



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:32 PM UTC

PDB ID : 2BFU / pdb\_00002bfu  
Title : X-ray structure of CPMV top component  
Authors : Ochoa, W.F.; Chatterji, A.; Lin, T.; Johnson, J.E.  
Deposited on : 2004-12-13  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

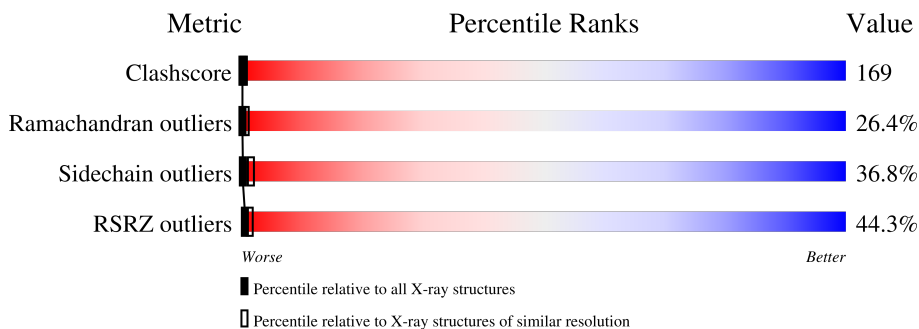
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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

Mol	Chain	Length	Quality of chain
1	L	369	
2	S	189	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5282 atoms, of which 939 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COWPEA MOSAIC VIRUS, LARGE (L) SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	L	369	3500	1822	634	480	542	22	0	0	0

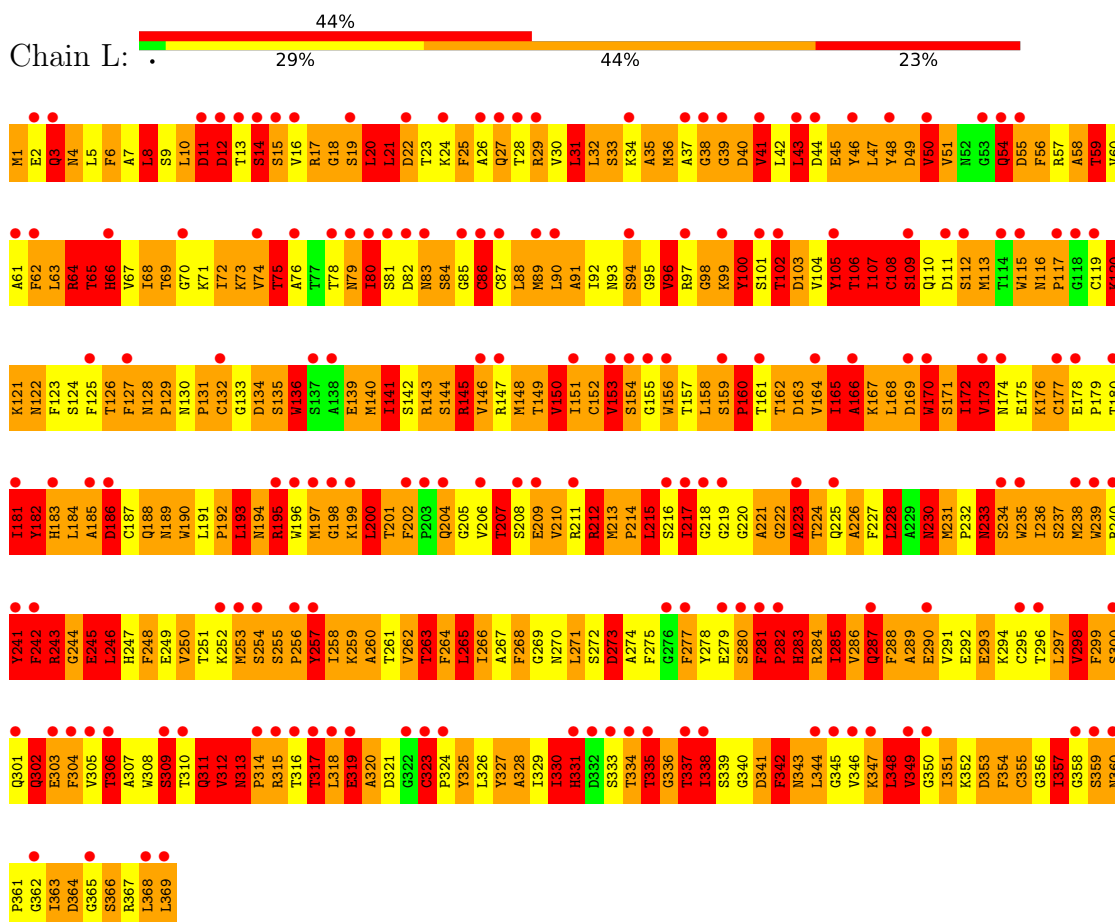
- Molecule 2 is a protein called COWPEA MOSAIC VIRUS, SMALL (S) SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	S	189	1782	944	305	247	277	9	0	0	0

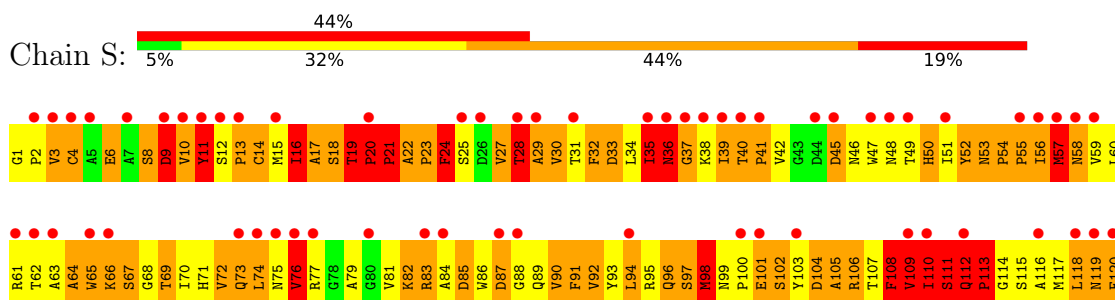
### 3 Residue-property plots

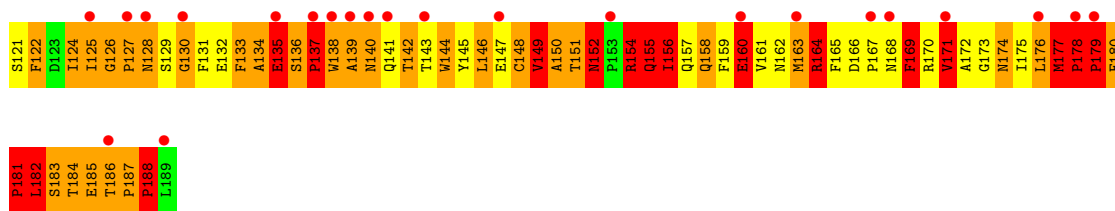
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: COWPEA MOSAIC VIRUS, LARGE (L) SUBUNIT



#### • Molecule 2: COWPEA MOSAIC VIRUS, SMALL (S) SUBUNIT





## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	311.41Å 311.41Å 311.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-4.00) 92.5 (30.00-4.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.45 (at 4.01Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.230 , (Not available) 0.497 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.027 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.38	EDS
Total number of atoms	5282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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	L	1.64	49/2933 (1.7%)	2.07	130/3983 (3.3%)
2	S	1.60	18/1524 (1.2%)	2.23	79/2089 (3.8%)
All	All	1.63	67/4457 (1.5%)	2.13	209/6072 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	6
2	S	0	1
All	All	0	7

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	20	PRO	CA-C	14.30	1.65	1.52
1	L	286	VAL	CA-CB	9.65	1.67	1.54
1	L	89	MET	SD-CE	-9.36	1.56	1.79
1	L	200	LEU	CA-C	9.09	1.63	1.53
2	S	57	MET	SD-CE	8.58	2.01	1.79
1	L	306	THR	CA-C	8.46	1.62	1.52
1	L	173	VAL	CA-C	8.46	1.62	1.52
1	L	338	ILE	CA-CB	8.18	1.65	1.54
2	S	178	PRO	CA-C	8.15	1.59	1.52
2	S	163	MET	SD-CE	8.00	1.99	1.79
2	S	98	MET	SD-CE	7.59	1.98	1.79
2	S	24	PHE	CA-C	7.46	1.62	1.52
1	L	1	MET	SD-CE	7.40	1.98	1.79
1	L	80	ILE	CA-CB	7.18	1.64	1.54
1	L	106	THR	CA-CB	7.09	1.65	1.53
1	L	312	VAL	CA-CB	7.01	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	22	ALA	CA-C	7.00	1.61	1.52
1	L	37	ALA	CA-CB	6.75	1.60	1.52
1	L	217	ILE	CA-CB	6.71	1.63	1.54
1	L	161	THR	CA-CB	6.67	1.64	1.53
2	S	72	VAL	CA-CB	6.67	1.60	1.54
1	L	115	TRP	CA-C	6.63	1.60	1.52
1	L	234	SER	CA-C	6.54	1.61	1.53
1	L	91	ALA	CA-CB	-6.53	1.43	1.53
1	L	178	GLU	CA-C	6.38	1.60	1.52
2	S	109	VAL	CA-CB	6.38	1.63	1.54
1	L	285	ILE	CA-CB	6.24	1.62	1.54
1	L	238	MET	SD-CE	-6.20	1.64	1.79
1	L	102	THR	CA-CB	6.15	1.59	1.53
2	S	30	VAL	CA-CB	6.10	1.61	1.54
2	S	128	ASN	CA-C	-6.10	1.45	1.52
1	L	148	MET	SD-CE	6.05	1.94	1.79
1	L	75	THR	CA-CB	6.04	1.63	1.52
1	L	122	ASN	N-CA	6.04	1.53	1.46
1	L	181	ILE	CA-CB	5.90	1.62	1.54
1	L	337	THR	CA-CB	5.82	1.62	1.53
2	S	24	PHE	N-CA	5.81	1.53	1.46
1	L	313	ASN	CA-C	5.73	1.57	1.52
1	L	51	VAL	CA-CB	5.71	1.62	1.54
1	L	122	ASN	CA-C	5.71	1.59	1.52
2	S	186	THR	CA-CB	5.61	1.62	1.53
1	L	300	SER	N-CA	5.59	1.53	1.46
2	S	151	THR	CA-CB	5.57	1.61	1.53
1	L	164	VAL	CA-CB	5.55	1.62	1.54
1	L	166	ALA	N-CA	5.52	1.53	1.46
1	L	217	ILE	CA-C	5.48	1.59	1.52
1	L	231	MET	CA-C	5.47	1.59	1.52
1	L	80	ILE	CA-C	5.34	1.59	1.52
2	S	22	ALA	CA-CB	5.34	1.61	1.53
1	L	16	VAL	CA-CB	5.29	1.60	1.54
2	S	152	ASN	CA-C	5.29	1.59	1.52
1	L	19	SER	CA-C	-5.26	1.46	1.52
1	L	323	CYS	CA-C	5.20	1.59	1.52
1	L	200	LEU	CA-CB	5.19	1.57	1.53
1	L	29	ARG	CG-CD	5.19	1.68	1.52
1	L	349	VAL	CA-C	5.18	1.59	1.52
1	L	100	TYR	CA-C	5.17	1.59	1.52
1	L	115	TRP	N-CA	5.15	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	37	ALA	CA-C	5.14	1.59	1.53
2	S	28	THR	CA-CB	5.12	1.62	1.53
1	L	228	LEU	CA-C	5.10	1.59	1.52
1	L	360	ASN	CA-C	-5.10	1.47	1.52
1	L	250	VAL	CA-C	-5.09	1.47	1.52
1	L	221	ALA	N-CA	5.09	1.51	1.46
1	L	230	ASN	CA-C	5.07	1.59	1.52
2	S	185	GLU	CA-C	5.03	1.58	1.52
1	L	266	ILE	CA-C	5.02	1.59	1.52

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	19	THR	CA-C-N	27.75	148.97	120.38
2	S	19	THR	C-N-CA	27.75	148.97	120.38
2	S	20	PRO	N-CA-C	21.75	137.23	110.70
1	L	302	GLN	N-CA-C	-18.49	91.13	111.28
1	L	16	VAL	N-CA-C	15.68	131.74	108.54
1	L	281	PHE	CA-C-N	13.75	137.03	119.84
1	L	281	PHE	C-N-CA	13.75	137.03	119.84
1	L	323	CYS	CA-C-N	12.90	135.96	119.84
1	L	323	CYS	C-N-CA	12.90	135.96	119.84
1	L	307	ALA	N-CA-C	12.36	127.66	110.24
1	L	309	SER	N-CA-C	12.15	129.12	108.23
2	S	58	ASN	N-CA-C	-12.00	97.91	111.71
1	L	233	ASN	N-CA-C	11.95	128.61	113.55
2	S	177	MET	N-CA-C	11.48	135.18	109.81
2	S	177	MET	CA-C-N	10.90	131.61	120.38
2	S	177	MET	C-N-CA	10.90	131.61	120.38
1	L	22	ASP	N-CA-C	-10.89	100.23	113.19
1	L	15	SER	N-CA-C	-10.85	91.85	108.67
1	L	256	PRO	N-CA-C	-10.78	100.88	114.68
1	L	335	THR	N-CA-C	10.64	121.86	108.45
1	L	328	ALA	N-CA-C	10.22	124.02	110.53
1	L	317	THR	N-CA-C	10.09	125.24	109.81
1	L	255	SER	CA-C-N	9.79	132.11	120.94
1	L	255	SER	C-N-CA	9.79	132.11	120.94
1	L	234	SER	N-CA-C	9.79	126.14	112.04
2	S	18	SER	N-CA-C	9.75	124.30	108.99
1	L	122	ASN	N-CA-C	9.59	123.18	108.42
2	S	8	SER	N-CA-C	9.40	130.82	110.80
1	L	153	VAL	N-CA-C	-9.35	89.89	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	235	TRP	N-CA-C	-9.07	101.47	112.54
2	S	36	ASN	N-CA-C	8.96	122.31	108.96
1	L	49	ASP	N-CA-C	-8.92	101.52	111.07
1	L	83	ASN	N-CA-C	8.90	121.88	111.02
1	L	19	SER	N-CA-C	-8.82	98.36	110.35
1	L	115	TRP	N-CA-C	8.81	123.18	109.52
2	S	158	GLN	N-CA-C	8.80	123.78	110.14
2	S	4	CYS	N-CA-C	-8.76	97.05	110.10
1	L	246	LEU	N-CA-C	-8.52	97.86	110.46
1	L	100	TYR	N-CA-C	8.50	128.90	110.80
1	L	354	PHE	N-CA-C	8.50	122.48	108.96
1	L	112	SER	N-CA-C	8.46	121.56	108.96
1	L	221	ALA	N-CA-C	8.43	120.91	108.60
1	L	136	TRP	N-CA-C	8.35	122.07	108.55
1	L	159	SER	CA-C-N	8.28	130.19	119.84
1	L	159	SER	C-N-CA	8.28	130.19	119.84
2	S	112	GLN	CA-C-N	8.24	130.14	119.84
2	S	112	GLN	C-N-CA	8.24	130.14	119.84
1	L	209	GLU	N-CA-C	8.23	120.54	110.41
2	S	154	ARG	N-CA-C	-8.16	100.37	110.65
1	L	126	THR	N-CA-C	8.15	122.35	109.39
1	L	202	PHE	N-CA-C	8.13	120.54	109.24
1	L	105	TYR	N-CA-C	-8.00	103.10	113.17
2	S	96	GLN	N-CA-C	7.97	122.31	112.59
2	S	163	MET	N-CA-C	7.88	122.07	108.76
1	L	33	SER	N-CA-C	7.87	121.38	109.41
1	L	143	ARG	N-CA-C	-7.81	104.69	112.97
2	S	152	ASN	CA-C-N	7.71	127.43	119.64
2	S	152	ASN	C-N-CA	7.71	127.43	119.64
1	L	149	THR	N-CA-C	7.67	118.66	108.07
2	S	22	ALA	C-N-CD	-7.61	103.85	120.60
1	L	58	ALA	N-CA-C	-7.55	97.70	109.25
1	L	255	SER	N-CA-C	7.54	129.26	107.84
2	S	65	TRP	N-CA-C	-7.54	98.66	109.96
2	S	142	THR	N-CA-C	-7.51	97.30	107.88
1	L	145	ARG	N-CA-C	7.46	126.70	110.80
1	L	300	SER	N-CA-C	7.44	126.65	110.80
2	S	183	SER	N-CA-C	-7.38	95.07	110.80
2	S	185	GLU	N-CA-C	7.31	120.00	107.93
2	S	79	ALA	N-CA-C	7.30	117.61	108.19
1	L	223	ALA	N-CA-C	-7.29	95.27	110.80
1	L	283	HIS	N-CA-C	7.28	126.30	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	285	ILE	N-CA-C	7.26	124.45	109.34
2	S	104	ASP	N-CA-C	7.26	120.92	110.10
1	L	228	LEU	N-CA-C	7.23	126.20	110.80
2	S	101	GLU	N-CA-C	-7.23	95.41	110.80
2	S	156	ILE	N-CA-C	7.22	119.37	107.24
1	L	12	ASP	N-CA-C	7.16	126.05	110.80
2	S	39	ILE	N-CA-C	7.13	119.19	111.77
2	S	182	LEU	N-CA-C	7.10	120.68	109.81
2	S	57	MET	N-CA-C	7.05	122.20	112.04
1	L	103	ASP	N-CA-C	7.00	118.73	108.86
1	L	290	GLU	N-CA-C	-6.99	103.66	111.28
2	S	76	VAL	N-CA-C	6.98	119.88	108.99
2	S	184	THR	N-CA-C	6.91	121.75	111.04
1	L	40	ASP	N-CA-C	6.89	122.38	107.49
1	L	36	MET	N-CA-C	6.86	120.71	109.06
1	L	169	ASP	N-CA-C	6.84	119.67	108.52
1	L	342	PHE	N-CA-C	6.78	118.60	110.19
2	S	1	GLY	CA-C-N	6.77	128.30	119.84
2	S	1	GLY	C-N-CA	6.77	128.30	119.84
1	L	61	ALA	N-CA-C	6.69	119.40	111.71
2	S	164	ARG	N-CA-C	6.69	120.19	107.75
1	L	258	ILE	N-CA-C	-6.68	99.53	108.35
1	L	73	LYS	N-CA-C	6.63	119.84	110.50
2	S	171	VAL	N-CA-C	6.62	123.10	109.34
1	L	109	SER	N-CA-C	6.61	124.87	110.80
1	L	212	ARG	N-CA-C	6.60	124.86	110.80
1	L	148	MET	N-CA-C	6.60	119.84	110.14
1	L	337	THR	N-CA-C	-6.52	104.91	112.86
2	S	137	PRO	N-CA-C	6.50	125.86	112.47
1	L	244	GLY	N-CA-C	6.50	120.59	110.91
1	L	226	ALA	N-CA-C	-6.45	98.72	108.52
2	S	25	SER	N-CA-C	6.44	124.52	110.80
1	L	368	LEU	N-CA-C	-6.39	97.19	110.80
2	S	39	ILE	CB-CA-C	-6.39	103.97	112.46
2	S	56	ILE	N-CA-C	-6.38	104.71	113.00
1	L	306	THR	N-CA-C	6.35	118.74	108.32
2	S	128	ASN	N-CA-C	-6.35	101.28	110.24
1	L	56	PHE	N-CA-C	6.35	116.65	108.34
1	L	4	ASN	N-CA-C	-6.33	104.58	113.20
1	L	188	GLN	N-CA-C	6.33	118.93	108.99
1	L	116	ASN	CA-C-N	6.30	127.72	119.84
1	L	116	ASN	C-N-CA	6.30	127.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	42	VAL	N-CA-C	6.28	118.98	108.81
1	L	32	LEU	N-CA-C	6.27	118.53	107.61
1	L	43	LEU	N-CA-C	6.27	124.15	110.80
2	S	85	ASP	N-CA-C	-6.26	102.80	111.81
1	L	18	GLY	N-CA-C	-6.20	104.14	112.14
2	S	22	ALA	CA-C-N	6.20	141.87	127.00
2	S	22	ALA	C-N-CA	6.20	141.87	127.00
2	S	108	PHE	N-CA-C	6.13	117.72	108.46
1	L	21	LEU	N-CA-C	-6.13	106.34	113.88
2	S	133	PHE	N-CA-C	6.12	123.83	110.80
2	S	66	LYS	N-CA-C	6.05	120.34	107.70
1	L	205	GLY	N-CA-C	-6.04	101.58	111.78
1	L	166	ALA	N-CA-C	6.02	123.62	110.80
2	S	54	PRO	N-CA-C	5.99	118.01	110.70
1	L	167	LYS	N-CA-C	5.99	118.66	108.90
1	L	165	ILE	N-CA-C	5.97	121.76	109.34
1	L	200	LEU	N-CA-C	5.93	120.44	109.24
1	L	28	THR	N-CA-C	5.92	118.05	107.80
2	S	37	GLY	N-CA-C	5.87	122.10	110.77
2	S	21	PRO	N-CA-C	5.87	124.56	112.47
1	L	347	LYS	N-CA-C	5.85	117.74	108.79
1	L	31	LEU	N-CA-C	5.85	117.84	110.24
2	S	186	THR	N-CA-C	-5.85	99.38	109.15
2	S	109	VAL	N-CA-C	5.84	121.49	109.34
1	L	245	GLU	CB-CG-CD	5.81	122.48	112.60
1	L	268	PHE	N-CA-C	5.79	117.03	107.20
1	L	94	SER	N-CA-C	5.77	118.90	108.69
1	L	280	SER	N-CA-C	5.76	120.55	112.72
1	L	215	LEU	N-CA-C	-5.75	98.55	110.80
1	L	242	PHE	CB-CA-C	5.74	119.87	109.37
2	S	139	ALA	CA-C-N	5.72	132.47	121.54
2	S	139	ALA	C-N-CA	5.72	132.47	121.54
2	S	149	VAL	N-CA-C	5.70	121.20	109.34
1	L	186	ASP	N-CA-C	5.68	122.90	110.80
1	L	282	PRO	CA-C-N	5.68	132.38	121.54
1	L	282	PRO	C-N-CA	5.68	132.38	121.54
2	S	160	GLU	N-CA-C	5.66	117.63	108.41
1	L	168	LEU	CA-CB-CG	-5.64	96.55	116.30
1	L	282	PRO	N-CA-C	5.63	124.07	112.47
2	S	10	VAL	N-CA-C	5.63	117.69	108.97
1	L	86	CYS	N-CA-C	5.63	116.81	108.60
2	S	187	PRO	N-CA-C	5.62	117.56	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14	SER	N-CA-C	5.61	122.75	110.80
2	S	136	SER	CA-C-N	5.61	126.85	119.84
2	S	136	SER	C-N-CA	5.61	126.85	119.84
2	S	178	PRO	N-CA-C	5.61	117.54	110.70
1	L	172	ILE	CA-C-N	5.60	129.46	121.96
1	L	172	ILE	C-N-CA	5.60	129.46	121.96
1	L	35	ALA	N-CA-C	-5.58	98.91	110.80
2	S	181	PRO	CA-C-N	-5.58	113.05	123.03
2	S	181	PRO	C-N-CA	-5.58	113.05	123.03
2	S	17	ALA	N-CA-C	5.57	116.72	108.86
1	L	265	LEU	N-CA-C	5.55	122.63	110.80
1	L	161	THR	N-CA-C	5.55	122.63	110.80
2	S	106	ARG	N-CA-C	5.54	118.29	109.81
1	L	113	MET	N-CA-CB	-5.54	102.65	111.62
1	L	160	PRO	N-CA-C	5.53	123.86	112.47
2	S	113	PRO	N-CA-C	5.51	123.83	112.47
1	L	84	SER	N-CA-C	5.51	117.77	109.23
1	L	127	PHE	N-CA-C	5.51	122.54	110.80
2	S	19	THR	C-N-CD	-5.50	102.47	125.00
1	L	128	ASN	CA-C-N	5.49	126.71	119.84
1	L	128	ASN	C-N-CA	5.49	126.71	119.84
2	S	9	ASP	N-CA-C	5.47	122.45	110.80
1	L	273	ASP	N-CA-C	5.46	122.44	110.80
1	L	170	TRP	N-CA-C	5.45	116.25	108.74
1	L	355	CYS	CB-CA-C	-5.44	102.05	111.30
2	S	24	PHE	N-CA-C	5.43	122.37	110.80
2	S	126	GLY	CA-C-N	-5.42	113.06	119.84
2	S	126	GLY	C-N-CA	-5.42	113.06	119.84
2	S	181	PRO	N-CA-C	-5.38	101.39	112.47
1	L	9	SER	N-CA-C	-5.36	102.19	109.54
2	S	169	PHE	N-CA-C	5.35	117.87	108.56
1	L	207	THR	N-CA-C	-5.31	102.67	110.42
1	L	222	GLY	CA-C-N	5.29	131.65	121.54
1	L	222	GLY	C-N-CA	5.29	131.65	121.54
1	L	41	VAL	N-CA-CB	5.28	116.56	110.49
1	L	348	LEU	CB-CA-C	-5.27	104.55	112.09
2	S	176	LEU	N-CA-C	5.27	117.29	108.23
1	L	183	HIS	N-CA-C	5.24	121.96	110.80
1	L	54	GLN	N-CA-C	5.23	118.20	107.37
1	L	39	GLY	N-CA-C	-5.20	100.85	113.18
2	S	11	TYR	N-CA-C	5.20	117.89	108.69
2	S	103	TYR	N-CA-C	-5.19	99.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	243	ARG	N-CA-C	5.19	118.61	107.67
1	L	248	PHE	N-CA-C	5.18	118.10	110.59
1	L	289	ALA	N-CA-C	5.17	116.93	109.07
1	L	264	PHE	CB-CA-C	-5.15	103.13	110.34
2	S	144	TRP	N-CA-C	5.12	118.30	110.20
1	L	168	LEU	N-CA-C	5.10	116.97	107.99
1	L	59	THR	N-CA-C	5.10	118.94	111.34
1	L	217	ILE	N-CA-C	5.09	119.93	109.34
1	L	343	ASN	N-CA-C	5.09	115.25	108.38
1	L	319	GLU	CA-C-N	5.03	131.14	121.54
1	L	319	GLU	C-N-CA	5.03	131.14	121.54
1	L	98	GLY	N-CA-C	-5.02	100.41	110.69

