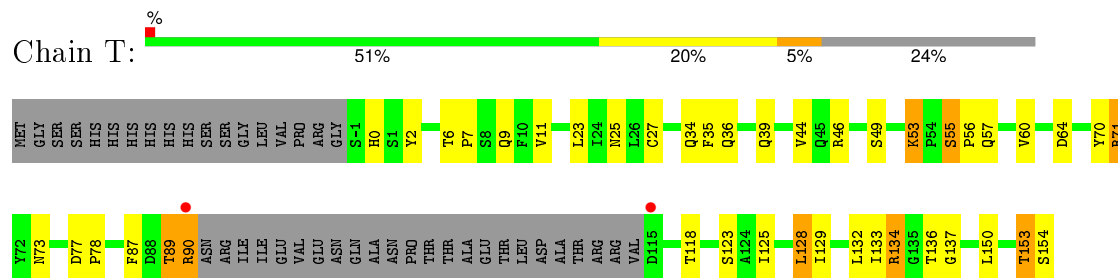
- Molecule 1: Capsid protein



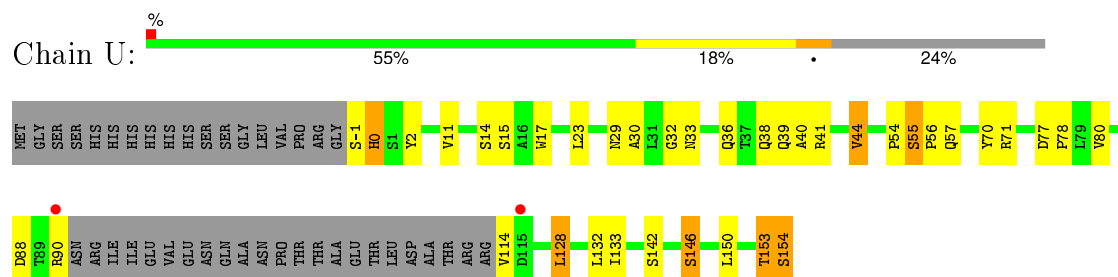
- Molecule 1: Capsid protein



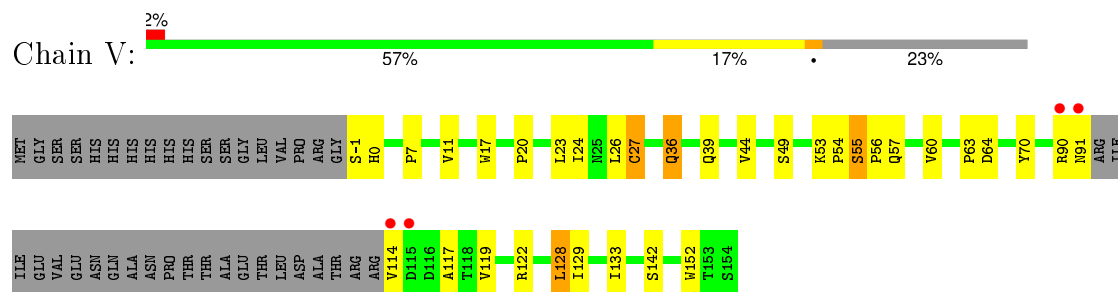
- Molecule 1: Capsid protein



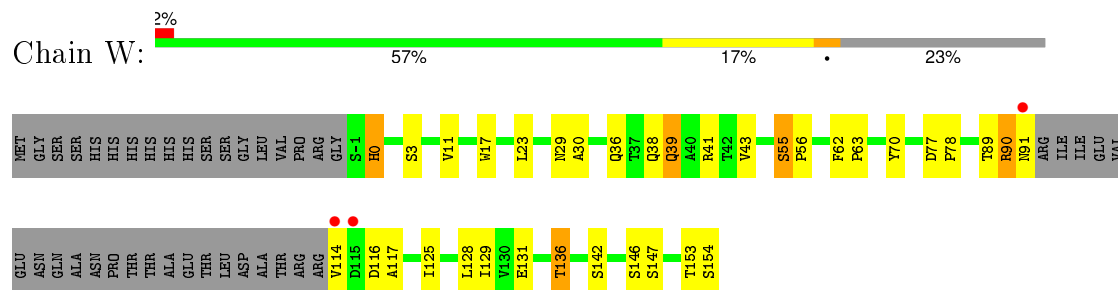
- Molecule 1: Capsid protein



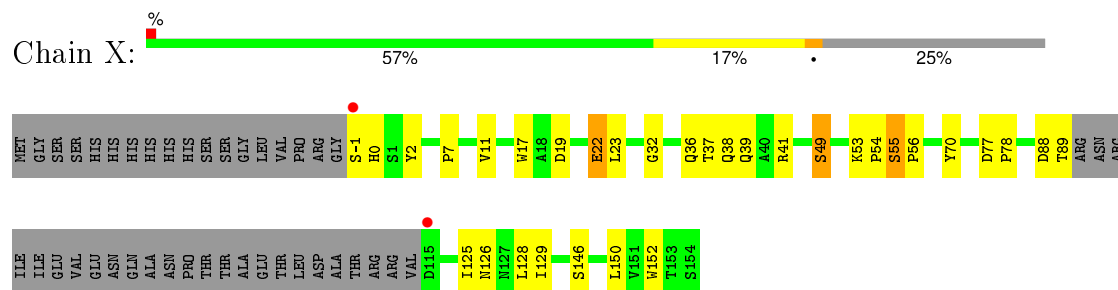
- Molecule 1: Capsid protein



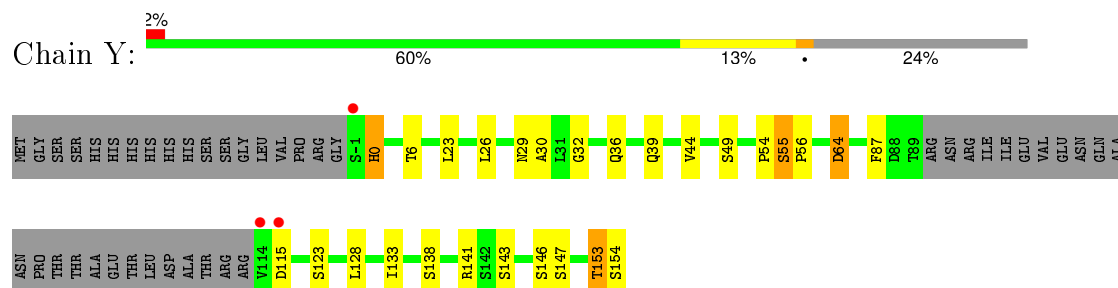
- Molecule 1: Capsid protein



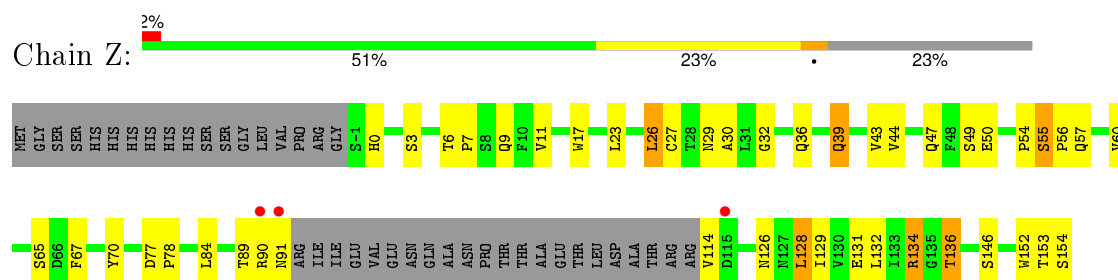
- Molecule 1: Capsid protein



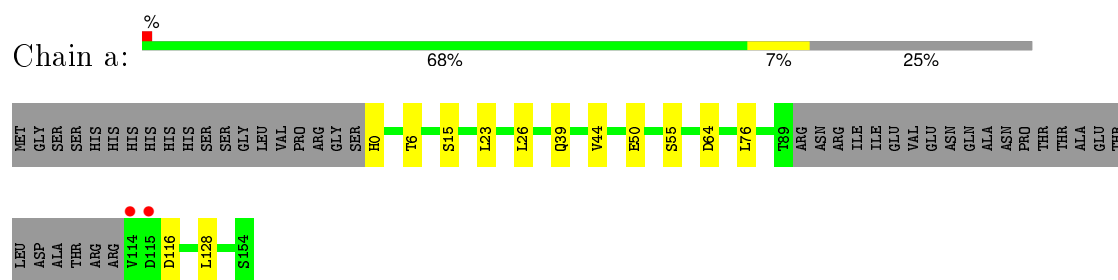
- Molecule 1: Capsid protein



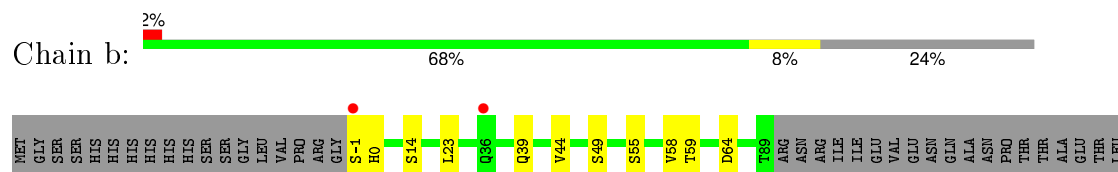
- Molecule 1: Capsid protein

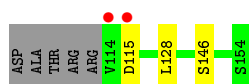


- Molecule 1: Capsid protein



- Molecule 1: Capsid protein

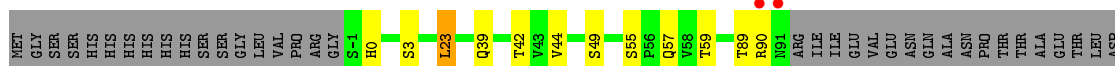




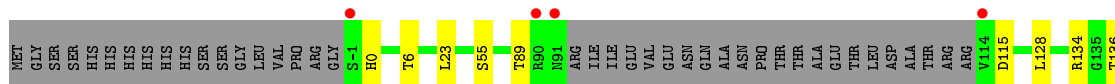
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

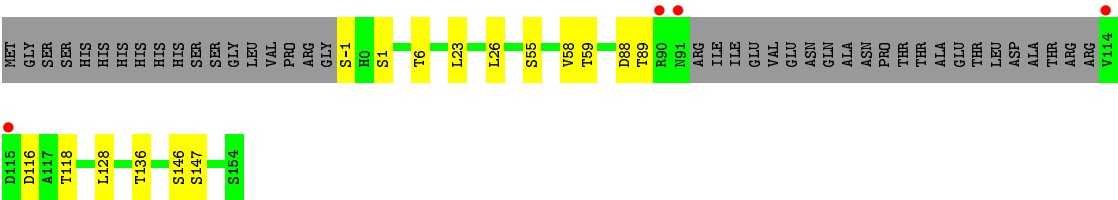


• Molecule 1: Capsid protein

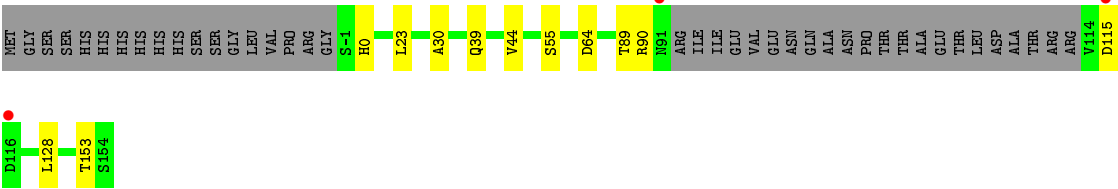


• Molecule 1: Capsid protein





● Molecule 1: Capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.07Å 221.68Å 225.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.06 49.91 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.06) 99.7 (49.91-3.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.90 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204 , 0.255 0.202 , 0.252	Depositor DCC
$R_{free}$ test set	8195 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 17.7	EDS
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 163217 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	36918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.64	0/1138	0.72	0/1552
1	B	0.62	0/1119	0.70	0/1526
1	C	0.67	0/1155	0.74	0/1576
1	D	0.65	0/1149	0.74	0/1566
1	E	0.64	0/1123	0.75	0/1531
1	F	0.63	0/1154	0.69	0/1573
1	G	0.63	0/1154	0.73	0/1573
1	H	0.61	0/1158	0.71	0/1578
1	I	0.58	0/1134	0.71	0/1547
1	J	0.61	0/1166	0.69	0/1590
1	K	0.66	0/1154	0.73	0/1573
1	L	0.62	0/1134	0.76	1/1547 (0.1%)
1	M	0.65	0/1145	0.71	0/1561
1	N	0.59	0/1145	0.70	0/1561
1	O	0.64	1/1123 (0.1%)	0.70	0/1531
1	P	0.65	0/1181	0.69	0/1611
1	Q	0.65	1/1173 (0.1%)	0.72	1/1600 (0.1%)
1	R	0.67	0/1069	0.73	0/1459
1	S	0.65	0/1069	0.74	0/1459
1	T	0.64	0/1062	0.73	1/1449 (0.1%)
1	U	0.61	0/1069	0.67	0/1459
1	V	0.69	1/1077 (0.1%)	0.78	1/1470 (0.1%)
1	W	0.65	0/1077	0.72	0/1470
1	X	0.63	0/1051	0.71	0/1435
1	Y	0.66	0/1058	0.72	0/1445
1	Z	0.64	0/1077	0.72	0/1470
1	a	0.61	0/1052	0.69	0/1437
1	b	0.63	0/1058	0.73	0/1445
1	c	0.67	1/1092 (0.1%)	0.73	0/1489
1	d	0.70	0/1077	0.79	1/1470 (0.1%)
1	e	0.65	0/1077	0.73	0/1470
1	f	0.66	0/1077	0.75	0/1470
1	h	0.61	0/1077	0.75	0/1470
1	i	0.68	0/1077	0.74	0/1470

