



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:46 AM GMT

PDB ID : 2BFU
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

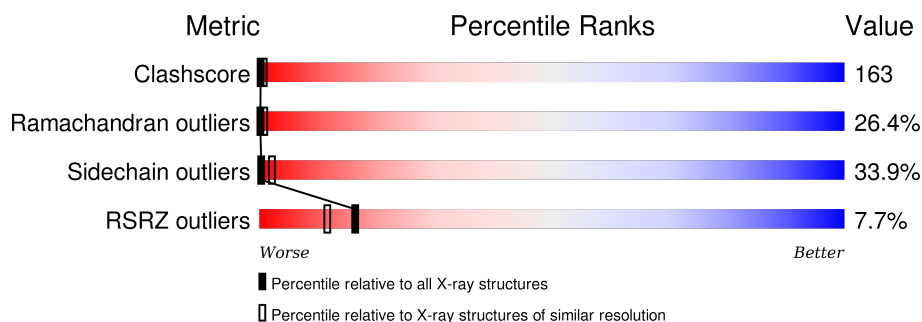
1 Overall quality at a glance

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	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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
1	L	369	Total	C	H	N	O	S	0	0	0
			3500	1822	634	480	542	22			

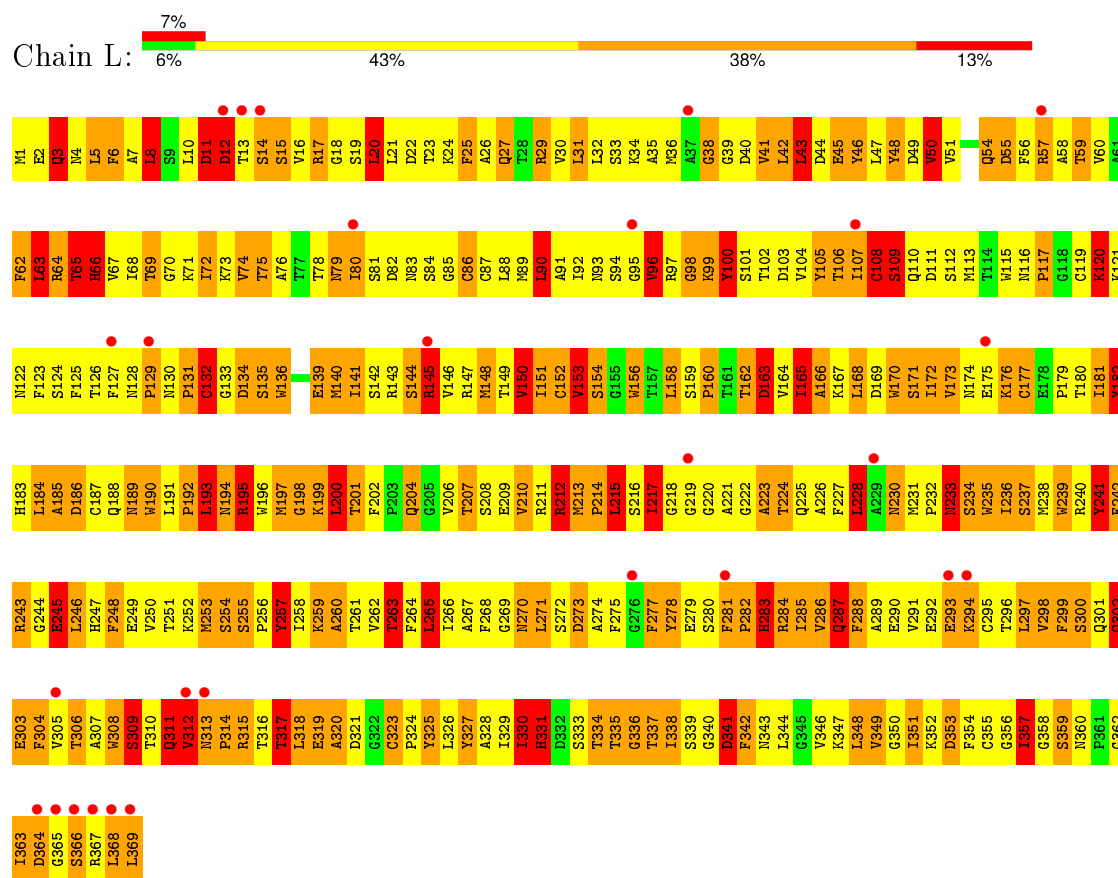
- Molecule 2 is a protein called COWPEA MOSAIC VIRUS, SMALL (S) SUBUNIT.

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

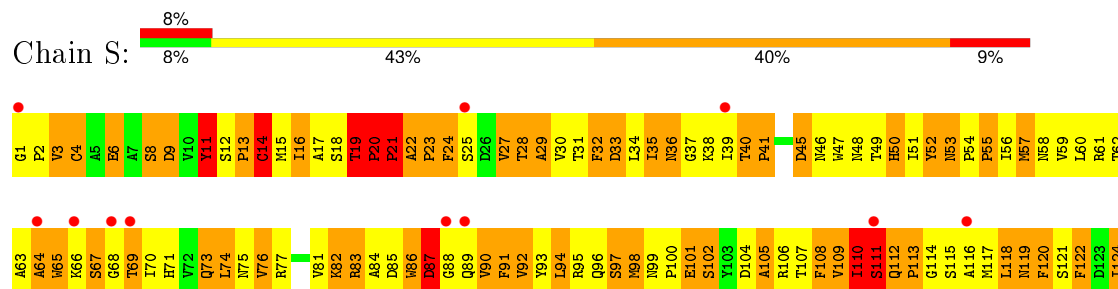
3 Residue-property plots

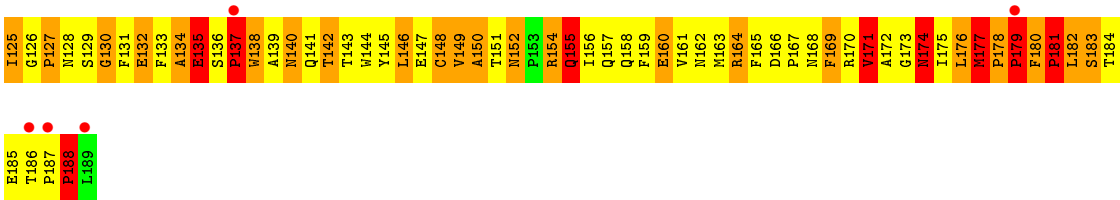
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	311.41Å 311.41Å 311.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 56.85 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-4.00) 92.8 (56.85-4.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.45 (at 4.01Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.230 , (Not available) 0.510 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	100.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , -4.6	EDS
Estimated twinning fraction	0.027 for -l,-k,-h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39472 reflections	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	5282	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.23	7/2933 (0.2%)	1.50	36/3983 (0.9%)
2	S	1.21	6/1524 (0.4%)	1.46	16/2089 (0.8%)
All	All	1.22	13/4457 (0.3%)	1.49	52/6072 (0.9%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	245	GLU	CB-CG	7.86	1.67	1.52
1	L	108	CYS	CB-SG	7.32	1.94	1.82
1	L	235	TRP	CB-CG	7.30	1.63	1.50
1	L	132	CYS	CB-SG	7.29	1.94	1.82
2	S	132	GLU	CB-CG	6.83	1.65	1.52
2	S	101	GLU	CB-CG	6.58	1.64	1.52
1	L	29	ARG	CG-CD	6.42	1.68	1.51
2	S	20	PRO	CA-C	6.31	1.65	1.52
2	S	132	GLU	CG-CD	6.16	1.61	1.51
1	L	286	VAL	CA-CB	6.11	1.67	1.54
2	S	11	TYR	CB-CG	5.72	1.60	1.51
2	S	86	TRP	CB-CG	5.55	1.60	1.50
1	L	308	TRP	CB-CG	-5.15	1.41	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	20	PRO	N-CA-C	9.67	137.23	112.10
2	S	177	MET	N-CA-C	8.96	135.18	111.00
2	S	19	THR	C-N-CD	-8.24	102.47	120.60
1	L	168	LEU	CA-CB-CG	-8.15	96.55	115.30
1	L	153	VAL	N-CA-C	-7.82	89.89	111.00
1	L	16	VAL	N-CA-C	7.68	131.74	111.00
2	S	22	ALA	C-N-CD	-7.61	103.85	120.60
1	L	302	GLN	N-CA-C	-7.36	91.13	111.00
2	S	8	SER	N-CA-C	7.34	130.82	111.00
1	L	5	LEU	CA-CB-CG	7.28	132.03	115.30
1	L	200	LEU	CA-CB-CG	7.11	131.65	115.30
1	L	15	SER	N-CA-C	-7.09	91.85	111.00
1	L	29	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	L	90	LEU	CA-CB-CG	6.78	130.89	115.30
1	L	255	SER	N-CA-C	6.76	129.26	111.00
1	L	309	SER	N-CA-C	6.71	129.12	111.00
1	L	100	TYR	N-CA-C	6.63	128.90	111.00
1	L	233	ASN	N-CA-C	6.52	128.61	111.00
2	S	19	THR	C-N-CA	6.42	148.97	122.00
1	L	132	CYS	CA-CB-SG	6.35	125.44	114.00
1	L	307	ALA	N-CA-C	6.17	127.66	111.00
1	L	193	LEU	CA-CB-CG	6.09	129.32	115.30
1	L	228	LEU	CA-CB-CG	6.04	129.19	115.30
1	L	212	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	S	4	CYS	CA-CB-SG	5.95	124.71	114.00
2	S	183	SER	N-CA-C	-5.90	95.07	111.00
1	L	42	LEU	CA-CB-CG	-5.88	101.78	115.30
1	L	223	ALA	N-CA-C	-5.83	95.27	111.00
1	L	145	ARG	N-CA-C	5.81	126.70	111.00
1	L	300	SER	N-CA-C	5.80	126.65	111.00
2	S	101	GLU	N-CA-C	-5.78	95.41	111.00
1	L	265	LEU	CA-CB-CG	5.72	128.47	115.30
1	L	283	HIS	N-CA-C	5.67	126.30	111.00
1	L	228	LEU	N-CA-C	5.63	126.20	111.00
1	L	234	SER	N-CA-C	5.61	126.14	111.00
1	L	12	ASP	N-CA-C	5.57	126.05	111.00
2	S	1	GLY	N-CA-C	-5.48	99.41	113.10
1	L	330	ILE	CG1-CB-CG2	5.45	123.40	111.40
2	S	137	PRO	N-CA-C	5.29	125.86	112.10
1	L	317	THR	N-CA-C	5.27	125.24	111.00
1	L	341	ASP	CB-CG-OD2	5.23	123.00	118.30
2	S	14	CYS	CA-CB-SG	5.19	123.35	114.00
1	L	163	ASP	CB-CG-OD1	5.18	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	4	CYS	N-CA-C	-5.17	97.05	111.00
1	L	109	SER	N-CA-C	5.14	124.87	111.00
1	L	212	ARG	N-CA-C	5.13	124.86	111.00
1	L	368	LEU	N-CA-C	-5.11	97.19	111.00
1	L	63	LEU	CA-CB-CG	5.08	126.99	115.30
1	L	98	GLY	N-CA-C	-5.08	100.41	113.10
2	S	142	THR	N-CA-C	-5.08	97.30	111.00
2	S	176	LEU	CA-C-N	-5.05	106.09	117.20
2	S	25	SER	N-CA-C	5.01	124.52	111.00

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 ⓘ

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	956	29
2	S	1477	305	1413	488	0
