



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2026 – 10:59 PM JST

PDB ID : 9UE8 / pdb_00009ue8
Title : Crystal structure of MPXV A35R in complex with a neutralizing antibody BA345
Authors : Sun, D.; Zhang, N.; Guo, Y.
Deposited on : 2025-04-08
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.48.1

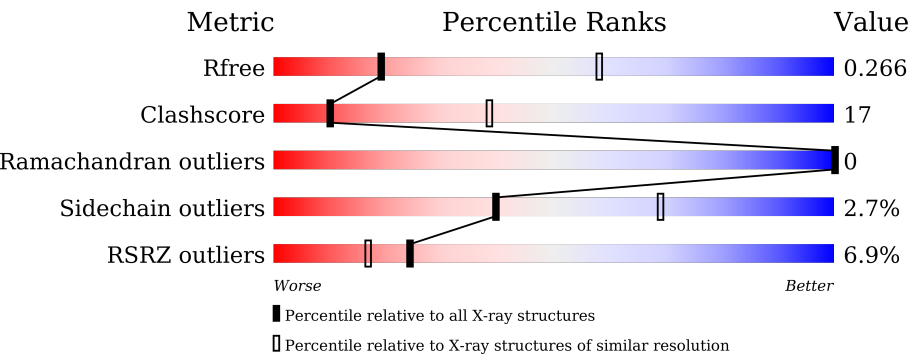
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	221	<div><div>3%</div><div>59%</div><div>39%</div><div>.</div></div>
1	E	221	<div><div>7%</div><div>73%</div><div>24%</div><div>.</div></div>
1	I	221	<div><div>5%</div><div>59%</div><div>41%</div><div>.</div></div>
1	M	221	<div><div>4%</div><div>65%</div><div>31%</div><div>.</div></div>
1	Q	221	<div><div>4%</div><div>71%</div><div>28%</div><div>.</div></div>
1	U	221	<div><div>10%</div><div>62%</div><div>38%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	B	215	
2	F	215	
2	J	215	
2	N	215	
2	R	215	
2	V	215	
3	C	152	
3	D	152	
3	G	152	
3	H	152	
3	K	152	
3	L	152	
3	O	152	
3	P	152	
3	S	152	
3	T	152	
3	W	152	
3	X	152	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27654 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 345 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			
1	E	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			
1	I	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			
1	M	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			
1	Q	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			
1	U	221	Total	C	N	O	S	0	0	0
			1632	1030	274	323	5			

- Molecule 2 is a protein called 345 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			
2	F	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			
2	J	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			
2	N	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			
2	R	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			
2	V	215	Total	C	N	O	S	0	0	0
			1649	1028	282	334	5			

- Molecule 3 is a protein called Protein OPG161.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	D	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	G	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	H	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	K	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	L	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	O	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	P	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	S	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	T	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	W	84	Total 664	C 412	N 103	O 145	S 4	0	0	0
3	X	84	Total 664	C 412	N 103	O 145	S 4	0	0	0

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	85	GLY	-	expression tag	UNP A0A7H0DND2
C	86	SER	-	expression tag	UNP A0A7H0DND2
C	87	GLY	-	expression tag	UNP A0A7H0DND2
C	88	LEU	-	expression tag	UNP A0A7H0DND2
C	89	ASN	-	expression tag	UNP A0A7H0DND2
C	90	ASP	-	expression tag	UNP A0A7H0DND2
C	91	ILE	-	expression tag	UNP A0A7H0DND2
C	92	PHE	-	expression tag	UNP A0A7H0DND2
C	93	GLU	-	expression tag	UNP A0A7H0DND2
C	94	ALA	-	expression tag	UNP A0A7H0DND2
C	95	GLN	-	expression tag	UNP A0A7H0DND2
C	96	LYS	-	expression tag	UNP A0A7H0DND2
C	97	ILE	-	expression tag	UNP A0A7H0DND2
C	98	GLU	-	expression tag	UNP A0A7H0DND2
C	99	TRP	-	expression tag	UNP A0A7H0DND2
C	100	HIS	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	101	GLU	-	expression tag	UNP A0A7H0DND2
C	102	ALA	-	expression tag	UNP A0A7H0DND2
C	103	ALA	-	expression tag	UNP A0A7H0DND2
C	104	ALA	-	expression tag	UNP A0A7H0DND2
C	105	HIS	-	expression tag	UNP A0A7H0DND2
C	106	HIS	-	expression tag	UNP A0A7H0DND2
C	107	HIS	-	expression tag	UNP A0A7H0DND2
C	108	HIS	-	expression tag	UNP A0A7H0DND2
C	109	HIS	-	expression tag	UNP A0A7H0DND2
C	110	HIS	-	expression tag	UNP A0A7H0DND2
C	111	HIS	-	expression tag	UNP A0A7H0DND2
C	112	HIS	-	expression tag	UNP A0A7H0DND2
D	85	GLY	-	expression tag	UNP A0A7H0DND2
D	86	SER	-	expression tag	UNP A0A7H0DND2
D	87	GLY	-	expression tag	UNP A0A7H0DND2
D	88	LEU	-	expression tag	UNP A0A7H0DND2
D	89	ASN	-	expression tag	UNP A0A7H0DND2
D	90	ASP	-	expression tag	UNP A0A7H0DND2
D	91	ILE	-	expression tag	UNP A0A7H0DND2
D	92	PHE	-	expression tag	UNP A0A7H0DND2
D	93	GLU	-	expression tag	UNP A0A7H0DND2
D	94	ALA	-	expression tag	UNP A0A7H0DND2
D	95	GLN	-	expression tag	UNP A0A7H0DND2
D	96	LYS	-	expression tag	UNP A0A7H0DND2
D	97	ILE	-	expression tag	UNP A0A7H0DND2
D	98	GLU	-	expression tag	UNP A0A7H0DND2
D	99	TRP	-	expression tag	UNP A0A7H0DND2
D	100	HIS	-	expression tag	UNP A0A7H0DND2
D	101	GLU	-	expression tag	UNP A0A7H0DND2
D	102	ALA	-	expression tag	UNP A0A7H0DND2
D	103	ALA	-	expression tag	UNP A0A7H0DND2
D	104	ALA	-	expression tag	UNP A0A7H0DND2
D	105	HIS	-	expression tag	UNP A0A7H0DND2
D	106	HIS	-	expression tag	UNP A0A7H0DND2
D	107	HIS	-	expression tag	UNP A0A7H0DND2
D	108	HIS	-	expression tag	UNP A0A7H0DND2
D	109	HIS	-	expression tag	UNP A0A7H0DND2
D	110	HIS	-	expression tag	UNP A0A7H0DND2
D	111	HIS	-	expression tag	UNP A0A7H0DND2
D	112	HIS	-	expression tag	UNP A0A7H0DND2
G	85	GLY	-	expression tag	UNP A0A7H0DND2
G	86	SER	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	87	GLY	-	expression tag	UNP A0A7H0DND2
G	88	LEU	-	expression tag	UNP A0A7H0DND2
G	89	ASN	-	expression tag	UNP A0A7H0DND2
G	90	ASP	-	expression tag	UNP A0A7H0DND2
G	91	ILE	-	expression tag	UNP A0A7H0DND2
G	92	PHE	-	expression tag	UNP A0A7H0DND2
G	93	GLU	-	expression tag	UNP A0A7H0DND2
G	94	ALA	-	expression tag	UNP A0A7H0DND2
G	95	GLN	-	expression tag	UNP A0A7H0DND2
G	96	LYS	-	expression tag	UNP A0A7H0DND2
G	97	ILE	-	expression tag	UNP A0A7H0DND2
G	98	GLU	-	expression tag	UNP A0A7H0DND2
G	99	TRP	-	expression tag	UNP A0A7H0DND2
G	100	HIS	-	expression tag	UNP A0A7H0DND2
G	101	GLU	-	expression tag	UNP A0A7H0DND2
G	102	ALA	-	expression tag	UNP A0A7H0DND2
G	103	ALA	-	expression tag	UNP A0A7H0DND2
G	104	ALA	-	expression tag	UNP A0A7H0DND2
G	105	HIS	-	expression tag	UNP A0A7H0DND2
G	106	HIS	-	expression tag	UNP A0A7H0DND2
G	107	HIS	-	expression tag	UNP A0A7H0DND2
G	108	HIS	-	expression tag	UNP A0A7H0DND2
G	109	HIS	-	expression tag	UNP A0A7H0DND2
G	110	HIS	-	expression tag	UNP A0A7H0DND2
G	111	HIS	-	expression tag	UNP A0A7H0DND2
G	112	HIS	-	expression tag	UNP A0A7H0DND2
H	85	GLY	-	expression tag	UNP A0A7H0DND2
H	86	SER	-	expression tag	UNP A0A7H0DND2
H	87	GLY	-	expression tag	UNP A0A7H0DND2
H	88	LEU	-	expression tag	UNP A0A7H0DND2
H	89	ASN	-	expression tag	UNP A0A7H0DND2
H	90	ASP	-	expression tag	UNP A0A7H0DND2
H	91	ILE	-	expression tag	UNP A0A7H0DND2
H	92	PHE	-	expression tag	UNP A0A7H0DND2
H	93	GLU	-	expression tag	UNP A0A7H0DND2
H	94	ALA	-	expression tag	UNP A0A7H0DND2
H	95	GLN	-	expression tag	UNP A0A7H0DND2
H	96	LYS	-	expression tag	UNP A0A7H0DND2
H	97	ILE	-	expression tag	UNP A0A7H0DND2
H	98	GLU	-	expression tag	UNP A0A7H0DND2
H	99	TRP	-	expression tag	UNP A0A7H0DND2
H	100	HIS	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	101	GLU	-	expression tag	UNP A0A7H0DND2
H	102	ALA	-	expression tag	UNP A0A7H0DND2
H	103	ALA	-	expression tag	UNP A0A7H0DND2
H	104	ALA	-	expression tag	UNP A0A7H0DND2
H	105	HIS	-	expression tag	UNP A0A7H0DND2
H	106	HIS	-	expression tag	UNP A0A7H0DND2
H	107	HIS	-	expression tag	UNP A0A7H0DND2
H	108	HIS	-	expression tag	UNP A0A7H0DND2
H	109	HIS	-	expression tag	UNP A0A7H0DND2
H	110	HIS	-	expression tag	UNP A0A7H0DND2
H	111	HIS	-	expression tag	UNP A0A7H0DND2
H	112	HIS	-	expression tag	UNP A0A7H0DND2
K	85	GLY	-	expression tag	UNP A0A7H0DND2
K	86	SER	-	expression tag	UNP A0A7H0DND2
K	87	GLY	-	expression tag	UNP A0A7H0DND2
K	88	LEU	-	expression tag	UNP A0A7H0DND2
K	89	ASN	-	expression tag	UNP A0A7H0DND2
K	90	ASP	-	expression tag	UNP A0A7H0DND2
K	91	ILE	-	expression tag	UNP A0A7H0DND2
K	92	PHE	-	expression tag	UNP A0A7H0DND2
K	93	GLU	-	expression tag	UNP A0A7H0DND2
K	94	ALA	-	expression tag	UNP A0A7H0DND2
K	95	GLN	-	expression tag	UNP A0A7H0DND2
K	96	LYS	-	expression tag	UNP A0A7H0DND2
K	97	ILE	-	expression tag	UNP A0A7H0DND2
K	98	GLU	-	expression tag	UNP A0A7H0DND2
K	99	TRP	-	expression tag	UNP A0A7H0DND2
K	100	HIS	-	expression tag	UNP A0A7H0DND2
K	101	GLU	-	expression tag	UNP A0A7H0DND2
K	102	ALA	-	expression tag	UNP A0A7H0DND2
K	103	ALA	-	expression tag	UNP A0A7H0DND2
K	104	ALA	-	expression tag	UNP A0A7H0DND2
K	105	HIS	-	expression tag	UNP A0A7H0DND2
K	106	HIS	-	expression tag	UNP A0A7H0DND2
K	107	HIS	-	expression tag	UNP A0A7H0DND2
K	108	HIS	-	expression tag	UNP A0A7H0DND2
K	109	HIS	-	expression tag	UNP A0A7H0DND2
K	110	HIS	-	expression tag	UNP A0A7H0DND2
K	111	HIS	-	expression tag	UNP A0A7H0DND2
K	112	HIS	-	expression tag	UNP A0A7H0DND2
L	85	GLY	-	expression tag	UNP A0A7H0DND2
L	86	SER	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	87	GLY	-	expression tag	UNP A0A7H0DND2
L	88	LEU	-	expression tag	UNP A0A7H0DND2
L	89	ASN	-	expression tag	UNP A0A7H0DND2
L	90	ASP	-	expression tag	UNP A0A7H0DND2
L	91	ILE	-	expression tag	UNP A0A7H0DND2
L	92	PHE	-	expression tag	UNP A0A7H0DND2
L	93	GLU	-	expression tag	UNP A0A7H0DND2
L	94	ALA	-	expression tag	UNP A0A7H0DND2
L	95	GLN	-	expression tag	UNP A0A7H0DND2
L	96	LYS	-	expression tag	UNP A0A7H0DND2
L	97	ILE	-	expression tag	UNP A0A7H0DND2
L	98	GLU	-	expression tag	UNP A0A7H0DND2
L	99	TRP	-	expression tag	UNP A0A7H0DND2
L	100	HIS	-	expression tag	UNP A0A7H0DND2
L	101	GLU	-	expression tag	UNP A0A7H0DND2
L	102	ALA	-	expression tag	UNP A0A7H0DND2
L	103	ALA	-	expression tag	UNP A0A7H0DND2
L	104	ALA	-	expression tag	UNP A0A7H0DND2
L	105	HIS	-	expression tag	UNP A0A7H0DND2
L	106	HIS	-	expression tag	UNP A0A7H0DND2
L	107	HIS	-	expression tag	UNP A0A7H0DND2
L	108	HIS	-	expression tag	UNP A0A7H0DND2
L	109	HIS	-	expression tag	UNP A0A7H0DND2
L	110	HIS	-	expression tag	UNP A0A7H0DND2
L	111	HIS	-	expression tag	UNP A0A7H0DND2
L	112	HIS	-	expression tag	UNP A0A7H0DND2
O	85	GLY	-	expression tag	UNP A0A7H0DND2
O	86	SER	-	expression tag	UNP A0A7H0DND2
O	87	GLY	-	expression tag	UNP A0A7H0DND2
O	88	LEU	-	expression tag	UNP A0A7H0DND2
O	89	ASN	-	expression tag	UNP A0A7H0DND2
O	90	ASP	-	expression tag	UNP A0A7H0DND2
O	91	ILE	-	expression tag	UNP A0A7H0DND2
O	92	PHE	-	expression tag	UNP A0A7H0DND2
O	93	GLU	-	expression tag	UNP A0A7H0DND2
O	94	ALA	-	expression tag	UNP A0A7H0DND2
O	95	GLN	-	expression tag	UNP A0A7H0DND2
O	96	LYS	-	expression tag	UNP A0A7H0DND2
O	97	ILE	-	expression tag	UNP A0A7H0DND2
O	98	GLU	-	expression tag	UNP A0A7H0DND2
O	99	TRP	-	expression tag	UNP A0A7H0DND2
O	100	HIS	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	101	GLU	-	expression tag	UNP A0A7H0DND2
O	102	ALA	-	expression tag	UNP A0A7H0DND2
O	103	ALA	-	expression tag	UNP A0A7H0DND2
O	104	ALA	-	expression tag	UNP A0A7H0DND2
O	105	HIS	-	expression tag	UNP A0A7H0DND2
O	106	HIS	-	expression tag	UNP A0A7H0DND2
O	107	HIS	-	expression tag	UNP A0A7H0DND2
O	108	HIS	-	expression tag	UNP A0A7H0DND2
O	109	HIS	-	expression tag	UNP A0A7H0DND2
O	110	HIS	-	expression tag	UNP A0A7H0DND2
O	111	HIS	-	expression tag	UNP A0A7H0DND2
O	112	HIS	-	expression tag	UNP A0A7H0DND2
P	85	GLY	-	expression tag	UNP A0A7H0DND2
P	86	SER	-	expression tag	UNP A0A7H0DND2
P	87	GLY	-	expression tag	UNP A0A7H0DND2
P	88	LEU	-	expression tag	UNP A0A7H0DND2
P	89	ASN	-	expression tag	UNP A0A7H0DND2
P	90	ASP	-	expression tag	UNP A0A7H0DND2
P	91	ILE	-	expression tag	UNP A0A7H0DND2
P	92	PHE	-	expression tag	UNP A0A7H0DND2
P	93	GLU	-	expression tag	UNP A0A7H0DND2
P	94	ALA	-	expression tag	UNP A0A7H0DND2
P	95	GLN	-	expression tag	UNP A0A7H0DND2
P	96	LYS	-	expression tag	UNP A0A7H0DND2
P	97	ILE	-	expression tag	UNP A0A7H0DND2
P	98	GLU	-	expression tag	UNP A0A7H0DND2
P	99	TRP	-	expression tag	UNP A0A7H0DND2
P	100	HIS	-	expression tag	UNP A0A7H0DND2
P	101	GLU	-	expression tag	UNP A0A7H0DND2
P	102	ALA	-	expression tag	UNP A0A7H0DND2
P	103	ALA	-	expression tag	UNP A0A7H0DND2
P	104	ALA	-	expression tag	UNP A0A7H0DND2
P	105	HIS	-	expression tag	UNP A0A7H0DND2
P	106	HIS	-	expression tag	UNP A0A7H0DND2
P	107	HIS	-	expression tag	UNP A0A7H0DND2
P	108	HIS	-	expression tag	UNP A0A7H0DND2
P	109	HIS	-	expression tag	UNP A0A7H0DND2
P	110	HIS	-	expression tag	UNP A0A7H0DND2
P	111	HIS	-	expression tag	UNP A0A7H0DND2
P	112	HIS	-	expression tag	UNP A0A7H0DND2
S	85	GLY	-	expression tag	UNP A0A7H0DND2
S	86	SER	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	87	GLY	-	expression tag	UNP A0A7H0DND2
S	88	LEU	-	expression tag	UNP A0A7H0DND2
S	89	ASN	-	expression tag	UNP A0A7H0DND2
S	90	ASP	-	expression tag	UNP A0A7H0DND2
S	91	ILE	-	expression tag	UNP A0A7H0DND2
S	92	PHE	-	expression tag	UNP A0A7H0DND2
S	93	GLU	-	expression tag	UNP A0A7H0DND2
S	94	ALA	-	expression tag	UNP A0A7H0DND2
S	95	GLN	-	expression tag	UNP A0A7H0DND2
S	96	LYS	-	expression tag	UNP A0A7H0DND2
S	97	ILE	-	expression tag	UNP A0A7H0DND2
S	98	GLU	-	expression tag	UNP A0A7H0DND2
S	99	TRP	-	expression tag	UNP A0A7H0DND2
S	100	HIS	-	expression tag	UNP A0A7H0DND2
S	101	GLU	-	expression tag	UNP A0A7H0DND2
S	102	ALA	-	expression tag	UNP A0A7H0DND2
S	103	ALA	-	expression tag	UNP A0A7H0DND2
S	104	ALA	-	expression tag	UNP A0A7H0DND2
S	105	HIS	-	expression tag	UNP A0A7H0DND2
S	106	HIS	-	expression tag	UNP A0A7H0DND2
S	107	HIS	-	expression tag	UNP A0A7H0DND2
S	108	HIS	-	expression tag	UNP A0A7H0DND2
S	109	HIS	-	expression tag	UNP A0A7H0DND2
S	110	HIS	-	expression tag	UNP A0A7H0DND2
S	111	HIS	-	expression tag	UNP A0A7H0DND2
S	112	HIS	-	expression tag	UNP A0A7H0DND2
T	85	GLY	-	expression tag	UNP A0A7H0DND2
T	86	SER	-	expression tag	UNP A0A7H0DND2
T	87	GLY	-	expression tag	UNP A0A7H0DND2
T	88	LEU	-	expression tag	UNP A0A7H0DND2
T	89	ASN	-	expression tag	UNP A0A7H0DND2
T	90	ASP	-	expression tag	UNP A0A7H0DND2
T	91	ILE	-	expression tag	UNP A0A7H0DND2
T	92	PHE	-	expression tag	UNP A0A7H0DND2
T	93	GLU	-	expression tag	UNP A0A7H0DND2
T	94	ALA	-	expression tag	UNP A0A7H0DND2
T	95	GLN	-	expression tag	UNP A0A7H0DND2
T	96	LYS	-	expression tag	UNP A0A7H0DND2
T	97	ILE	-	expression tag	UNP A0A7H0DND2
T	98	GLU	-	expression tag	UNP A0A7H0DND2
T	99	TRP	-	expression tag	UNP A0A7H0DND2
T	100	HIS	-	expression tag	UNP A0A7H0DND2

