



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2022 – 06:15 PM JST

PDB ID : 7EW5  
Title : immune complex of HPV6 L1 pentamer and neutralizing antibody 13H5  
Authors : Wang, Z.P.; Wang, D.N.; Gu, Y.; Li, S.W.  
Deposited on : 2021-05-24  
Resolution : 3.61 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

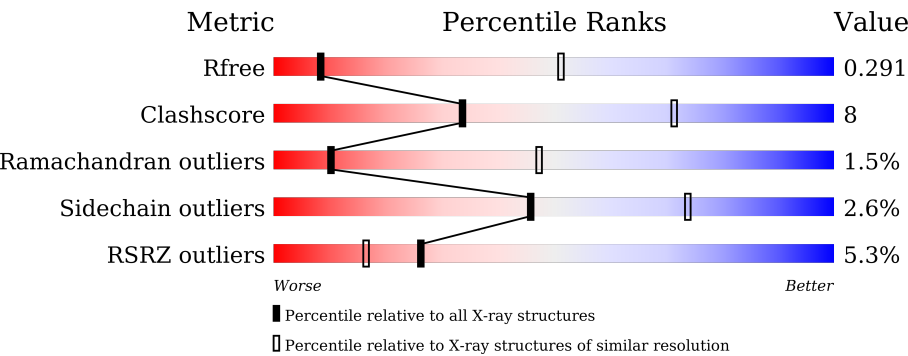
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.61 Å.

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






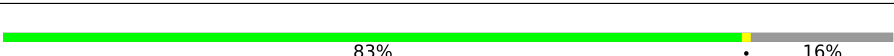
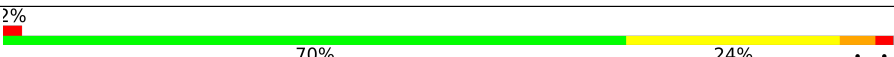
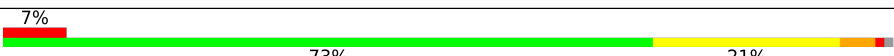
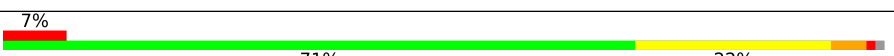
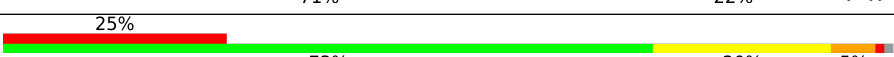

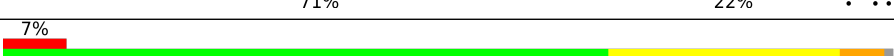
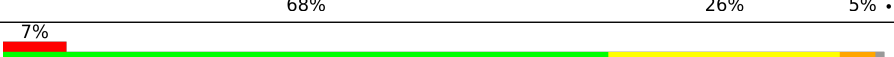

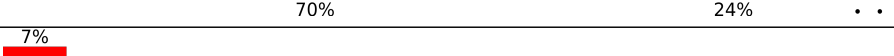
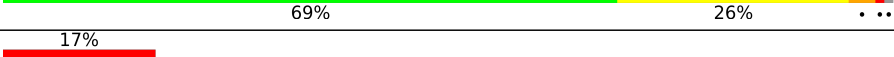
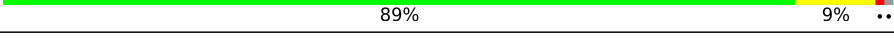
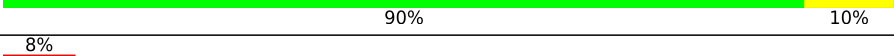



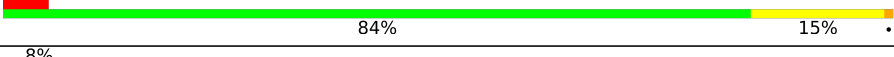

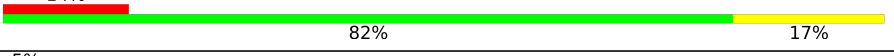

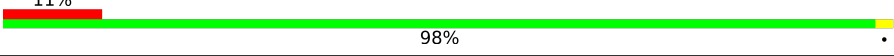
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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  $\geq 3$ , 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	496	<div><div>%</div><div><div></div><div>69%</div><div>14%</div><div>•</div><div>16%</div></div></div>
1	D	496	<div><div>%</div><div><div></div><div>69%</div><div>15%</div><div></div><div>16%</div></div></div>
1	G	496	<div><div>%</div><div><div></div><div>68%</div><div>15%</div><div>•</div><div>16%</div></div></div>
1	J	496	<div><div></div><div><div></div><div>69%</div><div>14%</div><div>•</div><div>16%</div></div></div>
1	M	496	<div><div></div><div><div></div><div>67%</div><div>16%</div><div>•</div><div>16%</div></div></div>
1	P	496	<div><div>2%</div><div><div></div><div>69%</div><div>14%</div><div>•</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	S	496	
1	V	496	
1	Y	496	
1	b	496	
2	B	221	
2	E	221	
2	H	221	
2	K	221	
2	N	221	
2	Q	221	
2	T	221	
2	W	221	
2	Z	221	
2	g	221	
3	C	214	
3	F	214	
3	I	214	
3	L	214	
3	O	214	
3	R	214	
3	U	214	
3	X	214	
3	a	214	
3	j	214	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 65550 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	D	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	G	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	J	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	M	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	P	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	S	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	V	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	Y	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			
1	b	416	Total	C	N	O	S	0	0	0
			3258	2069	548	622	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q9W9C6
A	376	VAL	MET	conflict	UNP Q9W9C6
D	-2	MET	-	initiating methionine	UNP Q9W9C6
D	376	VAL	MET	conflict	UNP Q9W9C6
G	-2	MET	-	initiating methionine	UNP Q9W9C6
G	376	VAL	MET	conflict	UNP Q9W9C6
J	-2	MET	-	initiating methionine	UNP Q9W9C6
J	376	VAL	MET	conflict	UNP Q9W9C6
M	-2	MET	-	initiating methionine	UNP Q9W9C6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	376	VAL	MET	conflict	UNP Q9W9C6
P	-2	MET	-	initiating methionine	UNP Q9W9C6
P	376	VAL	MET	conflict	UNP Q9W9C6
S	-2	MET	-	initiating methionine	UNP Q9W9C6
S	376	VAL	MET	conflict	UNP Q9W9C6
V	-2	MET	-	initiating methionine	UNP Q9W9C6
V	376	VAL	MET	conflict	UNP Q9W9C6
Y	-2	MET	-	initiating methionine	UNP Q9W9C6
Y	376	VAL	MET	conflict	UNP Q9W9C6
b	-2	MET	-	initiating methionine	UNP Q9W9C6
b	376	VAL	MET	conflict	UNP Q9W9C6

- Molecule 2 is a protein called Heavy chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	E	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	H	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	K	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	N	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	g	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Q	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	T	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	W	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			
2	Z	218	Total	C	N	O	S	0	0	0
			1643	1038	269	330	6			

- Molecule 3 is a protein called Light chain of 13H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	F	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

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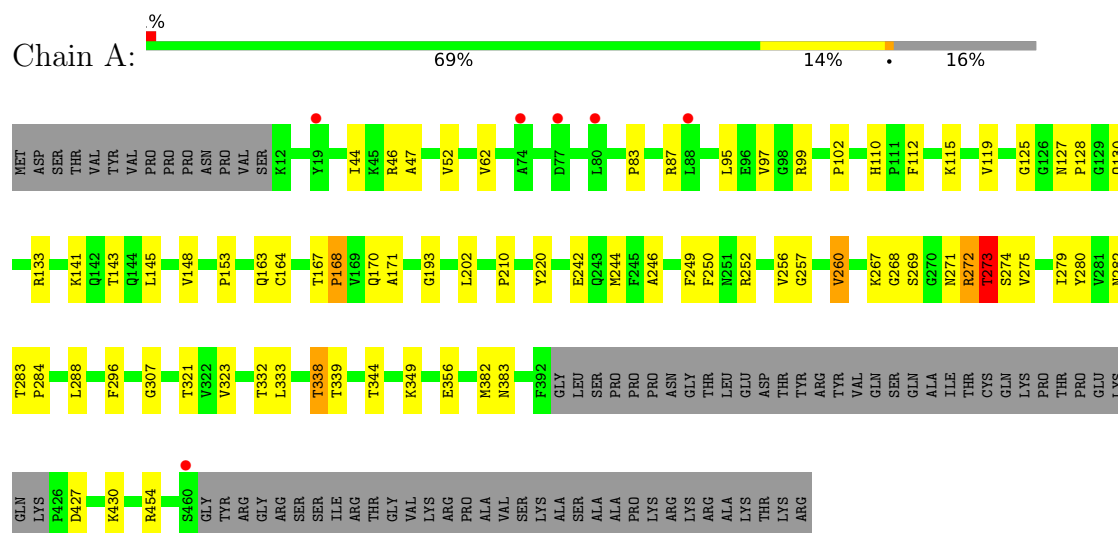
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	L	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	O	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	j	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	R	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	U	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	X	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			
3	a	214	Total	C	N	O	S	25	0	0
			1654	1026	277	341	10			

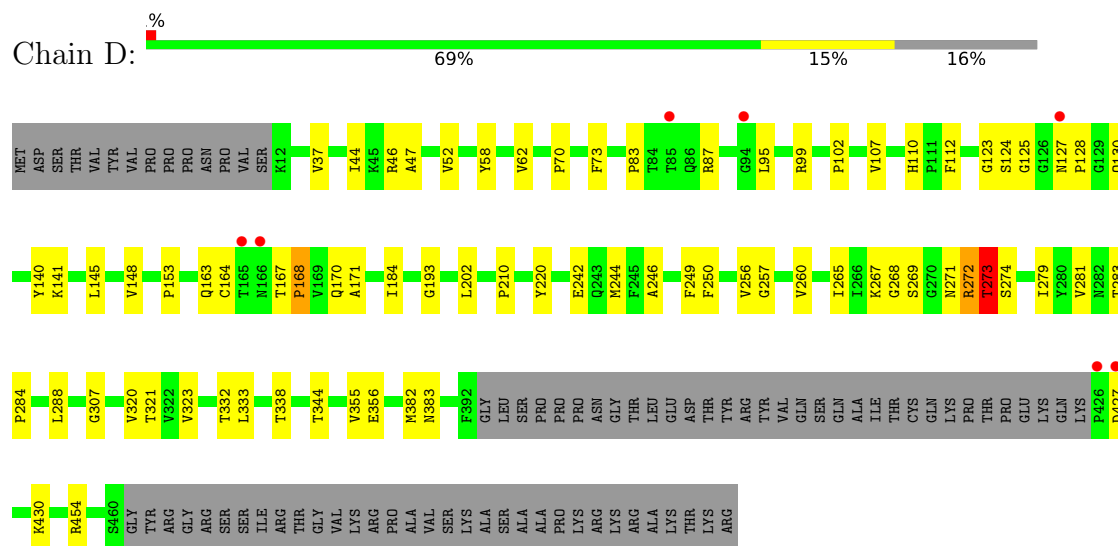
### 3 Residue-property plots [i](#)

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: Major capsid protein L1

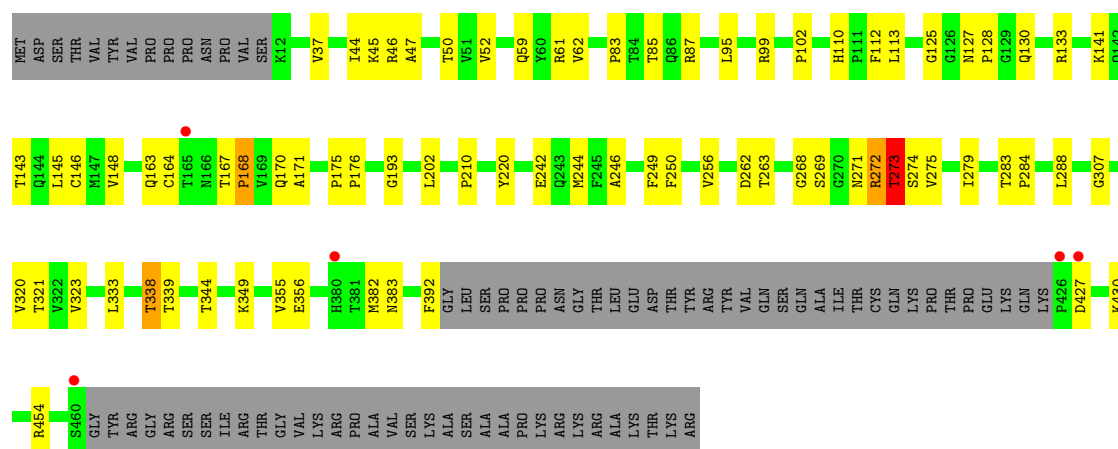


#### • Molecule 1: Major capsid protein L1



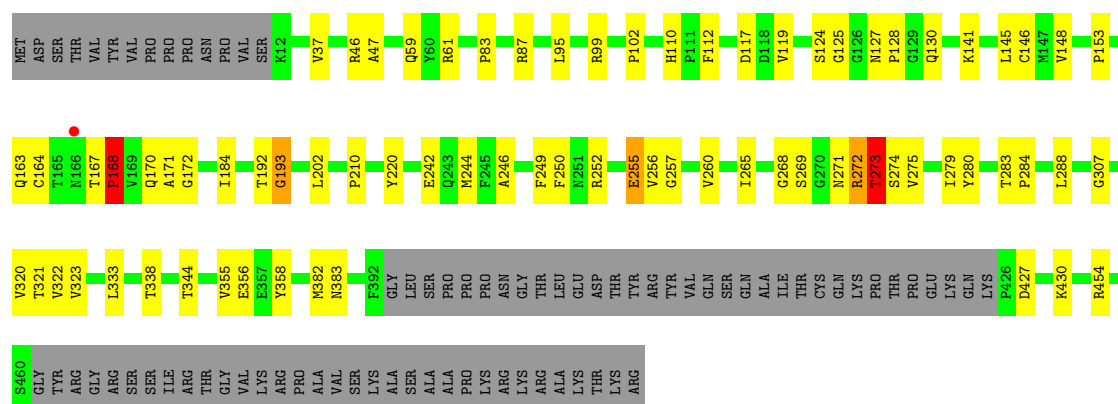
#### • Molecule 1: Major capsid protein L1





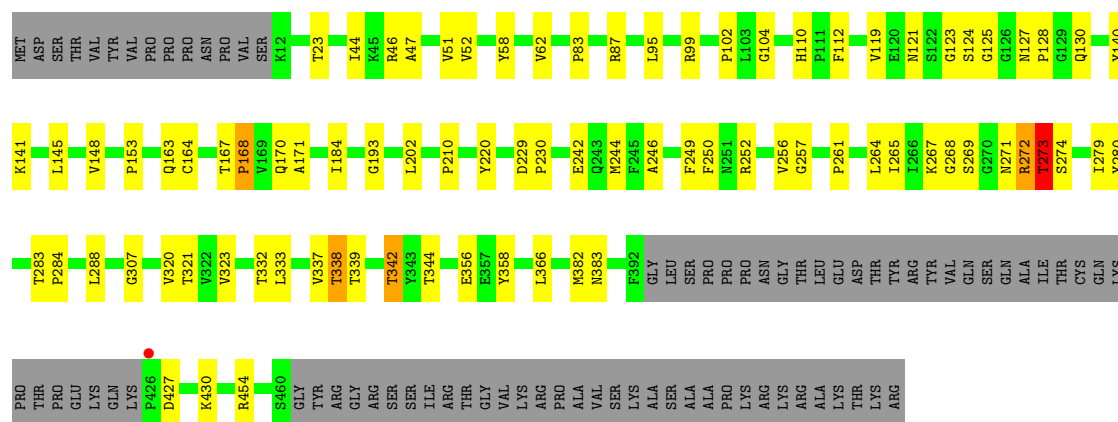
- Molecule 1: Major capsid protein L1

Chain J: 69% 14% 16%



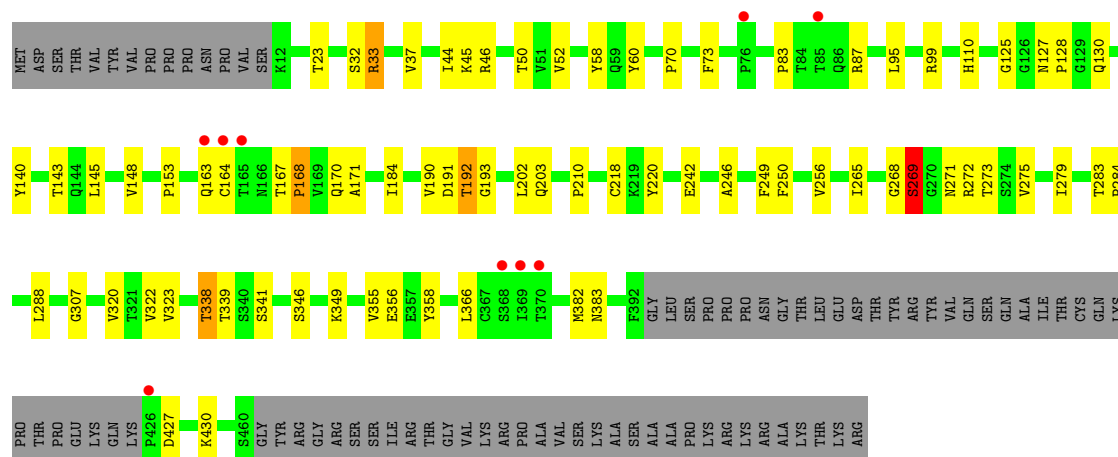
- Molecule 1: Major capsid protein L1

Chain M: 67% 16% 16%



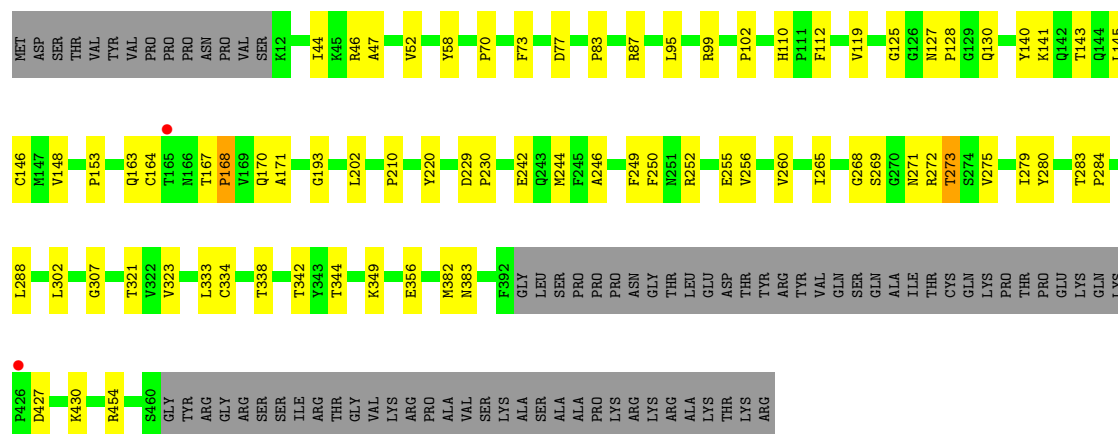
- Molecule 1: Major capsid protein L1

Chain P: 69% 14% 16%



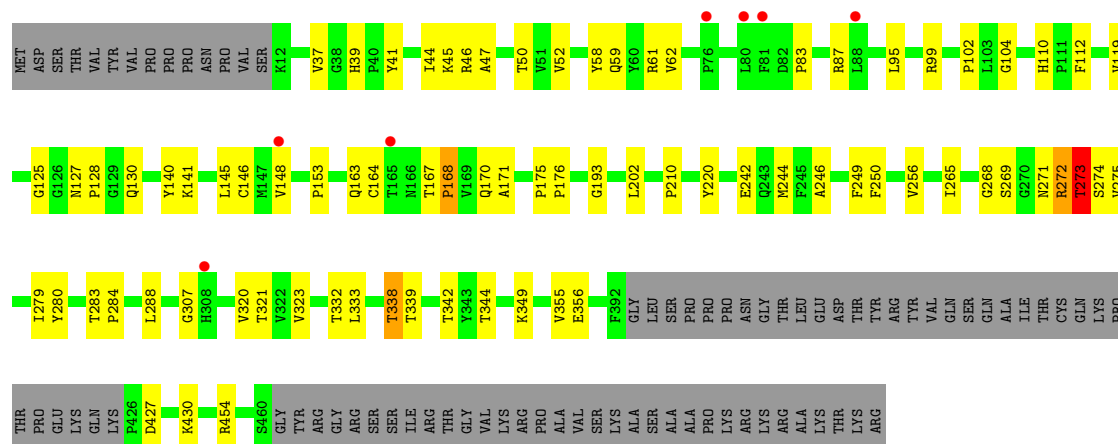
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Chain S: 69% 15% 16%