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.64	4/37701 (0.0%)	0.72	5/51433 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	d	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	27	CYS	CB-SG	-6.52	1.71	1.82
1	Q	103	THR	CB-OG1	5.65	1.54	1.43
1	O	50	GLU	CG-CD	5.38	1.60	1.51
1	c	27	CYS	CB-SG	-5.08	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	71	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	d	23	LEU	CA-CB-CG	5.63	128.24	115.30
1	L	152	TRP	C-N-CA	5.45	135.32	121.70
1	V	128	LEU	CA-CB-CG	5.28	127.45	115.30
1	Q	61	ARG	NE-CZ-NH1	-5.17	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	152	TRP	Peptide
1	d	153	THR	Peptide

## 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	1115	0	1092	32	0
1	B	1096	0	1071	45	0
1	C	1132	0	1107	43	0
1	D	1126	0	1105	41	0
1	E	1100	0	1074	46	0
1	F	1131	0	1108	39	0
1	G	1131	0	1117	30	0
1	H	1135	0	1111	52	0
1	I	1111	0	1089	39	0
1	J	1143	0	1120	19	0
1	K	1131	0	1108	27	0
1	L	1111	0	1089	25	0
1	M	1122	0	1102	27	0
1	N	1122	0	1102	33	0
1	O	1100	0	1074	21	0
1	P	1157	0	1135	29	0
1	Q	1150	0	1127	17	0
1	R	1046	0	1023	27	0
1	S	1046	0	1023	31	0
1	T	1039	0	1014	35	0
1	U	1046	0	1023	33	0
1	V	1054	0	1029	28	0
1	W	1054	0	1029	24	0
1	X	1028	0	1001	23	0
1	Y	1035	0	1010	16	0
1	Z	1054	0	1029	39	0
1	a	1029	0	1005	0	0
1	b	1035	0	1010	0	0
1	c	1069	0	1045	0	0
1	d	1054	0	1029	0	0
1	e	1054	0	1029	0	0
1	f	1054	0	1029	0	0
1	h	1054	0	1029	0	0
1	i	1054	0	1029	0	0
All	All	36918	0	36117	697	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (697) 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:Q:27:CYS:HB3	1:Q:129:ILE:HD11	1.27	1.15
1:E:27:CYS:HB3	1:E:129:ILE:HD11	1.19	1.14
1:H:27:CYS:HB3	1:H:129:ILE:HD11	1.31	1.12
1:E:0:HIS:HB3	1:E:153:THR:O	4.61	1.11
1:T:36:GLN:HB2	1:U:90:ARG:HD2	1.32	1.09
1:T:134:ARG:HH11	1:T:134:ARG:HG2	1.18	1.08
1:K:0:HIS:HB3	1:K:154:SER:HA	1.28	1.08
1:K:0:HIS:CB	1:K:154:SER:HA	1.89	1.03
1:H:55:SER:HB3	1:H:56:PRO:HD3	1.91	0.99
1:I:27:CYS:HB3	1:I:129:ILE:HD11	1.43	0.97
1:N:27:CYS:HB3	1:N:129:ILE:HD11	1.47	0.96
1:L:131:GLU:OE1	1:L:136:THR:HG21	1.65	0.96
1:Q:77:ASP:HB3	1:Q:78:PRO:HD3	1.49	0.95
1:R:36:GLN:HE21	1:T:89:THR:HA	1.29	0.94
1:N:57:GLN:HE22	1:P:57:GLN:HE22	1.12	0.93
1:Y:0:HIS:HB3	1:Y:153:THR:O	1.69	0.93
1:E:27:CYS:HB3	1:E:129:ILE:CD1	1.99	0.93
1:S:90:ARG:HD3	1:Z:36:GLN:HB2	1.49	0.92
1:E:27:CYS:CB	1:E:129:ILE:HD11	2.00	0.92
1:S:38:GLN:HE22	1:S:90:ARG:HG2	1.32	0.92
1:H:57:GLN:HE22	1:O:57:GLN:HE22	1.17	0.91
1:V:49:SER:OG	1:Y:32:GLY:HA3	1.70	0.91
1:E:55:SER:HB3	1:E:56:PRO:HD3	2.13	0.90
1:C:55:SER:HB3	1:C:56:PRO:HD3	2.07	0.89
1:I:55:SER:HB3	1:I:56:PRO:HD3	2.15	0.88
1:U:-1:SER:O	1:U:0:HIS:HB2	1.71	0.88
1:G:57:GLN:HE22	1:L:57:GLN:HE22	1.22	0.88
1:B:55:SER:HB3	1:B:56:PRO:CD	2.09	0.87
1:D:27:CYS:HB3	1:D:129:ILE:HD11	1.56	0.87
1:V:36:GLN:HA	1:V:36:GLN:NE2	1.89	0.87
1:A:55:SER:HB3	1:A:56:PRO:HD3	1.76	0.87
1:X:32:GLY:HA3	1:Y:49:SER:OG	1.74	0.87
1:X:36:GLN:HA	1:X:36:GLN:OE1	1.72	0.87
1:Z:55:SER:HB3	1:Z:56:PRO:CD	2.05	0.86
1:D:90:ARG:HH11	1:I:36:GLN:CB	40.22	0.86
1:F:27:CYS:HB3	1:F:129:ILE:HD11	1.58	0.84
1:H:55:SER:HB3	1:H:56:PRO:CD	2.22	0.84
1:V:36:GLN:HA	1:V:36:GLN:HE21	1.42	0.84
1:A:55:SER:HB3	1:A:56:PRO:CD	2.18	0.84
1:T:55:SER:HB3	1:T:56:PRO:HD3	1.59	0.84
1:D:57:GLN:HE22	1:E:57:GLN:HE22	1.22	0.84
1:Q:55:SER:HB3	1:Q:56:PRO:CD	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:ASN:O	1:N:92:ARG:NH1	2.12	0.83
1:F:55:SER:HB3	1:F:56:PRO:HD3	1.79	0.82
1:E:38:GLN:HE22	1:E:90:ARG:HA	1.43	0.82
1:E:89:THR:HA	1:U:36:GLN:HE21	54.62	0.81
1:Y:55:SER:HB3	1:Y:56:PRO:CD	2.10	0.81
1:C:90:ARG:HD2	1:H:36:GLN:HB2	75.78	0.81
1:W:55:SER:HB3	1:W:56:PRO:HD3	1.62	0.81
1:J:153:THR:HG22	1:J:154:SER:H	1.46	0.81
1:C:27:CYS:HB3	1:C:129:ILE:HD11	1.63	0.81
1:F:57:GLN:HE22	1:J:57:GLN:HE22	1.26	0.81
1:E:55:SER:HB3	1:E:56:PRO:CD	2.35	0.80
1:J:90:ARG:H	1:J:113:ARG:HH22	1.29	0.80
1:V:55:SER:HB3	1:V:56:PRO:CD	2.11	0.80
1:I:77:ASP:HB3	1:I:78:PRO:HD3	1.63	0.79
1:O:55:SER:HB3	1:O:56:PRO:CD	2.12	0.79
1:F:77:ASP:HB3	1:F:78:PRO:HD3	1.63	0.79
1:X:77:ASP:HB3	1:X:78:PRO:HD3	1.65	0.78
1:U:55:SER:HB3	1:U:56:PRO:HD3	1.64	0.78
1:S:142:SER:O	1:S:146:SER:HB2	1.84	0.78
1:D:77:ASP:HB3	1:D:78:PRO:HD3	1.66	0.77
1:B:55:SER:HB3	1:B:56:PRO:HD3	1.77	0.76
1:C:90:ARG:CD	1:H:36:GLN:HB2	74.94	0.76
1:F:75:VAL:HG22	1:Z:54:PRO:HD2	1.68	0.76
1:C:36:GLN:HB2	1:E:90:ARG:HG3	1.67	0.76
1:U:36:GLN:HA	1:U:36:GLN:OE1	1.84	0.75
1:I:57:GLN:HE22	1:K:57:GLN:HE22	1.34	0.75
1:E:77:ASP:HB3	1:E:78:PRO:HD3	1.67	0.75
1:H:77:ASP:HB3	1:H:78:PRO:HD3	1.69	0.75
1:R:32:GLY:HA3	1:T:49:SER:OG	1.87	0.75
1:Z:134:ARG:HG2	1:Z:134:ARG:HH11	1.50	0.75
1:Z:55:SER:HB3	1:Z:56:PRO:HD3	1.68	0.74
1:D:90:ARG:HH11	1:I:36:GLN:HB3	39.89	0.74
1:A:40:ALA:O	1:A:44:VAL:HG13	1.87	0.74
1:E:90:ARG:HG3	1:U:36:GLN:HG3	55.83	0.73
1:T:77:ASP:HB3	1:T:78:PRO:HD3	1.70	0.73
1:R:38:GLN:NE2	1:R:41:ARG:HH21	1.86	0.73
1:C:55:SER:HB3	1:C:56:PRO:CD	2.39	0.73
1:Z:77:ASP:HB3	1:Z:78:PRO:HD3	1.70	0.73
1:G:77:ASP:HB3	1:G:78:PRO:HD3	1.69	0.73
1:S:38:GLN:NE2	1:S:90:ARG:HG2	2.04	0.72
1:Q:153:THR:HG22	1:Q:154:SER:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:36:GLN:NE2	1:T:89:THR:HA	2.03	0.72
1:K:131:GLU:OE1	1:K:136:THR:HG21	1.90	0.72
1:V:55:SER:HB3	1:V:56:PRO:HD3	1.72	0.72
1:S:55:SER:HB3	1:S:56:PRO:CD	2.19	0.72
1:L:90:ARG:HG3	1:P:36:GLN:CB	2.20	0.72
1:F:90:ARG:HG3	1:V:36:GLN:HG3	74.99	0.72
1:T:36:GLN:HB2	1:U:90:ARG:CD	2.17	0.71
1:T:55:SER:HB3	1:T:56:PRO:CD	2.20	0.71
1:T:134:ARG:NH1	1:T:134:ARG:HG2	1.97	0.71
1:Z:153:THR:HG23	1:Z:154:SER:H	1.56	0.71
1:Q:55:SER:HB3	1:Q:56:PRO:HD3	1.72	0.71
1:Z:134:ARG:NH1	1:Z:134:ARG:HG2	2.04	0.71
1:S:90:ARG:HG3	1:Z:36:GLN:HG3	1.73	0.71
1:D:90:ARG:HH11	1:I:36:GLN:HB2	40.33	0.71
1:R:67:PHE:CE2	1:T:7:PRO:HG3	2.26	0.71
1:G:23:LEU:HD13	1:G:132:LEU:HD11	1.71	0.71
1:P:126:ASN:O	1:P:130:VAL:HG23	1.90	0.70
1:C:38:GLN:NE2	1:C:41:ARG:HH21	2.48	0.70
1:F:55:SER:HB3	1:F:56:PRO:CD	2.29	0.70
1:T:134:ARG:HH11	1:T:134:ARG:CG	2.02	0.70
1:Y:55:SER:HB3	1:Y:56:PRO:HD3	1.73	0.70
1:P:113:ARG:HB3	1:P:113:ARG:HH11	1.56	0.70
1:C:23:LEU:HD13	1:C:132:LEU:HD11	1.75	0.69
1:V:114:VAL:HA	1:V:117:ALA:HB3	1.73	0.69
1:D:38:GLN:NE2	1:D:41:ARG:HH21	2.37	0.69
1:J:153:THR:HG22	1:J:154:SER:N	2.06	0.69
1:D:55:SER:HB3	1:D:56:PRO:HD3	2.38	0.69
1:F:11:VAL:HG21	1:V:133:ILE:HA	115.86	0.69
1:H:38:GLN:NE2	1:H:41:ARG:HH21	2.44	0.69
1:C:36:GLN:CB	1:E:90:ARG:HG3	2.23	0.69
1:X:55:SER:HB3	1:X:56:PRO:CD	2.23	0.69
1:D:17:TRP:CZ3	1:D:70:TYR:HB2	2.54	0.68
1:M:38:GLN:HE22	1:M:90:ARG:HA	1.58	0.68
1:M:38:GLN:NE2	1:M:90:ARG:HA	2.09	0.68
1:S:35:PHE:CE1	1:S:44:VAL:HG21	2.29	0.68
1:M:27:CYS:HB3	1:M:129:ILE:HD11	1.76	0.68
1:C:83:LEU:HA	1:C:124:ALA:HB1	1.75	0.68
1:H:27:CYS:CB	1:H:129:ILE:HD11	2.18	0.67
1:R:55:SER:HB3	1:R:56:PRO:HD3	1.76	0.67
1:L:57:GLN:HB2	1:L:60:VAL:HB	1.75	0.67
1:V:17:TRP:CZ3	1:V:70:TYR:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:TRP:CZ3	1:O:70:TYR:HB2	2.30	0.67
1:R:55:SER:HB3	1:R:56:PRO:CD	2.25	0.67
1:A:23:LEU:HD13	1:A:132:LEU:HD11	1.74	0.67
1:A:0:HIS:HD2	1:A:153:THR:O	1.77	0.67
1:S:27:CYS:HB3	1:S:129:ILE:HD11	1.77	0.67
1:D:131:GLU:OE1	1:D:136:THR:HG21	2.21	0.67
1:D:40:ALA:O	1:D:44:VAL:HG13	1.94	0.66
1:P:55:SER:HB3	1:P:56:PRO:HD3	1.76	0.66
1:A:36:GLN:CB	1:C:90:ARG:HG3	2.26	0.66
1:R:36:GLN:HB3	1:T:90:ARG:HG3	1.77	0.66
1:K:0:HIS:HB2	1:K:153:THR:O	1.96	0.66
1:O:27:CYS:HB3	1:O:129:ILE:HD11	1.77	0.66
1:A:77:ASP:HB3	1:A:78:PRO:HD3	2.05	0.66
1:D:90:ARG:NH1	1:I:36:GLN:HB2	40.08	0.66
1:P:57:GLN:HB2	1:P:60:VAL:HB	1.76	0.66
1:J:153:THR:CG2	1:J:154:SER:H	2.10	0.65
1:B:13:LEU:HD22	1:B:57:GLN:O	3.14	0.65
1:M:90:ARG:HG3	1:N:36:GLN:HB2	1.78	0.65
1:K:134:ARG:HB2	1:K:136:THR:HG22	1.77	0.65
1:S:35:PHE:HE1	1:S:44:VAL:HG21	1.61	0.65
1:Z:26:LEU:HD21	1:Z:47:GLN:HB3	1.77	0.65
1:A:44:VAL:HA	1:A:47:GLN:HG3	3.20	0.65
1:X:55:SER:HB3	1:X:56:PRO:HD3	1.79	0.65
1:E:54:PRO:HD2	1:P:75:VAL:HG22	79.43	0.65
1:J:91:ASN:O	1:J:92:ARG:HD2	1.97	0.64
1:O:55:SER:HB3	1:O:56:PRO:HD2	1.79	0.64
1:W:153:THR:HG22	1:W:154:SER:N	2.12	0.64
1:Q:77:ASP:HB3	1:Q:78:PRO:CD	2.27	0.64
1:J:40:ALA:O	1:J:44:VAL:HG13	1.97	0.64
1:K:91:ASN:HD22	1:K:114:VAL:HG21	1.63	0.63
1:P:113:ARG:NH1	1:P:113:ARG:HB3	2.14	0.63
1:D:44:VAL:HA	1:D:47:GLN:HG3	2.75	0.63
1:W:77:ASP:HB3	1:W:78:PRO:CD	2.28	0.63
