



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:55 AM GMT

PDB ID : 1VU0
Title : Structure-function Analysis of Receptor-binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors : Xie, Q.
Deposited on : 2011-09-13
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

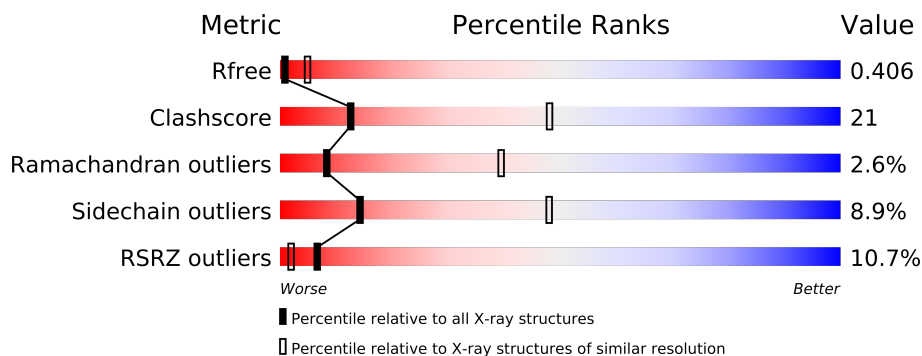
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	U	520	
1	V	520	
1	W	520	
1	X	520	
1	Y	520	
1	Z	520	
1	a	520	
1	b	520	
1	c	520	
1	d	520	
1	e	520	
1	f	520	
1	g	520	
1	h	520	

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Mol	Chain	Length	Quality of chain
1	i	520	
1	j	520	
1	k	520	
1	l	520	
1	m	520	
1	n	520	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 82420 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	V	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	W	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	X	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	Y	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	Z	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	a	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	b	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	c	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	d	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	e	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	f	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	g	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	h	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	i	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	j	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

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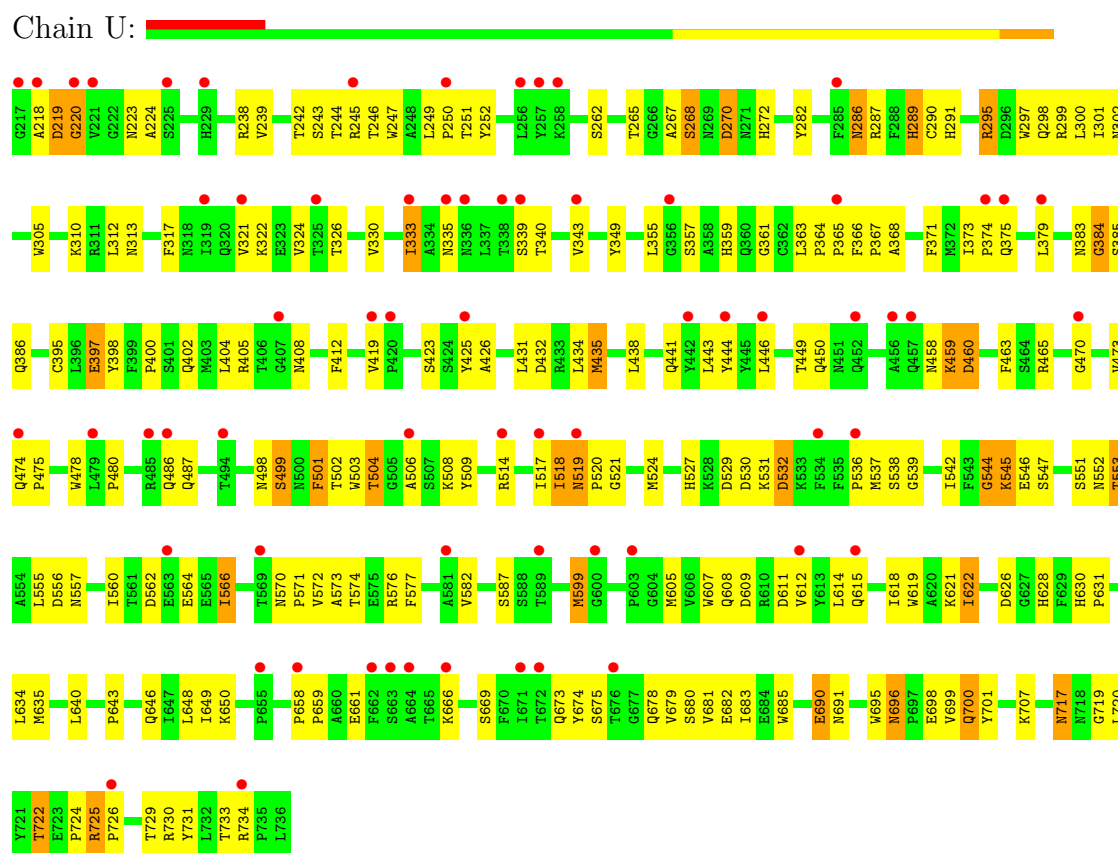
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	k	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	l	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	m	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	n	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0

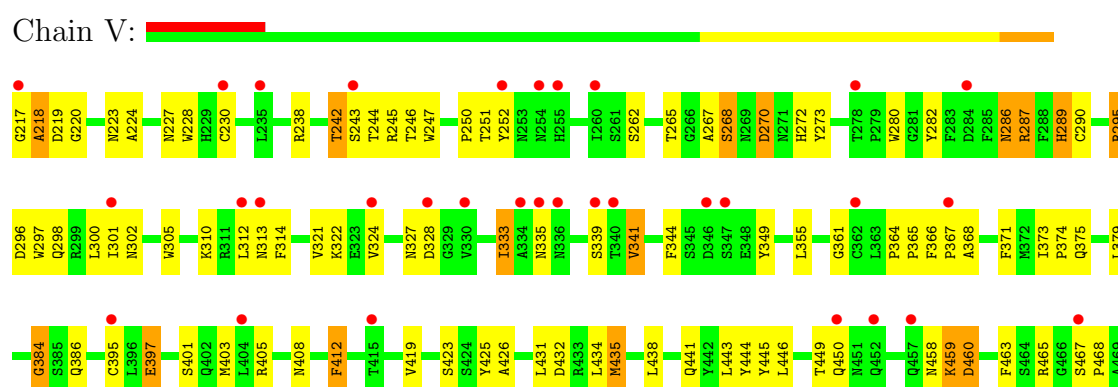
3 Residue-property plots

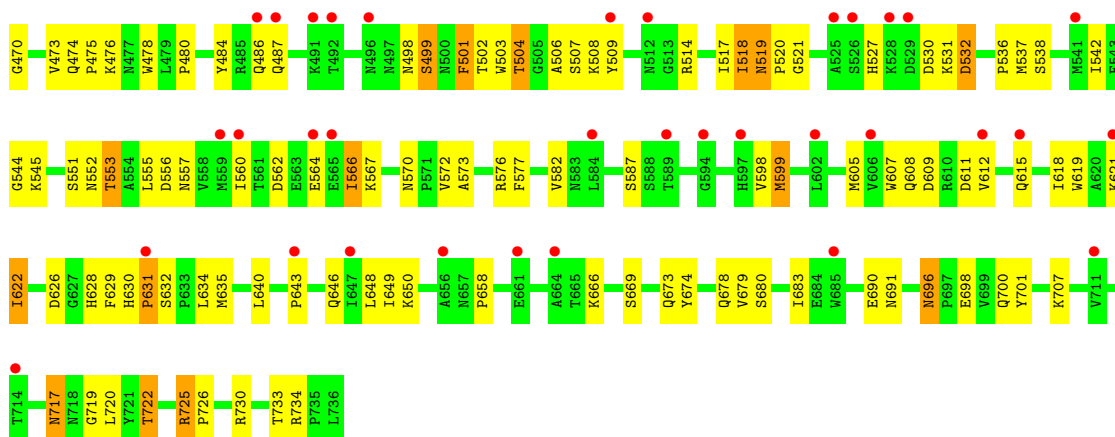
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Capsid protein VP1



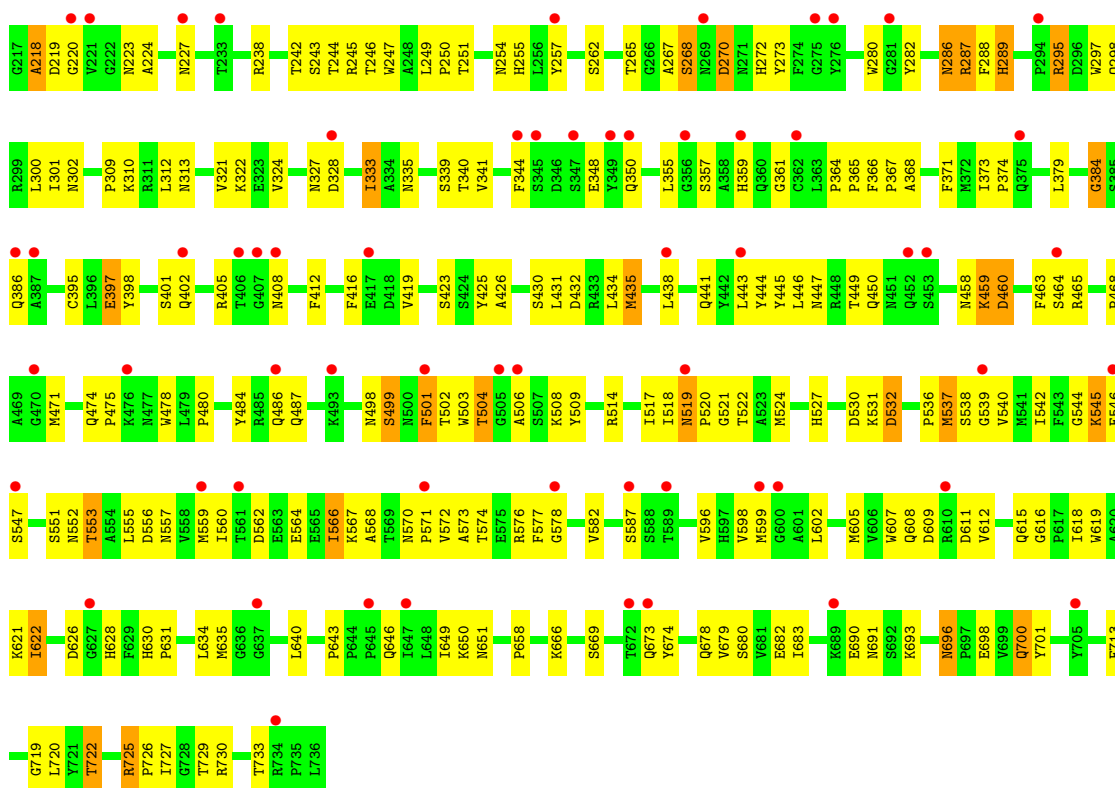
• Molecule 1: Capsid protein VP1





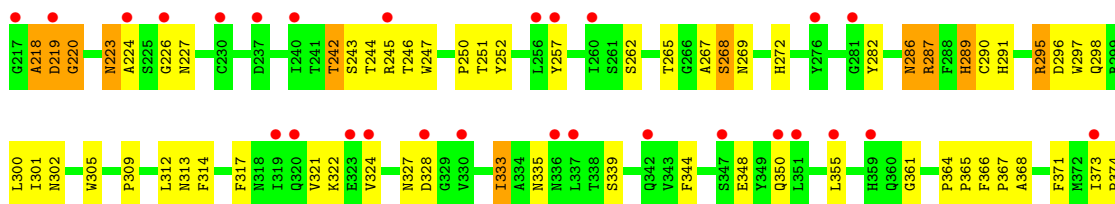
• Molecule 1: Capsid protein VP1

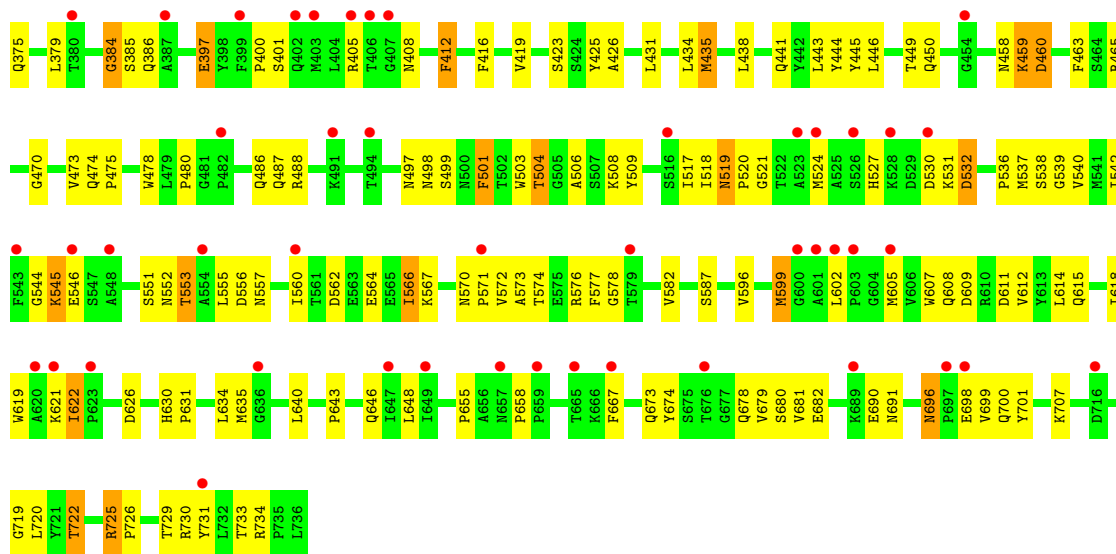
Chain W:



• Molecule 1: Capsid protein VP1

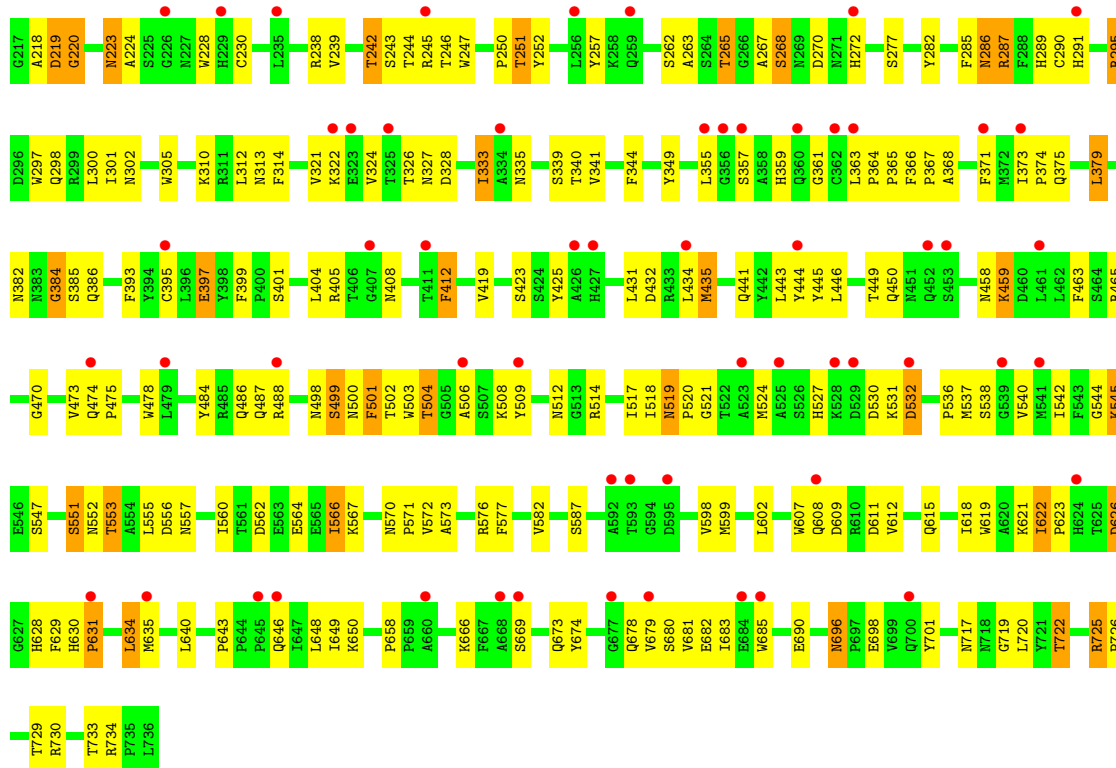
Chain X:





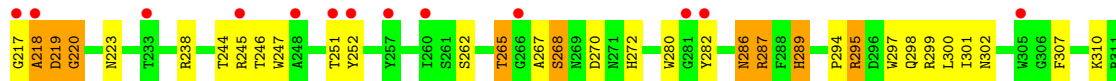
• Molecule 1: Capsid protein VP1

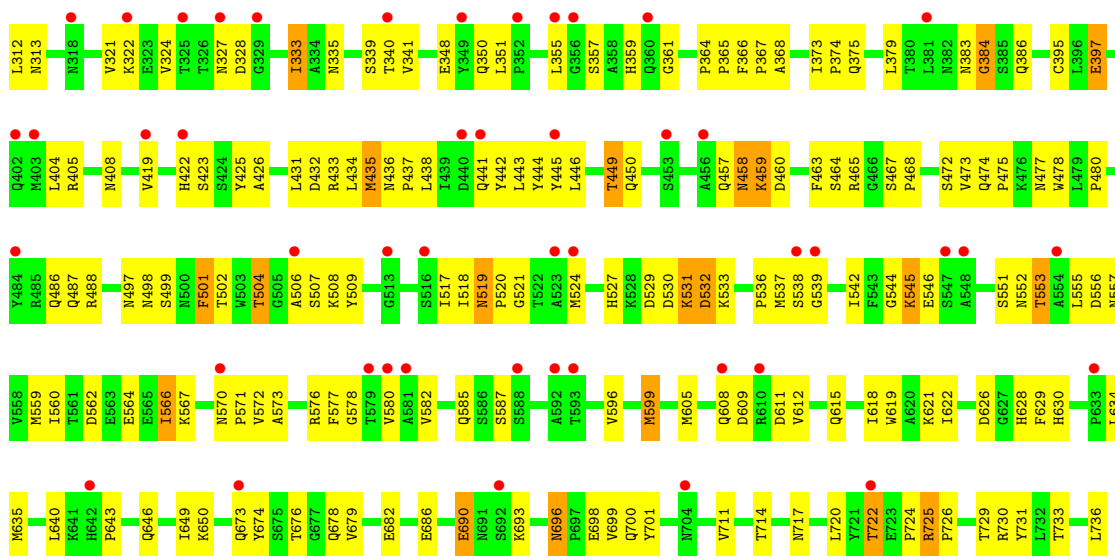
Chain Y:



• Molecule 1: Capsid protein VP1

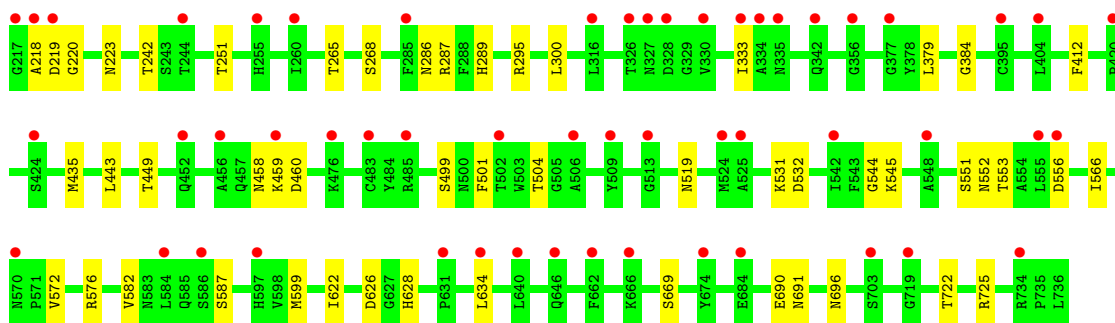
Chain Z:





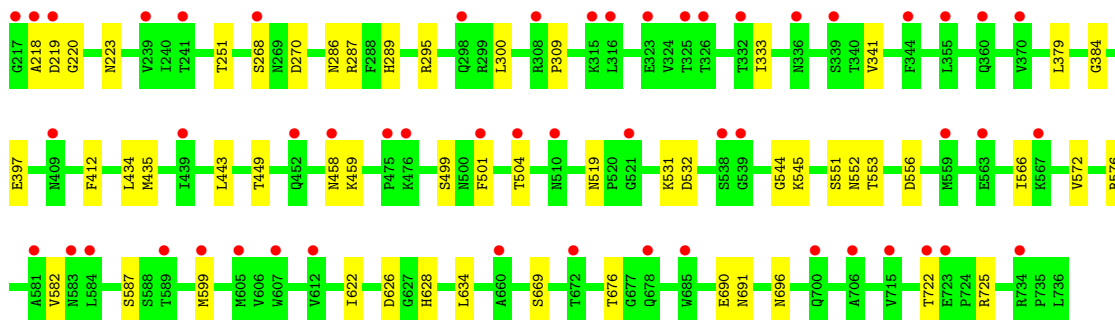
• Molecule 1: Capsid protein VP1

Chain a:



• Molecule 1: Capsid protein VP1

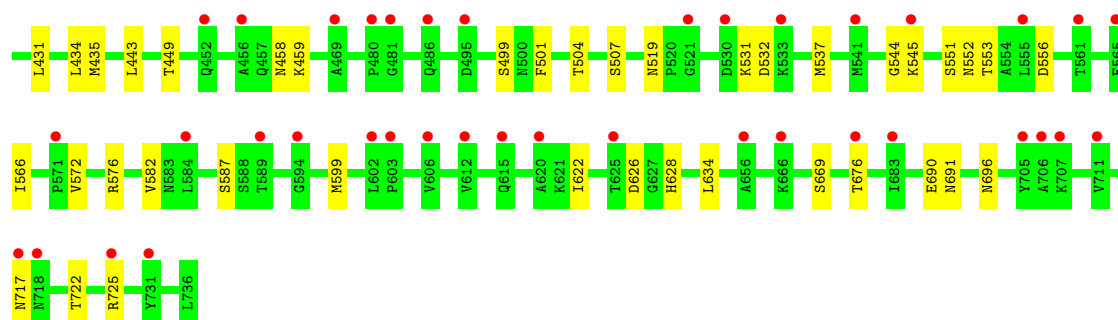
Chain b:



• Molecule 1: Capsid protein VP1

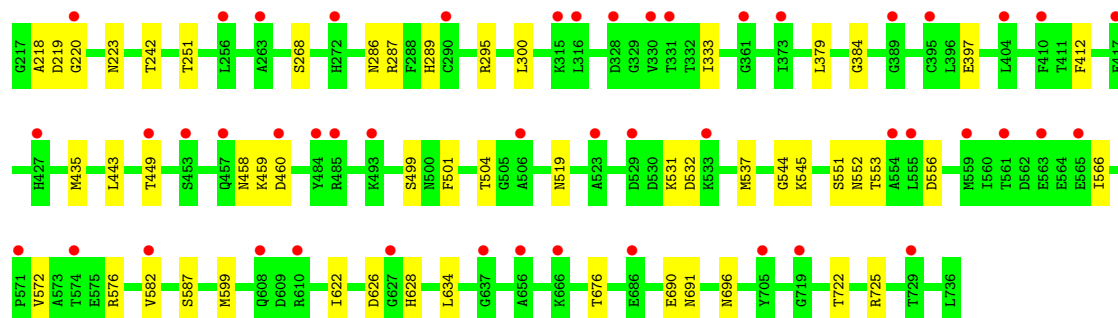
Chain c:





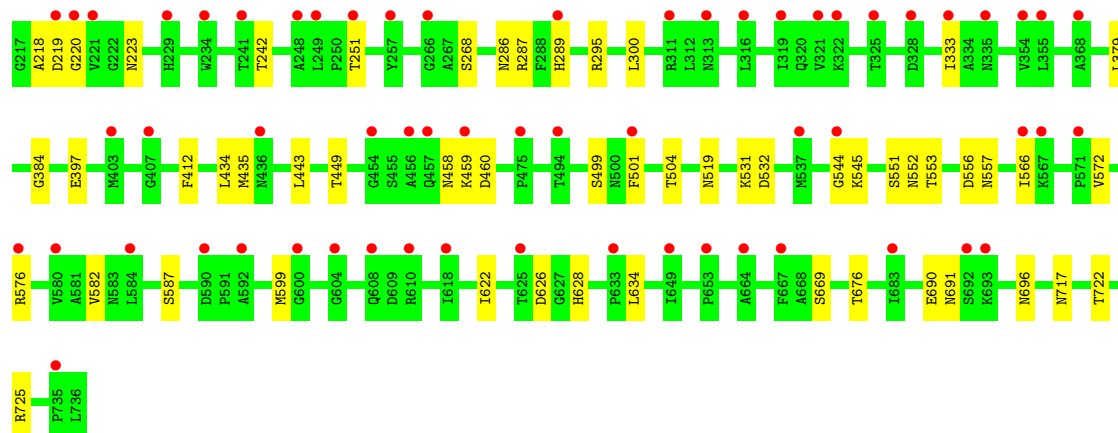
• Molecule 1: Capsid protein VP1

Chain d: 



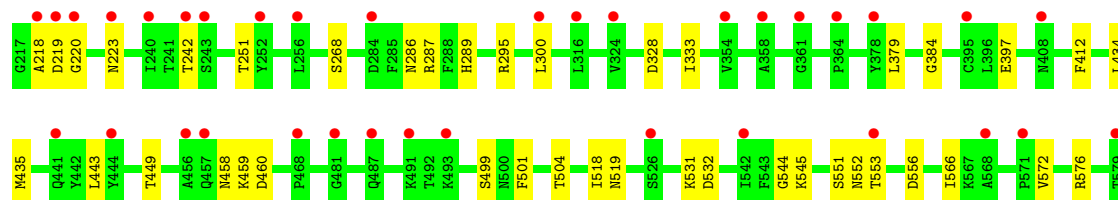
• Molecule 1: Capsid protein VP1

Chain e: 