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Chain	Residue	Modelled	Actual	Comment	Reference
T	101	GLU	-	expression tag	UNP A0A7H0DND2
T	102	ALA	-	expression tag	UNP A0A7H0DND2
T	103	ALA	-	expression tag	UNP A0A7H0DND2
T	104	ALA	-	expression tag	UNP A0A7H0DND2
T	105	HIS	-	expression tag	UNP A0A7H0DND2
T	106	HIS	-	expression tag	UNP A0A7H0DND2
T	107	HIS	-	expression tag	UNP A0A7H0DND2
T	108	HIS	-	expression tag	UNP A0A7H0DND2
T	109	HIS	-	expression tag	UNP A0A7H0DND2
T	110	HIS	-	expression tag	UNP A0A7H0DND2
T	111	HIS	-	expression tag	UNP A0A7H0DND2
T	112	HIS	-	expression tag	UNP A0A7H0DND2
W	85	GLY	-	expression tag	UNP A0A7H0DND2
W	86	SER	-	expression tag	UNP A0A7H0DND2
W	87	GLY	-	expression tag	UNP A0A7H0DND2
W	88	LEU	-	expression tag	UNP A0A7H0DND2
W	89	ASN	-	expression tag	UNP A0A7H0DND2
W	90	ASP	-	expression tag	UNP A0A7H0DND2
W	91	ILE	-	expression tag	UNP A0A7H0DND2
W	92	PHE	-	expression tag	UNP A0A7H0DND2
W	93	GLU	-	expression tag	UNP A0A7H0DND2
W	94	ALA	-	expression tag	UNP A0A7H0DND2
W	95	GLN	-	expression tag	UNP A0A7H0DND2
W	96	LYS	-	expression tag	UNP A0A7H0DND2
W	97	ILE	-	expression tag	UNP A0A7H0DND2
W	98	GLU	-	expression tag	UNP A0A7H0DND2
W	99	TRP	-	expression tag	UNP A0A7H0DND2
W	100	HIS	-	expression tag	UNP A0A7H0DND2
W	101	GLU	-	expression tag	UNP A0A7H0DND2
W	102	ALA	-	expression tag	UNP A0A7H0DND2
W	103	ALA	-	expression tag	UNP A0A7H0DND2
W	104	ALA	-	expression tag	UNP A0A7H0DND2
W	105	HIS	-	expression tag	UNP A0A7H0DND2
W	106	HIS	-	expression tag	UNP A0A7H0DND2
W	107	HIS	-	expression tag	UNP A0A7H0DND2
W	108	HIS	-	expression tag	UNP A0A7H0DND2
W	109	HIS	-	expression tag	UNP A0A7H0DND2
W	110	HIS	-	expression tag	UNP A0A7H0DND2
W	111	HIS	-	expression tag	UNP A0A7H0DND2
W	112	HIS	-	expression tag	UNP A0A7H0DND2
X	85	GLY	-	expression tag	UNP A0A7H0DND2
X	86	SER	-	expression tag	UNP A0A7H0DND2

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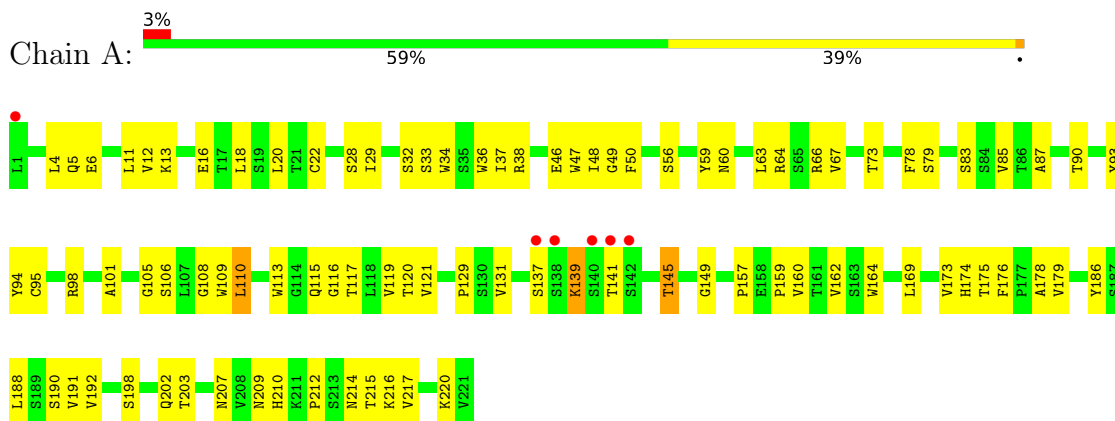
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Chain	Residue	Modelled	Actual	Comment	Reference
X	87	GLY	-	expression tag	UNP A0A7H0DND2
X	88	LEU	-	expression tag	UNP A0A7H0DND2
X	89	ASN	-	expression tag	UNP A0A7H0DND2
X	90	ASP	-	expression tag	UNP A0A7H0DND2
X	91	ILE	-	expression tag	UNP A0A7H0DND2
X	92	PHE	-	expression tag	UNP A0A7H0DND2
X	93	GLU	-	expression tag	UNP A0A7H0DND2
X	94	ALA	-	expression tag	UNP A0A7H0DND2
X	95	GLN	-	expression tag	UNP A0A7H0DND2
X	96	LYS	-	expression tag	UNP A0A7H0DND2
X	97	ILE	-	expression tag	UNP A0A7H0DND2
X	98	GLU	-	expression tag	UNP A0A7H0DND2
X	99	TRP	-	expression tag	UNP A0A7H0DND2
X	100	HIS	-	expression tag	UNP A0A7H0DND2
X	101	GLU	-	expression tag	UNP A0A7H0DND2
X	102	ALA	-	expression tag	UNP A0A7H0DND2
X	103	ALA	-	expression tag	UNP A0A7H0DND2
X	104	ALA	-	expression tag	UNP A0A7H0DND2
X	105	HIS	-	expression tag	UNP A0A7H0DND2
X	106	HIS	-	expression tag	UNP A0A7H0DND2
X	107	HIS	-	expression tag	UNP A0A7H0DND2
X	108	HIS	-	expression tag	UNP A0A7H0DND2
X	109	HIS	-	expression tag	UNP A0A7H0DND2
X	110	HIS	-	expression tag	UNP A0A7H0DND2
X	111	HIS	-	expression tag	UNP A0A7H0DND2
X	112	HIS	-	expression tag	UNP A0A7H0DND2

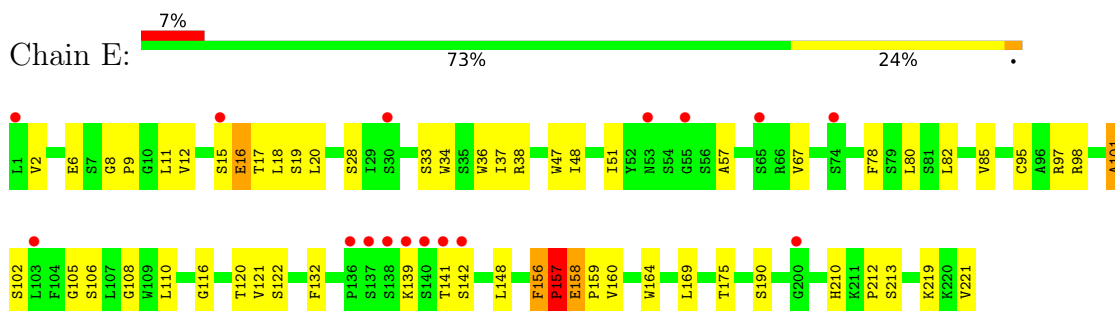
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