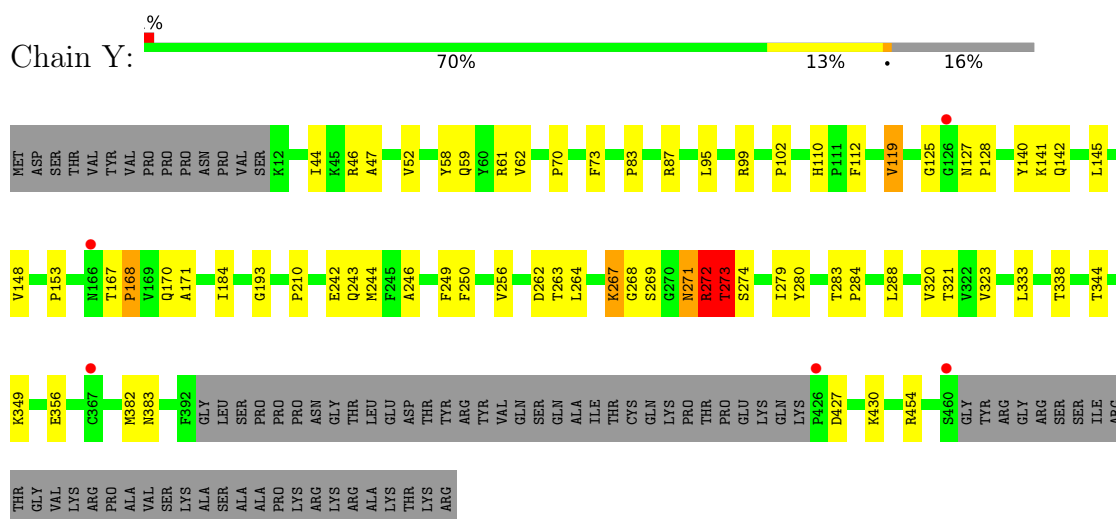


• Molecule 1: Major capsid protein L1

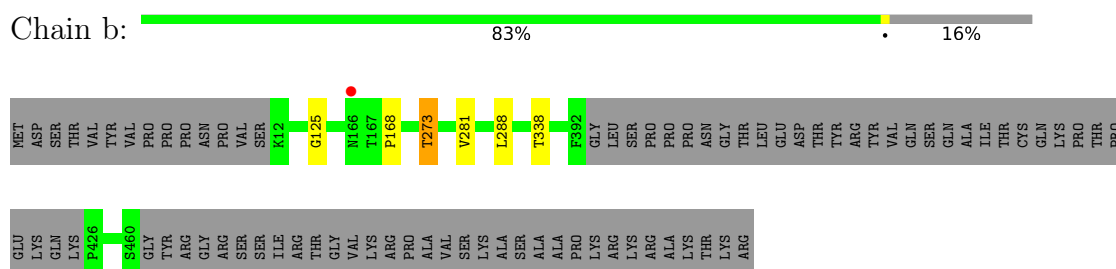
Chain V: 68% 15% 16%



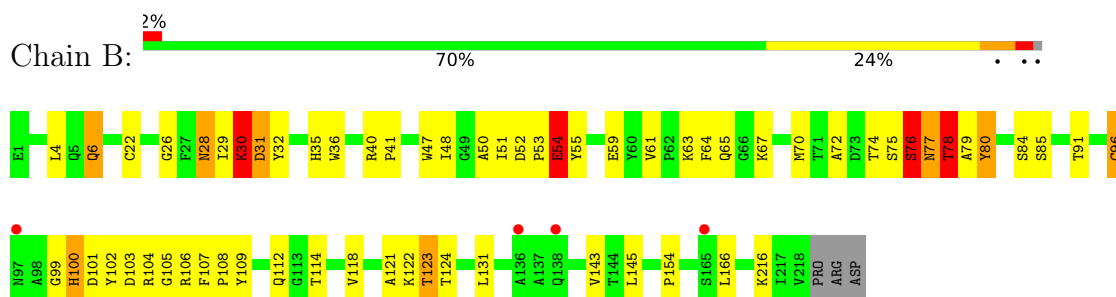
• Molecule 1: Major capsid protein L1



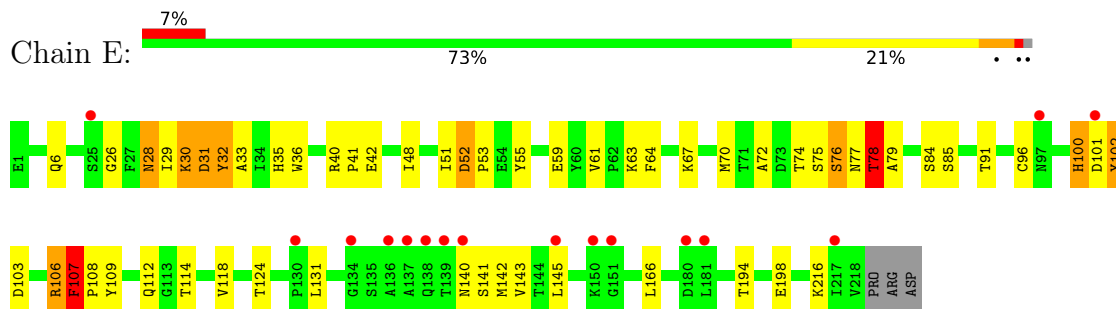
• Molecule 1: Major capsid protein L1



• Molecule 2: Heavy chain of 13H5

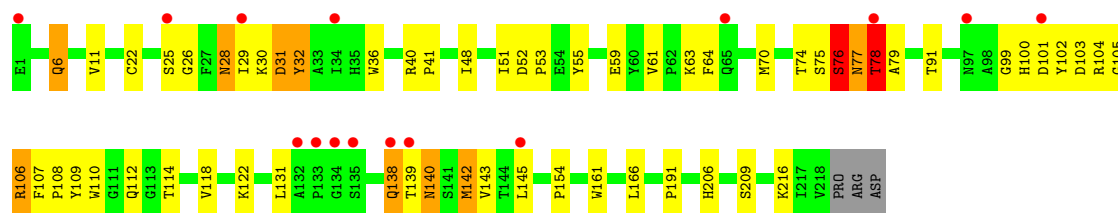


• Molecule 2: Heavy chain of 13H5

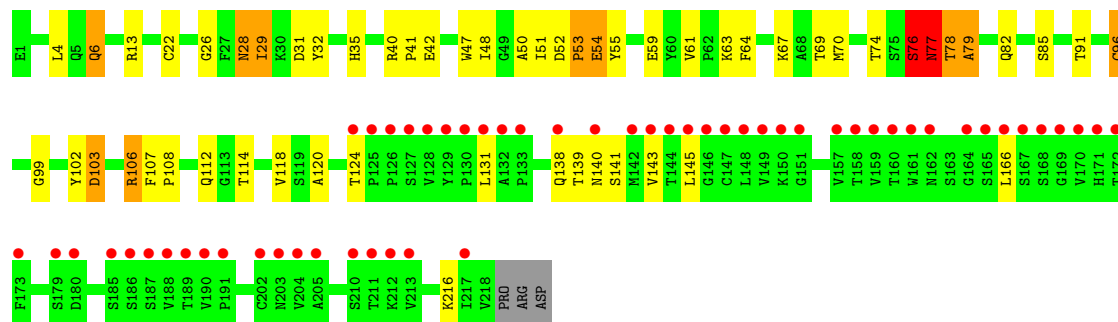
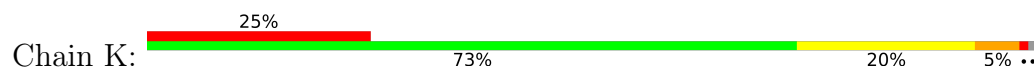


• Molecule 2: Heavy chain of 13H5

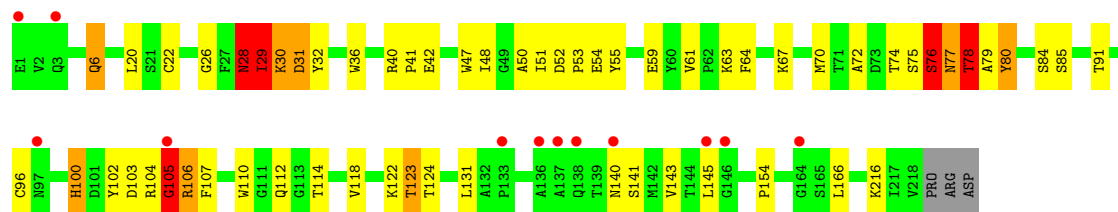




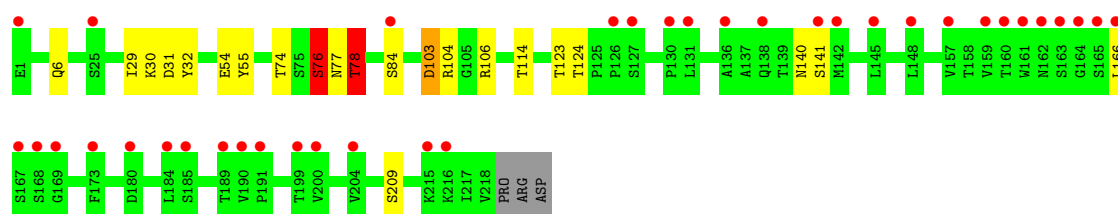
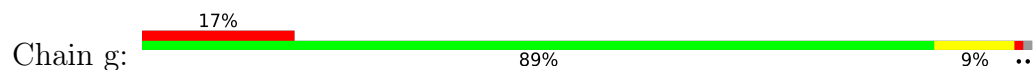
● Molecule 2: Heavy chain of 13H5



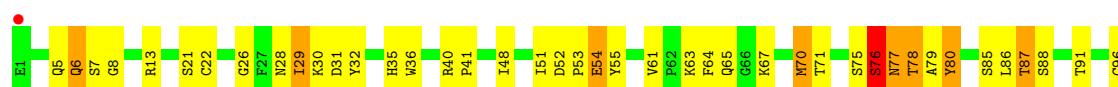
● Molecule 2: Heavy chain of 13H5

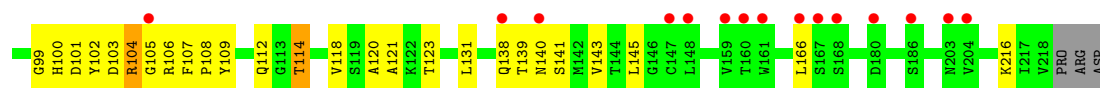


● Molecule 2: Heavy chain of 13H5

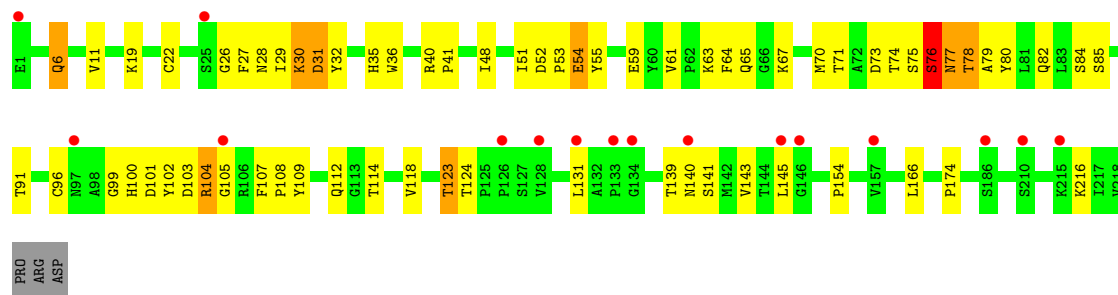


● Molecule 2: Heavy chain of 13H5

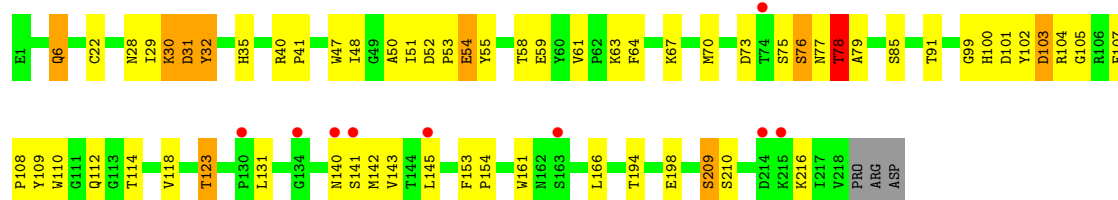




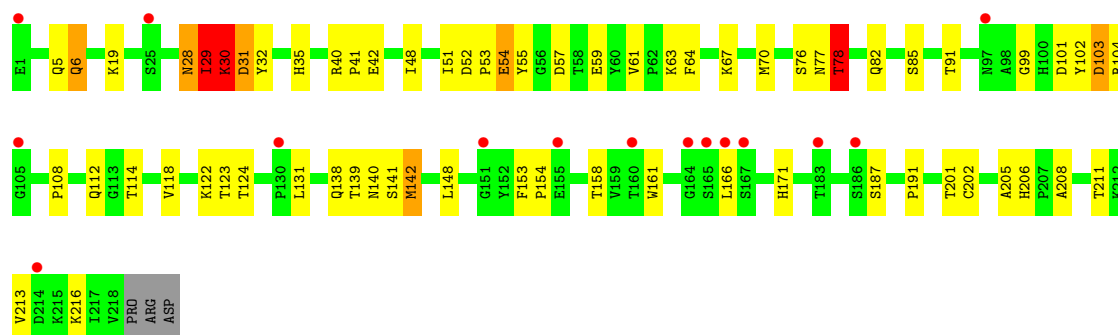
• Molecule 2: Heavy chain of 13H5



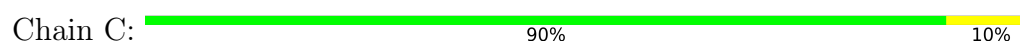
• Molecule 2: Heavy chain of 13H5



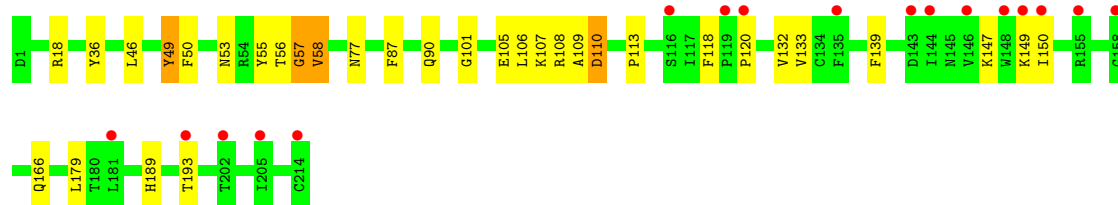
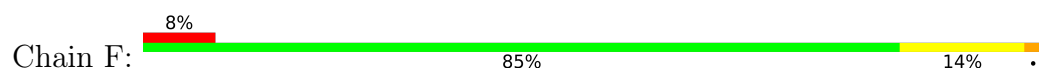
• Molecule 2: Heavy chain of 13H5



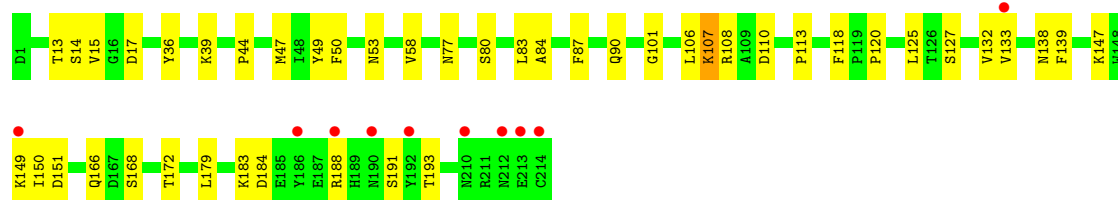
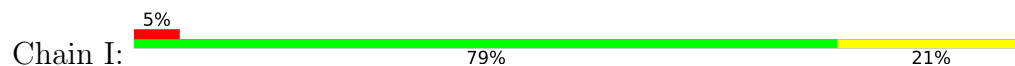
• Molecule 3: Light chain of 13H5



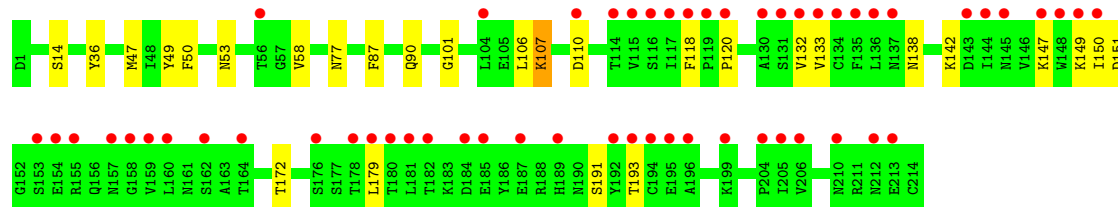
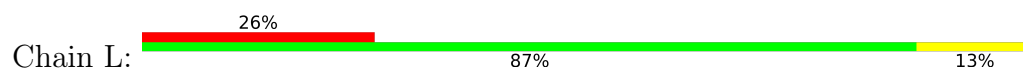
• Molecule 3: Light chain of 13H5



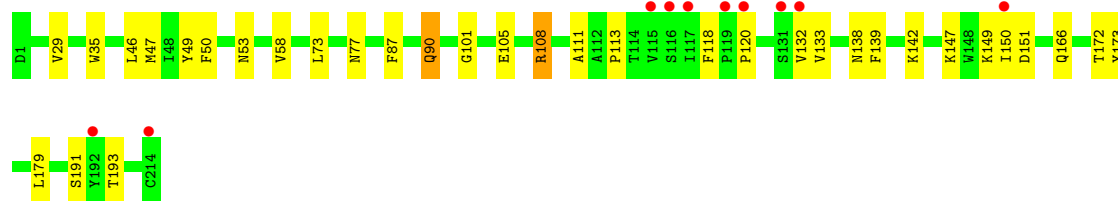
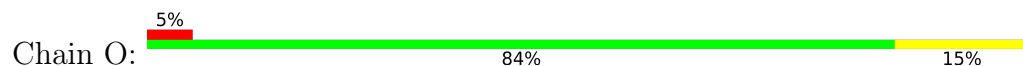
- Molecule 3: Light chain of 13H5