• Molecule 1: Capsid protein VP1

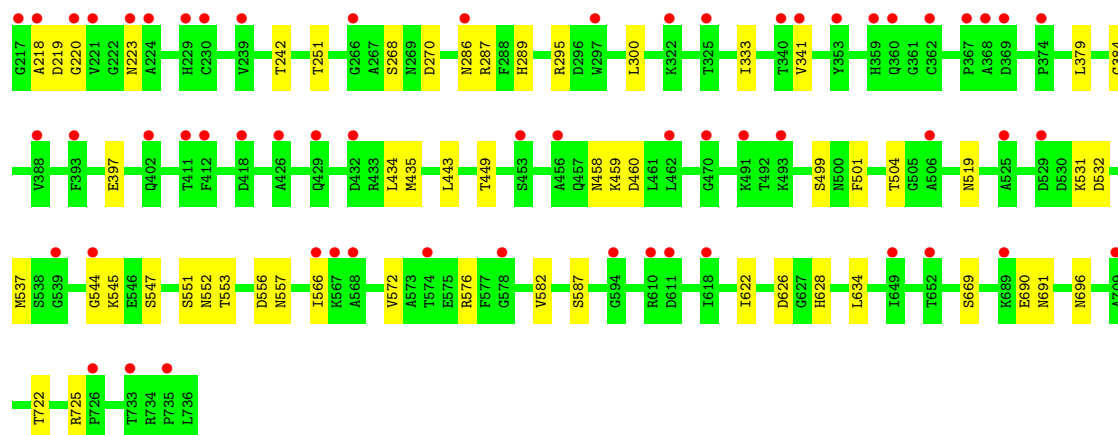
Chain f: 





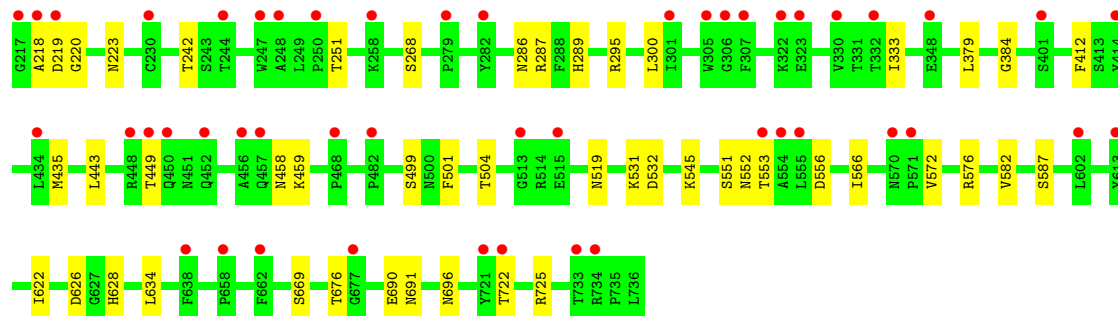
• Molecule 1: Capsid protein VP1

Chain g:



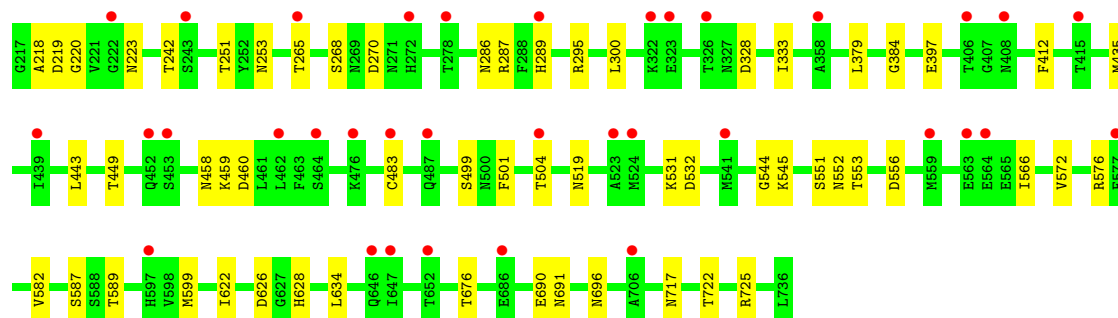
• Molecule 1: Capsid protein VP1

Chain h:



• Molecule 1: Capsid protein VP1

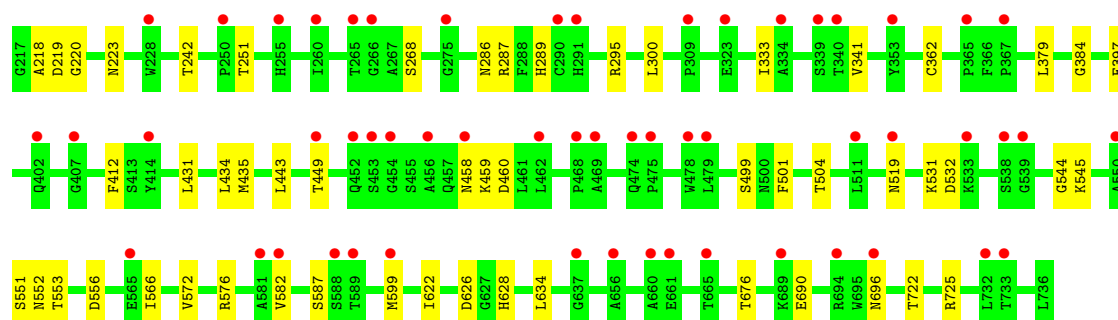
Chain i:



• Molecule 1: Capsid protein VP1

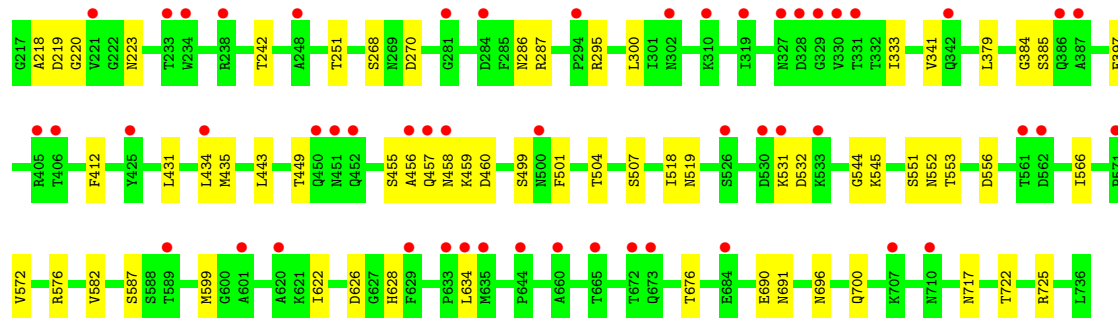
Chain j:





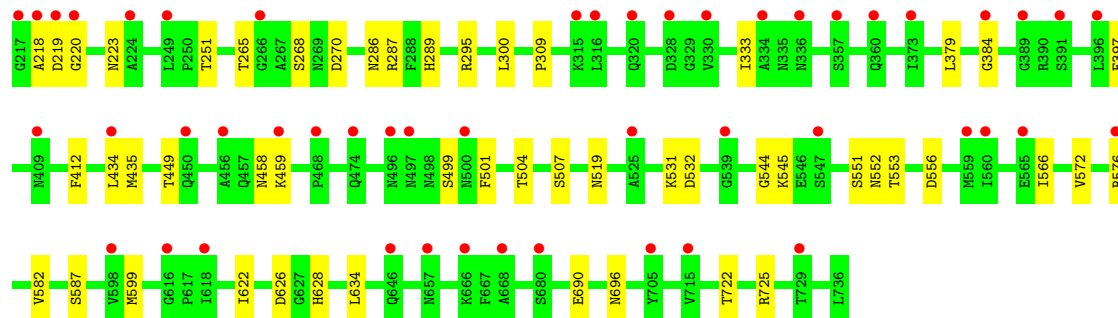
• Molecule 1: Capsid protein VP1

Chain k:



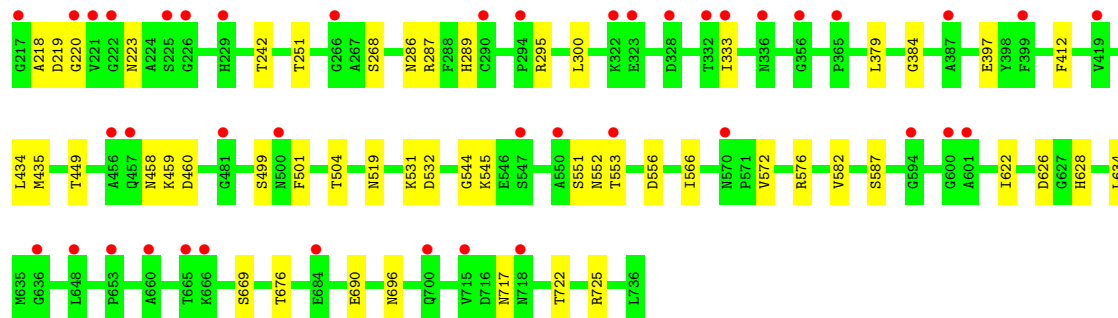
• Molecule 1: Capsid protein VP1

Chain l:



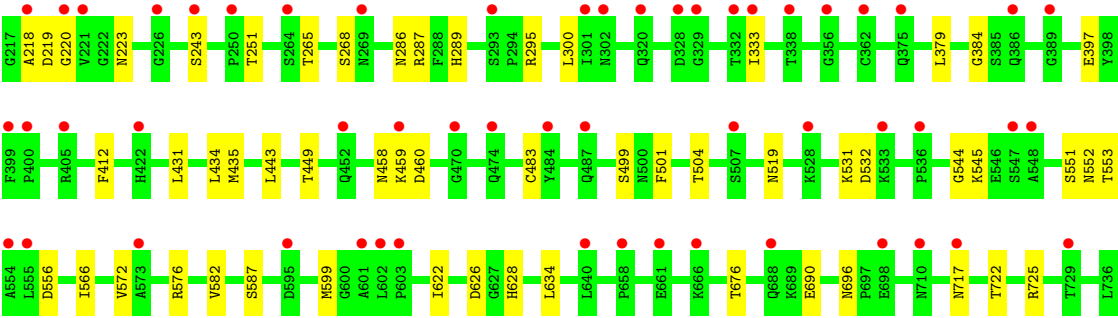
• Molecule 1: Capsid protein VP1

Chain m:



• Molecule 1: Capsid protein VP1

Chain n: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	354.79Å 363.90Å 371.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00 49.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	35.1 (49.21-3.00) 30.8 (49.21-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.251 , 0.286 0.407 , 0.406	Depositor DCC
R_{free} test set	3267 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , -2.9	EDS
Estimated twinning fraction	0.019 for -h,l,k 0.009 for -l,-k,-h 0.023 for k,h,-l 0.008 for k,l,h 0.008 for l,h,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 332221 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.56	EDS
Total number of atoms	82420	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	U	0.62	0/4247	0.63	0/5790
1	V	0.62	0/4247	0.62	0/5790
1	W	0.69	0/4247	0.64	0/5790
1	X	0.69	0/4247	0.65	0/5790
1	Y	0.64	0/4247	0.64	0/5790
1	Z	0.59	0/4247	0.62	0/5790
1	a	0.55	0/4247	0.61	0/5790
1	b	0.57	0/4247	0.60	0/5790
1	c	0.54	0/4247	0.62	0/5790
1	d	0.55	0/4247	0.61	0/5790
1	e	0.57	0/4247	0.61	0/5790
1	f	0.52	0/4247	0.60	0/5790
1	g	0.60	0/4247	0.62	0/5790
1	h	0.59	0/4247	0.61	0/5790
1	i	0.55	1/4247 (0.0%)	0.60	0/5790
1	j	0.58	1/4247 (0.0%)	0.61	0/5790
1	k	0.59	0/4247	0.61	0/5790
1	l	0.59	0/4247	0.60	0/5790
1	m	0.66	0/4247	0.63	0/5790
1	n	0.63	1/4247 (0.0%)	0.62	0/5790
All	All	0.60	3/84940 (0.0%)	0.62	0/115800