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	105	TYR	Sidechain
1	L	182	TYR	Sidechain
1	L	241	TYR	Sidechain
1	L	257	TYR	Sidechain
1	L	299	PHE	Sidechain
1	L	48	TYR	Sidechain
2	S	52	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2866	634	2813	995	29
2	S	1477	305	1413	506	0
All	All	4343	939	4226	1450	29

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 169.

All (1450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:308:TRP:HB3	1:L:323:CYS:SG	1.61	1.39
2:S:89:GLN:HA	2:S:111:SER:HA	1.19	1.16
2:S:54:PRO:HB2	2:S:57:MET:HB3	1.27	1.15
2:S:36:ASN:HB2	2:S:61:ARG:HA	1.16	1.13
1:L:73:LYS:HB2	1:L:126:THR:HG22	1.30	1.13
1:L:120:LYS:HG2	1:L:121:LYS:HG2	1.14	1.12
1:L:96:VAL:HA	2:S:176:LEU:HB2	1.27	1.11
1:L:256:PRO:HB3	1:L:290:GLU:HA	1.18	1.11
1:L:261:THR:HA	1:L:286:VAL:HB	1.26	1.11
2:S:112:GLN:HB2	2:S:113:PRO:HD2	1.27	1.10
1:L:60:VAL:HB	1:L:64:ARG:HD2	1.12	1.09
2:S:14:CYS:HA	2:S:57:MET:SD	1.93	1.08
1:L:241:TYR:HA	1:L:309:SER:HA	1.25	1.08
1:L:250:VAL:HG13	1:L:295:CYS:HB2	1.14	1.08
2:S:94:LEU:HB3	2:S:146:LEU:HG	1.29	1.07
1:L:267:ALA:HB3	1:L:327:TYR:HE1	1.15	1.07
1:L:193:LEU:HB2	1:L:232:PRO:HA	1.27	1.07
1:L:215:LEU:HB2	1:L:325:TYR:HB2	1.33	1.06
1:L:255:SER:HB3	1:L:258:ILE:HB	1.37	1.06
1:L:351:ILE:HD13	1:L:354:PHE:HB3	1.33	1.06
1:L:239:TRP:HA	1:L:358:GLY:O	1.55	1.06
2:S:13:PRO:HB3	2:S:162:ASN:ND2	1.70	1.05
1:L:258:ILE:HG12	1:L:336:GLY:HA2	1.39	1.04
2:S:27:VAL:HG13	2:S:151:THR:HA	1.38	1.04
1:L:273:ASP:HA	1:L:278:TYR:HE2	1.21	1.02
1:L:267:ALA:HB3	1:L:327:TYR:CE1	1.93	1.02
1:L:248:PHE:HA	1:L:347:LYS:O	1.59	1.01
1:L:93:ASN:HA	1:L:110:GLN:HB2	1.43	1.00
1:L:143:ARG:HB3	2:S:137:PRO:HB2	1.43	1.00
2:S:91:PHE:H	2:S:149:VAL:HG21	1.24	1.00
2:S:95:ARG:HE	2:S:98:MET:HG2	1.26	1.00
1:L:120:LYS:HE2	1:L:121:LYS:H	1.22	0.99
1:L:318:LEU:HA	1:L:321:ASP:HB2	1.45	0.99
1:L:266:ILE:HG12	1:L:304:PHE:CE1	1.98	0.99
1:L:93:ASN:HA	1:L:110:GLN:CB	1.91	0.99
1:L:266:ILE:HG23	1:L:324:PRO:HB2	1.46	0.98
1:L:48:TYR:CE2	1:L:62:PHE:HE2	1.81	0.98
1:L:74:VAL:HG13	1:L:170:TRP:CD1	1.99	0.98
1:L:250:VAL:CG1	1:L:295:CYS:HB2	1.94	0.97
1:L:210:VAL:HG11	1:L:278:TYR:CE2	2.00	0.97
1:L:308:TRP:CB	1:L:323:CYS:SG	2.52	0.97
1:L:297:LEU:HD12	1:L:299:PHE:HE1	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:PHE:HA	1:L:56:PHE:HB2	1.47	0.97
1:L:200:LEU:HB3	1:L:211:ARG:HD2	1.46	0.96
1:L:242:PHE:HB3	1:L:310:THR:OG1	1.65	0.95
1:L:242:PHE:CZ	1:L:246:LEU:HD21	2.01	0.94
1:L:88:LEU:HB3	1:L:115:TRP:CE2	2.01	0.94
1:L:338:ILE:HG22	1:L:339:SER:H	1.30	0.94
2:S:106:ARG:HG2	2:S:106:ARG:HH11	1.31	0.94
1:L:314:PRO:HG3	1:L:365:GLY:HA3	1.49	0.94
2:S:89:GLN:CA	2:S:111:SER:HA	1.97	0.94
2:S:73:GLN:HB2	2:S:118:LEU:O	1.66	0.94
1:L:44:ASP:HA	1:L:148:MET:O	1.66	0.94
1:L:68:ILE:HB	1:L:136:TRP:CZ3	2.02	0.94
1:L:73:LYS:HE2	1:L:173:VAL:HG13	1.50	0.94
2:S:149:VAL:HG12	2:S:150:ALA:H	1.31	0.94
1:L:212:ARG:O	1:L:327:TYR:HA	1.68	0.93
2:S:33:ASP:HA	2:S:145:TYR:HD2	1.31	0.93
1:L:227:PHE:CD2	2:S:181:PRO:HA	2.04	0.93
1:L:219:GLY:HA2	1:L:234:SER:OG	1.67	0.93
1:L:80:ILE:HD12	1:L:156:TRP:CH2	2.04	0.92
1:L:20:LEU:HG	1:L:73:LYS:HE2	1.51	0.92
2:S:13:PRO:HB3	2:S:162:ASN:HD22	1.27	0.92
2:S:96:GLN:HA	2:S:143:THR:O	1.67	0.92
2:S:20:PRO:HB3	2:S:21:PRO:HD2	1.52	0.91
1:L:213:MET:SD	1:L:326:LEU:O	2.28	0.91
2:S:16:ILE:HB	2:S:52:TYR:HE2	1.35	0.91
2:S:74:LEU:HB3	2:S:118:LEU:HD23	1.53	0.91
2:S:86:TRP:CZ2	2:S:88:GLY:HA3	2.05	0.91
1:L:168:LEU:HG	1:L:170:TRP:HE1	1.35	0.91
1:L:239:TRP:HB2	1:L:357:ILE:O	1.71	0.90
2:S:65:TRP:HB2	2:S:172:ALA:HB3	1.50	0.90
1:L:191:LEU:HB3	1:L:351:ILE:H	1.36	0.90
1:L:140:MET:O	1:L:140:MET:SD	2.30	0.90
1:L:199:LYS:HG3	1:L:343:ASN:HD21	1.36	0.90
1:L:268:PHE:CE1	1:L:324:PRO:HG3	2.07	0.90
2:S:177:MET:HB3	2:S:180:PHE:CZ	2.06	0.90
2:S:89:GLN:O	2:S:90:VAL:HG23	1.72	0.90
1:L:212:ARG:O	1:L:213:MET:SD	2.30	0.89
2:S:109:VAL:HG22	2:S:110:ILE:H	1.36	0.89
1:L:226:ALA:HA	2:S:181:PRO:HB3	1.52	0.89
1:L:249:GLU:HA	1:L:296:THR:HA	1.52	0.89
2:S:34:LEU:HB2	2:S:145:TYR:CA	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:ARG:HB3	1:L:355:CYS:HB3	1.54	0.89
1:L:273:ASP:HA	1:L:278:TYR:CE2	2.08	0.88
1:L:25:PHE:HA	1:L:56:PHE:CB	2.04	0.88
2:S:34:LEU:HD21	2:S:146:LEU:HD12	1.56	0.88
1:L:182:TYR:HD1	1:L:235:TRP:CZ3	1.93	0.87
1:L:195:ARG:HH21	1:L:217:ILE:HA	1.39	0.87
1:L:215:LEU:HD12	1:L:326:LEU:H	1.40	0.87
2:S:36:ASN:HB2	2:S:61:ARG:CA	2.02	0.87
1:L:187:CYS:SG	1:L:355:CYS:HA	2.15	0.86
1:L:165:ILE:HD13	1:L:165:ILE:H	1.39	0.86
2:S:32:PHE:HB3	2:S:41:PRO:HD3	1.56	0.85
2:S:71:HIS:HA	2:S:120:PHE:O	1.75	0.85
1:L:96:VAL:HA	2:S:176:LEU:CB	2.05	0.85
1:L:95:GLY:H	1:L:146:VAL:HG22	1.41	0.85
2:S:93:TYR:HA	2:S:106:ARG:O	1.77	0.85
2:S:34:LEU:N	2:S:145:TYR:HA	1.91	0.85
1:L:219:GLY:C	1:L:233:ASN:HB3	2.02	0.85
1:L:258:ILE:HG22	1:L:342:PHE:CD1	2.11	0.85
2:S:68:GLY:HA3	2:S:169:PHE:HA	1.59	0.85
2:S:62:THR:HG22	2:S:177:MET:HE2	1.57	0.85
1:L:303:GLU:HG2	1:L:304:PHE:H	1.42	0.85
2:S:36:ASN:CB	2:S:61:ARG:HA	2.04	0.85
1:L:60:VAL:CB	1:L:64:ARG:HD2	2.04	0.84
1:L:60:VAL:HB	1:L:64:ARG:CD	2.02	0.84
1:L:106:THR:HG23	1:L:228:LEU:HD13	1.57	0.84
1:L:248:PHE:HB3	1:L:347:LYS:H	1.42	0.84
1:L:269:GLY:HA3	1:L:325:TYR:CZ	2.11	0.84
2:S:68:GLY:HA3	2:S:169:PHE:CG	2.12	0.84
1:L:48:TYR:CE2	1:L:62:PHE:CE2	2.65	0.84
1:L:265:LEU:HD22	1:L:283:HIS:HA	1.58	0.84
2:S:54:PRO:HB2	2:S:57:MET:CB	2.07	0.84
1:L:235:TRP:CE3	2:S:171:VAL:HG12	2.11	0.84
2:S:35:ILE:HD12	2:S:36:ASN:H	1.38	0.84
1:L:215:LEU:HD12	1:L:326:LEU:N	1.93	0.84
1:L:351:ILE:HD13	1:L:354:PHE:CB	2.07	0.84
1:L:263:THR:HA	1:L:285:ILE:HB	1.60	0.83
1:L:250:VAL:HG13	1:L:295:CYS:CB	2.05	0.83
1:L:60:VAL:O	1:L:64:ARG:HB2	1.77	0.83
1:L:183:HIS:NE2	1:L:185:ALA:HB3	1.93	0.83
1:L:91:ALA:CB	1:L:107:ILE:HB	2.08	0.83
1:L:265:LEU:H	1:L:326:LEU:HG	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:ARG:CB	2:S:137:PRO:HB2	2.09	0.82
1:L:204:GLN:HE22	1:L:258:ILE:HD13	1.43	0.82
1:L:199:LYS:HG3	1:L:343:ASN:ND2	1.94	0.82
1:L:264:PHE:CE1	1:L:285:ILE:HA	2.13	0.82
1:L:120:LYS:HE2	1:L:121:LYS:N	1.95	0.82
1:L:243:ARG:HA	1:L:308:TRP:CH2	2.15	0.82
1:L:240:ARG:NH1	1:L:309:SER:OG	2.13	0.82
1:L:314:PRO:HG3	1:L:365:GLY:CA	2.10	0.82
2:S:57:MET:HG2	2:S:61:ARG:HH21	1.43	0.82
1:L:246:LEU:HG	1:L:351:ILE:HD12	1.62	0.82
1:L:23:THR:HG21	1:L:172:ILE:HG22	1.59	0.81
1:L:17:ARG:HH22	1:L:20:LEU:HD22	1.45	0.81
1:L:193:LEU:CB	1:L:232:PRO:HA	2.08	0.81
1:L:241:TYR:HB3	1:L:308:TRP:C	2.05	0.81
1:L:204:GLN:HG2	1:L:340:GLY:O	1.81	0.81
2:S:96:GLN:HB3	2:S:142:THR:OG1	1.80	0.81
1:L:252:LYS:NZ	1:L:256:PRO:HG3	1.94	0.81
2:S:135:GLU:HA	2:S:141:GLN:HB3	1.63	0.81
1:L:86:CYS:SG	1:L:117:PRO:HB2	2.22	0.80
2:S:53:ASN:HA	2:S:61:ARG:HH22	1.44	0.80
2:S:141:GLN:HG3	2:S:142:THR:H	1.44	0.80
2:S:12:SER:HB3	2:S:56:ILE:HD11	1.60	0.80
1:L:98:GLY:O	1:L:100:TYR:HD1	1.65	0.80
1:L:241:TYR:CA	1:L:309:SER:HA	2.11	0.80
1:L:258:ILE:HG12	1:L:336:GLY:CA	2.11	0.80
1:L:54:GLN:HG2	1:L:56:PHE:HE1	1.45	0.80
1:L:256:PRO:HB3	1:L:290:GLU:CA	2.07	0.80
1:L:92:ILE:HD12	1:L:125:PHE:HE2	1.46	0.79
1:L:120:LYS:CG	1:L:121:LYS:HG2	2.04	0.79
1:L:242:PHE:CZ	1:L:246:LEU:HD11	2.17	0.79
1:L:262:VAL:HG13	1:L:328:ALA:HB1	1.64	0.79
1:L:311:GLN:HE21	1:L:312:VAL:H	1.31	0.79
1:L:22:ASP:HA	1:L:57:ARG:HG2	1.64	0.79
1:L:113:MET:SD	1:L:123:PHE:CD2	2.75	0.79
1:L:248:PHE:HB2	1:L:297:LEU:HD23	1.62	0.79
2:S:13:PRO:HA	2:S:162:ASN:HA	1.63	0.79
1:L:32:LEU:H	1:L:165:ILE:HG22	1.46	0.79
1:L:182:TYR:HD1	1:L:235:TRP:CE3	2.01	0.79
1:L:270:ASN:HA	1:L:318:LEU:HG	1.63	0.79
1:L:134:ASP:CB	1:L:177:CYS:SG	2.71	0.79
1:L:195:ARG:H	1:L:232:PRO:CB	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:MET:SD	1:L:108:CYS:SG	2.81	0.79
1:L:278:TYR:CG	1:L:329:ILE:HG12	2.17	0.78
2:S:73:GLN:HG3	2:S:162:ASN:HB2	1.65	0.78
1:L:325:TYR:CE1	1:L:327:TYR:HB3	2.17	0.78
1:L:187:CYS:HA	1:L:354:PHE:O	1.83	0.78
1:L:236:ILE:HG22	1:L:236:ILE:O	1.83	0.78
2:S:69:THR:HB	2:S:166:ASP:CB	2.14	0.78
1:L:193:LEU:HB2	1:L:232:PRO:CA	2.13	0.78
2:S:94:LEU:HB3	2:S:146:LEU:CG	2.13	0.78
2:S:164:ARG:NH2	2:S:166:ASP:HA	1.98	0.78
1:L:96:VAL:HG13	2:S:176:LEU:HD12	1.66	0.78
2:S:94:LEU:HA	2:S:146:LEU:HA	1.64	0.78
1:L:219:GLY:O	1:L:233:ASN:HB3	1.83	0.78
2:S:27:VAL:CG1	2:S:151:THR:HA	2.13	0.78
1:L:100:TYR:O	2:S:178:PRO:HA	1.84	0.77
1:L:91:ALA:HB2	1:L:107:ILE:HB	1.66	0.77
1:L:198:GLY:HA2	1:L:346:VAL:HG23	1.67	0.77
2:S:74:LEU:HB3	2:S:118:LEU:CD2	2.15	0.77
2:S:90:VAL:HG22	2:S:149:VAL:HB	1.66	0.77
2:S:126:GLY:HA3	2:S:131:PHE:C	2.09	0.77
1:L:230:ASN:ND2	1:L:233:ASN:HB2	1.99	0.77
2:S:27:VAL:HG11	2:S:151:THR:HG23	1.66	0.77
1:L:188:GLN:O	1:L:353:ASP:HA	1.84	0.77
1:L:65:THR:O	1:L:66:HIS:HB2	1.85	0.77
2:S:91:PHE:CD1	2:S:93:TYR:HE2	2.02	0.77
1:L:71:LYS:HB3	1:L:126:THR:O	1.85	0.77
1:L:96:VAL:CA	2:S:176:LEU:HB2	2.12	0.76
1:L:242:PHE:CE2	1:L:246:LEU:HD21	2.20	0.76
1:L:262:VAL:H	1:L:286:VAL:CG2	1.99	0.76
2:S:68:GLY:CA	2:S:169:PHE:HA	2.15	0.76
2:S:95:ARG:NE	2:S:98:MET:HA	2.00	0.76
2:S:74:LEU:HD22	2:S:118:LEU:HD23	1.66	0.76
2:S:95:ARG:CZ	2:S:98:MET:HA	2.16	0.76
1:L:252:LYS:HB3	1:L:293:GLU:CB	2.15	0.76
1:L:149:THR:O	1:L:150:VAL:HG13	1.86	0.76
1:L:134:ASP:HB2	1:L:177:CYS:SG	2.26	0.76
2:S:29:ALA:HA	2:S:150:ALA:HB3	1.66	0.76
1:L:186:ASP:HB2	1:L:356:GLY:O	1.85	0.76
1:L:22:ASP:HA	1:L:57:ARG:CG	2.15	0.75
1:L:143:ARG:HB3	2:S:137:PRO:CB	2.15	0.75
1:L:251:THR:HA	1:L:293:GLU:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:134:ALA:HA	2:S:143:THR:OG1	1.86	0.75
1:L:20:LEU:HB3	1:L:73:LYS:NZ	2.00	0.75
1:L:245:GLU:C	1:L:351:ILE:HG13	2.11	0.75
1:L:269:GLY:HA3	1:L:325:TYR:OH	1.86	0.75
2:S:52:TYR:C	2:S:54:PRO:HD3	2.11	0.75
2:S:63:ALA:HB3	2:S:66:LYS:HE3	1.67	0.75
2:S:132:GLU:O	2:S:133:PHE:HB2	1.85	0.75
2:S:57:MET:O	2:S:60:LEU:HB2	1.86	0.75
1:L:256:PRO:HB2	1:L:290:GLU:OE2	1.86	0.75
2:S:16:ILE:HB	2:S:52:TYR:CE2	2.21	0.75
2:S:76:VAL:HG12	2:S:158:GLN:O	1.87	0.75
2:S:125:ILE:HG13	2:S:126:GLY:H	1.52	0.75
1:L:244:GLY:O	1:L:246:LEU:HD12	1.86	0.75
1:L:145:ARG:CZ	2:S:137:PRO:HG2	2.17	0.75
2:S:89:GLN:HA	2:S:111:SER:CA	2.11	0.75
1:L:247:HIS:HB2	1:L:297:LEU:HB3	1.67	0.75
1:L:314:PRO:CG	1:L:365:GLY:HA3	2.17	0.75
2:S:69:THR:HB	2:S:166:ASP:HB2	1.67	0.75
1:L:210:VAL:HG13	1:L:328:ALA:O	1.87	0.74
1:L:311:GLN:NE2	1:L:312:VAL:H	1.85	0.74
2:S:178:PRO:HB2	2:S:179:PRO:HD3	1.69	0.74
1:L:200:LEU:HD12	1:L:202:PHE:CZ	2.22	0.74
1:L:250:VAL:O	1:L:295:CYS:N	2.20	0.74
1:L:255:SER:CB	1:L:258:ILE:HB	2.16	0.74
2:S:32:PHE:CE2	2:S:148:CYS:SG	2.79	0.74
2:S:32:PHE:CZ	2:S:148:CYS:SG	2.79	0.74
1:L:288:PHE:HD2	1:L:342:PHE:CZ	2.06	0.74
2:S:19:THR:HA	2:S:47:TRP:CZ3	2.23	0.74
1:L:70:GLY:HA3	1:L:173:VAL:O	1.87	0.74
1:L:244:GLY:HA2	1:L:301:GLN:HE22	1.52	0.74
2:S:143:THR:HG22	2:S:144:TRP:H	1.53	0.74
1:L:182:TYR:CD1	1:L:235:TRP:CE3	2.76	0.74
2:S:58:ASN:HA	2:S:61:ARG:HB2	1.69	0.74
2:S:91:PHE:N	2:S:149:VAL:HG21	2.02	0.74
1:L:130:ASN:OD1	1:L:132:CYS:SG	2.44	0.73
1:L:197:MET:SD	1:L:347:LYS:HA	2.28	0.73
1:L:256:PRO:CB	1:L:290:GLU:HA	2.10	0.73
2:S:30:VAL:HG13	2:S:148:CYS:SG	2.28	0.73
1:L:210:VAL:HB	1:L:273:ASP:HB2	1.70	0.73
1:L:104:VAL:HG21	1:L:153:VAL:HG22	1.69	0.73
2:S:90:VAL:HB	2:S:110:ILE:HG21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:THR:HG22	1:L:171:SER:HB2	1.70	0.73
1:L:78:THR:O	1:L:79:ASN:HB2	1.86	0.73
2:S:20:PRO:HB3	2:S:21:PRO:CD	2.18	0.73
1:L:33:SER:HB3	1:L:36:MET:SD	2.28	0.72
1:L:355:CYS:SG	1:L:357:ILE:HD11	2.28	0.72
1:L:68:ILE:HB	1:L:136:TRP:CH2	2.23	0.72
1:L:218:GLY:H	1:L:233:ASN:HD21	1.37	0.72
1:L:88:LEU:HD23	1:L:115:TRP:CZ2	2.24	0.72
1:L:5:LEU:HA	1:L:8:LEU:HB2	1.70	0.72
1:L:230:ASN:HB2	1:L:232:PRO:HD2	1.72	0.72
2:S:19:THR:HB	2:S:156:ILE:O	1.89	0.72
2:S:21:PRO:C	2:S:24:PHE:HB2	2.15	0.72
2:S:71:HIS:CD2	2:S:164:ARG:HD3	2.24	0.72
2:S:127:PRO:HD2	2:S:132:GLU:HA	1.69	0.72
2:S:130:GLY:O	2:S:131:PHE:HD2	1.72	0.72
2:S:106:ARG:CD	2:S:107:THR:H	2.02	0.71
1:L:186:ASP:HB2	1:L:356:GLY:C	2.14	0.71
1:L:357:ILE:N	1:L:357:ILE:HD12	2.05	0.71
2:S:34:LEU:H	2:S:145:TYR:HA	1.54	0.71
2:S:94:LEU:HB2	2:S:145:TYR:O	1.91	0.71
1:L:46:TYR:OH	1:L:145:ARG:HB3	1.90	0.71
1:L:134:ASP:HB3	1:L:177:CYS:SG	2.31	0.71
1:L:32:LEU:N	1:L:165:ILE:HG22	2.05	0.71
1:L:215:LEU:HD21	1:L:248:PHE:HZ	1.55	0.71
1:L:262:VAL:C	1:L:285:ILE:HG13	2.15	0.71
1:L:4:ASN:OD1	1:L:6:PHE:CD1	2.44	0.71
1:L:25:PHE:CE2	1:L:171:SER:HA	2.26	0.71
1:L:21:LEU:C	1:L:23:THR:H	1.98	0.71
1:L:32:LEU:HD13	1:L:164:VAL:O	1.91	0.71
1:L:265:LEU:C	1:L:266:ILE:HD12	2.15	0.71
1:L:73:LYS:CE	1:L:173:VAL:HG13	2.21	0.71
1:L:183:HIS:CD2	1:L:185:ALA:HB3	2.26	0.70
1:L:200:LEU:HD12	1:L:202:PHE:HZ	1.55	0.70
1:L:218:GLY:N	1:L:233:ASN:HD21	1.89	0.70
1:L:261:THR:OG1	1:L:287:GLN:HG3	1.92	0.70
2:S:68:GLY:HA3	2:S:169:PHE:CD1	2.26	0.70
1:L:29:ARG:HA	1:L:166:ALA:O	1.91	0.70
1:L:246:LEU:HG	1:L:351:ILE:CD1	2.21	0.70
1:L:86:CYS:HG	1:L:156:TRP:CG	2.09	0.70
1:L:214:PRO:HA	1:L:325:TYR:CG	2.27	0.70
2:S:30:VAL:HG23	2:S:41:PRO:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:245:GLU:OE2	1:L:298:VAL:HG22	1.91	0.70
2:S:74:LEU:HA	2:S:160:GLU:O	1.90	0.70
2:S:34:LEU:HB2	2:S:145:TYR:HA	1.72	0.70
1:L:93:ASN:HB2	2:S:176:LEU:HD21	1.73	0.70
1:L:23:THR:HA	1:L:58:ALA:HB2	1.74	0.70
1:L:187:CYS:SG	1:L:355:CYS:CA	2.79	0.70
1:L:264:PHE:HB3	1:L:326:LEU:HD11	1.74	0.70
1:L:105:TYR:CD2	1:L:196:TRP:HB3	2.26	0.70
1:L:151:ILE:HG12	1:L:152:CYS:N	2.05	0.70
1:L:169:ASP:C	1:L:170:TRP:HD1	2.00	0.70
1:L:209:GLU:O	1:L:210:VAL:HG23	1.92	0.70
1:L:325:TYR:HE1	1:L:327:TYR:HB3	1.55	0.70
1:L:338:ILE:HG22	1:L:339:SER:N	2.07	0.70
1:L:200:LEU:CB	1:L:211:ARG:HD2	2.22	0.69
1:L:245:GLU:O	1:L:245:GLU:HG3	1.91	0.69
1:L:93:ASN:CA	1:L:110:GLN:HB2	2.21	0.69
1:L:108:CYS:SG	1:L:109:SER:N	2.65	0.69
2:S:55:PRO:O	2:S:59:VAL:HG23	1.93	0.69
2:S:112:GLN:CB	2:S:113:PRO:HD2	2.07	0.69
1:L:17:ARG:HH12	1:L:20:LEU:CD1	2.06	0.69
2:S:107:THR:HG22	2:S:108:PHE:N	2.07	0.69
1:L:219:GLY:HA2	1:L:234:SER:HG	1.56	0.69
1:L:264:PHE:CD1	1:L:285:ILE:HA	2.28	0.69
2:S:91:PHE:H	2:S:149:VAL:CG2	2.04	0.69
1:L:195:ARG:H	1:L:232:PRO:HB3	1.57	0.69
2:S:91:PHE:HA	2:S:108:PHE:O	1.93	0.69
2:S:95:ARG:HG2	2:S:98:MET:HG3	1.74	0.69
1:L:197:MET:C	1:L:346:VAL:HB	2.18	0.69
1:L:261:THR:HG23	1:L:286:VAL:O	1.92	0.69
1:L:271:LEU:HD11	1:L:275:PHE:CD2	2.28	0.69
2:S:178:PRO:HB2	2:S:179:PRO:CD	2.23	0.69
1:L:73:LYS:HA	1:L:126:THR:HA	1.75	0.68
1:L:86:CYS:H	1:L:116:ASN:ND2	1.92	0.68
1:L:96:VAL:CG1	2:S:176:LEU:HB2	2.23	0.68
1:L:148:MET:SD	1:L:148:MET:C	2.76	0.68
1:L:286:VAL:HG12	1:L:287:GLN:H	1.57	0.68
1:L:141:ILE:HA	1:L:144:SER:HB2	1.75	0.68
2:S:95:ARG:NE	2:S:98:MET:HG2	2.05	0.68
1:L:68:ILE:HG22	1:L:69:THR:H	1.58	0.68
2:S:33:ASP:HB3	2:S:39:ILE:HA	1.74	0.68
2:S:122:PHE:O	2:S:122:PHE:CD2	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:156:ILE:O	2:S:156:ILE:HG22	1.94	0.68
1:L:139:GLU:HA	1:L:142:SER:OG	1.94	0.68
1:L:262:VAL:H	1:L:286:VAL:HG23	1.56	0.68
2:S:109:VAL:CG2	2:S:110:ILE:H	2.07	0.68
1:L:252:LYS:HZ2	1:L:256:PRO:HG3	1.58	0.68
1:L:291:VAL:HG23	1:L:292:GLU:H	1.57	0.68
1:L:113:MET:CG	1:L:123:PHE:CE2	2.77	0.68
1:L:212:ARG:H	1:L:212:ARG:HD3	1.58	0.68
1:L:36:MET:HE1	1:L:42:LEU:HD21	1.76	0.68
1:L:202:PHE:HE2	1:L:211:ARG:HG2	1.58	0.68
1:L:261:THR:HG23	1:L:285:ILE:HG12	1.74	0.68
1:L:261:THR:CA	1:L:286:VAL:HB	2.15	0.68
2:S:54:PRO:HD2	2:S:57:MET:HG2	1.76	0.68
2:S:99:ASN:C	2:S:101:GLU:H	2.02	0.68
1:L:261:THR:HG22	1:L:285:ILE:HD11	1.76	0.67
1:L:264:PHE:HE1	1:L:285:ILE:HA	1.58	0.67
2:S:86:TRP:CE2	2:S:113:PRO:HA	2.28	0.67
2:S:48:ASN:ND2	2:S:50:HIS:ND1	2.42	0.67
2:S:127:PRO:HD2	2:S:132:GLU:CA	2.24	0.67
1:L:31:LEU:HB2	1:L:42:LEU:HB3	1.75	0.67
1:L:258:ILE:HD11	1:L:340:GLY:HA3	1.76	0.67
1:L:285:ILE:HG13	1:L:286:VAL:H	1.58	0.67
2:S:106:ARG:HG2	2:S:106:ARG:NH1	1.98	0.67