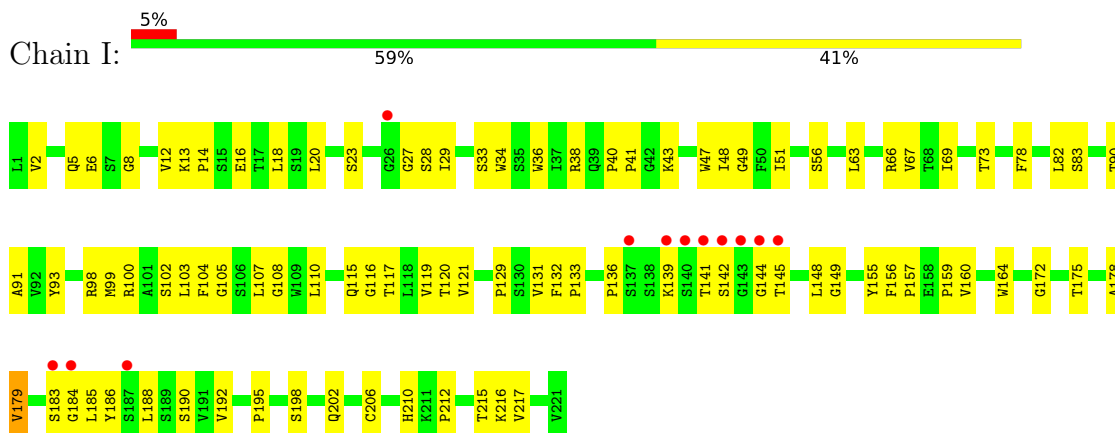
• Molecule 1: 345 Heavy Chain



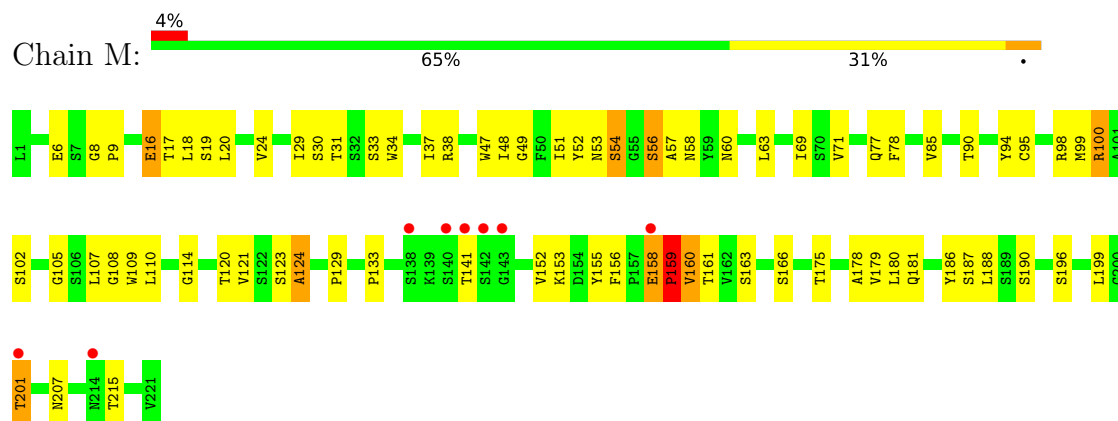
• Molecule 1: 345 Heavy Chain



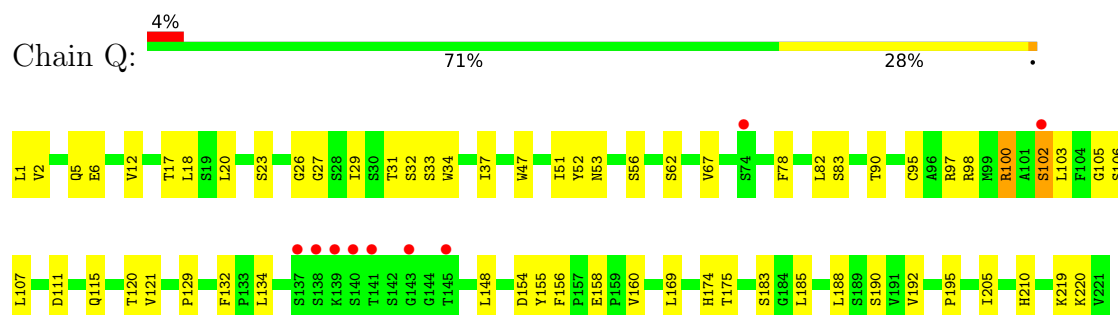
• Molecule 1: 345 Heavy Chain



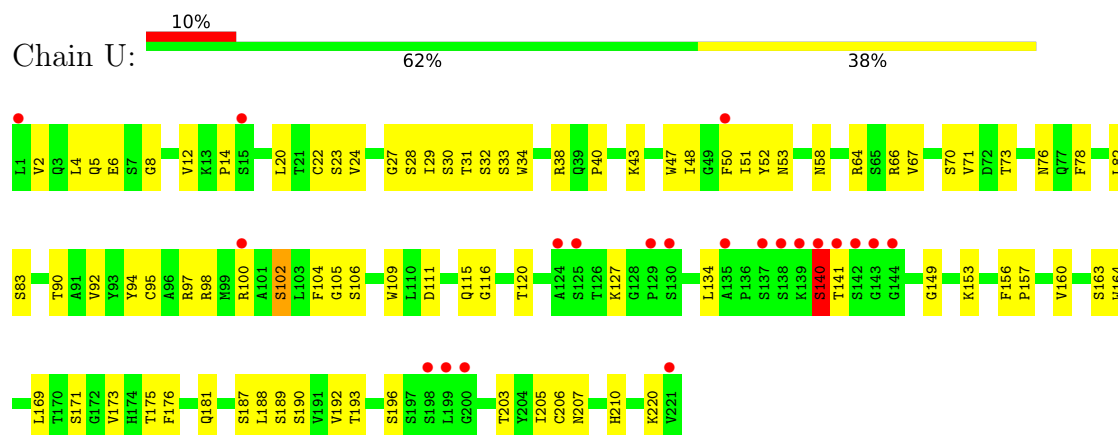
- Molecule 1: 345 Heavy Chain



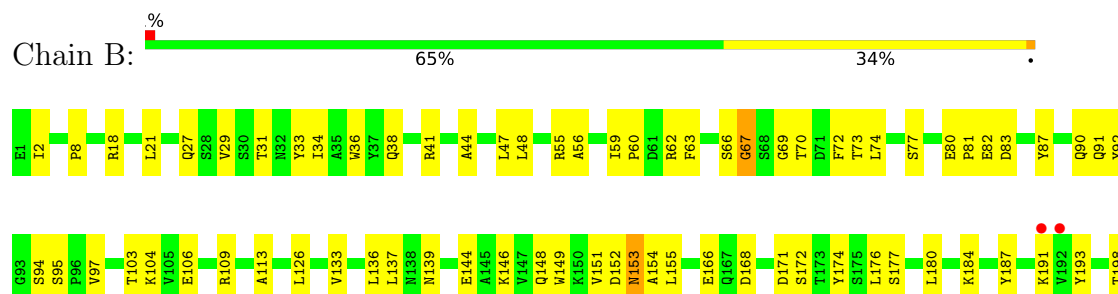
- Molecule 1: 345 Heavy Chain



- Molecule 1: 345 Heavy Chain

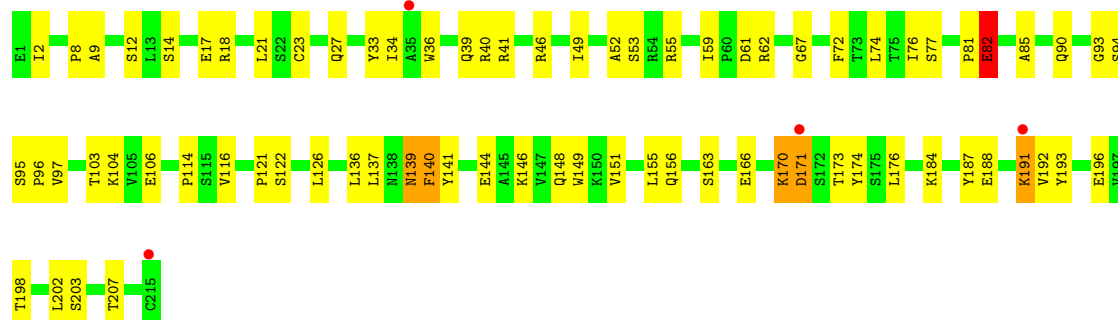


- Molecule 2: 345 Light Chain

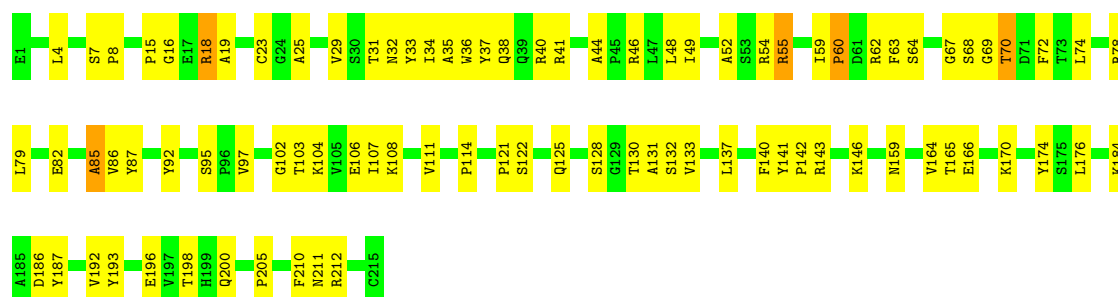




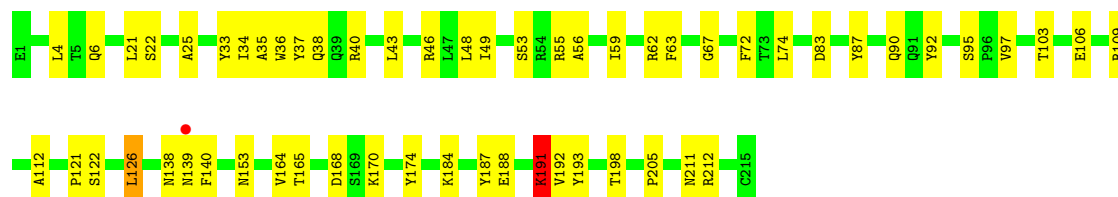
• Molecule 2: 345 Light Chain



• Molecule 2: 345 Light Chain



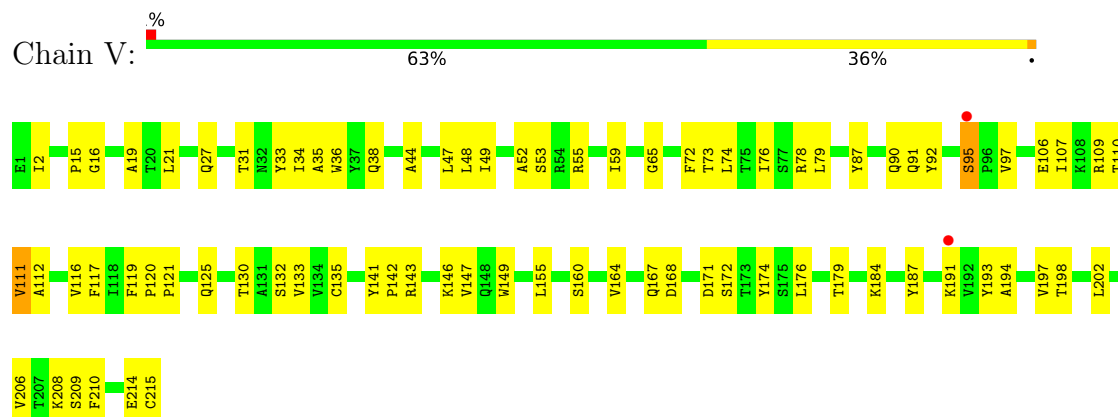
• Molecule 2: 345 Light Chain



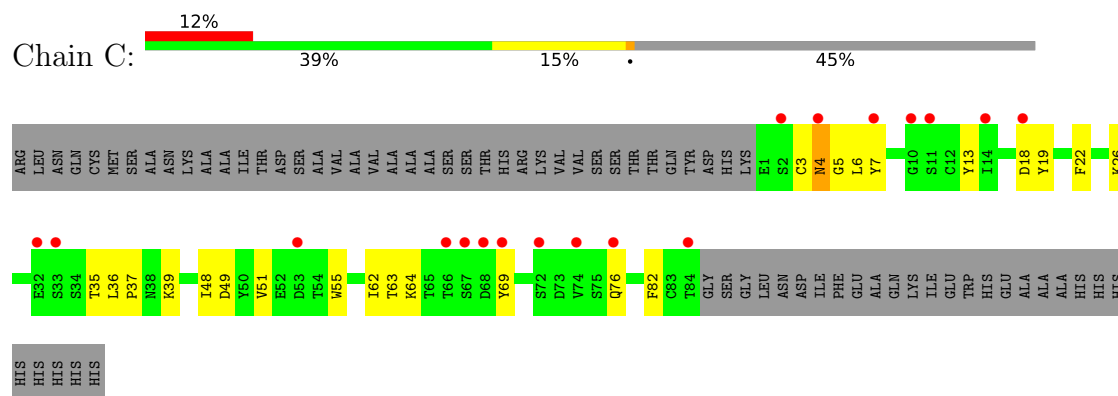
• Molecule 2: 345 Light Chain



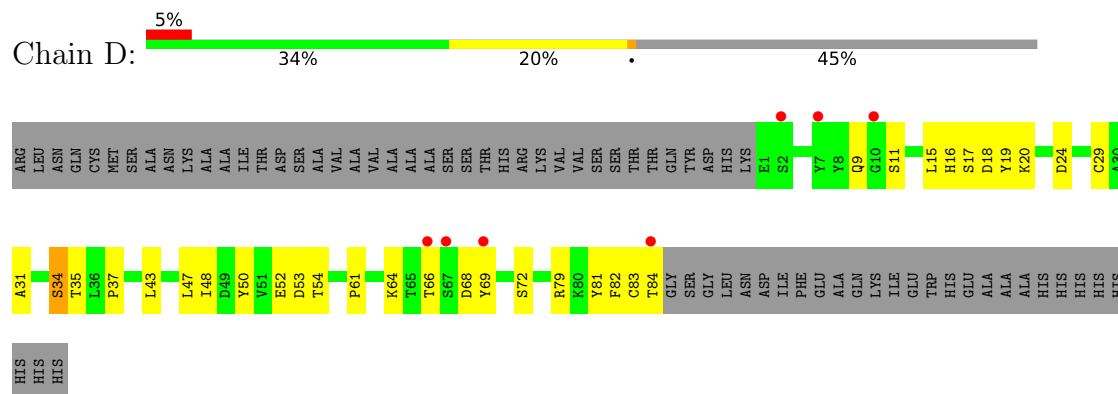
- Molecule 2: 345 Light Chain



- Molecule 3: Protein OPG161

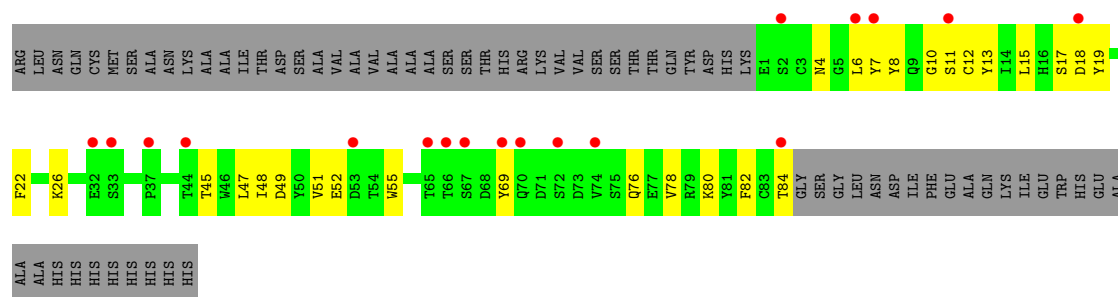


- Molecule 3: Protein OPG161

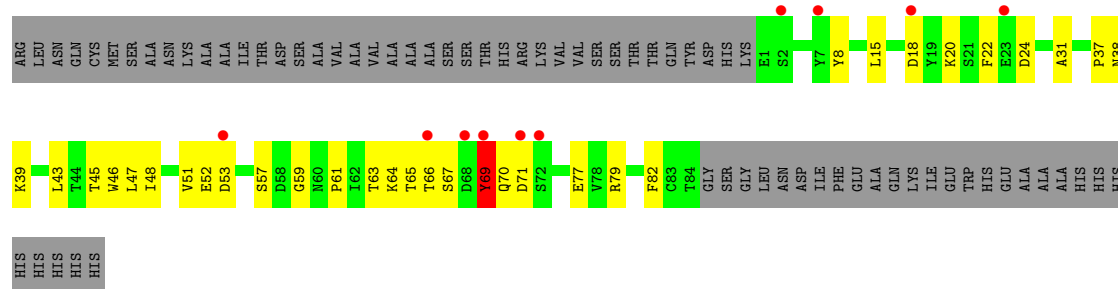
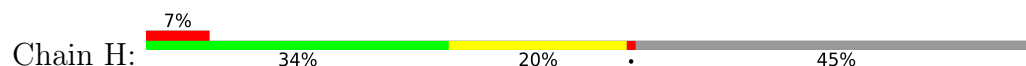


- Molecule 3: Protein OPG161

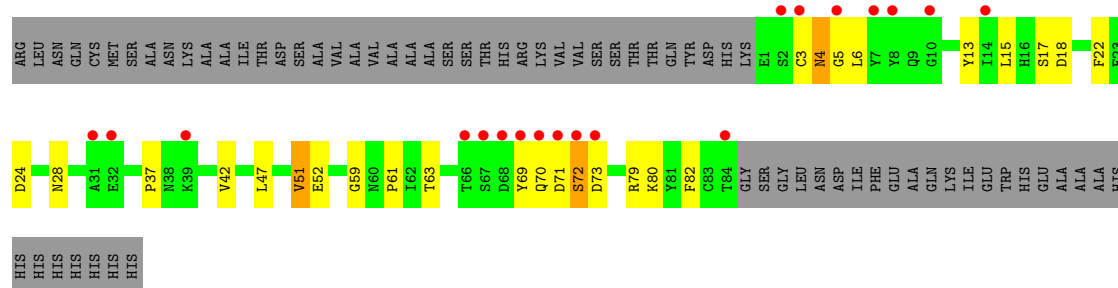
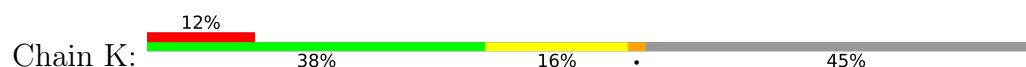




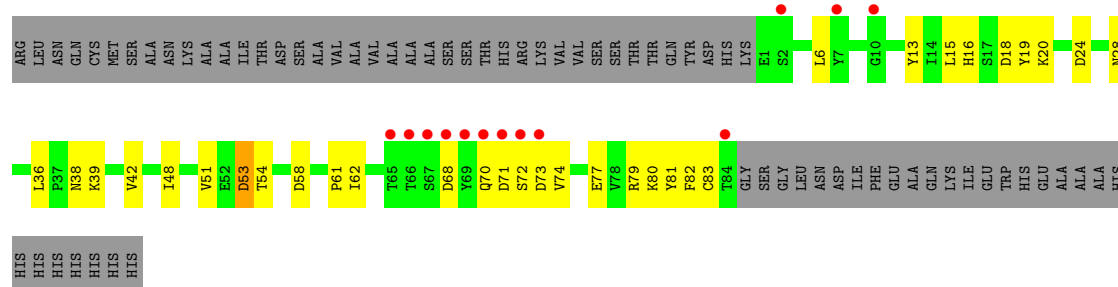
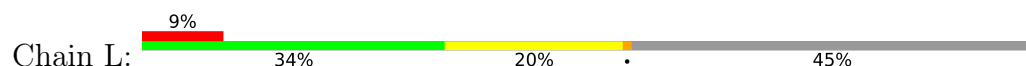
• Molecule 3: Protein OPG161



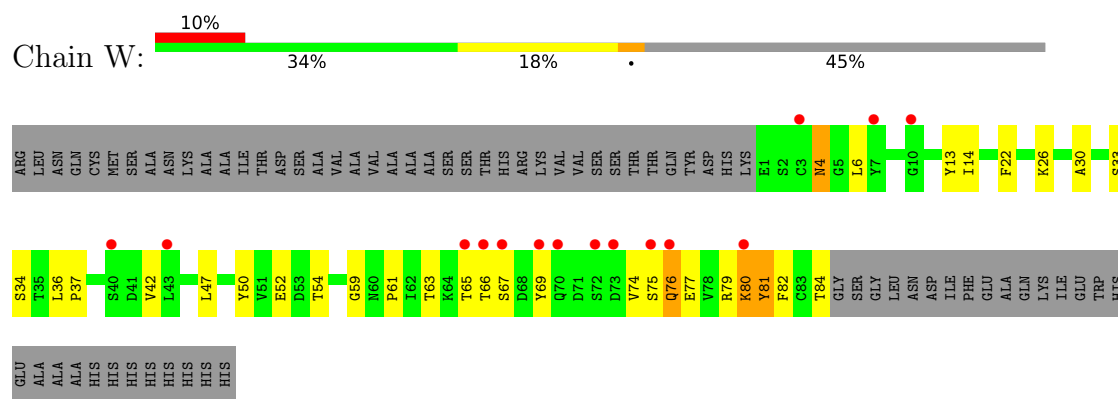
• Molecule 3: Protein OPG161



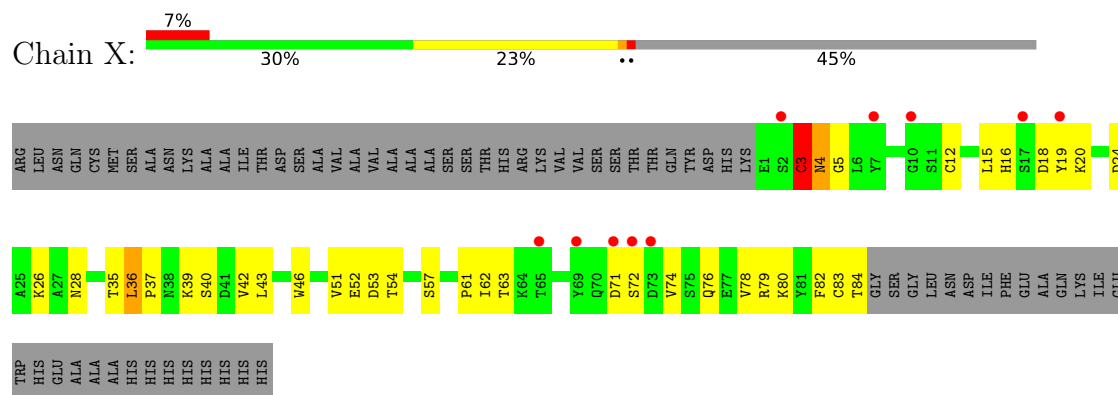
• Molecule 3: Protein OPG161



• Molecule 3: Protein OPG161



- Molecule 3: Protein OPG161



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	113.06Å 126.07Å 350.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.20 49.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.48-3.20) 99.5 (49.48-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.202 , 0.267 0.213 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27654	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5143e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.60	0/1672	0.98	5/2283 (0.2%)
1	E	0.84	1/1672 (0.1%)	1.09	10/2283 (0.4%)
1	I	0.69	0/1672	1.05	8/2283 (0.4%)
1	M	0.93	1/1672 (0.1%)	1.49	18/2283 (0.8%)
1	Q	0.55	0/1672	0.84	4/2283 (0.2%)
1	U	0.69	1/1672 (0.1%)	0.93	6/2283 (0.3%)
2	B	0.70	0/1683	0.92	3/2284 (0.1%)
2	F	0.72	0/1683	1.05	12/2284 (0.5%)
2	J	0.73	0/1683	0.94	7/2284 (0.3%)
2	N	0.67	0/1683	0.98	9/2284 (0.4%)
2	R	0.59	0/1683	0.91	6/2284 (0.3%)
2	V	0.64	0/1683	0.87	4/2284 (0.2%)
3	C	0.53	0/679	1.31	3/924 (0.3%)
3	D	0.42	0/679	0.74	3/924 (0.3%)
3	G	0.47	0/679	0.81	1/924 (0.1%)
3	H	0.52	0/679	0.85	3/924 (0.3%)
3	K	0.55	0/679	1.59	8/924 (0.9%)
3	L	0.61	0/679	1.17	5/924 (0.5%)
3	O	0.53	0/679	1.14	6/924 (0.6%)
3	P	0.43	0/679	0.75	3/924 (0.3%)
3	S	0.65	0/679	0.98	5/924 (0.5%)
3	T	0.70	0/679	0.95	1/924 (0.1%)
3	W	0.64	0/679	1.08	3/924 (0.3%)
3	X	0.57	0/679	1.33	5/924 (0.5%)
All	All	0.66	3/28278 (0.0%)	1.04	138/38490 (0.4%)

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	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
2	J	0	2
3	L	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	159	PRO	N-CD	26.84	1.85	1.47
1	E	157	PRO	N-CD	21.53	1.77	1.47
1	U	12	VAL	C-N	5.45	1.44	1.33

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	158	GLU	CB-CA-C	-28.92	68.49	108.68
3	K	72	SER	N-CA-C	-25.36	71.58	108.60
1	M	159	PRO	N-CA-CB	-24.04	76.16	102.60
3	C	4	ASN	N-CA-C	-23.33	74.27	110.42
3	K	4	ASN	N-CA-C	-21.73	75.89	109.79
1	M	159	PRO	N-CA-C	19.89	163.82	112.10
3	X	4	ASN	N-CA-C	-19.80	80.99	109.11
3	X	3	CYS	CB-CA-C	-19.49	81.04	110.67
1	A	137	SER	N-CA-C	-17.18	83.52	108.60
3	L	71	ASP	CB-CA-C	-17.18	82.10	111.30
3	C	4	ASN	CB-CA-C	15.92	136.06	109.80
1	M	158	GLU	N-CA-C	15.67	131.94	110.31
1	M	159	PRO	N-CD-CG	-15.46	85.25	103.80
1	I	183	SER	N-CA-C	15.06	142.88	110.80
3	O	73	ASP	N-CA-CB	14.93	135.12	110.79
1	E	157	PRO	N-CA-C	-14.84	81.91	112.47
3	K	4	ASN	CB-CA-C	14.63	146.39	113.33
1	I	183	SER	CB-CA-C	-13.98	82.60	110.42
3	K	5	GLY	N-CA-C	13.79	135.49	111.50
3	O	73	ASP	N-CA-C	-12.40	86.52	107.23
1	E	157	PRO	CA-N-CD	-11.73	95.57	112.00
1	E	157	PRO	CB-CA-C	11.47	130.49	111.56
3	P	66	THR	N-CA-C	-11.37	92.87	109.59
3	L	72	SER	N-CA-CB	-10.75	92.32	110.49
2	F	82	GLU	N-CA-C	10.61	123.91	111.71
1	M	199	LEU	CB-CA-C	10.20	127.72	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	75	SER	N-CA-C	10.17	123.32	111.11
3	O	72	SER	N-CA-C	-10.09	93.02	108.67
3	L	73	ASP	N-CA-C	-10.02	100.37	112.59
3	K	73	ASP	N-CA-C	-9.99	86.70	107.37
1	M	159	PRO	CA-N-CD	-9.70	97.92	111.50
1	E	157	PRO	N-CA-CB	9.67	113.40	103.25
2	N	191	LYS	CB-CA-C	-9.57	93.58	109.27
1	M	201	THR	N-CA-C	-9.56	99.93	111.69
2	R	70	THR	N-CA-C	9.39	124.00	112.54
2	F	171	ASP	N-CA-C	-9.38	100.73	113.30
3	K	52	GLU	N-CA-C	-9.36	94.71	109.50
2	F	81	PRO	CB-CA-C	-9.20	96.90	112.26
2	N	192	VAL	N-CA-CB	8.97	123.59	112.10
2	B	153	ASN	CB-CA-C	-8.95	98.73	111.80
2	R	23	CYS	N-CA-C	-8.94	93.46	108.75
1	E	17	THR	N-CA-C	8.77	122.67	109.25
1	A	110	LEU	N-CA-C	8.54	125.53	107.67
1	M	17	THR	N-CA-C	8.52	123.31	109.76
2	B	70	THR	N-CA-C	8.43	120.47	111.28
3	C	5	GLY	N-CA-C	8.35	126.75	112.22
1	A	145	THR	N-CA-CB	8.12	124.45	110.81
2	V	111	VAL	N-CA-C	-8.00	98.07	109.51
1	M	123	SER	N-CA-C	-7.97	92.99	107.98
1	A	145	THR	N-CA-C	-7.91	94.69	108.69
2	R	48	LEU	CB-CA-C	-7.75	96.00	109.02
1	M	124	ALA	N-CA-CB	7.61	125.68	111.52
1	M	77	GLN	CB-CA-C	-7.60	99.70	110.34
3	H	69	TYR	N-CA-C	7.59	120.51	111.02
3	T	4	ASN	CB-CA-C	7.55	126.09	110.31
2	F	81	PRO	N-CA-C	7.48	124.66	113.81
2	V	111	VAL	CB-CA-C	7.44	123.79	111.51
1	M	17	THR	N-CA-CB	-7.37	98.52	109.95
1	M	215	THR	N-CA-C	7.35	120.89	110.68
1	M	124	ALA	N-CA-C	-7.17	97.74	108.99
3	O	6	LEU	N-CA-C	7.16	121.04	110.30
1	U	141	THR	N-CA-C	7.07	121.20	109.46
1	U	141	THR	N-CA-CB	-6.94	98.71	110.16
2	J	70	THR	N-CA-C	6.92	121.55	113.18
2	R	23	CYS	CB-CA-C	6.92	123.37	109.68
1	U	140	SER	CB-CA-C	6.88	123.87	110.67
2	F	139	ASN	N-CA-C	6.84	120.93	112.58
2	J	18	ARG	CG-CD-NE	-6.71	97.23	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	156	PHE	N-CA-C	6.70	124.63	109.81
1	Q	158	GLU	C-N-CD	-6.68	105.90	120.60
2	F	81	PRO	CA-C-N	6.67	129.89	120.28
2	F	81	PRO	C-N-CA	6.67	129.89	120.28
3	X	4	ASN	N-CA-CB	-6.67	99.64	110.11
2	F	171	ASP	N-CA-CB	6.66	120.66	110.61
3	X	71	ASP	N-CA-C	-6.50	104.39	112.90
2	F	140	PHE	N-CA-C	6.48	120.62	110.32
1	I	142	SER	N-CA-C	-6.46	99.82	109.83
1	M	215	THR	N-CA-CB	-6.45	102.33	110.45
2	V	53	SER	N-CA-CB	-6.42	102.03	110.88
3	W	81	TYR	N-CA-CB	-6.41	101.24	111.62
3	D	34	SER	CB-CA-C	-6.38	96.04	109.38
1	E	16	GLU	CB-CA-C	-6.35	97.34	109.66
2	N	53	SER	CA-C-N	-6.29	114.03	122.72
2	N	53	SER	C-N-CA	-6.29	114.03	122.72
2	F	170	LYS	CB-CA-C	-6.23	98.61	109.07
3	L	72	SER	N-CA-C	-6.22	97.56	110.80
1	M	16	GLU	CB-CA-C	-6.19	98.57	109.71
1	E	102	SER	N-CA-C	-6.15	100.13	109.85
2	N	140	PHE	N-CA-CB	6.12	120.92	110.57
3	S	32	GLU	CB-CA-C	6.12	121.67	110.36
2	N	139	ASN	N-CA-C	-6.11	97.62	108.13
1	I	141	THR	CB-CA-C	6.05	118.91	109.84
3	P	66	THR	CB-CA-C	5.98	119.23	110.26
3	S	34	SER	CB-CA-C	-5.97	96.91	109.38
1	U	106	SER	N-CA-C	-5.96	106.04	113.55
2	J	60	PRO	CA-C-N	-5.87	107.79	121.52
2	J	60	PRO	C-N-CA	-5.87	107.79	121.52
2	N	153	ASN	CB-CA-C	-5.86	102.47	111.66
2	F	53	SER	N-CA-CB	-5.79	102.14	110.65
1	Q	158	GLU	CA-C-N	5.76	140.82	127.00
1	Q	158	GLU	C-N-CA	5.76	140.82	127.00
3	P	67	SER	N-CA-CB	5.74	119.79	110.32
3	X	36	LEU	N-CA-C	5.72	116.18	109.60
3	W	4	ASN	N-CA-C	-5.71	103.78	111.54
2	F	170	LYS	N-CA-C	5.70	121.27	113.97
3	S	78	VAL	N-CA-C	5.67	116.39	109.30
1	M	56	SER	N-CA-C	-5.63	96.38	107.69
2	R	69	GLY	N-CA-C	-5.62	100.57	111.02
2	N	192	VAL	N-CA-C	-5.61	97.81	107.24
2	V	112	ALA	N-CA-C	-5.61	98.75	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	35	THR	N-CA-C	5.61	118.77	110.46
2	B	67	GLY	CA-C-O	-5.58	118.38	122.23
2	J	170	LYS	N-CA-C	5.56	120.18	112.90
3	L	71	ASP	N-CA-C	-5.55	98.22	107.99
1	I	185	LEU	N-CA-C	-5.55	100.84	109.72
2	J	85	ALA	CB-CA-C	-5.55	98.52	110.45
2	J	18	ARG	CA-CB-CG	-5.53	103.03	114.10
1	E	17	THR	N-CA-CB	-5.52	100.87	109.87
3	H	65	THR	CB-CA-C	5.49	118.07	109.84
2	R	49	ILE	N-CA-CB	5.46	120.23	111.23
3	D	66	THR	N-CA-C	-5.41	106.52	113.01
3	K	51	VAL	N-CA-C	-5.38	98.14	109.34
1	E	101	ALA	CB-CA-C	-5.34	100.92	110.70
1	I	179	VAL	O-C-N	5.34	128.21	123.03
1	U	157	PRO	CA-C-N	5.32	127.60	120.58
1	U	157	PRO	C-N-CA	5.32	127.60	120.58
2	N	138	ASN	N-CA-C	5.31	118.92	112.23
1	A	110	LEU	CB-CA-C	-5.28	104.54	112.09
1	Q	195	PRO	N-CA-C	5.27	119.36	111.14
3	S	77	GLU	CB-CA-C	-5.26	102.75	110.06
1	I	185	LEU	N-CA-CB	5.25	120.06	111.08
1	I	184	GLY	N-CA-C	-5.22	108.04	115.30
3	H	66	THR	N-CA-C	-5.20	105.69	111.36
3	S	35	THR	N-CA-C	5.19	118.14	110.46
3	K	52	GLU	N-CA-CB	5.17	120.77	111.37
3	G	11	SER	CB-CA-C	-5.15	102.90	110.06
3	O	79	ARG	CG-CD-NE	-5.12	100.73	112.00
3	O	5	GLY	N-CA-C	-5.10	102.75	111.27