All	All	4343	939	4226	1394	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 163.

All (1394) 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
2:S:91:PHE:H	2:S:149:VAL:HG21	1.24	1.00
1:L:143:ARG:HB3	2:S:137:PRO:HB2	1.43	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:HH11	2:S:106:ARG:HG2	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:268:PHE:CE1	1:L:324:PRO:HG3	2.07	0.90
1:L:199:LYS:HG3	1:L:343:ASN:HD21	1.36	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:H	1:L:165:ILE:HD13	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: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
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:106:THR:HG23	1:L:228:LEU:HD13	1.57	0.84
1:L:60:VAL:HB	1:L:64:ARG:CD	2.02	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
1:L:204:GLN:HE22	1:L:258:ILE:HD13	1.43	0.82
1:L:143:ARG:CB	2:S:137:PRO:HB2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:308:TRP:HB3	1:L:323:CYS:HG	1.40	0.81
1:L:193:LEU:CB	1:L:232:PRO:HA	2.08	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:141:GLN:HG3	2:S:142:THR:H	1.44	0.80
2:S:53:ASN:HA	2:S:61:ARG:HH22	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:219:GLY:C	1:L:233:ASN:HB3	2.02	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:311:GLN:HE21	1:L:312:VAL:H	1.31	0.79
1:L:262:VAL:HG13	1:L:328:ALA:HB1	1.64	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:195:ARG:H	1:L:232:PRO:CB	1.95	0.79
1:L:134:ASP:CB	1:L:177:CYS:SG	2.71	0.79
1:L:89:MET:SD	1:L:108:CYS:SG	2.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:L:236:ILE:HG22	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:164:ARG:NH2	2:S:166:ASP:HA	1.98	0.78
2:S:94:LEU:HB3	2:S:146:LEU:CG	2.13	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
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:241:TYR:HB3	1:L:308:TRP:C	2.05	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
2:S:29:ALA:HA	2:S:150:ALA:HB3	1.66	0.76
1:L:134:ASP:HB2	1:L:177:CYS:SG	2.26	0.76
1:L:186:ASP:HB2	1:L:356:GLY:O	1.85	0.76
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
1:L:22:ASP:HA	1:L:57:ARG:CG	2.15	0.75
2:S:134:ALA:HA	2:S:143:THR:OG1	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:LEU:HB3	1:L:73:LYS:NZ	2.00	0.75
1:L:269:GLY:HA3	1:L:325:TYR:OH	1.86	0.75
2:S:132:GLU:O	2:S:133:PHE:HB2	1.85	0.75
2:S:63:ALA:HB3	2:S:66:LYS:HE3	1.67	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:125:ILE:HG13	2:S:126:GLY:H	1.52	0.75
2:S:76:VAL:HG12	2:S:158:GLN:O	1.87	0.75
2:S:16:ILE:HB	2:S:52:TYR:CE2	2.21	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:311:GLN:NE2	1:L:312:VAL:H	1.85	0.74
1:L:210:VAL:HG13	1:L:328:ALA:O	1.87	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:91:PHE:N	2:S:149:VAL:HG21	2.02	0.74
2:S:58:ASN:HA	2:S:61:ARG:HB2	1.69	0.74
1:L:130:ASN:OD1	1:L:132:CYS:SG	2.44	0.73
1:L:256:PRO:CB	1:L:290:GLU:HA	2.10	0.73
1:L:197:MET:SD	1:L:347:LYS:HA	2.28	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:252:LYS:HZ1	1:L:256:PRO:HG3	1.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:20:PRO:HB3	2:S:21:PRO:CD	2.18	0.73
2:S:126:GLY:HA3	2:S:131:PHE:C	2.09	0.72
1:L:355:CYS:SG	1:L:357:ILE:HD11	2.28	0.72
1:L:33:SER:HB3	1:L:36:MET:SD	2.28	0.72
1:L:218:GLY:H	1:L:233:ASN:HD21	1.37	0.72
1:L:68:ILE:HB	1:L:136:TRP:CH2	2.23	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:130:GLY:O	2:S:131:PHE:HD2	1.72	0.72
2:S:127:PRO:HD2	2:S:132:GLU:HA	1.69	0.72
2:S:71:HIS:CD2	2:S:164:ARG:HD3	2.24	0.72
2:S:19:THR:HB	2:S:156:ILE:O	1.89	0.72
1:L:36:MET:HE1	1:L:40:ASP:HB3	1.72	0.72
2:S:106:ARG:CD	2:S:107:THR:H	2.02	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:215:LEU:HD21	1:L:248:PHE:HZ	1.55	0.71
1:L:32:LEU:N	1:L:165:ILE:HG22	2.05	0.71
1:L:25:PHE:CE2	1:L:171:SER:HA	2.26	0.71
1:L:4:ASN:OD1	1:L:6:PHE:CD1	2.44	0.71
1:L:32:LEU:HD13	1:L:164:VAL:O	1.91	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:245:GLU:C	1:L:351:ILE:HG13	2.11	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
2:S:52:TYR:C	2:S:54:PRO:HD3	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:264:PHE:HB3	1:L:326:LEU:HD11	1.74	0.70
1:L:187:CYS:SG	1:L:355:CYS:CA	2.79	0.70
1:L:23:THR:HA	1:L:58:ALA:HB2	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:245:GLU:HG3	1:L:245:GLU:O	1.91	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:108:CYS:SG	1:L:109:SER:N	2.65	0.69
1:L:93:ASN:CA	1:L:110:GLN:HB2	2.21	0.69
2:S:112:GLN:CB	2:S:113:PRO:HD2	2.07	0.69