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	362	CYS	CB-SG	-6.32	1.71	1.82
1	n	483	CYS	CB-SG	-5.67	1.72	1.81
1	i	483	CYS	CB-SG	-5.08	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	4121	0	3896	190	0
1	V	4121	0	3896	176	0
1	W	4121	0	3896	191	0
1	X	4121	0	3896	173	0
1	Y	4121	0	3896	221	0
1	Z	4121	0	3896	202	0
1	a	4121	0	3896	0	0
1	b	4121	0	3896	0	0
1	c	4121	0	3896	0	0
1	d	4121	0	3896	0	0
1	e	4121	0	3896	0	0
1	f	4121	0	3896	0	0
1	g	4121	0	3896	0	2
1	h	4121	0	3896	0	0
1	i	4121	0	3896	0	0
1	j	4121	0	3896	0	0
1	k	4121	0	3896	0	2
1	l	4121	0	3896	0	0
1	m	4121	0	3896	0	0
1	n	4121	0	3896	0	0
All	All	82420	0	77920	1054	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (1054) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:551:SER:HA	1:Z:464:SER:HB3	1.50	0.94
1:Y:501:PHE:HE2	1:Z:449:THR:HG1	1.08	0.93
1:Y:500:ASN:HA	1:Z:449:THR:HG23	1.52	0.90
1:Y:393:PHE:H	1:Z:696:ASN:HD21	1.10	0.90
1:V:405:ARG:H	1:V:408:ASN:HD22	1.18	0.89
1:W:408:ASN:HD21	1:X:224:ALA:H	1.18	0.88
1:U:408:ASN:HD21	1:V:224:ALA:H	1.23	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:405:ARG:H	1:U:408:ASN:HD22	1.19	0.86
1:V:408:ASN:HD21	1:W:224:ALA:H	1.23	0.86
1:U:431:LEU:HD21	1:U:478:TRP:HB2	1.58	0.86
1:U:224:ALA:H	1:Y:408:ASN:HD21	1.24	0.85
1:Y:508:LYS:HB3	1:Y:517:ILE:HA	1.60	0.84
1:Y:519:ASN:HB3	1:Y:520:PRO:HD3	1.61	0.83
1:X:553:THR:HG23	1:X:557:ASN:HB2	1.61	0.82
1:V:286:ASN:ND2	1:V:618:ILE:H	1.78	0.81
1:Z:302:ASN:HD21	1:Z:701:TYR:H	1.26	0.81
1:V:297:TRP:NE1	1:V:301:ILE:HD11	1.96	0.81
1:X:519:ASN:HB3	1:X:520:PRO:HD3	1.63	0.81
1:X:509:TYR:HD1	1:X:518:ILE:HD13	1.46	0.80
1:V:431:LEU:HD21	1:V:478:TRP:HB2	1.63	0.80
1:W:286:ASN:HD21	1:W:619:TRP:H	1.29	0.80
1:W:431:LEU:HD21	1:W:478:TRP:HB2	1.64	0.80
1:U:519:ASN:HB3	1:U:520:PRO:HD3	1.64	0.80
1:U:286:ASN:ND2	1:U:618:ILE:H	1.80	0.80
1:W:405:ARG:H	1:W:408:ASN:HD22	1.28	0.80
1:X:408:ASN:HD21	1:Y:224:ALA:H	1.28	0.80
1:Y:245:ARG:NH1	1:Y:364:PRO:O	2.14	0.80
1:Y:322:LYS:HE2	1:Y:335:ASN:HD21	1.47	0.79
1:V:519:ASN:HB3	1:V:520:PRO:HD3	1.65	0.79
1:W:519:ASN:HB3	1:W:520:PRO:HD3	1.63	0.79
1:Y:501:PHE:CD2	1:Z:449:THR:HG21	2.17	0.79
1:X:297:TRP:NE1	1:X:301:ILE:HD11	1.98	0.79
1:U:509:TYR:HD1	1:U:518:ILE:HD13	1.47	0.79
1:Z:286:ASN:ND2	1:Z:618:ILE:H	1.81	0.79
1:W:542:ILE:HD12	1:W:560:ILE:HG13	1.65	0.78
1:Z:519:ASN:HB3	1:Z:520:PRO:HD3	1.64	0.78
1:X:405:ARG:H	1:X:408:ASN:HD22	1.29	0.78
1:W:302:ASN:HD21	1:W:701:TYR:H	1.32	0.77
1:Y:517:ILE:HG22	1:Z:473:VAL:HA	1.67	0.77
1:Y:393:PHE:H	1:Z:696:ASN:ND2	1.82	0.77
1:X:245:ARG:NH1	1:X:364:PRO:O	2.17	0.77
1:W:286:ASN:ND2	1:W:618:ILE:H	1.82	0.77
1:Z:405:ARG:H	1:Z:408:ASN:HD22	1.31	0.77
1:V:509:TYR:HD1	1:V:518:ILE:HD13	1.50	0.77
1:Y:405:ARG:H	1:Y:408:ASN:HD22	1.32	0.76
1:X:508:LYS:HB3	1:X:517:ILE:HA	1.67	0.76
1:U:542:ILE:HD12	1:U:560:ILE:HG13	1.67	0.76
1:Y:286:ASN:ND2	1:Y:618:ILE:H	1.84	0.76
1:U:322:LYS:HE2	1:U:335:ASN:ND2	1.99	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:286:ASN:HD21	1:X:619:TRP:H	1.34	0.76
1:Y:611:ASP:OD1	1:Y:730:ARG:HG3	1.85	0.76
1:V:322:LYS:HE2	1:V:335:ASN:HD21	1.49	0.76
1:Z:286:ASN:HD21	1:Z:619:TRP:H	1.33	0.75
1:U:322:LYS:HE2	1:U:335:ASN:HD21	1.49	0.75
1:Y:519:ASN:HB3	1:Z:475:PRO:HA	1.69	0.75
1:Y:431:LEU:HD21	1:Y:478:TRP:HB2	1.66	0.75
1:X:431:LEU:HD21	1:X:478:TRP:HB2	1.68	0.75
1:V:322:LYS:HE2	1:V:335:ASN:ND2	2.01	0.74
1:Y:322:LYS:HE2	1:Y:335:ASN:ND2	2.02	0.74
1:W:245:ARG:NH1	1:W:364:PRO:O	2.20	0.74
1:W:321:VAL:HG11	1:W:339:SER:HB3	1.68	0.74
1:Y:509:TYR:HD1	1:Y:518:ILE:HD13	1.52	0.74
1:Y:379:LEU:HD11	1:Z:437:PRO:HB3	1.70	0.74
1:W:508:LYS:HB3	1:W:517:ILE:HA	1.69	0.74
1:Z:245:ARG:NH1	1:Z:364:PRO:O	2.21	0.73
1:Z:508:LYS:HB3	1:Z:517:ILE:HA	1.69	0.73
1:U:361:GLY:HA3	1:U:374:PRO:HG3	1.70	0.73
1:X:542:ILE:HD12	1:X:560:ILE:HG13	1.70	0.73
1:V:542:ILE:HD12	1:V:560:ILE:HG13	1.70	0.73
1:U:297:TRP:NE1	1:U:301:ILE:HD11	2.04	0.73
1:Z:509:TYR:HD1	1:Z:518:ILE:HD13	1.54	0.73
1:Z:542:ILE:HD12	1:Z:560:ILE:HG13	1.70	0.72
1:Z:431:LEU:HD21	1:Z:478:TRP:HB2	1.70	0.72
1:Z:322:LYS:HE2	1:Z:335:ASN:ND2	2.05	0.72
1:W:322:LYS:HE2	1:W:335:ASN:ND2	2.04	0.72
1:W:562:ASP:OD1	1:W:564:GLU:OE2	2.07	0.72
1:U:508:LYS:HB3	1:U:517:ILE:HA	1.70	0.72
1:V:553:THR:HG23	1:V:557:ASN:HB2	1.72	0.72
1:V:302:ASN:HD21	1:V:701:TYR:H	1.37	0.72
1:Y:302:ASN:HD21	1:Y:701:TYR:H	1.35	0.72
1:Z:322:LYS:HE2	1:Z:335:ASN:HD21	1.55	0.71
1:Z:297:TRP:NE1	1:Z:301:ILE:HD11	2.04	0.71
1:Y:520:PRO:HG2	1:Y:635:MET:HG2	1.72	0.71
1:V:508:LYS:HB3	1:V:517:ILE:HA	1.73	0.71
1:X:286:ASN:ND2	1:X:618:ILE:H	1.89	0.71
1:W:509:TYR:HD1	1:W:518:ILE:HD13	1.55	0.71
1:Y:286:ASN:HD21	1:Y:619:TRP:H	1.38	0.71
1:U:501:PHE:HD2	1:U:501:PHE:H	1.36	0.71
1:Y:297:TRP:NE1	1:Y:301:ILE:HD11	2.06	0.71
1:Z:486:GLN:HE22	1:Z:538:SER:H	1.39	0.70
1:Y:562:ASP:OD2	1:Y:564:GLU:HG3	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:611:ASP:OD1	1:Z:730:ARG:HG3	1.91	0.70
1:W:487:GLN:HB3	1:W:537:MET:HE2	1.71	0.70
1:W:262:SER:O	1:W:265:THR:HG22	1.92	0.70
1:V:286:ASN:HD21	1:V:619:TRP:H	1.38	0.70
1:Y:450:GLN:HA	1:Y:459:LYS:O	1.92	0.70
1:V:486:GLN:HE22	1:V:538:SER:H	1.37	0.70
1:W:321:VAL:HG11	1:W:339:SER:CB	2.21	0.69
1:W:450:GLN:HA	1:W:459:LYS:O	1.93	0.69
1:U:611:ASP:OD1	1:U:730:ARG:HG3	1.92	0.69
1:U:486:GLN:HE22	1:U:538:SER:H	1.40	0.69
1:X:441:GLN:OE1	1:X:475:PRO:HD2	1.93	0.69
1:Y:361:GLY:HA3	1:Y:374:PRO:HG3	1.74	0.69
1:U:562:ASP:OD2	1:U:564:GLU:HG3	1.92	0.69
1:X:322:LYS:HE2	1:X:335:ASN:HD21	1.57	0.69
1:V:450:GLN:HA	1:V:459:LYS:O	1.93	0.69
1:W:553:THR:HG23	1:W:557:ASN:HB2	1.75	0.69
1:U:286:ASN:HD21	1:U:619:TRP:H	1.38	0.68
1:X:322:LYS:HE2	1:X:335:ASN:ND2	2.08	0.68
1:X:262:SER:O	1:X:265:THR:HG22	1.91	0.68
1:X:611:ASP:OD1	1:X:730:ARG:HG3	1.92	0.68
1:W:322:LYS:HE2	1:W:335:ASN:HD21	1.58	0.68
1:V:611:ASP:OD1	1:V:730:ARG:HG3	1.93	0.68
1:Z:553:THR:HG23	1:Z:557:ASN:HB2	1.75	0.68
1:Z:312:LEU:HD12	1:Z:313:ASN:H	1.58	0.68
1:U:245:ARG:NH1	1:U:364:PRO:O	2.27	0.68
1:Y:277:SER:HB2	1:Z:438:LEU:HD11	1.75	0.68
1:V:245:ARG:NH1	1:V:364:PRO:O	2.26	0.68
1:Z:562:ASP:OD1	1:Z:564:GLU:OE2	2.12	0.68
1:W:611:ASP:OD1	1:W:730:ARG:HG3	1.93	0.68
1:X:487:GLN:HB3	1:X:537:MET:HE2	1.76	0.67
1:U:553:THR:HG23	1:U:557:ASN:HB2	1.76	0.67
1:W:297:TRP:NE1	1:W:301:ILE:HD11	2.10	0.67
1:V:501:PHE:HA	1:V:504:THR:HG22	1.74	0.67
1:X:530:ASP:O	1:X:532:ASP:N	2.26	0.67
1:Z:555:LEU:HD23	1:Z:555:LEU:O	1.95	0.67
1:Y:519:ASN:HB3	1:Y:520:PRO:CD	2.24	0.67
1:Y:530:ASP:O	1:Y:532:ASP:N	2.24	0.67
1:U:696:ASN:H	1:U:696:ASN:ND2	1.93	0.67
1:X:611:ASP:HB2	1:X:730:ARG:NH1	2.10	0.67
1:W:361:GLY:HA3	1:W:374:PRO:HG3	1.74	0.67
1:X:520:PRO:HG2	1:X:635:MET:HG2	1.78	0.66
1:Y:501:PHE:HD2	1:Y:501:PHE:H	1.41	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:542:ILE:HD12	1:Y:560:ILE:HG13	1.78	0.66
1:V:501:PHE:HD2	1:V:501:PHE:H	1.43	0.66
1:W:408:ASN:ND2	1:X:224:ALA:H	1.93	0.66
1:Y:609:ASP:OD2	1:Y:630:HIS:HE1	1.77	0.66
1:U:487:GLN:HB3	1:U:537:MET:HE2	1.77	0.66
1:V:286:ASN:HD21	1:V:618:ILE:H	1.42	0.66
1:Z:446:LEU:HD13	1:Z:463:PHE:CE2	2.31	0.66
1:Y:562:ASP:OD1	1:Y:564:GLU:OE2	2.14	0.66
1:W:615:GLN:HE22	1:W:726:PRO:HA	1.61	0.66
1:Y:615:GLN:HE22	1:Y:726:PRO:HA	1.60	0.66
1:X:486:GLN:HE22	1:X:539:GLY:N	1.94	0.65
1:X:501:PHE:HA	1:X:504:THR:HG22	1.78	0.65
1:Z:289:HIS:CE1	1:Z:365:PRO:HG3	2.32	0.65
1:U:562:ASP:OD1	1:U:564:GLU:OE2	2.14	0.65
1:X:501:PHE:H	1:X:501:PHE:HD2	1.43	0.65
1:W:486:GLN:HE22	1:W:538:SER:H	1.44	0.65
1:U:450:GLN:HA	1:U:459:LYS:O	1.97	0.65
1:Z:501:PHE:H	1:Z:501:PHE:HD2	1.44	0.65
1:X:509:TYR:CD1	1:X:518:ILE:HD13	2.32	0.65
1:W:530:ASP:O	1:W:532:ASP:N	2.30	0.64
1:V:696:ASN:ND2	1:V:696:ASN:H	1.95	0.64
1:Y:553:THR:HG23	1:Y:557:ASN:HB2	1.78	0.64
1:X:322:LYS:O	1:X:673:GLN:HB2	1.97	0.64
1:V:487:GLN:HB3	1:V:537:MET:HE2	1.80	0.64
1:Z:487:GLN:HB3	1:Z:537:MET:HE2	1.79	0.64
1:Y:611:ASP:OD2	1:Y:612:VAL:N	2.29	0.64
1:U:696:ASN:H	1:U:696:ASN:HD22	1.47	0.63
1:X:361:GLY:HA3	1:X:374:PRO:HG3	1.79	0.63
1:Y:501:PHE:H	1:Z:449:THR:HG21	1.62	0.63
1:Y:551:SER:HA	1:Z:464:SER:CB	2.28	0.63
1:W:366:PHE:CE2	1:W:368:ALA:HB3	2.34	0.63
1:U:355:LEU:HD23	1:U:646:GLN:HG2	1.79	0.63
1:Y:246:THR:HG23	1:Y:678:GLN:HE21	1.64	0.63
1:Y:435:MET:HG2	1:Y:474:GLN:OE1	1.98	0.63
1:Z:615:GLN:HE22	1:Z:726:PRO:HA	1.62	0.63
1:U:577:PHE:CE1	1:U:599:MET:HG2	2.32	0.63
1:X:509:TYR:HD1	1:X:518:ILE:CD1	2.12	0.63
1:W:562:ASP:OD2	1:W:564:GLU:HG3	1.98	0.63
1:W:611:ASP:OD2	1:W:612:VAL:N	2.30	0.63
1:W:501:PHE:H	1:W:501:PHE:HD2	1.45	0.63
1:X:508:LYS:HA	1:X:518:ILE:HG12	1.80	0.63
1:X:517:ILE:HD11	1:X:538:SER:CB	2.29	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:312:LEU:HD12	1:Y:313:ASN:H	1.63	0.63
1:W:519:ASN:HB3	1:W:520:PRO:CD	2.29	0.63
1:V:435:MET:HG2	1:V:474:GLN:OE1	1.98	0.63
1:V:361:GLY:HA3	1:V:374:PRO:HG3	1.81	0.63
1:Y:262:SER:O	1:Y:265:THR:HG22	1.99	0.63
1:Y:486:GLN:HE22	1:Y:538:SER:H	1.47	0.62
1:V:446:LEU:HD13	1:V:463:PHE:CE2	2.34	0.62
1:Y:508:LYS:HA	1:Y:518:ILE:HG12	1.81	0.62
1:Y:725:ARG:HB2	1:Y:726:PRO:HD2	1.81	0.62
1:V:609:ASP:OD2	1:V:630:HIS:HE1	1.82	0.62
1:X:519:ASN:HB3	1:X:520:PRO:CD	2.29	0.62
1:Z:361:GLY:HA3	1:Z:374:PRO:HG3	1.82	0.62
1:X:562:ASP:OD1	1:X:564:GLU:OE2	2.17	0.62
1:X:312:LEU:HD12	1:X:313:ASN:H	1.64	0.62
1:V:611:ASP:OD2	1:V:612:VAL:N	2.33	0.62
1:U:520:PRO:HG2	1:U:635:MET:HG2	1.81	0.62
1:U:530:ASP:O	1:U:532:ASP:N	2.32	0.62
1:V:562:ASP:OD1	1:V:564:GLU:OE2	2.18	0.62
1:X:419:VAL:HG11	1:X:640:LEU:CD2	2.30	0.62
1:Z:441:GLN:OE1	1:Z:475:PRO:HD2	2.00	0.61
1:U:322:LYS:HB2	1:U:674:TYR:CE1	2.35	0.61
1:Y:527:HIS:CE1	1:Y:564:GLU:CD	2.73	0.61
1:Z:519:ASN:HB3	1:Z:520:PRO:CD	2.31	0.61
1:Z:501:PHE:HA	1:Z:504:THR:HG22	1.81	0.61
1:V:262:SER:O	1:V:265:THR:HG22	2.00	0.61
1:W:698:GLU:OE1	1:W:733:THR:HG23	2.00	0.61
1:X:302:ASN:HD21	1:X:701:TYR:H	1.48	0.61
1:V:312:LEU:HD12	1:V:313:ASN:H	1.64	0.61
1:V:698:GLU:OE1	1:V:733:THR:HG23	1.99	0.61
1:X:698:GLU:OE1	1:X:733:THR:HG23	2.00	0.61
1:W:246:THR:HG23	1:W:678:GLN:HE21	1.64	0.61
1:U:501:PHE:CD2	1:U:501:PHE:N	2.69	0.61
1:Y:487:GLN:HB3	1:Y:537:MET:HE2	1.82	0.61
1:V:562:ASP:OD2	1:V:564:GLU:HG3	2.00	0.61
1:Y:366:PHE:CE2	1:Y:368:ALA:HB3	2.35	0.61
1:V:405:ARG:H	1:V:408:ASN:ND2	1.94	0.61
1:U:508:LYS:HA	1:U:518:ILE:HG12	1.81	0.61
1:U:698:GLU:OE1	1:U:733:THR:HG23	2.01	0.61
1:V:267:ALA:O	1:V:268:SER:HB3	2.01	0.61
1:Y:517:ILE:CG2	1:Z:473:VAL:HA	2.31	0.61
1:Y:527:HIS:NE2	1:Y:564:GLU:OE2	2.31	0.61
1:V:530:ASP:O	1:V:532:ASP:N	2.34	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:246:THR:HG23	1:U:678:GLN:HE21	1.65	0.61
1:V:696:ASN:H	1:V:696:ASN:HD22	1.47	0.60
1:Y:512:ASN:HD21	1:Z:529:ASP:H	1.49	0.60
1:Z:696:ASN:ND2	1:Z:696:ASN:H	1.99	0.60
1:U:519:ASN:HB3	1:U:520:PRO:CD	2.31	0.60
1:Y:498:ASN:HD21	1:Z:457:GLN:HB3	1.66	0.60
1:U:527:HIS:NE2	1:U:564:GLU:OE2	2.33	0.60
1:W:419:VAL:HG11	1:W:640:LEU:CD2	2.30	0.60
1:U:555:LEU:O	1:U:555:LEU:HD23	2.01	0.60
1:U:302:ASN:HD21	1:U:701:TYR:H	1.48	0.60
1:Z:267:ALA:O	1:Z:268:SER:CB	2.50	0.60
1:U:322:LYS:O	1:U:673:GLN:HB2	2.01	0.60
1:W:527:HIS:CE1	1:W:564:GLU:CD	2.75	0.60
1:U:408:ASN:ND2	1:V:224:ALA:H	1.97	0.60
1:V:519:ASN:HB3	1:V:520:PRO:CD	2.30	0.60
1:Y:282:TYR:CE2	1:Y:374:PRO:HB2	2.36	0.60
1:W:527:HIS:NE2	1:W:564:GLU:OE2	2.28	0.60
1:W:696:ASN:H	1:W:696:ASN:ND2	2.00	0.60
1:V:289:HIS:CE1	1:V:365:PRO:HG3	2.36	0.60
1:U:501:PHE:HA	1:U:504:THR:HG22	1.83	0.60
1:Z:530:ASP:O	1:Z:532:ASP:N	2.32	0.60
1:U:262:SER:O	1:U:265:THR:HG22	2.00	0.60
1:V:508:LYS:HA	1:V:518:ILE:HG12	1.83	0.60
1:V:324:VAL:HB	1:V:333:ILE:HG23	1.84	0.60
1:U:321:VAL:HG11	1:U:339:SER:HB3	1.84	0.59
1:U:609:ASP:OD2	1:U:630:HIS:HE1	1.85	0.59
1:Z:508:LYS:HA	1:Z:518:ILE:HG12	1.84	0.59
1:Y:555:LEU:O	1:Y:555:LEU:HD23	2.02	0.59
1:Z:562:ASP:OD2	1:Z:564:GLU:HG3	2.02	0.59
1:X:450:GLN:HA	1:X:459:LYS:O	2.01	0.59
1:V:267:ALA:O	1:V:268:SER:CB	2.50	0.59
1:U:480:PRO:O	1:U:605:MET:HG2	2.03	0.59
1:U:286:ASN:HD21	1:U:618:ILE:H	1.48	0.59
1:V:395:CYS:SG	1:V:397:GLU:HG2	2.43	0.59
1:Z:696:ASN:H	1:Z:696:ASN:HD22	1.51	0.59
1:Z:267:ALA:O	1:Z:268:SER:HB3	2.03	0.59
1:U:611:ASP:OD2	1:U:612:VAL:N	2.35	0.59
1:Y:519:ASN:O	1:Y:521:GLY:N	2.36	0.59
1:W:501:PHE:HA	1:W:504:THR:HG22	1.85	0.59
1:U:621:LYS:HB2	1:U:643:PRO:HG3	1.85	0.59
1:Z:262:SER:O	1:Z:265:THR:HG22	2.03	0.59
1:Y:626:ASP:H	1:Z:608:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:509:TYR:HD1	1:Z:518:ILE:CD1	2.15	0.59
1:Y:696:ASN:H	1:Y:696:ASN:ND2	1.99	0.59
1:Y:399:PHE:CZ	1:Z:693:LYS:HG3	2.38	0.58
1:U:519:ASN:O	1:U:520:PRO:C	2.35	0.58
1:Z:419:VAL:HG11	1:Z:640:LEU:CD2	2.32	0.58
1:W:423:SER:CB	1:W:425:TYR:CE2	2.86	0.58
1:W:355:LEU:HD23	1:W:646:GLN:HG2	1.84	0.58
1:Y:621:LYS:HB2	1:Y:643:PRO:HG3	1.85	0.58
1:X:553:THR:HG23	1:X:557:ASN:CB	2.33	0.58
1:U:519:ASN:O	1:U:521:GLY:N	2.37	0.58
1:V:265:THR:HG23	1:V:267:ALA:H	1.68	0.58
1:X:607:TRP:HD1	1:X:608:GLN:O	1.87	0.58
1:Y:501:PHE:CD2	1:Y:501:PHE:N	2.70	0.58
1:Y:698:GLU:OE1	1:Y:733:THR:HG23	2.04	0.58
1:W:246:THR:HG23	1:W:678:GLN:NE2	2.18	0.58
1:V:289:HIS:CD2	1:V:365:PRO:HG3	2.39	0.58
1:V:419:VAL:HG11	1:V:640:LEU:CD2	2.33	0.58
1:W:267:ALA:O	1:W:268:SER:HB3	2.02	0.58
1:Y:500:ASN:HA	1:Z:449:THR:CG2	2.31	0.58
1:Z:238:ARG:HG2	1:Z:238:ARG:HH11	1.68	0.58
1:V:321:VAL:HG11	1:V:339:SER:HB3	1.83	0.58
1:V:408:ASN:ND2	1:W:224:ALA:H	1.99	0.58
1:Z:611:ASP:OD2	1:Z:612:VAL:N	2.35	0.58
1:U:701:TYR:C	1:U:701:TYR:CD2	2.77	0.58
1:X:611:ASP:OD2	1:X:612:VAL:N	2.36	0.58
1:Y:519:ASN:O	1:Y:520:PRO:C	2.38	0.58
1:Z:450:GLN:HA	1:Z:459:LYS:O	2.04	0.58
1:U:509:TYR:HD1	1:U:518:ILE:CD1	2.17	0.57
1:W:508:LYS:HA	1:W:518:ILE:HG12	1.86	0.57
1:Y:527:HIS:NE2	1:Y:564:GLU:CD	2.58	0.57
1:X:509:TYR:HB3	1:X:518:ILE:HD11	1.84	0.57
1:Y:265:THR:HG23	1:Y:267:ALA:H	1.69	0.57
1:W:696:ASN:HD22	1:W:696:ASN:H	1.52	0.57
1:Y:502:THR:HG23	1:Z:449:THR:HG22	1.84	0.57
1:Z:700:GLN:HA	1:Z:700:GLN:HE21	1.69	0.57
1:V:566:ILE:HG13	1:V:570:ASN:HB2	1.85	0.57
1:U:532:ASP:OD2	1:U:562:ASP:OD1	2.22	0.57
1:X:355:LEU:HD23	1:X:646:GLN:HG2	1.87	0.57
1:Z:486:GLN:HE22	1:Z:539:GLY:N	2.01	0.57
1:U:324:VAL:HB	1:U:333:ILE:HG23	1.85	0.57
1:W:486:GLN:HE22	1:W:539:GLY:N	2.02	0.57
1:Z:282:TYR:CE2	1:Z:374:PRO:HB2	2.39	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:267:ALA:O	1:U:268:SER:HB3	2.04	0.57
1:W:701:TYR:CD2	1:W:701:TYR:C	2.78	0.57
1:Y:286:ASN:HD21	1:Y:618:ILE:H	1.53	0.57
1:Z:486:GLN:NE2	1:Z:538:SER:H	2.02	0.57
1:W:265:THR:HG23	1:W:267:ALA:H	1.68	0.57
1:Y:696:ASN:HD22	1:Y:696:ASN:H	1.52	0.57
1:Z:423:SER:CB	1:Z:425:TYR:CE2	2.87	0.57
1:V:532:ASP:OD2	1:V:562:ASP:OD1	2.23	0.57
1:Z:517:ILE:HD11	1:Z:538:SER:CB	2.35	0.57
1:W:386:GLN:NE2	1:X:707:LYS:HD2	2.20	0.57
1:U:405:ARG:H	1:U:408:ASN:ND2	1.97	0.57
1:X:609:ASP:OD2	1:X:630:HIS:HE1	1.88	0.57
1:Y:501:PHE:HA	1:Y:504:THR:HG22	1.85	0.57
1:Z:609:ASP:OD2	1:Z:630:HIS:HE1	1.87	0.57
1:X:480:PRO:O	1:X:605:MET:HG2	2.05	0.56
1:Z:423:SER:HB2	1:Z:425:TYR:CE2	2.40	0.56
1:V:297:TRP:CD1	1:V:301:ILE:HD11	2.39	0.56
1:Z:609:ASP:O	1:Z:730:ARG:NH2	2.33	0.56
1:V:648:LEU:HD22	1:V:648:LEU:N	2.21	0.56
1:W:720:LEU:O	1:W:722:THR:HG22	2.06	0.56
1:U:532:ASP:OD1	1:U:564:GLU:OE2	2.24	0.56
1:V:441:GLN:OE1	1:V:475:PRO:HD2	2.05	0.56
1:W:289:HIS:CE1	1:W:365:PRO:HG3	2.40	0.56
1:Z:286:ASN:HD21	1:Z:618:ILE:H	1.53	0.56
1:Y:322:LYS:O	1:Y:673:GLN:HB2	2.05	0.56
1:V:621:LYS:HB2	1:V:643:PRO:HG3	1.87	0.56
1:X:621:LYS:HB2	1:X:643:PRO:HG3	1.87	0.56
1:W:520:PRO:HG2	1:W:635:MET:HG2	1.86	0.56
1:X:562:ASP:CG	1:X:564:GLU:HG3	2.26	0.56
1:Z:725:ARG:HB2	1:Z:726:PRO:HD2	1.88	0.56
1:Z:312:LEU:HD12	1:Z:313:ASN:N	2.21	0.56
1:Y:246:THR:HG23	1:Y:678:GLN:NE2	2.20	0.56
1:U:366:PHE:CE2	1:U:368:ALA:HB3	2.40	0.56
1:W:725:ARG:HB2	1:W:726:PRO:HD2	1.87	0.56
1:W:441:GLN:OE1	1:W:475:PRO:HD2	2.06	0.56
1:V:245:ARG:NE	1:V:367:PRO:HA	2.21	0.56
1:Y:267:ALA:O	1:Y:268:SER:HB3	2.06	0.56
1:V:321:VAL:HG11	1:V:339:SER:CB	2.36	0.56
1:U:615:GLN:HE22	1:U:726:PRO:HA	1.71	0.56
1:V:520:PRO:HG2	1:V:635:MET:HG2	1.87	0.56
1:Y:527:HIS:CE1	1:Y:532:ASP:OD1	2.59	0.55
1:W:267:ALA:O	1:W:268:SER:CB	2.53	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:562:ASP:CG	1:U:564:GLU:HG3	2.26	0.55
1:V:366:PHE:CE2	1:V:368:ALA:HB3	2.42	0.55
1:Z:519:ASN:O	1:Z:520:PRO:C	2.38	0.55
1:U:441:GLN:OE1	1:U:475:PRO:HD2	2.06	0.55
1:W:340:THR:HG22	1:W:405:ARG:HG2	1.88	0.55
1:V:519:ASN:O	1:V:521:GLY:N	2.39	0.55
1:X:297:TRP:CD1	1:X:301:ILE:HD11	2.40	0.55
1:Z:502:THR:O	1:Z:506:ALA:HB2	2.06	0.55
1:U:527:HIS:CE1	1:U:564:GLU:CD	2.80	0.55
1:X:578:GLY:O	1:X:596:VAL:HG12	2.05	0.55
1:X:272:HIS:HB3	1:X:384:GLY:HA2	1.89	0.55
1:W:322:LYS:HB2	1:W:674:TYR:CE1	2.42	0.55
1:X:701:TYR:CD2	1:X:701:TYR:C	2.80	0.55
1:V:432:ASP:O	1:V:435:MET:HE3	2.07	0.55
1:V:607:TRP:HD1	1:V:608:GLN:O	1.90	0.55
1:V:519:ASN:O	1:V:520:PRO:C	2.42	0.55
1:Y:532:ASP:OD2	1:Y:562:ASP:OD1	2.25	0.55
1:U:297:TRP:CD1	1:U:301:ILE:HD11	2.42	0.55
1:W:501:PHE:N	1:W:501:PHE:CD2	2.74	0.55
1:U:246:THR:HG23	1:U:678:GLN:NE2	2.22	0.55
1:Y:270:ASP:O	1:Z:472:SER:HB3	2.07	0.55
1:X:324:VAL:HB	1:X:333:ILE:HG23	1.88	0.55
1:Y:551:SER:CA	1:Z:464:SER:HB3	2.30	0.55
1:V:272:HIS:HB3	1:V:384:GLY:HA2	1.89	0.55
1:Y:247:TRP:HB2	1:Y:373:ILE:HD11	1.89	0.54
1:Z:426:ALA:O	1:Z:733:THR:HA	2.07	0.54
1:W:397:GLU:HB2	1:X:367:PRO:HB2	1.87	0.54
1:Z:509:TYR:CD1	1:Z:518:ILE:HD13	2.39	0.54
1:Z:322:LYS:O	1:Z:673:GLN:HB2	2.06	0.54
1:Y:379:LEU:HD13	1:Z:437:PRO:HD3	1.89	0.54
1:X:501:PHE:CD2	1:X:501:PHE:N	2.73	0.54
1:V:564:GLU:O	1:V:567:LYS:HG3	2.07	0.54
1:Y:446:LEU:HD13	1:Y:463:PHE:CE2	2.41	0.54
1:Y:444:TYR:CZ	1:Y:465:ARG:HB3	2.42	0.54
1:X:519:ASN:O	1:X:520:PRO:C	2.38	0.54
1:Z:536:PRO:HG3	1:Z:573:ALA:HB3	1.89	0.54
1:Z:321:VAL:HG11	1:Z:339:SER:HB3	1.89	0.54
1:V:444:TYR:CZ	1:V:465:ARG:HB3	2.43	0.54
1:X:615:GLN:HE22	1:X:726:PRO:HA	1.71	0.54
1:X:246:THR:HG23	1:X:678:GLN:HE21	1.72	0.54
1:W:423:SER:HB2	1:W:425:TYR:CE2	2.42	0.54
1:U:486:GLN:NE2	1:U:538:SER:H	2.04	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:322:LYS:O	1:V:673:GLN:HB2	2.07	0.54
1:U:527:HIS:CE1	1:U:532:ASP:OD1	2.61	0.54
1:Z:435:MET:HG2	1:Z:474:GLN:OE1	2.08	0.54
1:Y:322:LYS:HB2	1:Y:674:TYR:CE1	2.43	0.54
1:W:282:TYR:CE2	1:W:374:PRO:HB2	2.43	0.54
1:X:609:ASP:O	1:X:730:ARG:NH2	2.35	0.54
1:U:267:ALA:O	1:U:268:SER:CB	2.56	0.54
1:Y:648:LEU:HD22	1:Y:648:LEU:N	2.22	0.54
1:W:562:ASP:CG	1:W:564:GLU:HG3	2.28	0.54
1:U:367:PRO:HB2	1:Y:397:GLU:HB2	1.88	0.54
1:V:355:LEU:HD23	1:V:646:GLN:HG2	1.88	0.54
1:X:699:VAL:O	1:X:731:TYR:HB3	2.07	0.54
1:V:611:ASP:HB2	1:V:730:ARG:NH1	2.23	0.54
1:V:501:PHE:CD2	1:V:501:PHE:N	2.76	0.54
1:X:532:ASP:OD1	1:X:564:GLU:OE2	2.26	0.54
1:U:503:TRP:CD1	1:U:503:TRP:C	2.82	0.53
1:W:622:ILE:CD1	1:W:631:PRO:HB2	2.38	0.53
1:V:486:GLN:NE2	1:V:538:SER:H	2.04	0.53
1:Y:611:ASP:HB2	1:Y:730:ARG:NH1	2.23	0.53
1:Y:527:HIS:HE2	1:Y:564:GLU:CD	2.12	0.53
1:Y:564:GLU:O	1:Y:567:LYS:HG3	2.08	0.53
1:W:666:LYS:NZ	1:X:719:GLY:O	2.41	0.53
1:X:444:TYR:CZ	1:X:465:ARG:HB3	2.43	0.53
1:V:701:TYR:C	1:V:701:TYR:CD2	2.81	0.53
1:Z:562:ASP:CG	1:Z:564:GLU:HG3	2.28	0.53
1:Z:564:GLU:O	1:Z:567:LYS:HG3	2.07	0.53
1:V:289:HIS:CG	1:V:365:PRO:HG3	2.42	0.53
1:V:615:GLN:HE22	1:V:726:PRO:HA	1.74	0.53
1:Z:701:TYR:C	1:Z:701:TYR:CD2	2.82	0.53
1:Y:562:ASP:CG	1:Y:564:GLU:HG3	2.28	0.53
1:Y:599:MET:HE1	1:Y:602:LEU:HD11	1.90	0.53
1:V:725:ARG:HB2	1:V:726:PRO:HD2	1.89	0.53
1:X:564:GLU:O	1:X:567:LYS:HG3	2.08	0.53
1:X:426:ALA:O	1:X:733:THR:HA	2.08	0.53
1:Y:532:ASP:OD1	1:Y:564:GLU:OE2	2.27	0.53
1:U:265:THR:HG23	1:U:267:ALA:H	1.71	0.53
1:V:305:TRP:CE3	1:V:734:ARG:NH2	2.76	0.53
1:U:383:ASN:O	1:U:384:GLY:O	2.27	0.53
1:Y:247:TRP:HB3	1:Y:371:PHE:CE1	2.44	0.53
1:X:348:GLU:HB2	1:X:350:GLN:NE2	2.23	0.53
1:W:402:GLN:HG3	1:X:227:ASN:HD21	1.74	0.53
1:V:397:GLU:HB2	1:W:367:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:527:HIS:NE2	1:W:564:GLU:CD	2.62	0.53
1:V:501:PHE:CA	1:V:504:THR:HG22	2.39	0.53
1:U:272:HIS:HB3	1:U:384:GLY:HA2	1.90	0.53
1:X:696:ASN:H	1:X:696:ASN:ND2	2.06	0.53
1:X:435:MET:HG2	1:X:474:GLN:OE1	2.08	0.53
1:W:498:ASN:O	1:W:499:SER:CB	2.57	0.53
1:W:611:ASP:HB2	1:W:730:ARG:NH1	2.23	0.53
1:Y:626:ASP:H	1:Z:608:GLN:HE22	1.57	0.53
1:Z:280:TRP:CE2	1:Z:650:LYS:HD2	2.44	0.53
1:V:532:ASP:OD1	1:V:564:GLU:OE2	2.27	0.53
1:V:480:PRO:O	1:V:605:MET:HG2	2.09	0.53
1:U:312:LEU:HD12	1:U:313:ASN:H	1.74	0.53
1:W:577:PHE:CE1	1:W:599:MET:HG2	2.44	0.53
1:U:299:ARG:NH1	1:Z:690:GLU:OE2	2.42	0.53
1:Y:297:TRP:CD1	1:Y:301:ILE:HD11	2.43	0.53
1:Y:502:THR:O	1:Y:506:ALA:HB2	2.10	0.52
1:U:648:LEU:N	1:U:648:LEU:HD22	2.25	0.52
1:U:419:VAL:HG11	1:U:640:LEU:CD2	2.39	0.52
1:U:517:ILE:HD11	1:U:538:SER:CB	2.40	0.52
1:V:282:TYR:CE2	1:V:374:PRO:HB2	2.44	0.52
1:X:366:PHE:CE2	1:X:368:ALA:HB3	2.44	0.52
1:W:446:LEU:HD13	1:W:463:PHE:CE2	2.45	0.52
1:X:287:ARG:HG2	1:X:289:HIS:NE2	2.24	0.52
1:Z:444:TYR:CZ	1:Z:465:ARG:HB3	2.44	0.52
1:W:426:ALA:O	1:W:733:THR:HA	2.10	0.52
1:U:725:ARG:HB2	1:U:726:PRO:HD2	1.90	0.52
1:X:244:THR:HA	1:X:679:VAL:O	2.09	0.52
1:W:536:PRO:HG3	1:W:573:ALA:HB3	1.91	0.52
1:Y:419:VAL:HG11	1:Y:640:LEU:CD2	2.39	0.52
1:Y:399:PHE:CE2	1:Z:693:LYS:HG3	2.44	0.52
1:Y:577:PHE:CE1	1:Y:599:MET:HG2	2.44	0.52
1:X:321:VAL:HG11	1:X:339:SER:HB3	1.91	0.52
1:Z:532:ASP:OD2	1:Z:562:ASP:OD1	2.28	0.52
1:Y:701:TYR:C	1:Y:701:TYR:CD2	2.82	0.52
1:Y:519:ASN:CB	1:Z:475:PRO:HA	2.39	0.52
1:V:295:ARG:O	1:V:298:GLN:HB3	2.10	0.52
1:U:509:TYR:CD1	1:U:518:ILE:HD13	2.37	0.52
1:Z:519:ASN:O	1:Z:521:GLY:N	2.42	0.52
1:X:423:SER:CB	1:X:425:TYR:CE2	2.93	0.52
1:V:322:LYS:HB2	1:V:674:TYR:CE1	2.45	0.52
1:X:282:TYR:CE2	1:X:374:PRO:HB2	2.44	0.52
1:Z:247:TRP:HB2	1:Z:373:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:536:PRO:HG3	1:V:573:ALA:HB3	1.91	0.52
1:Y:598:VAL:HG23	1:Z:580:VAL:HG11	1.91	0.52
1:Y:287:ARG:HB3	1:Y:290:CYS:SG	2.50	0.52
1:V:562:ASP:CG	1:V:564:GLU:HG3	2.30	0.52
1:Z:322:LYS:HB2	1:Z:674:TYR:CE1	2.45	0.52
1:U:444:TYR:CZ	1:U:465:ARG:HB3	2.45	0.52
1:W:609:ASP:OD2	1:W:630:HIS:HE1	1.93	0.52
1:X:655:PRO:HB3	1:X:667:PHE:CE1	2.45	0.52
1:W:607:TRP:HD1	1:W:608:GLN:O	1.92	0.52
1:Y:441:GLN:OE1	1:Y:475:PRO:HD2	2.10	0.52
1:X:290:CYS:HB2	1:X:291:HIS:CD2	2.44	0.51
1:X:555:LEU:O	1:X:555:LEU:HD23	2.10	0.51
1:U:247:TRP:HB3	1:U:371:PHE:CE1	2.46	0.51
1:W:519:ASN:O	1:W:520:PRO:C	2.43	0.51
1:Y:252:TYR:CE1	1:Y:375:GLN:HB2	2.45	0.51
1:Y:520:PRO:HD3	1:Z:475:PRO:HB3	1.91	0.51
1:V:502:THR:O	1:V:506:ALA:HB2	2.10	0.51
1:X:545:LYS:O	1:X:546:GLU:HB2	2.11	0.51
1:V:405:ARG:N	1:V:408:ASN:HD22	1.99	0.51
1:W:622:ILE:HD12	1:W:631:PRO:HB2	1.91	0.51
1:X:408:ASN:ND2	1:Y:224:ALA:H	2.01	0.51
1:W:555:LEU:HD23	1:W:555:LEU:O	2.11	0.51
1:Y:312:LEU:HD12	1:Y:313:ASN:N	2.26	0.51
1:V:247:TRP:HB2	1:V:373:ILE:HD11	1.92	0.51
1:X:286:ASN:HD21	1:X:618:ILE:H	1.58	0.51
1:Z:219:ASP:O	1:Z:220:GLY:O	2.29	0.51
1:Z:395:CYS:SG	1:Z:397:GLU:HG2	2.51	0.51
1:V:509:TYR:HD1	1:V:518:ILE:CD1	2.23	0.51
1:X:446:LEU:HD13	1:X:463:PHE:CE2	2.46	0.51
1:Y:272:HIS:HB3	1:Y:384:GLY:HA2	1.93	0.51
1:X:218:ALA:HB1	1:Y:223:ASN:OD1	2.10	0.51
1:W:502:THR:O	1:W:506:ALA:HB2	2.11	0.51
1:X:562:ASP:OD2	1:X:564:GLU:HG3	2.11	0.51
1:U:555:LEU:HD23	1:U:555:LEU:C	2.31	0.51
1:Y:355:LEU:HD23	1:Y:646:GLN:HG2	1.93	0.51
1:V:246:THR:HG23	1:V:678:GLN:HE21	1.76	0.51
1:X:322:LYS:HB2	1:X:674:TYR:CE1	2.47	0.51
1:Z:438:LEU:HD23	1:Z:438:LEU:N	2.26	0.51
1:Y:321:VAL:HG11	1:Y:339:SER:HB3	1.92	0.51
1:Z:559:MET:SD	1:Z:725:ARG:HA	2.50	0.51
1:U:622:ILE:CD1	1:U:631:PRO:HB2	2.41	0.51
1:U:446:LEU:HD13	1:U:463:PHE:CE2	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:470:GLY:O	1:X:473:VAL:HG22	2.10	0.50
1:Y:503:TRP:C	1:Y:503:TRP:CD1	2.84	0.50
1:W:322:LYS:O	1:W:673:GLN:HB2	2.11	0.50
1:Y:537:MET:HG3	1:Z:446:LEU:HD23	1.93	0.50
1:Y:501:PHE:HE2	1:Z:449:THR:OG1	1.85	0.50
1:U:486:GLN:HE22	1:U:539:GLY:N	2.09	0.50