1:L:23:THR:HG22	1:L:171:SER:CB	2.25	0.67
1:L:266:ILE:CG2	1:L:324:PRO:HB2	2.23	0.67
2:S:55:PRO:HG2	2:S:56:ILE:H	1.60	0.67
1:L:364:ASP:HB3	2:S:182:LEU:HD13	1.75	0.67
2:S:34:LEU:HB2	2:S:145:TYR:C	2.19	0.67
1:L:312:VAL:HG22	1:L:316:THR:OG1	1.95	0.67
1:L:30:VAL:HG23	1:L:30:VAL:O	1.93	0.67
2:S:34:LEU:CD2	2:S:146:LEU:HD12	2.23	0.67
1:L:356:GLY:O	1:L:357:ILE:HG13	1.94	0.67
1:L:74:VAL:HA	1:L:169:ASP:O	1.95	0.67
2:S:177:MET:C	2:S:180:PHE:HZ	2.02	0.67
2:S:29:ALA:HA	2:S:150:ALA:CB	2.25	0.66
2:S:75:ASN:ND2	2:S:117:MET:HB3	2.09	0.66
1:L:25:PHE:CA	1:L:56:PHE:HB2	2.24	0.66
1:L:184:LEU:HD21	2:S:165:PHE:CE1	2.30	0.66
2:S:56:ILE:HD12	2:S:57:MET:N	2.10	0.66
1:L:314:PRO:O	1:L:315:ARG:HG3	1.96	0.66
2:S:22:ALA:HA	2:S:23:PRO:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:310:THR:O	1:L:311:GLN:HB3	1.94	0.66
1:L:289:ALA:HB3	1:L:292:GLU:HB2	1.77	0.66
2:S:122:PHE:O	2:S:122:PHE:HD2	1.79	0.66
1:L:140:MET:SD	2:S:65:TRP:CH2	2.89	0.66
1:L:266:ILE:HG21	1:L:304:PHE:CD1	2.30	0.66
2:S:141:GLN:HG3	2:S:142:THR:O	1.95	0.66
1:L:130:ASN:CG	1:L:132:CYS:HG	2.03	0.66
1:L:91:ALA:HB3	1:L:149:THR:HG23	1.77	0.66
1:L:92:ILE:HG21	1:L:127:PHE:CE2	2.30	0.66
2:S:106:ARG:HG3	2:S:107:THR:N	2.11	0.66
1:L:67:VAL:HG13	1:L:136:TRP:H	1.60	0.66
1:L:347:LYS:HG3	1:L:348:LEU:N	2.09	0.66
1:L:73:LYS:O	1:L:170:TRP:HB3	1.96	0.65
1:L:156:TRP:H	1:L:156:TRP:CD1	2.13	0.65
1:L:367:ARG:O	1:L:369:LEU:N	2.29	0.65
1:L:68:ILE:HD12	1:L:68:ILE:N	2.11	0.65
1:L:91:ALA:HB1	1:L:107:ILE:HB	1.77	0.65
1:L:100:TYR:HB3	2:S:176:LEU:O	1.96	0.65
1:L:113:MET:HG2	1:L:123:PHE:CE2	2.31	0.65
1:L:119:CYS:SG	1:L:293:GLU:OE1	2.55	0.65
2:S:33:ASP:HA	2:S:145:TYR:CD2	2.23	0.65
1:L:72:ILE:N	1:L:172:ILE:HD12	2.10	0.65
1:L:103:ASP:O	1:L:107:ILE:HG13	1.96	0.65
1:L:258:ILE:HG23	1:L:335:THR:O	1.96	0.65
1:L:262:VAL:O	1:L:264:PHE:CE1	2.50	0.65
1:L:267:ALA:O	1:L:324:PRO:HB3	1.94	0.65
2:S:40:THR:HG23	2:S:49:THR:HG21	1.77	0.65
2:S:92:VAL:HG22	2:S:146:LEU:HD21	1.78	0.65
1:L:86:CYS:O	1:L:116:ASN:HA	1.97	0.65
1:L:195:ARG:HH21	1:L:217:ILE:CA	2.07	0.65
1:L:195:ARG:HB3	1:L:197:MET:HE3	1.78	0.65
1:L:210:VAL:O	1:L:212:ARG:HD3	1.96	0.65
1:L:32:LEU:O	1:L:163:ASP:HA	1.97	0.65
1:L:73:LYS:HB3	1:L:173:VAL:HG22	1.77	0.65
1:L:105:TYR:HB2	1:L:196:TRP:CD1	2.32	0.65
1:L:3:GLN:O	1:L:5:LEU:HD23	1.96	0.65
1:L:78:THR:HG23	1:L:79:ASN:N	2.11	0.65
1:L:85:GLY:O	1:L:156:TRP:HA	1.96	0.65
1:L:86:CYS:HB3	1:L:156:TRP:N	2.12	0.65
1:L:75:THR:HG23	1:L:122:ASN:CG	2.22	0.65
1:L:193:LEU:HD23	1:L:232:PRO:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:218:GLY:H	1:L:233:ASN:ND2	1.95	0.65
1:L:308:TRP:HB3	1:L:323:CYS:HG	1.57	0.65
1:L:153:VAL:HG21	1:L:196:TRP:CH2	2.32	0.65
1:L:227:PHE:CD1	1:L:366:SER:HB2	2.32	0.65
1:L:265:LEU:N	1:L:326:LEU:HG	2.12	0.65
2:S:126:GLY:HA3	2:S:131:PHE:CA	2.26	0.65
1:L:199:LYS:O	1:L:200:LEU:HD23	1.96	0.64
2:S:53:ASN:HD21	2:S:182:LEU:HB2	1.61	0.64
1:L:210:VAL:HG21	1:L:278:TYR:CD2	2.33	0.64
2:S:171:VAL:HG13	2:S:172:ALA:N	2.11	0.64
1:L:71:LYS:HE2	1:L:126:THR:OG1	1.97	0.64
1:L:93:ASN:HA	1:L:110:GLN:CG	2.28	0.64
1:L:195:ARG:H	1:L:232:PRO:HB2	1.59	0.64
1:L:15:SER:CB	1:L:68:ILE:HA	2.26	0.64
1:L:183:HIS:CE1	1:L:185:ALA:H	2.16	0.64
1:L:338:ILE:CG2	1:L:339:SER:H	2.01	0.64
1:L:4:ASN:C	1:L:6:PHE:H	2.04	0.64
1:L:90:LEU:HD13	1:L:149:THR:O	1.97	0.64
1:L:187:CYS:SG	1:L:355:CYS:CB	2.86	0.64
1:L:191:LEU:HD12	1:L:192:PRO:N	2.13	0.64
1:L:215:LEU:HB2	1:L:325:TYR:CB	2.21	0.64
2:S:149:VAL:HG12	2:S:150:ALA:N	2.10	0.64
1:L:44:ASP:CB	1:L:149:THR:HG22	2.28	0.64
1:L:231:MET:HB2	2:S:174:ASN:HB2	1.80	0.64
2:S:91:PHE:CD1	2:S:93:TYR:CE2	2.85	0.64
1:L:31:LEU:O	1:L:42:LEU:HD13	1.97	0.64
1:L:71:LYS:HD3	1:L:175:GLU:HB2	1.79	0.64
1:L:171:SER:O	1:L:172:ILE:HB	1.96	0.64
1:L:278:TYR:C	1:L:280:SER:H	2.05	0.64
2:S:106:ARG:CG	2:S:107:THR:N	2.61	0.64
2:S:109:VAL:HG22	2:S:110:ILE:N	2.11	0.64
1:L:214:PRO:HA	1:L:325:TYR:CD2	2.33	0.64
1:L:218:GLY:N	1:L:233:ASN:ND2	2.46	0.64
1:L:245:GLU:O	1:L:245:GLU:CG	2.45	0.64
2:S:15:MET:HB2	2:S:50:HIS:O	1.97	0.64
1:L:13:THR:HA	1:L:65:THR:O	1.99	0.63
1:L:191:LEU:O	1:L:350:GLY:HA2	1.98	0.63
1:L:255:SER:O	1:L:258:ILE:O	2.16	0.63
2:S:165:PHE:HA	2:S:169:PHE:CE2	2.33	0.63
2:S:15:MET:HA	2:S:52:TYR:CD2	2.32	0.63
1:L:133:GLY:HA2	1:L:179:PRO:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:278:TYR:CE1	1:L:281:PHE:CE2	2.86	0.63
2:S:148:CYS:HB2	2:S:159:PHE:CE1	2.33	0.63
1:L:87:CYS:SG	1:L:88:LEU:N	2.71	0.63
1:L:87:CYS:O	1:L:152:CYS:HA	1.98	0.63
1:L:154:SER:HB2	1:L:253:MET:HG3	1.80	0.63
1:L:214:PRO:HA	1:L:325:TYR:CD1	2.33	0.63
1:L:217:ILE:HG12	1:L:242:PHE:CD1	2.34	0.63
1:L:62:PHE:HB3	1:L:63:LEU:HD12	1.80	0.63
1:L:90:LEU:HD22	1:L:150:VAL:HG13	1.79	0.63
1:L:191:LEU:HG	1:L:193:LEU:HD12	1.81	0.63
1:L:226:ALA:HA	2:S:181:PRO:CB	2.25	0.63
1:L:176:LYS:O	1:L:176:LYS:HG2	1.98	0.63
1:L:120:LYS:HB3	1:L:120:LYS:HZ2	1.63	0.63
1:L:191:LEU:HD13	1:L:354:PHE:CE2	2.33	0.63
2:S:53:ASN:HA	2:S:61:ARG:NH2	2.13	0.63
1:L:20:LEU:HB3	1:L:73:LYS:HZ3	1.63	0.63
1:L:262:VAL:O	1:L:285:ILE:HG13	1.98	0.63
2:S:31:THR:HG23	2:S:31:THR:O	1.98	0.63
2:S:53:ASN:HA	2:S:61:ARG:HH12	1.64	0.63
2:S:74:LEU:HD22	2:S:118:LEU:HB3	1.80	0.63
2:S:127:PRO:HG2	2:S:128:ASN:H	1.64	0.63
2:S:160:GLU:O	2:S:160:GLU:HG3	1.98	0.63
1:L:139:GLU:O	1:L:140:MET:HB2	1.97	0.63
2:S:93:TYR:CD1	2:S:107:THR:OG1	2.52	0.62
1:L:21:LEU:O	1:L:57:ARG:HB3	1.99	0.62
2:S:40:THR:HG23	2:S:49:THR:CG2	2.29	0.62
1:L:252:LYS:HB3	1:L:293:GLU:HB2	1.80	0.62
1:L:258:ILE:CD1	1:L:340:GLY:HA3	2.29	0.62
1:L:33:SER:OG	1:L:34:LYS:N	2.30	0.62
1:L:204:GLN:OE1	1:L:336:GLY:HA3	1.99	0.62
1:L:210:VAL:HG13	1:L:329:ILE:HG13	1.80	0.62
2:S:28:THR:O	2:S:29:ALA:HB2	1.99	0.62
2:S:106:ARG:HD2	2:S:107:THR:H	1.63	0.62
1:L:128:ASN:HD21	1:L:136:TRP:HE1	1.47	0.62
1:L:162:THR:OG1	1:L:163:ASP:N	2.32	0.62
1:L:188:GLN:O	1:L:188:GLN:HG3	1.97	0.62
1:L:351:ILE:HG21	1:L:354:PHE:HB3	1.80	0.62
2:S:74:LEU:C	2:S:74:LEU:HD23	2.24	0.62
2:S:110:ILE:HG23	2:S:111:SER:H	1.65	0.62
1:L:260:ALA:HB3	1:L:342:PHE:CD2	2.34	0.62
1:L:127:PHE:CZ	1:L:129:PRO:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:LYS:HG3	1:L:343:ASN:CG	2.23	0.62
1:L:278:TYR:CD1	1:L:281:PHE:CE2	2.87	0.62
1:L:193:LEU:HD22	1:L:195:ARG:N	2.15	0.62
2:S:91:PHE:O	2:S:93:TYR:CE2	2.53	0.62
2:S:29:ALA:HA	2:S:149:VAL:O	2.00	0.62
2:S:161:VAL:O	2:S:162:ASN:ND2	2.32	0.62
1:L:243:ARG:HG3	1:L:243:ARG:HH11	1.65	0.61
1:L:278:TYR:CE1	1:L:281:PHE:HE2	2.18	0.61
1:L:297:LEU:CD1	1:L:299:PHE:HE1	2.05	0.61
2:S:29:ALA:CA	2:S:150:ALA:HB3	2.29	0.61
2:S:34:LEU:O	2:S:35:ILE:HG23	1.99	0.61
2:S:90:VAL:HG13	2:S:149:VAL:HG23	1.81	0.61
2:S:177:MET:N	2:S:177:MET:SD	2.73	0.61
1:L:71:LYS:HE2	1:L:126:THR:CB	2.31	0.61
1:L:145:ARG:H	1:L:145:ARG:HD2	1.65	0.61
2:S:89:GLN:HB2	2:S:111:SER:OG	2.01	0.61
2:S:94:LEU:HD23	2:S:94:LEU:H	1.66	0.61
1:L:297:LEU:O	1:L:298:VAL:HG23	2.01	0.61
1:L:227:PHE:HE2	2:S:182:LEU:HB3	1.65	0.61
2:S:90:VAL:HG13	2:S:149:VAL:CG2	2.30	0.61
1:L:49:ASP:O	1:L:51:VAL:N	2.34	0.61
1:L:134:ASP:O	1:L:135:SER:O	2.19	0.61
1:L:258:ILE:CG1	1:L:336:GLY:HA2	2.22	0.61
2:S:14:CYS:CA	2:S:54:PRO:HG2	2.31	0.61
2:S:34:LEU:C	2:S:35:ILE:HG13	2.25	0.61
2:S:89:GLN:HG2	2:S:90:VAL:H	1.64	0.61
2:S:158:GLN:HG2	2:S:159:PHE:N	2.16	0.61
1:L:19:SER:O	1:L:21:LEU:N	2.33	0.61
1:L:246:LEU:HB2	1:L:348:LEU:HD11	1.81	0.61
1:L:261:THR:HG22	1:L:285:ILE:CD1	2.30	0.61
1:L:266:ILE:HD13	1:L:299:PHE:HB3	1.83	0.61
1:L:182:TYR:CD1	1:L:182:TYR:N	2.69	0.61
1:L:232:PRO:O	1:L:236:ILE:HG21	2.01	0.61
1:L:285:ILE:CG1	1:L:286:VAL:N	2.63	0.61
2:S:75:ASN:ND2	2:S:117:MET:SD	2.74	0.61
2:S:14:CYS:CA	2:S:57:MET:SD	2.80	0.61
1:L:199:LYS:HG3	1:L:343:ASN:OD1	2.00	0.60
1:L:305:VAL:O	1:L:306:THR:HG23	2.01	0.60
1:L:30:VAL:N	1:L:165:ILE:O	2.33	0.60
1:L:206:VAL:CG1	1:L:333:SER:HA	2.32	0.60
1:L:227:PHE:HB2	2:S:180:PHE:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:ASN:O	1:L:315:ARG:N	2.34	0.60
1:L:330:ILE:O	1:L:331:HIS:HD2	1.84	0.60
1:L:255:SER:HB3	1:L:258:ILE:CB	2.24	0.60
1:L:297:LEU:HD12	1:L:299:PHE:CE1	2.20	0.60
1:L:301:GLN:O	1:L:305:VAL:HB	2.01	0.60
1:L:92:ILE:O	1:L:108:CYS:O	2.19	0.60
1:L:169:ASP:C	1:L:170:TRP:CD1	2.78	0.60
2:S:177:MET:CB	2:S:180:PHE:CZ	2.83	0.60
1:L:21:LEU:C	1:L:23:THR:N	2.58	0.60
1:L:282:PRO:HA	1:L:283:HIS:ND1	2.17	0.60
2:S:35:ILE:HD12	2:S:36:ASN:N	2.15	0.60
2:S:112:GLN:HB2	2:S:113:PRO:CD	2.18	0.60
2:S:130:GLY:C	2:S:131:PHE:HD2	2.08	0.60
1:L:70:GLY:N	1:L:136:TRP:HZ2	1.99	0.60
1:L:101:SER:OG	1:L:106:THR:HG21	2.01	0.60
1:L:142:SER:C	1:L:144:SER:H	2.07	0.60
1:L:204:GLN:NE2	1:L:258:ILE:HD13	2.16	0.60
1:L:67:VAL:C	1:L:68:ILE:HD12	2.26	0.60
1:L:286:VAL:HG22	1:L:344:LEU:HD11	1.84	0.60
2:S:70:ILE:HD13	2:S:163:MET:SD	2.41	0.60
2:S:86:TRP:CD1	2:S:113:PRO:HD3	2.37	0.60
1:L:75:THR:HG23	1:L:122:ASN:ND2	2.15	0.60
1:L:88:LEU:HD23	1:L:115:TRP:CE2	2.36	0.60
1:L:88:LEU:HD23	1:L:115:TRP:NE1	2.16	0.60
1:L:188:GLN:C	1:L:353:ASP:HA	2.26	0.60
1:L:217:ILE:HG13	1:L:310:THR:HG23	1.84	0.60
1:L:252:LYS:C	1:L:254:SER:H	2.09	0.60
1:L:270:ASN:HA	1:L:318:LEU:CG	2.31	0.60
1:L:105:TYR:CD2	1:L:105:TYR:O	2.55	0.60
1:L:130:ASN:CG	1:L:132:CYS:SG	2.85	0.60
1:L:262:VAL:H	1:L:286:VAL:CB	2.15	0.60
1:L:311:GLN:HG2	1:L:360:ASN:ND2	2.17	0.60
2:S:45:ASP:C	2:S:47:TRP:HD1	2.09	0.60
1:L:31:LEU:O	1:L:32:LEU:HD12	2.01	0.60
1:L:100:TYR:OH	1:L:147:ARG:NH1	2.35	0.60
1:L:213:MET:O	1:L:327:TYR:HB3	2.02	0.60
2:S:34:LEU:HD13	2:S:146:LEU:HB2	1.84	0.60
1:L:82:ASP:OD1	1:L:83:ASN:ND2	2.35	0.59
2:S:92:VAL:O	2:S:107:THR:HA	2.02	0.59
1:L:88:LEU:HB3	1:L:115:TRP:CZ2	2.37	0.59
1:L:193:LEU:HD23	1:L:232:PRO:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:VAL:HG22	1:L:329:ILE:HA	1.83	0.59
1:L:285:ILE:CG1	1:L:286:VAL:H	2.15	0.59
2:S:92:VAL:HG22	2:S:146:LEU:CD2	2.33	0.59
2:S:93:TYR:HB3	2:S:104:ASP:CG	2.27	0.59
1:L:17:ARG:HG3	1:L:17:ARG:O	2.01	0.59
1:L:181:ILE:HD13	2:S:170:ARG:NH1	2.17	0.59
1:L:250:VAL:HG21	1:L:344:LEU:HG	1.84	0.59
1:L:73:LYS:CB	1:L:173:VAL:HG22	2.33	0.59
1:L:266:ILE:HA	1:L:325:TYR:O	2.01	0.59
1:L:317:THR:OG1	1:L:318:LEU:N	2.36	0.59
2:S:57:MET:HG2	2:S:61:ARG:NH2	2.15	0.59
2:S:95:ARG:HE	2:S:98:MET:CG	2.10	0.59
1:L:23:THR:CG2	1:L:172:ILE:HG22	2.31	0.59
1:L:46:TYR:CD1	1:L:147:ARG:HG2	2.37	0.59
1:L:272:SER:O	1:L:274:ALA:N	2.35	0.59
1:L:238:MET:O	1:L:239:TRP:O	2.21	0.59
2:S:35:ILE:HB	2:S:66:LYS:NZ	2.18	0.59
1:L:15:SER:OG	1:L:68:ILE:HA	2.03	0.59
1:L:95:GLY:N	1:L:146:VAL:HG22	2.15	0.59
1:L:288:PHE:HD2	1:L:342:PHE:CE2	2.21	0.59
2:S:18:SER:O	2:S:20:PRO:HD3	2.03	0.59
1:L:192:PRO:O	1:L:193:LEU:HB3	2.02	0.59
1:L:199:LYS:HA	1:L:343:ASN:OD1	2.02	0.59
1:L:311:GLN:NE2	1:L:312:VAL:N	2.49	0.59
1:L:119:CYS:O	1:L:120:LYS:NZ	2.29	0.59
2:S:83:ARG:HH11	2:S:83:ARG:HG3	1.68	0.58
1:L:89:MET:HE1	1:L:196:TRP:CE3	2.37	0.58
1:L:120:LYS:HB3	1:L:120:LYS:NZ	2.17	0.58
1:L:210:VAL:O	1:L:210:VAL:HG12	2.02	0.58
1:L:271:LEU:HD21	1:L:275:PHE:HD2	1.68	0.58
2:S:14:CYS:HA	2:S:54:PRO:HG2	1.84	0.58
2:S:64:ALA:HB3	2:S:173:GLY:HA2	1.85	0.58
2:S:107:THR:CG2	2:S:108:PHE:N	2.66	0.58
1:L:113:MET:HG3	1:L:124:SER:O	2.03	0.58
1:L:195:ARG:NH2	1:L:217:ILE:HA	2.15	0.58
2:S:53:ASN:CA	2:S:61:ARG:HH22	2.15	0.58
2:S:96:GLN:HB3	2:S:142:THR:CG2	2.33	0.58
1:L:44:ASP:HB2	1:L:149:THR:HG22	1.85	0.58
1:L:227:PHE:CD2	2:S:181:PRO:CA	2.84	0.58
1:L:240:ARG:NH1	1:L:241:TYR:CD1	2.71	0.58
1:L:250:VAL:CG2	1:L:251:THR:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:HIS:ND1	1:L:283:HIS:N	2.52	0.58
2:S:69:THR:CB	2:S:166:ASP:HB2	2.33	0.58
1:L:318:LEU:C	1:L:320:ALA:H	2.11	0.58
1:L:198:GLY:HA2	1:L:346:VAL:CG2	2.34	0.58
1:L:199:LYS:C	1:L:200:LEU:HD23	2.28	0.58
2:S:125:ILE:HD12	2:S:130:GLY:O	2.03	0.58
2:S:130:GLY:C	2:S:131:PHE:CD2	2.82	0.58
1:L:241:TYR:HA	1:L:310:THR:H	1.68	0.58
1:L:246:LEU:HD12	1:L:246:LEU:H	1.69	0.58
2:S:35:ILE:HB	2:S:66:LYS:HZ3	1.69	0.58
2:S:57:MET:CG	2:S:61:ARG:HH21	2.15	0.58
2:S:70:ILE:O	2:S:71:HIS:ND1	2.37	0.58
2:S:106:ARG:NH1	2:S:106:ARG:CG	2.64	0.58
1:L:215:LEU:CB	1:L:325:TYR:HB2	2.21	0.58
2:S:81:VAL:HG23	2:S:81:VAL:O	2.02	0.58
1:L:240:ARG:HD2	1:L:241:TYR:CD1	2.39	0.58
1:L:247:HIS:HB2	1:L:298:VAL:N	2.18	0.57
2:S:86:TRP:NE1	2:S:88:GLY:H	2.02	0.57
1:L:266:ILE:HD13	1:L:303:GLU:OE2	2.03	0.57
2:S:92:VAL:HB	2:S:108:PHE:HB2	1.86	0.57
1:L:20:LEU:HD12	1:L:172:ILE:O	2.05	0.57
1:L:140:MET:SD	2:S:65:TRP:HH2	2.27	0.57
1:L:212:ARG:C	1:L:327:TYR:HA	2.29	0.57
1:L:238:MET:O	1:L:359:SER:HA	2.05	0.57
1:L:17:ARG:HH12	1:L:20:LEU:HD13	1.69	0.57
1:L:264:PHE:O	1:L:265:LEU:HB3	2.05	0.57
1:L:95:GLY:C	1:L:96:VAL:HG22	2.30	0.57
1:L:278:TYR:CD1	1:L:281:PHE:HE2	2.22	0.57
1:L:243:ARG:HH22	1:L:305:VAL:HG23	1.70	0.57
1:L:270:ASN:HB3	1:L:321:ASP:HB3	1.85	0.57
1:L:305:VAL:O	1:L:305:VAL:HG22	2.04	0.57
2:S:70:ILE:HA	2:S:164:ARG:O	2.04	0.57
1:L:165:ILE:H	1:L:165:ILE:CD1	2.12	0.57
2:S:71:HIS:CA	2:S:120:PHE:O	2.50	0.57
2:S:89:GLN:HG2	2:S:90:VAL:N	2.20	0.57
1:L:36:MET:HE2	1:L:40:ASP:HB3	1.86	0.57
1:L:143:ARG:CA	2:S:137:PRO:HB2	2.34	0.57
2:S:106:ARG:CG	2:S:107:THR:H	2.16	0.57
1:L:15:SER:HA	1:L:68:ILE:HA	1.87	0.57
1:L:42:LEU:O	1:L:43:LEU:HB2	2.03	0.57
1:L:193:LEU:O	1:L:232:PRO:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:PHE:CE2	2:S:182:LEU:N	2.72	0.57
1:L:250:VAL:CG2	1:L:344:LEU:HG	2.35	0.57
1:L:73:LYS:CB	1:L:126:THR:HG22	2.21	0.57
1:L:210:VAL:HB	1:L:273:ASP:CB	2.35	0.57
2:S:94:LEU:CB	2:S:146:LEU:HG	2.20	0.57
1:L:10:LEU:HD13	1:L:10:LEU:C	2.30	0.56
2:S:86:TRP:CD1	2:S:87:ASP:N	2.73	0.56
1:L:248:PHE:O	1:L:296:THR:C	2.48	0.56
1:L:262:VAL:H	1:L:286:VAL:HB	1.69	0.56
1:L:268:PHE:N	1:L:327:TYR:CE1	2.73	0.56
1:L:19:SER:O	1:L:22:ASP:N	2.39	0.56
1:L:54:GLN:HG2	1:L:56:PHE:CE1	2.34	0.56
1:L:94:SER:O	2:S:176:LEU:HG	2.06	0.56
1:L:170:TRP:CD1	1:L:170:TRP:N	2.73	0.56
1:L:184:LEU:HG	1:L:235:TRP:CZ2	2.40	0.56
1:L:230:ASN:HD21	1:L:233:ASN:HB2	1.67	0.56
1:L:243:ARG:HH22	1:L:305:VAL:CG2	2.19	0.56
1:L:311:GLN:HE22	1:L:363:ILE:HD12	1.71	0.56
1:L:362:GLY:O	1:L:363:ILE:HG13	2.05	0.56
2:S:86:TRP:CG	2:S:87:ASP:N	2.72	0.56
2:S:95:ARG:HG3	2:S:96:GLN:N	2.20	0.56
2:S:96:GLN:HG2	2:S:142:THR:HG23	1.86	0.56
2:S:138:TRP:HE3	2:S:139:ALA:N	2.02	0.56
1:L:70:GLY:N	1:L:136:TRP:CZ2	2.73	0.56
1:L:89:MET:CA	1:L:115:TRP:CZ3	2.88	0.56
1:L:202:PHE:HB2	1:L:342:PHE:HB3	1.88	0.56
2:S:60:LEU:HD21	2:S:70:ILE:HD11	1.87	0.56
2:S:81:VAL:HB	2:S:85:ASP:O	2.05	0.56
2:S:127:PRO:HD3	2:S:132:GLU:HB3	1.88	0.56
1:L:120:LYS:O	1:L:121:LYS:HD3	2.06	0.56
1:L:242:PHE:HZ	1:L:246:LEU:HD11	1.68	0.56
1:L:263:THR:N	1:L:285:ILE:HD12	2.20	0.56
1:L:17:ARG:NH2	1:L:20:LEU:HD22	2.16	0.56
1:L:240:ARG:NH1	1:L:241:TYR:CE1	2.73	0.56
1:L:244:GLY:HA2	1:L:301:GLN:NE2	2.21	0.56
2:S:19:THR:CB	2:S:156:ILE:O	2.53	0.56
1:L:227:PHE:CZ	2:S:182:LEU:HD22	2.41	0.56
2:S:86:TRP:HH2	2:S:156:ILE:HD11	1.70	0.56
2:S:107:THR:CG2	2:S:108:PHE:H	2.18	0.56
1:L:184:LEU:HD21	2:S:165:PHE:HE1	1.69	0.56
1:L:220:GLY:HA2	1:L:230:ASN:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:336:GLY:O	1:L:338:ILE:HD12	2.06	0.56
1:L:337:THR:C	1:L:338:ILE:HG13	2.31	0.56
1:L:29:ARG:HD3	1:L:165:ILE:HD11	1.87	0.56
1:L:89:MET:CE	1:L:104:VAL:HB	2.36	0.56
1:L:264:PHE:CB	1:L:297:LEU:HD11	2.35	0.56
1:L:363:ILE:O	1:L:364:ASP:HB2	2.06	0.56
2:S:21:PRO:O	2:S:24:PHE:HB2	2.06	0.56
2:S:91:PHE:CD1	2:S:149:VAL:HG21	2.41	0.56
1:L:127:PHE:CE1	1:L:129:PRO:HD3	2.42	0.55
1:L:128:ASN:ND2	1:L:136:TRP:HE1	2.04	0.55
1:L:29:ARG:HG3	1:L:167:LYS:HE2	1.88	0.55
1:L:74:VAL:HG13	1:L:169:ASP:O	2.05	0.55
1:L:156:TRP:H	1:L:156:TRP:HD1	1.54	0.55
1:L:183:HIS:NE2	1:L:185:ALA:CB	2.69	0.55
1:L:235:TRP:CZ3	2:S:171:VAL:HG12	2.41	0.55
1:L:140:MET:HA	2:S:138:TRP:HD1	1.71	0.55
2:S:125:ILE:CG1	2:S:126:GLY:H	2.19	0.55
1:L:141:ILE:HG22	1:L:146:VAL:HG21	1.89	0.55