2:S:55:PRO:O	2:S:59:VAL:HG23	1.93	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
2:S:91:PHE:HA	2:S:108:PHE:O	1.93	0.69
1:L:195:ARG:H	1:L:232:PRO:HB3	1.57	0.69
2:S:95:ARG:HG2	2:S:98:MET:HG3	1.74	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:86:CYS:H	1:L:116:ASN:ND2	1.92	0.68
1:L:286:VAL:HG12	1:L:287:GLN:H	1.57	0.68
1:L:73:LYS:HA	1:L:126:THR:HA	1.75	0.68
1:L:96:VAL:CG1	2:S:176:LEU:HB2	2.23	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:122:PHE:O	2:S:122:PHE:CD2	2.46	0.68
2:S:156:ILE:HG22	2:S:156:ILE:O	1.94	0.68
2:S:33:ASP:HB3	2:S:39:ILE:HA	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:264:PHE:HE1	1:L:285:ILE:HA	1.58	0.67
1:L:261:THR:HG22	1:L:285:ILE:HD11	1.76	0.67
2:S:86:TRP:CE2	2:S:113:PRO:HA	2.28	0.67
2:S:127:PRO:HD2	2:S:132:GLU:CA	2.24	0.67
2:S:48:ASN:ND2	2:S:50:HIS:ND1	2.42	0.67
1:L:285:ILE:HG13	1:L:286:VAL:H	1.58	0.67
1:L:258:ILE:HD11	1:L:340:GLY:HA3	1.76	0.67
1:L:31:LEU:HB2	1:L:42:LEU:HB3	1.75	0.67
2:S:106:ARG:NH1	2:S:106:ARG:HG2	1.98	0.67
2:S:21:PRO:C	2:S:24:PHE:HB2	2.15	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
1:L:312:VAL:HG22	1:L:316:THR:OG1	1.95	0.67
1:L:186:ASP:HB2	1:L:356:GLY:C	2.14	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:75:ASN:ND2	2:S:117:MET:HB3	2.09	0.66
2:S:29:ALA:HA	2:S:150:ALA:CB	2.25	0.66
1:L:184:LEU:HD21	2:S:165:PHE:CE1	2.30	0.66
1:L:25:PHE:CA	1:L:56:PHE:HB2	2.24	0.66
2:S:56:ILE:HD12	2:S:57:MET:N	2.10	0.66
1:L:21:LEU:C	1:L:23:THR:H	1.98	0.66
1:L:262:VAL:C	1:L:285:ILE:HG13	2.15	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
1:L:265:LEU:C	1:L:266:ILE:HD12	2.15	0.66
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: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:140:MET:SD	2:S:65:TRP:CH2	2.89	0.66
1:L:91:ALA:HB3	1:L:149:THR:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:347:LYS:HG3	1:L:348:LEU:N	2.09	0.66
1:L:67:VAL:HG13	1:L:136:TRP:H	1.60	0.66
1:L:367:ARG:O	1:L:369:LEU:N	2.29	0.65
1:L:73:LYS:O	1:L:170:TRP:HB3	1.96	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: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
1:L:100:TYR:HB3	2:S:176:LEU:O	1.96	0.65
2:S:33:ASP:HA	2:S:145:TYR:CD2	2.23	0.65
1:L:103:ASP:O	1:L:107:ILE:HG13	1.96	0.65
1:L:72:ILE:N	1:L:172:ILE:HD12	2.10	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:92:VAL:HG22	2:S:146:LEU:HD21	1.78	0.65
2:S:40:THR:HG23	2:S:49:THR:HG21	1.77	0.65
1:L:195:ARG:HH21	1:L:217:ILE:CA	2.07	0.65
1:L:210:VAL:O	1:L:212:ARG:HD3	1.96	0.65
1:L:86:CYS:O	1:L:116:ASN:HA	1.97	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:33:SER:OG	1:L:34:LYS:N	2.30	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:78:THR:HG23	1:L:79:ASN:N	2.11	0.65
1:L:3:GLN:O	1:L:5:LEU:HD23	1.96	0.65
1:L:193:LEU:HD23	1:L:232:PRO:O	1.97	0.65
1:L:218:GLY:H	1:L:233:ASN:ND2	1.95	0.65
1:L:169:ASP:C	1:L:170:TRP:HD1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:ASN:HA	1:L:110:GLN:CG	2.28	0.64
1:L:71:LYS:HE2	1:L:126:THR:OG1	1.97	0.64
1:L:195:ARG:H	1:L:232:PRO:HB2	1.59	0.64
1:L:139:GLU:O	1:L:140:MET:HB2	1.97	0.64
1:L:15:SER:CB	1:L:68:ILE:HA	2.26	0.64
1:L:338:ILE:CG2	1:L:339:SER:H	2.01	0.64
1:L:183:HIS:CE1	1:L:185:ALA:H	2.16	0.64
1:L:90:LEU:HD13	1:L:149:THR:O	1.97	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
1:L:187:CYS:SG	1:L:355:CYS:CB	2.86	0.64
2:S:149:VAL:HG12	2:S:150:ALA:N	2.10	0.64
1:L:231:MET:HB2	2:S:174:ASN:HB2	1.80	0.64
1:L:197:MET:C	1:L:346:VAL:HB	2.18	0.64
1:L:44:ASP:CB	1:L:149:THR:HG22	2.28	0.64
2:S:91:PHE:CD1	2:S:93:TYR:CE2	2.85	0.64
1:L:148:MET:SD	1:L:148:MET:C	2.76	0.64
1:L:171:SER:O	1:L:172:ILE:HB	1.96	0.64
1:L:71:LYS:HD3	1:L:175:GLU:HB2	1.79	0.64
1:L:31:LEU:O	1:L:42:LEU:HD13	1.97	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:176:LYS:O	1:L:176:LYS:HG2	1.98	0.64
1:L:218:GLY:N	1:L:233:ASN:ND2	2.46	0.64
1:L:245:GLU:CG	1:L:245:GLU:O	2.45	0.64
1:L:214:PRO:HA	1:L:325:TYR:CD2	2.33	0.64
2:S:15:MET:HB2	2:S:50:HIS:O	1.97	0.64
1:L:255:SER:O	1:L:258:ILE:O	2.16	0.63
1:L:191:LEU:O	1:L:350:GLY:HA2	1.98	0.63
2:S:165:PHE:HA	2:S:169:PHE:CE2	2.33	0.63
1:L:13:THR:HA	1:L:65:THR:O	1.99	0.63
2:S:15:MET:HA	2:S:52:TYR:CD2	2.32	0.63
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:133:GLY:HA2	1:L:179:PRO:HB3	1.79	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:217:ILE:HG12	1:L:242:PHE:CD1	2.34	0.63
1:L:214:PRO:HA	1:L:325:TYR:CD1	2.33	0.63
1:L:87:CYS:SG	1:L:88:LEU:N	2.71	0.63