1:T:27:CYS:HB3	1:T:129:ILE:HD11	1.81	0.63
1:P:55:SER:HB3	1:P:56:PRO:CD	2.28	0.63
1:G:55:SER:HB3	1:G:56:PRO:CD	2.28	0.63
1:O:21:ILE:HG22	1:O:25:ASN:ND2	2.14	0.63
1:S:67:PHE:CE2	1:X:7:PRO:HG3	2.34	0.63
1:Z:55:SER:CB	1:Z:56:PRO:CD	2.77	0.63
1:N:55:SER:HB3	1:N:56:PRO:CD	2.28	0.63
1:Z:0:HIS:ND1	1:Z:153:THR:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:109:ASP:O	1:P:113:ARG:HB2	1.99	0.62
1:B:57:GLN:HB2	1:B:60:VAL:HB	2.28	0.62
1:E:91:ASN:ND2	1:E:114:VAL:HG21	2.56	0.62
1:B:32:GLY:HA3	1:Z:49:SER:OG	111.46	0.62
1:F:0:HIS:CD2	1:F:154:SER:HA	6.40	0.62
1:I:55:SER:CB	1:I:56:PRO:HD3	2.71	0.61
1:E:32:GLY:HA3	1:H:49:SER:OG	85.84	0.61
1:E:49:SER:HB2	1:U:32:GLY:HA3	65.32	0.61
1:X:126:ASN:HD22	1:X:129:ILE:HD12	1.66	0.61
1:B:77:ASP:HB3	1:B:78:PRO:HD3	2.05	0.61
1:Y:64:ASP:HA	1:Y:141:ARG:NH2	2.16	0.61
1:D:49:SER:OG	1:I:32:GLY:HA3	50.50	0.61
1:C:77:ASP:HB3	1:C:78:PRO:HD3	1.82	0.61
1:K:131:GLU:O	1:K:136:THR:HG23	2.01	0.61
1:K:7:PRO:HG3	1:M:67:PHE:CE2	2.36	0.61
1:C:34:GLN:HE21	1:E:90:ARG:NH1	1.99	0.61
1:Z:153:THR:HG23	1:Z:154:SER:N	2.15	0.61
1:B:55:SER:CB	1:B:56:PRO:CD	2.88	0.60
1:C:153:THR:HG22	1:C:154:SER:N	2.16	0.60
1:V:27:CYS:HB3	1:V:129:ILE:HD11	1.83	0.60
1:Z:131:GLU:OE1	1:Z:136:THR:HG21	2.01	0.60
1:H:57:GLN:HB2	1:H:60:VAL:HB	1.83	0.60
1:L:90:ARG:HG3	1:P:36:GLN:HB3	1.83	0.60
1:G:133:ILE:HA	1:N:11:VAL:HG21	1.83	0.60
1:O:40:ALA:O	1:O:44:VAL:HG13	2.01	0.60
1:M:-1:SER:O	1:M:0:HIS:HB2	2.00	0.60
1:S:55:SER:HB3	1:S:56:PRO:HD3	1.82	0.60
1:F:40:ALA:O	1:F:44:VAL:HG13	2.02	0.60
1:W:36:GLN:HA	1:W:36:GLN:OE1	2.02	0.60
1:D:36:GLN:HB3	1:R:90:ARG:HG3	55.47	0.60
1:A:36:GLN:HB3	1:C:90:ARG:HG3	1.84	0.59
1:E:90:ARG:HD2	1:U:36:GLN:HB3	55.08	0.59
1:S:90:ARG:CD	1:Z:36:GLN:HB2	2.29	0.59
1:O:55:SER:CB	1:O:56:PRO:CD	2.79	0.59
1:J:16:ALA:HB1	1:J:71:ARG:HB3	1.84	0.59
1:W:77:ASP:HB3	1:W:78:PRO:HD3	1.84	0.59
1:Z:17:TRP:CZ3	1:Z:70:TYR:HB2	2.37	0.59
1:M:151:VAL:HG12	1:M:153:THR:HG23	1.85	0.59
1:V:90:ARG:HG3	1:Y:36:GLN:HB3	1.85	0.59
1:C:40:ALA:O	1:C:44:VAL:HG13	2.03	0.59
1:F:4:ILE:HD12	1:F:4:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:27:CYS:HB3	1:K:129:ILE:HD11	1.84	0.58
1:C:0:HIS:HA	1:C:153:THR:O	4.43	0.58
1:M:17:TRP:CZ3	1:M:70:TYR:HB2	2.39	0.58
1:G:6:THR:O	1:G:9:GLN:HG3	2.04	0.58
1:K:91:ASN:ND2	1:K:114:VAL:HG21	2.18	0.58
1:C:24:ILE:HG12	1:E:11:VAL:HG13	1.85	0.58
1:W:142:SER:O	1:W:146:SER:HB2	2.03	0.58
1:G:17:TRP:CZ3	1:G:70:TYR:HB2	2.39	0.58
1:V:36:GLN:CA	1:V:36:GLN:HE21	2.16	0.58
1:M:55:SER:HB3	1:M:56:PRO:CD	2.33	0.58
1:K:17:TRP:CZ3	1:K:70:TYR:HB2	2.39	0.58
1:B:153:THR:HG23	1:B:154:SER:N	4.84	0.58
1:B:54:PRO:HD2	1:H:75:VAL:HG22	139.13	0.58
1:I:0:HIS:HD2	1:K:-1:SER:HB3	1.68	0.58
1:T:133:ILE:HA	1:U:11:VAL:HG21	1.86	0.58
1:D:131:GLU:O	1:D:136:THR:HG23	2.26	0.57
1:H:131:GLU:OE1	1:H:136:THR:HG21	2.40	0.57
1:I:17:TRP:CZ3	1:I:70:TYR:HB2	2.39	0.57
1:Z:134:ARG:HH11	1:Z:134:ARG:CG	2.16	0.57
1:E:131:GLU:HA	1:E:134:ARG:HG3	3.25	0.57
1:B:55:SER:HB3	1:B:56:PRO:HD2	1.93	0.57
1:F:27:CYS:CB	1:F:129:ILE:HD11	2.33	0.57
1:O:55:SER:HB3	1:O:56:PRO:HD3	1.86	0.57
1:M:90:ARG:HG3	1:N:36:GLN:CB	2.34	0.57
1:L:77:ASP:HB3	1:L:78:PRO:HD3	1.85	0.57
1:X:17:TRP:CZ3	1:X:70:TYR:HB2	2.39	0.57
1:P:38:GLN:NE2	1:P:41:ARG:HH21	2.03	0.57
1:T:153:THR:HG22	1:T:154:SER:H	1.70	0.56
1:B:131:GLU:OE1	1:B:136:THR:HG21	2.05	0.56
1:T:57:GLN:HB2	1:T:60:VAL:HB	1.87	0.56
1:M:23:LEU:HD13	1:M:132:LEU:HD11	1.87	0.56
1:Q:153:THR:HG22	1:Q:154:SER:N	2.20	0.56
1:G:55:SER:HB3	1:G:56:PRO:HD3	1.87	0.56
1:R:53:LYS:HB3	1:R:54:PRO:HD2	1.87	0.56
1:H:23:LEU:HD13	1:H:132:LEU:HD11	1.87	0.56
1:C:20:PRO:O	1:C:24:ILE:HG22	2.04	0.56
1:O:16:ALA:HB1	1:O:71:ARG:HB3	1.87	0.56
1:I:55:SER:HB3	1:I:56:PRO:CD	2.44	0.56
1:C:90:ARG:CD	1:H:36:GLN:CB	75.11	0.56
1:T:34:GLN:HA	1:U:88:ASP:OD1	2.06	0.56
1:P:153:THR:HG22	1:P:154:SER:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ARG:HD3	1:G:93:ILE:CG2	2.36	0.56
1:Z:55:SER:HB3	1:Z:56:PRO:HD2	1.87	0.56
1:P:91:ASN:ND2	1:P:114:VAL:HG21	2.21	0.56
1:F:38:GLN:NE2	1:F:41:ARG:HH21	2.29	0.56
1:D:134:ARG:HB2	1:D:136:THR:CG2	2.36	0.55
1:V:90:ARG:HG3	1:Y:36:GLN:CB	2.35	0.55
1:E:57:GLN:HB2	1:E:60:VAL:HB	1.89	0.55
1:D:153:THR:HG22	1:D:154:SER:N	2.20	0.55
1:H:57:GLN:NE2	1:O:57:GLN:HE22	1.97	0.55
1:Y:55:SER:CB	1:Y:56:PRO:CD	2.83	0.55
1:Q:53:LYS:HB3	1:Q:54:PRO:HD2	1.89	0.55
1:A:153:THR:HG22	1:A:154:SER:N	2.98	0.55
1:L:40:ALA:O	1:L:44:VAL:HG13	2.07	0.55
1:O:2:TYR:HB3	1:O:150:LEU:HD22	1.89	0.55
1:K:126:ASN:O	1:K:130:VAL:HG23	2.07	0.55
1:B:38:GLN:HA	1:B:41:ARG:NH2	2.71	0.55
1:M:77:ASP:HB3	1:M:78:PRO:HD3	1.88	0.55
1:K:0:HIS:HB2	1:K:154:SER:HA	1.82	0.55
1:L:131:GLU:O	1:L:136:THR:HG23	2.06	0.55
1:F:49:SER:OG	1:H:32:GLY:HA3	2.07	0.55
1:V:20:PRO:O	1:V:24:ILE:HG22	2.06	0.55
1:W:114:VAL:HG12	1:W:114:VAL:O	2.07	0.55
1:B:17:TRP:CZ3	1:B:70:TYR:HB2	2.42	0.55
1:U:40:ALA:O	1:U:44:VAL:HG13	2.07	0.55
1:E:0:HIS:HB3	1:E:153:THR:C	5.51	0.55
1:A:0:HIS:HD2	1:A:153:THR:C	2.11	0.54
1:D:36:GLN:CB	1:R:90:ARG:HG3	55.67	0.54
1:K:1:SER:HB2	1:K:58:VAL:O	2.06	0.54
1:T:128:LEU:HD13	1:T:132:LEU:HD11	1.88	0.54
1:G:36:GLN:OE1	1:N:89:THR:HA	2.07	0.54
1:F:17:TRP:CZ3	1:F:70:TYR:HB2	2.42	0.54
1:S:77:ASP:HB3	1:S:78:PRO:HD3	1.89	0.54
1:B:40:ALA:O	1:B:44:VAL:HG13	2.07	0.54
1:E:38:GLN:NE2	1:E:90:ARG:HA	2.17	0.54
1:D:11:VAL:HG22	1:K:24:ILE:HG12	1.90	0.54
1:B:153:THR:HG23	1:B:154:SER:H	4.61	0.54
1:S:7:PRO:HG3	1:Z:67:PHE:CE2	2.43	0.54
1:A:6:THR:O	1:A:9:GLN:HG3	2.08	0.54
1:E:153:THR:HG22	1:E:154:SER:N	2.23	0.53
1:H:41:ARG:HH12	1:H:114:VAL:HG22	4.55	0.53
1:G:34:GLN:HE21	1:N:90:ARG:NH1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ILE:O	1:H:125:ILE:HG13	2.07	0.53
1:C:113:ARG:C	1:C:115:ASP:H	3.33	0.53
1:Q:55:SER:HB3	1:Q:56:PRO:HD2	1.88	0.53
1:B:29:ASN:O	1:B:30:ALA:C	2.75	0.53
1:G:23:LEU:HD13	1:G:132:LEU:CD1	2.39	0.53
1:B:38:GLN:NE2	1:B:90:ARG:HG2	2.24	0.53
1:L:90:ARG:HG3	1:P:36:GLN:HB2	1.89	0.53
1:M:134:ARG:HB2	1:M:136:THR:HG23	1.91	0.53
1:F:133:ILE:HA	1:G:11:VAL:HG21	1.91	0.53
1:J:153:THR:CG2	1:J:154:SER:N	2.71	0.53
1:P:-1:SER:O	1:P:0:HIS:HB2	2.09	0.53
1:V:55:SER:CB	1:V:56:PRO:CD	2.85	0.53
1:B:27:CYS:HB3	1:B:129:ILE:HD11	1.90	0.53
1:W:153:THR:CG2	1:W:154:SER:N	2.72	0.52
1:Y:29:ASN:O	1:Y:30:ALA:C	2.48	0.52
1:U:153:THR:HG22	1:U:154:SER:H	1.75	0.52
1:E:75:VAL:HG22	1:R:54:PRO:HG2	1.92	0.52
1:S:133:ILE:HA	1:X:11:VAL:HG21	1.90	0.52
1:H:40:ALA:O	1:H:44:VAL:HG13	2.09	0.52
1:U:38:GLN:HE21	1:U:41:ARG:HH21	1.56	0.52
1:N:40:ALA:O	1:N:44:VAL:HG13	2.09	0.52
1:K:92:ARG:HH11	1:K:92:ARG:HA	1.73	0.52
1:A:17:TRP:CZ3	1:A:70:TYR:HB2	2.54	0.52
1:E:126:ASN:O	1:E:130:VAL:HG23	2.19	0.52
1:A:4:ILE:HD12	1:A:4:ILE:N	2.63	0.52
1:B:36:GLN:HB3	1:Z:90:ARG:HD2	91.82	0.52
1:U:77:ASP:HB3	1:U:78:PRO:HD3	1.91	0.52
1:H:53:LYS:HB3	1:H:54:PRO:HD2	1.91	0.52
1:B:6:THR:HB	1:B:7:PRO:HD2	3.84	0.52
1:N:55:SER:HB3	1:N:56:PRO:HD3	1.91	0.52
1:L:125:ILE:O	1:L:129:ILE:HG13	2.09	0.52
1:A:38:GLN:NE2	1:A:41:ARG:HH21	2.08	0.52
1:B:30:ALA:HB1	1:B:125:ILE:HD13	2.77	0.51
1:D:7:PRO:HG3	1:I:67:PHE:CE2	46.41	0.51
1:F:23:LEU:HD13	1:F:132:LEU:HD11	1.92	0.51
1:L:55:SER:HB3	1:L:56:PRO:CD	2.40	0.51
1:P:0:HIS:HA	1:P:153:THR:O	2.11	0.51
1:H:55:SER:CB	1:H:56:PRO:CD	2.91	0.51
1:D:77:ASP:HB3	1:D:78:PRO:CD	2.40	0.51
1:C:23:LEU:HD13	1:C:132:LEU:CD1	2.40	0.51
1:C:0:HIS:CD2	1:C:0:HIS:H	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:125:ILE:O	1:W:129:ILE:HG13	2.11	0.51
1:M:91:ASN:HD22	1:M:114:VAL:HG21	1.75	0.51
1:D:133:ILE:HA	1:R:11:VAL:HG21	63.49	0.51
1:G:36:GLN:CB	1:N:90:ARG:HG3	2.40	0.51
1:A:2:TYR:HB3	1:A:150:LEU:HD22	1.93	0.51
1:U:17:TRP:CZ3	1:U:70:TYR:HB2	2.46	0.51
1:X:36:GLN:CA	1:X:36:GLN:OE1	2.52	0.51
1:D:55:SER:HB3	1:D:56:PRO:CD	2.56	0.51
1:D:83:LEU:HA	1:D:124:ALA:HB1	1.93	0.51
1:A:15:SER:OG	1:A:54:PRO:HD3	2.56	0.51
1:F:19:ASP:HB3	1:F:22:GLU:HB3	1.92	0.51
1:I:45:GLN:HB2	1:I:87:PHE:CG	2.73	0.50
1:L:134:ARG:HB2	1:L:136:THR:HG22	1.94	0.50
1:A:153:THR:HG22	1:A:154:SER:H	2.29	0.50
1:D:2:TYR:HB3	1:D:150:LEU:HD22	1.93	0.50
1:O:126:ASN:O	1:O:130:VAL:HG23	2.11	0.50
1:X:2:TYR:CD1	1:X:150:LEU:HB3	2.46	0.50
1:S:142:SER:O	1:S:146:SER:CB	2.59	0.50
1:G:20:PRO:O	1:G:24:ILE:HG22	2.11	0.50
1:Y:44:VAL:HG23	1:Y:87:PHE:CE1	2.46	0.50
1:W:131:GLU:OE1	1:W:136:THR:HG21	2.11	0.50
1:C:17:TRP:CZ3	1:C:70:TYR:HB2	2.50	0.50