1:L:188:GLN:O	1:L:354:PHE:N	2.36	0.55
2:S:96:GLN:CA	2:S:143:THR:O	2.50	0.55
1:L:143:ARG:O	2:S:137:PRO:HD2	2.06	0.55
1:L:202:PHE:HD1	1:L:342:PHE:HB3	1.70	0.55
1:L:221:ALA:O	1:L:228:LEU:N	2.39	0.55
1:L:71:LYS:HE2	1:L:126:THR:HB	1.89	0.55
1:L:195:ARG:O	1:L:197:MET:SD	2.65	0.55
1:L:250:VAL:HG22	1:L:251:THR:N	2.20	0.55
2:S:14:CYS:SG	2:S:57:MET:HE1	2.46	0.55
1:L:108:CYS:O	1:L:110:GLN:N	2.40	0.55
1:L:262:VAL:O	1:L:286:VAL:HG23	2.07	0.55
2:S:166:ASP:HB3	2:S:167:PRO:CD	2.36	0.55
1:L:40:ASP:O	1:L:42:LEU:HG	2.06	0.55
1:L:200:LEU:O	1:L:202:PHE:CD2	2.60	0.55
2:S:68:GLY:HA3	2:S:169:PHE:CA	2.33	0.55
1:L:17:ARG:HH12	1:L:20:LEU:HD11	1.70	0.55
1:L:86:CYS:HA	1:L:253:MET:O	2.07	0.55
1:L:92:ILE:HG21	1:L:127:PHE:CD2	2.42	0.55
1:L:98:GLY:O	1:L:100:TYR:N	2.39	0.55
2:S:2:PRO:C	2:S:4:CYS:H	2.15	0.55
1:L:252:LYS:HZ1	1:L:256:PRO:HG3	1.71	0.55
2:S:64:ALA:H	2:S:173:GLY:HA2	1.72	0.55
2:S:127:PRO:CD	2:S:132:GLU:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:149:VAL:CG1	2:S:150:ALA:H	2.11	0.55
1:L:216:SER:OG	1:L:367:ARG:NH1	2.41	0.54
1:L:330:ILE:O	1:L:331:HIS:CD2	2.61	0.54
2:S:33:ASP:OD2	2:S:39:ILE:HG22	2.07	0.54
1:L:27:GLN:N	1:L:54:GLN:OE1	2.40	0.54
1:L:210:VAL:HG21	1:L:278:TYR:HD2	1.73	0.54
1:L:245:GLU:O	1:L:351:ILE:HG13	2.06	0.54
2:S:95:ARG:HD3	2:S:104:ASP:HA	1.89	0.54
1:L:140:MET:HE3	1:L:141:ILE:HG23	1.90	0.54
1:L:220:GLY:HA3	1:L:228:LEU:O	2.08	0.54
1:L:261:THR:CG2	1:L:285:ILE:HG12	2.37	0.54
2:S:71:HIS:NE2	2:S:166:ASP:OD1	2.39	0.54
1:L:17:ARG:NH2	1:L:19:SER:HA	2.22	0.54
1:L:143:ARG:HB3	2:S:137:PRO:C	2.32	0.54
2:S:35:ILE:CG1	2:S:144:TRP:HB2	2.38	0.54
2:S:63:ALA:O	2:S:66:LYS:HD2	2.07	0.54
2:S:71:HIS:CE1	2:S:121:SER:HG	2.21	0.54
1:L:318:LEU:HD23	1:L:319:GLU:OE2	2.08	0.54
2:S:55:PRO:HG2	2:S:56:ILE:HG13	1.90	0.54
1:L:202:PHE:HB2	1:L:342:PHE:CB	2.38	0.54
2:S:89:GLN:CG	2:S:90:VAL:H	2.20	0.54
1:L:23:THR:HG22	1:L:171:SER:OG	2.08	0.54
1:L:193:LEU:CD2	1:L:232:PRO:HB2	2.38	0.54
1:L:27:GLN:HB2	1:L:54:GLN:OE1	2.07	0.54
1:L:72:ILE:N	1:L:127:PHE:O	2.41	0.54
1:L:193:LEU:HD13	1:L:194:ASN:H	1.73	0.54
1:L:20:LEU:CG	1:L:73:LYS:HE2	2.31	0.54
1:L:46:TYR:CB	1:L:49:ASP:HB3	2.37	0.54
1:L:72:ILE:HB	1:L:127:PHE:O	2.08	0.54
1:L:248:PHE:CA	1:L:347:LYS:O	2.45	0.54
1:L:299:PHE:HD2	1:L:303:GLU:OE1	1.91	0.54
1:L:89:MET:HA	1:L:115:TRP:CZ3	2.43	0.53
1:L:187:CYS:HA	1:L:355:CYS:HA	1.89	0.53
1:L:191:LEU:CD1	1:L:193:LEU:HD12	2.38	0.53
1:L:240:ARG:HD2	1:L:241:TYR:CE1	2.43	0.53
1:L:202:PHE:O	1:L:342:PHE:N	2.41	0.53
1:L:234:SER:HB3	2:S:59:VAL:CG2	2.38	0.53
2:S:54:PRO:HD2	2:S:61:ARG:NH2	2.24	0.53
1:L:74:VAL:CG1	1:L:170:TRP:CD1	2.84	0.53
1:L:91:ALA:O	1:L:148:MET:HB2	2.07	0.53
1:L:184:LEU:HG	1:L:235:TRP:HZ2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:VAL:HG11	1:L:333:SER:HA	1.90	0.53
1:L:314:PRO:CD	1:L:365:GLY:HA3	2.39	0.53
2:S:19:THR:OG1	2:S:156:ILE:HG22	2.09	0.53
2:S:86:TRP:NE1	2:S:88:GLY:N	2.57	0.53
2:S:122:PHE:CE2	2:S:124:ILE:HG12	2.43	0.53
1:L:60:VAL:C	1:L:64:ARG:HB2	2.32	0.53
1:L:235:TRP:CD1	1:L:238:MET:HE2	2.44	0.53
1:L:310:THR:O	1:L:310:THR:HG22	2.08	0.53
2:S:14:CYS:O	2:S:52:TYR:HB2	2.08	0.53
2:S:171:VAL:HG22	2:S:172:ALA:H	1.74	0.53
1:L:300:SER:O	1:L:304:PHE:HD2	1.91	0.53
2:S:74:LEU:CD2	2:S:118:LEU:HD23	2.37	0.53
2:S:152:ASN:HB3	2:S:155:GLN:HE21	1.73	0.53
1:L:245:GLU:HB3	1:L:352:LYS:HB3	1.91	0.53
1:L:286:VAL:HG12	1:L:287:GLN:N	2.24	0.53
1:L:309:SER:O	1:L:311:GLN:N	2.42	0.53
1:L:351:ILE:HG21	1:L:354:PHE:HD2	1.73	0.53
2:S:141:GLN:CG	2:S:142:THR:H	2.14	0.53
1:L:30:VAL:O	1:L:30:VAL:CG2	2.57	0.53
1:L:193:LEU:HD21	1:L:195:ARG:HB2	1.91	0.53
1:L:197:MET:HG2	1:L:346:VAL:CG1	2.39	0.53
1:L:300:SER:OG	1:L:301:GLN:N	2.40	0.53
2:S:69:THR:OG1	2:S:168:ASN:HB2	2.09	0.53
1:L:31:LEU:C	1:L:32:LEU:HD12	2.34	0.53
1:L:72:ILE:CA	1:L:172:ILE:HD12	2.39	0.53
1:L:100:TYR:HA	2:S:178:PRO:HB3	1.89	0.53
1:L:262:VAL:HG22	1:L:330:ILE:HA	1.90	0.53
2:S:58:ASN:O	2:S:62:THR:N	2.39	0.53
1:L:91:ALA:O	1:L:148:MET:HA	2.09	0.53
1:L:201:THR:O	1:L:211:ARG:NH2	2.42	0.53
1:L:214:PRO:HG3	1:L:367:ARG:NE	2.24	0.53
2:S:110:ILE:HG23	2:S:111:SER:N	2.23	0.53
1:L:269:GLY:O	1:L:318:LEU:HD12	2.09	0.52
2:S:50:HIS:HB3	2:S:52:TYR:OH	2.09	0.52
2:S:67:SER:O	2:S:169:PHE:HA	2.08	0.52
2:S:74:LEU:CB	2:S:118:LEU:HD23	2.31	0.52
2:S:133:PHE:O	2:S:141:GLN:HG2	2.09	0.52
1:L:74:VAL:HG22	1:L:170:TRP:CD2	2.44	0.52
1:L:89:MET:HE3	1:L:104:VAL:HB	1.91	0.52
1:L:204:GLN:NE2	1:L:340:GLY:C	2.67	0.52
2:S:107:THR:HG22	2:S:108:PHE:H	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:109:VAL:O	2:S:110:ILE:HG22	2.08	0.52
1:L:47:LEU:HD21	1:L:146:VAL:HB	1.91	0.52
1:L:54:GLN:O	1:L:56:PHE:HD1	1.92	0.52
1:L:193:LEU:HD22	1:L:194:ASN:N	2.25	0.52
1:L:195:ARG:N	1:L:232:PRO:HB2	2.24	0.52
1:L:198:GLY:HA2	1:L:346:VAL:N	2.23	0.52
1:L:338:ILE:CG2	1:L:339:SER:N	2.71	0.52
1:L:354:PHE:O	1:L:354:PHE:CD1	2.62	0.52
1:L:85:GLY:C	1:L:86:CYS:SG	2.91	0.52
1:L:104:VAL:HG21	1:L:153:VAL:CG2	2.38	0.52
1:L:176:LYS:H	1:L:176:LYS:HD2	1.75	0.52
1:L:234:SER:HB3	2:S:59:VAL:HG22	1.91	0.52
2:S:69:THR:O	2:S:169:PHE:CE2	2.63	0.52
1:L:239:TRP:HB2	1:L:357:ILE:C	2.33	0.52
2:S:22:ALA:CB	2:S:154:ARG:NH1	2.73	0.52
2:S:112:GLN:CB	2:S:113:PRO:CD	2.85	0.52
1:L:128:ASN:HD21	1:L:136:TRP:NE1	2.06	0.52
1:L:256:PRO:C	1:L:259:LYS:HZ1	2.18	0.52
2:S:122:PHE:CD2	2:S:124:ILE:HG12	2.45	0.52
1:L:88:LEU:HD23	1:L:115:TRP:HE1	1.73	0.52
1:L:120:LYS:CE	1:L:121:LYS:H	2.10	0.52
1:L:168:LEU:HG	1:L:170:TRP:NE1	2.15	0.52
1:L:212:ARG:CB	1:L:327:TYR:HB2	2.40	0.52
1:L:311:GLN:CG	1:L:360:ASN:ND2	2.73	0.52
2:S:37:GLY:O	2:S:39:ILE:HG23	2.09	0.52
2:S:45:ASP:HA	2:S:47:TRP:CD1	2.45	0.52
2:S:86:TRP:CZ2	2:S:88:GLY:CA	2.88	0.52
1:L:92:ILE:O	1:L:110:GLN:HB3	2.10	0.52
1:L:4:ASN:C	1:L:6:PHE:N	2.66	0.52
1:L:224:THR:O	1:L:225:GLN:C	2.51	0.52
1:L:33:SER:CB	1:L:36:MET:SD	2.97	0.51
1:L:47:LEU:HG	1:L:141:ILE:HB	1.93	0.51
1:L:55:ASP:C	1:L:56:PHE:CD1	2.88	0.51
2:S:14:CYS:SG	2:S:57:MET:CE	2.98	0.51
1:L:88:LEU:HA	1:L:151:ILE:O	2.10	0.51
1:L:96:VAL:HG12	2:S:176:LEU:HB2	1.91	0.51
2:S:31:THR:H	2:S:41:PRO:HB3	1.74	0.51
2:S:151:THR:O	2:S:152:ASN:OD1	2.28	0.51
1:L:3:GLN:C	1:L:5:LEU:H	2.18	0.51
1:L:80:ILE:HD12	1:L:156:TRP:CZ2	2.45	0.51
1:L:265:LEU:O	1:L:266:ILE:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:96:GLN:C	2:S:145:TYR:HE1	2.19	0.51
1:L:42:LEU:O	1:L:150:VAL:HG23	2.11	0.51
1:L:242:PHE:HZ	1:L:246:LEU:CD1	2.23	0.51
1:L:251:THR:O	1:L:253:MET:SD	2.68	0.51
2:S:34:LEU:HD22	2:S:146:LEU:HB2	1.92	0.51
1:L:91:ALA:HB3	1:L:149:THR:N	2.26	0.51
1:L:214:PRO:HG3	1:L:367:ARG:CZ	2.41	0.51
1:L:259:LYS:HA	1:L:342:PHE:CZ	2.46	0.51
1:L:264:PHE:HD1	1:L:284:ARG:O	1.93	0.51
2:S:96:GLN:HB3	2:S:142:THR:HG23	1.92	0.51
1:L:266:ILE:HG12	1:L:304:PHE:HE1	1.69	0.51
2:S:58:ASN:HA	2:S:61:ARG:NE	2.25	0.51
1:L:22:ASP:OD2	1:L:57:ARG:HG2	2.11	0.51
1:L:32:LEU:O	1:L:163:ASP:CA	2.58	0.51
2:S:65:TRP:CD1	2:S:172:ALA:HB1	2.46	0.51
1:L:19:SER:C	1:L:21:LEU:N	2.69	0.51
1:L:25:PHE:HE2	1:L:171:SER:HA	1.74	0.51
1:L:30:VAL:O	1:L:165:ILE:C	2.54	0.51
1:L:186:ASP:HB3	1:L:239:TRP:CE3	2.45	0.51
1:L:236:ILE:O	1:L:236:ILE:CG2	2.56	0.51
1:L:72:ILE:HG22	1:L:170:TRP:HE3	1.76	0.51
1:L:127:PHE:CD1	1:L:129:PRO:HD3	2.45	0.51
1:L:136:TRP:HH2	1:L:172:ILE:HG12	1.76	0.51
1:L:242:PHE:CZ	1:L:246:LEU:CD2	2.85	0.51
1:L:41:VAL:HA	1:L:151:ILE:HB	1.93	0.51
1:L:165:ILE:HD13	1:L:165:ILE:N	2.16	0.51
1:L:278:TYR:HE1	1:L:281:PHE:CE2	2.29	0.51
2:S:13:PRO:CA	2:S:162:ASN:HA	2.39	0.51
2:S:30:VAL:CG2	2:S:41:PRO:HG3	2.41	0.51
2:S:35:ILE:HG13	2:S:144:TRP:HB2	1.93	0.51
1:L:31:LEU:HA	1:L:165:ILE:CG2	2.41	0.50
1:L:31:LEU:HA	1:L:165:ILE:HB	1.93	0.50
1:L:242:PHE:HB3	1:L:310:THR:HG1	1.75	0.50
1:L:284:ARG:NH2	1:L:298:VAL:O	2.43	0.50
1:L:136:TRP:CZ2	1:L:172:ILE:HD11	2.46	0.50
1:L:206:VAL:O	1:L:207:THR:C	2.54	0.50
2:S:29:ALA:N	2:S:150:ALA:HB3	2.26	0.50
2:S:112:GLN:NE2	2:S:113:PRO:HG2	2.26	0.50
2:S:167:PRO:C	2:S:169:PHE:H	2.17	0.50
1:L:238:MET:C	1:L:239:TRP:O	2.50	0.50
1:L:352:LYS:O	1:L:352:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:91:PHE:O	2:S:91:PHE:HD1	1.95	0.50
2:S:92:VAL:HB	2:S:108:PHE:CB	2.42	0.50
1:L:20:LEU:HB3	1:L:73:LYS:HZ1	1.72	0.50
1:L:194:ASN:OD1	1:L:349:VAL:HG22	2.12	0.50
2:S:35:ILE:HA	2:S:163:MET:HE1	1.93	0.50
2:S:126:GLY:HA3	2:S:131:PHE:HA	1.93	0.50
1:L:199:LYS:CG	1:L:343:ASN:HD21	2.14	0.50
1:L:245:GLU:O	1:L:351:ILE:HA	2.11	0.50
1:L:313:ASN:HA	1:L:363:ILE:HG21	1.93	0.50
2:S:92:VAL:O	2:S:107:THR:HG23	2.10	0.50
2:S:96:GLN:HB3	2:S:142:THR:CB	2.42	0.50
1:L:48:TYR:CZ	1:L:62:PHE:HE2	2.27	0.50
1:L:257:TYR:N	1:L:259:LYS:HZ1	2.09	0.50
1:L:284:ARG:HH22	1:L:298:VAL:HG12	1.76	0.50
1:L:359:SER:OG	1:L:360:ASN:N	2.45	0.50
2:S:55:PRO:O	2:S:59:VAL:CG2	2.60	0.50
2:S:94:LEU:HD22	2:S:146:LEU:HG	1.93	0.50
1:L:30:VAL:O	1:L:165:ILE:CA	2.60	0.50
1:L:76:ALA:HB2	1:L:168:LEU:CD1	2.41	0.50
1:L:123:PHE:CD2	1:L:124:SER:N	2.80	0.50
2:S:76:VAL:O	2:S:115:SER:HA	2.12	0.50
1:L:264:PHE:HB2	1:L:297:LEU:HD11	1.94	0.50
1:L:300:SER:O	1:L:304:PHE:CD2	2.64	0.50
1:L:325:TYR:HE1	1:L:327:TYR:CB	2.24	0.50
2:S:69:THR:HB	2:S:166:ASP:CG	2.36	0.50
2:S:90:VAL:O	2:S:110:ILE:HG22	2.12	0.50
1:L:314:PRO:HD3	1:L:365:GLY:HA3	1.93	0.50
1:L:362:GLY:C	1:L:363:ILE:HG13	2.37	0.50
1:L:19:SER:C	1:L:21:LEU:H	2.20	0.49
2:S:143:THR:HG22	2:S:144:TRP:N	2.24	0.49
1:L:71:LYS:O	1:L:173:VAL:HG23	2.12	0.49
1:L:199:LYS:CA	1:L:343:ASN:OD1	2.60	0.49
1:L:243:ARG:HH11	1:L:243:ARG:CG	2.25	0.49
1:L:248:PHE:O	1:L:296:THR:CA	2.60	0.49
1:L:258:ILE:HG22	1:L:342:PHE:CE1	2.47	0.49
2:S:180:PHE:N	2:S:181:PRO:HD3	2.27	0.49
1:L:20:LEU:HD22	1:L:20:LEU:H	1.78	0.49
1:L:73:LYS:HB2	1:L:173:VAL:CG2	2.42	0.49
1:L:210:VAL:CG1	1:L:328:ALA:O	2.60	0.49
2:S:57:MET:C	2:S:59:VAL:N	2.66	0.49
2:S:67:SER:OG	2:S:170:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:86:TRP:CZ2	2:S:113:PRO:HA	2.47	0.49
1:L:20:LEU:HG	1:L:73:LYS:CE	2.35	0.49
1:L:184:LEU:O	1:L:186:ASP:N	2.45	0.49
1:L:256:PRO:HB3	1:L:290:GLU:CG	2.43	0.49
2:S:70:ILE:C	2:S:71:HIS:ND1	2.70	0.49
2:S:77:ARG:HB2	2:S:158:GLN:HB3	1.93	0.49
2:S:158:GLN:CG	2:S:159:PHE:N	2.75	0.49
1:L:140:MET:SD	2:S:65:TRP:CZ3	3.05	0.49
1:L:237:SER:O	1:L:238:MET:HG2	2.12	0.49
2:S:18:SER:OG	2:S:158:GLN:HB2	2.12	0.49
2:S:53:ASN:HA	2:S:61:ARG:NH1	2.27	0.49
2:S:56:ILE:O	2:S:59:VAL:HB	2.13	0.49
2:S:177:MET:HB3	2:S:180:PHE:HZ	1.69	0.49
1:L:103:ASP:CG	1:L:106:THR:OG1	2.55	0.49
1:L:242:PHE:CE2	1:L:246:LEU:HD11	2.48	0.49
2:S:39:ILE:HD12	2:S:39:ILE:C	2.37	0.49
1:L:33:SER:HB3	1:L:36:MET:CE	2.42	0.49
1:L:195:ARG:HB2	1:L:348:LEU:HB2	1.93	0.49
1:L:210:VAL:CG1	1:L:329:ILE:HG13	2.42	0.49
1:L:245:GLU:CG	1:L:352:LYS:HB3	2.42	0.49
2:S:97:SER:O	2:S:98:MET:HB2	2.12	0.49
2:S:126:GLY:HA3	2:S:132:GLU:N	2.27	0.49
2:S:94:LEU:HD21	2:S:120:PHE:HZ	1.77	0.49
1:L:7:ALA:HA	1:L:11:ASP:OD2	2.13	0.49
1:L:191:LEU:HB2	1:L:354:PHE:CD2	2.48	0.49
1:L:202:PHE:HE2	1:L:211:ARG:CG	2.24	0.49
1:L:227:PHE:CE2	2:S:182:LEU:HD22	2.48	0.49
1:L:265:LEU:HD11	1:L:281:PHE:C	2.38	0.49
2:S:16:ILE:HG22	2:S:52:TYR:OH	2.13	0.49
1:L:151:ILE:CG1	1:L:152:CYS:N	2.75	0.48
1:L:189:ASN:HA	1:L:353:ASP:HA	1.94	0.48
1:L:268:PHE:HB3	1:L:270:ASN:OD1	2.13	0.48
2:S:60:LEU:O	2:S:66:LYS:HE3	2.13	0.48
2:S:75:ASN:HA	2:S:117:MET:HA	1.94	0.48
2:S:92:VAL:HG13	2:S:146:LEU:HD21	1.95	0.48
1:L:72:ILE:CB	1:L:127:PHE:O	2.61	0.48
1:L:202:PHE:HB2	1:L:342:PHE:CA	2.42	0.48
2:S:19:THR:HG23	2:S:47:TRP:CH2	2.48	0.48
1:L:32:LEU:HD13	1:L:165:ILE:HA	1.94	0.48
1:L:70:GLY:O	1:L:136:TRP:HZ2	1.96	0.48
1:L:153:VAL:HG11	1:L:196:TRP:HZ2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:ARG:HH12	1:L:305:VAL:HA	1.79	0.48
2:S:15:MET:C	2:S:52:TYR:CE2	2.91	0.48
2:S:19:THR:CA	2:S:47:TRP:CZ3	2.95	0.48
1:L:182:TYR:CD1	1:L:235:TRP:CZ3	2.85	0.48
1:L:252:LYS:HB3	1:L:293:GLU:HB3	1.90	0.48
1:L:284:ARG:HG2	1:L:284:ARG:HH11	1.79	0.48
2:S:92:VAL:CG2	2:S:146:LEU:HD21	2.43	0.48
2:S:177:MET:C	2:S:180:PHE:CZ	2.87	0.48
1:L:26:ALA:C	1:L:54:GLN:OE1	2.56	0.48
1:L:49:ASP:O	1:L:50:VAL:C	2.57	0.48
1:L:72:ILE:HA	1:L:172:ILE:HA	1.95	0.48
1:L:106:THR:HG23	1:L:228:LEU:CD1	2.36	0.48
1:L:197:MET:CE	1:L:348:LEU:HD22	2.44	0.48
1:L:262:VAL:CG2	1:L:330:ILE:HA	2.43	0.48
1:L:363:ILE:HG22	1:L:364:ASP:N	2.28	0.48
2:S:27:VAL:HG22	2:S:151:THR:C	2.38	0.48
2:S:90:VAL:HG12	2:S:91:PHE:N	2.28	0.48
2:S:164:ARG:HH21	2:S:166:ASP:HA	1.77	0.48
1:L:30:VAL:O	1:L:165:ILE:O	2.32	0.48
1:L:202:PHE:HB2	1:L:342:PHE:C	2.38	0.48
1:L:220:GLY:HA2	1:L:230:ASN:ND2	2.28	0.48
2:S:95:ARG:HG2	2:S:98:MET:CG	2.41	0.48
2:S:152:ASN:HD22	2:S:155:GLN:NE2	2.11	0.48
1:L:240:ARG:O	1:L:310:THR:HB	2.13	0.48
1:L:367:ARG:C	1:L:369:LEU:N	2.71	0.48
2:S:95:ARG:NH1	2:S:102:SER:HB3	2.29	0.48
1:L:110:GLN:OE1	2:S:174:ASN:HB3	2.13	0.48
1:L:207:THR:O	1:L:209:GLU:N	2.45	0.48
1:L:242:PHE:O	1:L:308:TRP:CZ2	2.67	0.48
2:S:75:ASN:HD22	2:S:117:MET:HB3	1.77	0.48
1:L:13:THR:O	1:L:65:THR:O	2.32	0.48
1:L:73:LYS:HB3	1:L:73:LYS:HE3	1.66	0.48
1:L:197:MET:SD	1:L:197:MET:N	2.87	0.48
1:L:214:PRO:HA	1:L:325:TYR:CE2	2.49	0.48
2:S:57:MET:HE3	2:S:60:LEU:CD1	2.43	0.48
1:L:268:PHE:CZ	1:L:324:PRO:HG3	2.47	0.48
1:L:299:PHE:HB3	1:L:303:GLU:OE2	2.14	0.48
2:S:16:ILE:HG22	2:S:16:ILE:O	2.13	0.48
2:S:74:LEU:O	2:S:117:MET:HA	2.14	0.48
2:S:90:VAL:CG1	2:S:91:PHE:N	2.77	0.48
2:S:122:PHE:CG	2:S:144:TRP:CZ3	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:154:ARG:O	2:S:155:GLN:NE2	2.46	0.48
1:L:100:TYR:OH	1:L:147:ARG:HD3	2.14	0.47
1:L:214:PRO:HB3	1:L:367:ARG:NH2	2.28	0.47
2:S:34:LEU:HB2	2:S:145:TYR:N	2.28	0.47
1:L:38:GLY:O	1:L:152:CYS:SG	2.67	0.47
1:L:197:MET:SD	1:L:346:VAL:C	2.98	0.47
1:L:302:GLN:OE1	1:L:302:GLN:N	2.47	0.47
1:L:351:ILE:HG23	1:L:352:LYS:N	2.27	0.47
2:S:77:ARG:O	2:S:157:GLN:N	2.47	0.47
2:S:91:PHE:CD1	2:S:91:PHE:N	2.79	0.47
1:L:148:MET:SD	1:L:149:THR:N	2.87	0.47
2:S:8:SER:O	2:S:9:ASP:O	2.33	0.47
2:S:155:GLN:O	2:S:156:ILE:HD13	2.15	0.47
2:S:165:PHE:CE1	2:S:169:PHE:HB3	2.49	0.47
1:L:67:VAL:HG22	1:L:136:TRP:C	2.40	0.47
1:L:227:PHE:HE2	2:S:182:LEU:N	2.12	0.47
1:L:256:PRO:CB	1:L:290:GLU:HG2	2.45	0.47
1:L:263:THR:C	1:L:264:PHE:CD1	2.93	0.47
2:S:17:ALA:O	2:S:158:GLN:HG3	2.15	0.47
2:S:58:ASN:CA	2:S:61:ARG:HB2	2.42	0.47
1:L:141:ILE:HD12	1:L:142:SER:N	2.29	0.47
1:L:216:SER:O	1:L:310:THR:HA	2.14	0.47
2:S:128:ASN:O	2:S:129:SER:C	2.57	0.47
1:L:86:CYS:H	1:L:116:ASN:CG	2.22	0.47
1:L:100:TYR:HA	2:S:178:PRO:CA	2.44	0.47
1:L:239:TRP:HA	1:L:358:GLY:C	2.34	0.47
1:L:363:ILE:HG22	1:L:364:ASP:H	1.79	0.47
2:S:19:THR:N	2:S:157:GLN:O	2.48	0.47
2:S:20:PRO:HB2	2:S:24:PHE:CZ	2.50	0.47
2:S:84:ALA:C	2:S:86:TRP:H	2.23	0.47
1:L:21:LEU:O	1:L:57:ARG:CB	2.63	0.47
1:L:30:VAL:O	1:L:165:ILE:HA	2.14	0.47
1:L:88:LEU:CD2	1:L:115:TRP:HE1	2.27	0.47
1:L:88:LEU:CD2	1:L:115:TRP:NE1	2.77	0.47
1:L:31:LEU:HB2	1:L:42:LEU:CB	2.44	0.47
1:L:39:GLY:CA	1:L:151:ILE:HD11	2.45	0.47
1:L:40:ASP:N	1:L:151:ILE:HG13	2.29	0.47
1:L:245:GLU:HB2	1:L:300:SER:HB2	1.97	0.47
1:L:283:HIS:O	1:L:284:ARG:HB2	2.15	0.47
2:S:45:ASP:C	2:S:47:TRP:CD1	2.92	0.47
2:S:99:ASN:C	2:S:101:GLU:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:122:PHE:HB2	2:S:144:TRP:CZ3	2.50	0.47
2:S:152:ASN:O	2:S:155:GLN:HB2	2.15	0.47
1:L:17:ARG:O	1:L:17:ARG:CG	2.62	0.47
1:L:46:TYR:HB2	1:L:49:ASP:HB3	1.96	0.47
1:L:50:VAL:HG13	1:L:51:VAL:HG23	1.97	0.47
1:L:107:ILE:O	1:L:108:CYS:HB3	2.14	0.47
1:L:141:ILE:CA	1:L:144:SER:HB2	2.45	0.47
1:L:227:PHE:HB3	1:L:366:SER:OG	2.15	0.47
2:S:35:ILE:HG22	2:S:60:LEU:HD22	1.97	0.47
2:S:184:THR:HG23	2:S:185:GLU:H	1.80	0.47
1:L:242:PHE:CZ	1:L:246:LEU:CD1	2.93	0.46
1:L:323:CYS:HA	1:L:324:PRO:HD3	1.59	0.46
2:S:13:PRO:O	2:S:14:CYS:SG	2.73	0.46
2:S:91:PHE:CD1	2:S:149:VAL:CG2	2.98	0.46
1:L:119:CYS:HG	1:L:293:GLU:CD	2.22	0.46
1:L:284:ARG:HH22	1:L:298:VAL:CB	2.29	0.46