1:L:90:LEU:HD22	1:L:150:VAL:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:191:LEU:HG	1:L:193:LEU:HD12	1.81	0.63
2:S:99:ASN:C	2:S:101:GLU:H	2.02	0.63
1:L:226:ALA:HA	2:S:181:PRO:CB	2.25	0.63
1:L:62:PHE:HB3	1:L:63:LEU:HD12	1.80	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:262:VAL:O	1:L:285:ILE:HG13	1.98	0.63
1:L:20:LEU:HB3	1:L:73:LYS:HZ3	1.63	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
2:S:31:THR:O	2:S:31:THR:HG23	1.98	0.63
2:S:53:ASN:HA	2:S:61:ARG:HH12	1.64	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:258:ILE:CD1	1:L:340:GLY:HA3	2.29	0.62
1:L:252:LYS:HB3	1:L:293:GLU:HB2	1.80	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:106:ARG:HD2	2:S:107:THR:H	1.63	0.62
2:S:34:LEU:HB2	2:S:145:TYR:C	2.19	0.62
2:S:28:THR:O	2:S:29:ALA:HB2	1.99	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:HG3	1:L:188:GLN:O	1.97	0.62
1:L:351:ILE:HG21	1:L:354:PHE:HB3	1.80	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
1:L:278:TYR:CD1	1:L:281:PHE:CE2	2.87	0.62
2:S:177:MET:C	2:S:180:PHE:HZ	2.02	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:161:VAL:O	2:S:162:ASN:ND2	2.32	0.62
2:S:29:ALA:HA	2:S:149:VAL:O	2.00	0.62
1:L:120:LYS:HZ2	1:L:120:LYS:HB3	1.64	0.61
1:L:243:ARG:HH11	1:L:243:ARG:HG3	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:90:VAL:HG13	2:S:149:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:177:MET:SD	2:S:177:MET:N	2.73	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
1:L:71:LYS:HE2	1:L:126:THR:CB	2.31	0.61
1:L:145:ARG:HD2	1:L:145:ARG:H	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
1:L:197:MET:HE2	1:L:248:PHE:CD2	2.35	0.61
2:S:90:VAL:HG13	2:S:149:VAL:CG2	2.30	0.61
1:L:130:ASN:CG	1:L:132:CYS:HG	2.03	0.61
1:L:258:ILE:CG1	1:L:336:GLY:HA2	2.22	0.61
1:L:49:ASP:O	1:L:51:VAL:N	2.34	0.61
2:S:14:CYS:CA	2:S:54:PRO:HG2	2.31	0.61
2:S:158:GLN:HG2	2:S:159:PHE:N	2.16	0.61
2:S:89:GLN:HG2	2:S:90:VAL:H	1.64	0.61
1:L:134:ASP:O	1:L:135:SER:O	2.19	0.61
1:L:19:SER:O	1:L:21:LEU:N	2.33	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:246:LEU:HB2	1:L:348:LEU:HD11	1.81	0.61
1:L:89:MET:HE3	1:L:104:VAL:HB	1.81	0.61
1:L:182:TYR:N	1:L:182:TYR:CD1	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: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:227:PHE:HB2	2:S:180:PHE:O	2.00	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
2:S:177:MET:CB	2:S:180:PHE:CZ	2.83	0.60
1:L:282:PRO:HA	1:L:283:HIS:ND1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:112:GLN:HB2	2:S:113:PRO:CD	2.18	0.60
2:S:35:ILE:HD12	2:S:36:ASN:N	2.15	0.60
1:L:101:SER:OG	1:L:106:THR:HG21	2.01	0.60
1:L:204:GLN:NE2	1:L:258:ILE:HD13	2.16	0.60
1:L:70:GLY:N	1:L:136:TRP:HZ2	1.99	0.60
1:L:286:VAL:HG22	1:L:344:LEU:HD11	1.84	0.60
2:S:86:TRP:CD1	2:S:113:PRO:HD3	2.37	0.60
2:S:70:ILE:HD13	2:S:163:MET:SD	2.41	0.60
1:L:217:ILE:HG13	1:L:310:THR:HG23	1.84	0.60
1:L:270:ASN:HA	1:L:318:LEU:CG	2.31	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:75:THR:HG23	1:L:122:ASN:ND2	2.15	0.60
1:L:105:TYR:CD2	1:L:105:TYR:O	2.55	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
1:L:75:THR:HG23	1:L:122:ASN:CG	2.22	0.60
1:L:100:TYR:OH	1:L:147:ARG:NH1	2.35	0.60
1:L:31:LEU:O	1:L:32:LEU:HD12	2.01	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
2:S:92:VAL:O	2:S:107:THR:HA	2.02	0.59
1:L:82:ASP:OD1	1:L:83:ASN:ND2	2.35	0.59
1:L:193:LEU:HD23	1:L:232:PRO:HB2	1.83	0.59
1:L:210:VAL:HG22	1:L:329:ILE:HA	1.83	0.59
1:L:88:LEU:HB3	1:L:115:TRP:CZ2	2.37	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
1:L:17:ARG:O	1:L:17:ARG:HG3	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:278:TYR:C	1:L:280:SER:H	2.05	0.59
1:L:317:THR:OG1	1:L:318:LEU:N	2.36	0.59
1:L:266:ILE:HA	1:L:325:TYR:O	2.01	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:46:TYR:CD1	1:L:147:ARG:HG2	2.37	0.59
1:L:23:THR:CG2	1:L:172:ILE:HG22	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:PHE:HD2	1:L:342:PHE:CE2	2.21	0.59
1:L:95:GLY:N	1:L:146:VAL:HG22	2.15	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:120:LYS:NZ	1:L:120:LYS:HB3	2.17	0.58
1:L:210:VAL:HG12	1:L:210:VAL:O	2.02	0.58
1:L:271:LEU:HD21	1:L:275:PHE:HD2	1.68	0.58
2:S:107:THR:CG2	2:S:108:PHE:N	2.66	0.58
2:S:64:ALA:HB3	2:S:173:GLY:HA2	1.85	0.58
2:S:14:CYS:HA	2:S:54:PRO:HG2	1.84	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:96:GLN:HB3	2:S:142:THR:CG2	2.33	0.58
2:S:53:ASN:CA	2:S:61:ARG:HH22	2.15	0.58