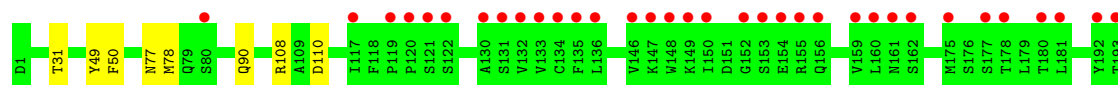
- Molecule 3: Light chain of 13H5

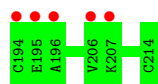


- Molecule 3: Light chain of 13H5

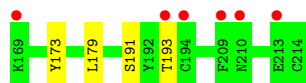
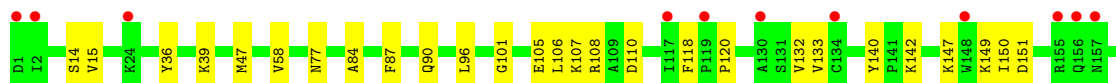
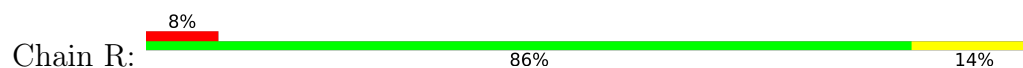


- Molecule 3: Light chain of 13H5

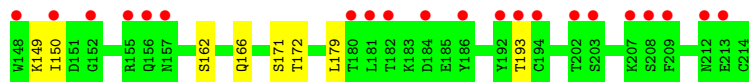
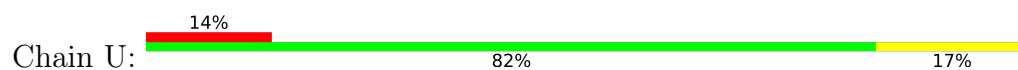




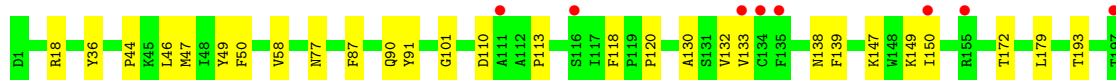
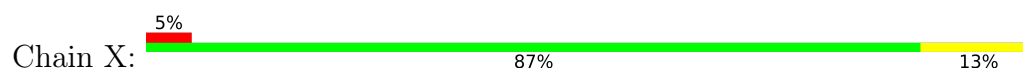
- Molecule 3: Light chain of 13H5



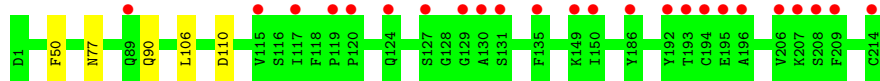
- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5



- Molecule 3: Light chain of 13H5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.09Å 208.31Å 205.95Å 90.00° 95.61° 90.00°	Depositor
Resolution (Å)	49.02 – 3.61 49.71 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-3.61) 99.5 (49.71-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.31	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.252 , 0.293 0.251 , 0.291	Depositor DCC
$R_{free}$ test set	6719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	65550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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, 0.333 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	0.26	0/3342	0.46	0/4544
1	D	0.25	0/3342	0.46	0/4544
1	G	0.26	0/3342	0.46	0/4544
1	J	0.26	0/3342	0.46	0/4544
1	M	0.26	0/3342	0.46	0/4544
1	P	0.26	0/3342	0.46	0/4544
1	S	0.26	0/3342	0.47	0/4544
1	V	0.25	0/3342	0.46	0/4544
1	Y	0.25	0/3342	0.46	0/4544
1	b	0.25	0/3342	0.46	0/4544
2	B	0.26	0/1686	0.58	2/2309 (0.1%)
2	E	0.27	0/1686	0.59	3/2309 (0.1%)
2	H	0.27	0/1686	0.56	1/2309 (0.0%)
2	K	0.26	0/1686	0.57	1/2309 (0.0%)
2	N	0.27	0/1686	0.58	3/2309 (0.1%)
2	Q	0.27	0/1686	0.57	1/2309 (0.0%)
2	T	0.27	0/1686	0.56	2/2309 (0.1%)
2	W	0.26	0/1686	0.57	2/2309 (0.1%)
2	Z	0.26	0/1686	0.55	1/2309 (0.0%)
2	g	0.28	0/1686	0.59	2/2309 (0.1%)
3	C	0.26	0/1688	0.47	0/2286
3	F	0.26	0/1688	0.52	2/2286 (0.1%)
3	I	0.25	0/1688	0.46	0/2286
3	L	0.25	0/1688	0.46	0/2286
3	O	0.25	0/1688	0.46	0/2286
3	R	0.26	0/1688	0.47	0/2286
3	U	0.26	0/1688	0.48	0/2286
3	X	0.25	0/1688	0.45	0/2286
3	a	0.26	0/1688	0.46	0/2286
3	j	0.26	0/1688	0.48	0/2286
All	All	0.26	0/67160	0.50	20/91390 (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
2	B	0	3
2	E	0	2
2	H	0	2
2	N	0	2
2	T	0	2
2	W	0	1
2	Z	0	2
2	g	0	2
3	F	0	1
All	All	0	17

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	58	VAL	N-CA-C	-7.51	90.72	111.00
2	K	76	SER	C-N-CA	7.11	139.48	121.70
2	E	107	PHE	C-N-CD	-6.65	105.98	120.60
2	Q	76	SER	C-N-CA	6.05	136.82	121.70
2	T	30	LYS	C-N-CA	5.99	136.67	121.70
2	B	76	SER	C-N-CA	5.75	136.07	121.70
2	g	30	LYS	C-N-CA	5.63	135.77	121.70
3	F	57	GLY	N-CA-C	-5.56	99.20	113.10
2	T	76	SER	C-N-CA	5.53	135.51	121.70
2	N	76	SER	C-N-CA	5.51	135.47	121.70
2	H	76	SER	C-N-CA	5.47	135.37	121.70
2	g	76	SER	C-N-CA	5.46	135.34	121.70
2	N	105	GLY	C-N-CA	5.41	135.22	121.70
2	N	30	LYS	C-N-CA	5.31	134.98	121.70
2	E	107	PHE	C-N-CA	5.28	144.16	122.00
2	W	76	SER	C-N-CA	5.25	134.82	121.70
2	E	30	LYS	C-N-CA	5.24	134.80	121.70
2	W	30	LYS	C-N-CA	5.22	134.75	121.70
2	Z	30	LYS	C-N-CA	5.13	134.51	121.70
2	B	30	LYS	C-N-CA	5.08	134.39	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	30	LYS	Peptide
2	B	76	SER	Peptide
2	B	78	THR	Peptide
2	E	76	SER	Peptide
2	E	78	THR	Peptide
3	F	57	GLY	Peptide
2	H	76	SER	Peptide
2	H	78	THR	Peptide
2	N	76	SER	Peptide
2	N	78	THR	Peptide
2	T	76	SER	Peptide
2	T	78	THR	Peptide
2	W	78	THR	Peptide
2	Z	30	LYS	Peptide
2	Z	78	THR	Peptide
2	g	76	SER	Peptide
2	g	78	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	3258	0	3150	52	0
1	D	3258	0	3150	52	0
1	G	3258	0	3150	53	0
1	J	3258	0	3150	54	0
1	M	3258	0	3150	61	0
1	P	3258	0	3150	52	0
1	S	3258	0	3150	53	1
1	V	3258	0	3150	58	0
1	Y	3258	0	3150	44	0
1	b	3258	0	3150	0	0
2	B	1643	0	1590	53	0
2	E	1643	0	1590	48	0
2	H	1643	0	1590	46	0
2	K	1643	0	1590	43	0
2	N	1643	0	1590	59	0
2	Q	1643	0	1590	48	1
2	T	1643	0	1590	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1643	0	1590	52	0
2	Z	1643	0	1590	43	0
2	g	1643	0	1590	0	0
3	C	1654	0	1582	14	0
3	F	1654	0	1582	21	1
3	I	1654	0	1582	29	1
3	L	1654	0	1582	17	0
3	O	1654	0	1582	24	0
3	R	1654	0	1582	19	0
3	U	1654	0	1582	26	0
3	X	1654	0	1582	20	0
3	a	1654	0	1582	0	0
3	j	1654	0	1582	0	0
All	All	65550	0	63220	941	2

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 8.