2:S:82:LYS:O	2:S:85:ASP:N	2.48	0.46
2:S:149:VAL:O	2:S:150:ALA:HB2	2.15	0.46
1:L:97:ARG:HH12	2:S:38:LYS:HG2	1.80	0.46
1:L:191:LEU:CG	1:L:193:LEU:HD12	2.46	0.46
1:L:194:ASN:HB3	1:L:347:LYS:HE3	1.97	0.46
1:L:249:GLU:HA	1:L:295:CYS:O	2.15	0.46
2:S:53:ASN:C	2:S:61:ARG:HH22	2.23	0.46
2:S:75:ASN:OD1	2:S:116:ALA:N	2.49	0.46
2:S:177:MET:CB	2:S:180:PHE:HZ	2.26	0.46
1:L:98:GLY:O	1:L:100:TYR:CD1	2.56	0.46
1:L:266:ILE:HG23	1:L:324:PRO:CB	2.32	0.46
1:L:278:TYR:CE1	1:L:281:PHE:CZ	3.04	0.46
2:S:22:ALA:HB2	2:S:154:ARG:NH1	2.30	0.46
2:S:65:TRP:CD1	2:S:65:TRP:H	2.33	0.46
1:L:269:GLY:HA3	1:L:325:TYR:HH	1.80	0.46
1:L:288:PHE:CD2	1:L:342:PHE:CE2	3.03	0.46
1:L:291:VAL:HG23	1:L:292:GLU:N	2.29	0.46
2:S:64:ALA:N	2:S:173:GLY:HA2	2.30	0.46
2:S:75:ASN:HB3	2:S:160:GLU:HG2	1.96	0.46
2:S:135:GLU:CA	2:S:141:GLN:HB3	2.41	0.46
1:L:36:MET:HE1	1:L:42:LEU:CD2	2.43	0.46
1:L:68:ILE:HD13	1:L:136:TRP:CZ3	2.51	0.46
1:L:89:MET:O	1:L:150:VAL:HA	2.15	0.46
1:L:278:TYR:HD1	1:L:281:PHE:CE2	2.32	0.46
1:L:313:ASN:HB2	1:L:363:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:67:SER:HB2	2:S:131:PHE:CD2	2.51	0.46
2:S:95:ARG:NE	2:S:98:MET:CG	2.74	0.46
1:L:329:ILE:O	1:L:330:ILE:O	2.33	0.46
2:S:126:GLY:HA2	2:S:132:GLU:HB3	1.96	0.46
2:S:186:THR:O	2:S:188:PRO:HD3	2.15	0.46
1:L:48:TYR:OH	1:L:63:LEU:HD23	2.14	0.46
1:L:55:ASP:O	1:L:56:PHE:CG	2.69	0.46
1:L:197:MET:SD	1:L:346:VAL:O	2.73	0.46
1:L:258:ILE:O	1:L:342:PHE:HE1	1.99	0.46
2:S:73:GLN:HB3	2:S:119:ASN:HA	1.97	0.46
2:S:178:PRO:O	2:S:180:PHE:CE2	2.69	0.46
1:L:48:TYR:CD2	1:L:62:PHE:HE2	2.28	0.46
1:L:92:ILE:HD12	1:L:125:PHE:CE2	2.38	0.46
1:L:184:LEU:HD21	2:S:165:PHE:CD1	2.51	0.46
1:L:193:LEU:CB	1:L:236:ILE:HG13	2.45	0.46
1:L:193:LEU:CA	1:L:232:PRO:HA	2.46	0.46
1:L:198:GLY:HA2	1:L:346:VAL:CB	2.46	0.46
1:L:202:PHE:O	1:L:341:ASP:HA	2.15	0.46
1:L:258:ILE:HG22	1:L:342:PHE:HD1	1.72	0.46
2:S:86:TRP:CG	2:S:87:ASP:H	2.34	0.46
2:S:86:TRP:HH2	2:S:156:ILE:CD1	2.29	0.46
2:S:133:PHE:O	2:S:134:ALA:C	2.59	0.46
1:L:96:VAL:HA	2:S:176:LEU:CA	2.45	0.45
2:S:45:ASP:CA	2:S:47:TRP:HD1	2.29	0.45
2:S:138:TRP:HE3	2:S:138:TRP:C	2.23	0.45
1:L:27:GLN:OE1	1:L:56:PHE:CE2	2.70	0.45
1:L:202:PHE:CD1	1:L:342:PHE:HB3	2.49	0.45
1:L:244:GLY:HA3	1:L:351:ILE:HD11	1.98	0.45
1:L:366:SER:O	1:L:367:ARG:C	2.59	0.45
2:S:9:ASP:O	2:S:11:TYR:CE1	2.68	0.45
1:L:34:LYS:HG2	1:L:35:ALA:N	2.30	0.45
1:L:206:VAL:HG13	1:L:333:SER:HA	1.98	0.45
1:L:252:LYS:C	1:L:254:SER:N	2.74	0.45
1:L:265:LEU:CD2	1:L:283:HIS:HA	2.40	0.45
1:L:190:TRP:C	1:L:351:ILE:HG22	2.41	0.45
1:L:193:LEU:HD23	1:L:232:PRO:CB	2.47	0.45
1:L:238:MET:HE3	2:S:56:ILE:HG22	1.97	0.45
1:L:313:ASN:OD1	1:L:313:ASN:C	2.59	0.45
1:L:351:ILE:HG21	1:L:354:PHE:CD2	2.51	0.45
1:L:364:ASP:HB3	2:S:182:LEU:CD1	2.44	0.45
2:S:56:ILE:HD12	2:S:56:ILE:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:148:CYS:CB	2:S:159:PHE:CE1	2.99	0.45
2:S:178:PRO:CB	2:S:179:PRO:CD	2.94	0.45
2:S:31:THR:N	2:S:41:PRO:HB3	2.32	0.45
2:S:54:PRO:HB2	2:S:57:MET:CG	2.47	0.45
2:S:89:GLN:CG	2:S:90:VAL:N	2.79	0.45
2:S:136:SER:O	2:S:138:TRP:N	2.49	0.45
1:L:191:LEU:O	1:L:349:VAL:O	2.35	0.45
1:L:200:LEU:H	1:L:343:ASN:CG	2.25	0.45
1:L:241:TYR:HA	1:L:310:THR:N	2.31	0.45
1:L:273:ASP:N	1:L:273:ASP:OD1	2.49	0.45
1:L:317:THR:O	1:L:321:ASP:HA	2.16	0.45
1:L:31:LEU:H	1:L:31:LEU:CD2	2.29	0.45
1:L:32:LEU:HB2	1:L:164:VAL:C	2.42	0.45
1:L:76:ALA:HA	1:L:167:LYS:O	2.17	0.45
1:L:80:ILE:CD1	1:L:156:TRP:CH2	2.89	0.45
1:L:86:CYS:N	1:L:116:ASN:ND2	2.64	0.45
1:L:87:CYS:SG	1:L:153:VAL:HG23	2.57	0.45
1:L:130:ASN:ND2	1:L:132:CYS:SG	2.89	0.45
1:L:246:LEU:HB2	1:L:348:LEU:CD1	2.46	0.45
2:S:83:ARG:HB3	2:S:83:ARG:CZ	2.46	0.45
2:S:86:TRP:CZ2	2:S:113:PRO:CA	3.00	0.45
1:L:119:CYS:SG	1:L:293:GLU:CD	2.99	0.45
1:L:72:ILE:HG13	1:L:127:PHE:O	2.17	0.45
1:L:200:LEU:O	1:L:201:THR:C	2.60	0.45
1:L:214:PRO:HA	1:L:325:TYR:CE1	2.52	0.45
1:L:241:TYR:HB3	1:L:308:TRP:O	2.17	0.45
1:L:243:ARG:CB	1:L:355:CYS:HB3	2.36	0.45
2:S:29:ALA:HB1	2:S:149:VAL:HA	1.99	0.45
1:L:68:ILE:HD13	1:L:136:TRP:HZ3	1.81	0.45
1:L:72:ILE:HA	1:L:172:ILE:HD12	1.98	0.45
1:L:262:VAL:N	1:L:286:VAL:HB	2.32	0.45
2:S:118:LEU:HD12	2:S:119:ASN:N	2.32	0.45
2:S:120:PHE:CD1	2:S:120:PHE:C	2.95	0.45
1:L:5:LEU:C	1:L:7:ALA:H	2.25	0.44
1:L:135:SER:C	1:L:136:TRP:CD1	2.96	0.44
1:L:286:VAL:CG2	1:L:344:LEU:HD11	2.47	0.44
2:S:29:ALA:HB1	2:S:147:GLU:OE2	2.16	0.44
2:S:35:ILE:HG12	2:S:144:TRP:HB2	2.00	0.44
2:S:56:ILE:HB	2:S:165:PHE:HB2	1.99	0.44
1:L:130:ASN:HA	1:L:131:PRO:HD3	1.79	0.44
1:L:173:VAL:HB	1:L:175:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:314:PRO:O	1:L:315:ARG:CG	2.63	0.44
2:S:94:LEU:O	2:S:105:ALA:HB3	2.17	0.44
2:S:95:ARG:HD2	2:S:98:MET:H	1.83	0.44
1:L:6:PHE:CD1	1:L:6:PHE:C	2.94	0.44
1:L:17:ARG:HH22	1:L:20:LEU:H	1.65	0.44
1:L:73:LYS:O	1:L:170:TRP:HA	2.17	0.44
1:L:91:ALA:O	1:L:148:MET:CA	2.65	0.44
1:L:176:LYS:H	1:L:176:LYS:NZ	2.14	0.44
1:L:246:LEU:N	1:L:351:ILE:HG13	2.32	0.44
1:L:248:PHE:O	1:L:296:THR:HA	2.16	0.44
2:S:82:LYS:C	2:S:84:ALA:N	2.75	0.44
2:S:108:PHE:HE2	2:S:120:PHE:CD2	2.36	0.44
1:L:90:LEU:HD12	1:L:92:ILE:HG13	2.00	0.44
1:L:197:MET:HE2	1:L:248:PHE:CD2	2.52	0.44
1:L:202:PHE:O	1:L:341:ASP:CA	2.65	0.44
1:L:202:PHE:CE2	1:L:211:ARG:HG2	2.47	0.44
2:S:93:TYR:HD1	2:S:107:THR:OG1	1.97	0.44
1:L:70:GLY:O	1:L:136:TRP:CZ2	2.70	0.44
1:L:74:VAL:CG1	1:L:169:ASP:O	2.65	0.44
1:L:127:PHE:CZ	1:L:129:PRO:CB	3.00	0.44
1:L:174:ASN:ND2	1:L:174:ASN:O	2.48	0.44
1:L:213:MET:O	1:L:326:LEU:O	2.35	0.44
1:L:258:ILE:HG12	1:L:335:THR:O	2.18	0.44
1:L:311:GLN:NE2	1:L:312:VAL:O	2.50	0.44
2:S:64:ALA:O	2:S:133:PHE:CD1	2.70	0.44
2:S:68:GLY:O	2:S:169:PHE:CE2	2.71	0.44
2:S:86:TRP:CE2	2:S:113:PRO:CA	2.98	0.44
2:S:91:PHE:O	2:S:93:TYR:CD2	2.71	0.44
2:S:165:PHE:HA	2:S:169:PHE:HE2	1.80	0.44
1:L:59:THR:CG2	1:L:60:VAL:N	2.80	0.44
1:L:113:MET:HE2	1:L:125:PHE:HB2	1.98	0.44
1:L:188:GLN:CD	1:L:354:PHE:CE2	2.96	0.44
1:L:189:ASN:N	1:L:189:ASN:ND2	2.65	0.44
1:L:235:TRP:C	1:L:237:SER:H	2.24	0.44
2:S:127:PRO:HD2	2:S:131:PHE:O	2.18	0.44
1:L:33:SER:HB3	1:L:36:MET:HE3	1.99	0.44
1:L:107:ILE:HD12	1:L:149:THR:HG21	2.00	0.44
2:S:19:THR:HA	2:S:20:PRO:HD3	1.47	0.44
2:S:20:PRO:CB	2:S:21:PRO:CD	2.94	0.44
2:S:68:GLY:O	2:S:124:ILE:HD12	2.17	0.44
2:S:86:TRP:CZ2	2:S:112:GLN:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:95:ARG:CB	2:S:105:ALA:H	2.30	0.44
1:L:88:LEU:HD23	1:L:115:TRP:HZ2	1.76	0.44
1:L:91:ALA:O	1:L:148:MET:CB	2.66	0.44
1:L:189:ASN:C	1:L:189:ASN:HD22	2.24	0.44
1:L:243:ARG:HH12	1:L:301:GLN:HG2	1.83	0.44
1:L:78:THR:HG23	1:L:79:ASN:H	1.78	0.44
1:L:154:SER:CB	1:L:253:MET:HG3	2.47	0.44
1:L:264:PHE:CE2	1:L:344:LEU:HD21	2.53	0.44
2:S:86:TRP:HE1	2:S:88:GLY:H	1.64	0.44
1:L:17:ARG:CZ	1:L:18:GLY:O	2.66	0.43
1:L:102:THR:C	1:L:107:ILE:HD11	2.43	0.43
1:L:255:SER:HA	1:L:256:PRO:HD3	1.41	0.43
1:L:316:THR:HG22	1:L:317:THR:N	2.33	0.43
2:S:86:TRP:CZ2	2:S:113:PRO:C	2.95	0.43
1:L:284:ARG:CB	1:L:299:PHE:HZ	2.30	0.43
2:S:53:ASN:ND2	2:S:182:LEU:HB2	2.30	0.43
1:L:244:GLY:O	1:L:246:LEU:CD1	2.64	0.43
1:L:304:PHE:HD2	1:L:304:PHE:O	2.02	0.43
1:L:88:LEU:HA	1:L:151:ILE:C	2.42	0.43
1:L:262:VAL:N	1:L:286:VAL:HG23	2.27	0.43
1:L:280:SER:O	1:L:281:PHE:CD1	2.71	0.43
1:L:311:GLN:HG2	1:L:360:ASN:HD21	1.83	0.43
1:L:337:THR:O	1:L:338:ILE:HG13	2.18	0.43
2:S:14:CYS:SG	2:S:57:MET:SD	3.16	0.43
2:S:48:ASN:O	2:S:50:HIS:N	2.51	0.43
2:S:57:MET:HE3	2:S:60:LEU:HD12	2.00	0.43
2:S:95:ARG:HG3	2:S:97:SER:H	1.82	0.43
1:L:75:THR:CG2	1:L:122:ASN:ND2	2.79	0.43
1:L:91:ALA:O	1:L:92:ILE:HG12	2.18	0.43
1:L:244:GLY:CA	1:L:351:ILE:HD11	2.49	0.43
2:S:32:PHE:HD2	2:S:32:PHE:C	2.27	0.43
2:S:39:ILE:H	2:S:39:ILE:HG13	1.61	0.43
2:S:65:TRP:HD1	2:S:173:GLY:N	2.17	0.43
2:S:109:VAL:CG2	2:S:110:ILE:N	2.78	0.43
2:S:110:ILE:HG12	2:S:111:SER:N	2.33	0.43
1:L:115:TRP:CH2	1:L:150:VAL:HG12	2.52	0.43
1:L:127:PHE:CZ	1:L:129:PRO:HD3	2.53	0.43
2:S:96:GLN:HG3	2:S:143:THR:C	2.44	0.43
2:S:122:PHE:O	2:S:124:ILE:N	2.51	0.43
1:L:86:CYS:HB3	1:L:155:GLY:C	2.43	0.43
1:L:120:LYS:C	1:L:121:LYS:HG2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:20:PRO:HD3	2:S:47:TRP:CE3	2.54	0.43
2:S:59:VAL:O	2:S:63:ALA:HB2	2.19	0.43
2:S:134:ALA:O	2:S:135:GLU:C	2.61	0.43
2:S:184:THR:C	2:S:185:GLU:HG2	2.43	0.43
1:L:71:LYS:HB3	1:L:126:THR:HB	2.01	0.43
1:L:195:ARG:HH21	1:L:217:ILE:N	2.16	0.43
1:L:239:TRP:HB2	1:L:357:ILE:H	1.84	0.43
1:L:245:GLU:OE1	1:L:246:LEU:O	2.37	0.43
1:L:314:PRO:HG3	1:L:365:GLY:HA2	1.94	0.43
2:S:6:GLU:O	2:S:6:GLU:HG3	2.19	0.43
2:S:30:VAL:HG12	2:S:148:CYS:O	2.19	0.43
2:S:151:THR:O	2:S:151:THR:HG22	2.18	0.43
1:L:62:PHE:C	1:L:62:PHE:CD2	2.97	0.43
1:L:73:LYS:CB	1:L:173:VAL:CG2	2.97	0.43
1:L:100:TYR:HA	2:S:178:PRO:CB	2.49	0.43
1:L:244:GLY:C	1:L:351:ILE:HD11	2.44	0.43
1:L:267:ALA:O	1:L:268:PHE:CG	2.72	0.43
2:S:13:PRO:HB2	2:S:14:CYS:H	1.46	0.43
2:S:86:TRP:CH2	2:S:113:PRO:C	2.97	0.43
1:L:79:ASN:O	1:L:80:ILE:HB	2.19	0.42
1:L:176:LYS:H	1:L:176:LYS:HZ3	1.67	0.42
1:L:212:ARG:CA	1:L:327:TYR:HB2	2.49	0.42
2:S:55:PRO:C	2:S:57:MET:N	2.76	0.42
2:S:106:ARG:HD2	2:S:107:THR:N	2.32	0.42
2:S:114:GLY:HA2	2:S:156:ILE:HD11	2.01	0.42
1:L:15:SER:CA	1:L:68:ILE:HA	2.49	0.42
1:L:47:LEU:N	1:L:47:LEU:HD22	2.34	0.42
1:L:59:THR:HG22	1:L:60:VAL:HG13	2.01	0.42
1:L:204:GLN:CD	1:L:340:GLY:H	2.27	0.42
1:L:214:PRO:HB2	1:L:215:LEU:H	1.46	0.42
1:L:221:ALA:O	1:L:227:PHE:C	2.62	0.42
1:L:265:LEU:O	1:L:326:LEU:HA	2.19	0.42
1:L:284:ARG:HG2	1:L:284:ARG:NH1	2.35	0.42
1:L:345:GLY:C	1:L:346:VAL:HG23	2.44	0.42
1:L:13:THR:CA	1:L:65:THR:O	2.67	0.42
1:L:131:PRO:O	1:L:179:PRO:HA	2.19	0.42
1:L:313:ASN:CB	1:L:363:ILE:HD13	2.50	0.42
2:S:63:ALA:O	2:S:133:PHE:CE1	2.71	0.42
2:S:83:ARG:HH11	2:S:83:ARG:CG	2.31	0.42
2:S:86:TRP:HZ2	2:S:112:GLN:O	2.02	0.42
1:L:34:LYS:HG3	1:L:159:SER:OG	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:LEU:HD12	1:L:63:LEU:N	2.35	0.42
1:L:156:TRP:O	1:L:157:THR:C	2.60	0.42
1:L:231:MET:N	1:L:232:PRO:HD2	2.34	0.42
1:L:260:ALA:O	1:L:286:VAL:CG1	2.67	0.42
1:L:29:ARG:HB3	1:L:165:ILE:CG1	2.49	0.42
1:L:128:ASN:ND2	1:L:136:TRP:NE1	2.66	0.42
1:L:168:LEU:HA	1:L:168:LEU:HD12	1.27	0.42
1:L:212:ARG:CZ	1:L:273:ASP:OD1	2.68	0.42
1:L:271:LEU:HD13	1:L:278:TYR:CE1	2.54	0.42
1:L:356:GLY:C	1:L:357:ILE:HG13	2.43	0.42
2:S:94:LEU:CA	2:S:146:LEU:HA	2.41	0.42
1:L:31:LEU:HD22	1:L:31:LEU:N	2.34	0.42
1:L:54:GLN:CG	1:L:56:PHE:HE1	2.21	0.42
1:L:86:CYS:H	1:L:116:ASN:HD21	1.67	0.42
1:L:99:LYS:O	2:S:178:PRO:HB3	2.19	0.42
1:L:278:TYR:CD1	1:L:329:ILE:HG12	2.55	0.42
1:L:284:ARG:HH12	1:L:298:VAL:N	2.18	0.42
1:L:296:THR:O	1:L:297:LEU:HD22	2.20	0.42
1:L:345:GLY:C	1:L:346:VAL:CG2	2.93	0.42
1:L:15:SER:HA	1:L:68:ILE:HG13	2.01	0.42
1:L:17:ARG:HH21	1:L:19:SER:HA	1.85	0.42
1:L:75:THR:OG1	1:L:122:ASN:ND2	2.43	0.42
1:L:89:MET:HB3	1:L:104:VAL:HG12	2.02	0.42
1:L:89:MET:C	1:L:115:TRP:CZ3	2.98	0.42
1:L:212:ARG:CZ	1:L:273:ASP:CG	2.93	0.42
1:L:265:LEU:HD22	1:L:283:HIS:CA	2.39	0.42
2:S:49:THR:O	2:S:51:ILE:HG13	2.20	0.42
2:S:68:GLY:HA2	2:S:169:PHE:HA	1.99	0.42
2:S:117:MET:HB2	2:S:118:LEU:H	1.64	0.42
1:L:122:ASN:CG	1:L:123:PHE:N	2.77	0.42
1:L:183:HIS:CE1	1:L:185:ALA:CB	3.02	0.42
1:L:190:TRP:CG	1:L:191:LEU:N	2.88	0.42
1:L:240:ARG:HB3	1:L:241:TYR:CD2	2.55	0.42
1:L:262:VAL:N	1:L:286:VAL:CG2	2.76	0.42
1:L:284:ARG:HH22	1:L:298:VAL:CG1	2.33	0.42
2:S:28:THR:O	2:S:29:ALA:CB	2.65	0.42
1:L:21:LEU:HA	1:L:24:LYS:HB2	2.02	0.42
1:L:73:LYS:HE3	1:L:172:ILE:O	2.20	0.42
1:L:183:HIS:CE1	1:L:185:ALA:HB3	2.53	0.42
1:L:189:ASN:N	1:L:189:ASN:HD22	2.17	0.42
1:L:275:PHE:HE1	1:L:277:PHE:HD2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:12:SER:HB3	2:S:56:ILE:CD1	2.42	0.42
2:S:57:MET:O	2:S:60:LEU:N	2.53	0.42
2:S:122:PHE:CD2	2:S:144:TRP:CZ2	3.08	0.42
1:L:67:VAL:HA	1:L:136:TRP:O	2.20	0.42
1:L:195:ARG:HB3	1:L:197:MET:CE	2.48	0.42
1:L:231:MET:N	1:L:232:PRO:CD	2.83	0.42
2:S:14:CYS:HB3	2:S:15:MET:H	1.64	0.42
2:S:86:TRP:CE2	2:S:88:GLY:N	2.87	0.42
1:L:59:THR:HG22	1:L:60:VAL:N	2.35	0.41
1:L:91:ALA:HB2	1:L:149:THR:OG1	2.19	0.41
1:L:193:LEU:HD23	1:L:232:PRO:C	2.44	0.41
1:L:71:LYS:O	1:L:73:LYS:N	2.53	0.41
1:L:165:ILE:O	1:L:166:ALA:O	2.37	0.41
1:L:188:GLN:CD	1:L:354:PHE:CZ	2.98	0.41
1:L:189:ASN:HB3	1:L:353:ASP:OD1	2.20	0.41
1:L:191:LEU:HG	1:L:193:LEU:CD1	2.48	0.41
1:L:301:GLN:HG3	1:L:305:VAL:HA	2.02	0.41
2:S:69:THR:HG22	2:S:71:HIS:HE1	1.85	0.41
1:L:197:MET:SD	1:L:346:VAL:HG12	2.59	0.41
1:L:230:ASN:HD22	1:L:233:ASN:HB2	1.80	0.41
1:L:252:LYS:HD3	1:L:289:ALA:O	2.20	0.41
2:S:94:LEU:CB	2:S:145:TYR:O	2.64	0.41
1:L:120:LYS:O	1:L:121:LYS:CD	2.68	0.41
1:L:141:ILE:HG22	1:L:146:VAL:CG2	2.50	0.41
1:L:246:LEU:HD23	1:L:348:LEU:HG	2.01	0.41
1:L:32:LEU:HB2	1:L:164:VAL:O	2.21	0.41
1:L:242:PHE:O	1:L:308:TRP:CE2	2.73	0.41
2:S:32:PHE:C	2:S:32:PHE:CD2	2.98	0.41
1:L:256:PRO:HB3	1:L:290:GLU:HG2	2.01	0.41
2:S:173:GLY:O	2:S:174:ASN:C	2.63	0.41
1:L:31:LEU:HA	1:L:165:ILE:CB	2.50	0.41
1:L:84:SER:HB3	1:L:158:LEU:HD12	2.03	0.41
1:L:97:ARG:N	2:S:176:LEU:O	2.54	0.41
1:L:136:TRP:CH2	1:L:172:ILE:HG12	2.55	0.41
1:L:170:TRP:O	1:L:171:SER:HB3	2.21	0.41
1:L:245:GLU:CG	1:L:352:LYS:CB	2.98	0.41
2:S:122:PHE:HE2	2:S:124:ILE:HD13	1.85	0.41
2:S:160:GLU:OE1	2:S:162:ASN:ND2	2.53	0.41
2:S:171:VAL:O	2:S:172:ALA:HB2	2.21	0.41
1:L:5:LEU:C	1:L:7:ALA:N	2.77	0.41
1:L:113:MET:HE2	1:L:125:PHE:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:SER:C	1:L:136:TRP:CG	2.97	0.41
1:L:189:ASN:HA	1:L:353:ASP:CA	2.51	0.41
1:L:191:LEU:HA	1:L:192:PRO:HD3	1.56	0.41
1:L:194:ASN:O	1:L:347:LYS:HE2	2.21	0.41
1:L:325:TYR:HE1	1:L:327:TYR:CG	2.39	0.41
2:S:57:MET:HB2	2:S:60:LEU:HD12	2.02	0.41
2:S:64:ALA:H	2:S:173:GLY:CA	2.32	0.41
2:S:125:ILE:CG1	2:S:126:GLY:N	2.83	0.41
1:L:20:LEU:HD11	1:L:173:VAL:HA	2.03	0.41
1:L:113:MET:HB3	1:L:113:MET:HE3	1.56	0.41
1:L:136:TRP:CH2	1:L:172:ILE:CD1	3.04	0.41
1:L:193:LEU:HD23	1:L:232:PRO:CA	2.51	0.41
1:L:250:VAL:CG2	1:L:251:THR:H	2.34	0.41
1:L:312:VAL:HG22	1:L:316:THR:CB	2.51	0.41
2:S:21:PRO:O	2:S:24:PHE:CB	2.68	0.41
2:S:119:ASN:N	2:S:119:ASN:ND2	2.69	0.41
2:S:148:CYS:O	2:S:149:VAL:O	2.38	0.41
1:L:313:ASN:O	1:L:313:ASN:CG	2.63	0.41
2:S:34:LEU:CB	2:S:145:TYR:HA	2.45	0.41
1:L:90:LEU:CD1	1:L:148:MET:SD	3.09	0.40
1:L:297:LEU:CD1	1:L:299:PHE:CE1	2.95	0.40
1:L:313:ASN:OD1	1:L:315:ARG:HB2	2.21	0.40
2:S:34:LEU:CD2	2:S:94:LEU:HD13	2.52	0.40
2:S:34:LEU:HB3	2:S:144:TRP:HB3	2.03	0.40
2:S:87:ASP:O	2:S:155:GLN:CG	2.69	0.40
1:L:22:ASP:HA	1:L:57:ARG:CB	2.51	0.40
1:L:91:ALA:HB1	1:L:107:ILE:CB	2.47	0.40
1:L:202:PHE:O	1:L:341:ASP:CG	2.64	0.40
1:L:217:ILE:CD1	1:L:242:PHE:CD1	3.04	0.40
1:L:223:ALA:O	1:L:224:THR:C	2.64	0.40
1:L:231:MET:HE1	1:L:235:TRP:HB3	2.03	0.40
1:L:364:ASP:OD1	1:L:365:GLY:N	2.55	0.40
2:S:101:GLU:O	2:S:102:SER:O	2.39	0.40
2:S:149:VAL:HG23	2:S:149:VAL:H	1.53	0.40
1:L:45:GLU:OE1	1:L:50:VAL:HG22	2.20	0.40
1:L:105:TYR:OH	1:L:220:GLY:HA2	2.21	0.40
1:L:186:ASP:CB	1:L:356:GLY:C	2.90	0.40
2:S:31:THR:C	2:S:41:PRO:HB3	2.46	0.40
2:S:96:GLN:CB	2:S:142:THR:OG1	2.60	0.40
2:S:166:ASP:O	2:S:169:PHE:HB2	2.21	0.40
1:L:74:VAL:HG22	1:L:170:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:CYS:C	1:L:117:PRO:HD2	2.46	0.40
1:L:90:LEU:CD1	1:L:148:MET:HB2	2.50	0.40
1:L:95:GLY:O	1:L:96:VAL:HG22	2.22	0.40
1:L:195:ARG:HH21	1:L:217:ILE:H	1.69	0.40
1:L:313:ASN:HB3	1:L:363:ILE:HD13	2.04	0.40
1:L:363:ILE:CG2	1:L:364:ASP:H	2.31	0.40
2:S:143:THR:O	2:S:145:TYR:CE1	2.74	0.40
1:L:88:LEU:HB3	1:L:115:TRP:CD2	2.54	0.40
1:L:235:TRP:HA	1:L:238:MET:SD	2.62	0.40
1:L:264:PHE:CZ	1:L:344:LEU:HD21	2.56	0.40
1:L:304:PHE:CD2	1:L:304:PHE:O	2.75	0.40
1:L:355:CYS:SG	1:L:355:CYS:O	2.77	0.40
2:S:12:SER:CB	2:S:56:ILE:HD11	2.42	0.40
2:S:86:TRP:CD2	2:S:113:PRO:HA	2.56	0.40