1:U:690:GLU:OE2	1:Z:299:ARG:NH1	2.44	0.50
1:X:295:ARG:O	1:X:298:GLN:HB3	2.11	0.50
1:W:348:GLU:HB2	1:W:350:GLN:NE2	2.26	0.50
1:W:532:ASP:OD1	1:W:564:GLU:OE2	2.28	0.50
1:X:527:HIS:CE1	1:X:564:GLU:CD	2.84	0.50
1:Z:555:LEU:C	1:Z:555:LEU:HD23	2.31	0.50
1:Z:698:GLU:OE1	1:Z:733:THR:HG23	2.11	0.50
1:W:486:GLN:NE2	1:W:538:SER:H	2.07	0.50
1:U:224:ALA:H	1:Y:408:ASN:ND2	2.01	0.50
1:Y:517:ILE:HD11	1:Y:538:SER:CB	2.42	0.50
1:X:725:ARG:HB2	1:X:726:PRO:HD2	1.94	0.50
1:V:312:LEU:HD13	1:V:683:ILE:HG12	1.94	0.50
1:Y:423:SER:HB2	1:Y:425:TYR:CE2	2.46	0.50
1:W:244:THR:HA	1:W:679:VAL:O	2.12	0.50
1:V:262:SER:OG	1:V:272:HIS:HD2	1.95	0.50
1:V:312:LEU:HD12	1:V:313:ASN:N	2.26	0.50
1:U:622:ILE:HD12	1:U:631:PRO:HB2	1.93	0.50
1:W:384:GLY:C	1:W:386:GLN:H	2.14	0.50
1:W:272:HIS:HB3	1:W:384:GLY:HA2	1.92	0.50
1:V:297:TRP:CD1	1:V:301:ILE:CD1	2.95	0.50
1:Y:423:SER:CB	1:Y:425:TYR:CE2	2.94	0.50
1:U:649:ILE:HG12	1:U:650:LYS:H	1.76	0.50
1:Y:520:PRO:CG	1:Y:635:MET:HG2	2.41	0.50
1:U:486:GLN:HE22	1:U:538:SER:N	2.10	0.50
1:Z:501:PHE:N	1:Z:501:PHE:CD2	2.73	0.50
1:U:577:PHE:CD1	1:U:599:MET:HG2	2.46	0.50
1:U:349:TYR:OH	1:U:643:PRO:O	2.20	0.49
1:Z:297:TRP:CD1	1:Z:301:ILE:HD11	2.46	0.49
1:Y:382:ASN:HD21	1:Z:433:ARG:HG3	1.77	0.49
1:U:321:VAL:HG11	1:U:339:SER:CB	2.41	0.49
1:Y:501:PHE:HD2	1:Y:501:PHE:N	2.08	0.49
1:V:555:LEU:O	1:V:555:LEU:HD23	2.13	0.49
1:X:622:ILE:HD12	1:X:631:PRO:HB2	1.94	0.49
1:X:527:HIS:CE1	1:X:532:ASP:OD1	2.65	0.49
1:U:607:TRP:HD1	1:U:608:GLN:O	1.95	0.49
1:U:289:HIS:CE1	1:U:365:PRO:HG3	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:287:ARG:HD2	1:Z:442:TYR:CZ	2.47	0.49
1:U:432:ASP:O	1:U:435:MET:HE3	2.13	0.49
1:W:509:TYR:CD1	1:W:518:ILE:HD13	2.43	0.49
1:Z:520:PRO:HG2	1:Z:635:MET:HG2	1.93	0.49
1:Z:629:PHE:O	1:Z:630:HIS:C	2.51	0.49
1:Y:536:PRO:HG3	1:Y:573:ALA:HB3	1.95	0.49
1:Y:519:ASN:HD22	1:Y:520:PRO:CD	2.25	0.49
1:W:519:ASN:O	1:W:521:GLY:N	2.46	0.49
1:Y:634:LEU:HB2	1:Z:477:ASN:O	2.13	0.49
1:X:267:ALA:O	1:X:268:SER:HB3	2.13	0.49
1:X:247:TRP:HB2	1:X:373:ILE:HD11	1.95	0.49
1:U:312:LEU:HD13	1:U:683:ILE:HG12	1.94	0.49
1:U:317:PHE:N	1:U:317:PHE:CD2	2.80	0.49
1:U:295:ARG:O	1:U:298:GLN:HB3	2.12	0.49
1:Y:379:LEU:CD1	1:Z:437:PRO:HB3	2.42	0.49
1:Y:289:HIS:CE1	1:Y:365:PRO:HG3	2.47	0.49
1:W:432:ASP:O	1:W:435:MET:HE3	2.12	0.49
1:X:501:PHE:CA	1:X:504:THR:HG22	2.42	0.49
1:U:247:TRP:HB2	1:U:373:ILE:HD11	1.94	0.49
1:W:564:GLU:O	1:W:567:LYS:HG3	2.12	0.49
1:Z:578:GLY:O	1:Z:596:VAL:HG12	2.12	0.49
1:W:312:LEU:HD13	1:W:683:ILE:HG12	1.94	0.49
1:W:384:GLY:O	1:W:386:GLN:N	2.46	0.49
1:X:577:PHE:CE1	1:X:599:MET:HG2	2.48	0.48
1:W:658:PRO:HG2	1:X:250:PRO:HB3	1.94	0.48
1:U:368:ALA:HB2	1:Y:397:GLU:HG3	1.95	0.48
1:Y:252:TYR:CZ	1:Y:375:GLN:HB2	2.47	0.48
1:Z:445:TYR:CD1	1:Z:445:TYR:N	2.81	0.48
1:Y:395:CYS:SG	1:Y:397:GLU:HG2	2.54	0.48
1:X:297:TRP:CD1	1:X:301:ILE:CD1	2.96	0.48
1:W:542:ILE:CD1	1:W:560:ILE:HG13	2.39	0.48
1:W:238:ARG:HG2	1:W:238:ARG:HH11	1.77	0.48
1:X:317:PHE:N	1:X:317:PHE:CD2	2.81	0.48
1:Y:720:LEU:O	1:Y:722:THR:HG22	2.13	0.48
1:X:519:ASN:O	1:X:521:GLY:N	2.46	0.48
1:X:696:ASN:HD22	1:X:696:ASN:H	1.62	0.48
1:U:524:MET:HG2	1:U:571:PRO:HG2	1.94	0.48
1:Z:527:HIS:CE1	1:Z:564:GLU:CD	2.87	0.48
1:Z:321:VAL:HG11	1:Z:339:SER:CB	2.44	0.48
1:X:423:SER:HB2	1:X:425:TYR:CE2	2.48	0.48
1:X:267:ALA:O	1:X:268:SER:CB	2.61	0.48
1:Y:289:HIS:CD2	1:Y:365:PRO:HG3	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:423:SER:CB	1:V:425:TYR:CE2	2.96	0.48
1:Y:359:HIS:CE1	1:Z:436:ASN:H	2.30	0.48
1:W:324:VAL:HB	1:W:333:ILE:HG23	1.95	0.48
1:Y:615:GLN:NE2	1:Y:726:PRO:HA	2.28	0.48
1:X:501:PHE:N	1:X:501:PHE:HD2	2.10	0.48
1:W:700:GLN:HE21	1:W:700:GLN:HA	1.78	0.48
1:W:444:TYR:CZ	1:W:465:ARG:HB3	2.49	0.48
1:Y:267:ALA:O	1:Y:268:SER:CB	2.62	0.48
1:V:408:ASN:HD21	1:W:224:ALA:N	2.02	0.48
1:V:444:TYR:CE2	1:V:465:ARG:HB3	2.48	0.48
1:V:286:ASN:HD21	1:V:618:ILE:N	2.10	0.48
1:U:700:GLN:HE21	1:U:700:GLN:HA	1.78	0.48
1:X:305:TRP:CE3	1:X:734:ARG:NH2	2.81	0.48
1:Y:286:ASN:HD22	1:Y:286:ASN:C	2.16	0.48
1:Z:649:ILE:HG12	1:Z:650:LYS:N	2.29	0.48
1:U:272:HIS:CB	1:U:384:GLY:HA2	2.43	0.48
1:U:498:ASN:O	1:U:499:SER:CB	2.61	0.48
1:X:536:PRO:HG3	1:X:573:ALA:HB3	1.95	0.48
1:Z:553:THR:HG23	1:Z:557:ASN:CB	2.42	0.48
1:Z:501:PHE:N	1:Z:501:PHE:HD2	2.11	0.48
1:W:615:GLN:NE2	1:W:726:PRO:HA	2.27	0.48
1:Y:444:TYR:CE2	1:Y:465:ARG:HB3	2.48	0.48
1:X:397:GLU:HB2	1:Y:367:PRO:HB2	1.94	0.48
1:X:486:GLN:O	1:X:574:THR:HA	2.14	0.48
1:W:517:ILE:HD11	1:W:538:SER:CB	2.44	0.48
1:W:249:LEU:HD23	1:W:651:ASN:OD1	2.14	0.48
1:Y:609:ASP:O	1:Y:730:ARG:NH2	2.44	0.48
1:W:532:ASP:OD2	1:W:562:ASP:OD1	2.32	0.48
1:Z:611:ASP:HB2	1:Z:730:ARG:NH1	2.29	0.48
1:Z:265:THR:HG23	1:Z:267:ALA:H	1.79	0.48
1:W:509:TYR:HD1	1:W:518:ILE:CD1	2.26	0.48
1:V:486:GLN:HE22	1:V:538:SER:N	2.08	0.48
1:X:309:PRO:HB2	1:X:416:PHE:CD2	2.49	0.48
1:W:559:MET:SD	1:W:725:ARG:HA	2.54	0.48
1:Z:432:ASP:O	1:Z:435:MET:HE3	2.14	0.47
1:Z:577:PHE:CE1	1:Z:599:MET:HG2	2.49	0.47
1:Z:621:LYS:HB2	1:Z:643:PRO:HG3	1.95	0.47
1:W:247:TRP:HB3	1:W:371:PHE:CE1	2.48	0.47
1:U:282:TYR:CE2	1:U:374:PRO:HB2	2.49	0.47
1:Y:499:SER:HA	1:Z:450:GLN:OE1	2.13	0.47
1:V:246:THR:HG23	1:V:678:GLN:NE2	2.29	0.47
1:Z:355:LEU:HD23	1:Z:646:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:286:ASN:HD21	1:W:618:ILE:H	1.58	0.47
1:W:312:LEU:HD12	1:W:313:ASN:H	1.79	0.47
1:V:426:ALA:O	1:V:733:THR:HA	2.14	0.47
1:V:553:THR:HG23	1:V:557:ASN:CB	2.43	0.47
1:V:252:TYR:CE1	1:V:375:GLN:HB2	2.49	0.47
1:Z:524:MET:HG2	1:Z:571:PRO:HG2	1.96	0.47
1:V:333:ILE:HG21	1:V:674:TYR:HE1	1.79	0.47
1:X:540:VAL:HG21	1:X:560:ILE:HG23	1.96	0.47
1:U:397:GLU:HB2	1:V:367:PRO:HB2	1.96	0.47
1:Z:501:PHE:CA	1:Z:504:THR:HG22	2.45	0.47
1:Y:327:ASN:O	1:Y:328:ASP:HB2	2.15	0.47
1:V:658:PRO:HG2	1:W:250:PRO:HB3	1.97	0.47
1:U:305:TRP:CE3	1:U:734:ARG:NH2	2.82	0.47
1:W:553:THR:HG23	1:W:557:ASN:CB	2.44	0.47
1:Z:301:ILE:HG12	1:Z:729:THR:HA	1.97	0.47
1:U:649:ILE:HG12	1:U:650:LYS:N	2.29	0.47
1:W:649:ILE:HG12	1:W:650:LYS:N	2.30	0.47
1:U:527:HIS:NE2	1:U:564:GLU:CD	2.68	0.47
1:U:423:SER:CB	1:U:425:TYR:CE2	2.98	0.47
1:Y:501:PHE:H	1:Z:449:THR:CG2	2.28	0.47
1:W:286:ASN:HD21	1:W:619:TRP:N	2.04	0.47
1:V:509:TYR:CD1	1:V:518:ILE:HD13	2.40	0.47
1:V:403:MET:HG3	1:W:227:ASN:HA	1.96	0.47
1:U:630:HIS:N	1:U:631:PRO:HD3	2.30	0.47
1:U:405:ARG:N	1:U:408:ASN:HD22	1.99	0.47
1:V:517:ILE:HD11	1:V:538:SER:CB	2.44	0.47
1:U:618:ILE:HB	1:U:619:TRP:CE3	2.50	0.47
1:W:313:ASN:HB3	1:W:682:GLU:HB3	1.97	0.47
1:V:341:VAL:HG23	1:V:650:LYS:O	2.13	0.47
1:X:486:GLN:HE22	1:X:538:SER:H	1.63	0.47
1:U:333:ILE:HG21	1:U:674:TYR:HE1	1.80	0.47
1:U:545:LYS:O	1:U:546:GLU:HB2	2.15	0.47
1:X:314:PHE:HB3	1:X:412:PHE:HD1	1.80	0.47
1:W:621:LYS:HB2	1:W:643:PRO:HG3	1.97	0.47
1:W:402:GLN:HG3	1:X:227:ASN:ND2	2.30	0.47
1:U:509:TYR:HB3	1:U:518:ILE:HD11	1.97	0.47
1:W:527:HIS:HE2	1:W:564:GLU:CD	2.17	0.47
1:Y:630:HIS:N	1:Y:631:PRO:HD3	2.30	0.47
1:V:649:ILE:HG12	1:V:650:LYS:N	2.30	0.47
1:X:700:GLN:HA	1:X:700:GLN:HE21	1.80	0.47
1:U:244:THR:HA	1:U:679:VAL:O	2.15	0.47
1:V:577:PHE:CE1	1:V:599:MET:HG2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:498:ASN:O	1:V:499:SER:CB	2.63	0.47
1:Z:649:ILE:HG12	1:Z:650:LYS:H	1.80	0.47
1:W:301:ILE:HG12	1:W:729:THR:HA	1.97	0.47
1:X:246:THR:HG23	1:X:678:GLN:NE2	2.31	0.46
1:Z:340:THR:HA	1:Z:404:LEU:O	2.15	0.46
1:U:501:PHE:CA	1:U:504:THR:HG22	2.45	0.46
1:V:527:HIS:ND1	1:V:527:HIS:O	2.49	0.46
1:U:313:ASN:HB3	1:U:682:GLU:HB3	1.97	0.46
1:U:444:TYR:CE2	1:U:465:ARG:HB3	2.51	0.46
1:Z:566:ILE:HG13	1:Z:570:ASN:HB2	1.98	0.46
1:V:470:GLY:O	1:V:473:VAL:HG22	2.15	0.46
1:X:384:GLY:O	1:X:386:GLN:N	2.49	0.46
1:X:444:TYR:CE2	1:X:465:ARG:HB3	2.50	0.46
1:Z:444:TYR:CE2	1:Z:465:ARG:HB3	2.50	0.46
1:V:649:ILE:HG12	1:V:650:LYS:H	1.79	0.46
1:W:364:PRO:CG	1:W:371:PHE:HB3	2.45	0.46
1:Y:607:TRP:HD1	1:Y:608:GLN:O	1.97	0.46
1:X:243:SER:O	1:X:680:SER:HA	2.15	0.46
1:W:333:ILE:HD12	1:W:333:ILE:H	1.79	0.46
1:Z:615:GLN:NE2	1:Z:726:PRO:HA	2.29	0.46
1:U:435:MET:HG2	1:U:474:GLN:OE1	2.14	0.46
1:Z:245:ARG:NE	1:Z:367:PRO:HA	2.31	0.46
1:V:527:HIS:CE1	1:V:564:GLU:CD	2.89	0.46
1:Y:517:ILE:HG22	1:Z:472:SER:O	2.16	0.46
1:X:658:PRO:HD3	1:Y:674:TYR:CD2	2.50	0.46
1:Z:246:THR:HG23	1:Z:678:GLN:HE21	1.81	0.46
1:W:218:ALA:HB1	1:X:223:ASN:OD1	2.16	0.46
1:V:243:SER:O	1:V:680:SER:HA	2.15	0.46
1:Y:487:GLN:HE21	1:Y:488:ARG:H	1.64	0.46
1:Y:498:ASN:O	1:Y:499:SER:CB	2.63	0.46
1:Y:509:TYR:HD1	1:Y:518:ILE:CD1	2.25	0.46
1:X:658:PRO:HG2	1:Y:250:PRO:HB3	1.98	0.46
1:Z:272:HIS:HB3	1:Z:384:GLY:HA2	1.97	0.46
1:U:290:CYS:HB2	1:U:291:HIS:CD2	2.51	0.46
1:W:322:LYS:CE	1:W:335:ASN:ND2	2.76	0.46
1:X:648:LEU:N	1:X:648:LEU:HD22	2.30	0.46
1:U:470:GLY:O	1:U:473:VAL:HG22	2.14	0.46
1:U:536:PRO:HG3	1:U:573:ALA:HB3	1.97	0.46
1:X:532:ASP:OD2	1:X:562:ASP:OD1	2.33	0.46
1:Z:324:VAL:HB	1:Z:333:ILE:HG23	1.97	0.46
1:X:599:MET:HE1	1:X:602:LEU:HD11	1.97	0.46
1:U:566:ILE:HG13	1:U:570:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:509:TYR:HB3	1:Z:518:ILE:HD11	1.98	0.46
1:Z:486:GLN:HE22	1:Z:538:SER:N	2.10	0.46
1:U:501:PHE:HD2	1:U:501:PHE:N	2.06	0.46
1:W:297:TRP:CD1	1:W:301:ILE:HD11	2.50	0.46
1:X:459:LYS:O	1:X:460:ASP:CB	2.64	0.46
1:V:566:ILE:HD12	1:V:570:ASN:ND2	2.31	0.45
1:X:438:LEU:HD23	1:X:438:LEU:N	2.31	0.45
1:V:287:ARG:HB3	1:V:290:CYS:SG	2.56	0.45
1:Y:230:CYS:HA	1:Y:242:THR:O	2.16	0.45
1:Y:243:SER:O	1:Y:680:SER:HA	2.15	0.45
1:W:322:LYS:CE	1:W:335:ASN:HD21	2.28	0.45
1:V:609:ASP:O	1:V:730:ARG:NH2	2.44	0.45
1:X:527:HIS:NE2	1:X:562:ASP:OD1	2.47	0.45
1:X:287:ARG:HB3	1:X:290:CYS:SG	2.56	0.45
1:Y:290:CYS:HB2	1:Y:291:HIS:CD2	2.51	0.45
1:U:666:LYS:NZ	1:V:719:GLY:O	2.50	0.45
1:W:357:SER:HB2	1:W:359:HIS:CD2	2.51	0.45
1:W:254:ASN:O	1:W:255:HIS:HB2	2.16	0.45
1:U:502:THR:O	1:U:506:ALA:HB2	2.15	0.45
1:W:333:ILE:HG21	1:W:674:TYR:HE1	1.82	0.45
1:V:423:SER:HB2	1:V:425:TYR:CE2	2.52	0.45
1:W:602:LEU:HD23	1:W:602:LEU:HA	1.83	0.45
1:Z:348:GLU:HB2	1:Z:350:GLN:NE2	2.31	0.45
1:Y:297:TRP:CD1	1:Y:301:ILE:CD1	3.00	0.45
1:X:312:LEU:HD11	1:X:681:VAL:HG13	1.99	0.45
1:Z:238:ARG:HG2	1:Z:238:ARG:NH1	2.30	0.45
1:X:384:GLY:C	1:X:386:GLN:H	2.20	0.45
1:V:333:ILE:HD12	1:V:333:ILE:H	1.81	0.45
1:U:614:LEU:O	1:U:614:LEU:HD12	2.17	0.45
1:U:545:LYS:O	1:U:547:SER:N	2.46	0.45
1:Y:301:ILE:HG12	1:Y:729:THR:HA	1.99	0.45
1:Y:503:TRP:CE2	1:Y:508:LYS:HE3	2.52	0.45
1:U:658:PRO:HG2	1:V:250:PRO:HB3	1.97	0.45
1:X:517:ILE:HD11	1:X:538:SER:OG	2.17	0.45
1:V:252:TYR:CZ	1:V:375:GLN:HB2	2.52	0.45
1:U:398:TYR:OH	1:V:296:ASP:OD1	2.32	0.45
1:Z:720:LEU:O	1:Z:722:THR:HG22	2.16	0.45
1:Z:366:PHE:CE2	1:Z:368:ALA:HB3	2.51	0.45
1:Z:252:TYR:CZ	1:Z:375:GLN:HB2	2.52	0.45
1:Y:536:PRO:HD2	1:Y:540:VAL:HG13	1.98	0.45
1:U:386:GLN:NE2	1:V:707:LYS:HD2	2.32	0.45
1:U:384:GLY:O	1:U:386:GLN:N	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:327:ASN:O	1:W:328:ASP:HB2	2.17	0.45
1:Z:297:TRP:CD1	1:Z:301:ILE:CD1	3.00	0.45
1:V:666:LYS:NZ	1:W:719:GLY:O	2.50	0.45
1:Y:239:VAL:CG1	1:Y:685:TRP:HB2	2.47	0.45
1:U:459:LYS:O	1:U:460:ASP:CB	2.64	0.45
1:V:622:ILE:HD12	1:V:631:PRO:HB2	1.98	0.45
1:U:426:ALA:O	1:U:733:THR:HA	2.17	0.45
1:Y:629:PHE:O	1:Y:630:HIS:C	2.54	0.44
1:Y:555:LEU:C	1:Y:555:LEU:HD23	2.36	0.44
1:X:272:HIS:CB	1:X:384:GLY:HA2	2.46	0.44
1:U:719:GLY:HA2	1:Y:257:TYR:O	2.18	0.44
1:V:272:HIS:CB	1:V:384:GLY:HA2	2.47	0.44
1:Z:459:LYS:O	1:Z:460:ASP:CB	2.65	0.44
1:Y:626:ASP:OD2	1:Z:423:SER:HB3	2.16	0.44
1:W:280:TRP:CE2	1:W:650:LYS:HD2	2.53	0.44
1:W:435:MET:HG2	1:W:474:GLN:OE1	2.17	0.44
1:U:498:ASN:O	1:U:499:SER:OG	2.33	0.44
1:V:280:TRP:CE2	1:V:650:LYS:HD2	2.52	0.44
1:X:445:TYR:CD1	1:X:445:TYR:N	2.85	0.44
1:Y:344:PHE:HB3	1:Y:401:SER:CB	2.47	0.44
1:U:239:VAL:CG1	1:U:685:TRP:HB2	2.47	0.44
1:U:384:GLY:C	1:U:386:GLN:H	2.20	0.44
1:Y:251:THR:HG22	1:Y:673:GLN:O	2.18	0.44
1:V:247:TRP:HB3	1:V:371:PHE:CE1	2.52	0.44
1:Z:384:GLY:C	1:Z:386:GLN:H	2.21	0.44
1:V:630:HIS:N	1:V:631:PRO:HD3	2.31	0.44
1:X:506:ALA:HA	1:X:537:MET:HE1	1.99	0.44
1:Y:405:ARG:H	1:Y:408:ASN:ND2	2.06	0.44
1:Y:314:PHE:HB3	1:Y:412:PHE:HD1	1.82	0.44
1:Y:540:VAL:HG21	1:Y:560:ILE:HG23	2.00	0.44
1:U:297:TRP:CD1	1:U:301:ILE:CD1	3.01	0.44
1:Y:340:THR:HG22	1:Y:405:ARG:HG2	1.99	0.44
1:Z:383:ASN:O	1:Z:384:GLY:O	2.36	0.44
1:U:722:THR:O	1:U:724:PRO:HD3	2.18	0.44
1:Z:244:THR:HA	1:Z:679:VAL:O	2.17	0.44
1:Y:649:ILE:HG12	1:Y:650:LYS:H	1.83	0.44
1:Z:286:ASN:HD21	1:Z:619:TRP:N	2.09	0.44
1:X:524:MET:HG2	1:X:571:PRO:HG2	2.00	0.44
1:X:508:LYS:CB	1:X:517:ILE:HA	2.44	0.44
1:U:286:ASN:HD21	1:U:618:ILE:N	2.14	0.44
1:W:364:PRO:HG3	1:W:371:PHE:HB3	2.00	0.44
1:X:536:PRO:HD2	1:X:540:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:219:ASP:O	1:X:220:GLY:O	2.36	0.44
1:Y:244:THR:HA	1:Y:679:VAL:O	2.18	0.44
1:V:438:LEU:HD23	1:V:438:LEU:N	2.33	0.44
1:W:468:PRO:O	1:W:471:MET:HG3	2.18	0.44
1:V:484:TYR:CD1	1:V:598:VAL:HG22	2.53	0.44
1:U:250:PRO:HB3	1:Y:658:PRO:HG2	2.00	0.44
1:Y:487:GLN:HE22	1:Z:585:GLN:H	1.66	0.44
1:Y:333:ILE:H	1:Y:333:ILE:HD12	1.83	0.44
1:Y:622:ILE:HG12	1:Y:622:ILE:H	1.64	0.44
1:V:720:LEU:O	1:V:722:THR:HG22	2.17	0.44
1:Z:527:HIS:CE1	1:Z:532:ASP:OD1	2.71	0.44
1:U:312:LEU:HD12	1:U:313:ASN:N	2.32	0.43
1:Y:649:ILE:HG12	1:Y:650:LYS:N	2.33	0.43
1:U:699:VAL:O	1:U:731:TYR:HB3	2.18	0.43
1:Z:307:PHE:HA	1:Z:686:GLU:O	2.18	0.43
1:W:501:PHE:N	1:W:501:PHE:HD2	2.13	0.43
1:X:242:THR:HG23	1:X:682:GLU:HB2	2.00	0.43
1:Y:305:TRP:CE3	1:Y:734:ARG:NH2	2.87	0.43
1:Y:545:LYS:O	1:Y:547:SER:N	2.43	0.43
1:Z:545:LYS:O	1:Z:546:GLU:HB2	2.18	0.43
1:U:695:TRP:CE2	1:Z:294:PRO:HD2	2.53	0.43
1:V:349:TYR:OH	1:V:643:PRO:O	2.22	0.43
1:V:441:GLN:HE22	1:V:474:GLN:HB3	1.84	0.43
1:W:309:PRO:HB2	1:W:416:PHE:CD2	2.54	0.43
1:U:520:PRO:CG	1:U:635:MET:HG2	2.46	0.43
1:Y:272:HIS:CB	1:Y:384:GLY:HA2	2.48	0.43
1:V:467:SER:OG	1:V:468:PRO:HD2	2.19	0.43
1:U:340:THR:HA	1:U:404:LEU:O	2.18	0.43
1:X:501:PHE:HA	1:X:504:THR:CG2	2.48	0.43
1:W:289:HIS:CD2	1:W:365:PRO:HG3	2.53	0.43
1:U:366:PHE:HA	1:U:367:PRO:HD3	1.87	0.43
1:X:333:ILE:H	1:X:333:ILE:HD12	1.82	0.43
1:W:486:GLN:O	1:W:574:THR:HA	2.19	0.43
1:X:301:ILE:HG12	1:X:729:THR:HA	2.01	0.43
1:Z:246:THR:HG23	1:Z:678:GLN:NE2	2.33	0.43
1:W:527:HIS:CE1	1:W:532:ASP:OD1	2.71	0.43
1:U:717:ASN:H	1:U:717:ASN:ND2	2.17	0.43
1:W:444:TYR:CE2	1:W:465:ARG:HB3	2.53	0.43
1:W:247:TRP:HB2	1:W:373:ILE:HD11	2.01	0.43
1:Y:310:LYS:HD2	1:Y:310:LYS:HA	1.84	0.43
1:U:249:LEU:HB3	1:U:675:SER:OG	2.19	0.43
1:W:524:MET:HG2	1:W:571:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:487:GLN:NE2	1:Z:585:GLN:H	2.17	0.43
1:X:313:ASN:HB3	1:X:682:GLU:HB3	2.01	0.43
1:W:447:ASN:HB2	1:W:464:SER:OG	2.19	0.43
1:X:312:LEU:HD12	1:X:313:ASN:N	2.31	0.43
1:X:419:VAL:HG11	1:X:640:LEU:HD23	2.01	0.43
1:Y:524:MET:HG2	1:Y:571:PRO:HG2	2.00	0.43
1:W:486:GLN:HE22	1:W:538:SER:N	2.15	0.43
1:Y:626:ASP:HB2	1:Z:608:GLN:HA	2.00	0.43
1:Y:501:PHE:CA	1:Y:504:THR:HG22	2.48	0.43
1:U:301:ILE:HG12	1:U:729:THR:HA	2.01	0.43
1:V:238:ARG:HG2	1:V:238:ARG:HH11	1.84	0.43
1:Y:326:THR:HG23	1:Y:326:THR:O	2.19	0.43
1:U:397:GLU:O	1:V:230:CYS:HB3	2.18	0.43
1:Z:422:HIS:NE2	1:Z:612:VAL:HG22	2.34	0.42
1:U:402:GLN:HG3	1:V:227:ASN:HD21	1.84	0.42
1:Z:480:PRO:O	1:Z:605:MET:HG2	2.18	0.42
1:U:243:SER:O	1:U:680:SER:HA	2.19	0.42
1:W:243:SER:O	1:W:680:SER:HA	2.19	0.42
1:W:540:VAL:HG21	1:W:560:ILE:HG23	2.00	0.42
1:V:509:TYR:HB3	1:V:518:ILE:HD11	2.02	0.42
1:Y:384:GLY:C	1:Y:386:GLN:H	2.22	0.42
1:Z:527:HIS:NE2	1:Z:564:GLU:CD	2.73	0.42
1:U:343:VAL:HA	1:U:648:LEU:O	2.20	0.42
1:X:289:HIS:CE1	1:X:365:PRO:HG3	2.54	0.42
1:W:519:ASN:O	1:W:538:SER:O	2.37	0.42
1:Z:467:SER:OG	1:Z:468:PRO:HD2	2.19	0.42
1:Y:270:ASP:HA	1:Y:514:ARG:HB2	2.00	0.42
1:W:397:GLU:HG3	1:X:368:ALA:HB2	2.01	0.42
1:U:720:LEU:O	1:U:722:THR:HG22	2.20	0.42
1:X:344:PHE:HB3	1:X:401:SER:HB3	2.02	0.42
1:V:700:GLN:HA	1:V:700:GLN:HE21	1.84	0.42
1:W:545:LYS:O	1:W:547:SER:N	2.49	0.42
1:W:295:ARG:O	1:W:298:GLN:HB3	2.19	0.42
1:Z:531:LYS:C	1:Z:533:LYS:H	2.22	0.42
1:Y:295:ARG:O	1:Y:298:GLN:HB3	2.20	0.42
1:W:459:LYS:O	1:W:460:ASP:CB	2.67	0.42
1:Y:285:PHE:CD2	1:Y:681:VAL:HG21	2.54	0.42
1:V:327:ASN:O	1:V:328:ASP:HB2	2.20	0.42
1:Z:357:SER:HB2	1:Z:359:HIS:CD2	2.55	0.42
1:U:363:LEU:HA	1:U:364:PRO:HD3	1.91	0.42
1:Z:287:ARG:NH1	1:Z:615:GLN:O	2.46	0.42
1:U:658:PRO:HD3	1:V:674:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:359:HIS:CE1	1:Z:436:ASN:HB3	2.55	0.42
1:X:327:ASN:O	1:X:328:ASP:HB2	2.20	0.42
1:U:310:LYS:HD2	1:U:310:LYS:HA	1.88	0.42
1:U:252:TYR:CZ	1:U:375:GLN:HB2	2.55	0.42
1:X:487:GLN:HE21	1:X:488:ARG:H	1.67	0.42
1:Z:693:LYS:HA	1:Z:693:LYS:HD3	1.82	0.42
1:U:441:GLN:HE22	1:U:474:GLN:HB3	1.84	0.42
1:W:408:ASN:HD21	1:X:224:ALA:N	1.99	0.42
1:Y:519:ASN:CB	1:Y:520:PRO:CD	2.95	0.42
1:W:622:ILE:HG12	1:W:622:ILE:H	1.69	0.42
1:W:286:ASN:OD1	1:W:619:TRP:O	2.38	0.42
1:U:286:ASN:ND2	1:U:618:ILE:HB	2.34	0.42
1:W:480:PRO:O	1:W:605:MET:HG2	2.19	0.42
1:U:270:ASP:HA	1:U:514:ARG:HB2	2.01	0.42
1:W:503:TRP:CD1	1:W:503:TRP:C	2.93	0.42
1:X:497:ASN:OD1	1:X:498:ASN:O	2.38	0.42
1:Y:566:ILE:HG13	1:Y:570:ASN:HB2	2.02	0.42
1:U:557:ASN:HA	1:U:557:ASN:HD22	1.70	0.42
1:W:438:LEU:N	1:W:438:LEU:HD23	2.35	0.42
1:V:527:HIS:CE1	1:V:532:ASP:OD1	2.73	0.42
1:X:486:GLN:NE2	1:X:539:GLY:N	2.67	0.42
1:Z:286:ASN:ND2	1:Z:618:ILE:HB	2.34	0.42
1:U:286:ASN:HD21	1:U:619:TRP:N	2.12	0.42
1:V:397:GLU:HG3	1:W:368:ALA:HB2	2.01	0.42
1:Z:436:ASN:HA	1:Z:437:PRO:HD2	1.92	0.42
1:V:273:TYR:CD1	1:V:273:TYR:O	2.73	0.42
1:Y:238:ARG:HG2	1:Y:238:ARG:HH11	1.84	0.42
1:W:398:TYR:OH	1:X:296:ASP:OD1	2.33	0.42
1:W:713:PHE:CZ	1:W:727:ILE:HD11	2.54	0.42
1:W:615:GLN:HE22	1:W:726:PRO:CA	2.31	0.42
1:X:622:ILE:CD1	1:X:631:PRO:HB2	2.50	0.42
1:Z:717:ASN:ND2	1:Z:717:ASN:H	2.17	0.42
1:Z:517:ILE:HD11	1:Z:538:SER:OG	2.19	0.42
1:V:270:ASP:HA	1:V:514:ARG:HB2	2.01	0.42
1:V:230:CYS:HA	1:V:242:THR:O	2.19	0.42
1:X:527:HIS:NE2	1:X:564:GLU:CD	2.72	0.42
1:Z:341:VAL:HG23	1:Z:650:LYS:O	2.20	0.42
1:U:312:LEU:HD11	1:U:681:VAL:HG13	2.01	0.42
1:W:521:GLY:O	1:W:522:THR:C	2.58	0.42
1:Z:351:LEU:HA	1:Z:351:LEU:HD23	1.86	0.42
1:U:486:GLN:O	1:U:574:THR:HA	2.19	0.42
1:W:430:SER:HA	1:W:568:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:503:TRP:CD1	1:X:503:TRP:C	2.93	0.42
1:Z:327:ASN:O	1:Z:328:ASP:HB2	2.20	0.42
1:X:720:LEU:O	1:X:722:THR:HG22	2.19	0.42
1:V:344:PHE:HB3	1:V:401:SER:HB3	2.02	0.42
1:Y:470:GLY:O	1:Y:473:VAL:HG22	2.20	0.42
1:Z:286:ASN:ND2	1:Z:618:ILE:N	2.60	0.42
1:V:289:HIS:NE2	1:V:365:PRO:HG3	2.35	0.42
1:Y:509:TYR:CD1	1:Y:518:ILE:HD13	2.42	0.41
1:W:397:GLU:HB2	1:X:367:PRO:CB	2.49	0.41
1:V:297:TRP:HE1	1:V:301:ILE:HD11	1.80	0.41
1:W:509:TYR:HB3	1:W:518:ILE:HD11	2.01	0.41
1:W:527:HIS:O	1:W:527:HIS:ND1	2.53	0.41
1:W:270:ASP:HA	1:W:514:ARG:HB2	2.01	0.41
1:V:310:LYS:HA	1:V:310:LYS:HD2	1.80	0.41
1:W:238:ARG:HG2	1:W:238:ARG:NH1	2.34	0.41
1:U:238:ARG:HH11	1:U:238:ARG:HG2	1.84	0.41
1:Y:623:PRO:HB3	1:Z:736:LEU:HD22	2.02	0.41
1:U:529:ASP:HB3	1:U:530:ASP:H	1.64	0.41
1:U:395:CYS:SG	1:U:397:GLU:HG2	2.60	0.41
1:Z:286:ASN:HD21	1:Z:618:ILE:N	2.17	0.41
1:X:400:PRO:HA	1:Y:228:TRP:O	2.19	0.41
1:Z:373:ILE:HA	1:Z:374:PRO:HD3	1.93	0.41
1:X:268:SER:O	1:X:269:ASN:C	2.56	0.41
1:U:544:GLY:O	1:U:545:LYS:HB2	2.21	0.41
1:W:484:TYR:CD1	1:W:598:VAL:HG22	2.55	0.41
1:X:614:LEU:HD12	1:X:614:LEU:O	2.19	0.41
1:V:459:LYS:O	1:V:460:ASP:CB	2.68	0.41
1:Y:366:PHE:HA	1:Y:367:PRO:HD3	1.91	0.41
1:W:257:TYR:O	1:X:719:GLY:HA2	2.21	0.41
1:W:245:ARG:NE	1:W:367:PRO:HA	2.36	0.41
1:U:402:GLN:NE2	1:U:404:LEU:HD21	2.35	0.41
1:X:257:TYR:O	1:Y:719:GLY:HA2	2.21	0.41
1:Y:344:PHE:HB3	1:Y:401:SER:HB3	2.02	0.41
1:V:503:TRP:CD1	1:V:503:TRP:C	2.93	0.41
1:V:629:PHE:O	1:V:630:HIS:C	2.58	0.41
1:Y:312:LEU:HD13	1:Y:683:ILE:HG12	2.03	0.41
1:W:419:VAL:HG11	1:W:640:LEU:HD23	2.01	0.41
1:Y:349:TYR:OH	1:Y:643:PRO:O	2.28	0.41
1:W:395:CYS:SG	1:W:397:GLU:HG2	2.60	0.41
1:Y:322:LYS:CE	1:Y:335:ASN:ND2	2.80	0.41
1:W:287:ARG:HG3	1:W:616:GLY:O	2.20	0.41
1:U:219:ASP:O	1:U:220:GLY:O	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Z:497:ASN:OD1	1:Z:498:ASN:O	2.39	0.41
1:U:553:THR:HG23	1:U:557:ASN:CB	2.47	0.41
1:V:501:PHE:HA	1:V:504:THR:CG2	2.46	0.41
1:V:527:HIS:NE2	1:V:564:GLU:CD	2.74	0.41
1:V:384:GLY:C	1:V:386:GLN:H	2.24	0.41
1:V:519:ASN:HD22	1:V:520:PRO:CD	2.34	0.41
1:Y:289:HIS:CG	1:Y:365:PRO:HG3	2.56	0.41
1:Z:217:GLY:O	1:Z:218:ALA:HB2	2.20	0.41
1:V:622:ILE:HG12	1:V:622:ILE:H	1.70	0.41
1:Z:313:ASN:HB3	1:Z:682:GLU:HB3	2.03	0.41
1:Z:289:HIS:NE2	1:Z:365:PRO:HG3	2.36	0.41
1:Y:553:THR:HG23	1:Y:557:ASN:CB	2.47	0.41
1:Y:312:LEU:HD11	1:Y:681:VAL:HG13	2.02	0.41
1:Y:313:ASN:HB3	1:Y:682:GLU:HB3	2.01	0.41
1:U:423:SER:HB2	1:U:425:TYR:CE2	2.55	0.41
1:Y:501:PHE:CE2	1:Z:449:THR:HG21	2.56	0.41
1:Y:340:THR:HA	1:Y:404:LEU:O	2.20	0.41
1:X:366:PHE:HA	1:X:367:PRO:HD3	1.93	0.41
1:W:288:PHE:CZ	1:W:618:ILE:HG23	2.56	0.41
1:U:322:LYS:CE	1:U:335:ASN:ND2	2.77	0.41
1:Z:722:THR:O	1:Z:724:PRO:HD3	2.21	0.41
1:Z:333:ILE:HG21	1:Z:674:TYR:HE1	1.85	0.41
1:U:707:LYS:HD2	1:Y:386:GLN:NE2	2.35	0.41
1:Y:357:SER:HB2	1:Y:359:HIS:CD2	2.55	0.41
1:X:252:TYR:CZ	1:X:375:GLN:HB2	2.56	0.41
1:X:566:ILE:HG13	1:X:570:ASN:HB2	2.01	0.41
1:V:314:PHE:HB3	1:V:412:PHE:HD1	1.85	0.41
1:U:357:SER:HB2	1:U:359:HIS:CD2	2.55	0.41
1:V:630:HIS:O	1:V:632:SER:N	2.47	0.41
1:Y:484:TYR:CD1	1:Y:598:VAL:HG22	2.56	0.41
1:Y:333:ILE:HG21	1:Y:674:TYR:HE1	1.85	0.41
1:U:441:GLN:NE2	1:U:474:GLN:HB3	2.36	0.41
1:W:273:TYR:O	1:W:273:TYR:CD1	2.74	0.41
1:U:326:THR:HG23	1:U:326:THR:O	2.21	0.41
1:V:445:TYR:CD1	1:V:445:TYR:N	2.87	0.41
1:W:566:ILE:HG13	1:W:570:ASN:HB2	2.03	0.41
1:V:217:GLY:O	1:V:218:ALA:HB2	2.21	0.41
1:U:400:PRO:HA	1:V:228:TRP:O	2.21	0.41
1:X:630:HIS:N	1:X:631:PRO:HD3	2.35	0.41
1:Y:432:ASP:O	1:Y:435:MET:HE3	2.21	0.41
1:W:272:HIS:CB	1:W:384:GLY:HA2	2.51	0.40
1:Z:618:ILE:HB	1:Z:619:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:312:LEU:HD12	1:W:313:ASN:N	2.36	0.40
1:X:226:GLY:HA3	1:X:317:PHE:CD1	2.57	0.40
1:X:286:ASN:HD21	1:X:619:TRP:N	2.09	0.40
1:W:445:TYR:CD1	1:W:445:TYR:N	2.89	0.40
1:W:693:LYS:HD3	1:W:693:LYS:HA	1.90	0.40
1:V:244:THR:HA	1:V:679:VAL:O	2.21	0.40
1:Y:263:ALA:HB2	1:Y:385:SER:OG	2.21	0.40
1:Z:711:VAL:HB	1:Z:714:THR:HG21	2.02	0.40
1:W:578:GLY:O	1:W:596:VAL:HG12	2.21	0.40
1:V:506:ALA:HA	1:V:537:MET:HE1	2.03	0.40
1:Z:487:GLN:HE21	1:Z:488:ARG:H	1.68	0.40
1:U:367:PRO:CB	1:Y:397:GLU:HB2	2.51	0.40
1:Y:324:VAL:HB	1:Y:333:ILE:HG23	2.01	0.40
1:X:247:TRP:HB3	1:X:371:PHE:CE1	2.56	0.40
1:Z:355:LEU:HD13	1:Z:355:LEU:HA	1.91	0.40
1:Z:272:HIS:CB	1:Z:384:GLY:HA2	2.52	0.40
1:Y:219:ASP:O	1:Y:220:GLY:O	2.39	0.40
1:W:501:PHE:CA	1:W:504:THR:HG22	2.50	0.40
1:Z:458:ASN:O	1:Z:459:LYS:C	2.60	0.40
1:U:408:ASN:HD21	1:V:224:ALA:N	2.03	0.40
1:W:508:LYS:HA	1:W:518:ILE:H	1.86	0.40
1:U:719:GLY:O	1:Y:666:LYS:NZ	2.54	0.40
1:Z:310:LYS:HA	1:Z:310:LYS:HD2	1.81	0.40
1:Y:445:TYR:CD1	1:Y:445:TYR:N	2.88	0.40
1:W:310:LYS:HD2	1:W:310:LYS:HA	1.85	0.40
1:U:659:PRO:HB2	1:U:661:GLU:O	2.21	0.40
1:U:438:LEU:HD23	1:U:438:LEU:N	2.36	0.40
1:W:386:GLN:HE22	1:X:707:LYS:HD2	1.84	0.40
1:Y:519:ASN:HD22	1:Y:520:PRO:HD3	1.87	0.40
1:Y:363:LEU:HA	1:Y:364:PRO:HD3	1.95	0.40
1:U:333:ILE:H	1:U:333:ILE:HD12	1.87	0.40
1:Z:699:VAL:O	1:Z:731:TYR:HB3	2.21	0.40
1:Z:295:ARG:O	1:Z:298:GLN:HB3	2.21	0.40
1:V:474:GLN:O	1:V:476:LYS:HG3	2.21	0.40
1:X:355:LEU:N	1:X:355:LEU:HD22	2.37	0.40
1:W:321:VAL:HG11	1:W:339:SER:HB2	2.02	0.40
1:W:545:LYS:O	1:W:546:GLU:HB2	2.20	0.40
1:V:717:ASN:ND2	1:V:717:ASN:H	2.19	0.40
1:W:344:PHE:HB3	1:W:401:SER:CB	2.51	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	Distance(Å)	Clash(Å)
1:g:547:SER:CB	1:k:455:SER:O[3_545]	1.91	0.29
1:g:557:ASN:OD1	1:k:457:GLN:NE2[3_545]	1.97	0.23