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	PRO	Peptide
2	B	203	SER	Peptide
2	F	203	SER	Peptide
2	J	18	ARG	Sidechain
2	J	55	ARG	Sidechain
3	L	53	ASP	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	1632	0	1621	67	0
1	E	1632	0	1621	49	0
1	I	1632	0	1621	70	0
1	M	1632	0	1621	62	1
1	Q	1632	0	1621	56	0
1	U	1632	0	1621	79	0
2	B	1649	0	1604	59	0
2	F	1649	0	1604	52	0
2	J	1649	0	1604	67	0
2	N	1649	0	1604	39	0
2	R	1649	0	1604	62	1
2	V	1649	0	1604	48	0
3	C	664	0	599	16	8
3	D	664	0	599	32	0
3	G	664	0	599	21	0
3	H	664	0	599	23	0
3	K	664	0	599	18	0
3	L	664	0	599	25	0
3	O	664	0	599	26	0
3	P	664	0	599	19	0
3	S	664	0	599	43	0
3	T	664	0	599	36	0
3	W	664	0	599	36	8
3	X	664	0	599	36	0
All	All	27654	0	26538	919	9

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 17.

All (919) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:PRO:N	1:E:157:PRO:CD	1.77	1.40
1:M:159:PRO:CD	1:M:159:PRO:N	1.85	1.32
1:U:140:SER:O	2:V:117:PHE:CD1	1.90	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:PHE:O	1:E:156:PHE:CD1	2.05	1.10
3:K:3:CYS:SG	3:K:4:ASN:O	2.09	1.09
3:S:46:TRP:CE3	3:T:4:ASN:O	2.06	1.08
1:U:28:SER:HB2	3:W:69:TYR:HD2	1.14	1.06
1:U:140:SER:O	2:V:117:PHE:HD1	1.27	1.05
3:S:46:TRP:CD2	3:T:4:ASN:O	2.14	1.00
1:U:28:SER:HB2	3:W:69:TYR:CD2	1.95	1.00
3:O:69:TYR:O	3:O:72:SER:O	1.82	0.97
1:E:141:THR:HG22	1:E:142:SER:H	1.31	0.96
2:J:16:GLY:HA2	2:J:78:ARG:HG3	1.49	0.94
3:O:51:VAL:HG23	3:O:51:VAL:O	1.68	0.94
3:K:51:VAL:HG23	3:K:51:VAL:O	1.68	0.93
3:C:3:CYS:SG	3:C:4:ASN:O	2.28	0.91
3:X:35:THR:O	3:X:84:THR:HG22	1.70	0.90
3:K:3:CYS:C	3:K:4:ASN:O	1.96	0.86
3:X:19:TYR:CE1	3:X:80:LYS:HG3	2.10	0.85
1:E:33:SER:HB2	1:E:98:ARG:HB3	1.59	0.85
1:M:16:GLU:O	1:M:85:VAL:HG22	1.78	0.83
1:E:156:PHE:C	1:E:157:PRO:CD	2.51	0.83
2:N:95:SER:HB3	3:P:79:ARG:HH22	1.45	0.82
2:F:106:GLU:OE1	2:F:174:TYR:OH	1.97	0.82
1:A:5:GLN:OE1	1:A:115:GLN:NE2	2.13	0.81
1:I:33:SER:HB2	1:I:98:ARG:HB3	1.62	0.81
1:E:156:PHE:O	1:E:156:PHE:CG	2.34	0.81
1:I:129:PRO:HB3	1:I:155:TYR:HB3	1.62	0.81
1:E:101:ALA:O	2:F:33:TYR:OH	1.99	0.81
2:J:146:LYS:HB3	2:J:198:THR:HB	1.62	0.80
3:D:69:TYR:O	3:D:72:SER:OG	1.98	0.80
1:E:157:PRO:HB2	1:E:212:PRO:HG2	1.62	0.80
1:E:16:GLU:O	1:E:85:VAL:HG22	1.82	0.80
2:B:67:GLY:HA3	2:B:72:PHE:HA	1.63	0.78
1:U:28:SER:CB	3:W:69:TYR:HD2	1.95	0.78
2:J:55:ARG:NH1	2:J:63:PHE:O	2.17	0.77
3:S:15:LEU:HD12	3:T:50:TYR:CE1	2.20	0.77
3:S:29:CYS:HB3	3:S:34:SER:O	1.86	0.76
2:B:55:ARG:HG2	2:B:59:ILE:HB	1.67	0.76
1:U:29:ILE:HG22	3:W:69:TYR:OH	1.86	0.75
1:U:30:SER:O	1:U:53:ASN:HB2	1.87	0.75
1:U:28:SER:CB	3:W:69:TYR:CD2	2.69	0.74
1:U:28:SER:HA	3:W:69:TYR:CD2	2.23	0.74
2:J:38:GLN:OE1	2:J:46:ARG:NH1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:95:SER:HB2	3:H:79:ARG:HH22	1.51	0.73
1:Q:115:GLN:HA	2:R:44:ALA:HB2	1.68	0.73
3:C:22:PHE:CZ	3:C:26:LYS:HD2	2.24	0.73
3:S:6:LEU:HB2	3:S:13:TYR:HB2	1.70	0.73
1:U:90:THR:HG23	1:U:120:THR:HA	1.71	0.72
1:Q:106:SER:OG	3:T:79:ARG:NH1	2.23	0.72
2:F:49:ILE:HG21	2:F:52:ALA:O	1.89	0.72
1:E:8:GLY:HA3	1:E:20:LEU:HD23	1.72	0.72
1:M:99:MET:O	1:M:108:GLY:HA3	1.90	0.72
3:S:29:CYS:C	3:S:34:SER:O	2.33	0.71
3:K:51:VAL:O	3:K:51:VAL:CG2	2.38	0.71
2:B:106:GLU:OE1	2:B:174:TYR:OH	2.03	0.71
2:R:69:GLY:O	2:R:72:PHE:CE1	2.44	0.71
3:L:48:ILE:HA	3:L:51:VAL:HG22	1.72	0.70
2:J:38:GLN:HB2	2:J:48:LEU:HD11	1.72	0.70
3:L:6:LEU:HB2	3:L:13:TYR:HB2	1.74	0.70
1:I:105:GLY:HA2	3:L:53:ASP:HB2	1.73	0.70
3:K:6:LEU:HB2	3:K:13:TYR:HB2	1.74	0.69
1:A:105:GLY:HA2	3:D:53:ASP:HB2	1.74	0.69
1:I:12:VAL:O	1:I:121:VAL:HA	1.93	0.68
1:M:8:GLY:HA3	1:M:20:LEU:HD23	1.75	0.68
1:M:52:TYR:OH	1:M:58:ASN:ND2	2.27	0.68
3:K:24:ASP:O	3:K:28:ASN:HB2	1.94	0.68
2:R:67:GLY:HA3	2:R:72:PHE:HA	1.74	0.68
1:A:33:SER:HB2	1:A:98:ARG:HB3	1.75	0.67
1:A:110:LEU:O	1:A:113:TRP:CD1	2.46	0.67
1:M:33:SER:HB2	1:M:98:ARG:HB3	1.77	0.67
1:M:133:PRO:HD2	2:N:122:SER:HB3	1.77	0.67
1:U:2:VAL:HG22	1:U:27:GLY:HA3	1.75	0.67
1:U:115:GLN:HA	2:V:44:ALA:HB2	1.77	0.67
1:M:152:VAL:HG11	1:M:160:VAL:HG11	1.74	0.67
1:U:28:SER:OG	1:U:31:THR:OG1	2.05	0.67
2:V:146:LYS:HB3	2:V:198:THR:HB	1.77	0.67
1:Q:33:SER:HB2	1:Q:98:ARG:HB3	1.76	0.67
3:X:53:ASP:OD1	3:X:79:ARG:NH1	2.26	0.67
3:P:38:ASN:HB3	3:P:41:ASP:CG	2.20	0.66
2:N:21:LEU:HD23	2:N:103:THR:HB	1.76	0.66
2:N:67:GLY:HA3	2:N:72:PHE:HA	1.76	0.66
1:U:52:TYR:CZ	3:X:19:TYR:CE1	2.82	0.66
2:J:54:ARG:HH12	3:K:18:ASP:HA	1.60	0.66
1:Q:5:GLN:HB3	1:Q:23:SER:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:146:LYS:HB3	2:R:198:THR:HB	1.77	0.66
3:S:20:LYS:HD2	3:S:81:TYR:CE1	2.30	0.66
3:D:20:LYS:HB3	3:D:24:ASP:HB2	1.78	0.66
1:U:28:SER:CA	3:W:69:TYR:CD2	2.79	0.66
3:H:20:LYS:HB3	3:H:24:ASP:HB2	1.77	0.65
1:Q:205:ILE:HG12	1:Q:220:LYS:HA	1.79	0.65
2:F:137:LEU:HB2	2:F:176:LEU:HB3	1.78	0.65
2:V:147:VAL:HG22	2:V:197:VAL:HG22	1.79	0.65
3:P:77:GLU:OE1	3:P:79:ARG:NH2	2.30	0.65
1:U:30:SER:H	3:W:69:TYR:HE2	1.43	0.64
1:Q:5:GLN:OE1	1:Q:115:GLN:NE2	2.28	0.64
1:U:50:PHE:CE2	1:U:58:ASN:HB2	2.32	0.64
2:J:40:ARG:NH2	2:J:82:GLU:HG3	2.12	0.64
3:G:22:PHE:CZ	3:G:26:LYS:HD2	2.32	0.64
2:J:121:PRO:HG3	2:J:131:ALA:HB1	1.79	0.64
3:S:15:LEU:HG	3:T:50:TYR:CZ	2.32	0.64
3:G:12:CYS:O	3:G:84:THR:HA	1.97	0.64
1:U:67:VAL:HG23	1:U:82:LEU:HD13	1.80	0.64
3:O:51:VAL:O	3:O:51:VAL:CG2	2.37	0.63
2:B:90:GLN:HE21	2:B:97:VAL:HG13	1.64	0.63
2:R:121:PRO:HD3	2:R:133:VAL:HG22	1.81	0.63
1:Q:2:VAL:HG22	1:Q:27:GLY:HA3	1.81	0.63
1:E:141:THR:HG22	1:E:142:SER:N	2.07	0.62
3:L:54:THR:HB	3:L:81:TYR:HA	1.80	0.62
1:U:8:GLY:HA3	1:U:20:LEU:HD23	1.80	0.62
2:B:146:LYS:HB3	2:B:198:THR:HB	1.80	0.62
3:X:19:TYR:CD1	3:X:80:LYS:HG3	2.33	0.62
1:A:106:SER:OG	3:D:79:ARG:NH1	2.32	0.62
1:I:38:ARG:HB3	1:I:48:ILE:HD11	1.80	0.62
1:E:106:SER:OG	3:H:79:ARG:NH1	2.33	0.62
1:Q:5:GLN:CD	1:Q:115:GLN:HE22	2.07	0.62
1:U:38:ARG:HB3	1:U:48:ILE:HD11	1.81	0.62
1:Q:103:LEU:HD22	3:S:15:LEU:HD21	1.80	0.62
3:P:6:LEU:HB2	3:P:13:TYR:HB2	1.80	0.62
1:A:214:ASN:HB3	1:M:30:SER:HB2	1.82	0.62
2:N:38:GLN:OE1	2:N:46:ARG:NH1	2.32	0.62
3:S:37:PRO:HD3	3:S:82:PHE:O	2.00	0.62
1:I:8:GLY:HA3	1:I:20:LEU:HD23	1.82	0.61
2:N:198:THR:HG23	2:N:205:PRO:HG3	1.82	0.61
3:O:24:ASP:O	3:O:28:ASN:HB2	2.00	0.61
1:U:50:PHE:HZ	1:U:52:TYR:CE2	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:LEU:HB2	3:C:13:TYR:HB2	1.82	0.61
1:A:28:SER:HB3	3:C:69:TYR:OH	2.00	0.61
1:E:105:GLY:HA2	3:H:53:ASP:HB2	1.81	0.61
3:C:51:VAL:HG12	3:C:82:PHE:CD1	2.35	0.61
3:D:29:CYS:C	3:D:34:SER:O	2.44	0.61
3:H:52:GLU:HG3	3:H:63:THR:HA	1.83	0.61
1:I:2:VAL:HG22	1:I:27:GLY:HA3	1.83	0.61
1:I:34:TRP:HB3	1:I:78:PHE:CZ	2.36	0.61
2:R:48:LEU:O	2:R:49:ILE:HD13	2.01	0.60
3:X:42:VAL:HG21	3:X:51:VAL:HG21	1.82	0.60
1:A:56:SER:HB3	3:D:19:TYR:HB2	1.83	0.60
2:J:143:ARG:HG2	2:J:143:ARG:HH11	1.66	0.60
1:M:38:ARG:HB3	1:M:48:ILE:HD11	1.82	0.60
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.82	0.60
2:J:36:TRP:CD2	2:J:74:LEU:HB2	2.36	0.60
1:U:29:ILE:N	3:W:69:TYR:CE2	2.70	0.60
1:M:56:SER:HB3	3:P:19:TYR:HB2	1.84	0.60
2:V:48:LEU:HA	2:V:59:ILE:HG13	1.84	0.60
2:B:2:ILE:HG12	2:B:27:GLN:HG3	1.83	0.60
1:U:76:ASN:HD21	3:W:69:TYR:HE1	1.48	0.60
1:A:110:LEU:O	1:A:113:TRP:NE1	2.34	0.60
1:I:178:ALA:HB1	1:I:186:TYR:HB3	1.84	0.60
3:C:49:ASP:HB3	3:D:15:LEU:HD23	1.82	0.59
1:I:156:PHE:CD1	1:I:157:PRO:HA	2.37	0.59
2:R:94:SER:HB2	3:T:69:TYR:CE2	2.37	0.59
1:A:29:ILE:HG21	1:A:73:THR:HA	1.85	0.59
3:D:48:ILE:HG13	3:D:64:LYS:HG2	1.83	0.59
1:E:28:SER:HB3	3:G:69:TYR:CE1	2.37	0.59
3:S:35:THR:O	3:S:84:THR:HG22	2.02	0.59
1:M:158:GLU:C	1:M:159:PRO:CD	2.71	0.59
2:N:55:ARG:NH1	2:N:63:PHE:O	2.36	0.59
3:T:61:PRO:HB3	3:T:79:ARG:HD2	1.84	0.59
1:U:40:PRO:HB2	1:U:43:LYS:HB2	1.85	0.59
1:U:50:PHE:CZ	1:U:52:TYR:CE2	2.90	0.59
1:Q:29:ILE:HA	1:Q:34:TRP:HZ2	1.67	0.59
1:E:18:LEU:HB2	1:E:85:VAL:HG11	1.84	0.59
3:D:43:LEU:HA	3:D:48:ILE:HD13	1.84	0.59
1:U:5:GLN:HB3	1:U:23:SER:HB2	1.84	0.59
3:S:29:CYS:CB	3:S:34:SER:O	2.51	0.58
2:F:184:LYS:HE2	2:F:188:GLU:OE2	2.04	0.58
1:I:160:VAL:HG22	1:I:188:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:90:GLN:HG2	2:R:91:GLN:N	2.18	0.58
2:R:55:ARG:HD3	2:R:60:PRO:O	2.02	0.58
1:M:105:GLY:HA2	3:P:53:ASP:HB3	1.84	0.58
2:N:191:LYS:O	2:N:211:ASN:HA	2.04	0.58
3:P:37:PRO:HD3	3:P:82:PHE:O	2.04	0.58
3:C:18:ASP:OD1	3:C:18:ASP:N	2.33	0.58
3:O:55:TRP:HD1	3:O:81:TYR:HB3	1.68	0.58
1:E:37:ILE:HD11	1:E:110:LEU:HD22	1.86	0.58
1:M:34:TRP:HB3	1:M:78:PHE:CZ	2.39	0.58
3:D:15:LEU:HD21	3:D:17:SER:HB3	1.86	0.58
3:X:19:TYR:CZ	3:X:80:LYS:HE3	2.38	0.58
1:I:90:THR:HG23	1:I:120:THR:HA	1.86	0.57
3:W:54:THR:HA	3:W:80:LYS:O	2.05	0.57
1:E:141:THR:CG2	1:E:142:SER:H	2.11	0.57
1:I:34:TRP:HB2	1:I:51:ILE:CG2	2.34	0.57
3:X:35:THR:O	3:X:84:THR:CG2	2.49	0.57
1:E:101:ALA:O	2:F:33:TYR:CZ	2.57	0.57
2:F:14:SER:N	2:F:17:GLU:OE1	2.36	0.57
2:F:2:ILE:HG12	2:F:27:GLN:CG	2.34	0.57
2:J:69:GLY:O	2:J:72:PHE:CE1	2.57	0.57
2:V:90:GLN:HG2	2:V:91:GLN:N	2.20	0.57
1:E:158:GLU:N	1:E:159:PRO:HD2	2.19	0.57
1:A:216:LYS:HD3	1:M:53:ASN:HA	1.87	0.57
1:M:48:ILE:HG23	1:M:63:LEU:HD13	1.87	0.56
1:A:176:PHE:CE2	2:B:177:SER:HB3	2.40	0.56
3:O:37:PRO:HD3	3:O:82:PHE:O	2.06	0.56
2:R:2:ILE:HG12	2:R:27:GLN:HG3	1.85	0.56
2:R:15:PRO:HD3	2:R:107:ILE:HG23	1.87	0.56
2:V:167:GLN:HG2	2:V:172:SER:HA	1.86	0.56
3:X:16:HIS:NE2	3:X:83:CYS:SG	2.78	0.56
2:F:148:GLN:HB3	2:F:155:LEU:CD1	2.36	0.56
2:J:121:PRO:HD3	2:J:133:VAL:HG22	1.87	0.56
1:Q:102:SER:HB2	1:Q:105:GLY:HA3	1.86	0.56
3:W:61:PRO:HG3	3:W:79:ARG:HG3	1.87	0.56
1:Q:102:SER:HB3	3:T:52:GLU:HG3	1.88	0.56
1:Q:31:THR:HG22	3:S:52:GLU:OE2	2.06	0.56
3:W:54:THR:HB	3:W:81:TYR:HA	1.88	0.56
1:A:198:SER:HB2	1:A:202:GLN:HB3	1.88	0.55
3:D:31:ALA:HA	3:H:31:ALA:HA	1.87	0.55
2:R:48:LEU:HD11	2:R:87:TYR:HE1	1.70	0.55
1:U:78:PHE:CZ	1:U:95:CYS:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:SER:HB2	3:D:79:ARG:HH22	1.71	0.55
2:J:23:CYS:HB2	2:J:36:TRP:CH2	2.41	0.55
2:R:113:ALA:HB2	2:R:201:GLY:O	2.06	0.55
2:R:167:GLN:HG2	2:R:172:SER:HA	1.86	0.55
1:U:173:VAL:HG22	1:U:192:VAL:HB	1.89	0.55
3:H:51:VAL:HG12	3:H:82:PHE:CD2	2.41	0.55
2:J:67:GLY:HA3	2:J:72:PHE:HA	1.88	0.55
3:K:22:PHE:CE1	3:K:59:GLY:HA2	2.41	0.55
1:U:52:TYR:CE2	3:X:19:TYR:CD1	2.95	0.55
3:W:6:LEU:HB2	3:W:13:TYR:HB2	1.88	0.55
2:N:62:ARG:NH2	2:N:83:ASP:OD1	2.26	0.55
3:S:3:CYS:HB2	3:S:7:TYR:HD2	1.72	0.55
1:U:134:LEU:HB3	2:V:119:PHE:CD1	2.41	0.55
1:I:216:LYS:HZ2	3:X:40:SER:HB3	1.72	0.55
2:J:4:LEU:HD23	2:J:25:ALA:HA	1.88	0.55
1:A:173:VAL:HG22	1:A:192:VAL:HB	1.89	0.55
1:I:67:VAL:HG23	1:I:82:LEU:HD13	1.89	0.55
1:I:144:GLY:HA2	1:I:195:PRO:HA	1.89	0.55
2:J:48:LEU:HD23	2:J:59:ILE:HD12	1.89	0.55
3:L:77:GLU:OE1	3:L:79:ARG:NH2	2.39	0.55
1:M:47:TRP:O	1:M:60:ASN:HB2	2.07	0.55
3:L:61:PRO:HG3	3:L:79:ARG:CZ	2.37	0.54
1:U:205:ILE:HG12	1:U:220:LYS:HA	1.88	0.54
1:A:174:HIS:NE2	2:B:139:ASN:OD1	2.39	0.54
1:E:156:PHE:HB3	1:E:157:PRO:HD3	1.88	0.54
2:J:106:GLU:OE1	2:J:174:TYR:OH	2.14	0.54
1:U:2:VAL:HG22	1:U:27:GLY:CA	2.37	0.54
3:C:39:LYS:HE3	3:C:63:THR:O	2.07	0.54
1:A:207:ASN:HB3	1:M:54:SER:HB3	1.89	0.54
3:G:6:LEU:N	3:G:13:TYR:O	2.38	0.54
2:N:168:ASP:OD1	2:N:170:LYS:N	2.40	0.54
1:U:33:SER:HB2	1:U:98:ARG:HB3	1.89	0.54
1:I:156:PHE:CG	1:I:157:PRO:HA	2.43	0.54
1:U:50:PHE:HE1	1:U:52:TYR:CG	2.26	0.54
1:I:13:LYS:O	1:I:16:GLU:HB2	2.08	0.54
2:B:34:ILE:HD13	2:B:91:GLN:HA	1.90	0.54
1:I:99:MET:O	1:I:108:GLY:HA3	2.08	0.54
2:N:164:VAL:HG12	2:N:165:THR:O	2.08	0.54
2:B:95:SER:HB2	3:D:79:ARG:NH2	2.22	0.53
1:I:33:SER:CB	1:I:98:ARG:HE	2.21	0.53
2:J:60:PRO:HB2	2:J:62:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:33:TYR:HB3	2:N:92:TYR:CD1	2.43	0.53
3:S:13:TYR:HE1	3:S:37:PRO:HB3	1.72	0.53
2:V:36:TRP:HB2	2:V:49:ILE:HB	1.88	0.53
2:N:36:TRP:CD2	2:N:74:LEU:HB2	2.43	0.53
3:P:69:TYR:HB3	3:P:72:SER:OG	2.08	0.53
1:U:115:GLN:HA	2:V:44:ALA:CB	2.37	0.53
3:D:54:THR:HB	3:D:81:TYR:HA	1.90	0.53
1:I:107:LEU:HD22	2:J:97:VAL:HG23	1.90	0.53
1:M:31:THR:HG21	3:O:63:THR:HG22	1.89	0.53
1:M:107:LEU:HD22	2:N:97:VAL:HG23	1.90	0.53
3:W:54:THR:HB	3:W:80:LYS:O	2.08	0.53
1:M:47:TRP:CZ2	1:M:49:GLY:HA2	2.43	0.53
3:S:9:GLN:NE2	3:S:45:THR:HG21	2.24	0.53
1:A:90:THR:HG23	1:A:120:THR:HA	1.90	0.53
3:X:37:PRO:HD3	3:X:82:PHE:O	2.08	0.53
2:J:164:VAL:HG12	2:J:165:THR:O	2.08	0.53
1:M:33:SER:CB	1:M:98:ARG:HE	2.21	0.53
1:M:24:VAL:HG11	1:M:34:TRP:CH2	2.44	0.53
2:N:95:SER:CB	3:P:79:ARG:HH22	2.17	0.53
3:H:37:PRO:HD3	3:H:82:PHE:O	2.09	0.53
1:I:216:LYS:NZ	3:X:40:SER:HB3	2.24	0.53
2:V:38:GLN:HG3	2:V:87:TYR:CE1	2.43	0.53
2:V:125:GLN:HE22	2:V:132:SER:CB	2.22	0.53
3:W:22:PHE:CE1	3:W:59:GLY:HA2	2.44	0.53
2:J:187:TYR:CE2	2:J:212:ARG:HG3	2.44	0.52
3:T:22:PHE:CE1	3:T:59:GLY:HA2	2.44	0.52
1:U:164:TRP:HB3	1:U:169:LEU:HD23	1.91	0.52
2:B:144:GLU:H	2:B:144:GLU:CD	2.17	0.52
1:E:38:ARG:HB3	1:E:48:ILE:HD11	1.91	0.52
1:U:4:LEU:HB3	1:U:22:CYS:SG	2.50	0.52
1:A:149:GLY:HA2	1:A:164:TRP:CZ2	2.44	0.52
2:F:46:ARG:NH2	3:S:24:ASP:OD1	2.43	0.52
2:V:120:PRO:HB3	2:V:210:PHE:CE1	2.44	0.52
1:E:28:SER:HB3	3:G:69:TYR:HE1	1.75	0.52
2:F:146:LYS:HB3	2:F:198:THR:HB	1.91	0.52
2:V:33:TYR:HB3	2:V:92:TYR:CD2	2.44	0.52
2:V:160:SER:HA	2:V:179:THR:O	2.09	0.52
2:J:49:ILE:HG21	2:J:52:ALA:O	2.10	0.52
1:Q:132:PHE:HB3	2:R:122:SER:OG	2.10	0.52
2:R:69:GLY:O	2:R:72:PHE:CZ	2.63	0.52
1:M:180:LEU:HD13	1:M:186:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:PHE:CE2	2:J:125:GLN:HG3	2.44	0.52
1:I:41:PRO:HD3	1:I:90:THR:O	2.10	0.51
2:N:35:ALA:HA	2:N:49:ILE:O	2.10	0.51
3:O:15:LEU:HB2	3:O:82:PHE:CE2	2.45	0.51
3:S:45:THR:O	3:S:48:ILE:HG22	2.09	0.51
2:V:121:PRO:HD3	2:V:133:VAL:HG22	1.91	0.51