2:S:81:VAL:O	2:S:81:VAL:HG23	2.02	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
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:198:GLY:HA2	1:L:346:VAL:CG2	2.34	0.58
2:S:125:ILE:HD12	2:S:130:GLY:O	2.03	0.58
1:L:246:LEU:H	1:L:246:LEU:HD12	1.69	0.58
1:L:241:TYR:HA	1:L:310:THR:H	1.68	0.58
2:S:106:ARG:NH1	2:S:106:ARG:CG	2.64	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
1:L:215:LEU:CB	1:L:325:TYR:HB2	2.21	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
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:140:MET:SD	2:S:65:TRP:HH2	2.27	0.57
1:L:20:LEU:HD12	1:L:172:ILE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:238:MET:O	1:L:359:SER:HA	2.05	0.57
2:S:74:LEU:HD23	2:S:74:LEU:C	2.24	0.57
1:L:4:ASN:C	1:L:6:PHE:H	2.04	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:305:VAL:HG22	1:L:305:VAL:O	2.04	0.57
1:L:199:LYS:HG3	1:L:343:ASN:CG	2.23	0.57
1:L:278:TYR:CD1	1:L:281:PHE:HE2	2.22	0.57
1:L:270:ASN:HB3	1:L:321:ASP:HB3	1.85	0.57
1:L:243:ARG:HH22	1:L:305:VAL:HG23	1.70	0.57
2:S:70:ILE:HA	2:S:164:ARG:O	2.04	0.57
2:S:86:TRP:CG	2:S:87:ASP:N	2.72	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
2:S:106:ARG:CG	2:S:107:THR:H	2.16	0.57
1:L:143:ARG:CA	2:S:137:PRO:HB2	2.34	0.57
1:L:15:SER:HA	1:L:68:ILE:HA	1.87	0.57
1:L:193:LEU:O	1:L:232:PRO:HB3	2.05	0.57
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:42:LEU:O	1:L:43:LEU:HB2	2.03	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
2:S:86:TRP:CD1	2:S:87:ASP:N	2.73	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:170:TRP:N	1:L:170:TRP:CD1	2.73	0.56
1:L:230:ASN:HD21	1:L:233:ASN:HB2	1.67	0.56
1:L:184:LEU:HG	1:L:235:TRP:CZ2	2.40	0.56
1:L:54:GLN:HG2	1:L:56:PHE:CE1	2.34	0.56
2:S:138:TRP:HE3	2:S:139:ALA:N	2.02	0.56
1:L:94:SER:O	2:S:176:LEU:HG	2.06	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
1:L:113:MET:HE2	1:L:125:PHE:HB2	1.87	0.56
1:L:19:SER:O	1:L:22:ASP:N	2.39	0.56
1:L:243:ARG:HH22	1:L:305:VAL:CG2	2.19	0.56
1:L:362:GLY:O	1:L:363:ILE:HG13	2.05	0.56
1:L:311:GLN:HE22	1:L:363:ILE:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:34:LEU:C	2:S:35:ILE:HG13	2.25	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
1:L:70:GLY:N	1:L:136:TRP:CZ2	2.73	0.56
2:S:127:PRO:HD3	2:S:132:GLU: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
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:71:HIS:CE1	2:S:121:SER:HG	2.19	0.56
2:S:19:THR:CB	2:S:156:ILE:O	2.53	0.56
1:L:169:ASP:C	1:L:170:TRP:CD1	2.78	0.56
2:S:107:THR:CG2	2:S:108:PHE:H	2.18	0.56
2:S:86:TRP:HH2	2:S:156:ILE:HD11	1.70	0.56
1:L:227:PHE:CZ	2:S:182:LEU:HD22	2.41	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
1:L:336:GLY:O	1:L:338:ILE:HD12	2.06	0.56
1:L:142:SER:C	1:L:144:SER:H	2.07	0.56
1:L:29:ARG:HD3	1:L:165:ILE:HD11	1.87	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
1:L:89:MET:CE	1:L:104:VAL:HB	2.36	0.56
2:S:91:PHE:CD1	2:S:149:VAL:HG21	2.41	0.56
2:S:21:PRO:O	2:S:24:PHE:HB2	2.06	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
2:S:130:GLY:C	2:S:131:PHE:HD2	2.08	0.55
1:L:156:TRP:H	1:L:156:TRP:HD1	1.54	0.55
1:L:29:ARG:HG3	1:L:167:LYS:HE2	1.88	0.55
1:L:235:TRP:CZ3	2:S:171:VAL:HG12	2.41	0.55
1:L:74:VAL:HG13	1:L:169:ASP:O	2.05	0.55
1:L:183:HIS:NE2	1:L:185:ALA:CB	2.69	0.55
1:L:67:VAL:C	1:L:68:ILE:HD12	2.26	0.55
2:S:125:ILE:CG1	2:S:126:GLY:H	2.19	0.55
1:L:140:MET:HA	2:S:138:TRP:HD1	1.71	0.55
2:S:62:THR:HG22	2:S:177:MET:HE2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:188:GLN:C	1:L:353:ASP:HA	2.26	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:221:ALA:O	1:L:228:LEU:N	2.39	0.55
1:L:202:PHE:HD1	1:L:342:PHE:HB3	1.70	0.55
2:S:45:ASP:C	2:S:47:TRP:HD1	2.09	0.55
1:L:130:ASN:CG	1:L:132:CYS:SG	2.85	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
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:200:LEU:O	1:L:202:PHE:CD2	2.60	0.55
1:L:21:LEU:C	1:L:23:THR:N	2.58	0.55
1:L:40:ASP:O	1:L:42:LEU:HG	2.06	0.55
2:S:68:GLY:HA3	2:S:169:PHE:CA	2.33	0.55
1:L:98:GLY:O	1:L:100:TYR:N	2.39	0.55
1:L:92:ILE:HG21	1:L:127:PHE:CD2	2.42	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
2:S:127:PRO:CD	2:S:132:GLU:HB3	2.37	0.55
2:S:149:VAL:CG1	2:S:150:ALA:H	2.11	0.55
2:S:64:ALA:H	2:S:173:GLY:HA2	1.72	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:210:VAL:HG21	1:L:278:TYR:HD2	1.73	0.54
1:L:27:GLN:N	1:L:54:GLN:OE1	2.40	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:PHE:HB2	1:L:342:PHE:CB	2.38	0.54