1:I:57:GLN:HB2	1:I:60:VAL:HB	1.93	0.50
1:S:15:SER:OG	1:S:54:PRO:HD3	2.12	0.50
1:F:7:PRO:CB	1:H:138:SER:HB2	2.42	0.50
1:M:40:ALA:O	1:M:44:VAL:HG13	2.11	0.50
1:V:122:ARG:HH11	1:V:122:ARG:HG2	1.77	0.50
1:E:55:SER:CB	1:E:56:PRO:CD	3.00	0.50
1:H:54:PRO:HG2	1:L:75:VAL:HG22	45.61	0.50
1:E:130:VAL:O	1:E:134:ARG:HG2	4.06	0.50
1:L:7:PRO:HD3	1:P:67:PHE:CE2	2.47	0.50
1:U:30:ALA:O	1:U:33:ASN:HB2	2.12	0.50
1:C:53:LYS:HB3	1:C:54:PRO:HD2	1.94	0.50
1:A:77:ASP:HB3	1:A:78:PRO:CD	2.42	0.49
1:T:134:ARG:NH1	1:T:134:ARG:CG	2.68	0.49
1:F:0:HIS:HD2	1:F:154:SER:HA	6.77	0.49
1:X:125:ILE:O	1:X:129:ILE:HG13	2.12	0.49
1:H:44:VAL:HG22	1:H:87:PHE:CE1	2.70	0.49
1:Q:33:ASN:O	1:Q:122:ARG:NH2	2.46	0.49
1:M:91:ASN:ND2	1:M:114:VAL:HG21	2.27	0.49
1:F:29:ASN:O	1:F:30:ALA:C	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:2:TYR:CD1	1:U:150:LEU:HB3	2.48	0.49
1:F:90:ARG:HG3	1:H:36:GLN:HB2	1.93	0.49
1:J:90:ARG:O	1:J:113:ARG:NH1	2.45	0.49
1:F:6:THR:HB	1:F:7:PRO:HD2	2.56	0.49
1:Y:0:HIS:H	1:Y:0:HIS:CD2	2.30	0.49
1:E:40:ALA:O	1:E:44:VAL:HG13	2.11	0.49
1:L:11:VAL:HG21	1:P:133:ILE:HA	1.95	0.49
1:T:36:GLN:CB	1:U:90:ARG:HD2	2.21	0.49
1:P:153:THR:CG2	1:P:154:SER:N	2.76	0.49
1:M:2:TYR:HB3	1:M:150:LEU:HD22	1.94	0.49
1:R:153:THR:HG23	1:R:154:SER:N	2.28	0.49
1:D:125:ILE:O	1:D:129:ILE:HG13	2.82	0.49
1:I:13:LEU:HD22	1:I:57:GLN:HA	2.37	0.49
1:J:27:CYS:HB3	1:J:129:ILE:HD11	1.95	0.49
1:Q:134:ARG:HB2	1:Q:136:THR:HG23	1.95	0.49
1:D:17:TRP:CD1	1:D:56:PRO:HD2	2.48	0.49
1:B:38:GLN:HA	1:B:41:ARG:HH21	2.70	0.49
1:A:18:ALA:HB3	1:A:69:VAL:HB	1.94	0.49
1:W:29:ASN:O	1:W:30:ALA:C	2.51	0.49
1:E:11:VAL:HG21	1:U:133:ILE:HA	80.71	0.48
1:A:11:VAL:HG21	1:B:133:ILE:HA	1.95	0.48
1:A:130:VAL:O	1:A:134:ARG:HG3	2.40	0.48
1:H:38:GLN:HE22	1:H:90:ARG:HA	1.78	0.48
1:F:39:GLN:O	1:F:43:VAL:HG23	2.65	0.48
1:X:2:TYR:HB3	1:X:150:LEU:HD22	1.95	0.48
1:L:16:ALA:HB1	1:L:71:ARG:HB3	1.95	0.48
1:D:38:GLN:HE22	1:D:90:ARG:HA	1.79	0.48
1:Q:55:SER:CB	1:Q:56:PRO:CD	2.83	0.48
1:V:11:VAL:HG21	1:Y:133:ILE:HA	1.95	0.48
1:G:61:ARG:HD3	1:G:141:ARG:NH1	2.29	0.48
1:D:19:ASP:HB3	1:D:22:GLU:HB3	2.32	0.48
1:E:2:TYR:CD1	1:E:150:LEU:HB3	2.78	0.48
1:G:90:ARG:HD3	1:G:93:ILE:HG21	1.96	0.48
1:W:11:VAL:HG12	1:W:70:TYR:OH	2.13	0.48
1:O:117:ALA:O	1:O:121:ILE:HG13	2.14	0.48
1:J:57:GLN:HB2	1:J:60:VAL:HB	1.96	0.48
1:X:55:SER:CB	1:X:56:PRO:CD	2.91	0.48
1:B:38:GLN:NE2	1:B:41:ARG:HH21	2.29	0.48
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.77	0.48
1:H:38:GLN:NE2	1:H:90:ARG:HA	2.29	0.48
1:B:36:GLN:OE1	1:B:114:VAL:HG12	4.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:17:TRP:CZ3	1:W:70:TYR:HB2	2.48	0.48
1:I:131:GLU:OE2	1:T:53:LYS:HE2	2.14	0.48
1:F:16:ALA:HB1	1:F:71:ARG:HB3	2.25	0.48
1:I:27:CYS:O	1:I:28:THR:C	2.52	0.47
1:D:67:PHE:HA	1:D:139:TYR:O	2.14	0.47
1:Q:75:VAL:HG22	1:U:54:PRO:HG2	1.96	0.47
1:D:64:ASP:HA	1:D:141:ARG:NH2	2.98	0.47
1:F:131:GLU:OE1	1:F:136:THR:HG21	2.14	0.47
1:Y:55:SER:HB3	1:Y:56:PRO:HD2	1.94	0.47
1:A:27:CYS:HB3	1:A:129:ILE:HD11	2.47	0.47
1:H:27:CYS:HB3	1:H:129:ILE:CD1	2.22	0.47
1:A:38:GLN:HE22	1:A:90:ARG:HA	1.80	0.47
1:Q:17:TRP:CZ3	1:Q:70:TYR:HB2	2.48	0.47
1:W:41:ARG:HH22	1:W:91:ASN:ND2	2.12	0.47
1:W:62:PHE:CD1	1:W:63:PRO:HD2	2.48	0.47
1:A:91:ASN:ND2	1:A:114:VAL:HG21	2.29	0.47
1:I:0:HIS:O	1:I:153:THR:O	2.33	0.47
1:N:38:GLN:HE22	1:N:90:ARG:HA	1.79	0.47
1:H:131:GLU:O	1:H:136:THR:HG23	2.42	0.47
1:X:126:ASN:HA	1:X:129:ILE:HD12	1.95	0.47
1:B:13:LEU:HD13	1:B:57:GLN:O	4.03	0.47
1:T:35:PHE:CE1	1:T:44:VAL:HG21	2.49	0.47
1:U:128:LEU:HD13	1:U:132:LEU:HD11	1.96	0.47
1:R:67:PHE:HE2	1:T:7:PRO:HG3	1.75	0.47
1:P:90:ARG:H	1:P:113:ARG:HH22	1.62	0.47
1:G:2:TYR:HB3	1:G:150:LEU:HD22	1.97	0.47
1:M:61:ARG:HD3	1:M:141:ARG:CZ	2.45	0.47
1:B:133:ILE:HA	1:Z:11:VAL:HG21	145.43	0.47
1:W:39:GLN:O	1:W:43:VAL:HG23	2.14	0.47
1:L:9:GLN:HG2	1:L:150:LEU:HG	1.97	0.47
1:C:2:TYR:HB3	1:C:150:LEU:HD22	1.97	0.47
1:L:131:GLU:OE1	1:L:136:THR:CG2	2.52	0.47
1:I:55:SER:CB	1:I:56:PRO:CD	2.98	0.47
1:N:90:ARG:H	1:N:113:ARG:HH22	1.63	0.47
1:R:77:ASP:HB3	1:R:78:PRO:HD3	1.95	0.47
1:D:34:GLN:HA	1:R:88:ASP:OD1	55.74	0.47
1:K:38:GLN:HA	1:K:41:ARG:NH2	2.31	0.46
1:H:143:SER:O	1:H:147:SER:OG	2.74	0.46
1:N:16:ALA:HB1	1:N:71:ARG:HB3	1.97	0.46
1:X:-1:SER:OG	1:X:0:HIS:N	2.45	0.46
1:Z:6:THR:O	1:Z:9:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HD3	1:A:141:ARG:NH1	2.30	0.46
1:A:62:PHE:O	1:A:63:PRO:C	2.68	0.46
1:H:92:ARG:CZ	1:H:110:ALA:HB2	2.45	0.46
1:R:38:GLN:NE2	1:R:41:ARG:NH2	2.60	0.46
1:N:-1:SER:O	1:N:154:SER:O	2.34	0.46
1:C:73:ASN:ND2	1:C:137:GLY:HA2	2.53	0.46
1:T:11:VAL:HG12	1:T:70:TYR:OH	2.16	0.46
1:Q:91:ASN:O	1:Q:92:ARG:HD2	2.15	0.46
1:Z:27:CYS:HB3	1:Z:129:ILE:HD11	1.97	0.46
1:H:73:ASN:ND2	1:H:137:GLY:HA2	2.87	0.46
1:P:2:TYR:HB3	1:P:150:LEU:HD22	1.98	0.46
1:C:90:ARG:H	1:C:113:ARG:HH22	1.64	0.46
1:D:153:THR:HB	1:D:154:SER:H	2.63	0.46
1:B:36:GLN:HG3	1:Z:90:ARG:HG3	94.35	0.46
1:W:38:GLN:NE2	1:W:41:ARG:HH21	2.13	0.46
1:O:-1:SER:O	1:O:154:SER:HB2	2.16	0.46
1:I:29:ASN:O	1:I:30:ALA:C	2.66	0.46
1:H:57:GLN:HE22	1:O:57:GLN:NE2	1.99	0.46
1:V:55:SER:HB3	1:V:56:PRO:HD2	1.97	0.46
1:K:38:GLN:NE2	1:K:41:ARG:HH21	2.14	0.46
1:F:5:THR:N	1:F:9:GLN:OE1	2.42	0.46
1:I:77:ASP:HB3	1:I:78:PRO:CD	2.40	0.46
1:D:134:ARG:HB2	1:D:136:THR:HG23	1.98	0.46
1:W:0:HIS:ND1	1:W:153:THR:O	2.36	0.46
1:X:38:GLN:HA	1:X:41:ARG:NH2	2.30	0.46
1:B:142:SER:O	1:B:146:SER:HB3	2.96	0.46
1:B:21:ILE:HA	1:B:24:ILE:HG22	1.98	0.46
1:H:57:GLN:O	1:H:59:THR:N	2.81	0.46
1:X:77:ASP:HB3	1:X:78:PRO:CD	2.43	0.46
1:S:44:VAL:HG23	1:S:87:PHE:CE1	2.51	0.46
1:C:153:THR:CG2	1:C:154:SER:N	2.82	0.46
1:G:9:GLN:NE2	1:G:148:SER:O	2.47	0.46
1:G:36:GLN:HB2	1:N:90:ARG:HG3	1.98	0.46
1:U:142:SER:O	1:U:146:SER:HB3	2.16	0.46
1:P:19:ASP:HB3	1:P:22:GLU:HB2	1.97	0.46
1:I:61:ARG:HD2	1:I:152:TRP:CD2	2.51	0.46
1:H:57:GLN:O	1:H:58:VAL:C	2.55	0.45
1:E:91:ASN:HD22	1:E:114:VAL:HG21	2.36	0.45
1:N:107:THR:HA	1:N:110:ALA:HB3	1.97	0.45
1:F:36:GLN:HB2	1:W:90:ARG:HH11	74.72	0.45
1:E:90:ARG:O	1:E:113:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:ASN:O	1:L:77:ASP:HB2	2.16	0.45
1:W:90:ARG:O	1:W:114:VAL:HG21	2.16	0.45
1:F:90:ARG:HD2	1:V:36:GLN:HB3	74.13	0.45
1:B:125:ILE:O	1:B:129:ILE:HG13	2.46	0.45
1:N:112:ARG:HA	1:N:115:ASP:HB2	1.98	0.45
1:H:21:ILE:O	1:H:24:ILE:HG22	2.15	0.45
1:G:91:ASN:O	1:G:92:ARG:HD2	2.15	0.45
1:I:129:ILE:O	1:I:130:VAL:C	2.54	0.45
1:S:38:GLN:NE2	1:S:41:ARG:HH21	2.15	0.45
1:C:133:ILE:HA	1:E:11:VAL:HG21	1.98	0.45
1:K:77:ASP:HB3	1:K:78:PRO:HD3	1.97	0.45
1:V:57:GLN:HB2	1:V:60:VAL:HB	1.98	0.45
1:M:8:SER:HB2	1:N:133:ILE:O	2.16	0.45
1:M:11:VAL:HG21	1:N:133:ILE:HA	1.98	0.45
1:D:90:ARG:CG	1:I:36:GLN:HB3	40.67	0.45
1:E:38:GLN:NE2	1:E:41:ARG:HH21	2.64	0.45
1:Z:0:HIS:HB3	1:Z:152:TRP:CZ2	2.51	0.45
1:L:11:VAL:O	1:L:14:SER:OG	2.26	0.45
1:Z:57:GLN:HB2	1:Z:60:VAL:HB	1.99	0.45
1:Z:84:LEU:HA	1:Z:84:LEU:HD23	1.84	0.45
1:E:24:ILE:HG12	1:I:11:VAL:HG22	1.97	0.45
1:F:90:ARG:HG3	1:H:36:GLN:CB	2.47	0.45
1:B:129:ILE:HG22	1:B:133:ILE:CD1	2.91	0.45
1:T:2:TYR:CD1	1:T:150:LEU:HB3	2.52	0.45
1:N:2:TYR:HB3	1:N:150:LEU:HD22	1.99	0.45
1:S:11:VAL:HG12	1:S:70:TYR:OH	2.16	0.45
1:N:131:GLU:OE1	1:N:136:THR:HG21	2.16	0.45
1:S:38:GLN:HA	1:S:41:ARG:NH2	2.33	0.44
1:H:114:VAL:O	1:H:114:VAL:HG12	2.17	0.44
1:H:35:PHE:O	1:H:41:ARG:NH1	2.48	0.44
1:G:133:ILE:O	1:N:8:SER:HB2	2.17	0.44
1:W:90:ARG:O	1:W:114:VAL:CG2	2.66	0.44
1:L:55:SER:HB3	1:L:56:PRO:HD3	1.99	0.44
1:J:129:ILE:O	1:J:130:VAL:C	2.55	0.44
1:X:53:LYS:HB3	1:X:54:PRO:HD2	1.98	0.44
1:P:11:VAL:HG21	1:Q:133:ILE:HA	1.99	0.44
1:I:26:LEU:HD11	1:I:47:GLN:HE21	4.65	0.44
1:S:90:ARG:HD3	1:Z:36:GLN:CB	2.35	0.44
1:A:55:SER:CB	1:A:56:PRO:CD	2.95	0.44
1:K:134:ARG:HB2	1:K:136:THR:CG2	2.43	0.44
1:H:128:LEU:HD22	1:H:132:LEU:HG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:7:PRO:HB3	1:Y:138:SER:HB2	1.99	0.44
1:R:131:GLU:OE1	1:R:136:THR:HG21	2.18	0.44
1:P:103:THR:H	1:P:106:GLU:HB3	1.82	0.44
1:P:77:ASP:HB3	1:P:78:PRO:HD3	1.99	0.44
1:C:61:ARG:HD2	1:C:152:TRP:CD2	2.52	0.44
1:B:53:LYS:HB3	1:B:54:PRO:CD	2.78	0.44
1:M:17:TRP:CD1	1:M:56:PRO:HD2	2.52	0.44
1:N:20:PRO:O	1:N:24:ILE:HG22	2.17	0.44
1:N:55:SER:CB	1:N:56:PRO:CD	2.95	0.44
1:N:17:TRP:CZ3	1:N:70:TYR:HB2	2.52	0.44
1:C:18:ALA:O	1:C:69:VAL:HG23	2.17	0.44
1:G:121:ILE:O	1:G:125:ILE:HG13	2.17	0.44