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	U	518/520 (100%)	471 (91%)	31 (6%)	16 (3%)	7	34
1	V	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	W	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	9	40
1	X	518/520 (100%)	461 (89%)	43 (8%)	14 (3%)	8	38
1	Y	518/520 (100%)	461 (89%)	44 (8%)	13 (2%)	9	40
1	Z	518/520 (100%)	462 (89%)	44 (8%)	12 (2%)	10	43
1	a	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
1	b	518/520 (100%)	467 (90%)	39 (8%)	12 (2%)	10	43
1	c	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	10	43
1	d	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	9	40
1	e	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	9	40
1	f	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	7	34
1	g	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	h	518/520 (100%)	463 (89%)	44 (8%)	11 (2%)	11	47
1	i	518/520 (100%)	466 (90%)	37 (7%)	15 (3%)	7	35
1	j	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	k	518/520 (100%)	465 (90%)	37 (7%)	16 (3%)	7	34
1	l	518/520 (100%)	468 (90%)	38 (7%)	12 (2%)	10	43
1	m	518/520 (100%)	468 (90%)	37 (7%)	13 (2%)	9	40
1	n	518/520 (100%)	469 (90%)	36 (7%)	13 (2%)	9	40
All	All	10360/10400 (100%)	9315 (90%)	777 (8%)	268 (3%)	8	39