All (29) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:PHE:O	1:L:60:VAL:CG1[2_555]	1.34	0.86
1:L:59:THR:CG2	1:L:59:THR:CG2[2_555]	1.38	0.82
1:L:1:MET:N	1:L:124:SER:OG[2_555]	1.42	0.78
1:L:1:MET:O	1:L:122:ASN:ND2[2_555]	1.50	0.70
1:L:1:MET:H2	1:L:124:SER:CA[2_555]	0.94	0.66
1:L:1:MET:CE	1:L:123:PHE:CZ[2_555]	1.55	0.65
1:L:1:MET:CE	1:L:123:PHE:CE2[2_555]	1.59	0.61
1:L:10:LEU:CD2	1:L:21:LEU:CD1[2_555]	1.70	0.50
1:L:1:MET:H2	1:L:124:SER:CB[2_555]	1.11	0.49
1:L:12:ASP:OD1	1:L:57:ARG:HE[2_555]	1.18	0.42
1:L:12:ASP:CG	1:L:57:ARG:NE[2_555]	1.78	0.42
1:L:1:MET:N	1:L:124:SER:HG[2_555]	1.21	0.39
1:L:1:MET:N	1:L:124:SER:CB[2_555]	1.82	0.38
1:L:1:MET:CG	1:L:124:SER:H[2_555]	1.24	0.36
1:L:1:MET:N	1:L:124:SER:CA[2_555]	1.87	0.33
1:L:14:SER:OG	1:L:57:ARG:HH22[2_555]	1.27	0.33
1:L:1:MET:O	1:L:122:ASN:HD21[2_555]	1.30	0.30
1:L:12:ASP:CG	1:L:57:ARG:HE[2_555]	1.32	0.28
1:L:55:ASP:OD2	1:L:64:ARG:HH12[2_555]	1.32	0.28
1:L:14:SER:OG	1:L:57:ARG:NH2[2_555]	1.99	0.21
1:L:12:ASP:CB	1:L:57:ARG:NE[2_555]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:MET:CA	1:L:124:SER:N[2_555]	2.03	0.17
1:L:1:MET:O	1:L:122:ASN:HD22[2_555]	1.47	0.13
1:L:1:MET:N	1:L:124:SER:N[2_555]	2.09	0.11
1:L:59:THR:CB	1:L:59:THR:CG2[2_555]	2.11	0.09
1:L:12:ASP:OD1	1:L:57:ARG:NE[2_555]	2.12	0.08
1:L:1:MET:CA	1:L:123:PHE:C[2_555]	2.13	0.07
1:L:1:MET:CG	1:L:124:SER:N[2_555]	2.15	0.05
1:L:55:ASP:OD2	1:L:64:ARG:NH1[2_555]	2.16	0.04