1:K:0:HIS:HB3	1:K:154:SER:CA	2.21	0.44
1:D:11:VAL:HG21	1:I:133:ILE:HA	55.71	0.44
1:K:3:SER:HB3	1:K:153:THR:CG2	2.48	0.44
1:U:38:GLN:NE2	1:U:41:ARG:HH21	2.15	0.44
1:M:14:SER:HB2	1:N:25:ASN:OD1	2.18	0.44
1:B:69:VAL:CG1	1:B:76:LEU:CD1	3.38	0.44
1:V:53:LYS:HB3	1:V:54:PRO:HD2	2.00	0.44
1:Z:77:ASP:HB3	1:Z:78:PRO:CD	2.44	0.44
1:H:38:GLN:HE21	1:H:41:ARG:HH21	2.61	0.44
1:U:128:LEU:HD23	1:U:128:LEU:HA	1.81	0.44
1:E:83:LEU:HA	1:E:124:ALA:HB1	1.99	0.44
1:M:75:VAL:HG22	1:Y:54:PRO:HD2	2.00	0.44
1:R:36:GLN:CB	1:T:90:ARG:HG3	2.44	0.44
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.77	0.44
1:S:32:GLY:HA3	1:X:49:SER:OG	2.18	0.43
1:E:90:ARG:CD	1:U:36:GLN:HB3	54.24	0.43
1:J:90:ARG:H	1:J:113:ARG:NH2	2.07	0.43
1:M:55:SER:HB3	1:M:56:PRO:HD3	2.00	0.43
1:B:131:GLU:O	1:B:136:THR:HG23	2.17	0.43
1:O:57:GLN:HB2	1:O:60:VAL:HB	2.00	0.43
1:B:129:ILE:O	1:B:130:VAL:C	2.77	0.43
1:R:29:ASN:O	1:R:30:ALA:C	2.56	0.43
1:E:131:GLU:OE1	1:E:136:THR:HG21	2.19	0.43
1:U:15:SER:OG	1:U:54:PRO:HD3	2.19	0.43
1:H:30:ALA:O	1:H:33:ASN:HB2	2.18	0.43
1:B:26:LEU:HD12	1:B:26:LEU:HA	1.87	0.43
1:U:29:ASN:O	1:U:30:ALA:C	2.57	0.43
1:I:134:ARG:HB2	1:I:136:THR:CG2	2.48	0.43
1:B:36:GLN:CB	1:Z:90:ARG:HG3	93.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:17:TRP:CZ3	1:S:70:TYR:HB2	2.53	0.43
1:P:77:ASP:HB3	1:P:78:PRO:CD	2.49	0.43
1:R:30:ALA:HB1	1:R:125:ILE:HD13	1.99	0.43
1:Z:0:HIS:HB3	1:Z:152:TRP:CE2	2.54	0.43
1:R:57:GLN:O	1:R:58:VAL:C	2.55	0.43
1:Z:39:GLN:O	1:Z:43:VAL:HG23	2.18	0.43
1:L:134:ARG:HB2	1:L:136:THR:CG2	2.49	0.43
1:D:57:GLN:HB2	1:D:60:VAL:HB	2.09	0.43
1:R:17:TRP:CD1	1:R:56:PRO:HD2	2.53	0.43
1:R:17:TRP:CZ3	1:R:70:TYR:HB2	2.54	0.43
1:I:45:GLN:HB2	1:I:87:PHE:CB	2.79	0.43
1:X:0:HIS:HB2	1:X:152:TRP:CE2	2.54	0.43
1:X:19:ASP:HB3	1:X:22:GLU:HB2	2.00	0.43
1:C:62:PHE:CD1	1:C:141:ARG:HA	2.58	0.43
1:F:122:ARG:NH2	1:G:88:ASP:OD2	2.41	0.43
1:T:73:ASN:ND2	1:T:137:GLY:HA2	2.33	0.43
1:H:0:HIS:HB3	1:H:152:TRP:CE2	3.79	0.43
1:D:23:LEU:HD13	1:D:132:LEU:HD13	2.34	0.43
1:N:62:PHE:CD1	1:N:141:ARG:HA	2.54	0.43
1:L:2:TYR:CD1	1:L:150:LEU:HB3	2.54	0.43
1:C:71:ARG:NH1	1:C:71:ARG:HG3	2.34	0.43
1:H:17:TRP:CZ3	1:H:70:TYR:HB2	2.74	0.43
1:F:2:TYR:HB3	1:F:150:LEU:HD22	2.01	0.43
1:O:111:THR:HG22	1:O:112:ARG:N	2.33	0.43
1:C:90:ARG:HD3	1:H:36:GLN:CB	74.60	0.42
1:J:113:ARG:HB3	1:J:113:ARG:NH1	2.34	0.42
1:I:38:GLN:NE2	1:I:90:ARG:HG2	2.33	0.42
1:H:16:ALA:HB1	1:H:71:ARG:HB3	2.23	0.42
1:E:126:ASN:HD22	1:E:129:ILE:HD12	4.60	0.42
1:E:73:ASN:O	1:E:77:ASP:HB2	2.19	0.42
1:S:40:ALA:O	1:S:44:VAL:HG22	2.19	0.42
1:A:6:THR:HG22	1:A:7:PRO:HD2	2.45	0.42
1:V:0:HIS:HB3	1:V:152:TRP:CE2	2.54	0.42
1:A:75:VAL:HG22	1:I:54:PRO:HG2	71.03	0.42
1:F:77:ASP:HB3	1:F:78:PRO:CD	2.44	0.42
1:F:140:ASN:O	1:F:141:ARG:C	2.56	0.42
1:N:9:GLN:O	1:N:12:PHE:HB2	2.20	0.42
1:H:75:VAL:O	1:H:78:PRO:HD2	2.54	0.42
1:W:89:THR:HG22	1:W:90:ARG:N	2.35	0.42
1:M:92:ARG:NH1	1:M:110:ALA:HA	2.35	0.42
1:B:114:VAL:HA	1:B:117:ALA:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:77:ASP:HB3	1:O:78:PRO:CD	2.49	0.42
1:Z:126:ASN:HA	1:Z:126:ASN:HD22	1.71	0.42
1:F:36:GLN:CB	1:W:90:ARG:HH11	74.25	0.42
1:M:130:VAL:O	1:M:134:ARG:HG3	2.20	0.42
1:V:122:ARG:NH1	1:V:122:ARG:HG2	2.35	0.42
1:T:25:ASN:OD1	1:U:14:SER:HB2	2.19	0.42
1:F:90:ARG:HG3	1:V:36:GLN:CG	74.94	0.42
1:B:36:GLN:HB3	1:Z:90:ARG:HG3	92.76	0.42
1:B:91:ASN:HD22	1:B:114:VAL:HG21	1.85	0.42
1:C:150:LEU:HD23	1:C:150:LEU:HA	2.30	0.42
1:G:147:SER:HA	1:S:59:THR:HB	2.02	0.42
1:R:31:LEU:HD12	1:T:71:ARG:HH22	1.85	0.42
1:E:29:ASN:O	1:E:30:ALA:C	2.62	0.42
1:G:77:ASP:HB3	1:G:78:PRO:CD	2.45	0.42
1:T:125:ILE:O	1:T:129:ILE:HG13	2.20	0.42
1:K:11:VAL:HG21	1:M:133:ILE:HA	2.00	0.42
1:O:84:LEU:HA	1:O:84:LEU:HD23	1.94	0.42
1:S:36:GLN:HG2	1:X:88:ASP:OD1	2.19	0.42
1:S:9:GLN:HG2	1:S:150:LEU:HG	2.02	0.42
1:H:91:ASN:HD22	1:H:114:VAL:HG21	5.29	0.41
1:J:61:ARG:HD3	1:J:141:ARG:NH1	2.35	0.41
1:N:62:PHE:CG	1:N:63:PRO:HD2	2.55	0.41
1:Z:128:LEU:HD22	1:Z:132:LEU:HG	2.02	0.41
1:U:71:ARG:NH1	1:U:80:VAL:HB	2.35	0.41
1:E:24:ILE:O	1:E:27:CYS:HB2	2.19	0.41
1:J:90:ARG:N	1:J:113:ARG:HH22	2.07	0.41
1:H:41:ARG:HG3	1:H:41:ARG:HH11	1.85	0.41
1:I:38:GLN:HA	1:I:41:ARG:NH2	2.94	0.41
1:Q:6:THR:HB	1:Q:7:PRO:HD2	2.02	0.41
1:V:91:ASN:HA	1:V:114:VAL:HG21	2.01	0.41
1:T:44:VAL:HG23	1:T:87:PHE:CZ	2.55	0.41
1:S:19:ASP:HB3	1:S:22:GLU:HB3	2.02	0.41
1:S:84:LEU:HA	1:S:84:LEU:HD23	1.89	0.41
1:E:49:SER:CB	1:U:32:GLY:HA3	66.18	0.41
1:Z:6:THR:HB	1:Z:7:PRO:HD2	2.02	0.41
1:N:17:TRP:CD1	1:N:56:PRO:HD2	2.56	0.41
1:F:153:THR:OG1	1:F:154:SER:N	2.53	0.41
1:W:114:VAL:HA	1:W:117:ALA:CB	2.50	0.41
1:K:3:SER:HB3	1:K:153:THR:HG21	2.01	0.41
1:I:56:PRO:HG3	1:I:62:PHE:HD2	2.74	0.41
1:V:114:VAL:HA	1:V:117:ALA:CB	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LEU:HD11	1:H:137:GLY:HA3	2.02	0.41
1:G:91:ASN:HD22	1:G:114:VAL:HG21	1.86	0.41
1:C:140:ASN:O	1:C:141:ARG:C	2.59	0.41
1:A:32:GLY:HA3	1:B:49:SER:OG	39.85	0.41
1:T:77:ASP:HB3	1:T:78:PRO:CD	2.47	0.41
1:B:126:ASN:O	1:B:130:VAL:HG23	2.21	0.41
1:T:9:GLN:HB3	1:T:150:LEU:HD21	2.03	0.41
1:S:49:SER:HB2	1:Z:32:GLY:HA3	2.01	0.41
1:F:110:ALA:O	1:F:114:VAL:HB	2.21	0.41
1:I:56:PRO:HG3	1:I:62:PHE:CD2	3.56	0.41
1:D:90:ARG:HH12	1:I:34:GLN:HE21	42.38	0.41
1:E:90:ARG:HD2	1:U:36:GLN:CB	55.54	0.41
1:G:76:LEU:O	1:G:77:ASP:C	2.59	0.41
1:I:26:LEU:HD11	1:I:47:GLN:NE2	4.61	0.41
1:C:62:PHE:CD1	1:C:63:PRO:HD2	2.90	0.41
1:J:2:TYR:HB3	1:J:150:LEU:HD22	2.03	0.41
1:P:16:ALA:HB1	1:P:71:ARG:HB3	2.03	0.41
1:L:70:TYR:CZ	1:L:72:TYR:HB2	2.56	0.41
1:B:91:ASN:ND2	1:B:114:VAL:HG21	2.36	0.40
1:R:24:ILE:HG12	1:T:11:VAL:HG22	2.03	0.40
1:V:-1:SER:HB3	1:V:0:HIS:H	1.50	0.40
1:C:43:VAL:O	1:C:47:GLN:HG3	2.65	0.40
1:G:126:ASN:HA	1:G:126:ASN:HD22	1.71	0.40
1:L:12:PHE:HB3	1:L:144:PHE:HE1	1.86	0.40
1:D:129:ILE:O	1:D:130:VAL:C	2.59	0.40
1:B:13:LEU:HD13	1:B:58:VAL:HG22	2.59	0.40
1:C:153:THR:O	1:C:154:SER:HB2	2.21	0.40
1:O:62:PHE:O	1:O:63:PRO:C	2.59	0.40
1:K:23:LEU:HD13	1:K:132:LEU:HD11	2.03	0.40
1:G:16:ALA:HB1	1:G:71:ARG:HB3	2.04	0.40
1:N:72:TYR:O	1:N:73:ASN:C	2.60	0.40
1:C:128:LEU:HD22	1:C:132:LEU:HG	2.22	0.40
1:H:91:ASN:HD22	1:H:91:ASN:HA	3.13	0.40
1:U:36:GLN:OE1	1:U:36:GLN:CA	2.61	0.40
1:I:57:GLN:O	1:I:58:VAL:C	2.59	0.40
1:P:129:ILE:O	1:P:130:VAL:C	2.60	0.40
1:C:38:GLN:NE2	1:C:41:ARG:NH2	3.25	0.40
1:F:114:VAL:C	1:F:116:ASP:H	2.92	0.40
1:Z:29:ASN:O	1:Z:30:ALA:C	2.60	0.40
1:J:30:ALA:O	1:J:33:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 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	138/174 (79%)	129 (94%)	7 (5%)	2 (1%)	14	46
1	B	135/174 (78%)	129 (96%)	5 (4%)	1 (1%)	26	64
1	C	140/174 (80%)	130 (93%)	9 (6%)	1 (1%)	26	64
1	D	139/174 (80%)	128 (92%)	10 (7%)	1 (1%)	26	64
1	E	136/174 (78%)	126 (93%)	7 (5%)	3 (2%)	8	34
1	F	139/174 (80%)	127 (91%)	10 (7%)	2 (1%)	14	46
1	G	139/174 (80%)	129 (93%)	8 (6%)	2 (1%)	14	46
1	H	140/174 (80%)	126 (90%)	10 (7%)	4 (3%)	6	27
1	I	137/174 (79%)	121 (88%)	11 (8%)	5 (4%)	4	22
1	J	141/174 (81%)	129 (92%)	11 (8%)	1 (1%)	26	64
1	K	139/174 (80%)	128 (92%)	9 (6%)	2 (1%)	14	46
1	L	137/174 (79%)	128 (93%)	7 (5%)	2 (2%)	13	44
1	M	138/174 (79%)	131 (95%)	4 (3%)	3 (2%)	8	34
1	N	138/174 (79%)	129 (94%)	8 (6%)	1 (1%)	26	64
1	O	136/174 (78%)	127 (93%)	7 (5%)	2 (2%)	13	44
1	P	143/174 (82%)	131 (92%)	8 (6%)	4 (3%)	6	28
1	Q	142/174 (82%)	132 (93%)	7 (5%)	3 (2%)	9	35
1	R	129/174 (74%)	122 (95%)	5 (4%)	2 (2%)	12	42
1	S	129/174 (74%)	121 (94%)	6 (5%)	2 (2%)	12	42
1	T	128/174 (74%)	122 (95%)	5 (4%)	1 (1%)	24	61
1	U	129/174 (74%)	118 (92%)	9 (7%)	2 (2%)	12	42
1	V	130/174 (75%)	122 (94%)	6 (5%)	2 (2%)	13	44
1	W	130/174 (75%)	119 (92%)	10 (8%)	1 (1%)	24	61
1	X	127/174 (73%)	117 (92%)	9 (7%)	1 (1%)	24	61
1	Y	128/174 (74%)	118 (92%)	9 (7%)	1 (1%)	24	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	130/174 (75%)	123 (95%)	6 (5%)	1 (1%)	24	61
1	a	127/174 (73%)	117 (92%)	8 (6%)	2 (2%)	12	42
1	b	128/174 (74%)	115 (90%)	10 (8%)	3 (2%)	8	32
1	c	132/174 (76%)	120 (91%)	9 (7%)	3 (2%)	8	32
1	d	130/174 (75%)	119 (92%)	10 (8%)	1 (1%)	24	61
1	e	130/174 (75%)	116 (89%)	13 (10%)	1 (1%)	24	61
1	f	130/174 (75%)	121 (93%)	8 (6%)	1 (1%)	24	61
1	h	130/174 (75%)	122 (94%)	6 (5%)	2 (2%)	13	44
1	i	130/174 (75%)	116 (89%)	11 (8%)	3 (2%)	8	32
All	All	4554/5916 (77%)	4208 (92%)	278 (6%)	68 (2%)	13	44