1:L:318:LEU:C	1:L:320:ALA:H	2.11	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:193:LEU:HD13	1:L:194:ASN:H	1.73	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
2:S:93:TYR:HB3	2:S:104:ASP:CG	2.27	0.54
1:L:252:LYS:C	1:L:254:SER:H	2.09	0.54
1:L:299:PHE:HD2	1:L:303:GLU:OE1	1.91	0.54
1:L:248:PHE:CA	1:L:347:LYS:O	2.45	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:20:LEU:CG	1:L:73:LYS:HE2	2.31	0.54
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:187:CYS:HA	1:L:355:CYS:HA	1.89	0.53
1:L:89:MET:HA	1:L:115:TRP:CZ3	2.43	0.53
1:L:199:LYS:C	1:L:200:LEU:HD23	2.28	0.53
1:L:202:PHE:O	1:L:342:PHE:N	2.41	0.53
2:S:54:PRO:HD2	2:S:61:ARG:NH2	2.24	0.53
1:L:234:SER:HB3	2:S:59:VAL:CG2	2.38	0.53
1:L:91:ALA:O	1:L:148:MET:HB2	2.07	0.53
1:L:74:VAL:CG1	1:L:170:TRP:CD1	2.84	0.53
1:L:184:LEU:HG	1:L:235:TRP:HZ2	1.72	0.53
1:L:314:PRO:CD	1:L:365:GLY:HA3	2.39	0.53
1:L:206:VAL:HG11	1:L:333:SER:HA	1.90	0.53
2:S:122:PHE:CE2	2:S:124:ILE:HG12	2.43	0.53
2:S:130:GLY:C	2:S:131:PHE:CD2	2.82	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
1:L:310:THR:HG22	1:L:310:THR:O	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:152:ASN:HB3	2:S:155:GLN:HE21	1.73	0.53
2:S:74:LEU:CD2	2:S:118:LEU:HD23	2.37	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:245:GLU:HB3	1:L:352:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:30:VAL:O	1:L:30:VAL:CG2	2.57	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:197:MET:HE2	1:L:248:PHE:HD2	1.73	0.53
1:L:262:VAL:HG22	1:L:330:ILE:HA	1.90	0.53
1:L:212:ARG:C	1:L:327:TYR:HA	2.29	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
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
1:L:95:GLY:C	1:L:96:VAL:HG22	2.30	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
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
1:L:74:VAL:HG22	1:L:170:TRP:CD2	2.44	0.52
2:S:107:THR:HG22	2:S:108:PHE:H	1.72	0.52
2:S:109:VAL:O	2:S:110:ILE:HG22	2.08	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: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:354:PHE:CD1	1:L:354:PHE:O	2.62	0.52
1:L:104:VAL:HG21	1:L:153:VAL:CG2	2.38	0.52
1:L:234:SER:HB3	2:S:59:VAL:HG22	1.91	0.52
1:L:248:PHE:O	1:L:296:THR:C	2.48	0.52
2:S:69:THR:O	2:S:169:PHE:CE2	2.63	0.52
1:L:176:LYS:HD2	1:L:176:LYS:H	1.75	0.52
2:S:112:GLN:CB	2:S:113:PRO:CD	2.85	0.52
2:S:22:ALA:CB	2:S:154:ARG:NH1	2.73	0.52
2:S:122:PHE:CD2	2:S:124:ILE:HG12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:88:LEU:HD23	1:L:115:TRP:HE1	1.73	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:10:LEU:HD13	1:L:10:LEU:C	2.30	0.52
1:L:92:ILE:O	1:L:110:GLN:HB3	2.10	0.52
1:L:47:LEU:HG	1:L:141:ILE:HB	1.93	0.51
1:L:257:TYR:N	1:L:259:LYS:HZ1	2.08	0.51
1:L:33:SER:CB	1:L:36:MET:SD	2.97	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:151:THR:O	2:S:152:ASN:OD1	2.28	0.51
2:S:31:THR:H	2:S:41:PRO:HB3	1.74	0.51
1:L:265:LEU:O	1:L:266:ILE:HD12	2.10	0.51
1:L:80:ILE:HD12	1:L:156:TRP:CZ2	2.45	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
1:L:42:LEU:O	1:L:150:VAL:HG23	2.11	0.51
2:S:34:LEU:HD22	2:S:146:LEU:HB2	1.92	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
1:L:337:THR:C	1:L:338:ILE:HG13	2.31	0.51
1:L:214:PRO:HG3	1:L:367:ARG:CZ	2.41	0.51
1:L:91:ALA:HB3	1:L:149:THR:N	2.26	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:32:LEU:O	1:L:163:ASP:CA	2.58	0.51
1:L:22:ASP:OD2	1:L:57:ARG:HG2	2.11	0.51
2:S:65:TRP:CD1	2:S:172:ALA:HB1	2.46	0.51
2:S:96:GLN:O	2:S:142:THR:OG1	2.26	0.51
1:L:25:PHE:HE2	1:L:171:SER:HA	1.74	0.51
1:L:186:ASP:HB3	1:L:239:TRP:CE3	2.45	0.51
1:L:236:ILE:CG2	1:L:236:ILE:O	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:242:PHE:CZ	1:L:246:LEU:CD2	2.85	0.51
1:L:72:ILE:HG22	1:L:170:TRP:HE3	1.76	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
1:L:41:VAL:HA	1:L:151:ILE:HB	1.93	0.51
2:S:13:PRO:CA	2:S:162:ASN:HA	2.39	0.51
2:S:35:ILE:HG13	2:S:144:TRP:HB2	1.93	0.51
2:S:30:VAL:CG2	2:S:41:PRO:HG3	2.41	0.51
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:31:LEU:HA	1:L:165:ILE:CG2	2.41	0.50
1:L:136:TRP:CZ2	1:L:172:ILE:HD11	2.46	0.50
2:S:112:GLN:NE2	2:S:113:PRO:HG2	2.26	0.50
2:S:29:ALA:N	2:S:150:ALA:HB3	2.26	0.50
1:L:352:LYS:O	1:L:352:LYS:HD3	2.11	0.50
2:S:92:VAL:HB	2:S:108:PHE:CB	2.42	0.50
2:S:91:PHE:O	2:S:91:PHE:HD1	1.95	0.50
1:L:194:ASN:OD1	1:L:349:VAL:HG22	2.12	0.50
1:L:20:LEU:HB3	1:L:73:LYS:HZ1	1.72	0.50
2:S:126:GLY:HA3	2:S:131:PHE:HA	1.93	0.50