All (941) 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)
2:H:30:LYS:HA	2:H:31:ASP:HB2	1.52	0.90
3:U:83:LEU:HD21	3:U:106:LEU:HG	1.53	0.89
2:E:30:LYS:HA	2:E:31:ASP:HB2	1.55	0.86
2:W:30:LYS:HA	2:W:31:ASP:HB2	1.57	0.86
3:U:106:LEU:HB2	3:U:166:GLN:HE22	1.37	0.85
2:W:91:THR:HG22	2:W:118:VAL:H	1.42	0.84
1:S:349:LYS:HE2	2:T:101:ASP:OD2	1.79	0.83
3:I:83:LEU:HD21	3:I:106:LEU:HG	1.60	0.83
2:Z:142:MET:HG2	2:Z:191:PRO:HA	1.61	0.83
2:H:76:SER:HB2	2:H:77:ASN:HB2	1.62	0.82
2:B:91:THR:HG22	2:B:118:VAL:H	1.43	0.82
2:Z:91:THR:HG22	2:Z:118:VAL:H	1.45	0.82
1:Y:349:LYS:HE2	2:Z:101:ASP:OD2	1.80	0.81
2:Q:91:THR:HG22	2:Q:118:VAL:H	1.45	0.81
2:T:91:THR:HG22	2:T:118:VAL:H	1.45	0.80
3:R:105:GLU:OE2	3:R:173:TYR:OH	2.00	0.80
2:H:91:THR:HG22	2:H:118:VAL:H	1.46	0.79
1:G:349:LYS:HE2	2:H:101:ASP:OD2	1.83	0.79
2:N:91:THR:HG22	2:N:118:VAL:H	1.46	0.79
2:T:30:LYS:HA	2:T:31:ASP:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ALA:HB1	2:B:122:LYS:HA	1.65	0.78
2:B:28:ASN:OD1	2:B:28:ASN:N	2.17	0.78
2:E:91:THR:HG22	2:E:118:VAL:H	1.48	0.77
2:H:28:ASN:N	2:H:28:ASN:OD1	2.17	0.77
2:B:6:GLN:HG3	2:B:112:GLN:HG2	1.66	0.77
2:K:6:GLN:HG3	2:K:112:GLN:HG2	1.67	0.77
2:T:22:CYS:HB3	2:T:79:ALA:H	1.49	0.77
1:A:349:LYS:HE2	2:B:101:ASP:OD2	1.85	0.77
2:E:108:PRO:HB3	3:F:46:LEU:HB3	1.67	0.76
1:P:349:LYS:HE2	2:Q:101:ASP:OD2	1.86	0.76
1:Y:272:ARG:O	1:Y:274:SER:N	2.18	0.75
3:I:106:LEU:HB2	3:I:166:GLN:HE22	1.50	0.75
2:K:91:THR:HG22	2:K:118:VAL:H	1.51	0.75
2:E:6:GLN:HG3	2:E:112:GLN:HG2	1.69	0.74
2:N:30:LYS:HA	2:N:31:ASP:HB2	1.69	0.74
2:N:28:ASN:O	2:N:30:LYS:N	2.20	0.74
1:A:275:VAL:HG22	1:D:112:PHE:HE2	1.53	0.74
2:K:77:ASN:O	2:K:78:THR:OG1	2.04	0.74
1:P:341:SER:O	1:Y:267:LYS:NZ	2.20	0.73
2:W:6:GLN:HG3	2:W:112:GLN:HG2	1.70	0.73
2:E:100:HIS:HB3	2:E:109:TYR:HE2	1.52	0.73
2:Z:6:GLN:HG3	2:Z:112:GLN:HG2	1.71	0.73
2:W:209:SER:OG	2:W:210:SER:N	2.21	0.72
2:K:26:GLY:HA3	2:K:78:THR:HG21	1.71	0.72
2:W:76:SER:HB3	2:W:77:ASN:HB2	1.71	0.72
2:K:28:ASN:OD1	2:K:28:ASN:N	2.20	0.71
1:V:349:LYS:HE2	2:W:101:ASP:OD2	1.90	0.70
2:Q:75:SER:O	2:Q:77:ASN:HB2	1.92	0.70
2:T:30:LYS:HA	2:T:31:ASP:CB	2.20	0.70
1:G:193:GLY:HA3	1:G:284:PRO:HG3	1.74	0.70
1:V:275:VAL:HG22	1:Y:112:PHE:HE2	1.56	0.70
2:Z:67:LYS:NZ	2:Z:85:SER:O	2.24	0.70
1:D:202:LEU:HB3	1:G:333:LEU:HD22	1.73	0.69
2:T:78:THR:HB	2:T:79:ALA:HA	1.73	0.69
2:K:131:LEU:HD13	3:L:133:VAL:HG21	1.75	0.69
2:T:6:GLN:HG3	2:T:112:GLN:HG2	1.75	0.69
1:S:255:GLU:OE2	2:W:102:TYR:HB3	1.93	0.69
2:N:6:GLN:HG3	2:N:112:GLN:HG2	1.73	0.69
2:N:131:LEU:HD13	3:O:133:VAL:HG21	1.74	0.69
1:J:427:ASP:HB3	1:J:430:LYS:HG3	1.75	0.68
2:T:73:ASP:H	2:T:78:THR:HG21	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:ARG:HH11	3:C:109:ALA:H	1.41	0.68
1:D:272:ARG:O	1:D:274:SER:N	2.23	0.68
1:S:273:THR:HG21	2:W:59:GLU:OE2	1.94	0.68
1:V:193:GLY:HA3	1:V:284:PRO:HG3	1.75	0.68
2:B:131:LEU:HD13	3:C:133:VAL:HG21	1.74	0.68
2:E:131:LEU:HD13	3:F:133:VAL:HG21	1.76	0.68
2:Q:6:GLN:HG3	2:Q:112:GLN:HG2	1.75	0.68
1:A:250:PHE:HE1	1:A:283:THR:HG23	1.60	0.67
1:J:275:VAL:HG22	1:M:112:PHE:HE2	1.58	0.67
1:A:193:GLY:HA3	1:A:284:PRO:HG3	1.77	0.67
2:H:6:GLN:HG3	2:H:112:GLN:HG2	1.75	0.67
2:W:131:LEU:HD13	3:X:133:VAL:HG21	1.75	0.67
2:E:108:PRO:HB3	3:F:46:LEU:CB	2.25	0.67
2:Q:131:LEU:HD13	3:R:133:VAL:HG21	1.76	0.66
1:G:272:ARG:O	1:G:274:SER:N	2.26	0.66
1:J:272:ARG:O	1:J:274:SER:N	2.22	0.66
2:T:131:LEU:HD13	3:U:133:VAL:HG21	1.76	0.66
2:E:198:GLU:OE2	2:Z:5:GLN:NE2	2.28	0.65
1:S:99:ARG:NH2	1:S:356:GLU:OE1	2.30	0.65
2:H:131:LEU:HD13	3:I:133:VAL:HG21	1.78	0.65
1:A:272:ARG:O	1:A:274:SER:N	2.28	0.65
2:T:77:ASN:HB3	2:T:78:THR:HG23	1.78	0.64
2:Q:120:ALA:HB1	2:Q:121:ALA:HB2	1.78	0.64
1:J:202:LEU:HB3	1:M:333:LEU:HD22	1.80	0.64
1:J:141:LYS:HB3	1:J:192:THR:O	1.97	0.64
2:N:105:GLY:HA3	2:N:106:ARG:HG3	1.79	0.64
2:N:22:CYS:HB3	2:N:79:ALA:H	1.62	0.64
1:G:83:PRO:O	1:G:87:ARG:NH1	2.31	0.64
2:K:22:CYS:HB3	2:K:79:ALA:HB3	1.80	0.64
1:V:250:PHE:HE1	1:V:283:THR:HG23	1.63	0.64
1:Y:193:GLY:HA3	1:Y:284:PRO:HG3	1.78	0.63
1:A:115:LYS:NZ	1:M:121:ASN:O	2.30	0.63
2:Q:40:ARG:HH11	2:Q:41:PRO:HD2	1.63	0.63
2:E:51:ILE:HG13	2:E:70:MET:HE2	1.79	0.63
1:G:275:VAL:HG22	1:J:112:PHE:HE2	1.63	0.63
2:B:107:PHE:HB2	3:C:36:TYR:HE1	1.63	0.62
1:S:193:GLY:HA3	1:S:284:PRO:HG3	1.81	0.62
3:R:105:GLU:OE2	3:R:142:LYS:HD3	1.99	0.62
1:J:99:ARG:NH2	1:J:356:GLU:OE1	2.33	0.62
1:P:265:ILE:HD11	2:T:55:TYR:CE1	2.34	0.62
2:K:61:VAL:HG12	2:K:63:LYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:269:SER:HB2	1:P:272:ARG:HG3	1.82	0.62
1:J:167:THR:HB	1:J:168:PRO:HB3	1.82	0.62
1:S:141:LYS:HE3	1:S:242:GLU:HB3	1.82	0.61
2:N:61:VAL:HG12	2:N:63:LYS:H	1.65	0.61
2:Z:76:SER:OG	2:Z:77:ASN:N	2.33	0.61
1:J:130:GLN:HG3	1:M:344:THR:HG22	1.82	0.61
2:B:51:ILE:HG13	2:B:70:MET:HE2	1.82	0.61
2:T:51:ILE:HG13	2:T:70:MET:HE2	1.82	0.61
1:V:202:LEU:HB3	1:Y:333:LEU:HD22	1.83	0.61
1:V:272:ARG:O	1:V:274:SER:N	2.25	0.61
1:D:250:PHE:HE1	1:D:283:THR:HG23	1.65	0.61
2:T:73:ASP:H	2:T:78:THR:CG2	2.13	0.61
2:W:40:ARG:HH11	2:W:41:PRO:HD2	1.65	0.61
2:T:40:ARG:HH11	2:T:41:PRO:HD2	1.65	0.61
1:D:141:LYS:HE3	1:D:242:GLU:HB3	1.82	0.61
2:B:40:ARG:HH11	2:B:41:PRO:HD2	1.64	0.61
2:H:140:ASN:N	2:H:140:ASN:OD1	2.33	0.61
2:Z:61:VAL:HG12	2:Z:63:LYS:H	1.65	0.61
2:E:30:LYS:HA	2:E:31:ASP:CB	2.31	0.61
3:U:120:PRO:HD3	3:U:132:VAL:HG22	1.82	0.61
2:Z:29:ILE:O	2:Z:30:LYS:HE3	2.01	0.61
3:F:120:PRO:HD3	3:F:132:VAL:HG22	1.83	0.60
2:K:102:TYR:CG	2:K:103:ASP:N	2.68	0.60
1:Y:250:PHE:HE1	1:Y:283:THR:HG23	1.64	0.60
1:A:333:LEU:HD22	1:M:202:LEU:HB3	1.82	0.60
1:M:250:PHE:HE1	1:M:283:THR:HG23	1.66	0.60
1:M:272:ARG:O	1:M:274:SER:N	2.27	0.60
2:Z:40:ARG:HH11	2:Z:41:PRO:HD2	1.65	0.60
2:H:61:VAL:HG12	2:H:63:LYS:H	1.66	0.60
2:T:61:VAL:HG12	2:T:63:LYS:H	1.67	0.60
3:U:46:LEU:HD21	3:U:49:TYR:HD2	1.65	0.60
2:Z:30:LYS:HA	2:Z:31:ASP:CB	2.31	0.60
3:L:147:LYS:HD2	3:L:149:LYS:HZ1	1.66	0.60
2:Q:61:VAL:HG12	2:Q:63:LYS:H	1.66	0.60
2:W:61:VAL:HG12	2:W:63:LYS:H	1.67	0.60
1:P:202:LEU:HB3	1:S:333:LEU:HD22	1.84	0.60
2:E:40:ARG:HH11	2:E:41:PRO:HD2	1.67	0.60
2:T:67:LYS:NZ	2:T:85:SER:O	2.34	0.60
1:S:202:LEU:HB3	1:V:333:LEU:HD22	1.83	0.60
2:K:40:ARG:HH11	2:K:41:PRO:HD2	1.67	0.60
1:A:99:ARG:NH2	1:A:356:GLU:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:GLN:HG3	1:J:344:THR:HG22	1.84	0.60
1:M:83:PRO:O	1:M:87:ARG:NH1	2.33	0.59
1:S:250:PHE:HE1	1:S:283:THR:HG23	1.67	0.59
2:E:78:THR:HG22	2:E:79:ALA:HA	1.82	0.59
2:E:106:ARG:HD2	3:F:49:TYR:HD1	1.68	0.59
3:U:118:PHE:HB2	3:U:133:VAL:HG22	1.84	0.59
2:W:107:PHE:HB2	3:X:36:TYR:HE1	1.67	0.59
2:B:61:VAL:HG12	2:B:63:LYS:H	1.67	0.59
2:E:61:VAL:HG12	2:E:63:LYS:H	1.67	0.59
3:L:118:PHE:HB2	3:L:133:VAL:HG22	1.84	0.59
2:N:105:GLY:HA3	2:N:106:ARG:HB2	1.84	0.59
3:R:120:PRO:HD3	3:R:132:VAL:HG22	1.84	0.59
3:X:120:PRO:HD3	3:X:132:VAL:HG22	1.83	0.59
1:J:250:PHE:HE1	1:J:283:THR:HG23	1.67	0.59
3:I:120:PRO:HD3	3:I:132:VAL:HG22	1.85	0.59
3:O:120:PRO:HD3	3:O:132:VAL:HG22	1.85	0.59
1:D:193:GLY:HA3	1:D:284:PRO:HG3	1.84	0.59
1:S:265:ILE:HD11	2:W:55:TYR:CE1	2.38	0.59
2:N:40:ARG:HH11	2:N:41:PRO:HD2	1.68	0.59
2:N:105:GLY:HA3	2:N:106:ARG:CB	2.33	0.59
1:A:141:LYS:HE3	1:A:242:GLU:HB3	1.85	0.59
1:P:99:ARG:NH2	1:P:356:GLU:OE1	2.36	0.59
2:E:106:ARG:HA	2:E:107:PHE:HB2	1.84	0.59
2:N:30:LYS:HA	2:N:31:ASP:CB	2.33	0.59
2:B:76:SER:CB	2:B:77:ASN:HB2	2.33	0.59
1:J:265:ILE:HD11	2:N:55:TYR:CE1	2.38	0.59
1:P:250:PHE:HE1	1:P:283:THR:HG23	1.66	0.59
1:S:275:VAL:HG22	1:V:112:PHE:HE2	1.68	0.59
2:T:107:PHE:HB2	3:U:36:TYR:HE1	1.67	0.59
2:W:99:GLY:HA2	2:W:108:PRO:HD2	1.85	0.59
2:B:30:LYS:HA	2:B:31:ASP:HB2	1.85	0.58
3:F:106:LEU:H	3:F:166:GLN:HE22	1.51	0.58
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.85	0.58
2:T:22:CYS:HB3	2:T:79:ALA:N	2.17	0.58
1:M:141:LYS:HE3	1:M:242:GLU:HB3	1.86	0.58
2:B:22:CYS:HB3	2:B:79:ALA:H	1.68	0.58
2:Q:107:PHE:HB2	3:R:36:TYR:HE1	1.68	0.58
3:C:118:PHE:HB2	3:C:133:VAL:HG22	1.85	0.58
3:O:149:LYS:HB2	3:O:193:THR:HB	1.86	0.58
3:F:109:ALA:HB1	3:F:110:ASP:HB3	1.84	0.58
3:I:106:LEU:HB2	3:I:166:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ARG:NH2	1:G:356:GLU:OE1	2.37	0.58
1:Y:427:ASP:HB3	1:Y:430:LYS:HG3	1.84	0.58
1:M:47:ALA:HB1	2:N:28:ASN:HD21	1.67	0.58
2:E:67:LYS:NZ	2:E:85:SER:O	2.36	0.58
1:A:130:GLN:HG3	1:D:344:THR:HG22	1.86	0.58
1:Y:148:VAL:HG22	1:Y:320:VAL:HG22	1.85	0.58
2:E:28:ASN:OD1	2:E:28:ASN:N	2.32	0.58
2:H:22:CYS:HB3	2:H:79:ALA:H	1.69	0.58
1:M:99:ARG:NH2	1:M:356:GLU:OE1	2.37	0.58
2:H:40:ARG:HH11	2:H:41:PRO:HD2	1.67	0.58
2:Z:158:THR:HB	2:Z:205:ALA:HB3	1.85	0.58
1:P:275:VAL:HG22	1:S:112:PHE:HE2	1.69	0.58
1:M:257:GLY:O	2:B:30:LYS:HE2	2.04	0.57
1:V:265:ILE:HD11	2:Z:55:TYR:CE1	2.38	0.57
3:C:120:PRO:HD3	3:C:132:VAL:HG22	1.86	0.57
2:N:103:ASP:HB3	2:N:106:ARG:NH2	2.19	0.57
1:A:344:THR:HG22	1:M:130:GLN:HG3	1.86	0.57
1:J:193:GLY:HA3	1:J:284:PRO:HG3	1.85	0.57
1:V:62:VAL:HG22	1:V:321:THR:HG23	1.86	0.57
3:I:13:THR:O	3:I:107:LYS:N	2.37	0.57
2:W:76:SER:HB3	2:W:77:ASN:CB	2.33	0.57
1:G:202:LEU:HB3	1:J:333:LEU:HD22	1.86	0.57
2:B:99:GLY:HA2	2:B:108:PRO:HD2	1.86	0.57
2:N:52:ASP:OD2	2:N:55:TYR:HB2	2.03	0.57
2:Q:48:ILE:HG23	2:Q:64:PHE:HD1	1.69	0.57
2:W:30:LYS:HA	2:W:31:ASP:CB	2.33	0.57
1:V:130:GLN:HG3	1:Y:344:THR:HG22	1.86	0.57
1:V:141:LYS:HE3	1:V:242:GLU:HB3	1.85	0.57
2:W:48:ILE:HG23	2:W:64:PHE:HD1	1.69	0.57
1:A:145:LEU:HG	1:A:323:VAL:HB	1.87	0.57
1:M:193:GLY:HA3	1:M:284:PRO:HG3	1.86	0.57
3:I:118:PHE:HB2	3:I:133:VAL:HG22	1.87	0.57
3:R:118:PHE:HB2	3:R:133:VAL:HG22	1.86	0.57
2:W:102:TYR:CG	2:W:103:ASP:N	2.73	0.57
3:X:149:LYS:HB2	3:X:193:THR:HB	1.87	0.57
2:Z:102:TYR:CG	2:Z:103:ASP:N	2.72	0.57
1:A:83:PRO:O	1:A:87:ARG:NH1	2.36	0.56
1:D:344:THR:HG21	3:F:53:ASN:ND2	2.20	0.56
1:P:143:THR:HG23	1:P:242:GLU:HG2	1.86	0.56
1:V:110:HIS:HB2	1:V:210:PRO:HA	1.86	0.56
3:U:149:LYS:HB2	3:U:193:THR:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HB3	1:D:333:LEU:HD22	1.85	0.56
1:V:99:ARG:NH2	1:V:356:GLU:OE1	2.38	0.56
1:J:83:PRO:O	1:J:87:ARG:NH1	2.38	0.56
1:Y:271:ASN:O	1:Y:273:THR:N	2.38	0.56
1:G:62:VAL:HG22	1:G:321:THR:HG23	1.87	0.56
1:G:141:LYS:HE3	1:G:242:GLU:HB3	1.87	0.56
1:Y:268:GLY:HA3	1:Y:269:SER:HB2	1.87	0.56
2:H:107:PHE:HB2	3:I:36:TYR:HE1	1.70	0.56
3:U:147:LYS:HD2	3:U:149:LYS:HZ1	1.71	0.56
1:P:130:GLN:HG3	1:S:344:THR:HG22	1.86	0.56
1:Y:141:LYS:HB2	1:Y:244:MET:HB3	1.87	0.56
2:K:51:ILE:HG13	2:K:70:MET:HE2	1.88	0.56
1:M:167:THR:HB	1:M:168:PRO:HB3	1.88	0.56
2:B:131:LEU:H	2:B:216:LYS:HZ3	1.53	0.56
2:W:73:ASP:H	2:W:78:THR:HG21	1.71	0.56
2:Z:51:ILE:HG13	2:Z:70:MET:HE2	1.86	0.56
1:V:148:VAL:HG22	1:V:320:VAL:HG22	1.88	0.56
1:V:83:PRO:O	1:V:87:ARG:NH1	2.38	0.56
2:Q:76:SER:HB3	2:Q:77:ASN:CB	2.36	0.56
2:H:145:LEU:HD13	2:H:216:LYS:HD3	1.88	0.55
3:X:118:PHE:HB2	3:X:133:VAL:HG22	1.87	0.55
1:G:85:THR:H	1:G:392:PHE:HE2	1.53	0.55
2:T:99:GLY:HA2	2:T:108:PRO:HD2	1.88	0.55
3:O:118:PHE:HB2	3:O:133:VAL:HG22	1.87	0.55
2:T:40:ARG:HD2	2:T:41:PRO:HD2	1.89	0.55
3:U:107:LYS:HA	3:U:140:TYR:OH	2.07	0.55
2:K:145:LEU:HD13	2:K:216:LYS:HD3	1.89	0.55
3:L:149:LYS:HB2	3:L:193:THR:HB	1.89	0.55
2:Q:76:SER:HB3	2:Q:77:ASN:HB2	1.89	0.55
2:N:106:ARG:HG2	3:O:49:TYR:HB2	1.87	0.55
1:D:272:ARG:HG2	1:G:112:PHE:HE1	1.72	0.55
1:J:141:LYS:HE3	1:J:242:GLU:HB3	1.88	0.55
3:X:113:PRO:HB3	3:X:139:PHE:HB3	1.88	0.55
1:G:273:THR:HG21	2:K:59:GLU:OE2	2.07	0.55
2:E:52:ASP:OD2	2:E:55:TYR:HB2	2.06	0.55
2:K:40:ARG:HD2	2:K:41:PRO:HD2	1.88	0.55
2:Z:52:ASP:OD2	2:Z:55:TYR:HB2	2.05	0.55
1:P:307:GLY:HA2	1:S:454:ARG:NH1	2.22	0.55
2:N:105:GLY:HA3	2:N:106:ARG:CG	2.36	0.55
3:U:166:GLN:HE21	3:U:171:SER:HB3	1.72	0.55
1:P:145:LEU:HG	1:P:323:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:GLY:O	3:I:36:TYR:OH	2.25	0.54
3:R:15:VAL:HG23	3:R:106:LEU:HD21	1.88	0.54
2:Z:40:ARG:HD2	2:Z:41:PRO:HD2	1.88	0.54
1:D:130:GLN:HG3	1:G:344:THR:HG22	1.87	0.54
1:G:427:ASP:HB3	1:G:430:LYS:HG3	1.89	0.54
1:D:62:VAL:HG22	1:D:321:THR:HG23	1.88	0.54
2:E:40:ARG:HD2	2:E:41:PRO:HD2	1.89	0.54
3:I:15:VAL:HG22	3:I:106:LEU:HD13	1.89	0.54
2:Q:40:ARG:HD2	2:Q:41:PRO:HD2	1.89	0.54
1:M:427:ASP:HB3	1:M:430:LYS:HG3	1.89	0.54
1:Y:83:PRO:O	1:Y:87:ARG:NH1	2.41	0.54
2:B:30:LYS:HA	2:B:31:ASP:CB	2.38	0.54
2:B:105:GLY:O	3:C:36:TYR:OH	2.24	0.54
2:Q:32:TYR:O	2:Q:53:PRO:HD2	2.07	0.54
1:V:275:VAL:HG22	1:Y:112:PHE:CE2	2.41	0.54
1:Y:262:ASP:O	1:Y:264:LEU:N	2.41	0.54
2:B:40:ARG:HD2	2:B:41:PRO:HD2	1.89	0.54
2:B:102:TYR:CG	2:B:103:ASP:N	2.75	0.54
3:F:118:PHE:HB2	3:F:133:VAL:HG22	1.89	0.54
2:T:52:ASP:OD2	2:T:55:TYR:HB2	2.08	0.54
1:J:307:GLY:HA2	1:M:454:ARG:NH1	2.23	0.54
3:C:149:LYS:HB2	3:C:193:THR:HB	1.90	0.54
3:F:150:ILE:HD11	3:F:179:LEU:HD21	1.89	0.54
3:L:106:LEU:HD22	3:L:107:LYS:H	1.73	0.54
2:N:107:PHE:O	2:N:110:TRP:NE1	2.41	0.54
1:G:141:LYS:HB2	1:G:244:MET:HB3	1.89	0.54
1:M:273:THR:HG21	2:B:59:GLU:OE2	2.07	0.54
3:F:149:LYS:HB2	3:F:193:THR:HB	1.90	0.54
2:W:40:ARG:HD2	2:W:41:PRO:HD2	1.89	0.54
2:T:32:TYR:O	2:T:53:PRO:HD2	2.08	0.53
1:V:427:ASP:HB3	1:V:430:LYS:HG3	1.90	0.53
2:Q:102:TYR:CG	2:Q:103:ASP:N	2.76	0.53
2:Z:99:GLY:HA2	2:Z:108:PRO:HD2	1.91	0.53
1:D:273:THR:HG21	2:H:59:GLU:OE2	2.08	0.53
1:J:170:GLN:HB3	1:J:171:ALA:HA	1.89	0.53
1:V:145:LEU:HG	1:V:323:VAL:HB	1.90	0.53
1:D:427:ASP:HB3	1:D:430:LYS:HG3	1.91	0.53
1:P:265:ILE:HD11	2:T:55:TYR:HE1	1.74	0.53
2:E:75:SER:O	2:E:77:ASN:HB2	2.09	0.53
1:J:273:THR:HG21	2:N:59:GLU:OE2	2.09	0.53
1:M:145:LEU:HG	1:M:323:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:39:LYS:HG2	3:U:84:ALA:HB2	1.91	0.53
3:I:149:LYS:HB2	3:I:193:THR:HB	1.90	0.53
2:Q:87:THR:OG1	2:Q:88:SER:N	2.42	0.53
3:R:149:LYS:HB2	3:R:193:THR:HB	1.90	0.53
1:Y:99:ARG:NH2	1:Y:356:GLU:OE1	2.42	0.53
1:D:170:GLN:HB3	1:D:171:ALA:HA	1.91	0.53
1:J:127:ASN:N	1:J:128:PRO:HD3	2.24	0.53
2:B:145:LEU:HD13	2:B:216:LYS:HD3	1.90	0.53
2:H:102:TYR:CG	2:H:103:ASP:N	2.77	0.53
1:Y:145:LEU:HG	1:Y:323:VAL:HB	1.91	0.53
1:Y:170:GLN:HB3	1:Y:171:ALA:HA	1.90	0.53
1:G:59:GLN:OE1	1:G:61:ARG:NH2	2.42	0.53
1:J:110:HIS:HB2	1:J:210:PRO:HA	1.90	0.53
1:P:246:ALA:HB1	1:P:249:PHE:HE2	1.74	0.53
2:B:48:ILE:HG23	2:B:64:PHE:HD1	1.74	0.53
2:K:31:ASP:OD2	2:K:32:TYR:N	2.42	0.53
2:Q:52:ASP:OD1	2:Q:55:TYR:HB2	2.09	0.53
1:D:260:VAL:O	2:H:55:TYR:OH	2.22	0.52
1:J:252:ARG:HE	1:M:332:THR:HG21	1.74	0.52
2:N:145:LEU:HD13	2:N:216:LYS:HD3	1.90	0.52
2:T:65:GLN:O	3:X:18:ARG:NH2	2.33	0.52
1:J:145:LEU:HG	1:J:323:VAL:HB	1.91	0.52
2:K:107:PHE:HB2	3:L:36:TYR:HE1	1.73	0.52
2:Z:19:LYS:HG3	2:Z:82:GLN:HB3	1.90	0.52
1:D:110:HIS:HB2	1:D:210:PRO:HA	1.92	0.52
1:D:141:LYS:HB2	1:D:244:MET:HB3	1.91	0.52
1:G:170:GLN:HB3	1:G:171:ALA:HA	1.92	0.52
1:P:192:THR:HG22	1:P:193:GLY:H	1.75	0.52
1:S:170:GLN:HB3	1:S:171:ALA:HA	1.92	0.52
2:E:102:TYR:CG	2:E:103:ASP:N	2.76	0.52
2:H:40:ARG:HD2	2:H:41:PRO:HD2	1.90	0.52
2:K:48:ILE:HG23	2:K:64:PHE:HD1	1.75	0.52
2:N:76:SER:CB	2:N:77:ASN:HB2	2.39	0.52
1:P:191:ASP:HA	1:P:218:CYS:HB3	1.90	0.52
2:H:30:LYS:HA	2:H:31:ASP:CB	2.30	0.52
2:H:106:ARG:HD2	3:I:49:TYR:CD1	2.44	0.52
2:Q:7:SER:HB2	2:Q:21:SER:H	1.74	0.52
2:Q:67:LYS:NZ	2:Q:85:SER:O	2.42	0.52
2:T:102:TYR:CG	2:T:103:ASP:N	2.78	0.52
2:W:145:LEU:HD13	2:W:216:LYS:HD3	1.92	0.52
1:S:127:ASN:N	1:S:128:PRO:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:ARG:HD2	2:N:41:PRO:HD2	1.91	0.52
2:T:76:SER:CB	2:T:77:ASN:HB2	2.40	0.52
1:G:145:LEU:HG	1:G:323:VAL:HB	1.92	0.52
1:M:110:HIS:HB2	1:M:210:PRO:HA	1.91	0.52
2:W:52:ASP:OD2	2:W:55:TYR:HB2	2.09	0.52
1:V:170:GLN:HB3	1:V:171:ALA:HA	1.92	0.52
1:Y:127:ASN:N	1:Y:128:PRO:HD3	2.25	0.52
2:H:78:THR:HG22	2:H:79:ALA:HB2	1.92	0.52
2:K:76:SER:CB	2:K:77:ASN:HB2	2.39	0.52
1:A:260:VAL:HG23	2:E:55:TYR:OH	2.10	0.52
1:S:167:THR:HB	1:S:168:PRO:HB3	1.92	0.52
1:V:167:THR:HB	1:V:168:PRO:HB3	1.92	0.52
1:D:127:ASN:N	1:D:128:PRO:HD3	2.25	0.52
1:P:170:GLN:HB3	1:P:171:ALA:HA	1.92	0.52
2:H:51:ILE:HG13	2:H:70:MET:HE2	1.91	0.52
2:K:67:LYS:NZ	2:K:85:SER:O	2.43	0.52
2:W:51:ILE:HG22	2:W:58:THR:HG22	1.91	0.52
2:W:67:LYS:NZ	2:W:85:SER:O	2.43	0.52
1:D:145:LEU:HG	1:D:323:VAL:HB	1.92	0.51
1:M:141:LYS:HB2	1:M:244:MET:HB3	1.92	0.51
1:V:265:ILE:HD11	2:Z:55:TYR:HE1	1.75	0.51
2:T:105:GLY:O	3:U:36:TYR:OH	2.28	0.51
3:X:46:LEU:HD21	3:X:49:TYR:HD2	1.75	0.51
3:O:47:MET:HA	3:O:58:VAL:HG21	1.92	0.51
1:M:170:GLN:HB3	1:M:171:ALA:HA	1.92	0.51
2:B:32:TYR:O	2:B:53:PRO:HD2	2.10	0.51
2:B:35:HIS:CE1	2:B:104:ARG:HA	2.45	0.51
2:T:11:VAL:HG21	2:T:154:PRO:HG3	1.93	0.51
1:A:62:VAL:HG22	1:A:321:THR:HG23	1.92	0.51
2:N:51:ILE:HG13	2:N:70:MET:HE2	1.91	0.51
2:Q:76:SER:HB3	2:Q:77:ASN:CA	2.40	0.51
2:Q:105:GLY:O	3:R:36:TYR:OH	2.29	0.51
1:D:268:GLY:HA3	1:D:269:SER:HB2	1.92	0.51
1:M:127:ASN:N	1:M:128:PRO:HD3	2.26	0.51
2:Q:145:LEU:HD13	2:Q:216:LYS:HD3	1.92	0.51
1:D:167:THR:HB	1:D:168:PRO:HB3	1.92	0.51
2:T:35:HIS:CE1	2:T:104:ARG:HA	2.45	0.51
1:G:127:ASN:N	1:G:128:PRO:HD3	2.25	0.51
1:J:141:LYS:HB2	1:J:244:MET:HB3	1.93	0.51
1:P:268:GLY:HA3	1:P:269:SER:OG	2.11	0.51
1:S:141:LYS:HB2	1:S:244:MET:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:ALA:HA	2:E:78:THR:HG23	1.93	0.51
1:P:167:THR:HB	1:P:168:PRO:HB3	1.93	0.51
2:K:31:ASP:O	2:K:53:PRO:HG2	2.11	0.51
3:L:14:SER:HA	3:L:106:LEU:HD23	1.93	0.51
3:U:150:ILE:HD11	3:U:179:LEU:HD21	1.93	0.51
1:M:58:TYR:CZ	1:M:140:TYR:HB2	2.46	0.50
1:Y:110:HIS:HB2	1:Y:210:PRO:HA	1.94	0.50
1:Y:246:ALA:HB1	1:Y:249:PHE:HE2	1.76	0.50
2:W:76:SER:HB2	2:W:78:THR:OG1	2.12	0.50
1:A:102:PRO:HG3	1:M:220:TYR:CG	2.46	0.50
1:G:167:THR:HB	1:G:168:PRO:HB3	1.93	0.50
1:P:44:ILE:HD12	1:P:52:VAL:HB	1.91	0.50
1:V:127:ASN:N	1:V:128:PRO:HD3	2.26	0.50
2:E:194:THR:HG23	2:E:198:GLU:OE2	2.12	0.50
3:C:87:PHE:HE1	3:C:101:GLY:HA2	1.76	0.50
2:H:75:SER:O	2:H:77:ASN:HB2	2.12	0.50
3:O:46:LEU:HD21	3:O:49:TYR:HD2	1.75	0.50
3:R:147:LYS:HD2	3:R:149:LYS:HZ1	1.75	0.50
1:P:58:TYR:CZ	1:P:140:TYR:HB2	2.46	0.50
1:S:83:PRO:O	1:S:87:ARG:NH1	2.44	0.50
1:S:427:ASP:HB3	1:S:430:LYS:HG3	1.91	0.50
1:V:273:THR:HG21	2:Z:59:GLU:OE2	2.12	0.50
2:Z:48:ILE:HG23	2:Z:64:PHE:HD1	1.76	0.50
1:Y:141:LYS:HE3	1:Y:242:GLU:HB3	1.92	0.50
2:W:32:TYR:H	2:W:32:TYR:HD2	1.59	0.50
1:M:229:ASP:OD1	1:M:230:PRO:HD2	2.12	0.50
1:P:273:THR:HG21	2:T:59:GLU:OE2	2.11	0.50
1:S:344:THR:HG21	3:U:53:ASN:ND2	2.27	0.50
1:A:127:ASN:N	1:A:128:PRO:HD3	2.26	0.50
1:A:170:GLN:HB3	1:A:171:ALA:HA	1.94	0.50
1:D:246:ALA:HB1	1:D:249:PHE:HE2	1.77	0.50
1:J:172:GLY:HA3	1:M:337:VAL:HG22	1.94	0.50
1:P:44:ILE:HG23	2:Q:29:ILE:HD11	1.94	0.50
1:P:127:ASN:N	1:P:128:PRO:HD3	2.26	0.50
1:S:145:LEU:HG	1:S:323:VAL:HB	1.93	0.50
1:V:246:ALA:HB1	1:V:249:PHE:HE2	1.75	0.50
2:B:123:THR:HG23	2:B:154:PRO:HD3	1.93	0.50
2:H:76:SER:HB2	2:H:77:ASN:CB	2.40	0.50
2:H:131:LEU:H	2:H:216:LYS:HZ3	1.59	0.50
1:A:268:GLY:HA3	1:A:269:SER:HB2	1.94	0.50
1:A:273:THR:HG21	2:E:59:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:VAL:HG22	1:G:320:VAL:HG22	1.94	0.50
1:G:246:ALA:HB1	1:G:249:PHE:HE2	1.77	0.50
1:S:307:GLY:HA2	1:V:454:ARG:NH1	2.27	0.50
2:H:145:LEU:HB3	2:H:216:LYS:HE2	1.94	0.50
2:W:22:CYS:HB3	2:W:79:ALA:HB3	1.94	0.50
1:A:167:THR:HB	1:A:168:PRO:HB3	1.94	0.49
1:A:427:ASP:HB3	1:A:430:LYS:HG3	1.92	0.49
1:D:256:VAL:HG13	1:D:279:ILE:HD11	1.94	0.49
1:J:271:ASN:CG	1:J:272:ARG:H	2.15	0.49
1:M:46:ARG:CB	2:N:29:ILE:HG12	2.42	0.49
1:V:307:GLY:HA2	1:Y:454:ARG:NH1	2.26	0.49
2:T:73:ASP:N	2:T:78:THR:HG21	2.25	0.49
2:T:145:LEU:HD13	2:T:216:LYS:HD3	1.93	0.49
1:A:307:GLY:HA2	1:D:454:ARG:NH1	2.27	0.49
2:B:100:HIS:HD2	2:B:106:ARG:NH2	2.09	0.49
2:Q:104:ARG:HB3	3:R:96:LEU:HD11	1.94	0.49
2:W:131:LEU:H	2:W:216:LYS:NZ	2.10	0.49
2:W:131:LEU:H	2:W:216:LYS:HZ3	1.60	0.49
1:D:148:VAL:HG22	1:D:320:VAL:HG22	1.93	0.49
2:E:145:LEU:HB3	2:E:216:LYS:HE2	1.94	0.49
2:K:53:PRO:O	2:K:54:GLU:HB3	2.12	0.49
2:N:67:LYS:NZ	2:N:85:SER:O	2.45	0.49
2:T:22:CYS:CB	2:T:79:ALA:H	2.21	0.49
1:S:229:ASP:OD1	1:S:230:PRO:HD2	2.12	0.49
2:Q:65:GLN:O	3:U:18:ARG:NH2	2.38	0.49
3:R:47:MET:HA	3:R:58:VAL:HG21	1.95	0.49
2:T:19:LYS:HG3	2:T:82:GLN:HB3	1.95	0.49
1:A:141:LYS:HB2	1:A:244:MET:HB3	1.94	0.49
1:G:275:VAL:HG22	1:J:112:PHE:CE2	2.46	0.49
3:I:39:LYS:HG2	3:I:84:ALA:HB2	1.94	0.49
2:K:145:LEU:HB3	2:K:216:LYS:HE2	1.95	0.49
2:Q:131:LEU:H	2:Q:216:LYS:NZ	2.11	0.49
1:D:272:ARG:NH2	1:G:133:ARG:O	2.46	0.49
1:G:143:THR:HG23	1:G:242:GLU:HG2	1.94	0.49
1:J:47:ALA:HB1	2:K:28:ASN:ND2	2.28	0.49
1:M:246:ALA:HB1	1:M:249:PHE:HE2	1.77	0.49
2:B:65:GLN:O	3:F:18:ARG:NH2	2.37	0.49
2:Q:145:LEU:HB3	2:Q:216:LYS:HE2	1.95	0.49
2:W:100:HIS:HB3	2:W:109:TYR:HE2	1.78	0.49