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	SER
1	G	55	SER
1	I	1	SER
1	L	153	THR
1	M	0	HIS
1	N	55	SER
1	O	55	SER
1	P	64	ASP
1	Q	64	ASP
1	S	64	ASP
1	U	0	HIS
1	b	55	SER
1	c	114	VAL
1	e	55	SER
1	h	55	SER
1	i	64	ASP
1	B	55	SER
1	D	55	SER
1	L	55	SER
1	M	55	SER
1	P	0	HIS
1	P	91	ASN
1	Q	55	SER
1	R	55	SER
1	R	64	ASP

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Mol	Chain	Res	Type
1	S	55	SER
1	V	55	SER
1	X	55	SER
1	Z	55	SER
1	a	55	SER
1	b	58	VAL
1	c	55	SER
1	f	55	SER
1	i	55	SER
1	C	55	SER
1	E	55	SER
1	F	55	SER
1	H	55	SER
1	H	64	ASP
1	H	91	ASN
1	I	55	SER
1	J	55	SER
1	K	55	SER
1	P	55	SER
1	Q	91	ASN
1	T	55	SER
1	U	55	SER
1	V	64	ASP
1	W	55	SER
1	Y	55	SER
1	b	64	ASP
1	d	55	SER
1	h	58	VAL
1	A	0	HIS
1	E	64	ASP
1	I	64	ASP
1	M	63	PRO
1	c	64	ASP
1	i	30	ALA
1	E	63	PRO
1	a	64	ASP
1	F	63	PRO
1	K	63	PRO
1	O	63	PRO
1	I	63	PRO
1	G	63	PRO
1	H	77	ASP