All (268) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	384	GLY
1	U	459	LYS
1	U	519	ASN
1	U	531	LYS
1	U	545	LYS
1	V	459	LYS
1	V	519	ASN
1	V	531	LYS
1	V	553	THR
1	W	384	GLY
1	W	459	LYS
1	W	519	ASN
1	W	531	LYS
1	X	459	LYS
1	X	519	ASN
1	X	531	LYS
1	X	553	THR
1	Y	459	LYS
1	Y	519	ASN
1	Y	531	LYS
1	Y	545	LYS
1	Y	553	THR
1	Z	459	LYS
1	Z	519	ASN
1	Z	531	LYS
1	Z	552	ASN
1	a	459	LYS
1	a	519	ASN
1	a	531	LYS
1	a	553	THR
1	b	459	LYS
1	b	519	ASN
1	b	531	LYS
1	b	545	LYS
1	b	553	THR
1	c	519	ASN
1	c	531	LYS
1	c	545	LYS
1	d	459	LYS
1	d	519	ASN
1	d	531	LYS
1	d	545	LYS
1	d	553	THR

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Mol	Chain	Res	Type
1	e	459	LYS
1	e	519	ASN
1	e	531	LYS
1	e	545	LYS
1	e	553	THR
1	f	459	LYS
1	f	519	ASN
1	f	531	LYS
1	g	459	LYS
1	g	519	ASN
1	g	531	LYS
1	g	552	ASN
1	h	459	LYS
1	h	519	ASN
1	h	531	LYS
1	h	553	THR
1	i	459	LYS
1	i	519	ASN
1	i	531	LYS
1	i	545	LYS
1	i	553	THR
1	j	268	SER
1	j	459	LYS
1	j	519	ASN
1	j	531	LYS
1	k	384	GLY
1	k	459	LYS
1	k	519	ASN
1	k	531	LYS
1	l	459	LYS
1	l	519	ASN
1	l	531	LYS
1	l	553	THR
1	m	459	LYS
1	m	519	ASN
1	m	531	LYS
1	m	553	THR
1	n	459	LYS
1	n	519	ASN
1	n	531	LYS
1	n	545	LYS
1	n	553	THR

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Mol	Chain	Res	Type
1	U	220	GLY
1	U	268	SER
1	U	499	SER
1	U	544	GLY
1	U	552	ASN
1	U	553	THR
1	V	220	GLY
1	V	268	SER
1	V	384	GLY
1	V	499	SER
1	V	544	GLY
1	V	545	LYS
1	V	552	ASN
1	W	220	GLY
1	W	268	SER
1	W	499	SER
1	W	544	GLY
1	W	545	LYS
1	W	552	ASN
1	W	553	THR
1	X	220	GLY
1	X	268	SER
1	X	384	GLY
1	X	545	LYS
1	X	552	ASN
1	Y	220	GLY
1	Y	268	SER
1	Y	384	GLY
1	Y	499	SER
1	Y	544	GLY
1	Z	220	GLY
1	Z	268	SER
1	Z	384	GLY
1	Z	553	THR
1	a	220	GLY
1	a	268	SER
1	a	384	GLY
1	a	545	LYS
1	a	552	ASN
1	b	220	GLY
1	b	268	SER
1	b	384	GLY

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Mol	Chain	Res	Type
1	b	544	GLY
1	c	220	GLY
1	c	268	SER
1	c	384	GLY
1	c	459	LYS
1	c	544	GLY
1	c	552	ASN
1	c	553	THR
1	d	220	GLY
1	d	268	SER
1	d	384	GLY
1	d	544	GLY
1	d	552	ASN
1	e	220	GLY
1	e	268	SER
1	e	384	GLY
1	e	544	GLY
1	f	220	GLY
1	f	268	SER
1	f	384	GLY
1	f	545	LYS
1	f	552	ASN
1	f	553	THR
1	g	220	GLY
1	g	268	SER
1	g	384	GLY
1	g	544	GLY
1	g	545	LYS
1	g	553	THR
1	h	220	GLY
1	h	268	SER
1	h	384	GLY
1	h	545	LYS
1	h	552	ASN
1	i	220	GLY
1	i	268	SER
1	i	384	GLY
1	i	499	SER
1	j	220	GLY
1	j	384	GLY
1	j	544	GLY
1	j	545	LYS

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Mol	Chain	Res	Type
1	j	552	ASN
1	j	553	THR
1	k	220	GLY
1	k	268	SER
1	k	544	GLY
1	k	545	LYS
1	k	552	ASN
1	k	553	THR
1	l	220	GLY
1	l	268	SER
1	l	384	GLY
1	l	545	LYS
1	l	552	ASN
1	m	220	GLY
1	m	268	SER
1	m	384	GLY
1	m	544	GLY
1	m	545	LYS
1	n	220	GLY
1	n	268	SER
1	n	384	GLY
1	n	499	SER
1	U	218	ALA
1	V	218	ALA
1	W	218	ALA
1	X	218	ALA
1	X	499	SER
1	Y	218	ALA
1	Y	552	ASN
1	Z	218	ALA
1	Z	545	LYS
1	a	218	ALA
1	a	499	SER
1	b	218	ALA
1	b	499	SER
1	b	552	ASN
1	c	218	ALA
1	c	499	SER
1	d	218	ALA
1	d	499	SER
1	e	218	ALA
1	e	499	SER

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Mol	Chain	Res	Type
1	e	552	ASN
1	f	218	ALA
1	f	499	SER
1	g	218	ALA
1	g	499	SER
1	h	218	ALA
1	h	499	SER
1	i	552	ASN
1	j	218	ALA
1	k	218	ALA
1	k	385	SER
1	k	456	ALA
1	k	499	SER
1	l	218	ALA
1	l	499	SER
1	l	544	GLY
1	m	218	ALA
1	m	499	SER
1	m	552	ASN
1	n	218	ALA
1	n	544	GLY
1	n	552	ASN
1	X	385	SER
1	Z	499	SER
1	a	460	ASP
1	f	544	GLY
1	i	218	ALA
1	j	499	SER
1	n	460	ASP
1	U	460	ASP
1	U	518	ILE
1	X	460	ASP
1	Z	544	GLY
1	d	460	ASP
1	f	328	ASP
1	g	460	ASP
1	i	253	ASN
1	i	328	ASP
1	i	460	ASP
1	j	460	ASP
1	k	460	ASP
1	U	330	VAL

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Mol	Chain	Res	Type
1	U	385	SER
1	V	460	ASP
1	W	460	ASP
1	e	460	ASP
1	f	460	ASP
1	m	460	ASP
1	V	631	PRO
1	f	518	ILE
1	X	544	GLY
1	i	544	GLY
1	V	518	ILE
1	f	631	PRO
1	k	518	ILE
1	Y	631	PRO
1	a	544	GLY

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	U	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	V	452/452 (100%)	409 (90%)	43 (10%)	12	44
1	W	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	X	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	Y	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	Z	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	a	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	b	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	c	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	d	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	e	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	f	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	g	452/452 (100%)	412 (91%)	40 (9%)	14	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	i	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	j	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	k	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	l	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	m	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	n	452/452 (100%)	411 (91%)	41 (9%)	14	46
All	All	9040/9040 (100%)	8235 (91%)	805 (9%)	14	48

All (805) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	219	ASP
1	U	223	ASN
1	U	242	THR
1	U	251	THR
1	U	270	ASP
1	U	286	ASN
1	U	287	ARG
1	U	289	HIS
1	U	295	ARG
1	U	300	LEU
1	U	333	ILE
1	U	379	LEU
1	U	397	GLU
1	U	412	PHE
1	U	434	LEU
1	U	435	MET
1	U	443	LEU
1	U	449	THR
1	U	458	ASN
1	U	501	PHE
1	U	504	THR
1	U	532	ASP
1	U	551	SER
1	U	556	ASP
1	U	566	ILE
1	U	572	VAL
1	U	576	ARG
1	U	582	VAL

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Mol	Chain	Res	Type
1	U	587	SER
1	U	599	MET
1	U	622	ILE
1	U	626	ASP
1	U	628	HIS
1	U	634	LEU
1	U	669	SER
1	U	690	GLU
1	U	691	ASN
1	U	696	ASN
1	U	700	GLN
1	U	717	ASN
1	U	722	THR
1	U	725	ARG
1	V	219	ASP
1	V	223	ASN
1	V	242	THR
1	V	251	THR
1	V	270	ASP
1	V	286	ASN
1	V	287	ARG
1	V	289	HIS
1	V	295	ARG
1	V	300	LEU
1	V	333	ILE
1	V	341	VAL
1	V	379	LEU
1	V	397	GLU
1	V	412	PHE
1	V	434	LEU
1	V	435	MET
1	V	443	LEU
1	V	449	THR
1	V	458	ASN
1	V	501	PHE
1	V	504	THR
1	V	507	SER
1	V	532	ASP
1	V	551	SER
1	V	556	ASP
1	V	566	ILE
1	V	572	VAL

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Mol	Chain	Res	Type
1	V	576	ARG
1	V	582	VAL
1	V	587	SER
1	V	599	MET
1	V	622	ILE
1	V	626	ASP
1	V	628	HIS
1	V	634	LEU
1	V	669	SER
1	V	690	GLU
1	V	691	ASN
1	V	696	ASN
1	V	717	ASN
1	V	722	THR
1	V	725	ARG
1	W	219	ASP
1	W	223	ASN
1	W	242	THR
1	W	251	THR
1	W	270	ASP
1	W	286	ASN
1	W	287	ARG
1	W	289	HIS
1	W	295	ARG
1	W	300	LEU
1	W	333	ILE
1	W	341	VAL
1	W	379	LEU
1	W	397	GLU
1	W	412	PHE
1	W	434	LEU
1	W	435	MET
1	W	443	LEU
1	W	449	THR
1	W	458	ASN
1	W	501	PHE
1	W	504	THR
1	W	532	ASP
1	W	537	MET
1	W	551	SER
1	W	556	ASP
1	W	566	ILE

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Mol	Chain	Res	Type
1	W	572	VAL
1	W	576	ARG
1	W	582	VAL
1	W	587	SER
1	W	622	ILE
1	W	626	ASP
1	W	628	HIS
1	W	634	LEU
1	W	669	SER
1	W	690	GLU
1	W	691	ASN
1	W	696	ASN
1	W	700	GLN
1	W	722	THR
1	W	725	ARG
1	X	219	ASP
1	X	223	ASN
1	X	242	THR
1	X	251	THR
1	X	286	ASN
1	X	287	ARG
1	X	289	HIS
1	X	295	ARG
1	X	300	LEU
1	X	333	ILE
1	X	379	LEU
1	X	397	GLU
1	X	412	PHE
1	X	434	LEU
1	X	435	MET
1	X	443	LEU
1	X	449	THR
1	X	458	ASN
1	X	501	PHE
1	X	504	THR
1	X	532	ASP
1	X	551	SER
1	X	556	ASP
1	X	566	ILE
1	X	572	VAL
1	X	576	ARG
1	X	582	VAL

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Mol	Chain	Res	Type
1	X	587	SER
1	X	599	MET
1	X	622	ILE
1	X	626	ASP
1	X	634	LEU
1	X	690	GLU
1	X	691	ASN
1	X	696	ASN
1	X	722	THR
1	X	725	ARG
1	Y	219	ASP
1	Y	223	ASN
1	Y	242	THR
1	Y	251	THR
1	Y	265	THR
1	Y	286	ASN
1	Y	287	ARG
1	Y	295	ARG
1	Y	300	LEU
1	Y	333	ILE
1	Y	341	VAL
1	Y	379	LEU
1	Y	397	GLU
1	Y	412	PHE
1	Y	434	LEU
1	Y	435	MET
1	Y	443	LEU
1	Y	449	THR
1	Y	458	ASN
1	Y	501	PHE
1	Y	504	THR
1	Y	532	ASP
1	Y	551	SER
1	Y	556	ASP
1	Y	566	ILE
1	Y	572	VAL
1	Y	576	ARG
1	Y	582	VAL
1	Y	587	SER
1	Y	622	ILE
1	Y	626	ASP
1	Y	628	HIS

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Mol	Chain	Res	Type
1	Y	634	LEU
1	Y	669	SER
1	Y	690	GLU
1	Y	696	ASN
1	Y	717	ASN
1	Y	722	THR
1	Y	725	ARG
1	Z	219	ASP
1	Z	223	ASN
1	Z	251	THR
1	Z	265	THR
1	Z	270	ASP
1	Z	286	ASN
1	Z	287	ARG
1	Z	289	HIS
1	Z	295	ARG
1	Z	300	LEU
1	Z	333	ILE
1	Z	379	LEU
1	Z	397	GLU
1	Z	434	LEU
1	Z	435	MET
1	Z	443	LEU
1	Z	449	THR
1	Z	458	ASN
1	Z	501	PHE
1	Z	504	THR
1	Z	507	SER
1	Z	532	ASP
1	Z	551	SER
1	Z	556	ASP
1	Z	566	ILE
1	Z	572	VAL
1	Z	576	ARG
1	Z	582	VAL
1	Z	587	SER
1	Z	599	MET
1	Z	622	ILE
1	Z	626	ASP
1	Z	628	HIS
1	Z	634	LEU
1	Z	676	THR

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Mol	Chain	Res	Type
1	Z	690	GLU
1	Z	696	ASN
1	Z	722	THR
1	Z	725	ARG
1	a	219	ASP
1	a	223	ASN
1	a	242	THR
1	a	251	THR
1	a	265	THR
1	a	286	ASN
1	a	287	ARG
1	a	289	HIS
1	a	295	ARG
1	a	300	LEU
1	a	333	ILE
1	a	379	LEU
1	a	412	PHE
1	a	435	MET
1	a	443	LEU
1	a	449	THR
1	a	458	ASN
1	a	501	PHE
1	a	504	THR
1	a	532	ASP
1	a	551	SER
1	a	556	ASP
1	a	566	ILE
1	a	572	VAL
1	a	576	ARG
1	a	582	VAL
1	a	587	SER
1	a	599	MET
1	a	622	ILE
1	a	626	ASP
1	a	628	HIS
1	a	634	LEU
1	a	669	SER
1	a	690	GLU
1	a	691	ASN
1	a	696	ASN
1	a	722	THR
1	a	725	ARG

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Mol	Chain	Res	Type
1	b	219	ASP
1	b	223	ASN
1	b	251	THR
1	b	270	ASP
1	b	286	ASN
1	b	287	ARG
1	b	289	HIS
1	b	295	ARG
1	b	300	LEU
1	b	309	PRO
1	b	333	ILE
1	b	341	VAL
1	b	379	LEU
1	b	397	GLU
1	b	412	PHE
1	b	434	LEU
1	b	435	MET
1	b	443	LEU
1	b	449	THR
1	b	458	ASN
1	b	501	PHE
1	b	504	THR
1	b	532	ASP
1	b	551	SER
1	b	556	ASP
1	b	566	ILE
1	b	572	VAL
1	b	576	ARG
1	b	582	VAL
1	b	587	SER
1	b	599	MET
1	b	622	ILE
1	b	626	ASP
1	b	628	HIS
1	b	634	LEU
1	b	669	SER
1	b	676	THR
1	b	690	GLU
1	b	691	ASN
1	b	696	ASN
1	b	722	THR
1	b	725	ARG

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Mol	Chain	Res	Type
1	c	219	ASP
1	c	223	ASN
1	c	242	THR
1	c	251	THR
1	c	286	ASN
1	c	287	ARG
1	c	289	HIS
1	c	295	ARG
1	c	300	LEU
1	c	333	ILE
1	c	379	LEU
1	c	397	GLU
1	c	412	PHE
1	c	431	LEU
1	c	434	LEU
1	c	435	MET
1	c	443	LEU
1	c	449	THR
1	c	458	ASN
1	c	501	PHE
1	c	504	THR
1	c	507	SER
1	c	532	ASP
1	c	537	MET
1	c	551	SER
1	c	556	ASP
1	c	566	ILE
1	c	572	VAL
1	c	576	ARG
1	c	582	VAL
1	c	587	SER
1	c	599	MET
1	c	622	ILE
1	c	626	ASP
1	c	628	HIS
1	c	634	LEU
1	c	669	SER
1	c	676	THR
1	c	690	GLU
1	c	691	ASN
1	c	696	ASN
1	c	717	ASN

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Mol	Chain	Res	Type
1	c	722	THR
1	c	725	ARG
1	d	219	ASP
1	d	223	ASN
1	d	242	THR
1	d	251	THR
1	d	286	ASN
1	d	287	ARG
1	d	289	HIS
1	d	295	ARG
1	d	300	LEU
1	d	333	ILE
1	d	379	LEU
1	d	397	GLU
1	d	412	PHE
1	d	435	MET
1	d	443	LEU
1	d	449	THR
1	d	458	ASN
1	d	501	PHE
1	d	504	THR
1	d	532	ASP
1	d	537	MET
1	d	551	SER
1	d	556	ASP
1	d	566	ILE
1	d	572	VAL
1	d	576	ARG
1	d	582	VAL
1	d	587	SER
1	d	599	MET
1	d	622	ILE
1	d	626	ASP
1	d	628	HIS
1	d	634	LEU
1	d	676	THR
1	d	690	GLU
1	d	691	ASN
1	d	696	ASN
1	d	722	THR
1	d	725	ARG
1	e	219	ASP

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Mol	Chain	Res	Type
1	e	223	ASN
1	e	242	THR
1	e	251	THR
1	e	286	ASN
1	e	287	ARG
1	e	289	HIS
1	e	295	ARG
1	e	300	LEU
1	e	333	ILE
1	e	379	LEU
1	e	397	GLU
1	e	412	PHE
1	e	434	LEU
1	e	435	MET
1	e	443	LEU
1	e	449	THR
1	e	458	ASN
1	e	501	PHE
1	e	504	THR
1	e	532	ASP
1	e	551	SER
1	e	556	ASP
1	e	557	ASN
1	e	566	ILE
1	e	572	VAL
1	e	576	ARG
1	e	582	VAL
1	e	587	SER
1	e	599	MET
1	e	622	ILE
1	e	626	ASP
1	e	628	HIS
1	e	634	LEU
1	e	669	SER
1	e	676	THR
1	e	690	GLU
1	e	691	ASN
1	e	696	ASN
1	e	717	ASN
1	e	722	THR
1	e	725	ARG
1	f	219	ASP

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Mol	Chain	Res	Type
1	f	223	ASN
1	f	242	THR
1	f	251	THR
1	f	286	ASN
1	f	287	ARG
1	f	289	HIS
1	f	295	ARG
1	f	300	LEU
1	f	333	ILE
1	f	379	LEU
1	f	397	GLU
1	f	412	PHE
1	f	434	LEU
1	f	435	MET
1	f	443	LEU
1	f	449	THR
1	f	458	ASN
1	f	501	PHE
1	f	504	THR
1	f	532	ASP
1	f	551	SER
1	f	556	ASP
1	f	566	ILE
1	f	572	VAL
1	f	576	ARG
1	f	582	VAL
1	f	587	SER
1	f	626	ASP
1	f	628	HIS
1	f	634	LEU
1	f	676	THR
1	f	690	GLU
1	f	691	ASN
1	f	696	ASN
1	f	722	THR
1	f	725	ARG
1	g	219	ASP
1	g	223	ASN
1	g	242	THR
1	g	251	THR
1	g	270	ASP
1	g	286	ASN

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Mol	Chain	Res	Type
1	g	287	ARG
1	g	289	HIS
1	g	295	ARG
1	g	300	LEU
1	g	333	ILE
1	g	341	VAL
1	g	379	LEU
1	g	397	GLU
1	g	434	LEU
1	g	435	MET
1	g	443	LEU
1	g	449	THR
1	g	458	ASN
1	g	501	PHE
1	g	504	THR
1	g	532	ASP
1	g	537	MET
1	g	551	SER
1	g	556	ASP
1	g	566	ILE
1	g	572	VAL
1	g	576	ARG
1	g	582	VAL
1	g	587	SER
1	g	622	ILE
1	g	626	ASP
1	g	628	HIS
1	g	634	LEU
1	g	669	SER
1	g	690	GLU
1	g	691	ASN
1	g	696	ASN
1	g	722	THR
1	g	725	ARG
1	h	219	ASP
1	h	223	ASN
1	h	242	THR
1	h	251	THR
1	h	286	ASN
1	h	287	ARG
1	h	289	HIS
1	h	295	ARG

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Mol	Chain	Res	Type
1	h	300	LEU
1	h	333	ILE
1	h	379	LEU
1	h	412	PHE
1	h	435	MET
1	h	443	LEU
1	h	449	THR
1	h	458	ASN
1	h	501	PHE
1	h	504	THR
1	h	532	ASP
1	h	551	SER
1	h	556	ASP
1	h	566	ILE
1	h	572	VAL
1	h	576	ARG
1	h	582	VAL
1	h	587	SER
1	h	622	ILE
1	h	626	ASP
1	h	628	HIS
1	h	634	LEU
1	h	669	SER
1	h	676	THR
1	h	690	GLU
1	h	691	ASN
1	h	696	ASN
1	h	722	THR
1	h	725	ARG
1	i	219	ASP
1	i	223	ASN
1	i	242	THR
1	i	251	THR
1	i	265	THR
1	i	270	ASP
1	i	286	ASN
1	i	287	ARG
1	i	289	HIS
1	i	295	ARG
1	i	300	LEU
1	i	333	ILE
1	i	379	LEU

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Mol	Chain	Res	Type
1	i	397	GLU
1	i	412	PHE
1	i	435	MET
1	i	443	LEU
1	i	449	THR
1	i	458	ASN
1	i	501	PHE
1	i	504	THR
1	i	532	ASP
1	i	551	SER
1	i	556	ASP
1	i	566	ILE
1	i	572	VAL
1	i	576	ARG
1	i	582	VAL
1	i	587	SER
1	i	589	THR
1	i	599	MET
1	i	622	ILE
1	i	626	ASP
1	i	628	HIS
1	i	634	LEU
1	i	676	THR
1	i	690	GLU
1	i	691	ASN
1	i	696	ASN
1	i	717	ASN
1	i	722	THR
1	i	725	ARG
1	j	219	ASP
1	j	223	ASN
1	j	242	THR
1	j	251	THR
1	j	286	ASN
1	j	287	ARG
1	j	289	HIS
1	j	295	ARG
1	j	300	LEU
1	j	333	ILE
1	j	341	VAL
1	j	379	LEU
1	j	397	GLU

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Mol	Chain	Res	Type
1	j	412	PHE
1	j	431	LEU
1	j	434	LEU
1	j	435	MET
1	j	443	LEU
1	j	449	THR
1	j	458	ASN
1	j	501	PHE
1	j	504	THR
1	j	532	ASP
1	j	551	SER
1	j	556	ASP
1	j	566	ILE
1	j	572	VAL
1	j	576	ARG
1	j	582	VAL
1	j	587	SER
1	j	599	MET
1	j	622	ILE
1	j	626	ASP
1	j	628	HIS
1	j	634	LEU
1	j	676	THR
1	j	690	GLU
1	j	696	ASN
1	j	722	THR
1	j	725	ARG
1	k	219	ASP
1	k	223	ASN
1	k	242	THR
1	k	251	THR
1	k	270	ASP
1	k	286	ASN
1	k	287	ARG
1	k	295	ARG
1	k	300	LEU
1	k	333	ILE
1	k	341	VAL
1	k	379	LEU
1	k	397	GLU
1	k	412	PHE
1	k	431	LEU

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Mol	Chain	Res	Type
1	k	434	LEU
1	k	435	MET
1	k	443	LEU
1	k	449	THR
1	k	458	ASN
1	k	501	PHE
1	k	504	THR
1	k	507	SER
1	k	532	ASP
1	k	551	SER
1	k	556	ASP
1	k	566	ILE
1	k	572	VAL
1	k	576	ARG
1	k	582	VAL
1	k	587	SER
1	k	599	MET
1	k	622	ILE
1	k	626	ASP
1	k	628	HIS
1	k	634	LEU
1	k	676	THR
1	k	690	GLU
1	k	691	ASN
1	k	696	ASN
1	k	700	GLN
1	k	717	ASN
1	k	722	THR
1	k	725	ARG
1	l	219	ASP
1	l	223	ASN
1	l	251	THR
1	l	265	THR
1	l	270	ASP
1	l	286	ASN
1	l	287	ARG
1	l	289	HIS
1	l	295	ARG
1	l	300	LEU
1	l	309	PRO
1	l	333	ILE
1	l	379	LEU

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Mol	Chain	Res	Type
1	l	397	GLU
1	l	412	PHE
1	l	434	LEU
1	l	435	MET
1	l	449	THR
1	l	458	ASN
1	l	501	PHE
1	l	504	THR
1	l	507	SER
1	l	532	ASP
1	l	551	SER
1	l	556	ASP
1	l	566	ILE
1	l	572	VAL
1	l	576	ARG
1	l	582	VAL
1	l	587	SER
1	l	599	MET
1	l	622	ILE
1	l	626	ASP
1	l	628	HIS
1	l	634	LEU
1	l	690	GLU
1	l	696	ASN
1	l	722	THR
1	l	725	ARG
1	m	219	ASP
1	m	223	ASN
1	m	242	THR
1	m	251	THR
1	m	286	ASN
1	m	287	ARG
1	m	289	HIS
1	m	295	ARG
1	m	300	LEU
1	m	333	ILE
1	m	379	LEU
1	m	397	GLU
1	m	412	PHE
1	m	434	LEU
1	m	435	MET
1	m	449	THR

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Mol	Chain	Res	Type
1	m	458	ASN
1	m	501	PHE
1	m	504	THR
1	m	532	ASP
1	m	551	SER
1	m	556	ASP
1	m	566	ILE
1	m	572	VAL
1	m	576	ARG
1	m	582	VAL
1	m	587	SER
1	m	622	ILE
1	m	626	ASP
1	m	628	HIS
1	m	634	LEU
1	m	669	SER
1	m	676	THR
1	m	690	GLU
1	m	696	ASN
1	m	717	ASN
1	m	722	THR
1	m	725	ARG
1	n	219	ASP
1	n	223	ASN
1	n	243	SER
1	n	251	THR
1	n	265	THR
1	n	286	ASN
1	n	287	ARG
1	n	289	HIS
1	n	295	ARG
1	n	300	LEU
1	n	333	ILE
1	n	379	LEU
1	n	397	GLU
1	n	412	PHE
1	n	431	LEU
1	n	434	LEU
1	n	435	MET
1	n	443	LEU
1	n	449	THR
1	n	458	ASN