1:A:269:SER:O	1:A:269:SER:OG	2.30	0.49
1:Y:167:THR:HB	1:Y:168:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:142:LYS:HE3	3:O:142:LYS:HB2	1.55	0.49
2:T:53:PRO:O	2:T:54:GLU:HB3	2.13	0.49
1:J:257:GLY:O	2:N:30:LYS:HE2	2.13	0.48
1:S:246:ALA:HB1	1:S:249:PHE:HE2	1.77	0.48
2:H:131:LEU:H	2:H:216:LYS:NZ	2.11	0.48
1:D:265:ILE:HD11	2:H:55:TYR:CE1	2.49	0.48
1:P:23:THR:OG1	1:P:366:LEU:O	2.26	0.48
1:S:265:ILE:HD11	2:W:55:TYR:HE1	1.77	0.48
2:E:145:LEU:HD13	2:E:216:LYS:HD3	1.93	0.48
3:U:13:THR:O	3:U:106:LEU:HA	2.13	0.48
2:W:145:LEU:HB3	2:W:216:LYS:HE2	1.95	0.48
1:G:307:GLY:HA2	1:J:454:ARG:NH1	2.28	0.48
1:J:59:GLN:OE1	1:J:61:ARG:NH2	2.47	0.48
1:Y:193:GLY:HA3	1:Y:284:PRO:CG	2.42	0.48
2:H:26:GLY:HA2	2:H:53:PRO:HG3	1.96	0.48
3:I:113:PRO:HB3	3:I:139:PHE:HB3	1.96	0.48
1:A:110:HIS:HB2	1:A:210:PRO:HA	1.95	0.48
1:V:271:ASN:CG	1:V:272:ARG:H	2.17	0.48
2:B:53:PRO:O	2:B:54:GLU:HB3	2.13	0.48
3:F:87:PHE:HE1	3:F:101:GLY:HA2	1.79	0.48
2:N:28:ASN:OD1	2:N:28:ASN:N	2.34	0.48
2:Q:53:PRO:O	2:Q:54:GLU:HB3	2.14	0.48
2:T:11:VAL:CG2	2:T:154:PRO:HG3	2.44	0.48
1:D:271:ASN:CG	1:D:272:ARG:H	2.17	0.48
1:D:307:GLY:HA2	1:G:454:ARG:NH1	2.29	0.48
1:G:268:GLY:HA2	1:M:342:THR:HG22	1.95	0.48
1:V:220:TYR:CG	1:Y:102:PRO:HG3	2.48	0.48
2:B:72:ALA:HA	2:B:78:THR:OG1	2.13	0.48
2:E:100:HIS:HB3	2:E:109:TYR:CE2	2.42	0.48
2:H:138:GLN:HE22	2:H:143:VAL:HG23	1.79	0.48
2:N:72:ALA:HA	2:N:78:THR:OG1	2.13	0.48
2:N:145:LEU:HB3	2:N:216:LYS:HE2	1.96	0.48
3:O:108:ARG:HH12	3:O:111:ALA:HB2	1.78	0.48
3:X:46:LEU:HD21	3:X:49:TYR:CD2	2.49	0.48
1:V:272:ARG:HG2	1:Y:112:PHE:HE1	1.78	0.48
2:B:131:LEU:H	2:B:216:LYS:NZ	2.10	0.48
2:H:52:ASP:OD2	2:H:55:TYR:HB2	2.14	0.48
2:B:103:ASP:OD1	2:B:104:ARG:HG2	2.13	0.48
2:H:100:HIS:HB3	2:H:109:TYR:HE2	1.79	0.48
3:L:150:ILE:HD11	3:L:179:LEU:HD21	1.96	0.48
1:J:246:ALA:HB1	1:J:249:PHE:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:ILE:HG23	2:E:64:PHE:HD1	1.78	0.48
2:W:99:GLY:HA2	2:W:108:PRO:CD	2.44	0.48
1:D:153:PRO:HG2	1:D:184:ILE:HB	1.96	0.48
1:G:110:HIS:HB2	1:G:210:PRO:HA	1.96	0.48
2:B:52:ASP:OD2	2:B:55:TYR:HB2	2.14	0.48
3:I:47:MET:HA	3:I:58:VAL:HG21	1.95	0.48
1:A:246:ALA:HB1	1:A:249:PHE:HE2	1.79	0.48
1:P:110:HIS:HB2	1:P:210:PRO:HA	1.96	0.48
2:N:22:CYS:HB3	2:N:79:ALA:N	2.28	0.48
2:Q:131:LEU:H	2:Q:216:LYS:HZ3	1.62	0.48
2:N:36:TRP:CH2	2:N:96:CYS:HB3	2.48	0.47
2:Z:206:HIS:CE1	2:Z:208:ALA:HB3	2.49	0.47
1:J:170:GLN:HB3	1:J:171:ALA:CA	2.43	0.47
1:S:95:LEU:HD22	1:S:148:VAL:HG21	1.95	0.47
1:S:130:GLN:HG3	1:V:344:THR:HG22	1.96	0.47
1:V:119:VAL:HG21	1:V:280:TYR:HE1	1.79	0.47
1:V:170:GLN:HB3	1:V:171:ALA:CA	2.45	0.47
2:B:145:LEU:HB3	2:B:216:LYS:HE2	1.96	0.47
1:A:44:ILE:HD12	1:A:52:VAL:HB	1.96	0.47
1:A:275:VAL:HG22	1:D:112:PHE:CE2	2.41	0.47
1:D:95:LEU:HD22	1:D:148:VAL:HG21	1.96	0.47
1:D:170:GLN:HB3	1:D:171:ALA:CA	2.44	0.47
1:V:44:ILE:HD12	1:V:52:VAL:HB	1.96	0.47
2:N:102:TYR:CG	2:N:103:ASP:N	2.81	0.47
3:X:147:LYS:HD2	3:X:149:LYS:HZ1	1.79	0.47
2:K:29:ILE:HD12	2:K:29:ILE:HA	1.77	0.47
2:Q:99:GLY:HA2	2:Q:108:PRO:HD2	1.97	0.47
2:T:131:LEU:H	2:T:216:LYS:NZ	2.12	0.47
1:J:95:LEU:HD22	1:J:148:VAL:HG21	1.97	0.47
1:M:46:ARG:HA	1:M:47:ALA:HA	1.60	0.47
1:Y:95:LEU:HD22	1:Y:148:VAL:HG21	1.97	0.47
1:Y:170:GLN:HB3	1:Y:171:ALA:CA	2.44	0.47
2:T:100:HIS:HB3	2:T:109:TYR:HE2	1.79	0.47
2:E:32:TYR:H	2:E:32:TYR:HD2	1.63	0.47
1:J:46:ARG:HA	1:J:47:ALA:HA	1.56	0.47
1:J:256:VAL:HG13	1:J:279:ILE:HD11	1.97	0.47
1:M:271:ASN:CG	1:M:272:ARG:H	2.18	0.47
1:P:95:LEU:HD22	1:P:148:VAL:HG21	1.96	0.47
1:V:256:VAL:HG13	1:V:279:ILE:HD11	1.97	0.47
2:Q:31:ASP:HB3	2:Q:54:GLU:HB3	1.97	0.47
2:Z:138:GLN:O	2:Z:139:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:148:VAL:HG22	1:M:320:VAL:HG22	1.95	0.47
1:M:170:GLN:HB3	1:M:171:ALA:CA	2.45	0.47
1:M:261:PRO:HD2	1:M:264:LEU:HD12	1.95	0.47
1:V:95:LEU:HD22	1:V:148:VAL:HG21	1.97	0.47
2:Z:201:THR:HG21	2:Z:213:VAL:HG13	1.97	0.47
1:A:95:LEU:HD22	1:A:148:VAL:HG21	1.97	0.47
1:M:268:GLY:HA3	1:M:269:SER:HB2	1.96	0.47
2:B:80:TYR:CD2	2:B:80:TYR:N	2.83	0.47
3:C:150:ILE:HD11	3:C:179:LEU:HD21	1.96	0.47
2:H:22:CYS:HB3	2:H:79:ALA:N	2.29	0.47
2:N:131:LEU:H	2:N:216:LYS:HZ3	1.63	0.47
3:R:150:ILE:HD11	3:R:179:LEU:HD21	1.96	0.47
3:X:147:LYS:HD2	3:X:149:LYS:NZ	2.30	0.47
1:P:427:ASP:HB3	1:P:430:LYS:HG3	1.96	0.47
2:N:53:PRO:O	2:N:54:GLU:HB3	2.15	0.47
2:T:145:LEU:HB3	2:T:216:LYS:HE2	1.97	0.47
3:U:47:MET:HA	3:U:58:VAL:HG21	1.97	0.47
1:M:46:ARG:HB3	2:N:29:ILE:HG12	1.97	0.46
2:E:106:ARG:HA	2:E:107:PHE:CB	2.44	0.46
3:I:80:SER:HB3	3:I:168:SER:O	2.14	0.46
2:K:76:SER:HB2	2:K:77:ASN:HB2	1.96	0.46
1:P:37:VAL:HG22	1:P:355:VAL:HG12	1.97	0.46
1:S:44:ILE:HD12	1:S:52:VAL:HB	1.98	0.46
1:S:170:GLN:HB3	1:S:171:ALA:CA	2.45	0.46
3:I:150:ILE:HD11	3:I:179:LEU:HD21	1.97	0.46
2:K:99:GLY:HA2	2:K:108:PRO:HD2	1.98	0.46
2:Z:140:ASN:HA	2:Z:141:SER:HA	1.55	0.46
1:A:119:VAL:HG21	1:A:280:TYR:HE1	1.80	0.46
1:A:332:THR:HG21	1:M:252:ARG:HE	1.80	0.46
1:J:268:GLY:HA3	1:J:269:SER:HB2	1.96	0.46
1:M:95:LEU:HD22	1:M:148:VAL:HG21	1.97	0.46
2:B:121:ALA:CB	2:B:122:LYS:HA	2.41	0.46
2:E:140:ASN:HA	2:E:141:SER:HA	1.66	0.46
3:F:55:TYR:O	3:F:58:VAL:HG23	2.15	0.46
3:I:147:LYS:HD2	3:I:149:LYS:HZ1	1.80	0.46
1:J:37:VAL:HG22	1:J:355:VAL:HG12	1.97	0.46
2:E:131:LEU:H	2:E:216:LYS:NZ	2.14	0.46
2:K:131:LEU:H	2:K:216:LYS:NZ	2.14	0.46
2:T:99:GLY:HA2	2:T:108:PRO:CD	2.44	0.46
1:P:170:GLN:HB3	1:P:171:ALA:CA	2.45	0.46
1:Y:46:ARG:HA	1:Y:47:ALA:HA	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:TYR:H	2:H:32:TYR:HD2	1.62	0.46
2:K:106:ARG:HD2	3:L:49:TYR:HB2	1.98	0.46
2:N:123:THR:HG23	2:N:154:PRO:HD3	1.98	0.46
2:Q:138:GLN:O	2:Q:139:THR:HG22	2.16	0.46
2:Q:140:ASN:HA	2:Q:141:SER:HA	1.69	0.46
3:U:106:LEU:HB2	3:U:166:GLN:NE2	2.19	0.46
1:A:271:ASN:CG	1:A:272:ARG:H	2.17	0.46
1:D:44:ILE:HD12	1:D:52:VAL:HB	1.98	0.46
1:D:46:ARG:HA	1:D:47:ALA:HA	1.56	0.46
1:D:220:TYR:CG	1:G:102:PRO:HG3	2.50	0.46
1:G:170:GLN:HB3	1:G:171:ALA:CA	2.45	0.46
1:G:250:PHE:HE1	1:G:283:THR:HG23	1.80	0.46
1:V:338:THR:HG22	1:V:339:THR:H	1.81	0.46
3:O:138:ASN:HA	3:O:172:THR:HB	1.98	0.46
1:V:37:VAL:HG22	1:V:355:VAL:HG12	1.97	0.46
2:N:100:HIS:HE1	3:O:49:TYR:CZ	2.33	0.46
1:J:344:THR:HG21	3:L:53:ASN:ND2	2.31	0.46
1:P:220:TYR:CG	1:S:102:PRO:HG3	2.51	0.46
3:O:46:LEU:HD21	3:O:49:TYR:CD2	2.51	0.46
1:D:83:PRO:O	1:D:87:ARG:NH1	2.48	0.46
1:M:44:ILE:HD12	1:M:52:VAL:HB	1.98	0.46
1:Y:62:VAL:HG22	1:Y:321:THR:HG23	1.98	0.46
2:E:107:PHE:HB3	2:E:108:PRO:HA	1.98	0.46
1:P:322:VAL:HG11	1:P:358:TYR:HE1	1.82	0.45
1:S:268:GLY:HA3	1:S:269:SER:HB2	1.98	0.45
1:S:271:ASN:CG	1:S:272:ARG:H	2.19	0.45
1:Y:59:GLN:OE1	1:Y:61:ARG:NH2	2.49	0.45
3:O:147:LYS:HD2	3:O:149:LYS:NZ	2.31	0.45
1:D:163:GLN:HA	1:D:164:CYS:HA	1.72	0.45
1:V:141:LYS:HB2	1:V:244:MET:HB3	1.97	0.45
2:E:131:LEU:H	2:E:216:LYS:HZ3	1.63	0.45
2:N:26:GLY:HA2	2:N:53:PRO:HG3	1.98	0.45
2:Q:100:HIS:HB3	2:Q:109:TYR:HE2	1.81	0.45
1:A:170:GLN:HB3	1:A:171:ALA:CA	2.46	0.45
1:A:220:TYR:CG	1:D:102:PRO:HG3	2.50	0.45
1:G:271:ASN:CG	1:G:272:ARG:H	2.20	0.45
1:P:203:GLN:HA	1:S:334:CYS:HB3	1.97	0.45
2:T:36:TRP:CZ2	2:T:96:CYS:HB3	2.51	0.45
2:H:48:ILE:HG23	2:H:64:PHE:HD1	1.82	0.45
3:L:147:LYS:HD2	3:L:149:LYS:NZ	2.32	0.45
2:N:36:TRP:HZ2	2:N:79:ALA:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:48:ILE:HG23	2:N:64:PHE:HD1	1.81	0.45
2:K:4:LEU:HD23	2:K:96:CYS:SG	2.56	0.45
3:R:14:SER:HA	3:R:106:LEU:HD23	1.97	0.45
2:W:105:GLY:O	3:X:36:TYR:OH	2.34	0.45
1:P:338:THR:HG22	1:P:339:THR:H	1.82	0.45
1:V:193:GLY:HA3	1:V:284:PRO:CG	2.43	0.45
1:V:268:GLY:HA3	1:V:269:SER:HB2	1.99	0.45
2:Q:78:THR:HB	2:Q:79:ALA:HB2	1.98	0.45
2:Z:53:PRO:O	2:Z:54:GLU:HB3	2.16	0.45
1:M:119:VAL:HG21	1:M:280:TYR:HE1	1.82	0.45
1:P:140:TYR:CD1	1:P:192:THR:HG21	2.52	0.45
2:B:99:GLY:HA2	2:B:108:PRO:CD	2.46	0.45
3:I:151:ASP:HA	3:I:191:SER:HB3	1.98	0.45
3:X:87:PHE:HE1	3:X:101:GLY:HA2	1.81	0.45
1:P:140:TYR:CG	1:P:192:THR:HG21	2.51	0.45
1:S:220:TYR:CG	1:V:102:PRO:HG3	2.51	0.45
1:Y:44:ILE:HD12	1:Y:52:VAL:HB	1.99	0.45
2:B:75:SER:OG	2:W:123:THR:HB	2.16	0.45
2:N:32:TYR:O	2:N:53:PRO:HD2	2.17	0.45
2:Q:13:ARG:HH21	2:Q:121:ALA:HB1	1.82	0.45
3:R:147:LYS:HD2	3:R:149:LYS:NZ	2.32	0.45
3:U:87:PHE:HE1	3:U:101:GLY:HA2	1.82	0.45
1:J:119:VAL:HG21	1:J:280:TYR:HE1	1.81	0.45
2:N:131:LEU:H	2:N:216:LYS:NZ	2.14	0.45
2:Q:22:CYS:H	2:Q:79:ALA:H	1.65	0.45
3:U:113:PRO:HB3	3:U:139:PHE:HB3	1.99	0.45
2:E:36:TRP:CH2	2:E:96:CYS:HB3	2.51	0.45
2:K:140:ASN:HA	2:K:141:SER:HA	1.67	0.45
3:R:87:PHE:HE1	3:R:101:GLY:HA2	1.82	0.45
2:Z:30:LYS:HA	2:Z:31:ASP:HB2	1.98	0.45
1:A:112:PHE:HE1	1:M:272:ARG:HG2	1.82	0.44
1:A:272:ARG:HG2	1:D:112:PHE:HE1	1.81	0.44
1:D:58:TYR:CE1	1:D:140:TYR:HB2	2.52	0.44
1:M:153:PRO:HG2	1:M:184:ILE:HB	1.99	0.44
1:V:163:GLN:HA	1:V:164:CYS:HA	1.72	0.44
1:V:349:LYS:CE	2:W:101:ASP:OD2	2.64	0.44
2:K:52:ASP:OD2	2:K:53:PRO:O	2.35	0.44
2:T:174:PRO:O	3:U:162:SER:OG	2.29	0.44
3:X:47:MET:HA	3:X:58:VAL:HG21	1.99	0.44
1:S:143:THR:HG23	1:S:242:GLU:HG2	1.99	0.44
2:B:78:THR:HG23	2:B:79:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:78:THR:HG23	2:N:79:ALA:HB2	1.98	0.44
2:W:53:PRO:O	2:W:54:GLU:HB3	2.16	0.44
2:W:161:TRP:HZ3	2:W:216:LYS:HD2	1.82	0.44
1:A:338:THR:HG22	1:A:339:THR:H	1.82	0.44
1:S:163:GLN:HA	1:S:164:CYS:HA	1.70	0.44
2:B:100:HIS:HB3	2:B:109:TYR:HE2	1.83	0.44
2:H:206:HIS:ND1	2:H:209:SER:HB2	2.33	0.44
3:I:147:LYS:HD2	3:I:149:LYS:NZ	2.33	0.44
2:Q:80:TYR:N	2:Q:80:TYR:CD2	2.84	0.44
2:T:26:GLY:HA2	2:T:53:PRO:HG3	1.99	0.44
1:P:163:GLN:HA	1:P:164:CYS:HA	1.71	0.44
3:C:147:LYS:HD2	3:C:149:LYS:NZ	2.32	0.44
3:I:125:LEU:O	3:I:183:LYS:HD3	2.17	0.44
3:I:138:ASN:HA	3:I:172:THR:HB	1.99	0.44
3:U:46:LEU:HD21	3:U:49:TYR:CD2	2.50	0.44
1:J:163:GLN:HA	1:J:164:CYS:HA	1.70	0.44
1:S:260:VAL:N	2:W:55:TYR:OH	2.51	0.44
1:Y:271:ASN:O	1:Y:273:THR:OG1	2.33	0.44
2:E:107:PHE:HD2	3:F:36:TYR:CE1	2.36	0.44
2:H:161:TRP:HZ3	2:H:216:LYS:HD2	1.83	0.44
2:K:76:SER:HB2	2:K:77:ASN:CB	2.48	0.44
3:O:150:ILE:HD11	3:O:179:LEU:HD21	2.00	0.44
1:G:44:ILE:HD12	1:G:52:VAL:HB	2.00	0.44
1:S:46:ARG:HA	1:S:47:ALA:HA	1.55	0.44
1:V:46:ARG:HA	1:V:47:ALA:HA	1.55	0.44
2:H:25:SER:O	2:H:78:THR:HB	2.16	0.44
1:P:153:PRO:HG2	1:P:184:ILE:HB	2.00	0.44
1:P:256:VAL:HG13	1:P:279:ILE:HD11	2.00	0.44
3:C:47:MET:HA	3:C:58:VAL:HG21	2.00	0.44
3:O:105:GLU:OE1	3:O:173:TYR:OH	2.36	0.44
3:R:151:ASP:HA	3:R:191:SER:HB3	2.00	0.44
3:X:150:ILE:HD11	3:X:179:LEU:HD21	1.99	0.44
1:G:46:ARG:HA	1:G:47:ALA:HA	1.58	0.44
1:G:268:GLY:HA3	1:G:269:SER:HB2	1.99	0.44
1:M:356:GLU:HB3	1:M:358:TYR:HE2	1.83	0.44
2:B:67:LYS:NZ	2:B:85:SER:O	2.49	0.44
2:B:76:SER:HB2	2:B:77:ASN:HB2	1.99	0.44
2:B:107:PHE:HB2	3:C:36:TYR:CE1	2.47	0.44
3:L:87:PHE:HE1	3:L:101:GLY:HA2	1.83	0.44
1:A:97:VAL:O	1:A:296:PHE:HB3	2.18	0.44
1:J:220:TYR:CG	1:M:102:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:35:HIS:CD2	2:K:107:PHE:HE1	2.36	0.44
2:T:29:ILE:HG23	2:T:30:LYS:HG3	2.00	0.44
2:W:48:ILE:HG12	2:W:64:PHE:CE1	2.53	0.44
1:G:220:TYR:CG	1:J:102:PRO:HG3	2.53	0.43
1:M:256:VAL:HG13	1:M:279:ILE:HD11	1.99	0.43
1:P:46:ARG:CZ	2:Q:29:ILE:HG21	2.48	0.43
2:E:35:HIS:HB2	2:E:107:PHE:HE1	1.83	0.43
2:W:47:TRP:HZ2	2:W:50:ALA:HB2	1.82	0.43
2:B:47:TRP:HZ2	2:B:50:ALA:HB2	1.82	0.43
2:T:36:TRP:HZ2	2:T:79:ALA:O	2.01	0.43
3:U:147:LYS:HD2	3:U:149:LYS:NZ	2.31	0.43
2:Z:29:ILE:HG12	2:Z:30:LYS:HG2	2.00	0.43
2:Z:31:ASP:OD2	2:Z:101:ASP:HB3	2.19	0.43
1:G:256:VAL:HG13	1:G:279:ILE:HD11	2.00	0.43
1:P:265:ILE:HG22	1:S:110:HIS:CE1	2.53	0.43
2:H:36:TRP:HZ2	2:H:79:ALA:O	2.02	0.43
2:T:48:ILE:HG23	2:T:64:PHE:HD1	1.82	0.43
1:S:349:LYS:HZ3	2:T:30:LYS:HD3	1.83	0.43
3:F:113:PRO:HB3	3:F:139:PHE:HB3	2.00	0.43
3:F:147:LYS:HD2	3:F:149:LYS:NZ	2.34	0.43
2:Z:48:ILE:HG12	2:Z:64:PHE:CE1	2.53	0.43
1:M:163:GLN:HA	1:M:164:CYS:HA	1.70	0.43
1:Y:256:VAL:HG13	1:Y:279:ILE:HD11	2.00	0.43
2:B:26:GLY:HA2	2:B:53:PRO:HG3	1.99	0.43
2:H:28:ASN:C	2:H:30:LYS:H	2.22	0.43
2:N:75:SER:O	2:N:77:ASN:HB2	2.18	0.43
2:Z:28:ASN:C	2:Z:29:ILE:HG23	2.39	0.43
1:A:454:ARG:NH1	1:M:307:GLY:HA2	2.33	0.43
1:D:382:MET:HG2	1:D:383:ASN:H	1.84	0.43
1:P:346:SER:O	2:Q:100:HIS:NE2	2.51	0.43
2:B:36:TRP:HZ2	2:B:79:ALA:O	2.01	0.43
2:K:48:ILE:HG12	2:K:64:PHE:CE1	2.53	0.43
2:E:6:GLN:NE2	2:E:114:THR:OG1	2.47	0.43
2:K:138:GLN:O	2:K:139:THR:HG22	2.18	0.43
3:O:147:LYS:HD2	3:O:149:LYS:HZ1	1.83	0.43
2:Z:77:ASN:OD1	2:Z:78:THR:N	2.45	0.43
1:A:193:GLY:HA3	1:A:284:PRO:CG	2.47	0.43
1:G:193:GLY:HA3	1:G:284:PRO:CG	2.46	0.43
1:P:268:GLY:HA2	1:V:342:THR:OG1	2.19	0.43
1:S:119:VAL:HG21	1:S:280:TYR:HE1	1.84	0.43
2:N:78:THR:OG1	2:N:79:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:35:HIS:CE1	2:Q:104:ARG:HA	2.53	0.43
3:U:140:TYR:CG	3:U:141:PRO:HA	2.53	0.43
2:W:32:TYR:O	2:W:53:PRO:HD2	2.18	0.43
1:A:382:MET:HG2	1:A:383:ASN:H	1.84	0.43
1:D:99:ARG:NH2	1:D:356:GLU:OE1	2.50	0.43
1:G:344:THR:HG21	3:I:53:ASN:ND2	2.33	0.43
1:J:322:VAL:HG11	1:J:358:TYR:HE1	1.84	0.43
1:M:46:ARG:HG2	1:M:51:VAL:HG21	2.01	0.43
1:S:70:PRO:HA	1:S:73:PHE:HB2	2.00	0.43
1:A:257:GLY:O	2:E:30:LYS:HE2	2.18	0.43
1:G:338:THR:HG22	1:G:339:THR:H	1.84	0.43
1:J:153:PRO:HG2	1:J:184:ILE:HB	2.00	0.43
1:J:255:GLU:OE2	2:N:102:TYR:HB3	2.18	0.43
1:M:338:THR:HG22	1:M:339:THR:H	1.84	0.43
2:E:106:ARG:HD2	3:F:49:TYR:CD1	2.52	0.43
2:H:99:GLY:HA2	2:H:108:PRO:HD2	2.00	0.43
2:K:53:PRO:O	2:K:55:TYR:N	2.52	0.43
1:A:252:ARG:HE	1:D:332:THR:HG21	1.84	0.42
1:J:275:VAL:HG22	1:M:112:PHE:CE2	2.46	0.42
2:E:101:ASP:O	2:E:102:TYR:HB2	2.19	0.42
2:K:13:ARG:HE	2:K:120:ALA:HB1	1.83	0.42
2:N:36:TRP:CZ2	2:N:96:CYS:HB3	2.54	0.42
2:Z:131:LEU:H	2:Z:216:LYS:NZ	2.16	0.42
1:M:123:GLY:HA2	1:M:124:SER:HA	1.76	0.42
1:S:110:HIS:HB2	1:S:210:PRO:HA	2.00	0.42
3:O:87:PHE:HE1	3:O:101:GLY:HA2	1.84	0.42
3:O:151:ASP:HA	3:O:191:SER:HB3	2.00	0.42
2:Q:26:GLY:HA2	2:Q:53:PRO:HG3	1.99	0.42
1:A:143:THR:HG23	1:A:242:GLU:HG2	2.01	0.42
1:S:193:GLY:HA3	1:S:284:PRO:CG	2.47	0.42
1:S:382:MET:HG2	1:S:383:ASN:H	1.84	0.42
1:V:269:SER:O	1:V:269:SER:OG	2.28	0.42
3:I:87:PHE:HE1	3:I:101:GLY:HA2	1.83	0.42
2:N:106:ARG:HG2	3:O:49:TYR:CB	2.50	0.42
3:O:105:GLU:HB3	3:O:166:GLN:OE1	2.19	0.42
1:P:193:GLY:HA3	1:P:284:PRO:HG3	2.02	0.42
1:D:123:GLY:HA2	1:D:124:SER:HA	1.79	0.42
1:G:269:SER:O	1:G:269:SER:OG	2.30	0.42
2:N:103:ASP:OD1	2:N:104:ARG:HG2	2.20	0.42
2:Q:36:TRP:CZ2	2:Q:96:CYS:HB3	2.55	0.42
2:W:32:TYR:HA	2:W:101:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:140:ASN:HA	2:W:141:SER:HA	1.68	0.42
1:P:83:PRO:O	1:P:87:ARG:NH1	2.50	0.42
2:T:140:ASN:HA	2:T:141:SER:HA	1.69	0.42
2:W:110:TRP:CE3	3:X:44:PRO:HD2	2.55	0.42
1:Y:153:PRO:HG2	1:Y:184:ILE:HB	2.00	0.42
2:B:76:SER:OG	2:B:77:ASN:HB2	2.19	0.42
3:I:107:LYS:HE2	3:I:107:LYS:HB3	1.83	0.42
2:K:47:TRP:HZ2	2:K:50:ALA:HB2	1.84	0.42
2:W:51:ILE:HG21	2:W:70:MET:HB3	2.01	0.42
1:S:256:VAL:HG12	1:S:279:ILE:HD11	2.01	0.42
1:Y:58:TYR:CE1	1:Y:140:TYR:HB2	2.54	0.42
3:F:105:GLU:HB3	3:F:166:GLN:OE1	2.20	0.42
2:H:11:VAL:HG22	2:H:154:PRO:HG3	2.02	0.42
2:Q:8:GLY:H	2:Q:114:THR:HG22	1.85	0.42
1:P:46:ARG:O	1:P:46:ARG:HG3	2.20	0.42
1:S:252:ARG:HE	1:V:332:THR:HG21	1.84	0.42
3:I:106:LEU:HD23	3:I:106:LEU:HA	1.85	0.42
3:L:47:MET:HA	3:L:58:VAL:HG21	2.01	0.42
2:Q:8:GLY:H	2:Q:114:THR:CG2	2.32	0.42
2:Q:29:ILE:HG23	2:Q:30:LYS:HG2	2.02	0.42
2:Z:161:TRP:CZ3	2:Z:202:CYS:HB3	2.55	0.42
1:D:193:GLY:HA3	1:D:284:PRO:CG	2.49	0.42
1:G:95:LEU:HD22	1:G:148:VAL:HG21	2.01	0.42
1:P:70:PRO:HA	1:P:73:PHE:HB2	2.02	0.42
1:S:265:ILE:HG22	1:V:110:HIS:CE1	2.55	0.42
1:V:39:HIS:CE1	1:V:41:TYR:HB2	2.55	0.42
1:V:58:TYR:CE1	1:V:140:TYR:HB2	2.55	0.42
2:B:36:TRP:CH2	2:B:96:CYS:HB2	2.55	0.42
2:E:33:ALA:HB2	2:E:102:TYR:HD1	1.85	0.42
3:F:109:ALA:HA	3:F:110:ASP:HA	1.86	0.42
1:A:112:PHE:O	1:A:133:ARG:HD2	2.20	0.41
1:J:146:CYS:HA	1:J:321:THR:O	2.20	0.41
1:P:32:SER:OG	1:P:33:ARG:N	2.53	0.41
1:V:273:THR:HG22	2:Z:57:ASP:HB3	2.03	0.41
1:Y:193:GLY:HA3	1:Y:284:PRO:HB3	2.01	0.41
1:Y:267:LYS:H	1:Y:267:LYS:HG3	1.46	0.41
2:B:22:CYS:HB3	2:B:79:ALA:N	2.35	0.41
2:K:31:ASP:O	2:K:32:TYR:HB2	2.19	0.41
3:L:151:ASP:HA	3:L:191:SER:HB3	2.01	0.41
2:N:47:TRP:HZ2	2:N:50:ALA:HB2	1.85	0.41
1:A:256:VAL:HG13	1:A:279:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:70:PRO:HA	1:Y:73:PHE:HB2	2.02	0.41
2:B:48:ILE:HG12	2:B:64:PHE:CE1	2.54	0.41
2:E:36:TRP:CZ2	2:E:96:CYS:HB3	2.56	0.41
1:G:163:GLN:HA	1:G:164:CYS:HA	1.69	0.41
1:P:45:LYS:HG2	1:P:50:THR:HG22	2.01	0.41
1:S:153:PRO:HG3	1:S:321:THR:OG1	2.20	0.41
1:V:153:PRO:HG3	1:V:321:THR:OG1	2.20	0.41
2:B:4:LEU:HD23	2:B:96:CYS:SG	2.60	0.41
3:I:14:SER:HB3	3:I:17:ASP:OD1	2.20	0.41
2:Z:40:ARG:HG3	2:Z:42:GLU:H	1.85	0.41
1:A:163:GLN:HA	1:A:164:CYS:HA	1.72	0.41
1:D:37:VAL:HG22	1:D:355:VAL:HG12	2.02	0.41
1:G:175:PRO:HA	1:G:176:PRO:HD3	1.97	0.41
1:M:382:MET:HG2	1:M:383:ASN:H	1.86	0.41
3:C:87:PHE:CE1	3:C:101:GLY:HA2	2.55	0.41
2:H:110:TRP:CE3	3:I:44:PRO:HD2	2.55	0.41
3:L:138:ASN:HA	3:L:172:THR:HB	2.02	0.41
3:L:142:LYS:HB2	3:L:142:LYS:HE3	1.85	0.41
2:T:71:THR:OG1	2:T:80:TYR:HB2	2.20	0.41
1:M:265:ILE:HD11	2:B:55:TYR:CD1	2.56	0.41
1:M:344:THR:HG21	3:O:53:ASN:ND2	2.35	0.41
1:V:175:PRO:HA	1:V:176:PRO:HD3	1.97	0.41
2:E:40:ARG:HG3	2:E:42:GLU:H	1.84	0.41
2:K:131:LEU:H	2:K:216:LYS:HZ3	1.68	0.41
2:Q:51:ILE:HG13	2:Q:70:MET:HB3	2.02	0.41
1:A:46:ARG:HA	1:A:47:ALA:HA	1.57	0.41
1:V:59:GLN:OE1	1:V:61:ARG:NH2	2.54	0.41
2:H:103:ASP:HB3	2:H:106:ARG:NH1	2.36	0.41
2:N:20:LEU:O	2:N:80:TYR:HA	2.21	0.41
2:N:100:HIS:N	2:N:100:HIS:CD2	2.88	0.41
1:J:117:ASP:OD2	1:J:124:SER:HB3	2.20	0.41
1:J:272:ARG:HB2	1:J:273:THR:H	1.71	0.41
1:M:46:ARG:CZ	2:N:29:ILE:HG21	2.50	0.41
2:Q:86:LEU:HA	2:Q:86:LEU:HD23	1.87	0.41
2:T:28:ASN:OD1	2:T:28:ASN:N	2.51	0.41
2:T:76:SER:HB2	2:T:77:ASN:CA	2.51	0.41
1:A:282:ASN:HB3	1:D:107:VAL:HG11	2.03	0.41
1:J:244:MET:SD	1:M:104:GLY:HA2	2.60	0.41
1:M:62:VAL:HG22	1:M:321:THR:HG23	2.03	0.41
1:P:148:VAL:HG22	1:P:320:VAL:HG22	2.03	0.41
1:S:58:TYR:CE1	1:S:140:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:45:LYS:HG2	1:V:50:THR:HG22	2.03	0.41
1:V:146:CYS:HA	1:V:321:THR:O	2.21	0.41
3:C:83:LEU:HD11	3:C:106:LEU:HG	2.01	0.41
3:I:184:ASP:O	3:I:188:ARG:HG3	2.21	0.41
2:N:40:ARG:HG3	2:N:42:GLU:H	1.85	0.41
2:T:78:THR:CB	2:T:79:ALA:HA	2.46	0.41
2:W:107:PHE:HB2	3:X:36:TYR:CE1	2.51	0.41
2:Z:35:HIS:CE1	2:Z:104:ARG:HA	2.56	0.41
2:Z:153:PHE:HA	2:Z:154:PRO:HA	1.88	0.41
1:A:153:PRO:HG3	1:A:321:THR:OG1	2.20	0.41
1:D:70:PRO:HA	1:D:73:PHE:HB2	2.02	0.41
1:D:257:GLY:O	2:H:30:LYS:HE2	2.21	0.41
1:D:268:GLY:O	1:D:273:THR:HA	2.20	0.41
1:G:382:MET:HG2	1:G:383:ASN:H	1.85	0.41
1:S:244:MET:SD	1:V:104:GLY:HA2	2.61	0.41
2:E:108:PRO:HB3	3:F:46:LEU:HB2	2.02	0.41
2:K:40:ARG:HG3	2:K:42:GLU:H	1.85	0.41
2:N:140:ASN:HA	2:N:141:SER:HA	1.70	0.41
3:O:29:VAL:HG11	3:O:90:GLN:HG3	2.03	0.41
2:T:123:THR:HG23	2:T:154:PRO:HD3	2.02	0.41
3:U:138:ASN:HA	3:U:172:THR:HB	2.02	0.41
2:W:104:ARG:HG3	3:X:91:TYR:HB2	2.03	0.41
3:X:120:PRO:HG2	3:X:130:ALA:HB1	2.02	0.41
2:Z:131:LEU:H	2:Z:216:LYS:HZ3	1.69	0.41
1:G:146:CYS:HA	1:G:321:THR:O	2.21	0.41
1:G:262:ASP:OD2	1:G:263:THR:N	2.54	0.41
1:M:23:THR:OG1	1:M:366:LEU:O	2.26	0.41
1:S:146:CYS:HA	1:S:321:THR:O	2.21	0.41
1:Y:142:GLN:OE1	1:Y:243:GLN:NE2	2.54	0.41
3:O:35:TRP:CD2	3:O:73:LEU:HD12	2.56	0.41
3:R:107:LYS:HA	3:R:140:TYR:OH	2.21	0.41
2:W:153:PHE:HA	2:W:154:PRO:HA	1.85	0.41
3:X:138:ASN:HA	3:X:172:THR:HB	2.03	0.41
2:Z:32:TYR:O	2:Z:53:PRO:HD2	2.20	0.41
1:G:37:VAL:HG22	1:G:355:VAL:HG12	2.03	0.40
1:G:45:LYS:HG2	1:G:50:THR:HG22	2.04	0.40
1:P:60:TYR:CE2	1:P:190:VAL:HA	2.57	0.40
3:O:113:PRO:HB3	3:O:139:PHE:HB3	2.03	0.40
2:W:194:THR:HG23	2:W:198:GLU:OE2	2.21	0.40
1:G:110:HIS:HB3	1:G:113:LEU:HB2	2.03	0.40
1:Y:119:VAL:HG21	1:Y:280:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:HIS:N	2:B:106:ARG:HH12	2.18	0.40
2:E:26:GLY:HA2	2:E:53:PRO:HG3	2.02	0.40
2:H:142:MET:HA	2:H:191:PRO:HA	2.03	0.40
3:R:39:LYS:HG2	3:R:84:ALA:HB2	2.02	0.40
2:W:28:ASN:C	2:W:30:LYS:H	2.25	0.40
1:Y:382:MET:HG2	1:Y:383:ASN:H	1.86	0.40
2:K:69:THR:HB	2:K:82:GLN:HG2	2.04	0.40
2:K:76:SER:HB2	2:K:77:ASN:CA	2.51	0.40
2:Z:171:HIS:HB2	2:Z:187:SER:OG	2.22	0.40
1:J:148:VAL:HG22	1:J:320:VAL:HG22	2.02	0.40
2:E:77:ASN:HB3	2:E:78:THR:H	1.63	0.40
2:N:48:ILE:HG12	2:N:64:PHE:CE1	2.55	0.40
2:T:75:SER:O	2:T:77:ASN:HB2	2.21	0.40
2:Z:131:LEU:HD11	2:Z:148:LEU:HB2	2.03	0.40
1:J:260:VAL:N	2:N:55:TYR:OH	2.55	0.40
1:J:382:MET:HG2	1:J:383:ASN:H	1.85	0.40
1:M:46:ARG:HB2	2:N:29:ILE:HG12	2.04	0.40
1:P:382:MET:HG2	1:P:383:ASN:H	1.86	0.40
2:W:35:HIS:CE1	2:W:104:ARG:HA	2.57	0.40