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Mol	Chain	Res	Type
1	I	58	VAL

### 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	125/153 (82%)	115 (92%)	10 (8%)	15	46
1	B	123/153 (80%)	111 (90%)	12 (10%)	10	34
1	C	127/153 (83%)	118 (93%)	9 (7%)	18	52
1	D	126/153 (82%)	112 (89%)	14 (11%)	8	28
1	E	123/153 (80%)	109 (89%)	14 (11%)	7	26
1	F	127/153 (83%)	114 (90%)	13 (10%)	9	31
1	G	127/153 (83%)	110 (87%)	17 (13%)	5	19
1	H	127/153 (83%)	108 (85%)	19 (15%)	3	14
1	I	125/153 (82%)	111 (89%)	14 (11%)	7	28
1	J	128/153 (84%)	118 (92%)	10 (8%)	16	47
1	K	127/153 (83%)	113 (89%)	14 (11%)	8	29
1	L	125/153 (82%)	114 (91%)	11 (9%)	12	41
1	M	126/153 (82%)	114 (90%)	12 (10%)	11	36
1	N	126/153 (82%)	115 (91%)	11 (9%)	13	42
1	O	123/153 (80%)	113 (92%)	10 (8%)	15	45
1	P	130/153 (85%)	120 (92%)	10 (8%)	16	48
1	Q	129/153 (84%)	116 (90%)	13 (10%)	9	32
1	R	118/153 (77%)	103 (87%)	15 (13%)	5	20
1	S	118/153 (77%)	110 (93%)	8 (7%)	20	53
1	T	117/153 (76%)	102 (87%)	15 (13%)	5	20
1	U	118/153 (77%)	109 (92%)	9 (8%)	16	49
1	V	119/153 (78%)	110 (92%)	9 (8%)	16	49
1	W	119/153 (78%)	110 (92%)	9 (8%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	116/153 (76%)	108 (93%)	8 (7%)	19	52
1	Y	117/153 (76%)	103 (88%)	14 (12%)	6	23
1	Z	119/153 (78%)	105 (88%)	14 (12%)	6	24
1	a	116/153 (76%)	105 (90%)	11 (10%)	11	36
1	b	117/153 (76%)	106 (91%)	11 (9%)	11	37
1	c	120/153 (78%)	110 (92%)	10 (8%)	14	44
1	d	119/153 (78%)	102 (86%)	17 (14%)	4	16
1	e	119/153 (78%)	109 (92%)	10 (8%)	14	43
1	f	119/153 (78%)	107 (90%)	12 (10%)	9	32
1	h	119/153 (78%)	105 (88%)	14 (12%)	6	24
1	i	119/153 (78%)	110 (92%)	9 (8%)	16	49
All	All	4153/5202 (80%)	3745 (90%)	408 (10%)	10	34

All (408) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	6	THR
1	A	19	ASP
1	A	23	LEU
1	A	44	VAL
1	A	107	THR
1	A	112	ARG
1	A	115	ASP
1	A	128	LEU
1	A	153	THR
1	B	-1	SER
1	B	3	SER
1	B	6	THR
1	B	23	LEU
1	B	26	LEU
1	B	42	THR
1	B	49	SER
1	B	50	GLU
1	B	64	ASP
1	B	89	THR
1	B	128	LEU
1	B	136	THR

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Mol	Chain	Res	Type
1	C	0	HIS
1	C	23	LEU
1	C	44	VAL
1	C	69	VAL
1	C	89	THR
1	C	107	THR
1	C	123	SER
1	C	128	LEU
1	C	147	SER
1	D	0	HIS
1	D	3	SER
1	D	6	THR
1	D	8	SER
1	D	15	SER
1	D	23	LEU
1	D	44	VAL
1	D	89	THR
1	D	91	ASN
1	D	92	ARG
1	D	128	LEU
1	D	136	THR
1	D	142	SER
1	D	146	SER
1	E	0	HIS
1	E	23	LEU
1	E	39	GLN
1	E	44	VAL
1	E	63	PRO
1	E	89	THR
1	E	90	ARG
1	E	91	ASN
1	E	113	ARG
1	E	114	VAL
1	E	128	LEU
1	E	129	ILE
1	E	136	THR
1	E	146	SER
1	F	-1	SER
1	F	4	ILE
1	F	23	LEU
1	F	39	GLN
1	F	49	SER

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Mol	Chain	Res	Type
1	F	92	ARG
1	F	111	THR
1	F	112	ARG
1	F	114	VAL
1	F	115	ASP
1	F	116	ASP
1	F	128	LEU
1	F	136	THR
1	G	-1	SER
1	G	3	SER
1	G	4	ILE
1	G	5	THR
1	G	23	LEU
1	G	39	GLN
1	G	44	VAL
1	G	63	PRO
1	G	89	THR
1	G	92	ARG
1	G	93	ILE
1	G	112	ARG
1	G	113	ARG
1	G	128	LEU
1	G	136	THR
1	G	146	SER
1	G	153	THR
1	H	0	HIS
1	H	3	SER
1	H	6	THR
1	H	22	GLU
1	H	23	LEU
1	H	26	LEU
1	H	39	GLN
1	H	49	SER
1	H	63	PRO
1	H	92	ARG
1	H	106	GLU
1	H	107	THR
1	H	112	ARG
1	H	113	ARG
1	H	128	LEU
1	H	136	THR
1	H	146	SER

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Mol	Chain	Res	Type
1	H	153	THR
1	H	154	SER
1	I	0	HIS
1	I	1	SER
1	I	4	ILE
1	I	23	LEU
1	I	26	LEU
1	I	44	VAL
1	I	49	SER
1	I	90	ARG
1	I	107	THR
1	I	113	ARG
1	I	128	LEU
1	I	136	THR
1	I	147	SER
1	I	153	THR
1	J	15	SER
1	J	23	LEU
1	J	26	LEU
1	J	39	GLN
1	J	89	THR
1	J	92	ARG
1	J	108	LEU
1	J	128	LEU
1	J	146	SER
1	J	154	SER
1	K	0	HIS
1	K	3	SER
1	K	4	ILE
1	K	15	SER
1	K	22	GLU
1	K	23	LEU
1	K	39	GLN
1	K	42	THR
1	K	44	VAL
1	K	64	ASP
1	K	92	ARG
1	K	128	LEU
1	K	136	THR
1	K	146	SER
1	L	0	HIS
1	L	3	SER

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Mol	Chain	Res	Type
1	L	23	LEU
1	L	39	GLN
1	L	44	VAL
1	L	49	SER
1	L	64	ASP
1	L	128	LEU
1	L	136	THR
1	L	153	THR
1	L	154	SER
1	M	0	HIS
1	M	4	ILE
1	M	6	THR
1	M	23	LEU
1	M	26	LEU
1	M	39	GLN
1	M	44	VAL
1	M	92	ARG
1	M	115	ASP
1	M	128	LEU
1	M	136	THR
1	M	154	SER
1	N	0	HIS
1	N	23	LEU
1	N	26	LEU
1	N	89	THR
1	N	92	ARG
1	N	107	THR
1	N	112	ARG
1	N	128	LEU
1	N	136	THR
1	N	142	SER
1	N	153	THR
1	O	0	HIS
1	O	3	SER
1	O	6	THR
1	O	23	LEU
1	O	44	VAL
1	O	49	SER
1	O	89	THR
1	O	111	THR
1	O	128	LEU
1	O	153	THR

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Mol	Chain	Res	Type
1	P	22	GLU
1	P	23	LEU
1	P	44	VAL
1	P	92	ARG
1	P	103	THR
1	P	104	THR
1	P	112	ARG
1	P	113	ARG
1	P	128	LEU
1	P	146	SER
1	Q	0	HIS
1	Q	3	SER
1	Q	23	LEU
1	Q	26	LEU
1	Q	44	VAL
1	Q	50	GLU
1	Q	89	THR
1	Q	91	ASN
1	Q	92	ARG
1	Q	112	ARG
1	Q	128	LEU
1	Q	146	SER
1	Q	153	THR
1	R	-1	SER
1	R	0	HIS
1	R	6	THR
1	R	22	GLU
1	R	23	LEU
1	R	39	GLN
1	R	44	VAL
1	R	89	THR
1	R	114	VAL
1	R	118	THR
1	R	123	SER
1	R	128	LEU
1	R	136	THR
1	R	153	THR
1	R	154	SER
1	S	6	THR
1	S	15	SER
1	S	23	LEU
1	S	39	GLN

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Mol	Chain	Res	Type
1	S	128	LEU
1	S	136	THR
1	S	153	THR
1	S	154	SER
1	T	0	HIS
1	T	6	THR
1	T	23	LEU
1	T	39	GLN
1	T	46	ARG
1	T	53	LYS
1	T	64	ASP
1	T	89	THR
1	T	90	ARG
1	T	118	THR
1	T	123	SER
1	T	128	LEU
1	T	134	ARG
1	T	136	THR
1	T	153	THR
1	U	23	LEU
1	U	39	GLN
1	U	44	VAL
1	U	57	GLN
1	U	114	VAL
1	U	128	LEU
1	U	146	SER
1	U	153	THR
1	U	154	SER
1	V	23	LEU
1	V	26	LEU
1	V	36	GLN
1	V	39	GLN
1	V	44	VAL
1	V	63	PRO
1	V	119	VAL
1	V	128	LEU
1	V	142	SER
1	W	0	HIS
1	W	3	SER
1	W	23	LEU
1	W	39	GLN
1	W	90	ARG

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Mol	Chain	Res	Type
1	W	116	ASP
1	W	128	LEU
1	W	136	THR
1	W	147	SER
1	X	22	GLU
1	X	23	LEU
1	X	37	THR
1	X	39	GLN
1	X	49	SER
1	X	89	THR
1	X	128	LEU
1	X	146	SER
1	Y	0	HIS
1	Y	6	THR
1	Y	23	LEU
1	Y	26	LEU
1	Y	39	GLN
1	Y	64	ASP
1	Y	115	ASP
1	Y	123	SER
1	Y	128	LEU
1	Y	143	SER
1	Y	146	SER
1	Y	147	SER
1	Y	153	THR
1	Y	154	SER
1	Z	3	SER
1	Z	23	LEU
1	Z	26	LEU
1	Z	39	GLN
1	Z	44	VAL
1	Z	50	GLU
1	Z	65	SER
1	Z	89	THR
1	Z	91	ASN
1	Z	114	VAL
1	Z	128	LEU
1	Z	134	ARG
1	Z	136	THR
1	Z	146	SER
1	a	0	HIS
1	a	6	THR

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Mol	Chain	Res	Type
1	a	15	SER
1	a	23	LEU
1	a	26	LEU
1	a	39	GLN
1	a	44	VAL
1	a	50	GLU
1	a	76	LEU
1	a	116	ASP
1	a	128	LEU
1	b	-1	SER
1	b	0	HIS
1	b	14	SER
1	b	23	LEU
1	b	39	GLN
1	b	44	VAL
1	b	49	SER
1	b	59	THR
1	b	115	ASP
1	b	128	LEU
1	b	146	SER
1	c	3	SER
1	c	6	THR
1	c	23	LEU
1	c	39	GLN
1	c	88	ASP
1	c	113	ARG
1	c	115	ASP
1	c	128	LEU
1	c	136	THR
1	c	154	SER
1	d	0	HIS
1	d	3	SER
1	d	23	LEU
1	d	39	GLN
1	d	42	THR
1	d	44	VAL
1	d	49	SER
1	d	57	GLN
1	d	59	THR
1	d	89	THR
1	d	90	ARG
1	d	115	ASP

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Mol	Chain	Res	Type
1	d	123	SER
1	d	128	LEU
1	d	136	THR
1	d	142	SER
1	d	153	THR
1	e	0	HIS
1	e	6	THR
1	e	23	LEU
1	e	89	THR
1	e	115	ASP
1	e	128	LEU
1	e	134	ARG
1	e	136	THR
1	e	146	SER
1	e	153	THR
1	f	3	SER
1	f	4	ILE
1	f	23	LEU
1	f	26	LEU
1	f	39	GLN
1	f	88	ASP
1	f	89	THR
1	f	115	ASP
1	f	128	LEU
1	f	136	THR
1	f	146	SER
1	f	153	THR
1	h	-1	SER
1	h	1	SER
1	h	6	THR
1	h	23	LEU
1	h	26	LEU
1	h	59	THR
1	h	88	ASP
1	h	89	THR
1	h	116	ASP
1	h	118	THR
1	h	128	LEU
1	h	136	THR
1	h	146	SER
1	h	147	SER
1	i	0	HIS