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Mol	Chain	Res	Type
1	n	501	PHE
1	n	504	THR
1	n	532	ASP
1	n	551	SER
1	n	556	ASP
1	n	566	ILE
1	n	572	VAL
1	n	576	ARG
1	n	582	VAL
1	n	587	SER
1	n	599	MET
1	n	622	ILE
1	n	626	ASP
1	n	628	HIS
1	n	634	LEU
1	n	676	THR
1	n	690	GLU
1	n	696	ASN
1	n	717	ASN
1	n	722	THR
1	n	725	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (507) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	253	ASN
1	U	255	HIS
1	U	259	GLN
1	U	272	HIS
1	U	286	ASN
1	U	302	ASN
1	U	320	GLN
1	U	335	ASN
1	U	350	GLN
1	U	359	HIS
1	U	375	GLN
1	U	386	GLN
1	U	408	ASN
1	U	427	HIS
1	U	458	ASN
1	U	486	GLN
1	U	487	GLN

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Mol	Chain	Res	Type
1	U	497	ASN
1	U	498	ASN
1	U	519	ASN
1	U	557	ASN
1	U	608	GLN
1	U	630	HIS
1	U	691	ASN
1	U	696	ASN
1	U	717	ASN
1	V	253	ASN
1	V	255	HIS
1	V	259	GLN
1	V	272	HIS
1	V	286	ASN
1	V	302	ASN
1	V	320	GLN
1	V	335	ASN
1	V	350	GLN
1	V	375	GLN
1	V	386	GLN
1	V	408	ASN
1	V	458	ASN
1	V	486	GLN
1	V	487	GLN
1	V	497	ASN
1	V	498	ASN
1	V	519	ASN
1	V	557	ASN
1	V	630	HIS
1	V	691	ASN
1	V	696	ASN
1	V	700	GLN
1	V	717	ASN
1	W	253	ASN
1	W	255	HIS
1	W	272	HIS
1	W	286	ASN
1	W	302	ASN
1	W	320	GLN
1	W	335	ASN
1	W	350	GLN
1	W	375	GLN

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Mol	Chain	Res	Type
1	W	386	GLN
1	W	408	ASN
1	W	458	ASN
1	W	486	GLN
1	W	487	GLN
1	W	497	ASN
1	W	519	ASN
1	W	557	ASN
1	W	630	HIS
1	W	691	ASN
1	W	696	ASN
1	W	700	GLN
1	W	717	ASN
1	X	227	ASN
1	X	253	ASN
1	X	255	HIS
1	X	259	GLN
1	X	272	HIS
1	X	286	ASN
1	X	302	ASN
1	X	320	GLN
1	X	335	ASN
1	X	350	GLN
1	X	359	HIS
1	X	375	GLN
1	X	386	GLN
1	X	408	ASN
1	X	458	ASN
1	X	486	GLN
1	X	487	GLN
1	X	497	ASN
1	X	519	ASN
1	X	557	ASN
1	X	630	HIS
1	X	691	ASN
1	X	696	ASN
1	X	700	GLN
1	X	717	ASN
1	Y	255	HIS
1	Y	259	GLN
1	Y	272	HIS
1	Y	286	ASN

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Mol	Chain	Res	Type
1	Y	302	ASN
1	Y	320	GLN
1	Y	335	ASN
1	Y	375	GLN
1	Y	382	ASN
1	Y	383	ASN
1	Y	386	GLN
1	Y	408	ASN
1	Y	458	ASN
1	Y	486	GLN
1	Y	487	GLN
1	Y	497	ASN
1	Y	498	ASN
1	Y	512	ASN
1	Y	519	ASN
1	Y	557	ASN
1	Y	630	HIS
1	Y	691	ASN
1	Y	696	ASN
1	Y	700	GLN
1	Y	717	ASN
1	Z	253	ASN
1	Z	255	HIS
1	Z	259	GLN
1	Z	272	HIS
1	Z	286	ASN
1	Z	302	ASN
1	Z	320	GLN
1	Z	335	ASN
1	Z	350	GLN
1	Z	375	GLN
1	Z	386	GLN
1	Z	408	ASN
1	Z	458	ASN
1	Z	486	GLN
1	Z	487	GLN
1	Z	497	ASN
1	Z	498	ASN
1	Z	519	ASN
1	Z	557	ASN
1	Z	608	GLN
1	Z	630	HIS

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Mol	Chain	Res	Type
1	Z	691	ASN
1	Z	696	ASN
1	Z	717	ASN
1	a	253	ASN
1	a	255	HIS
1	a	259	GLN
1	a	272	HIS
1	a	286	ASN
1	a	302	ASN
1	a	320	GLN
1	a	335	ASN
1	a	350	GLN
1	a	359	HIS
1	a	375	GLN
1	a	386	GLN
1	a	408	ASN
1	a	458	ASN
1	a	486	GLN
1	a	487	GLN
1	a	497	ASN
1	a	519	ASN
1	a	557	ASN
1	a	585	GLN
1	a	624	HIS
1	a	630	HIS
1	a	691	ASN
1	a	696	ASN
1	a	700	GLN
1	b	259	GLN
1	b	272	HIS
1	b	286	ASN
1	b	302	ASN
1	b	320	GLN
1	b	335	ASN
1	b	350	GLN
1	b	386	GLN
1	b	408	ASN
1	b	458	ASN
1	b	486	GLN
1	b	487	GLN
1	b	497	ASN
1	b	498	ASN

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Mol	Chain	Res	Type
1	b	519	ASN
1	b	557	ASN
1	b	624	HIS
1	b	630	HIS
1	b	691	ASN
1	b	696	ASN
1	b	700	GLN
1	b	717	ASN
1	c	227	ASN
1	c	253	ASN
1	c	255	HIS
1	c	259	GLN
1	c	272	HIS
1	c	286	ASN
1	c	302	ASN
1	c	320	GLN
1	c	335	ASN
1	c	350	GLN
1	c	359	HIS
1	c	375	GLN
1	c	386	GLN
1	c	408	ASN
1	c	458	ASN
1	c	486	GLN
1	c	487	GLN
1	c	497	ASN
1	c	498	ASN
1	c	519	ASN
1	c	557	ASN
1	c	624	HIS
1	c	630	HIS
1	c	691	ASN
1	c	696	ASN
1	c	700	GLN
1	c	717	ASN
1	d	253	ASN
1	d	255	HIS
1	d	259	GLN
1	d	272	HIS
1	d	286	ASN
1	d	302	ASN
1	d	320	GLN

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Mol	Chain	Res	Type
1	d	335	ASN
1	d	360	GLN
1	d	375	GLN
1	d	382	ASN
1	d	386	GLN
1	d	408	ASN
1	d	458	ASN
1	d	486	GLN
1	d	487	GLN
1	d	497	ASN
1	d	498	ASN
1	d	512	ASN
1	d	519	ASN
1	d	557	ASN
1	d	630	HIS
1	d	691	ASN
1	d	696	ASN
1	d	700	GLN
1	d	717	ASN
1	e	253	ASN
1	e	255	HIS
1	e	259	GLN
1	e	272	HIS
1	e	286	ASN
1	e	302	ASN
1	e	320	GLN
1	e	335	ASN
1	e	350	GLN
1	e	359	HIS
1	e	375	GLN
1	e	383	ASN
1	e	386	GLN
1	e	408	ASN
1	e	427	HIS
1	e	458	ASN
1	e	486	GLN
1	e	487	GLN
1	e	497	ASN
1	e	498	ASN
1	e	519	ASN
1	e	557	ASN
1	e	608	GLN

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Mol	Chain	Res	Type
1	e	624	HIS
1	e	630	HIS
1	e	691	ASN
1	e	696	ASN
1	e	717	ASN
1	f	253	ASN
1	f	255	HIS
1	f	259	GLN
1	f	272	HIS
1	f	286	ASN
1	f	302	ASN
1	f	320	GLN
1	f	335	ASN
1	f	350	GLN
1	f	359	HIS
1	f	375	GLN
1	f	386	GLN
1	f	408	ASN
1	f	458	ASN
1	f	486	GLN
1	f	487	GLN
1	f	497	ASN
1	f	519	ASN
1	f	557	ASN
1	f	624	HIS
1	f	630	HIS
1	f	691	ASN
1	f	696	ASN
1	f	700	GLN
1	f	717	ASN
1	g	253	ASN
1	g	255	HIS
1	g	259	GLN
1	g	272	HIS
1	g	286	ASN
1	g	302	ASN
1	g	320	GLN
1	g	335	ASN
1	g	350	GLN
1	g	375	GLN
1	g	386	GLN
1	g	408	ASN

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Mol	Chain	Res	Type
1	g	458	ASN
1	g	486	GLN
1	g	487	GLN
1	g	497	ASN
1	g	498	ASN
1	g	519	ASN
1	g	557	ASN
1	g	630	HIS
1	g	691	ASN
1	g	696	ASN
1	g	700	GLN
1	g	717	ASN
1	h	253	ASN
1	h	255	HIS
1	h	259	GLN
1	h	272	HIS
1	h	286	ASN
1	h	302	ASN
1	h	320	GLN
1	h	335	ASN
1	h	350	GLN
1	h	375	GLN
1	h	383	ASN
1	h	386	GLN
1	h	408	ASN
1	h	458	ASN
1	h	486	GLN
1	h	487	GLN
1	h	497	ASN
1	h	519	ASN
1	h	557	ASN
1	h	624	HIS
1	h	630	HIS
1	h	691	ASN
1	h	696	ASN
1	h	700	GLN
1	h	717	ASN
1	i	253	ASN
1	i	259	GLN
1	i	272	HIS
1	i	286	ASN
1	i	302	ASN

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Mol	Chain	Res	Type
1	i	320	GLN
1	i	335	ASN
1	i	375	GLN
1	i	382	ASN
1	i	386	GLN
1	i	408	ASN
1	i	458	ASN
1	i	486	GLN
1	i	487	GLN
1	i	497	ASN
1	i	498	ASN
1	i	512	ASN
1	i	519	ASN
1	i	557	ASN
1	i	585	GLN
1	i	624	HIS
1	i	630	HIS
1	i	691	ASN
1	i	696	ASN
1	i	700	GLN
1	i	717	ASN
1	j	253	ASN
1	j	255	HIS
1	j	259	GLN
1	j	272	HIS
1	j	286	ASN
1	j	302	ASN
1	j	320	GLN
1	j	335	ASN
1	j	350	GLN
1	j	359	HIS
1	j	375	GLN
1	j	383	ASN
1	j	386	GLN
1	j	408	ASN
1	j	427	HIS
1	j	458	ASN
1	j	486	GLN
1	j	487	GLN
1	j	497	ASN
1	j	498	ASN
1	j	519	ASN

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Mol	Chain	Res	Type
1	j	557	ASN
1	j	608	GLN
1	j	624	HIS
1	j	630	HIS
1	j	691	ASN
1	j	696	ASN
1	j	717	ASN
1	k	253	ASN
1	k	255	HIS
1	k	259	GLN
1	k	272	HIS
1	k	286	ASN
1	k	302	ASN
1	k	320	GLN
1	k	335	ASN
1	k	350	GLN
1	k	359	HIS
1	k	375	GLN
1	k	383	ASN
1	k	386	GLN
1	k	408	ASN
1	k	458	ASN
1	k	486	GLN
1	k	487	GLN
1	k	497	ASN
1	k	498	ASN
1	k	519	ASN
1	k	557	ASN
1	k	585	GLN
1	k	624	HIS
1	k	630	HIS
1	k	691	ASN
1	k	696	ASN
1	k	700	GLN
1	k	717	ASN
1	l	253	ASN
1	l	255	HIS
1	l	259	GLN
1	l	272	HIS
1	l	286	ASN
1	l	302	ASN
1	l	320	GLN

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Mol	Chain	Res	Type
1	l	335	ASN
1	l	350	GLN
1	l	375	GLN
1	l	383	ASN
1	l	386	GLN
1	l	408	ASN
1	l	458	ASN
1	l	486	GLN
1	l	487	GLN
1	l	497	ASN
1	l	498	ASN
1	l	519	ASN
1	l	557	ASN
1	l	585	GLN
1	l	630	HIS
1	l	691	ASN
1	l	696	ASN
1	l	700	GLN
1	l	717	ASN
1	m	253	ASN
1	m	259	GLN
1	m	272	HIS
1	m	286	ASN
1	m	302	ASN
1	m	320	GLN
1	m	335	ASN
1	m	350	GLN
1	m	359	HIS
1	m	375	GLN
1	m	383	ASN
1	m	386	GLN
1	m	408	ASN
1	m	458	ASN
1	m	486	GLN
1	m	487	GLN
1	m	497	ASN
1	m	519	ASN
1	m	557	ASN
1	m	624	HIS
1	m	630	HIS
1	m	691	ASN
1	m	696	ASN

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Mol	Chain	Res	Type
1	m	700	GLN
1	m	717	ASN
1	n	253	ASN
1	n	255	HIS
1	n	259	GLN
1	n	272	HIS
1	n	286	ASN
1	n	302	ASN
1	n	320	GLN
1	n	335	ASN
1	n	375	GLN
1	n	382	ASN
1	n	386	GLN
1	n	408	ASN
1	n	458	ASN
1	n	486	GLN
1	n	487	GLN
1	n	497	ASN
1	n	498	ASN
1	n	512	ASN
1	n	519	ASN
1	n	557	ASN
1	n	624	HIS
1	n	630	HIS
1	n	691	ASN
1	n	696	ASN
1	n	700	GLN
1	n	717	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	U	520/520 (100%)	1.05	67 (12%) 4 1	45, 60, 91, 139	0
1	V	520/520 (100%)	1.04	66 (12%) 4 1	45, 61, 92, 140	0
1	W	520/520 (100%)	1.04	61 (11%) 5 2	46, 61, 93, 139	0
1	X	520/520 (100%)	1.04	74 (14%) 3 1	44, 61, 93, 141	0
1	Y	520/520 (100%)	1.00	59 (11%) 6 2	45, 61, 92, 139	0
1	Z	520/520 (100%)	1.04	60 (11%) 5 2	44, 60, 91, 140	0
1	a	520/520 (100%)	0.99	53 (10%) 7 2	44, 59, 92, 139	0
1	b	520/520 (100%)	0.96	53 (10%) 7 2	42, 58, 90, 137	0
1	c	520/520 (100%)	0.98	60 (11%) 5 2	44, 59, 90, 141	0
1	d	520/520 (100%)	0.96	48 (9%) 9 2	45, 60, 91, 141	0
1	e	520/520 (100%)	1.00	60 (11%) 5 2	43, 58, 89, 141	0
1	f	520/520 (100%)	0.96	57 (10%) 6 2	45, 59, 92, 141	0
1	g	520/520 (100%)	1.00	60 (11%) 5 2	46, 60, 92, 134	0
1	h	520/520 (100%)	0.95	48 (9%) 9 2	45, 60, 91, 140	0
1	i	520/520 (100%)	0.89	35 (6%) 17 4	43, 59, 90, 138	0
1	j	520/520 (100%)	1.05	55 (10%) 7 2	43, 58, 90, 139	0
1	k	520/520 (100%)	1.01	52 (10%) 8 2	41, 58, 90, 135	0
1	l	520/520 (100%)	0.95	49 (9%) 9 2	42, 57, 90, 138	0
1	m	520/520 (100%)	0.92	42 (8%) 12 3	42, 57, 89, 138	0
1	n	520/520 (100%)	1.01	54 (10%) 7 2	42, 57, 90, 139	0
All	All	10400/10400 (100%)	0.99	1113 (10%) 6 2	41, 59, 91, 141	0