All (2) 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)
1:S:77:ASP:OD2	3:F:189:HIS:NE2[2_545]	2.05	0.15
3:I:127:SER:OG	2:Q:5:GLN:OE1[1_565]	2.11	0.09

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15	55
1	G	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15	55
1	J	412/496 (83%)	383 (93%)	24 (6%)	5 (1%)	13	51
1	M	412/496 (83%)	384 (93%)	24 (6%)	4 (1%)	15	55
1	P	412/496 (83%)	386 (94%)	22 (5%)	4 (1%)	15	55
1	S	412/496 (83%)	382 (93%)	28 (7%)	2 (0%)	29	68
1	V	412/496 (83%)	382 (93%)	26 (6%)	4 (1%)	15	55
1	Y	412/496 (83%)	381 (92%)	26 (6%)	5 (1%)	13	51
1	b	412/496 (83%)	382 (93%)	27 (7%)	3 (1%)	22	61
2	B	216/221 (98%)	189 (88%)	20 (9%)	7 (3%)	4	31
2	E	216/221 (98%)	187 (87%)	20 (9%)	9 (4%)	3	25
2	H	216/221 (98%)	187 (87%)	22 (10%)	7 (3%)	4	31
2	K	216/221 (98%)	190 (88%)	18 (8%)	8 (4%)	3	28
2	N	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	3	25
2	Q	216/221 (98%)	191 (88%)	21 (10%)	4 (2%)	8	42
2	T	216/221 (98%)	191 (88%)	20 (9%)	5 (2%)	6	38
2	W	216/221 (98%)	186 (86%)	21 (10%)	9 (4%)	3	25
2	Z	216/221 (98%)	186 (86%)	23 (11%)	7 (3%)	4	31
2	g	216/221 (98%)	188 (87%)	18 (8%)	10 (5%)	2	23
3	C	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	F	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	I	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	17	57
3	L	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	O	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	R	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	29	68
3	U	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	17	57
3	X	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	a	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	68
3	j	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29	68
All	All	8400/9310 (90%)	7731 (92%)	543 (6%)	126 (2%)	10	47