3:X:12:CYS:O	3:X:84:THR:HA	2.10	0.51
1:A:101:ALA:HB2	1:A:108:GLY:HA2	1.91	0.51
2:B:69:GLY:O	2:B:72:PHE:CE2	2.62	0.51
2:F:67:GLY:HA3	2:F:72:PHE:HA	1.91	0.51
2:F:139:ASN:O	2:F:173:THR:HG21	2.10	0.51
2:F:39:GLN:O	2:F:85:ALA:HB1	2.11	0.51
3:K:15:LEU:HB2	3:K:82:PHE:CE2	2.46	0.51
1:Q:78:PHE:CZ	1:Q:95:CYS:HB2	2.45	0.51
2:R:120:PRO:HB3	2:R:210:PHE:CE2	2.45	0.51
2:R:126:LEU:O	2:R:184:LYS:HD2	2.10	0.51
1:U:156:PHE:O	1:U:210:HIS:HE1	1.93	0.51
1:A:12:VAL:O	1:A:121:VAL:HA	2.10	0.51
2:F:126:LEU:O	2:F:184:LYS:HD2	2.10	0.51
1:I:29:ILE:HG23	1:I:73:THR:HG22	1.92	0.51
2:J:16:GLY:HA2	2:J:78:ARG:CG	2.33	0.51
1:Q:115:GLN:H	1:Q:115:GLN:CD	2.19	0.51
2:B:148:GLN:HB3	2:B:155:LEU:HD13	1.92	0.51
3:D:48:ILE:CG1	3:D:64:LYS:HG2	2.41	0.51
1:E:78:PHE:CZ	1:E:95:CYS:HB2	2.45	0.51
3:G:15:LEU:HB2	3:G:82:PHE:CE2	2.46	0.51
2:B:34:ILE:HG13	2:B:72:PHE:CE2	2.46	0.51
3:T:48:ILE:O	3:T:52:GLU:HB2	2.10	0.51
1:M:133:PRO:HD2	2:N:122:SER:CB	2.40	0.51
3:O:69:TYR:C	3:O:72:SER:O	2.54	0.51
1:A:175:THR:HA	1:A:190:SER:HA	1.92	0.51
3:G:6:LEU:HB2	3:G:13:TYR:HB2	1.93	0.51
2:J:114:PRO:CA	2:J:140:PHE:HB3	2.41	0.51
1:M:34:TRP:HB2	1:M:51:ILE:HG22	1.91	0.51
2:N:126:LEU:HD21	2:N:187:TYR:CD2	2.46	0.51
1:U:105:GLY:HA2	3:X:53:ASP:HB2	1.92	0.51
1:A:78:PHE:CZ	1:A:95:CYS:HB2	2.46	0.51
3:D:20:LYS:HD3	3:D:24:ASP:HB3	1.92	0.51
2:R:171:ASP:O	2:R:173:THR:HG23	2.11	0.50
1:U:164:TRP:CH2	1:U:206:CYS:HB3	2.46	0.50
2:R:95:SER:HB2	3:T:79:ARG:HH22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:CYS:HB2	2:F:36:TRP:CH2	2.46	0.50
3:H:8:TYR:HD1	3:H:46:TRP:HE1	1.60	0.50
2:R:21:LEU:HD23	2:R:103:THR:HB	1.92	0.50
2:R:134:VAL:HG22	2:R:179:THR:HG23	1.93	0.50
1:A:18:LEU:HB2	1:A:85:VAL:HG11	1.92	0.50
1:A:162:VAL:HG11	1:A:190:SER:HB3	1.94	0.50
2:B:94:SER:HA	3:D:69:TYR:HE2	1.77	0.50
3:S:22:PHE:CZ	3:S:59:GLY:HA2	2.46	0.50
1:U:176:PHE:HD2	1:U:189:SER:O	1.93	0.50
3:X:78:VAL:C	3:X:79:ARG:HG3	2.37	0.50
1:A:38:ARG:HB3	1:A:48:ILE:HD11	1.92	0.50
1:M:37:ILE:O	1:M:94:TYR:N	2.44	0.50
1:M:90:THR:HG23	1:M:120:THR:HA	1.94	0.50
2:R:106:GLU:OE2	2:R:141:TYR:OH	2.17	0.50
1:U:34:TRP:HB3	1:U:78:PHE:CE2	2.47	0.50
1:U:175:THR:HG23	1:U:190:SER:HB2	1.93	0.50
2:B:62:ARG:NH2	2:B:82:GLU:OE2	2.44	0.50
3:K:37:PRO:HD3	3:K:82:PHE:O	2.11	0.50
1:U:67:VAL:CG2	1:U:82:LEU:HD13	2.42	0.50
1:A:179:VAL:HG23	1:A:179:VAL:O	2.11	0.50
1:I:34:TRP:HB2	1:I:51:ILE:HG22	1.93	0.50
2:J:104:LYS:NZ	2:J:166:GLU:OE1	2.40	0.50
2:J:198:THR:HG23	2:J:205:PRO:HG3	1.93	0.50
1:Q:98:ARG:NH1	1:Q:105:GLY:O	2.43	0.50
3:D:47:LEU:O	3:D:50:TYR:N	2.41	0.50
1:M:175:THR:HG23	1:M:190:SER:HB2	1.93	0.50
3:X:15:LEU:HB2	3:X:82:PHE:CE2	2.47	0.50
3:H:43:LEU:HA	3:H:48:ILE:HD13	1.94	0.49
1:I:6:GLU:HB3	1:I:117:THR:HG22	1.94	0.49
3:T:8:TYR:HB2	3:T:47:LEU:HD11	1.93	0.49
1:A:63:LEU:HB3	1:A:67:VAL:CG2	2.42	0.49
1:U:4:LEU:HD22	1:U:24:VAL:HG22	1.95	0.49
3:X:39:LYS:HE3	3:X:63:THR:O	2.12	0.49
1:Q:51:ILE:HD12	1:Q:56:SER:O	2.12	0.49
1:U:181:GLN:CD	1:U:187:SER:HB2	2.36	0.49
2:B:149:TRP:O	2:B:155:LEU:HD12	2.13	0.49
3:D:52:GLU:OE1	3:D:64:LYS:HE3	2.12	0.49
1:I:115:GLN:HA	2:J:44:ALA:HB2	1.94	0.49
3:S:15:LEU:HG	3:T:50:TYR:OH	2.12	0.49
3:X:20:LYS:HB3	3:X:24:ASP:HB2	1.93	0.49
2:V:125:GLN:HG2	2:V:130:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:43:LEU:HD11	3:D:64:LYS:O	2.11	0.49
1:E:34:TRP:HB2	1:E:51:ILE:CG2	2.43	0.49
1:E:47:TRP:CZ3	2:F:96:PRO:HB2	2.47	0.49
1:I:105:GLY:HA2	3:L:53:ASP:CB	2.39	0.49
2:R:4:LEU:HD11	2:R:91:GLN:N	2.27	0.49
3:S:15:LEU:CD1	3:T:50:TYR:CZ	2.96	0.49
2:F:33:TYR:HD2	2:F:93:GLY:HA2	1.77	0.49
1:Q:37:ILE:HG13	1:Q:47:TRP:HA	1.95	0.49
2:J:125:GLN:HE22	2:J:132:SER:HB2	1.77	0.49
2:J:192:VAL:HG22	2:J:211:ASN:OD1	2.13	0.49
1:M:34:TRP:HB2	1:M:51:ILE:CG2	2.43	0.49
2:R:156:GLN:HB3	2:R:159:ASN:HD21	1.77	0.49
3:W:4:ASN:HA	3:X:46:TRP:CE2	2.48	0.49
3:W:34:SER:HB3	3:W:84:THR:H	1.76	0.49
2:F:116:VAL:HA	2:F:136:LEU:O	2.12	0.48
3:L:74:VAL:HA	3:L:77:GLU:HG3	1.95	0.48
1:U:32:SER:HB2	1:U:34:TRP:CZ2	2.48	0.48
3:X:18:ASP:OD1	3:X:18:ASP:N	2.46	0.48
2:F:2:ILE:HG12	2:F:27:GLN:HG3	1.94	0.48
2:F:61:ASP:OD1	2:R:55:ARG:HB3	2.13	0.48
2:N:48:LEU:HA	2:N:59:ILE:HG13	1.95	0.48
3:T:18:ASP:OD1	3:T:18:ASP:N	2.44	0.48
3:X:61:PRO:HB3	3:X:79:ARG:CD	2.43	0.48
3:D:34:SER:HB3	3:D:84:THR:N	2.28	0.48
2:F:104:LYS:HE2	2:F:106:GLU:HB3	1.94	0.48
3:G:51:VAL:HG12	3:G:82:PHE:CD1	2.47	0.48
3:H:63:THR:HG21	3:H:69:TYR:HE2	1.78	0.48
2:J:95:SER:CB	3:L:79:ARG:HH22	2.26	0.48
1:M:129:PRO:HA	1:M:155:TYR:HB3	1.95	0.48
3:T:47:LEU:HD12	3:T:47:LEU:H	1.78	0.48
3:W:54:THR:CB	3:W:80:LYS:O	2.60	0.48
2:B:146:LYS:HE2	2:B:148:GLN:CD	2.39	0.48
1:I:159:PRO:O	1:I:210:HIS:HD2	1.95	0.48
2:J:7:SER:HA	2:J:8:PRO:C	2.37	0.48
2:J:122:SER:OG	2:J:125:GLN:HB2	2.13	0.48
2:J:125:GLN:HE22	2:J:132:SER:CB	2.25	0.48
1:M:99:MET:HE3	3:O:19:TYR:CE2	2.48	0.48
1:M:153:LYS:NZ	1:M:181:GLN:OE1	2.46	0.48
2:N:56:ALA:HB3	2:N:59:ILE:HG12	1.96	0.48
3:O:42:VAL:HG21	3:O:51:VAL:HG21	1.96	0.48
3:T:61:PRO:HB3	3:T:79:ARG:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:GLY:HA2	1:I:164:TRP:CZ2	2.49	0.48
1:Q:90:THR:HG23	1:Q:120:THR:HA	1.95	0.48
2:R:36:TRP:CD2	2:R:74:LEU:HB2	2.49	0.48
2:V:135:CYS:HB2	2:V:149:TRP:CZ2	2.48	0.48
1:A:11:LEU:HD12	1:A:120:THR:O	2.14	0.48
1:E:6:GLU:CD	1:E:116:GLY:H	2.20	0.48
3:G:8:TYR:HB3	3:G:47:LEU:HD11	1.94	0.48
2:N:34:ILE:HG13	2:N:72:PHE:CD1	2.49	0.48
3:X:43:LEU:HD12	3:X:43:LEU:HA	1.62	0.48
1:M:6:GLU:HG3	1:M:95:CYS:SG	2.53	0.48
1:M:179:VAL:HG22	1:M:187:SER:O	2.13	0.48
3:G:17:SER:HB2	3:G:80:LYS:NZ	2.29	0.48
1:M:6:GLU:OE2	1:M:114:GLY:HA3	2.13	0.48
1:M:178:ALA:HB1	1:M:186:TYR:HB3	1.96	0.48
2:N:187:TYR:HA	2:N:193:TYR:OH	2.14	0.48
3:O:3:CYS:SG	3:O:5:GLY:O	2.72	0.48
2:B:198:THR:HG23	2:B:205:PRO:HG3	1.94	0.48
3:O:54:THR:O	3:O:61:PRO:HA	2.13	0.47
1:Q:6:GLU:HG3	1:Q:95:CYS:SG	2.54	0.47
1:Q:105:GLY:HA2	3:T:53:ASP:HB3	1.96	0.47
1:E:12:VAL:O	1:E:121:VAL:HA	2.14	0.47
1:M:85:VAL:HB	1:M:121:VAL:HG21	1.97	0.47
2:B:133:VAL:HB	2:B:180:LEU:HB3	1.96	0.47
3:C:36:LEU:HD13	3:C:55:TRP:HB3	1.95	0.47
2:F:18:ARG:HG3	2:F:77:SER:HA	1.96	0.47
3:L:20:LYS:HB3	3:L:24:ASP:HB2	1.97	0.47
2:V:31:THR:HG22	2:V:31:THR:O	2.14	0.47
1:A:18:LEU:HG	1:A:119:VAL:HG11	1.95	0.47
3:C:48:ILE:HG23	3:C:64:LYS:HE2	1.97	0.47
3:H:22:PHE:CZ	3:H:59:GLY:HA2	2.50	0.47
2:R:48:LEU:C	2:R:49:ILE:HG12	2.38	0.47
3:S:20:LYS:N	3:S:78:VAL:HG23	2.30	0.47
2:V:110:THR:O	2:V:111:VAL:C	2.58	0.47
2:B:41:ARG:NE	2:B:166:GLU:HG3	2.29	0.47
3:S:8:TYR:HD2	3:S:9:GLN:CD	2.22	0.47
1:U:64:ARG:NH1	3:X:76:GLN:HB2	2.28	0.47
1:A:6:GLU:CD	1:A:116:GLY:H	2.23	0.47
1:U:66:ARG:HD2	1:U:83:SER:O	2.14	0.47
2:V:106:GLU:OE1	2:V:174:TYR:OH	2.33	0.47
3:L:24:ASP:O	3:L:28:ASN:HB2	2.14	0.47
1:M:18:LEU:HB2	1:M:85:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:90:GLN:HB2	2:R:99:PHE:CD1	2.49	0.47
3:T:35:THR:O	3:T:83:CYS:HA	2.14	0.47
3:X:36:LEU:O	3:X:57:SER:HB3	2.15	0.47
1:A:105:GLY:HA2	3:D:53:ASP:CB	2.42	0.47
2:B:36:TRP:CE2	2:B:74:LEU:HB2	2.50	0.47
2:J:32:ASN:HB3	2:J:52:ALA:HB2	1.97	0.47
1:A:59:TYR:HB2	1:A:64:ARG:HG3	1.97	0.47
1:A:94:TYR:CE1	2:B:44:ALA:HA	2.50	0.47
2:B:109:ARG:HD2	2:B:171:ASP:O	2.14	0.47
2:R:55:ARG:NH1	2:R:63:PHE:O	2.48	0.47
2:F:139:ASN:C	2:F:173:THR:HB	2.40	0.47
2:N:36:TRP:CE3	2:N:74:LEU:HB2	2.50	0.47
1:Q:102:SER:CB	3:T:52:GLU:HG3	2.45	0.47
1:U:203:THR:HG23	1:U:220:LYS:HE3	1.97	0.47
3:C:49:ASP:OD1	3:C:64:LYS:NZ	2.43	0.46
3:D:68:ASP:O	3:D:69:TYR:HD1	1.97	0.46
2:F:114:PRO:HB3	2:F:140:PHE:CD1	2.51	0.46
2:F:137:LEU:HB3	2:F:140:PHE:CE1	2.50	0.46
1:M:163:SER:OG	1:M:207:ASN:HB2	2.14	0.46
1:U:24:VAL:HG11	1:U:34:TRP:CH2	2.49	0.46
1:U:102:SER:HB3	3:X:52:GLU:HB3	1.97	0.46
1:U:160:VAL:HG21	1:U:188:LEU:HD21	1.97	0.46
2:V:202:LEU:HD13	2:V:206:VAL:H	1.79	0.46
1:I:133:PRO:HD2	2:J:122:SER:CB	2.46	0.46
2:J:86:VAL:HA	2:J:103:THR:O	2.15	0.46
3:L:16:HIS:HB3	3:L:18:ASP:OD1	2.14	0.46
1:M:180:LEU:HD13	1:M:186:TYR:CZ	2.50	0.46
3:O:55:TRP:CD1	3:O:81:TYR:HB3	2.50	0.46
1:Q:29:ILE:HA	1:Q:34:TRP:CZ2	2.49	0.46
2:R:8:PRO:O	2:R:103:THR:HG23	2.15	0.46
2:B:94:SER:HB2	3:D:69:TYR:CE2	2.51	0.46
2:F:9:ALA:HB2	2:J:196:GLU:OE2	2.16	0.46
1:I:67:VAL:CG2	1:I:82:LEU:HD13	2.46	0.46
3:P:73:ASP:C	3:P:75:SER:H	2.23	0.46
2:V:143:ARG:HB2	2:V:174:TYR:CE2	2.50	0.46
3:G:17:SER:HB2	3:G:80:LYS:HZ2	1.81	0.46
2:J:87:TYR:O	2:J:102:GLY:HA2	2.15	0.46
2:V:19:ALA:HB3	2:V:76:ILE:HB	1.97	0.46
1:A:109:TRP:HH2	3:C:19:TYR:CD1	2.34	0.46
3:D:18:ASP:OD1	3:D:18:ASP:N	2.36	0.46
2:R:1:GLU:HG3	2:R:98:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:42:VAL:HG12	3:W:47:LEU:HD12	1.97	0.46
3:X:61:PRO:HB3	3:X:79:ARG:HD3	1.97	0.46
1:E:101:ALA:HB1	2:F:33:TYR:CE2	2.50	0.46
1:U:6:GLU:HG3	1:U:95:CYS:SG	2.55	0.46
2:F:146:LYS:HE2	2:F:148:GLN:CD	2.41	0.46
3:H:77:GLU:OE1	3:H:79:ARG:NH2	2.48	0.46
3:L:39:LYS:HG3	3:L:62:ILE:HG23	1.97	0.46
3:O:35:THR:O	3:O:84:THR:HG22	2.15	0.46
1:Q:90:THR:HG1	1:Q:121:VAL:H	1.61	0.46
1:Q:107:LEU:HD22	2:R:97:VAL:HG23	1.97	0.46
3:T:15:LEU:HD13	3:T:82:PHE:CZ	2.51	0.46
3:D:34:SER:HB3	3:D:84:THR:H	1.81	0.46
1:E:164:TRP:HB3	1:E:169:LEU:HB3	1.98	0.46
3:G:55:TRP:HA	3:G:55:TRP:CE3	2.51	0.46
3:O:8:TYR:HB3	3:O:47:LEU:HD11	1.97	0.46
3:S:15:LEU:HD12	3:T:50:TYR:CD1	2.50	0.46
1:A:157:PRO:HD2	1:A:212:PRO:CB	2.45	0.46
2:F:187:TYR:HA	2:F:193:TYR:OH	2.15	0.46
3:H:20:LYS:HB3	3:H:24:ASP:CB	2.44	0.46
1:I:129:PRO:HB3	1:I:155:TYR:CB	2.39	0.46
3:K:15:LEU:HD21	3:K:17:SER:HB3	1.98	0.46
3:K:42:VAL:HG12	3:K:47:LEU:HD12	1.97	0.46
1:Q:26:GLY:HA2	3:S:71:ASP:HB2	1.97	0.46
2:B:36:TRP:CD2	2:B:74:LEU:HB2	2.50	0.46
3:L:54:THR:HA	3:L:80:LYS:O	2.16	0.46
3:L:58:ASP:N	3:L:58:ASP:OD1	2.49	0.46
1:M:9:PRO:HD2	1:M:19:SER:O	2.16	0.46
1:M:51:ILE:HD12	1:M:57:ALA:HB2	1.98	0.46
3:S:15:LEU:HA	3:S:15:LEU:HD23	1.69	0.46
3:S:36:LEU:HD13	3:S:55:TRP:HB3	1.98	0.46
3:T:17:SER:HB2	3:T:80:LYS:NZ	2.31	0.46
2:V:95:SER:HB2	3:X:79:ARG:HH22	1.81	0.46
2:V:194:ALA:HA	2:V:209:SER:HA	1.98	0.46
1:I:164:TRP:CH2	1:I:206:CYS:HB3	2.50	0.45
2:J:141:TYR:CD1	2:J:142:PRO:HA	2.51	0.45
2:F:41:ARG:NE	2:F:166:GLU:HG3	2.31	0.45
2:F:151:VAL:HG22	2:F:193:TYR:CD2	2.51	0.45
1:I:34:TRP:HB3	1:I:78:PHE:CE2	2.51	0.45
3:S:46:TRP:CZ3	3:T:4:ASN:O	2.65	0.45
1:U:160:VAL:CG2	1:U:188:LEU:HD21	2.46	0.45
3:X:39:LYS:HG3	3:X:62:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LEU:HB3	1:E:221:VAL:HG11	1.98	0.45
1:I:104:PHE:HB3	3:L:80:LYS:HD2	1.98	0.45
1:I:131:VAL:HB	1:I:217:VAL:HG11	1.97	0.45
1:I:198:SER:HB2	1:I:202:GLN:HB3	1.98	0.45
2:J:19:ALA:HB2	2:J:79:LEU:HD11	1.98	0.45
2:J:37:TYR:HA	2:J:46:ARG:O	2.16	0.45
2:J:187:TYR:CZ	2:J:212:ARG:HG3	2.51	0.45
1:Q:154:ASP:HB3	1:Q:185:LEU:HD12	1.98	0.45
1:Q:174:HIS:CE1	2:R:139:ASN:OD1	2.69	0.45
2:B:34:ILE:HD13	2:B:91:GLN:CA	2.46	0.45
1:I:93:TYR:O	1:I:116:GLY:HA2	2.15	0.45
2:J:29:VAL:HG11	2:J:34:ILE:HG12	1.98	0.45
3:K:61:PRO:O	3:K:63:THR:HG23	2.17	0.45
3:L:15:LEU:HB2	3:L:82:PHE:CE2	2.51	0.45
3:L:53:ASP:OD1	3:L:79:ARG:NH1	2.49	0.45
1:M:141:THR:HG23	1:M:196:SER:OG	2.16	0.45
3:S:15:LEU:HD12	3:T:50:TYR:CZ	2.52	0.45
1:A:28:SER:HB3	3:C:69:TYR:CZ	2.51	0.45
2:F:114:PRO:HD2	2:F:202:LEU:HG	1.98	0.45
1:I:164:TRP:CZ2	1:I:206:CYS:HB3	2.52	0.45
1:Q:31:THR:O	1:Q:53:ASN:HB3	2.16	0.45
1:U:31:THR:HA	1:U:53:ASN:HD22	1.82	0.45
1:U:34:TRP:HB3	1:U:78:PHE:CZ	2.52	0.45
3:X:72:SER:HB2	3:X:74:VAL:HG13	1.98	0.45
1:A:131:VAL:HG21	1:A:217:VAL:HB	1.97	0.45
2:B:47:LEU:HD23	2:B:56:ALA:HB2	1.99	0.45
2:B:63:PHE:HZ	2:B:83:ASP:OD1	1.98	0.45
1:I:40:PRO:HB2	1:I:43:LYS:HD2	1.98	0.45
2:N:90:GLN:HE21	2:N:97:VAL:HG13	1.81	0.45
1:U:29:ILE:HG22	3:W:69:TYR:HH	1.78	0.45
1:E:101:ALA:HB2	1:E:108:GLY:HA2	1.98	0.45
3:G:76:GLN:HE21	1:Q:1:LEU:HB2	1.82	0.45
2:B:34:ILE:CD1	2:B:91:GLN:HB3	2.47	0.45
1:E:210:HIS:CD2	1:E:212:PRO:HD2	2.52	0.45
1:I:38:ARG:NH2	1:I:63:LEU:HD21	2.32	0.45
1:I:155:TYR:CE1	1:I:160:VAL:HG13	2.52	0.45
2:N:34:ILE:HG13	2:N:72:PHE:CE1	2.52	0.45
2:V:2:ILE:HG12	2:V:27:GLN:HG2	1.98	0.45
1:A:36:TRP:O	1:A:48:ILE:HB	2.16	0.45
2:B:137:LEU:HB2	2:B:176:LEU:HB3	1.98	0.45
2:F:114:PRO:CA	2:F:140:PHE:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:LYS:HB3	2:F:191:LYS:HE3	1.80	0.45
2:J:34:ILE:HG13	2:J:72:PHE:CZ	2.52	0.45
2:R:154:ALA:O	2:R:156:GLN:NE2	2.50	0.45
3:S:29:CYS:HB3	3:S:34:SER:C	2.41	0.45
2:V:34:ILE:HG13	2:V:72:PHE:CG	2.52	0.45
3:H:45:THR:OG1	3:H:47:LEU:HB2	2.17	0.45
2:J:41:ARG:CZ	2:J:166:GLU:HB2	2.47	0.45
1:M:29:ILE:HA	1:M:34:TRP:HZ2	1.82	0.45
1:E:169:LEU:HD12	1:E:169:LEU:HA	1.84	0.44
2:F:126:LEU:HA	2:F:126:LEU:HD23	1.69	0.44
3:O:22:PHE:CE1	3:O:59:GLY:HA2	2.52	0.44
3:P:23:GLU:OE1	3:P:26:LYS:HE3	2.17	0.44
1:Q:102:SER:HB2	1:Q:105:GLY:CA	2.46	0.44
1:Q:115:GLN:HA	2:R:44:ALA:CB	2.44	0.44
3:T:3:CYS:HB2	3:T:7:TYR:HD2	1.81	0.44
1:U:5:GLN:NE2	1:U:6:GLU:O	2.43	0.44
1:U:94:TYR:CE1	1:U:116:GLY:HA3	2.52	0.44
3:D:16:HIS:CE1	3:D:83:CYS:SG	3.10	0.44
3:P:38:ASN:HB3	3:P:41:ASP:OD2	2.17	0.44
2:R:48:LEU:O	2:R:49:ILE:CD1	2.66	0.44
2:R:48:LEU:HD11	2:R:87:TYR:CE1	2.51	0.44
2:R:95:SER:CB	3:T:79:ARG:HH22	2.30	0.44
1:U:4:LEU:HD21	1:U:34:TRP:CZ3	2.52	0.44
1:U:175:THR:HA	1:U:190:SER:HA	1.98	0.44
1:E:219:LYS:HD2	1:E:219:LYS:HA	1.73	0.44
2:F:8:PRO:O	2:F:103:THR:HG23	2.16	0.44
3:G:19:TYR:HD2	3:G:78:VAL:HG23	1.83	0.44
3:H:45:THR:O	3:H:48:ILE:HG22	2.17	0.44
1:I:20:LEU:HD11	1:I:119:VAL:HG21	2.00	0.44
1:I:175:THR:HG23	1:I:190:SER:HB2	1.99	0.44
2:J:64:SER:O	2:J:74:LEU:HD12	2.17	0.44
2:J:111:VAL:HG11	2:J:200:GLN:HG2	1.99	0.44
2:J:137:LEU:HD13	2:J:176:LEU:HD22	2.00	0.44
1:Q:17:THR:HG23	1:Q:83:SER:HA	2.00	0.44
1:M:129:PRO:HB2	1:M:152:VAL:HG13	1.99	0.44
2:N:121:PRO:HG2	2:N:187:TYR:CZ	2.53	0.44