All (1113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	217	GLY	11.9
1	h	217	GLY	11.0
1	a	217	GLY	10.5
1	a	218	ALA	8.1
1	k	456	ALA	8.1
1	W	407	GLY	8.0
1	X	406	THR	7.9
1	j	469	ALA	7.9
1	Y	334	ALA	7.6
1	V	452	GLN	7.5
1	m	387	ALA	7.0
1	d	561	THR	7.0
1	j	454	GLY	6.9
1	j	275	GLY	6.7
1	V	612	VAL	6.7
1	U	338	THR	6.6
1	n	218	ALA	6.5
1	i	322	LYS	6.2
1	h	332	THR	6.2
1	V	560	ILE	6.0
1	c	452	GLN	6.0
1	a	483	CYS	6.0
1	Z	218	ALA	5.9
1	a	719	GLY	5.8
1	g	374	PRO	5.8
1	Z	523	ALA	5.8
1	Z	281	GLY	5.7
1	i	323	GLU	5.7
1	W	294	PRO	5.5
1	n	452	GLN	5.5
1	V	339	SER	5.5
1	k	457	GLN	5.5
1	j	339	SER	5.4
1	h	218	ALA	5.4
1	m	481	GLY	5.4
1	e	544	GLY	5.4
1	i	487	GLN	5.3
1	b	218	ALA	5.2
1	n	601	ALA	5.2
1	b	241	THR	5.2
1	c	656	ALA	5.2
1	m	456	ALA	5.2
1	j	453	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	c	612	VAL	5.1
1	k	561	THR	5.1
1	Z	381	LEU	5.1
1	n	389	GLY	5.0
1	a	452	GLN	5.0
1	h	219	ASP	5.0
1	h	457	GLN	5.0
1	i	652	THR	5.0
1	e	328	ASP	4.9
1	e	600	GLY	4.9
1	d	656	ALA	4.8
1	V	656	ALA	4.8
1	U	600	GLY	4.8
1	Y	624	HIS	4.7
1	i	563	GLU	4.7
1	n	487	GLN	4.7
1	h	248	ALA	4.7
1	Y	272	HIS	4.7
1	c	267	ALA	4.6
1	l	315	LYS	4.6
1	n	320	GLN	4.6
1	W	417	GLU	4.6
1	f	242	THR	4.6
1	n	554	ALA	4.5
1	c	521	GLY	4.5
1	f	219	ASP	4.5
1	l	666	LYS	4.5
1	h	258	LYS	4.5
1	Z	673	GLN	4.5
1	c	625	THR	4.4
1	e	618	ILE	4.4
1	Z	327	ASN	4.4
1	V	328	ASP	4.4
1	X	491	LYS	4.4
1	g	568	ALA	4.4
1	X	731	TYR	4.4
1	U	506	ALA	4.3
1	V	334	ALA	4.3
1	g	218	ALA	4.3
1	d	220	GLY	4.3
1	X	620	ALA	4.3
1	Y	506	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	l	474	GLN	4.3
1	g	594	GLY	4.3
1	m	500	ASN	4.3
1	V	541	MET	4.3
1	f	589	THR	4.3
1	W	672	THR	4.2
1	a	420	PRO	4.2
1	W	470	GLY	4.2
1	k	284	ASP	4.1
1	b	332	THR	4.1
1	X	665	THR	4.1
1	Z	402	GLN	4.1
1	k	634	LEU	4.1
1	j	365	PRO	4.1
1	Y	322	LYS	4.0
1	U	517	ILE	4.0
1	U	336	ASN	4.0
1	U	365	PRO	4.0
1	Y	434	LEU	4.0
1	g	574	THR	4.0
1	h	244	THR	3.9
1	V	564	GLU	3.9
1	W	539	GLY	3.9
1	b	715	VAL	3.9
1	m	636	GLY	3.9
1	l	559	MET	3.9
1	e	333	ILE	3.9
1	b	722	THR	3.9
1	g	362	CYS	3.9
1	d	571	PRO	3.9
1	U	446	LEU	3.8
1	Y	528	LYS	3.8
1	e	266	GLY	3.8
1	Z	554	ALA	3.8
1	V	526	SER	3.8
1	g	340	THR	3.8
1	i	265	THR	3.8
1	d	485	ARG	3.8
1	U	374	PRO	3.8
1	U	218	ALA	3.8
1	U	229	HIS	3.8
1	U	663	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	U	671	ILE	3.8
1	h	452	GLN	3.8
1	Y	362	CYS	3.8
1	U	419	VAL	3.7
1	U	456	ALA	3.7
1	h	555	LEU	3.7
1	V	487	GLN	3.7
1	d	484	TYR	3.7
1	c	328	ASP	3.7
1	f	542	ILE	3.7
1	j	334	ALA	3.7
1	W	362	CYS	3.7
1	c	217	GLY	3.7
1	V	346	ASP	3.7
1	e	576	ARG	3.7
1	n	243	SER	3.7
1	i	452	GLN	3.7
1	m	356	GLY	3.7
1	X	347	SER	3.7
1	b	476	LYS	3.7
1	d	533	LYS	3.7
1	X	454	GLY	3.7
1	Y	355	LEU	3.7
1	U	672	THR	3.7
1	U	534	PHE	3.6
1	k	450	GLN	3.6
1	d	637	GLY	3.6
1	W	501	PHE	3.6
1	X	600	GLY	3.6
1	c	377	GLY	3.6
1	V	525	ALA	3.6
1	d	331	THR	3.6
1	a	509	TYR	3.6
1	c	731	TYR	3.6
1	Z	266	GLY	3.6
1	j	732	LEU	3.6
1	W	673	GLN	3.6
1	d	608	GLN	3.6
1	U	442	TYR	3.5
1	c	364	PRO	3.5
1	W	220	GLY	3.5
1	c	561	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	l	334	ALA	3.5
1	U	474	GLN	3.5
1	a	244	THR	3.5
1	Y	363	LEU	3.5
1	c	333	ILE	3.5
1	U	470	GLY	3.5
1	g	221	VAL	3.5
1	d	361	GLY	3.5
1	g	325	THR	3.5
1	W	387	ALA	3.5
1	e	567	LYS	3.5
1	Y	525	ALA	3.5
1	a	328	ASP	3.5
1	g	367	PRO	3.4
1	U	257	TYR	3.4
1	V	395	CYS	3.4
1	b	323	GLU	3.4
1	d	449	THR	3.4
1	W	519	ASN	3.4
1	j	228	TRP	3.4
1	k	221	VAL	3.4
1	Z	349	TYR	3.4
1	V	312	LEU	3.4
1	W	561	THR	3.4
1	m	665	THR	3.4
1	g	229	HIS	3.4
1	X	402	GLN	3.4
1	d	389	GLY	3.4
1	j	533	LYS	3.4
1	W	406	THR	3.4
1	e	368	ALA	3.4
1	g	709	ALA	3.4
1	k	387	ALA	3.4
1	n	293	SER	3.4
1	U	356	GLY	3.4
1	c	666	LYS	3.4
1	k	329	GLY	3.4
1	d	457	GLN	3.4
1	d	395	CYS	3.4
1	Z	513	GLY	3.4
1	d	705	TYR	3.4
1	k	620	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	V	589	THR	3.4
1	h	554	ALA	3.4
1	i	559	MET	3.4
1	e	475	PRO	3.4
1	Z	282	TYR	3.4
1	V	714	THR	3.4
1	d	373	ILE	3.4
1	U	225	SER	3.4
1	g	462	LEU	3.4
1	f	252	TYR	3.3
1	f	491	LYS	3.3
1	a	219	ASP	3.3
1	U	221	VAL	3.3
1	c	486	GLN	3.3
1	m	457	GLN	3.3
1	Z	548	ALA	3.3
1	a	459	LYS	3.3
1	f	650	LYS	3.3
1	i	646	GLN	3.3
1	e	229	HIS	3.3
1	U	325	THR	3.3
1	X	623	PRO	3.3
1	Y	356	GLY	3.3
1	e	735	PRO	3.3
1	m	217	GLY	3.3
1	i	243	SER	3.3
1	k	452	GLN	3.3
1	c	717	ASN	3.3
1	b	599	MET	3.3
1	Y	474	GLN	3.3
1	V	664	ALA	3.3
1	c	481	GLY	3.3
1	f	218	ALA	3.3
1	j	694	ARG	3.3
1	Y	541	MET	3.3
1	X	526	SER	3.2
1	g	223	ASN	3.2
1	h	323	GLU	3.2
1	f	395	CYS	3.2
1	l	539	GLY	3.2
1	X	355	LEU	3.2
1	h	553	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	d	460	ASP	3.2
1	n	602	LEU	3.2
1	X	224	ALA	3.2
1	V	491	LYS	3.2
1	k	710	ASN	3.2
1	k	635	MET	3.2
1	c	313	ASN	3.2
1	V	301	ILE	3.2
1	X	257	TYR	3.2
1	U	420	PRO	3.2
1	W	600	GLY	3.2
1	c	706	ALA	3.2
1	j	582	VAL	3.2
1	Y	323	GLU	3.2
1	f	441	GLN	3.2
1	k	328	ASP	3.2
1	W	453	SER	3.2
1	X	359	HIS	3.2
1	j	462	LEU	3.2
1	m	229	HIS	3.2
1	e	653	PRO	3.2
1	d	315	LYS	3.2
1	g	220	GLY	3.2
1	X	657	ASN	3.2
1	W	587	SER	3.2
1	c	324	VAL	3.2
1	c	456	ALA	3.2
1	b	581	ALA	3.2
1	U	519	ASN	3.2
1	b	239	VAL	3.2
1	m	323	GLU	3.2
1	V	255	HIS	3.2
1	j	588	SER	3.1
1	e	664	ALA	3.1
1	U	217	GLY	3.1
1	h	279	PRO	3.1
1	b	678	GLN	3.1
1	e	592	ALA	3.1
1	l	459	LYS	3.1
1	X	281	GLY	3.1
1	n	658	PRO	3.1
1	j	581	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	c	254	ASN	3.1
1	a	260	ILE	3.1
1	a	556	ASP	3.1
1	e	456	ALA	3.1
1	d	453	SER	3.1
1	a	548	ALA	3.1
1	j	474	GLN	3.1
1	X	330	VAL	3.1
1	U	563	GLU	3.1
1	a	634	LEU	3.1
1	k	406	THR	3.1
1	V	367	PRO	3.1
1	j	696	ASN	3.1
1	j	266	GLY	3.1
1	X	528	LYS	3.1
1	V	340	THR	3.1
1	V	606	VAL	3.1
1	V	661	GLU	3.1
1	k	707	LYS	3.1
1	j	661	GLU	3.1
1	k	673	GLN	3.1
1	a	255	HIS	3.1
1	e	649	ILE	3.1
1	e	325	THR	3.1
1	a	584	LEU	3.1
1	X	328	ASP	3.1
1	k	425	TYR	3.1
1	Z	352	PRO	3.1
1	W	375	GLN	3.1
1	a	395	CYS	3.1
1	d	574	THR	3.1
1	e	257	TYR	3.0
1	e	604	GLY	3.0
1	Z	360	GLN	3.0
1	g	217	GLY	3.0
1	m	220	GLY	3.0
1	Y	373	ILE	3.0
1	m	226	GLY	3.0
1	Y	325	THR	3.0
1	d	563	GLU	3.0
1	d	554	ALA	3.0
1	i	524	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	m	333	ILE	3.0
1	e	692	SER	3.0
1	n	533	LYS	3.0
1	d	719	GLY	3.0
1	k	601	ALA	3.0
1	c	705	TYR	3.0
1	h	282	TYR	3.0
1	U	569	THR	3.0
1	h	456	ALA	3.0
1	X	351	LEU	3.0
1	f	457	GLN	3.0
1	a	570	ASN	3.0
1	Y	407	GLY	3.0
1	W	645	PRO	3.0
1	j	367	PRO	3.0
1	m	601	ALA	3.0
1	Z	305	TRP	3.0
1	a	330	VAL	3.0
1	d	330	VAL	3.0
1	Y	593	THR	3.0
1	e	234	TRP	3.0
1	j	565	GLU	3.0
1	e	354	VAL	3.0
1	l	560	ILE	3.0
1	m	266	GLY	3.0
1	U	603	PRO	3.0
1	b	217	GLY	3.0
1	j	260	ILE	3.0
1	c	707	LYS	3.0
1	f	593	THR	3.0
1	g	388	VAL	3.0
1	V	243	SER	3.0
1	n	332	THR	3.0
1	V	492	THR	3.0
1	W	505	GLY	3.0
1	W	589	THR	3.0
1	k	331	THR	3.0
1	l	217	GLY	3.0
1	Y	532	ASP	3.0
1	k	327	ASN	3.0
1	l	576	ARG	3.0
1	g	611	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	j	291	HIS	2.9
1	l	336	ASN	2.9
1	a	525	ALA	2.9
1	j	402	GLN	2.9
1	X	276	TYR	2.9
1	g	544	GLY	2.9
1	V	597	HIS	2.9
1	m	328	ASP	2.9
1	V	278	THR	2.9
1	V	647	ILE	2.9
1	e	335	ASN	2.9
1	l	360	GLN	2.9
1	e	219	ASP	2.9
1	V	643	PRO	2.9
1	l	316	LEU	2.9
1	b	521	GLY	2.9
1	a	333	ILE	2.9
1	Y	360	GLN	2.9
1	b	268	SER	2.9
1	X	482	PRO	2.9
1	f	602	LEU	2.9
1	U	581	ALA	2.9
1	X	387	ALA	2.9
1	U	321	VAL	2.9
1	e	220	GLY	2.9
1	W	599	MET	2.9
1	i	415	THR	2.9
1	j	550	ALA	2.9
1	n	666	LYS	2.9
1	W	647	ILE	2.9
1	c	571	PRO	2.9
1	X	405	ARG	2.9
1	n	221	VAL	2.9
1	c	264	SER	2.9
1	U	285	PHE	2.9
1	W	233	THR	2.9
1	g	432	ASP	2.9
1	U	494	THR	2.9
1	g	429	GLN	2.9
1	c	262	SER	2.9
1	c	270	ASP	2.9
1	f	256	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	g	610	ARG	2.8
1	k	530	ASP	2.8
1	e	571	PRO	2.8
1	h	658	PRO	2.8
1	X	219	ASP	2.8
1	X	237	ASP	2.8
1	a	316	LEU	2.8
1	e	566	ILE	2.8
1	g	539	GLY	2.8
1	a	734	ARG	2.8
1	V	336	ASN	2.8
1	Y	452	GLN	2.8
1	k	562	ASP	2.8
1	e	313	ASN	2.8
1	m	399	PHE	2.8
1	Y	371	PHE	2.8
1	Z	592	ALA	2.8
1	Y	595	ASP	2.8
1	W	221	VAL	2.8
1	V	565	GLU	2.8
1	Z	322	LYS	2.8
1	b	723	GLU	2.8
1	b	584	LEU	2.8
1	c	606	VAL	2.8
1	f	284	ASP	2.8
1	i	523	ALA	2.8
1	l	224	ALA	2.8
1	W	464	SER	2.8
1	U	655	PRO	2.8
1	j	250	PRO	2.8
1	k	281	GLY	2.8
1	e	241	THR	2.8
1	g	286	ASN	2.8
1	j	733	THR	2.8
1	Z	506	ALA	2.8
1	V	313	ASN	2.8
1	W	349	TYR	2.8
1	V	496	ASN	2.8
1	Y	427	HIS	2.8
1	g	341	VAL	2.8
1	W	610	ARG	2.8
1	Y	488	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	b	475	PRO	2.8
1	l	616	GLY	2.8
1	l	218	ALA	2.8
1	d	559	MET	2.8
1	c	310	LYS	2.8
1	j	539	GLY	2.8
1	f	444	TYR	2.8
1	b	504	THR	2.8
1	f	361	GLY	2.8
1	h	348	GLU	2.8
1	j	468	PRO	2.8
1	V	509	TYR	2.8
1	b	325	THR	2.8
1	l	391	SER	2.8
1	Y	357	SER	2.7
1	b	409	ASN	2.7
1	d	627	GLY	2.7
1	W	356	GLY	2.7
1	m	715	VAL	2.7
1	X	350	GLN	2.7
1	h	247	TRP	2.7
1	j	323	GLU	2.7
1	n	698	GLU	2.7
1	X	516	SER	2.7
1	Y	256	LEU	2.7
1	m	666	LYS	2.7
1	a	506	ALA	2.7
1	g	266	GLY	2.7
1	X	403	MET	2.7
1	b	538	SER	2.7
1	n	547	SER	2.7
1	X	649	ILE	2.7
1	h	450	GLN	2.7
1	X	494	THR	2.7
1	f	683	ILE	2.7
1	d	555	LEU	2.7
1	h	513	GLY	2.7
1	f	243	SER	2.7
1	c	584	LEU	2.7
1	e	457	GLN	2.7
1	f	616	GLY	2.7
1	Z	570	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	d	290	CYS	2.7
1	n	661	GLU	2.7
1	h	306	GLY	2.7
1	U	734	ARG	2.7
1	V	230	CYS	2.7
1	j	255	HIS	2.7
1	m	547	SER	2.7
1	b	559	MET	2.7
1	X	373	ILE	2.7
1	f	354	VAL	2.7
1	m	221	VAL	2.7
1	V	330	VAL	2.7
1	i	406	THR	2.7
1	d	493	LYS	2.7
1	e	580	VAL	2.7
1	b	219	ASP	2.7
1	l	328	ASP	2.7
1	b	660	ALA	2.7
1	j	479	LEU	2.7
1	W	275	GLY	2.6
1	Z	248	ALA	2.6
1	Z	441	GLN	2.6
1	Z	588	SER	2.6
1	l	266	GLY	2.6
1	W	637	GLY	2.6
1	i	464	SER	2.6
1	g	733	THR	2.6
1	h	613	TYR	2.6
1	n	484	TYR	2.6
1	l	219	ASP	2.6
1	l	565	GLU	2.6
1	g	493	LYS	2.6
1	n	573	ALA	2.6
1	V	615	GLN	2.6
1	Y	461	LEU	2.6
1	h	677	GLY	2.6
1	n	386	GLN	2.6
1	V	559	MET	2.6
1	W	347	SER	2.6
1	Z	257	TYR	2.6
1	m	594	GLY	2.6
1	k	500	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	700	GLN	2.6
1	h	570	ASN	2.6
1	l	384	GLY	2.6
1	n	595	ASP	2.6
1	j	519	ASN	2.6
1	X	319	ILE	2.6
1	i	326	THR	2.6
1	X	667	PHE	2.6
1	Z	356	GLY	2.6
1	d	523	ALA	2.6
1	a	666	LYS	2.6
1	c	565	GLU	2.6
1	d	404	LEU	2.6
1	X	554	ALA	2.6
1	V	528	LYS	2.6
1	g	689	LYS	2.6
1	k	405	ARG	2.6
1	k	434	LEU	2.6
1	Z	252	TYR	2.6
1	a	646	GLN	2.6
1	b	589	THR	2.6
1	m	553	THR	2.6
1	e	459	LYS	2.6
1	f	597	HIS	2.6
1	Y	631	PRO	2.6
1	c	620	ALA	2.6
1	i	541	MET	2.6
1	j	407	GLY	2.6
1	g	353	TYR	2.6
1	h	305	TRP	2.6
1	X	336	ASN	2.6
1	k	672	THR	2.6
1	f	456	ALA	2.6
1	Z	547	SER	2.6
1	W	345	SER	2.6
1	W	408	ASN	2.6
1	n	302	ASN	2.6
1	n	710	ASN	2.6
1	a	542	ILE	2.6
1	k	660	ALA	2.6
1	n	250	PRO	2.6
1	X	543	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	i	647	ILE	2.6
1	f	603	PRO	2.6
1	c	289	HIS	2.6
1	h	721	TYR	2.5
1	l	357	SER	2.5
1	b	539	GLY	2.5
1	V	529	ASP	2.5
1	a	285	PHE	2.5
1	d	565	GLU	2.5
1	g	453	SER	2.5
1	k	629	PHE	2.5
1	m	365	PRO	2.5
1	l	705	TYR	2.5
1	f	358	ALA	2.5
1	Z	403	MET	2.5
1	k	330	VAL	2.5
1	l	220	GLY	2.5
1	b	734	ARG	2.5
1	f	615	GLN	2.5
1	b	339	SER	2.5
1	Y	245	ARG	2.5
1	V	254	ASN	2.5
1	m	648	LEU	2.5
1	X	621	LYS	2.5
1	X	689	LYS	2.5
1	k	310	LYS	2.5
1	X	524	MET	2.5
1	i	706	ALA	2.5
1	X	523	ALA	2.5
1	a	555	LEU	2.5
1	m	322	LYS	2.5
1	f	324	VAL	2.5
1	n	536	PRO	2.5
1	Z	260	ILE	2.5
1	c	589	THR	2.5
1	j	265	THR	2.5
1	U	375	GLN	2.5
1	e	494	THR	2.5
1	f	618	ILE	2.5
1	Z	440	ASP	2.5
1	l	409	ASN	2.5
1	n	470	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	f	697	PRO	2.5
1	k	342	GLN	2.5
1	n	688	GLN	2.5
1	f	223	ASN	2.5
1	U	536	PRO	2.5
1	k	633	PRO	2.5
1	U	444	TYR	2.5
1	X	676	THR	2.5
1	e	436	ASN	2.5
1	n	555	LEU	2.5
1	Y	669	SER	2.5
1	Y	668	ALA	2.5
1	j	475	PRO	2.5
1	l	320	GLN	2.5
1	V	324	VAL	2.5
1	Z	251	THR	2.5
1	a	356	GLY	2.5
1	c	242	THR	2.5
1	n	329	GLY	2.5
1	U	514	ARG	2.5
1	j	456	ALA	2.5
1	X	560	ILE	2.5
1	f	579	THR	2.5
1	e	501	PHE	2.5
1	Z	642	HIS	2.5
1	X	579	THR	2.5
1	Y	229	HIS	2.5
1	m	653	PRO	2.5
1	Y	226	GLY	2.5
1	Z	419	VAL	2.5
1	j	656	ALA	2.5
1	m	419	VAL	2.5
1	U	379	LEU	2.5
1	Y	645	PRO	2.5
1	k	294	PRO	2.5
1	V	347	SER	2.5
1	b	439	ILE	2.5
1	f	553	THR	2.4
1	j	353	TYR	2.4
1	c	555	LEU	2.4
1	U	407	GLY	2.4
1	n	362	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	252	TYR	2.4
1	V	404	LEU	2.4
1	Z	704	ASN	2.4
1	e	610	ARG	2.4
1	f	300	LEU	2.4
1	h	482	PRO	2.4
1	Y	523	ALA	2.4
1	i	577	PHE	2.4
1	j	290	CYS	2.4
1	k	533	LYS	2.4
1	a	326	THR	2.4
1	U	343	VAL	2.4
1	c	469	ALA	2.4
1	U	486	GLN	2.4
1	U	666	LYS	2.4
1	f	568	ALA	2.4
1	g	224	ALA	2.4
1	Z	453	SER	2.4
1	m	336	ASN	2.4
1	b	308	ARG	2.4
1	U	425	TYR	2.4
1	k	526	SER	2.4
1	m	660	ALA	2.4
1	d	427	HIS	2.4
1	m	294	PRO	2.4
1	n	405	ARG	2.4
1	W	257	TYR	2.4
1	W	276	TYR	2.4
1	U	658	PRO	2.4
1	b	605	MET	2.4
1	X	399	PHE	2.4
1	k	458	ASN	2.4
1	W	734	ARG	2.4
1	b	326	THR	2.4
1	i	453	SER	2.4
1	f	364	PRO	2.4
1	U	319	ILE	2.4
1	b	510	ASN	2.4
1	c	718	ASN	2.4
1	j	340	THR	2.4
1	f	594	GLY	2.4
1	h	250	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	380	THR	2.4
1	Z	318	ASN	2.4
1	X	226	GLY	2.4
1	W	359	HIS	2.4
1	a	502	THR	2.4
1	X	571	PRO	2.4
1	a	640	LEU	2.4
1	a	684	GLU	2.4
1	e	221	VAL	2.4
1	e	355	LEU	2.4
1	j	589	THR	2.4
1	m	550	ALA	2.4
1	n	422	HIS	2.4
1	g	369	ASP	2.4
1	n	640	LEU	2.4
1	Z	233	THR	2.4
1	Z	484	TYR	2.4
1	Y	453	SER	2.4
1	b	360	GLN	2.4
1	n	356	GLY	2.4
1	U	250	PRO	2.4
1	W	386	GLN	2.4
1	Y	426	ALA	2.4
1	k	238	ARG	2.4
1	k	684	GLU	2.4
1	g	618	ILE	2.4
1	k	386	GLN	2.4
1	f	666	LYS	2.4
1	e	608	GLN	2.4
1	c	398	TYR	2.4
1	f	378	TYR	2.4
1	i	289	HIS	2.4
1	j	511	LEU	2.4
1	n	548	ALA	2.4
1	f	714	THR	2.3
1	X	602	LEU	2.3
1	X	546	GLU	2.3
1	Z	633	PRO	2.3
1	W	350	GLN	2.3
1	b	501	PHE	2.3
1	e	251	THR	2.3
1	b	355	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	W	705	TYR	2.3
1	e	311	ARG	2.3
1	g	359	HIS	2.3
1	W	486	GLN	2.3
1	Z	608	GLN	2.3
1	j	599	MET	2.3
1	Z	340	THR	2.3
1	b	700	GLN	2.3
1	X	337	LEU	2.3
1	Y	539	GLY	2.3
1	Z	538	SER	2.3
1	c	603	PRO	2.3
1	c	725	ARG	2.3
1	b	452	GLN	2.3
1	e	454	GLY	2.3
1	e	667	PHE	2.3
1	g	652	THR	2.3
1	b	316	LEU	2.3
1	h	468	PRO	2.3
1	i	439	ILE	2.3
1	Y	529	ASP	2.3
1	d	263	ALA	2.3
1	Y	679	VAL	2.3
1	c	337	LEU	2.3
1	d	256	LEU	2.3
1	e	321	VAL	2.3
1	l	646	GLN	2.3
1	a	476	LYS	2.3
1	i	686	GLU	2.3
1	k	233	THR	2.3
1	n	528	LYS	2.3
1	U	452	GLN	2.3
1	Z	581	ALA	2.3
1	c	530	ASP	2.3
1	h	571	PRO	2.3
1	X	245	ARG	2.3
1	a	327	ASN	2.3
1	U	479	LEU	2.3
1	a	586	SER	2.3
1	Z	580	VAL	2.3
1	n	717	ASN	2.3
1	c	397	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	n	220	GLY	2.3
1	f	635	MET	2.3
1	e	316	LEU	2.3
1	b	298	GLN	2.3
1	d	666	LYS	2.3
1	g	322	LYS	2.3
1	h	322	LYS	2.3
1	a	404	LEU	2.3
1	f	408	ASN	2.3
1	j	414	TYR	2.3
1	Z	325	THR	2.3
1	d	729	THR	2.3
1	W	559	MET	2.3
1	b	612	VAL	2.3
1	d	417	GLU	2.3
1	d	686	GLU	2.3
1	l	330	VAL	2.3
1	c	676	THR	2.3
1	g	230	CYS	2.3
1	V	621	LYS	2.3
1	f	657	ASN	2.3
1	h	515	GLU	2.3
1	W	281	GLY	2.3
1	n	375	GLN	2.3
1	W	689	LYS	2.3
1	g	491	LYS	2.3
1	W	571	PRO	2.3
1	U	612	VAL	2.3
1	W	402	GLN	2.3
1	X	636	GLY	2.3
1	Y	259	GLN	2.3
1	g	456	ALA	2.3
1	n	264	SER	2.3
1	m	600	GLY	2.3
1	X	601	ALA	2.3
1	g	368	ALA	2.3
1	b	672	THR	2.3
1	h	449	THR	2.3
1	l	468	PRO	2.3
1	U	726	PRO	2.3
1	c	711	VAL	2.2
1	n	474	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	662	PHE	2.2
1	W	227	ASN	2.2
1	W	627	GLY	2.2
1	c	495	ASP	2.2
1	a	631	PRO	2.2
1	X	647	ILE	2.2
1	U	335	ASN	2.2
1	V	457	GLN	2.2
1	a	334	ALA	2.2
1	c	318	ASN	2.2
1	i	462	LEU	2.2
1	k	531	LYS	2.2
1	Z	422	HIS	2.2
1	b	336	ASN	2.2
1	g	393	PHE	2.2
1	f	721	TYR	2.2
1	n	226	GLY	2.2
1	Y	235	LEU	2.2
1	V	284	ASP	2.2
1	W	443	LEU	2.2
1	e	289	HIS	2.2
1	k	319	ILE	2.2
1	V	584	LEU	2.2
1	W	493	LYS	2.2
1	W	328	ASP	2.2
1	l	598	VAL	2.2
1	n	399	PHE	2.2
1	Z	329	GLY	2.2
1	a	513	GLY	2.2
1	a	597	HIS	2.2
1	U	258	LYS	2.2
1	X	324	VAL	2.2
1	Y	509	TYR	2.2
1	l	547	SER	2.2
1	b	583	ASN	2.2
1	Y	291	HIS	2.2
1	X	407	GLY	2.2
1	Z	579	THR	2.2
1	Z	722	THR	2.2
1	Z	524	MET	2.2
1	a	703	SER	2.2
1	e	633	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	g	529	ASP	2.2
1	Z	692	SER	2.2
1	c	683	ILE	2.2
1	d	410	PHE	2.2
1	l	618	ILE	2.2
1	Z	456	ALA	2.2
1	U	220	GLY	2.2
1	a	377	GLY	2.2
1	i	408	ASN	2.2
1	k	302	ASN	2.2
1	Z	539	GLY	2.2
1	a	424	SER	2.2
1	j	458	ASN	2.2
1	a	342	GLN	2.2
1	i	358	ALA	2.2
1	h	434	LEU	2.2
1	c	325	THR	2.2
1	g	566	ILE	2.2
1	l	729	THR	2.2
1	X	320	GLN	2.2
1	f	481	GLY	2.2
1	U	339	SER	2.2
1	X	260	ILE	2.2
1	e	683	ILE	2.2
1	X	530	ASP	2.2
1	Y	685	TRP	2.2
1	k	644	PRO	2.2
1	f	588	SER	2.2
1	n	459	LYS	2.2
1	n	507	SER	2.2
1	U	615	GLN	2.2
1	b	685	TRP	2.2
1	j	637	GLY	2.2
1	g	360	GLN	2.2
1	e	693	LYS	2.2
1	l	434	LEU	2.2
1	X	716	ASP	2.2
1	f	220	GLY	2.2
1	a	456	ALA	2.2
1	k	571	PRO	2.2
1	X	230	CYS	2.2
1	d	582	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	m	570	ASN	2.2
1	V	486	GLN	2.2
1	f	487	GLN	2.2
1	k	248	ALA	2.2
1	i	597	HIS	2.2
1	U	245	ARG	2.2
1	V	335	ASN	2.1
1	W	438	LEU	2.1
1	Y	395	CYS	2.1
1	j	452	GLN	2.1
1	l	389	GLY	2.1
1	m	700	GLN	2.1
1	Z	445	TYR	2.1
1	n	333	ILE	2.1
1	n	603	PRO	2.1
1	e	407	GLY	2.1
1	V	415	THR	2.1
1	W	452	GLN	2.1
1	j	665	THR	2.1
1	l	373	ILE	2.1
1	b	706	ALA	2.1
1	e	584	LEU	2.1
1	n	729	THR	2.1
1	h	734	ARG	2.1
1	V	594	GLY	2.1
1	c	480	PRO	2.1
1	m	290	CYS	2.1
1	g	412	PHE	2.1
1	h	638	PHE	2.1
1	W	506	ALA	2.1
1	X	256	LEU	2.1
1	e	590	ASP	2.1
1	f	240	ILE	2.1
1	h	307	PHE	2.1
1	i	504	THR	2.1
1	k	589	THR	2.1
1	l	249	LEU	2.1
1	m	718	ASN	2.1
1	V	685	TRP	2.1
1	Y	592	ALA	2.1
1	Y	635	MET	2.1
1	l	525	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	W	269	ASN	2.1
1	b	458	ASN	2.1
1	h	602	LEU	2.1
1	h	662	PHE	2.1
1	h	733	THR	2.1
1	l	497	ASN	2.1
1	W	476	LYS	2.1
1	n	338	THR	2.1
1	i	483	CYS	2.1
1	l	680	SER	2.1
1	X	697	PRO	2.1
1	f	571	PRO	2.1
1	e	249	LEU	2.1
1	V	512	ASN	2.1
1	l	657	ASN	2.1
1	Y	411	THR	2.1
1	c	545	LYS	2.1
1	f	526	SER	2.1
1	j	689	LYS	2.1
1	n	328	ASP	2.1
1	V	260	ILE	2.1
1	h	301	ILE	2.1
1	a	485	ARG	2.1
1	W	578	GLY	2.1
1	f	591	PRO	2.1
1	g	297	TRP	2.1
1	g	567	LYS	2.1
1	h	401	SER	2.1
1	k	234	TRP	2.1
1	U	485	ARG	2.1
1	X	217	GLY	2.1
1	Y	660	ALA	2.1
1	f	468	PRO	2.1
1	g	239	VAL	2.1
1	h	414	TYR	2.1
1	X	342	GLN	2.1
1	Y	646	GLN	2.1
1	j	538	SER	2.1
1	d	316	LEU	2.1
1	e	248	ALA	2.1
1	i	272	HIS	2.1
1	b	344	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	c	371	PHE	2.1
1	l	456	ALA	2.1
1	Z	593	THR	2.1
1	f	316	LEU	2.1
1	Z	516	SER	2.1
1	c	533	LYS	2.1
1	b	563	GLU	2.1
1	n	301	ILE	2.1
1	U	256	LEU	2.1
1	l	450	GLN	2.1
1	b	370	VAL	2.1
1	d	328	ASP	2.1
1	g	470	GLY	2.1
1	a	335	ASN	2.1
1	c	541	MET	2.1
1	g	726	PRO	2.1
1	V	235	LEU	2.1
1	l	715	VAL	2.1
1	a	674	TYR	2.1
1	V	631	PRO	2.1
1	e	319	ILE	2.1
1	j	309	PRO	2.1
1	m	222	GLY	2.1
1	W	344	PHE	2.1
1	X	603	PRO	2.1
1	Z	355	LEU	2.1
1	d	272	HIS	2.1
1	h	448	ARG	2.1
1	i	278	THR	2.1
1	c	615	GLN	2.1
1	d	529	ASP	2.1
1	e	322	LYS	2.1
1	e	403	MET	2.1
1	g	402	GLN	2.1
1	g	649	ILE	2.1
1	h	230	CYS	2.1
1	l	396	LEU	2.1
1	m	225	SER	2.1
1	U	457	GLN	2.0
1	V	450	GLN	2.0
1	X	605	MET	2.0
1	X	240	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	j	660	ALA	2.0
1	X	659	PRO	2.0
1	V	362	CYS	2.0
1	V	602	LEU	2.0
1	j	449	THR	2.0
1	m	332	THR	2.0
1	n	400	PRO	2.0
1	U	664	ALA	2.0
1	a	524	MET	2.0
1	b	315	LYS	2.0
1	f	592	ALA	2.0
1	n	269	ASN	2.0
1	g	578	GLY	2.0
1	V	467	SER	2.0
1	k	665	THR	2.0
1	X	323	GLU	2.0
1	X	698	GLU	2.0
1	a	662	PHE	2.0
1	f	493	LYS	2.0
1	i	564	GLU	2.0
1	X	548	ALA	2.0
1	l	668	ALA	2.0
1	g	411	THR	2.0
1	l	500	ASN	2.0
1	Y	444	TYR	2.0
1	f	731	TYR	2.0
1	h	330	VAL	2.0
1	d	506	ALA	2.0
1	i	476	LYS	2.0
1	U	589	THR	2.0
1	V	217	GLY	2.0
1	U	333	ILE	2.0
1	f	698	GLU	2.0
1	g	426	ALA	2.0
1	l	496	ASN	2.0
1	V	711	VAL	2.0
1	e	625	THR	2.0
1	g	418	ASP	2.0
1	Y	677	GLY	2.0
1	Z	610	ARG	2.0
1	e	537	MET	2.0
1	g	735	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	c	594	GLY	2.0
1	i	222	GLY	2.0
1	W	546	GLU	2.0
1	b	567	LYS	2.0
1	W	547	SER	2.0
1	h	722	THR	2.0
1	j	478	TRP	2.0
1	Y	479	LEU	2.0
1	c	602	LEU	2.0
1	Y	684	GLU	2.0
1	c	263	ALA	2.0
1	m	684	GLU	2.0
1	Y	608	GLN	2.0
1	b	607	TRP	2.0
1	Z	245	ARG	2.0
1	d	610	ARG	2.0
1	k	451	ASN	2.0
1	g	506	ALA	2.0
1	g	525	ALA	2.0
1	U	676	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.