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	273	THR
1	Y	263	THR
1	Y	273	THR
2	B	31	ASP
2	B	77	ASN
2	E	29	ILE
2	E	31	ASP
2	E	32	TYR
2	E	102	TYR
2	H	29	ILE
2	H	31	ASP
2	H	32	TYR
2	H	77	ASN
2	K	29	ILE
2	K	77	ASN
2	N	77	ASN
2	N	106	ARG
2	g	29	ILE
2	g	32	TYR
2	g	77	ASN
2	Q	29	ILE
2	Q	77	ASN
2	T	31	ASP
2	T	77	ASN
2	W	29	ILE
2	W	32	TYR
2	Z	29	ILE
2	Z	122	LYS
1	A	125	GLY
1	A	273	THR
1	D	125	GLY
1	D	273	THR
1	G	125	GLY
1	J	125	GLY
1	M	125	GLY
1	M	273	THR
1	P	125	GLY
1	S	125	GLY
1	V	125	GLY
1	V	273	THR
1	Y	125	GLY
1	Y	272	ARG
1	b	125	GLY

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Mol	Chain	Res	Type
2	B	29	ILE
2	N	31	ASP
2	N	105	GLY
2	g	31	ASP
3	j	108	ARG
3	U	108	ARG
2	W	31	ASP
2	W	75	SER
2	W	103	ASP
2	W	209	SER
2	Z	31	ASP
3	a	77	ASN
1	G	273	THR
1	b	273	THR
2	H	78	THR
2	K	78	THR
2	K	79	ALA
2	N	28	ASN
2	N	122	LYS
2	g	54	GLU
2	g	103	ASP
1	D	168	PRO
1	D	272	ARG
1	G	168	PRO
1	J	168	PRO
1	J	272	ARG
1	M	168	PRO
1	P	168	PRO
1	P	271	ASN
1	V	168	PRO
1	V	272	ARG
1	b	168	PRO
2	B	54	GLU
2	E	78	THR
2	E	107	PHE
2	E	166	LEU
3	I	108	ARG
2	N	166	LEU
3	O	77	ASN
2	g	78	THR
2	Q	54	GLU
2	Z	142	MET

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Mol	Chain	Res	Type
1	A	272	ARG
1	G	272	ARG
1	M	272	ARG
1	P	269	SER
1	S	168	PRO
1	Y	168	PRO
2	B	78	THR
2	B	166	LEU
3	C	77	ASN
2	H	142	MET
3	I	77	ASN
2	K	54	GLU
2	K	166	LEU
2	g	55	TYR
2	g	84	SER
2	g	166	LEU
2	Q	166	LEU
2	T	54	GLU
2	T	166	LEU
2	W	54	GLU
2	W	166	LEU
3	X	77	ASN
2	Z	54	GLU
2	Z	103	ASP
2	Z	166	LEU
1	A	168	PRO
2	B	84	SER
2	E	84	SER
2	E	142	MET
3	F	77	ASN
2	H	166	LEU
2	K	103	ASP
3	L	77	ASN
2	N	84	SER
3	R	77	ASN
2	T	84	SER
3	U	77	ASN
2	W	142	MET
1	J	193	GLY
2	K	53	PRO
2	N	29	ILE

### 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	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	D	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	G	363/432 (84%)	360 (99%)	3 (1%)	81	91
1	J	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	M	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	P	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	S	363/432 (84%)	358 (99%)	5 (1%)	67	85
1	V	363/432 (84%)	360 (99%)	3 (1%)	81	91
1	Y	363/432 (84%)	356 (98%)	7 (2%)	57	80
1	b	363/432 (84%)	359 (99%)	4 (1%)	73	88
2	B	184/187 (98%)	171 (93%)	13 (7%)	14	48
2	E	184/187 (98%)	175 (95%)	9 (5%)	25	59
2	H	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	K	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	N	184/187 (98%)	172 (94%)	12 (6%)	17	51
2	Q	184/187 (98%)	171 (93%)	13 (7%)	14	48
2	T	184/187 (98%)	174 (95%)	10 (5%)	22	57
2	W	184/187 (98%)	179 (97%)	5 (3%)	44	73
2	Z	184/187 (98%)	176 (96%)	8 (4%)	29	63
2	g	184/187 (98%)	171 (93%)	13 (7%)	14	48
3	C	189/189 (100%)	187 (99%)	2 (1%)	73	88
3	F	189/189 (100%)	182 (96%)	7 (4%)	34	66
3	I	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	L	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	O	189/189 (100%)	186 (98%)	3 (2%)	62	83
3	R	189/189 (100%)	186 (98%)	3 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	U	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	X	189/189 (100%)	186 (98%)	3 (2%)	62	83
3	a	189/189 (100%)	185 (98%)	4 (2%)	53	78
3	j	189/189 (100%)	182 (96%)	7 (4%)	34	66
All	All	7360/8080 (91%)	7169 (97%)	191 (3%)	46	74

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	VAL
1	A	267	LYS
1	A	273	THR
1	A	288	LEU
1	A	338	THR
1	D	267	LYS
1	D	273	THR
1	D	281	VAL
1	D	288	LEU
1	D	338	THR
1	G	273	THR
1	G	288	LEU
1	G	338	THR
1	J	168	PRO
1	J	255	GLU
1	J	273	THR
1	J	288	LEU
1	J	338	THR
1	M	267	LYS
1	M	273	THR
1	M	288	LEU
1	M	338	THR
1	M	342	THR
1	P	33	ARG
1	P	192	THR
1	P	269	SER
1	P	288	LEU
1	P	338	THR
1	S	273	THR
1	S	288	LEU
1	S	302	LEU
1	S	338	THR

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Mol	Chain	Res	Type
1	S	342	THR
1	V	273	THR
1	V	288	LEU
1	V	338	THR
1	Y	119	VAL
1	Y	267	LYS
1	Y	271	ASN
1	Y	272	ARG
1	Y	273	THR
1	Y	288	LEU
1	Y	338	THR
1	b	273	THR
1	b	281	VAL
1	b	288	LEU
1	b	338	THR
2	B	6	GLN
2	B	28	ASN
2	B	54	GLU
2	B	74	THR
2	B	76	SER
2	B	78	THR
2	B	80	TYR
2	B	96	CYS
2	B	100	HIS
2	B	114	THR
2	B	123	THR
2	B	124	THR
2	B	143	VAL
3	C	50	PHE
3	C	90	GLN
2	E	28	ASN
2	E	52	ASP
2	E	74	THR
2	E	76	SER
2	E	78	THR
2	E	100	HIS
2	E	106	ARG
2	E	124	THR
2	E	143	VAL
3	F	49	TYR
3	F	50	PHE
3	F	56	THR

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Mol	Chain	Res	Type
3	F	90	GLN
3	F	107	LYS
3	F	108	ARG
3	F	110	ASP
2	H	6	GLN
2	H	28	ASN
2	H	74	THR
2	H	104	ARG
2	H	106	ARG
2	H	114	THR
2	H	122	LYS
2	H	138	GLN
2	H	139	THR
2	H	140	ASN
3	I	50	PHE
3	I	90	GLN
3	I	107	LYS
3	I	110	ASP
2	K	6	GLN
2	K	28	ASN
2	K	74	THR
2	K	76	SER
2	K	77	ASN
2	K	96	CYS
2	K	106	ARG
2	K	114	THR
2	K	124	THR
2	K	143	VAL
3	L	50	PHE
3	L	90	GLN
3	L	107	LYS
3	L	110	ASP
2	N	6	GLN
2	N	28	ASN
2	N	29	ILE
2	N	74	THR
2	N	76	SER
2	N	78	THR
2	N	80	TYR
2	N	100	HIS
2	N	114	THR
2	N	123	THR

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Mol	Chain	Res	Type
2	N	124	THR
2	N	143	VAL
3	O	50	PHE
3	O	90	GLN
3	O	108	ARG
2	g	6	GLN
2	g	74	THR
2	g	76	SER
2	g	78	THR
2	g	103	ASP
2	g	104	ARG
2	g	106	ARG
2	g	114	THR
2	g	123	THR
2	g	124	THR
2	g	140	ASN
2	g	141	SER
2	g	209	SER
3	j	31	THR
3	j	49	TYR
3	j	50	PHE
3	j	77	ASN
3	j	78	MET
3	j	90	GLN
3	j	110	ASP
2	Q	6	GLN
2	Q	28	ASN
2	Q	70	MET
2	Q	71	THR
2	Q	76	SER
2	Q	78	THR
2	Q	80	TYR
2	Q	87	THR
2	Q	104	ARG
2	Q	106	ARG
2	Q	114	THR
2	Q	123	THR
2	Q	143	VAL
3	R	90	GLN
3	R	108	ARG
3	R	110	ASP
2	T	6	GLN