1:L:245:GLU:O	1:L:351:ILE:HA	2.11	0.50
1:L:199:LYS:CG	1:L:343:ASN:HD21	2.14	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: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:48:TYR:CZ	1:L:62:PHE:HE2	2.27	0.50
1:L:123:PHE:CD2	1:L:124:SER:N	2.80	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
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: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
2:S:2:PRO:C	2:S:4:CYS:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:143:ARG:HB3	2:S:137:PRO:C	2.32	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:243:ARG:CG	1:L:243:ARG:HH11	2.25	0.49
1:L:258:ILE:HG22	1:L:342:PHE:CE1	2.47	0.49
1:L:248:PHE:O	1:L:296:THR:CA	2.60	0.49
1:L:199:LYS:CA	1:L:343:ASN:OD1	2.60	0.49
2:S:180:PHE:N	2:S:181:PRO:HD3	2.27	0.49
1:L:20:LEU:H	1:L:20:LEU:HD22	1.78	0.49
1:L:210:VAL:CG1	1:L:328:ALA:O	2.60	0.49
1:L:73:LYS:HB2	1:L:173:VAL:CG2	2.42	0.49
2:S:67:SER:OG	2:S:170:ARG:HB2	2.12	0.49
2:S:86:TRP:CZ2	2:S:113:PRO:HA	2.47	0.49
1:L:184:LEU:O	1:L:186:ASP:N	2.45	0.49
1:L:20:LEU:HG	1:L:73:LYS:CE	2.35	0.49
1:L:256:PRO:HB3	1:L:290:GLU:CG	2.43	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: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:177:MET:HB3	2:S:180:PHE:HZ	1.69	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
1:L:140:MET:SD	2:S:65:TRP:CZ3	3.05	0.49
1:L:242:PHE:CE2	1:L:246:LEU:HD11	2.48	0.49
1:L:195:ARG:HB2	1:L:348:LEU:HB2	1.93	0.49
1:L:245:GLU:CG	1:L:352:LYS:HB3	2.42	0.49
1:L:210:VAL:CG1	1:L:329:ILE:HG13	2.42	0.49
1:L:33:SER:HB3	1:L:36:MET:CE	2.42	0.49
2:S:126:GLY:HA3	2:S:132:GLU:N	2.27	0.49
2:S:97:SER:O	2:S:98:MET:HB2	2.12	0.49
2:S:94:LEU:HD21	2:S:120:PHE:HZ	1.77	0.49
1:L:202:PHE:HE2	1:L:211:ARG:CG	2.24	0.49
1:L:191:LEU:HB2	1:L:354:PHE:CD2	2.48	0.49
1:L:227:PHE:CE2	2:S:182:LEU:HD22	2.48	0.49
1:L:7:ALA:HA	1:L:11:ASP:OD2	2.13	0.49
1:L:238:MET:C	1:L:239:TRP:O	2.50	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:268:PHE:HB3	1:L:270:ASN:OD1	2.13	0.48
1:L:189:ASN:HA	1:L:353:ASP:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:92:VAL:HG13	2:S:146:LEU:HD21	1.95	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
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:60:VAL:C	1:L:64:ARG:HB2	2.32	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
1:L:32:LEU:HD13	1:L:165:ILE:HA	1.94	0.48
1:L:243:ARG:HH12	1:L:305:VAL:HA	1.79	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
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
1:L:72:ILE:HA	1:L:172:ILE:HA	1.95	0.48
2:S:164:ARG:HH21	2:S:166:ASP:HA	1.77	0.48
2:S:90:VAL:HG12	2:S:91:PHE:N	2.28	0.48
1:L:220:GLY:HA2	1:L:230:ASN:ND2	2.28	0.48
1:L:30:VAL:O	1:L:165:ILE:O	2.32	0.48
2:S:152:ASN:HD22	2:S:155:GLN:NE2	2.11	0.48
2:S:95:ARG:HG2	2:S:98:MET:CG	2.41	0.48
1:L:4:ASN:C	1:L:6:PHE:N	2.66	0.48
1:L:240:ARG:O	1:L:310:THR:HB	2.13	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
1:L:31:LEU:C	1:L:32:LEU:HD12	2.34	0.48
2:S:75:ASN:HD22	2:S:117:MET:HB3	1.77	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
1:L:73:LYS:HB3	1:L:73:LYS:HE3	1.66	0.48
2:S:16:ILE:HG22	2:S:16:ILE:O	2.13	0.48
1:L:13:THR:O	1:L:65:THR:O	2.32	0.48
1:L:148:MET:SD	1:L:149:THR:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:GLN:NE2	1:L:340:GLY:C	2.67	0.48
1:L:299:PHE:HB3	1:L:303:GLU:OE2	2.14	0.48
1:L:268:PHE:CZ	1:L:324:PRO:HG3	2.47	0.48
2:S:74:LEU:O	2:S:117:MET:HA	2.14	0.48
2:S:122:PHE:CG	2:S:144:TRP:CZ3	3.01	0.48
2:S:154:ARG:O	2:S:155:GLN:NE2	2.46	0.48
2:S:90:VAL:CG1	2:S:91:PHE:N	2.77	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: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:302:GLN:OE1	1:L:302:GLN:N	2.47	0.47
1:L:239:TRP:HB2	1:L:357:ILE:C	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
2:S:8:SER:O	2:S:9:ASP:O	2.33	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
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
1:L:85:GLY:C	1:L:86:CYS:SG	2.91	0.47
1:L:283:HIS:O	1:L:284:ARG:HB2	2.15	0.47
1:L:89:MET:HE1	1:L:196:TRP:CE3	2.50	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
1:L:100:TYR:HA	2:S:178:PRO:CA	2.44	0.47
1:L:363:ILE:HG22	1:L:364:ASP:H	1.79	0.47
2:S:167:PRO:C	2:S:169:PHE:H	2.17	0.47
1:L:224:THR:O	1:L:225:GLN:C	2.51	0.47
1:L:30:VAL:O	1:L:165:ILE:HA	2.14	0.47
1:L:21:LEU:O	1:L:57:ARG:CB	2.63	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:245:GLU:HB2	1:L:300:SER:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:ASP:N	1:L:151:ILE:HG13	2.29	0.47