1:Q:97:ARG:HB3	1:Q:111:ASP:O	2.18	0.44
2:R:135:CYS:HB2	2:R:149:TRP:CZ2	2.53	0.44
3:W:22:PHE:CZ	3:W:59:GLY:HA2	2.53	0.44
1:A:191:VAL:HG21	2:B:136:LEU:HD22	1.98	0.44
2:B:34:ILE:HA	2:B:90:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:GLU:N	2:F:144:GLU:OE1	2.50	0.44
1:I:13:LYS:HB2	1:I:16:GLU:OE1	2.18	0.44
1:I:178:ALA:HA	1:I:188:LEU:HB3	2.00	0.44
2:N:38:GLN:HB2	2:N:48:LEU:HD11	2.00	0.44
1:U:50:PHE:HE1	1:U:52:TYR:CD2	2.36	0.44
1:U:109:TRP:CD1	2:V:47:LEU:HD22	2.53	0.44
3:W:66:THR:HG22	3:W:66:THR:O	2.17	0.44
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.53	0.44
1:A:198:SER:O	1:A:202:GLN:N	2.50	0.44
2:B:187:TYR:HA	2:B:193:TYR:OH	2.17	0.44
2:J:15:PRO:HD3	2:J:107:ILE:HG23	1.99	0.44
2:J:85:ALA:O	2:J:87:TYR:CD1	2.71	0.44
1:Q:160:VAL:CG1	1:Q:188:LEU:HD21	2.47	0.44
2:R:34:ILE:HG13	2:R:72:PHE:CG	2.53	0.44
3:S:26:LYS:HB3	3:S:26:LYS:HE2	1.70	0.44
2:V:168:ASP:HB3	2:V:171:ASP:OD1	2.17	0.44
3:W:37:PRO:HD3	3:W:82:PHE:O	2.18	0.44
1:A:87:ALA:HA	1:A:121:VAL:HB	1.99	0.44
2:J:187:TYR:O	2:J:212:ARG:HD3	2.17	0.44
2:N:4:LEU:HD23	2:N:25:ALA:HA	2.00	0.44
1:Q:175:THR:HG23	1:Q:190:SER:HB2	1.99	0.44
2:R:12:SER:C	2:R:108:LYS:HB2	2.43	0.44
2:V:109:ARG:HD2	2:V:171:ASP:O	2.18	0.44
2:J:95:SER:HB2	3:L:79:ARG:HH22	1.82	0.44
1:M:166:SER:N	1:M:207:ASN:OD1	2.50	0.44
2:N:126:LEU:HD21	2:N:187:TYR:HD2	1.82	0.44
3:D:68:ASP:C	3:D:69:TYR:HD1	2.26	0.44
3:T:37:PRO:HD3	3:T:82:PHE:O	2.18	0.44
3:D:53:ASP:OD1	3:D:79:ARG:NH1	2.51	0.43
3:G:4:ASN:HB3	3:H:46:TRP:CG	2.53	0.43
1:Q:134:LEU:HB3	2:R:119:PHE:CD2	2.53	0.43
2:R:19:ALA:HB2	2:R:79:LEU:HD11	2.00	0.43
2:R:144:GLU:O	2:R:199:HIS:HD2	2.01	0.43
2:R:192:VAL:HG22	2:R:211:ASN:OD1	2.18	0.43
1:U:104:PHE:HZ	3:W:50:TYR:HA	1.82	0.43
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.78	0.43
2:B:148:GLN:HB3	2:B:155:LEU:CD1	2.48	0.43
3:D:37:PRO:HD3	3:D:82:PHE:O	2.18	0.43
1:I:28:SER:HB2	3:K:69:TYR:CE2	2.53	0.43
2:N:6:GLN:HA	2:N:22:SER:O	2.19	0.43
1:Q:67:VAL:HG22	1:Q:82:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:58:ASP:N	3:S:58:ASP:OD1	2.51	0.43
1:A:6:GLU:HB3	1:A:117:THR:HG22	2.01	0.43
1:A:178:ALA:HB1	1:A:186:TYR:HB3	1.99	0.43
2:B:33:TYR:HB3	2:B:92:TYR:CD2	2.53	0.43
3:H:61:PRO:HB3	3:H:79:ARG:CD	2.48	0.43
3:O:74:VAL:HB	3:O:77:GLU:HG3	2.00	0.43
1:Q:100:ARG:H	1:Q:100:ARG:HG3	1.55	0.43
3:T:54:THR:HB	3:T:81:TYR:HA	2.00	0.43
1:U:29:ILE:HG12	1:U:71:VAL:CG2	2.48	0.43
2:B:18:ARG:HG3	2:B:77:SER:HA	2.00	0.43
2:B:144:GLU:CD	2:B:144:GLU:N	2.74	0.43
1:E:132:PHE:HB3	2:F:122:SER:OG	2.18	0.43
2:R:41:ARG:CZ	2:R:166:GLU:HB3	2.48	0.43
1:U:163:SER:OG	1:U:207:ASN:HB2	2.17	0.43
2:V:164:VAL:HG22	2:V:176:LEU:HD12	2.00	0.43
2:B:126:LEU:O	2:B:184:LYS:HD2	2.18	0.43
2:F:149:TRP:HB2	2:F:156:GLN:HB2	2.01	0.43
2:R:152:ASP:O	2:R:153:ASN:HB2	2.18	0.43
2:V:49:ILE:HG21	2:V:65:GLY:HA3	1.99	0.43
3:G:49:ASP:HB3	3:H:15:LEU:HD23	2.01	0.43
1:I:66:ARG:HD2	1:I:83:SER:O	2.19	0.43
3:K:22:PHE:CZ	3:K:59:GLY:HA2	2.53	0.43
1:Q:205:ILE:HG12	1:Q:220:LYS:CA	2.45	0.43
2:R:113:ALA:HB1	2:R:202:LEU:CD2	2.49	0.43
2:R:160:SER:HA	2:R:179:THR:O	2.17	0.43
1:A:50:PHE:CZ	2:B:97:VAL:HG21	2.53	0.43
3:C:48:ILE:CG1	3:C:64:LYS:HG2	2.49	0.43
1:I:14:PRO:C	1:I:16:GLU:H	2.25	0.43
1:I:36:TRP:CD1	1:I:69:ILE:HG12	2.54	0.43
2:J:159:ASN:OD1	2:J:159:ASN:N	2.51	0.43
2:B:152:ASP:O	2:B:153:ASN:C	2.62	0.43
1:I:29:ILE:HA	1:I:34:TRP:CZ2	2.53	0.43
2:N:109:ARG:NH2	2:N:112:ALA:HB2	2.34	0.43
3:O:37:PRO:HD2	3:O:55:TRP:O	2.19	0.43
2:R:114:PRO:HB3	2:R:140:PHE:HB3	2.00	0.43
1:E:36:TRP:CD1	1:E:80:LEU:HB2	2.54	0.43
2:F:62:ARG:O	2:F:76:ILE:HA	2.19	0.43
1:M:158:GLU:HA	1:M:159:PRO:HA	1.93	0.43
1:Q:129:PRO:HB3	1:Q:155:TYR:HB3	2.01	0.43
1:Q:148:LEU:HA	2:R:119:PHE:HE2	1.83	0.43
3:S:19:TYR:HD1	3:S:78:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:58:ASN:OD1	3:X:78:VAL:HG22	2.18	0.43
1:E:18:LEU:HD23	1:E:19:SER:N	2.34	0.43
1:E:210:HIS:ND1	1:E:213:SER:OG	2.45	0.43
1:I:56:SER:HB3	3:L:19:TYR:HB2	2.00	0.43
1:I:172:GLY:O	1:I:192:VAL:HA	2.19	0.43
3:K:61:PRO:HB3	3:K:79:ARG:HD2	2.00	0.43
1:Q:12:VAL:HB	1:Q:121:VAL:HG22	2.01	0.43
1:Q:156:PHE:O	1:Q:210:HIS:HE1	2.02	0.43
2:R:114:PRO:HD3	2:R:199:HIS:ND1	2.33	0.43
3:S:29:CYS:O	3:S:34:SER:O	2.37	0.43
2:V:35:ALA:HA	2:V:49:ILE:O	2.19	0.43
3:W:54:THR:CA	3:W:80:LYS:O	2.67	0.43
1:A:203:THR:HG23	1:A:220:LYS:HE3	2.01	0.42
2:B:29:VAL:HG21	2:B:34:ILE:HD11	2.01	0.42
2:B:48:LEU:HD11	2:B:87:TYR:HE2	1.84	0.42
3:C:37:PRO:HB2	3:C:62:ILE:HD11	2.00	0.42
2:J:4:LEU:HD23	2:J:4:LEU:HA	1.85	0.42
2:N:83:ASP:O	2:N:87:TYR:OH	2.32	0.42
3:O:61:PRO:O	3:O:63:THR:HG23	2.19	0.42
3:P:54:THR:HB	3:P:81:TYR:HA	2.01	0.42
2:V:19:ALA:HB2	2:V:79:LEU:HD11	2.01	0.42
2:R:182:LEU:HD11	2:R:193:TYR:HE2	1.84	0.42
3:S:51:VAL:HG23	3:S:62:ILE:HG21	2.00	0.42
1:U:22:CYS:HB3	1:U:78:PHE:CE1	2.54	0.42
2:V:21:LEU:O	2:V:73:THR:HA	2.18	0.42
2:B:149:TRP:CE2	2:B:180:LEU:HB2	2.54	0.42
2:J:25:ALA:HB3	2:J:70:THR:HA	2.01	0.42
2:J:33:TYR:HB3	2:J:92:TYR:CD2	2.54	0.42
2:N:184:LYS:O	2:N:188:GLU:HG3	2.19	0.42
1:Q:148:LEU:HA	2:R:119:PHE:CE2	2.54	0.42
2:R:50:TYR:O	2:R:51:ASP:C	2.63	0.42
2:R:55:ARG:HG2	2:R:59:ILE:HB	2.01	0.42
3:S:6:LEU:CD1	3:S:47:LEU:HD23	2.49	0.42
3:W:34:SER:HB3	3:W:84:THR:N	2.35	0.42
1:E:67:VAL:HG23	1:E:82:LEU:HD13	2.00	0.42
2:F:36:TRP:CD2	2:F:74:LEU:HB2	2.54	0.42
2:F:55:ARG:HD2	2:F:59:ILE:O	2.19	0.42
3:G:45:THR:O	3:G:48:ILE:HG22	2.19	0.42
1:I:18:LEU:HG	1:I:119:VAL:HG11	2.00	0.42
3:K:15:LEU:HD13	3:K:82:PHE:CZ	2.55	0.42
1:M:188:LEU:HD12	1:M:188:LEU:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:121:PRO:HD2	2:N:187:TYR:OH	2.19	0.42
1:Q:20:LEU:HD23	1:Q:20:LEU:HA	1.76	0.42
3:T:42:VAL:HG21	3:T:51:VAL:HG21	2.00	0.42
1:U:51:ILE:CD1	1:U:70:SER:HA	2.49	0.42
3:X:16:HIS:HE2	3:X:83:CYS:HB2	1.84	0.42
1:A:16:GLU:O	1:A:85:VAL:HG22	2.19	0.42
1:A:18:LEU:CD2	1:A:20:LEU:HG	2.50	0.42
2:F:49:ILE:CG2	2:F:52:ALA:O	2.64	0.42
2:F:90:GLN:HE21	2:F:97:VAL:HG13	1.85	0.42
1:I:5:GLN:HB3	1:I:23:SER:HB2	2.01	0.42
1:I:102:SER:HA	3:K:80:LYS:HZ1	1.84	0.42
1:I:149:GLY:HA2	1:I:164:TRP:CH2	2.55	0.42
1:M:180:LEU:HA	1:M:180:LEU:HD12	1.81	0.42
3:O:15:LEU:HD13	3:O:82:PHE:CZ	2.54	0.42
3:P:48:ILE:HA	3:P:51:VAL:HG22	2.01	0.42
1:Q:18:LEU:HD21	1:Q:20:LEU:HG	2.02	0.42
1:U:181:GLN:NE2	1:U:187:SER:HB2	2.35	0.42
3:W:30:ALA:O	3:W:33:SER:N	2.45	0.42
2:B:168:ASP:O	2:B:172:SER:HA	2.19	0.42
1:I:144:GLY:CA	1:I:195:PRO:HA	2.47	0.42
3:P:48:ILE:HA	3:P:48:ILE:HD12	1.77	0.42
1:Q:2:VAL:HG22	1:Q:27:GLY:CA	2.47	0.42
2:R:115:SER:HB3	2:R:117:PHE:CE1	2.54	0.42
2:V:15:PRO:HD3	2:V:107:ILE:HG23	2.01	0.42
2:F:12:SER:HB3	2:F:141:TYR:OH	2.20	0.42
1:I:47:TRP:CZ2	1:I:49:GLY:HA2	2.55	0.42
2:J:19:ALA:HB2	2:J:79:LEU:HD21	2.01	0.42
2:J:114:PRO:HA	2:J:140:PHE:HB3	2.00	0.42
3:O:22:PHE:CZ	3:O:59:GLY:HA2	2.55	0.42
1:A:60:ASN:O	1:A:64:ARG:N	2.53	0.42
1:A:63:LEU:HB3	1:A:67:VAL:HG21	2.01	0.42
3:D:61:PRO:HB3	3:D:79:ARG:CD	2.50	0.42
1:I:14:PRO:HG3	1:I:121:VAL:HG12	2.02	0.42
2:J:125:GLN:HG2	2:J:130:THR:O	2.20	0.42
1:M:6:GLU:CD	1:M:114:GLY:HA3	2.45	0.42
2:N:187:TYR:O	2:N:212:ARG:HD3	2.20	0.42
3:P:26:LYS:HG3	3:P:27:ALA:N	2.32	0.42
1:U:71:VAL:HA	1:U:78:PHE:HA	2.02	0.42
3:W:6:LEU:HD21	3:W:50:TYR:CB	2.50	0.42
3:W:13:TYR:HE2	3:W:37:PRO:HB3	1.85	0.42
3:X:3:CYS:C	3:X:5:GLY:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:ILE:HG13	2:F:94:SER:OG	2.20	0.42
1:Q:219:LYS:HD2	1:Q:219:LYS:HA	1.73	0.42
1:U:97:ARG:HB3	1:U:111:ASP:O	2.20	0.42
3:C:37:PRO:HD3	3:C:82:PHE:O	2.19	0.42
1:E:9:PRO:HD2	1:E:19:SER:O	2.19	0.42
2:J:33:TYR:HD1	2:J:33:TYR:HA	1.70	0.42
1:M:29:ILE:HG13	1:M:34:TRP:NE1	2.35	0.42
1:M:124:ALA:HB3	1:M:156:PHE:CE2	2.54	0.42
3:S:22:PHE:CE1	3:S:59:GLY:HA2	2.55	0.42
1:U:50:PHE:CE1	1:U:52:TYR:CD2	3.07	0.42
2:B:8:PRO:O	2:B:103:THR:HG23	2.20	0.41
1:E:160:VAL:HG12	1:E:210:HIS:HB2	2.02	0.41
1:M:31:THR:HG21	3:O:63:THR:CG2	2.49	0.41
2:R:90:GLN:HB2	2:R:99:PHE:CE1	2.54	0.41
2:V:16:GLY:HA2	2:V:78:ARG:HG3	2.02	0.41
1:A:20:LEU:O	1:A:79:SER:HB2	2.20	0.41
1:A:37:ILE:HG23	1:A:46:GLU:O	2.19	0.41
1:A:66:ARG:HD2	1:A:83:SER:O	2.19	0.41
2:F:196:GLU:HA	2:F:207:THR:HA	2.02	0.41
1:I:136:PRO:HD3	1:I:148:LEU:HB3	2.02	0.41
3:O:36:LEU:HD13	3:O:55:TRP:HB3	2.02	0.41
3:W:61:PRO:O	3:W:63:THR:HG23	2.20	0.41
2:B:2:ILE:HG12	2:B:27:GLN:CG	2.47	0.41
1:E:2:VAL:HG21	1:E:97:ARG:NH1	2.35	0.41
2:F:121:PRO:HD2	2:F:187:TYR:OH	2.20	0.41
3:H:18:ASP:OD1	3:H:18:ASP:N	2.46	0.41
2:J:193:TYR:HB2	2:J:210:PHE:CZ	2.55	0.41
1:M:71:VAL:HA	1:M:78:PHE:HA	2.01	0.41
3:S:43:LEU:HD21	3:S:66:THR:HG22	2.01	0.41
2:V:141:TYR:CG	2:V:142:PRO:HA	2.56	0.41
2:V:155:LEU:HD12	2:V:155:LEU:HA	1.79	0.41
1:A:176:PHE:CZ	2:B:177:SER:HB3	2.56	0.41
1:E:51:ILE:HD12	1:E:57:ALA:HB2	2.03	0.41
1:E:122:SER:HB3	1:E:156:PHE:CZ	2.56	0.41
2:F:40:ARG:NH2	2:F:82:GLU:HG3	2.36	0.41
1:M:29:ILE:HA	1:M:34:TRP:CZ2	2.56	0.41
2:N:37:TYR:HA	2:N:46:ARG:O	2.20	0.41
3:O:25:ALA:HB1	3:O:81:TYR:CG	2.55	0.41
1:Q:32:SER:OG	1:Q:97:ARG:HD2	2.21	0.41
1:Q:52:TYR:OH	1:Q:106:SER:HB2	2.20	0.41
1:E:34:TRP:HB3	1:E:78:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:ASN:HD22	3:H:46:TRP:CD1	2.39	0.41
3:L:24:ASP:O	3:L:28:ASN:N	2.46	0.41
3:L:38:ASN:O	3:L:42:VAL:HG22	2.20	0.41
2:N:106:GLU:OE1	2:N:174:TYR:OH	2.23	0.41
2:R:41:ARG:O	2:R:41:ARG:HG3	2.21	0.41
3:S:15:LEU:CG	3:T:50:TYR:CZ	3.01	0.41
3:T:43:LEU:HA	3:T:43:LEU:HD12	1.78	0.41
1:U:105:GLY:HA2	3:X:53:ASP:CB	2.50	0.41
1:A:48:ILE:HG23	1:A:67:VAL:HG21	2.03	0.41
1:A:209:ASN:OD1	1:A:216:LYS:HG2	2.21	0.41
3:D:9:GLN:C	3:D:11:SER:H	2.29	0.41
3:G:18:ASP:N	3:G:18:ASP:OD1	2.51	0.41
3:H:39:LYS:HE2	3:H:43:LEU:HD22	2.02	0.41
2:J:125:GLN:O	2:J:128:SER:OG	2.27	0.41
3:L:36:LEU:HD23	3:L:82:PHE:O	2.20	0.41
3:P:55:TRP:HZ2	3:P:77:GLU:O	2.03	0.41
2:R:151:VAL:HG22	2:R:193:TYR:CD2	2.55	0.41
1:U:29:ILE:CG2	1:U:73:THR:HA	2.51	0.41
2:V:49:ILE:CG2	2:V:52:ALA:O	2.68	0.41
2:V:116:VAL:O	2:V:208:LYS:HE3	2.20	0.41
1:A:139:LYS:HD2	1:A:139:LYS:HA	1.78	0.41
2:B:60:PRO:HB2	2:B:62:ARG:HG2	2.03	0.41
2:B:90:GLN:HG2	2:B:91:GLN:N	2.35	0.41
3:H:38:ASN:HA	3:H:57:SER:OG	2.21	0.41
1:I:144:GLY:C	1:I:195:PRO:HA	2.46	0.41
3:P:18:ASP:OD1	3:P:18:ASP:N	2.54	0.41
3:W:81:TYR:CD1	3:W:81:TYR:N	2.88	0.41
1:I:33:SER:HB2	1:I:98:ARG:HE	1.84	0.41
1:I:91:ALA:HB3	1:I:93:TYR:CE1	2.56	0.41
1:I:100:ARG:HD2	1:I:103:LEU:O	2.20	0.41
3:L:16:HIS:NE2	3:L:83:CYS:SG	2.94	0.41
1:Q:34:TRP:HB3	1:Q:78:PHE:CE2	2.56	0.41
3:T:55:TRP:HE1	3:T:79:ARG:H	1.69	0.41
1:U:149:GLY:HA2	1:U:164:TRP:CH2	2.55	0.41
3:W:52:GLU:C	3:W:54:THR:H	2.29	0.41
3:X:24:ASP:O	3:X:28:ASN:HB2	2.21	0.41
1:A:32:SER:HB2	1:A:34:TRP:CZ2	2.56	0.41
2:B:80:GLU:O	2:B:81:PRO:C	2.63	0.41
1:I:157:PRO:HD2	1:I:212:PRO:CB	2.50	0.41
2:J:35:ALA:HA	2:J:49:ILE:O	2.21	0.41
2:J:141:TYR:CG	2:J:142:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:54:THR:HG21	3:L:82:PHE:CE1	2.56	0.41
1:M:109:TRP:CH2	3:O:19:TYR:CE1	3.09	0.41
2:N:33:TYR:HD1	2:N:33:TYR:HA	1.72	0.41
2:N:40:ARG:HB2	2:N:43:LEU:HD12	2.02	0.41
1:Q:169:LEU:HD21	1:Q:192:VAL:HG11	2.03	0.41
3:S:6:LEU:HD13	3:S:47:LEU:HD23	2.02	0.41
3:S:36:LEU:HD23	3:S:36:LEU:HA	1.87	0.41
3:T:6:LEU:HB3	3:T:46:TRP:CH2	2.56	0.41
2:V:36:TRP:CD2	2:V:74:LEU:HB2	2.55	0.41
2:V:49:ILE:HG21	2:V:52:ALA:O	2.21	0.41
3:W:65:THR:C	3:W:67:SER:H	2.27	0.41
1:A:34:TRP:O	1:A:50:PHE:HA	2.20	0.41
1:A:160:VAL:HG12	1:A:210:HIS:HB2	2.02	0.41
2:B:137:LEU:HD13	2:B:176:LEU:HD22	2.03	0.41
1:M:100:ARG:H	1:M:100:ARG:HG3	1.63	0.41
1:Q:115:GLN:OE1	1:Q:115:GLN:N	2.52	0.41
3:T:47:LEU:O	3:T:50:TYR:N	2.45	0.41
1:U:47:TRP:CD2	2:V:97:VAL:HB	2.56	0.41
1:U:153:LYS:HE3	2:V:130:THR:HG21	2.03	0.41
3:X:54:THR:HA	3:X:80:LYS:O	2.20	0.41
1:A:78:PHE:HZ	1:A:95:CYS:HB2	1.85	0.40
1:A:188:LEU:C	1:A:188:LEU:HD12	2.46	0.40
2:B:104:LYS:HE2	2:B:106:GLU:HB3	2.02	0.40
2:B:151:VAL:O	2:B:154:ALA:HB3	2.20	0.40
1:E:175:THR:HA	1:E:190:SER:HA	2.02	0.40
3:G:7:TYR:CZ	3:G:10:GLY:HA2	2.55	0.40
1:Q:183:SER:C	1:Q:185:LEU:H	2.29	0.40
2:B:66:SER:OG	2:B:73:THR:HB	2.21	0.40
2:B:113:ALA:HB1	2:B:202:LEU:CD2	2.52	0.40
3:G:51:VAL:HG12	3:G:82:PHE:CE1	2.55	0.40
1:A:129:PRO:HD2	1:A:215:THR:HG21	2.02	0.40
1:E:11:LEU:HD21	1:E:156:PHE:HE2	1.87	0.40
1:E:141:THR:CG2	1:E:142:SER:N	2.77	0.40
2:F:21:LEU:HD12	2:F:21:LEU:N	2.36	0.40
2:J:68:SER:O	2:J:69:GLY:C	2.64	0.40
2:J:108:LYS:HA	2:J:141:TYR:OH	2.20	0.40
1:M:34:TRP:HB3	1:M:78:PHE:CE1	2.56	0.40
1:M:99:MET:HG3	1:M:109:TRP:NE1	2.37	0.40
1:E:11:LEU:HA	1:E:120:THR:O	2.22	0.40
1:I:6:GLU:CD	1:I:116:GLY:H	2.29	0.40
1:M:181:GLN:NE2	1:M:187:SER:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:53:ASP:CG	3:P:79:ARG:HH11	2.28	0.40
3:S:8:TYR:HB3	3:S:9:GLN:OE1	2.20	0.40
3:T:8:TYR:CB	3:T:47:LEU:HD11	2.52	0.40
3:W:36:LEU:HD23	3:W:36:LEU:HA	1.91	0.40
1:A:4:LEU:HB3	1:A:22:CYS:SG	2.61	0.40
1:A:13:LYS:O	1:A:16:GLU:HB2	2.20	0.40
1:A:93:TYR:O	1:A:116:GLY:HA2	2.21	0.40
2:B:21:LEU:N	2:B:21:LEU:HD12	2.37	0.40
1:I:129:PRO:HD2	1:I:215:THR:HG21	2.02	0.40
1:M:51:ILE:HB	1:M:69:ILE:HG22	2.03	0.40
2:R:34:ILE:HA	2:R:90:GLN:O	2.21	0.40
3:S:19:TYR:HB3	3:S:78:VAL:CG2	2.51	0.40
2:V:187:TYR:CD1	2:V:193:TYR:CZ	3.10	0.40
3:W:14:ILE:HD13	3:W:14:ILE:HG21	1.84	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:GLN:OE1	3:W:76:GLN:NE2[1_455]	1.07	1.13
3:C:76:GLN:CD	3:W:76:GLN:OE1[1_455]	1.38	0.82
3:C:76:GLN:NE2	3:W:76:GLN:OE1[1_455]	1.41	0.79
3:C:76:GLN:CD	3:W:76:GLN:CD[1_455]	1.51	0.69
3:C:76:GLN:CD	3:W:76:GLN:NE2[1_455]	1.61	0.59
3:C:76:GLN:CG	3:W:76:GLN:OE1[1_455]	1.67	0.53
3:C:76:GLN:NE2	3:W:76:GLN:CD[1_455]	1.68	0.52
1:M:201:THR:O	2:R:68:SER:OG[3_645]	1.81	0.39
3:C:76:GLN:OE1	3:W:76:GLN:CD[1_455]	1.94	0.26