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Mol	Chain	Res	Type
2	T	27	PHE
2	T	74	THR
2	T	76	SER
2	T	104	ARG
2	T	114	THR
2	T	123	THR
2	T	124	THR
2	T	139	THR
2	T	143	VAL
3	U	50	PHE
3	U	90	GLN
3	U	107	LYS
3	U	110	ASP
2	W	6	GLN
2	W	78	THR
2	W	114	THR
2	W	123	THR
2	W	143	VAL
3	X	50	PHE
3	X	90	GLN
3	X	110	ASP
2	Z	6	GLN
2	Z	28	ASN
2	Z	29	ILE
2	Z	78	THR
2	Z	114	THR
2	Z	123	THR
2	Z	124	THR
2	Z	211	THR
3	a	50	PHE
3	a	90	GLN
3	a	106	LEU
3	a	110	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	185	GLN
1	G	248	HIS
3	C	77	ASN
3	F	77	ASN
3	F	166	GLN

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Mol	Chain	Res	Type
3	I	77	ASN
3	L	77	ASN
3	O	38	GLN
3	O	77	ASN
3	R	77	ASN
3	U	77	ASN
3	U	166	GLN
3	a	166	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	416/496 (83%)	-0.08	6 (1%) 75 61	27, 62, 124, 168	0
1	D	416/496 (83%)	-0.11	7 (1%) 70 55	37, 70, 124, 189	0
1	G	416/496 (83%)	-0.05	5 (1%) 79 66	41, 70, 132, 183	0
1	J	416/496 (83%)	-0.17	1 (0%) 95 91	31, 64, 122, 185	0
1	M	416/496 (83%)	-0.21	1 (0%) 95 91	28, 59, 118, 184	0
1	P	416/496 (83%)	-0.01	9 (2%) 62 45	34, 64, 123, 186	0
1	S	416/496 (83%)	-0.13	2 (0%) 91 83	31, 60, 119, 174	0
1	V	416/496 (83%)	-0.06	7 (1%) 70 55	30, 64, 118, 183	0
1	Y	416/496 (83%)	-0.11	5 (1%) 79 66	40, 71, 132, 169	0
1	b	416/496 (83%)	-0.08	1 (0%) 95 91	43, 69, 124, 163	0
2	B	218/221 (98%)	0.05	4 (1%) 68 53	34, 63, 123, 163	0
2	E	218/221 (98%)	0.47	16 (7%) 15 9	52, 109, 174, 217	0
2	H	218/221 (98%)	0.46	15 (6%) 16 10	52, 91, 133, 172	0
2	K	218/221 (98%)	1.38	56 (25%) 0 0	40, 108, 220, 258	0
2	N	218/221 (98%)	0.28	12 (5%) 25 15	38, 73, 144, 204	0
2	Q	218/221 (98%)	0.45	16 (7%) 15 9	53, 98, 148, 174	0
2	T	218/221 (98%)	0.52	16 (7%) 15 9	47, 109, 171, 191	0
2	W	218/221 (98%)	0.29	9 (4%) 37 24	35, 70, 161, 191	0
2	Z	218/221 (98%)	0.52	15 (6%) 16 10	49, 99, 157, 210	0
2	g	218/221 (98%)	0.76	37 (16%) 1 1	58, 105, 196, 218	0
3	C	214/214 (100%)	-0.03	0 100 100	27, 59, 102, 125	12 (5%)
3	F	214/214 (100%)	0.48	17 (7%) 12 7	35, 98, 175, 211	12 (5%)
3	I	214/214 (100%)	0.35	10 (4%) 31 19	47, 104, 154, 191	12 (5%)
3	L	214/214 (100%)	1.20	56 (26%) 0 0	44, 118, 223, 275	12 (5%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	O	214/214 (100%)	0.51	10 (4%) 31 19	30, 78, 140, 193	12 (5%)
3	R	214/214 (100%)	0.48	17 (7%) 12 7	51, 97, 150, 195	12 (5%)
3	U	214/214 (100%)	0.75	30 (14%) 2 2	46, 113, 202, 229	12 (5%)
3	X	214/214 (100%)	0.19	10 (4%) 31 19	29, 80, 141, 189	12 (5%)
3	a	214/214 (100%)	0.52	24 (11%) 5 3	35, 77, 142, 194	12 (5%)
3	j	214/214 (100%)	0.78	39 (18%) 1 0	53, 114, 183, 218	12 (5%)
All	All	8480/9310 (91%)	0.22	453 (5%) 26 16	27, 75, 167, 275	120 (1%)

All (453) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	132	ALA	12.1
2	K	147	CYS	9.9
2	K	186	SER	9.3
2	K	158	THR	9.2
2	K	187	SER	9.1
3	L	119	PRO	9.1
3	L	131	SER	8.9
2	K	165	SER	7.6
2	K	203	ASN	7.3
2	K	130	PRO	7.2
2	K	159	VAL	7.2
2	K	169	GLY	7.0
3	L	180	THR	7.0
2	K	148	LEU	6.9
2	T	146	GLY	6.5
2	K	205	ALA	6.4
3	j	154	GLU	6.0
2	K	170	VAL	5.8
3	L	181	LEU	5.8
3	U	156	GLN	5.8
2	K	166	LEU	5.7
3	j	150	ILE	5.6
3	L	114	THR	5.6
3	I	214	CYS	5.6
3	L	130	ALA	5.5
2	K	171	HIS	5.4
2	K	188	VAL	5.4
3	L	133	VAL	5.1
2	K	128	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
2	H	133	PRO	5.0
2	K	204	VAL	5.0
3	a	131	SER	5.0
3	j	152	GLY	5.0
3	L	148	TRP	4.9
3	U	155	ARG	4.9
3	R	148	TRP	4.9
3	L	196	ALA	4.9
3	L	135	PHE	4.8
1	A	77	ASP	4.8
3	R	157	ASN	4.8
3	L	118	PHE	4.7
3	X	135	PHE	4.7
3	L	136	LEU	4.7
2	E	101	ASP	4.6
3	U	180	THR	4.6
2	Z	164	GLY	4.6
3	L	195	GLU	4.5
3	j	153	SER	4.5
2	K	144	THR	4.5
3	j	121	SER	4.5
2	K	212	LYS	4.5
2	K	180	ASP	4.4
2	K	129	TYR	4.4
2	K	133	PRO	4.4
3	L	160	LEU	4.4
3	L	179	LEU	4.4
3	L	137	ASN	4.4
3	L	213	GLU	4.3
3	U	131	SER	4.3
3	j	160	LEU	4.3
2	Q	180	ASP	4.2
3	j	131	SER	4.2
3	L	132	VAL	4.2
3	L	158	GLY	4.2
2	K	161	TRP	4.2
2	Z	1	GLU	4.2
2	g	167	SER	4.2
2	E	136	ALA	4.2
2	E	139	THR	4.2
3	L	210	ASN	4.2
3	j	149	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
3	L	134	CYS	4.1
3	U	117	ILE	4.1
2	Q	140	ASN	4.1
2	K	157	VAL	4.0
2	K	124	THR	4.0
1	P	426	PRO	4.0
2	N	138	GLN	4.0
3	j	120	PRO	4.0
3	L	149	LYS	4.0
3	L	182	THR	4.0
3	U	213	GLU	4.0
2	K	138	GLN	3.9
2	g	163	SER	3.9
2	E	145	LEU	3.9
2	Q	138	GLN	3.9
3	j	156	GLN	3.9
2	K	143	VAL	3.8
3	L	120	PRO	3.8
3	U	192	TYR	3.8
3	U	120	PRO	3.8
2	K	127	SER	3.8
3	U	181	LEU	3.8
1	Y	426	PRO	3.8
2	g	127	SER	3.7
2	T	145	LEU	3.7
2	N	1	GLU	3.7
3	j	161	ASN	3.7
3	U	202	THR	3.7
3	a	208	SER	3.7
2	W	145	LEU	3.7
2	g	159	VAL	3.7
2	K	168	SER	3.7
3	L	144	ILE	3.7
3	j	155	ARG	3.7
2	H	97	ASN	3.6
2	K	146	GLY	3.6
3	L	159	VAL	3.6
1	D	426	PRO	3.6
2	g	142	MET	3.6
3	j	148	TRP	3.5
3	j	180	THR	3.5
2	K	191	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
3	O	214	CYS	3.5
2	T	134	GLY	3.5
3	O	150	ILE	3.5
2	g	166	LEU	3.5
1	Y	126	GLY	3.5
3	j	147	LYS	3.5
2	E	140	ASN	3.4
3	U	148	TRP	3.4
3	j	193	THR	3.4
3	L	155	ARG	3.4
2	E	97	ASN	3.4
1	P	163	GLN	3.4
3	F	155	ARG	3.4
3	j	117	ILE	3.4
2	Z	105	GLY	3.4
3	U	152	GLY	3.4
3	a	149	LYS	3.3
2	T	131	LEU	3.3
3	U	182	THR	3.3
2	K	190	VAL	3.3
3	j	133	VAL	3.3
3	j	146	VAL	3.3
3	L	117	ILE	3.3
2	K	145	LEU	3.3
3	L	184	ASP	3.3
2	K	164	GLY	3.3
3	L	150	ILE	3.3
1	A	80	LEU	3.3
3	j	80	SER	3.3
3	U	186	TYR	3.2
2	N	136	ALA	3.2
2	g	165	SER	3.2
1	P	369	ILE	3.2
2	H	132	ALA	3.2
3	U	212	ASN	3.2
2	W	215	LYS	3.2
2	Q	166	LEU	3.2
3	L	178	THR	3.2
2	H	65	GLN	3.2
2	g	168	SER	3.2
2	g	216	LYS	3.2
2	Z	130	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	R	117	ILE	3.2
3	U	130	ALA	3.2
3	j	132	VAL	3.2
2	H	78	THR	3.2
3	j	178	THR	3.2
2	B	165	SER	3.1
2	Q	147	CYS	3.1
3	I	212	ASN	3.1
3	a	192	TYR	3.1
3	j	119	PRO	3.1
2	Z	183	THR	3.1
3	I	133	VAL	3.1
3	L	193	THR	3.1
2	Z	25	SER	3.1
2	W	163	SER	3.1
3	I	210	ASN	3.1
2	W	140	ASN	3.1
3	R	210	ASN	3.1
2	K	185	SER	3.1
2	K	125	PRO	3.1
2	g	148	LEU	3.1
3	a	127	SER	3.1
2	g	126	PRO	3.0
2	H	138	GLN	3.0
2	g	180	ASP	3.0
1	V	308	HIS	3.0
2	Q	167	SER	3.0
3	O	131	SER	3.0
3	j	194	CYS	3.0
2	N	137	ALA	3.0
3	F	116	SER	3.0
2	K	210	SER	3.0
3	L	212	ASN	3.0
2	g	162	ASN	3.0
3	X	155	ARG	3.0
2	H	101	ASP	3.0
2	K	150	LYS	3.0
2	g	200	VAL	3.0
2	g	190	VAL	3.0
3	L	143	ASP	3.0
2	T	133	PRO	2.9
3	j	162	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	L	199	LYS	2.9
3	F	214	CYS	2.9
3	L	194	CYS	2.9
3	R	156	GLN	2.9
3	L	185	GLU	2.9
2	K	173	PHE	2.9
3	X	134	CYS	2.9
3	F	202	THR	2.9
3	R	193	THR	2.9
2	E	137	ALA	2.9
2	T	215	LYS	2.9
3	L	192	TYR	2.9
3	U	122	SER	2.9
2	K	167	SER	2.9
2	Z	165	SER	2.9
2	g	1	GLU	2.9
3	j	122	SER	2.9
2	Q	1	GLU	2.9
3	U	150	ILE	2.9
3	L	189	HIS	2.8
2	Q	203	ASN	2.8
2	K	172	THR	2.8
3	a	195	GLU	2.8
3	a	214	CYS	2.8
2	K	162	ASN	2.8
3	j	159	VAL	2.8
2	T	97	ASN	2.8
2	Q	204	VAL	2.8
3	U	209	PHE	2.8
3	X	133	VAL	2.8
3	j	181	LEU	2.8
3	j	195	GLU	2.8
2	N	105	GLY	2.8
2	Q	168	SER	2.8
2	K	131	LEU	2.8
3	L	116	SER	2.8
1	V	165	THR	2.8
2	g	199	THR	2.8
3	O	115	VAL	2.7
2	Z	97	ASN	2.7
1	V	88	LEU	2.7
3	R	134	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	Q	186	SER	2.7
3	R	194	CYS	2.7
2	H	134	GLY	2.7
3	F	120	PRO	2.7
3	L	162	SER	2.7
1	P	165	THR	2.7
2	H	25	SER	2.7
3	U	119	PRO	2.7
1	V	80	LEU	2.7
1	b	166	ASN	2.7
3	a	117	ILE	2.7
2	K	179	SER	2.7
3	F	181	LEU	2.7
2	T	140	ASN	2.7
2	Z	214	ASP	2.7
3	F	143	ASP	2.7
3	L	187	GLU	2.7
2	E	138	GLN	2.7
2	Q	159	VAL	2.6
2	E	217	ILE	2.6
2	K	151	GLY	2.6
2	g	184	LEU	2.6
2	g	130	PRO	2.6
2	B	138	GLN	2.6
3	L	154	GLU	2.6
3	X	116	SER	2.6
3	j	134	CYS	2.6
3	a	119	PRO	2.6
1	M	426	PRO	2.6
2	K	149	VAL	2.6
2	g	84	SER	2.6
3	U	208	SER	2.6
3	U	193	THR	2.6
3	j	135	PHE	2.6
3	a	194	CYS	2.6
3	U	157	ASN	2.6
2	N	3	GLN	2.6
3	j	207	LYS	2.6
2	W	141	SER	2.6
3	I	186	TYR	2.5
3	O	132	VAL	2.5
2	N	97	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
3	X	214	CYS	2.5
2	g	169	GLY	2.5
2	g	141	SER	2.5
1	D	427	ASP	2.5
1	G	427	ASP	2.5
2	K	160	THR	2.5
2	T	1	GLU	2.5
2	g	189	THR	2.5
3	L	164	THR	2.5
2	E	25	SER	2.5
3	R	24	LYS	2.5
3	O	117	ILE	2.5
3	U	194	CYS	2.5
2	H	145	LEU	2.5
2	T	157	VAL	2.5
1	G	380	HIS	2.5
1	P	164	CYS	2.5
3	L	147	LYS	2.5
1	G	426	PRO	2.5
3	j	136	LEU	2.5
1	D	166	ASN	2.5
1	G	460	SER	2.5
3	O	119	PRO	2.5
2	K	213	VAL	2.5
2	g	136	ALA	2.5
3	F	144	ILE	2.5
2	Q	148	LEU	2.4
3	R	155	ARG	2.4
2	T	186	SER	2.4
3	F	150	ILE	2.4
3	R	213	GLU	2.4
2	K	126	PRO	2.4
3	L	56	THR	2.4
3	U	203	SER	2.4
3	j	177	SER	2.4
3	I	190	ASN	2.4
2	K	211	THR	2.4
2	N	140	ASN	2.4
3	L	115	VAL	2.4
3	a	193	THR	2.4
3	R	2	ILE	2.4
2	Z	167	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	j	130	ALA	2.4
1	G	165	THR	2.4
3	F	193	THR	2.4
2	Z	155	GLU	2.3
3	a	120	PRO	2.3
2	T	128	VAL	2.3
3	F	158	GLY	2.3
3	j	196	ALA	2.3
1	J	166	ASN	2.3
3	j	192	TYR	2.3
2	H	1	GLU	2.3
2	K	142	MET	2.3
3	F	149	LYS	2.3
1	Y	166	ASN	2.3
1	V	76	PRO	2.3
2	E	134	GLY	2.3
2	E	150	LYS	2.3
2	Q	161	TRP	2.3
1	P	76	PRO	2.3
1	D	85	THR	2.3
1	P	85	THR	2.3
3	L	104	LEU	2.3
3	a	130	ALA	2.3
2	W	130	PRO	2.3
1	D	165	THR	2.3
2	N	146	GLY	2.3
2	W	134	GLY	2.3
3	L	205	ILE	2.3
1	D	127	ASN	2.3
2	T	25	SER	2.3
3	L	206	VAL	2.3
3	O	116	SER	2.3
2	Q	105	GLY	2.3
3	a	129	GLY	2.3
1	S	426	PRO	2.2
2	N	133	PRO	2.2
2	T	210	SER	2.2
3	R	130	ALA	2.2
3	a	206	VAL	2.2
2	K	189	THR	2.2
2	g	173	PHE	2.2
3	F	146	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	Z	151	GLY	2.2
1	V	148	VAL	2.2
2	H	139	THR	2.2
1	A	460	SER	2.2
3	a	209	PHE	2.2
3	a	150	ILE	2.2
2	B	136	ALA	2.2
3	L	145	ASN	2.2
1	Y	367	CYS	2.2
3	F	119	PRO	2.2
2	E	151	GLY	2.2
2	g	131	LEU	2.2
2	B	97	ASN	2.2
2	g	145	LEU	2.2
2	T	126	PRO	2.2
2	T	105	GLY	2.2
2	W	214	ASP	2.2
3	U	86	TYR	2.2
3	a	115	VAL	2.2
1	Y	460	SER	2.2
3	a	124	GLN	2.2
2	g	25	SER	2.2
2	g	185	SER	2.2
1	A	19	TYR	2.2
1	V	81	PHE	2.2
3	X	150	ILE	2.2
3	j	206	VAL	2.1
1	P	370	THR	2.1
2	Q	160	THR	2.1
3	a	186	TYR	2.1
3	U	184	ASP	2.1
2	g	138	GLN	2.1
2	g	161	TRP	2.1
3	a	196	ALA	2.1
2	K	202	CYS	2.1
2	g	164	GLY	2.1
3	F	135	PHE	2.1
2	K	140	ASN	2.1
2	Z	160	THR	2.1
3	L	176	SER	2.1
3	X	197	THR	2.1
2	E	180	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	g	215	LYS	2.1
3	L	157	ASN	2.1
3	X	111	ALA	2.1
3	O	120	PRO	2.1
2	K	217	ILE	2.1
2	g	204	VAL	2.1
2	Z	186	SER	2.1
3	j	175	MET	2.1
3	U	76	SER	2.1
3	I	213	GLU	2.1
2	N	164	GLY	2.1
1	A	88	LEU	2.1
3	a	89	GLN	2.1
3	L	110	ASP	2.1
1	A	74	ALA	2.1
3	L	153	SER	2.1
3	R	1	ASP	2.1
3	O	192	TYR	2.1
1	S	165	THR	2.1
2	Z	166	LEU	2.1
3	F	205	ILE	2.1
3	U	146	VAL	2.1
2	H	34	ILE	2.1
3	X	206	VAL	2.1
2	E	130	PRO	2.1
2	H	135	SER	2.1
3	R	169	LYS	2.1
2	H	29	ILE	2.1
3	I	188	ARG	2.1
3	a	207	LYS	2.0
2	W	74	THR	2.0
2	g	191	PRO	2.0
3	R	119	PRO	2.0
2	g	157	VAL	2.0
3	R	209	PHE	2.0
2	g	160	THR	2.0
3	I	149	LYS	2.0
3	a	135	PHE	2.0
1	P	368	SER	2.0
2	N	145	LEU	2.0
3	L	204	PRO	2.0
2	E	181	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	148	TRP	2.0
3	U	207	LYS	2.0
1	D	94	GLY	2.0
3	I	192	TYR	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 monosaccharides 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.