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Mol	Chain	Res	Type
1	i	23	LEU
1	i	39	GLN
1	i	44	VAL
1	i	89	THR
1	i	90	ARG
1	i	115	ASP
1	i	128	LEU
1	i	153	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	36	GLN
1	A	38	GLN
1	A	91	ASN
1	A	126	ASN
1	B	34	GLN
1	B	38	GLN
1	B	91	ASN
1	B	126	ASN
1	C	34	GLN
1	C	38	GLN
1	D	38	GLN
1	D	57	GLN
1	D	91	ASN
1	D	126	ASN
1	E	34	GLN
1	E	38	GLN
1	E	126	ASN
1	F	36	GLN
1	F	38	GLN
1	F	91	ASN
1	F	126	ASN
1	G	34	GLN
1	G	38	GLN
1	G	57	GLN
1	G	91	ASN
1	G	126	ASN
1	H	0	HIS
1	H	38	GLN
1	H	57	GLN

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Mol	Chain	Res	Type
1	H	126	ASN
1	I	34	GLN
1	I	38	GLN
1	I	91	ASN
1	I	126	ASN
1	J	34	GLN
1	J	36	GLN
1	J	38	GLN
1	J	57	GLN
1	J	126	ASN
1	K	34	GLN
1	K	38	GLN
1	K	57	GLN
1	K	91	ASN
1	K	126	ASN
1	L	0	HIS
1	L	34	GLN
1	L	36	GLN
1	L	126	ASN
1	M	38	GLN
1	M	91	ASN
1	M	126	ASN
1	N	34	GLN
1	N	38	GLN
1	N	57	GLN
1	N	91	ASN
1	N	126	ASN
1	O	25	ASN
1	O	91	ASN
1	O	126	ASN
1	P	36	GLN
1	P	38	GLN
1	P	91	ASN
1	P	126	ASN
1	Q	34	GLN
1	Q	38	GLN
1	Q	91	ASN
1	Q	126	ASN
1	R	36	GLN
1	R	38	GLN
1	R	126	ASN
1	S	34	GLN

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Mol	Chain	Res	Type
1	S	38	GLN
1	S	126	ASN
1	T	34	GLN
1	T	38	GLN
1	U	34	GLN
1	U	38	GLN
1	U	39	GLN
1	U	57	GLN
1	U	126	ASN
1	V	0	HIS
1	V	36	GLN
1	V	38	GLN
1	V	57	GLN
1	V	126	ASN
1	W	38	GLN
1	W	39	GLN
1	W	57	GLN
1	W	91	ASN
1	W	126	ASN
1	X	0	HIS
1	X	38	GLN
1	X	126	ASN
1	Y	0	HIS
1	Y	34	GLN
1	Y	39	GLN
1	Y	126	ASN
1	Z	34	GLN
1	Z	38	GLN
1	Z	91	ASN
1	Z	126	ASN
1	a	34	GLN
1	a	38	GLN
1	a	39	GLN
1	a	57	GLN
1	b	34	GLN
1	b	38	GLN
1	b	126	ASN
1	c	38	GLN
1	c	91	ASN
1	c	126	ASN
1	d	34	GLN
1	d	38	GLN

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Mol	Chain	Res	Type
1	d	91	ASN
1	d	126	ASN
1	e	34	GLN
1	e	38	GLN
1	e	91	ASN
1	e	126	ASN
1	f	0	HIS
1	f	34	GLN
1	f	38	GLN
1	f	91	ASN
1	f	126	ASN
1	h	0	HIS
1	h	34	GLN
1	h	38	GLN
1	h	91	ASN
1	h	126	ASN
1	i	34	GLN
1	i	38	GLN
1	i	47	GLN
1	i	57	GLN
1	i	91	ASN
1	i	126	ASN

### 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 carbohydrates 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	142/174 (81%)	-0.27	6 (4%) 40 18	35, 41, 84, 113	0
1	B	139/174 (79%)	-0.35	4 (2%) 55 29	34, 41, 76, 107	0
1	C	144/174 (82%)	-0.16	10 (6%) 20 7	33, 41, 105, 128	0
1	D	143/174 (82%)	-0.21	10 (6%) 19 7	31, 40, 87, 111	0
1	E	140/174 (80%)	-0.28	5 (3%) 46 21	33, 40, 80, 108	0
1	F	143/174 (82%)	-0.18	9 (6%) 23 9	35, 44, 92, 121	0
1	G	143/174 (82%)	-0.18	10 (6%) 19 7	36, 42, 101, 117	0
1	H	144/174 (82%)	-0.22	7 (4%) 33 14	35, 45, 93, 116	0
1	I	141/174 (81%)	-0.31	7 (4%) 32 13	35, 44, 88, 114	0
1	J	145/174 (83%)	-0.13	10 (6%) 20 7	34, 44, 105, 124	0
1	K	143/174 (82%)	-0.20	9 (6%) 23 9	32, 40, 90, 116	0
1	L	141/174 (81%)	-0.24	6 (4%) 39 17	35, 43, 84, 112	0
1	M	142/174 (81%)	-0.28	7 (4%) 33 14	34, 43, 90, 112	0
1	N	142/174 (81%)	-0.22	6 (4%) 40 18	35, 44, 88, 106	0
1	O	140/174 (80%)	-0.31	4 (2%) 55 29	37, 45, 79, 107	0
1	P	147/174 (84%)	-0.11	12 (8%) 14 5	36, 45, 114, 130	0
1	Q	146/174 (83%)	-0.14	11 (7%) 17 6	36, 44, 110, 129	0
1	R	133/174 (76%)	-0.45	3 (2%) 64 38	32, 40, 65, 86	0
1	S	133/174 (76%)	-0.46	3 (2%) 64 38	33, 42, 63, 87	0
1	T	132/174 (75%)	-0.35	2 (1%) 76 55	36, 44, 62, 83	0
1	U	133/174 (76%)	-0.33	2 (1%) 76 55	36, 47, 69, 89	0
1	V	134/174 (77%)	-0.38	4 (2%) 54 27	29, 40, 65, 86	0
1	W	134/174 (77%)	-0.36	3 (2%) 65 40	35, 42, 67, 88	0
1	X	131/174 (75%)	-0.39	2 (1%) 76 55	36, 44, 59, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	132/174 (75%)	-0.39	3 (2%) 64 38	33, 43, 61, 85	0
1	Z	134/174 (77%)	-0.44	3 (2%) 65 40	34, 42, 69, 87	0
1	a	131/174 (75%)	-0.37	2 (1%) 76 55	37, 47, 64, 89	0
1	b	132/174 (75%)	-0.37	4 (3%) 54 27	37, 47, 67, 83	0
1	c	136/174 (78%)	-0.34	4 (2%) 55 29	36, 45, 76, 95	0
1	d	134/174 (77%)	-0.43	3 (2%) 65 40	30, 41, 68, 85	0
1	e	134/174 (77%)	-0.32	4 (2%) 54 27	37, 46, 68, 88	0
1	f	134/174 (77%)	-0.44	3 (2%) 65 40	30, 41, 65, 84	0
1	h	134/174 (77%)	-0.42	4 (2%) 54 27	35, 45, 69, 89	0
1	i	134/174 (77%)	-0.31	3 (2%) 65 40	34, 43, 68, 86	0
All	All	4690/5916 (79%)	-0.30	185 (3%) 43 20	29, 43, 82, 130	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	109	ASP	7.7
1	L	107	THR	7.6
1	Q	104	THR	7.0
1	A	107	THR	6.7
1	N	107	THR	6.5
1	G	109	ASP	6.0
1	Q	109	ASP	6.0
1	I	107	THR	5.9
1	C	104	THR	5.9
1	D	107	THR	5.7
1	M	107	THR	5.7
1	F	107	THR	5.6
1	J	106	GLU	5.6
1	E	109	ASP	5.4
1	Q	103	THR	5.3
1	L	109	ASP	5.2
1	V	91	ASN	5.2
1	J	109	ASP	5.1
1	J	107	THR	5.0
1	A	111	THR	5.0
1	P	106	GLU	4.8
1	Z	91	ASN	4.8
1	P	102	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	P	105	ALA	4.7
1	K	107	THR	4.7
1	P	109	ASP	4.6
1	Q	107	THR	4.6
1	E	110	ALA	4.6
1	H	107	THR	4.6
1	P	104	THR	4.6
1	Q	110	ALA	4.5
1	M	109	ASP	4.5
1	C	109	ASP	4.4
1	A	109	ASP	4.4
1	C	107	THR	4.4
1	F	106	GLU	4.4
1	T	90	ARG	4.3
1	K	109	ASP	4.3
1	G	92	ARG	4.3
1	M	92	ARG	4.2
1	I	109	ASP	4.1
1	N	92	ARG	4.1
1	L	91	ASN	4.1
1	P	107	THR	4.1
1	X	115	ASP	4.1
1	B	109	ASP	3.9
1	Q	91	ASN	3.9
1	D	109	ASP	3.9
1	P	110	ALA	3.9
1	G	94	ILE	3.9
1	F	92	ARG	3.9
1	N	91	ASN	3.9
1	Q	106	GLU	3.8
1	B	111	THR	3.8
1	H	109	ASP	3.8
1	P	103	THR	3.8
1	J	105	ALA	3.8
1	A	110	ALA	3.7
1	G	111	THR	3.6
1	C	111	THR	3.6
1	h	91	ASN	3.6
1	G	110	ALA	3.6
1	E	111	THR	3.6
1	P	91	ASN	3.6
1	H	92	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	108	LEU	3.5
1	D	92	ARG	3.5
1	e	90	ARG	3.5
1	C	105	ALA	3.4
1	N	109	ASP	3.4
1	A	91	ASN	3.4
1	Q	111	THR	3.4
1	F	110	ALA	3.4
1	Q	92	ARG	3.4
1	c	91	ASN	3.4
1	R	115	ASP	3.3
1	C	91	ASN	3.3
1	K	108	LEU	3.3
1	K	106	GLU	3.3
1	O	91	ASN	3.3
1	f	91	ASN	3.2
1	V	90	ARG	3.2
1	F	109	ASP	3.2
1	J	92	ARG	3.2
1	I	108	LEU	3.2
1	A	108	LEU	3.1
1	G	93	ILE	3.1
1	H	110	ALA	3.1
1	L	111	THR	3.1
1	P	92	ARG	3.1
1	f	90	ARG	3.1
1	c	115	ASP	3.1
1	J	91	ASN	3.0
1	Q	105	ALA	3.0
1	d	91	ASN	3.0
1	M	108	LEU	3.0
1	D	91	ASN	3.0
1	i	91	ASN	3.0
1	F	111	THR	3.0
1	R	90	ARG	2.9
1	K	110	ALA	2.9
1	J	104	THR	2.9
1	d	114	VAL	2.9
1	N	110	ALA	2.9
1	K	92	ARG	2.9
1	L	108	LEU	2.9
1	O	111	THR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	W	91	ASN	2.9
1	I	91	ASN	2.9
1	b	114	VAL	2.9
1	h	115	ASP	2.9
1	J	108	LEU	2.9
1	P	111	THR	2.9
1	B	91	ASN	2.8
1	I	110	ALA	2.8
1	M	91	ASN	2.8
1	Y	114	VAL	2.8
1	U	90	ARG	2.8
1	Z	90	ARG	2.8
1	B	110	ALA	2.8
1	O	110	ALA	2.8
1	i	115	ASP	2.7
1	E	91	ASN	2.7
1	C	106	GLU	2.7
1	c	90	ARG	2.7
1	H	91	ASN	2.7
1	H	106	GLU	2.7
1	W	115	ASP	2.7
1	I	111	THR	2.7
1	a	114	VAL	2.7
1	D	110	ALA	2.7
1	S	114	VAL	2.6
1	S	90	ARG	2.6
1	C	110	ALA	2.6
1	Z	115	ASP	2.6
1	R	114	VAL	2.6
1	K	91	ASN	2.5
1	d	90	ARG	2.5
1	a	115	ASP	2.5
1	J	110	ALA	2.5
1	M	110	ALA	2.5
1	e	91	ASN	2.5
1	h	90	ARG	2.5
1	S	115	ASP	2.5
1	e	-1	SER	2.4
1	J	111	THR	2.4
1	W	114	VAL	2.4
1	F	108	LEU	2.4
1	T	115	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	115	ASP	2.4
1	f	114	VAL	2.4
1	L	110	ALA	2.4
1	i	116	ASP	2.3
1	G	91	ASN	2.3
1	c	-2	GLY	2.3
1	D	111	THR	2.3
1	P	108	LEU	2.3
1	G	0	HIS	2.3
1	M	111	THR	2.3
1	H	108	LEU	2.3
1	F	91	ASN	2.2
1	h	114	VAL	2.2
1	N	111	THR	2.2
1	E	113	ARG	2.2
1	G	112	ARG	2.2
1	C	108	LEU	2.2
1	V	115	ASP	2.2
1	C	0	HIS	2.2
1	I	90	ARG	2.2
1	Y	-1	SER	2.2
1	D	113	ARG	2.1
1	V	114	VAL	2.1
1	e	114	VAL	2.1
1	b	115	ASP	2.1
1	K	0	HIS	2.1
1	D	108	LEU	2.1
1	X	-1	SER	2.1
1	D	90	ARG	2.1
1	b	36	GLN	2.1
1	K	154	SER	2.0
1	Q	90	ARG	2.0
1	Y	115	ASP	2.0
1	F	90	ARG	2.0
1	b	-1	SER	2.0
1	D	-1	SER	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.