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	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
1	E	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
1	I	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
1	M	219/221 (99%)	209 (95%)	10 (5%)	0	100	100
1	Q	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
1	U	219/221 (99%)	211 (96%)	8 (4%)	0	100	100
2	B	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
2	F	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	J	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	N	213/215 (99%)	208 (98%)	5 (2%)	0	100	100
2	R	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
2	V	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
3	C	82/152 (54%)	74 (90%)	8 (10%)	0	100	100
3	D	82/152 (54%)	73 (89%)	9 (11%)	0	100	100
3	G	82/152 (54%)	77 (94%)	5 (6%)	0	100	100
3	H	82/152 (54%)	75 (92%)	7 (8%)	0	100	100
3	K	82/152 (54%)	79 (96%)	3 (4%)	0	100	100
3	L	82/152 (54%)	77 (94%)	5 (6%)	0	100	100
3	O	82/152 (54%)	77 (94%)	5 (6%)	0	100	100
3	P	82/152 (54%)	78 (95%)	4 (5%)	0	100	100
3	S	82/152 (54%)	78 (95%)	4 (5%)	0	100	100
3	T	82/152 (54%)	74 (90%)	8 (10%)	0	100	100
3	W	82/152 (54%)	74 (90%)	8 (10%)	0	100	100
3	X	82/152 (54%)	75 (92%)	7 (8%)	0	100	100
All	All	3576/4440 (80%)	3398 (95%)	178 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	186 (98%)	3 (2%)	58	79
1	E	189/189 (100%)	185 (98%)	4 (2%)	48	74
1	I	189/189 (100%)	185 (98%)	4 (2%)	48	74
1	M	189/189 (100%)	182 (96%)	7 (4%)	29	62
1	Q	189/189 (100%)	186 (98%)	3 (2%)	58	79
1	U	189/189 (100%)	180 (95%)	9 (5%)	21	55
2	B	185/185 (100%)	183 (99%)	2 (1%)	70	86
2	F	185/185 (100%)	178 (96%)	7 (4%)	28	60
2	J	185/185 (100%)	182 (98%)	3 (2%)	58	79
2	N	185/185 (100%)	183 (99%)	2 (1%)	70	86
2	R	185/185 (100%)	181 (98%)	4 (2%)	47	73
2	V	185/185 (100%)	179 (97%)	6 (3%)	34	65
3	C	76/130 (58%)	74 (97%)	2 (3%)	41	70
3	D	76/130 (58%)	76 (100%)	0	100	100
3	G	76/130 (58%)	75 (99%)	1 (1%)	65	83
3	H	76/130 (58%)	71 (93%)	5 (7%)	14	45
3	K	76/130 (58%)	73 (96%)	3 (4%)	27	60
3	L	76/130 (58%)	74 (97%)	2 (3%)	41	70
3	O	76/130 (58%)	73 (96%)	3 (4%)	27	60
3	P	76/130 (58%)	76 (100%)	0	100	100
3	S	76/130 (58%)	71 (93%)	5 (7%)	14	45
3	T	76/130 (58%)	73 (96%)	3 (4%)	27	60
3	W	76/130 (58%)	71 (93%)	5 (7%)	14	45
3	X	76/130 (58%)	73 (96%)	3 (4%)	27	60
All	All	3156/3804 (83%)	3070 (97%)	86 (3%)	40	69