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	367/369 (100%)	174 (47%)	94 (26%)	99 (27%)	<b>0</b> <b>0</b>
2	S	187/189 (99%)	87 (46%)	53 (28%)	47 (25%)	<b>0</b> <b>1</b>
All	All	554/558 (99%)	261 (47%)	147 (26%)	146 (26%)	<b>0</b> <b>1</b>

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	8	LEU
1	L	14	SER
1	L	50	VAL
1	L	55	ASP
1	L	66	HIS
1	L	79	ASN
1	L	80	ILE
1	L	99	LYS
1	L	100	TYR
1	L	108	CYS
1	L	109	SER
1	L	135	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	140	MET
1	L	145	ARG
1	L	153	VAL
1	L	166	ALA
1	L	172	ILE
1	L	190	TRP
1	L	193	LEU
1	L	195	ARG
1	L	199	LYS
1	L	201	THR
1	L	210	VAL
1	L	212	ARG
1	L	215	LEU
1	L	217	ILE
1	L	222	GLY
1	L	223	ALA
1	L	273	ASP
1	L	282	PRO
1	L	283	HIS
1	L	284	ARG
1	L	287	GLN
1	L	288	PHE
1	L	298	VAL
1	L	315	ARG
1	L	320	ALA
1	L	330	ILE
1	L	363	ILE
1	L	364	ASP
1	L	366	SER
1	L	368	LEU
2	S	6	GLU
2	S	9	ASP
2	S	13	PRO
2	S	14	CYS
2	S	20	PRO
2	S	21	PRO
2	S	23	PRO
2	S	27	VAL
2	S	35	ILE
2	S	87	ASP
2	S	102	SER
2	S	109	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	S	110	ILE
2	S	113	PRO
2	S	125	ILE
2	S	127	PRO
2	S	137	PRO
2	S	149	VAL
2	S	150	ALA
1	L	11	ASP
1	L	12	ASP
1	L	20	LEU
1	L	38	GLY
1	L	65	THR
1	L	69	THR
1	L	72	ILE
1	L	81	SER
1	L	96	VAL
1	L	107	ILE
1	L	117	PRO
1	L	132	CYS
1	L	171	SER
1	L	194	ASN
1	L	214	PRO
1	L	260	ALA
1	L	265	LEU
1	L	331	HIS
1	L	338	ILE
1	L	351	ILE
2	S	29	ALA
2	S	64	ALA
2	S	83	ARG
2	S	90	VAL
2	S	97	SER
2	S	134	ALA
2	S	135	GLU
2	S	140	ASN
2	S	174	ASN
2	S	178	PRO
1	L	3	GLN
1	L	43	LEU
1	L	64	ARG
1	L	120	LYS
1	L	129	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	152	CYS
1	L	154	SER
1	L	192	PRO
1	L	198	GLY
1	L	208	SER
1	L	237	SER
1	L	239	TRP
1	L	279	GLU
1	L	293	GLU
1	L	311	GLN
1	L	312	VAL
1	L	314	PRO
1	L	357	ILE
2	S	55	PRO
2	S	82	LYS
2	S	111	SER
1	L	45	GLU
1	L	162	THR
1	L	185	ALA
1	L	353	ASP
2	S	3	VAL
2	S	171	VAL
2	S	187	PRO
1	L	131	PRO
1	L	134	ASP
1	L	204	GLN
1	L	224	THR
1	L	236	ILE
2	S	45	ASP
2	S	105	ALA
2	S	130	GLY
2	S	155	GLN
1	L	160	PRO
1	L	263	THR
1	L	303	GLU
1	L	334	THR
1	L	336	GLY
2	S	98	MET
2	S	100	PRO
1	L	165	ILE
1	L	349	VAL
2	S	41	PRO

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Mol	Chain	Res	Type
2	S	181	PRO
2	S	188	PRO
1	L	285	ILE
2	S	152	ASN
1	L	141	ILE
1	L	150	VAL
2	S	179	PRO
2	S	16	ILE

### 5.3.2 Protein sidechains [i](#)

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	L	318/318 (100%)	197 (62%)	121 (38%)	0	1
2	S	163/163 (100%)	107 (66%)	56 (34%)	0	2
All	All	481/481 (100%)	304 (63%)	177 (37%)	0	1

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	GLU
1	L	3	GLN
1	L	6	PHE
1	L	8	LEU
1	L	10	LEU
1	L	11	ASP
1	L	17	ARG
1	L	20	LEU
1	L	21	LEU
1	L	25	PHE
1	L	27	GLN
1	L	31	LEU
1	L	41	VAL
1	L	43	LEU
1	L	46	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	47	LEU
1	L	50	VAL
1	L	54	GLN
1	L	59	THR
1	L	62	PHE
1	L	63	LEU
1	L	64	ARG
1	L	65	THR
1	L	66	HIS
1	L	68	ILE
1	L	74	VAL
1	L	75	THR
1	L	80	ILE
1	L	86	CYS
1	L	88	LEU
1	L	90	LEU
1	L	96	VAL
1	L	102	THR
1	L	106	THR
1	L	107	ILE
1	L	108	CYS
1	L	111	ASP
1	L	112	SER
1	L	120	LYS
1	L	121	LYS
1	L	136	TRP
1	L	139	GLU
1	L	141	ILE
1	L	144	SER
1	L	145	ARG
1	L	146	VAL
1	L	150	VAL
1	L	151	ILE
1	L	156	TRP
1	L	158	LEU
1	L	160	PRO
1	L	163	ASP
1	L	165	ILE
1	L	170	TRP
1	L	173	VAL
1	L	176	LYS
1	L	177	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	180	THR
1	L	181	ILE
1	L	182	TYR
1	L	184	LEU
1	L	186	ASP
1	L	189	ASN
1	L	193	LEU
1	L	195	ARG
1	L	197	MET
1	L	200	LEU
1	L	207	THR
1	L	212	ARG
1	L	213	MET
1	L	215	LEU
1	L	217	ILE
1	L	228	LEU
1	L	230	ASN
1	L	233	ASN
1	L	241	TYR
1	L	242	PHE
1	L	243	ARG
1	L	245	GLU
1	L	246	LEU
1	L	253	MET
1	L	254	SER
1	L	257	TYR
1	L	259	LYS
1	L	262	VAL
1	L	263	THR
1	L	265	LEU
1	L	271	LEU
1	L	277	PHE
1	L	281	PHE
1	L	283	HIS
1	L	287	GLN
1	L	294	LYS
1	L	297	LEU
1	L	298	VAL
1	L	302	GLN
1	L	304	PHE
1	L	306	THR
1	L	309	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	311	GLN
1	L	312	VAL
1	L	313	ASN
1	L	317	THR
1	L	318	LEU
1	L	319	GLU
1	L	323	CYS
1	L	325	TYR
1	L	327	TYR
1	L	330	ILE
1	L	331	HIS
1	L	334	THR
1	L	335	THR
1	L	337	THR
1	L	341	ASP
1	L	342	PHE
1	L	344	LEU
1	L	348	LEU
1	L	357	ILE
1	L	359	SER
1	L	361	PRO
1	L	369	LEU
2	S	3	VAL
2	S	10	VAL
2	S	11	TYR
2	S	16	ILE
2	S	19	THR
2	S	20	PRO
2	S	21	PRO
2	S	24	PHE
2	S	28	THR
2	S	32	PHE
2	S	33	ASP
2	S	35	ILE
2	S	36	ASN
2	S	40	THR
2	S	46	ASN
2	S	50	HIS
2	S	53	ASN
2	S	57	MET
2	S	67	SER
2	S	69	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	S	72	VAL
2	S	73	GLN
2	S	74	LEU
2	S	76	VAL
2	S	91	PHE
2	S	92	VAL
2	S	94	LEU
2	S	108	PHE
2	S	110	ILE
2	S	111	SER
2	S	112	GLN
2	S	118	LEU
2	S	119	ASN
2	S	120	PHE
2	S	122	PHE
2	S	124	ILE
2	S	135	GLU
2	S	138	TRP
2	S	140	ASN
2	S	146	LEU
2	S	148	CYS
2	S	154	ARG
2	S	155	GLN
2	S	156	ILE
2	S	160	GLU
2	S	164	ARG
2	S	169	PHE
2	S	171	VAL
2	S	175	ILE
2	S	177	MET
2	S	179	PRO
2	S	180	PHE
2	S	181	PRO
2	S	182	LEU
2	S	183	SER
2	S	188	PRO

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	83	ASN
1	L	116	ASN

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Mol	Chain	Res	Type
1	L	128	ASN
1	L	188	GLN
1	L	189	ASN
1	L	233	ASN
1	L	247	HIS
1	L	311	GLN
1	L	331	HIS
1	L	360	ASN
2	S	48	ASN
2	S	58	ASN
2	S	112	GLN
2	S	119	ASN
2	S	141	GLN
2	S	152	ASN
2	S	155	GLN
2	S	158	GLN
2	S	174	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	369/369 (100%)	1.98	163 (44%) 0   1	10, 13, 14, 15	0
2	S	189/189 (100%)	2.05	84 (44%) 0   1	9, 13, 15, 15	0
All	All	558/558 (100%)	2.01	247 (44%) 0   1	9, 13, 15, 15	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	15	SER	9.9
1	L	41	VAL	7.9
2	S	137	PRO	7.5
2	S	109	VAL	6.8
1	L	241	TYR	5.9
1	L	125	PHE	5.9
1	L	12	ASP	5.8
1	L	13	THR	5.8
2	S	189	LEU	5.7
2	S	55	PRO	5.5
1	L	82	ASP	5.5
1	L	37	ALA	5.4
1	L	99	LYS	5.1
1	L	316	THR	5.1
1	L	151	ILE	5.1
1	L	2	GLU	5.0
2	S	37	GLY	5.0
1	L	281	PHE	4.9
2	S	56	ILE	4.9
1	L	252	LYS	4.9
1	L	154	SER	4.8
1	L	296	THR	4.8
2	S	26	ASP	4.8
1	L	322	GLY	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	146	VAL	4.8
1	L	38	GLY	4.7
2	S	41	PRO	4.7
1	L	287	GLN	4.6
2	S	77	ARG	4.5
1	L	81	SER	4.5
1	L	16	VAL	4.4
1	L	203	PRO	4.4
1	L	333	SER	4.4
1	L	86	CYS	4.4
2	S	73	GLN	4.4
1	L	368	LEU	4.3
1	L	78	THR	4.3
1	L	279	GLU	4.3
1	L	83	ASN	4.3
2	S	36	ASN	4.2
2	S	103	TYR	4.2
2	S	128	ASN	4.2
2	S	83	ARG	4.1
1	L	102	THR	4.1
1	L	240	ARG	4.1
1	L	254	SER	4.1
1	L	74	VAL	4.0
1	L	257	TYR	3.9
1	L	198	GLY	3.8
1	L	48	TYR	3.8
1	L	335	THR	3.8
1	L	300	SER	3.8
2	S	100	PRO	3.8
1	L	239	TRP	3.7
2	S	9	ASP	3.7
1	L	43	LEU	3.7
2	S	44	ASP	3.7
1	L	90	LEU	3.7
2	S	25	SER	3.7
1	L	161	THR	3.7
2	S	65	TRP	3.7
1	L	317	THR	3.6
1	L	350	GLY	3.6
1	L	204	GLN	3.6
2	S	57	MET	3.6
2	S	20	PRO	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	347	LYS	3.5
1	L	138	ALA	3.5
1	L	196	TRP	3.5
2	S	80	GLY	3.5
1	L	3	GLN	3.5
1	L	119	CYS	3.5
2	S	62	THR	3.5
2	S	38	LYS	3.5
2	S	127	PRO	3.5
1	L	53	GLY	3.4
2	S	118	LEU	3.4
2	S	12	SER	3.4
2	S	179	PRO	3.4
1	L	323	CYS	3.4
1	L	331	HIS	3.4
1	L	44	ASP	3.4
1	L	137	SER	3.4
2	S	120	PHE	3.4
1	L	169	ASP	3.4
1	L	295	CYS	3.4
1	L	309	SER	3.3
1	L	180	THR	3.3
1	L	235	TRP	3.3
1	L	334	THR	3.3
1	L	132	CYS	3.3
2	S	138	TRP	3.3
1	L	50	VAL	3.3
2	S	110	ILE	3.3
1	L	223	ALA	3.2
1	L	89	MET	3.2
1	L	34	LYS	3.2
1	L	174	ASN	3.2
1	L	127	PHE	3.2
1	L	195	ARG	3.2
2	S	153	PRO	3.2
1	L	14	SER	3.2
1	L	39	GLY	3.2
1	L	209	GLU	3.2
1	L	177	CYS	3.2
1	L	211	ARG	3.2
1	L	315	ARG	3.2
2	S	168	ASN	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	55	ASP	3.2
2	S	59	VAL	3.2
1	L	319	GLU	3.1
1	L	80	ILE	3.1
1	L	111	ASP	3.1
2	S	74	LEU	3.1
1	L	97	ARG	3.1
1	L	238	MET	3.1
2	S	66	LYS	3.1
1	L	183	HIS	3.1
1	L	197	MET	3.1
1	L	345	GLY	3.0
2	S	13	PRO	3.0
2	S	160	GLU	3.0
2	S	3	VAL	3.0
1	L	166	ALA	3.0
1	L	170	TRP	3.0
2	S	61	ARG	3.0
1	L	310	THR	2.9
2	S	49	THR	2.9
1	L	54	GLN	2.9
2	S	47	TRP	2.9
1	L	216	SER	2.9
2	S	116	ALA	2.9
1	L	79	ASN	2.9
1	L	369	LEU	2.9
1	L	234	SER	2.9
2	S	147	GLU	2.9
2	S	35	ILE	2.9
2	S	84	ALA	2.9
1	L	114	THR	2.8
1	L	181	ILE	2.8
2	S	39	ILE	2.8
2	S	125	ILE	2.8
2	S	140	ASN	2.8
2	S	163	MET	2.8
1	L	349	VAL	2.8
2	S	31	THR	2.8
2	S	40	THR	2.8
2	S	58	ASN	2.8
2	S	119	ASN	2.7
1	L	61	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	217	ILE	2.7
1	L	147	ARG	2.7
1	L	301	GLN	2.7
2	S	15	MET	2.7
1	L	94	SER	2.7
1	L	218	GLY	2.7
1	L	306	THR	2.7
2	S	88	GLY	2.6
2	S	76	VAL	2.6
2	S	178	PRO	2.6
1	L	118	GLY	2.6
1	L	105	TYR	2.6
2	S	139	ALA	2.6
1	L	19	SER	2.6
2	S	143	THR	2.6
1	L	324	PRO	2.6
1	L	305	VAL	2.6
1	L	208	SER	2.5
1	L	66	HIS	2.5
2	S	186	THR	2.5
1	L	109	SER	2.5
1	L	280	SER	2.5
1	L	346	VAL	2.5
1	L	277	PHE	2.5
1	L	185	ALA	2.5
2	S	63	ALA	2.5
1	L	62	PHE	2.4
2	S	11	TYR	2.4
2	S	112	GLN	2.4
1	L	359	SER	2.4
1	L	24	LYS	2.4
1	L	276	GLY	2.4
1	L	11	ASP	2.4
2	S	51	ILE	2.4
1	L	153	VAL	2.4
1	L	290	GLU	2.4
1	L	303	GLU	2.4
1	L	87	CYS	2.4
2	S	2	PRO	2.4
2	S	101	GLU	2.4
1	L	101	SER	2.4
1	L	46	TYR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	164	VAL	2.4
1	L	27	GLN	2.4
2	S	4	CYS	2.3
2	S	176	LEU	2.3
1	L	365	GLY	2.3
1	L	360	ASN	2.3
1	L	304	PHE	2.3
1	L	219	GLY	2.3
1	L	26	ALA	2.3
1	L	344	LEU	2.3
1	L	253	MET	2.3
1	L	115	TRP	2.3
1	L	337	THR	2.3
1	L	155	GLY	2.3
1	L	29	ARG	2.3
1	L	314	PRO	2.3
1	L	173	VAL	2.3
1	L	178	GLU	2.2
1	L	225	GLN	2.3
2	S	28	THR	2.2
1	L	85	GLY	2.2
2	S	171	VAL	2.2
1	L	242	PHE	2.2
1	L	318	LEU	2.2
2	S	7	ALA	2.2
2	S	130	GLY	2.2
1	L	202	PHE	2.2
1	L	199	LYS	2.2
2	S	135	GLU	2.2
2	S	87	ASP	2.2
2	S	94	LEU	2.2
1	L	76	ALA	2.1
2	S	167	PRO	2.1
2	S	75	ASN	2.1
1	L	206	VAL	2.1
2	S	10	VAL	2.1
1	L	70	GLY	2.1
1	L	358	GLY	2.1
1	L	28	THR	2.1
1	L	332	ASP	2.1
2	S	29	ALA	2.1
1	L	256	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	282	PRO	2.1
1	L	338	ILE	2.1
1	L	362	GLY	2.1
1	L	22	ASP	2.0
1	L	186	ASP	2.0
2	S	45	ASP	2.0
2	S	48	ASN	2.0
2	S	5	ALA	2.0
1	L	117	PRO	2.0
1	L	156	TRP	2.0
2	S	141	GLN	2.0
1	L	112	SER	2.0
1	L	159	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.