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	141	THR
1	A	145	THR
2	B	31	THR

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Mol	Chain	Res	Type
2	B	191	LYS
3	C	7	TYR
3	C	35	THR
1	E	15	SER
1	E	139	LYS
1	E	157	PRO
1	E	158	GLU
2	F	34	ILE
2	F	82	GLU
2	F	163	SER
2	F	170	LYS
2	F	171	ASP
2	F	191	LYS
2	F	192	VAL
3	G	52	GLU
3	H	64	LYS
3	H	67	SER
3	H	69	TYR
3	H	70	GLN
3	H	71	ASP
1	I	110	LEU
1	I	139	LYS
1	I	145	THR
1	I	179	VAL
2	J	31	THR
2	J	184	LYS
2	J	186	ASP
3	K	70	GLN
3	K	71	ASP
3	K	72	SER
3	L	68	ASP
3	L	70	GLN
1	M	54	SER
1	M	100	ARG
1	M	102	SER
1	M	110	LEU
1	M	159	PRO
1	M	160	VAL
1	M	161	THR
2	N	126	LEU
2	N	191	LYS
3	O	52	GLU

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Mol	Chain	Res	Type
3	O	70	GLN
3	O	74	VAL
1	Q	62	SER
1	Q	100	ARG
1	Q	102	SER
2	R	22	SER
2	R	27	GLN
2	R	49	ILE
2	R	51	ASP
3	S	26	LYS
3	S	32	GLU
3	S	68	ASP
3	S	69	TYR
3	S	75	SER
3	T	6	LEU
3	T	43	LEU
3	T	76	GLN
1	U	14	PRO
1	U	92	VAL
1	U	100	ARG
1	U	102	SER
1	U	127	LYS
1	U	140	SER
1	U	171	SER
1	U	193	THR
1	U	196	SER
2	V	55	ARG
2	V	95	SER
2	V	184	LYS
2	V	191	LYS
2	V	214	GLU
2	V	215	CYS
3	W	26	LYS
3	W	74	VAL
3	W	76	GLN
3	W	77	GLU
3	W	80	LYS
3	X	3	CYS
3	X	4	ASN
3	X	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
3	D	16	HIS
3	D	60	ASN
3	G	28	ASN
3	H	38	ASN
3	K	16	HIS
3	L	60	ASN
1	M	58	ASN
1	M	76	ASN
1	Q	5	GLN
1	Q	115	GLN
1	Q	174	HIS
1	Q	209	ASN
3	S	60	ASN
3	T	16	HIS
3	T	28	ASN
1	U	76	ASN
3	W	76	GLN
3	X	60	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	221/221 (100%)	-0.12	6 (2%) 56 40	17, 34, 62, 99	0
1	E	221/221 (100%)	0.12	16 (7%) 23 16	17, 35, 71, 105	0
1	I	221/221 (100%)	-0.12	12 (5%) 32 22	15, 26, 49, 112	0
1	M	221/221 (100%)	-0.13	8 (3%) 46 32	14, 27, 49, 107	0
1	Q	221/221 (100%)	0.30	9 (4%) 42 28	26, 48, 74, 110	0
1	U	221/221 (100%)	0.66	21 (9%) 15 10	27, 50, 82, 117	0
2	B	215/215 (100%)	-0.35	3 (1%) 73 58	12, 25, 44, 67	0
2	F	215/215 (100%)	-0.26	4 (1%) 66 50	12, 25, 46, 74	0
2	J	215/215 (100%)	-0.40	0 100 100	11, 23, 44, 72	0
2	N	215/215 (100%)	-0.38	1 (0%) 87 78	11, 22, 44, 69	0
2	R	215/215 (100%)	-0.19	1 (0%) 87 78	22, 34, 52, 77	0
2	V	215/215 (100%)	-0.14	2 (0%) 81 68	20, 34, 54, 86	0
3	C	84/152 (55%)	1.15	18 (21%) 3 2	40, 65, 119, 135	0
3	D	84/152 (55%)	0.86	7 (8%) 19 13	49, 66, 100, 108	0
3	G	84/152 (55%)	1.45	18 (21%) 3 2	48, 78, 126, 135	0
3	H	84/152 (55%)	1.03	10 (11%) 10 7	49, 70, 109, 113	0
3	K	84/152 (55%)	1.16	19 (22%) 3 2	41, 69, 107, 124	0
3	L	84/152 (55%)	0.94	13 (15%) 6 4	30, 58, 95, 106	0
3	O	84/152 (55%)	1.07	16 (19%) 4 3	38, 69, 104, 111	0
3	P	84/152 (55%)	0.69	8 (9%) 15 10	31, 63, 97, 105	0
3	S	84/152 (55%)	0.88	15 (17%) 4 4	32, 51, 104, 109	0
3	T	84/152 (55%)	1.15	19 (22%) 3 2	31, 54, 91, 122	0
3	W	84/152 (55%)	0.86	15 (17%) 4 4	30, 50, 108, 126	0
3	X	84/152 (55%)	0.61	10 (11%) 10 7	34, 53, 90, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3624/4440 (81%)	0.22	251 (6%) 24 17	11, 38, 90, 135	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	140	SER	7.7
1	U	125	SER	6.5
1	U	140	SER	6.5
1	U	141	THR	5.9
3	L	70	GLN	5.8
3	T	2	SER	5.7
3	O	69	TYR	5.6
1	U	137	SER	5.6
1	U	130	SER	5.6
1	E	136	PRO	5.4
3	L	68	ASP	5.3
3	L	67	SER	5.3
3	K	69	TYR	5.2
3	W	76	GLN	5.1
3	L	69	TYR	5.1
3	T	7	TYR	5.1
3	T	3	CYS	5.0
1	A	142	SER	4.9
3	S	7	TYR	4.9
1	U	142	SER	4.8
1	M	140	SER	4.8
3	C	69	TYR	4.7
3	S	74	VAL	4.7
1	U	143	GLY	4.6
3	W	69	TYR	4.6
1	A	141	THR	4.5
3	S	75	SER	4.5
3	K	66	THR	4.4
3	W	7	TYR	4.4
3	C	76	GLN	4.4
3	S	9	GLN	4.4
3	H	71	ASP	4.3
3	O	70	GLN	4.3
1	I	144	GLY	4.3
3	X	69	TYR	4.3
3	T	69	TYR	4.2
3	O	7	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
3	G	69	TYR	4.1
3	S	71	ASP	4.1
3	L	10	GLY	4.1
3	K	70	GLN	4.1
3	C	7	TYR	4.1
3	O	66	THR	4.1
3	S	66	THR	4.0
1	Q	141	THR	4.0
1	U	129	PRO	4.0
3	S	68	ASP	3.9
2	B	191	LYS	3.9
3	P	66	THR	3.9
1	U	15	SER	3.8
3	O	67	SER	3.8
3	G	11	SER	3.8
1	I	143	GLY	3.7
1	I	145	THR	3.7
3	D	7	TYR	3.7
1	U	138	SER	3.7
3	C	66	THR	3.7
1	M	143	GLY	3.6
1	M	158	GLU	3.6
3	S	72	SER	3.6
3	K	10	GLY	3.6
3	G	7	TYR	3.6
1	I	141	THR	3.6
3	H	66	THR	3.6
3	K	71	ASP	3.6
3	W	75	SER	3.6
3	P	69	TYR	3.6
3	T	5	GLY	3.6
1	E	15	SER	3.6
3	C	53	ASP	3.5
1	U	50	PHE	3.5
1	A	138	SER	3.5
1	E	142	SER	3.5
3	T	1	GLU	3.5
3	X	19	TYR	3.5
3	D	10	GLY	3.5
3	O	74	VAL	3.5
3	H	68	ASP	3.5
3	W	72	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	R	68	SER	3.4
3	G	72	SER	3.4
3	T	72	SER	3.4
2	F	191	LYS	3.4
3	H	7	TYR	3.4
3	O	2	SER	3.4
3	H	72	SER	3.3
3	T	66	THR	3.3
3	T	65	THR	3.3
1	E	141	THR	3.2
1	E	138	SER	3.2
3	K	67	SER	3.2
3	S	8	TYR	3.2
2	N	139	ASN	3.2
1	U	124	ALA	3.2
3	L	66	THR	3.2
3	G	33	SER	3.1
3	L	65	THR	3.1
3	O	5	GLY	3.1
3	X	73	ASP	3.1
3	C	32	GLU	3.1
1	U	144	GLY	3.1
3	W	73	ASP	3.1
1	Q	138	SER	3.1
3	L	71	ASP	3.0
3	C	33	SER	3.0
1	U	139	LYS	3.0
1	A	137	SER	3.0
3	X	72	SER	3.0
3	L	72	SER	3.0
3	X	2	SER	3.0
3	W	66	THR	3.0
3	H	53	ASP	3.0
3	C	11	SER	3.0
2	V	191	LYS	2.9
2	B	192	VAL	2.9
3	T	32	GLU	2.9
3	G	53	ASP	2.9
3	L	73	ASP	2.9
3	O	10	GLY	2.9
3	G	44	THR	2.9
1	Q	74	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	K	68	ASP	2.9
1	A	140	SER	2.9
3	G	2	SER	2.9
3	O	71	ASP	2.8
3	G	66	THR	2.8
1	E	55	GLY	2.8
1	Q	143	GLY	2.8
3	K	2	SER	2.7
3	G	70	GLN	2.7
1	E	139	LYS	2.7
1	E	140	SER	2.7
1	I	142	SER	2.7
1	U	198	SER	2.7
3	H	2	SER	2.7
1	M	214	ASN	2.7
3	K	7	TYR	2.7
1	Q	137	SER	2.7
3	C	67	SER	2.7
3	D	67	SER	2.7
3	K	39	LYS	2.7
1	M	141	THR	2.7
1	M	142	SER	2.6
3	P	72	SER	2.6
3	T	71	ASP	2.6
3	W	67	SER	2.6
3	K	31	ALA	2.6
1	E	200	GLY	2.6
3	T	67	SER	2.6
3	C	4	ASN	2.6
3	G	6	LEU	2.6
3	G	74	VAL	2.6
3	C	72	SER	2.6
3	C	74	VAL	2.6
3	W	70	GLN	2.6
3	G	32	GLU	2.6
3	G	37	PRO	2.6
3	C	18	ASP	2.6
3	S	69	TYR	2.5
1	E	74	SER	2.5
1	M	201	THR	2.5
1	E	1	LEU	2.5
1	I	184	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	65	THR	2.5
3	X	17	SER	2.5
3	C	84	THR	2.5
3	D	84	THR	2.5
3	W	10	GLY	2.5
3	K	84	THR	2.5
3	C	10	GLY	2.5
3	P	2	SER	2.5
3	O	53	ASP	2.5
3	T	18	ASP	2.5
1	E	137	SER	2.4
1	I	183	SER	2.4
3	O	72	SER	2.4
3	X	71	ASP	2.4
2	B	215	CYS	2.4
3	G	84	THR	2.4
3	K	73	ASP	2.4
3	P	10	GLY	2.4
3	S	84	THR	2.4
3	L	7	TYR	2.4
1	E	30	SER	2.4
1	M	138	SER	2.4
3	X	65	THR	2.4
3	K	8	TYR	2.4
3	S	34	SER	2.4
3	K	3	CYS	2.4
3	D	69	TYR	2.3
1	U	135	ALA	2.3
1	U	1	LEU	2.3
3	G	67	SER	2.3
2	F	171	ASP	2.3
3	T	74	VAL	2.3
3	X	10	GLY	2.3
3	K	32	GLU	2.3
3	O	68	ASP	2.3
3	T	73	ASP	2.3
1	U	221	VAL	2.3
3	O	39	LYS	2.3
1	E	103	LEU	2.3
3	W	3	CYS	2.3
3	W	43	LEU	2.3
3	W	40	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	139	LYS	2.3
3	S	10	GLY	2.3
1	U	200	GLY	2.3
1	E	65	SER	2.3
3	G	18	ASP	2.2
3	H	18	ASP	2.2
3	D	66	THR	2.2
2	F	35	ALA	2.2
3	S	67	SER	2.2
3	C	68	ASP	2.2
3	P	71	ASP	2.2
3	S	70	GLN	2.2
3	W	80	LYS	2.2
3	X	7	TYR	2.2
1	A	1	LEU	2.2
3	L	2	SER	2.2
3	H	69	TYR	2.2
1	I	140	SER	2.2
3	T	64	LYS	2.2
1	Q	145	THR	2.2
3	L	84	THR	2.2
3	W	65	THR	2.2
3	K	5	GLY	2.2
3	P	1	GLU	2.2
3	T	30	ALA	2.1
3	C	14	ILE	2.1
1	U	199	LEU	2.1
3	T	76	GLN	2.1
3	O	43	LEU	2.1
3	D	2	SER	2.1
3	K	72	SER	2.1
2	F	215	CYS	2.1
3	O	65	THR	2.1
1	I	187	SER	2.1
3	C	2	SER	2.1
1	E	53	ASN	2.1
1	U	100	ARG	2.0
1	I	26	GLY	2.0
1	Q	102	SER	2.0
2	V	95	SER	2.0
3	T	70	GLN	2.0
3	H	23	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	137	SER	2.0
3	P	4	ASN	2.0
1	Q	139	LYS	2.0
3	K	14	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.