1:L:55:ASP:C	1:L:56:PHE:CD1	2.88	0.47
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: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:17:ARG:CG	1:L:17:ARG:O	2.62	0.47
1:L:227:PHE:HB3	1:L:366:SER:OG	2.15	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
2:S:96:GLN:C	2:S:145:TYR:HE1	2.19	0.47
2:S:57:MET:C	2:S:59:VAL:N	2.66	0.47
2:S:35:ILE:HG22	2:S:60:LEU:HD22	1.97	0.47
1:L:3:GLN:C	1:L:5:LEU:H	2.18	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:284:ARG:HH22	1:L:298:VAL:CB	2.29	0.46
2:S:149:VAL:O	2:S:150:ALA:HB2	2.15	0.46
2:S:82:LYS:O	2:S:85:ASP:N	2.48	0.46
1:L:113:MET:HE2	1:L:125:PHE:CB	2.45	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:97:ARG:HH12	2:S:38:LYS:HG2	1.80	0.46
1:L:249:GLU:HA	1:L:295:CYS:O	2.15	0.46
1:L:30:VAL:O	1:L:165:ILE:C	2.54	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:19:SER:C	1:L:21:LEU:N	2.69	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
1:L:98:GLY:O	1:L:100:TYR:CD1	2.56	0.46
2:S:22:ALA:HB2	2:S:154:ARG:NH1	2.30	0.46
1:L:269:GLY:HA3	1:L:325:TYR:HH	1.80	0.46
1:L:291:VAL:HG23	1:L:292:GLU:N	2.29	0.46
1:L:288:PHE:CD2	1:L:342:PHE:CE2	3.03	0.46
2:S:135:GLU:CA	2:S:141:GLN:HB3	2.41	0.46
2:S:75:ASN:HB3	2:S:160:GLU:HG2	1.96	0.46
2:S:64:ALA:N	2:S:173:GLY:HA2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:68:ILE:HD13	1:L:136:TRP:CZ3	2.51	0.46
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:197:MET:SD	1:L:346:VAL:O	2.73	0.46
1:L:206:VAL:O	1:L:207:THR:C	2.54	0.46
1:L:258:ILE:O	1:L:342:PHE:HE1	1.99	0.46
1:L:55:ASP:O	1:L:56:PHE:CG	2.69	0.46
2:S:178:PRO:O	2:S:180:PHE:CE2	2.69	0.46
2:S:35:ILE:HB	2:S:66:LYS:HZ3	1.80	0.46
2:S:73:GLN:HB3	2:S:119:ASN:HA	1.97	0.46
1:L:48:TYR:OH	1:L:63:LEU:HD23	2.14	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:258:ILE:HG22	1:L:342:PHE:HD1	1.72	0.46
1:L:202:PHE:O	1:L:341:ASP:HA	2.15	0.46
1:L:198:GLY:HA2	1:L:346:VAL:CB	2.46	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
2:S:86:TRP:HH2	2:S:156:ILE:CD1	2.29	0.46
1:L:48:TYR:CD2	1:L:62:PHE:HE2	2.28	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
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:27:GLN:OE1	1:L:56:PHE:CE2	2.70	0.45
2:S:9:ASP:O	2:S:11:TYR:CE1	2.68	0.45
1:L:265:LEU:CD2	1:L:283:HIS:HA	2.40	0.45
1:L:206:VAL:HG13	1:L:333:SER:HA	1.98	0.45
1:L:34:LYS:HG2	1:L:35:ALA:N	2.30	0.45
1:L:193:LEU:HD23	1:L:232:PRO:CB	2.47	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: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:136:SER:O	2:S:138:TRP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:THR:HB	2:S:166:ASP:CG	2.36	0.45
2:S:89:GLN:CG	2:S:90:VAL:N	2.79	0.45
1:L:241:TYR:HA	1:L:310:THR:N	2.31	0.45
1:L:273:ASP:OD1	1:L:273:ASP:N	2.49	0.45
1:L:317:THR:O	1:L:321:ASP:HA	2.16	0.45
1:L:191:LEU:O	1:L:349:VAL:O	2.35	0.45
1:L:362:GLY:C	1:L:363:ILE:HG13	2.37	0.45
1:L:86:CYS:N	1:L:116:ASN:ND2	2.64	0.45
1:L:80:ILE:CD1	1:L:156:TRP:CH2	2.89	0.45
1:L:19:SER:C	1:L:21:LEU:H	2.20	0.45
1:L:246:LEU:HB2	1:L:348:LEU:CD1	2.46	0.45
1:L:31:LEU:CD2	1:L:31:LEU:H	2.29	0.45
1:L:76:ALA:HA	1:L:167:LYS:O	2.17	0.45
1:L:87:CYS:SG	1:L:153:VAL:HG23	2.57	0.45
2:S:86:TRP:CZ2	2:S:113:PRO:CA	3.00	0.45
1:L:130:ASN:ND2	1:L:132:CYS:SG	2.89	0.45
2:S:83:ARG:HB3	2:S:83:ARG:CZ	2.46	0.45
2:S:39:ILE:C	2:S:39:ILE:HD12	2.37	0.45
1:L:241:TYR:HB3	1:L:308:TRP:O	2.17	0.45
1:L:214:PRO:HA	1:L:325:TYR:CE1	2.52	0.45
1:L:243:ARG:CB	1:L:355:CYS:HB3	2.36	0.45
1:L:72:ILE:HG13	1:L:127:PHE:O	2.17	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:70:ILE:C	2:S:71:HIS:ND1	2.70	0.45
1:L:189:ASN:ND2	1:L:189:ASN:N	2.65	0.44
1:L:286:VAL:CG2	1:L:344:LEU:HD11	2.47	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
2:S:29:ALA:HB1	2:S:147:GLU:OE2	2.16	0.44
1:L:103:ASP:CG	1:L:106:THR:OG1	2.55	0.44
1:L:173:VAL:HB	1:L:175:GLU:HG3	1.99	0.44
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:130:ASN:HA	1:L:131:PRO:HD3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:LYS:O	1:L:170:TRP:HA	2.17	0.44
1:L:17:ARG:HH22	1:L:20:LEU:H	1.65	0.44
1:L:248:PHE:O	1:L:296:THR:HA	2.16	0.44
1:L:246:LEU:N	1:L:351:ILE:HG13	2.32	0.44
1:L:91:ALA:O	1:L:148:MET:CA	2.65	0.44
2:S:108:PHE:HE2	2:S:120:PHE:CD2	2.36	0.44
2:S:15:MET:C	2:S:52:TYR:CE2	2.91	0.44
1:L:176:LYS:NZ	1:L:176:LYS:H	2.14	0.44
1:L:202:PHE:CE2	1:L:211:ARG:HG2	2.47	0.44
1:L:202:PHE:O	1:L:341:ASP:CA	2.65	0.44
1:L:90:LEU:HD12	1:L:92:ILE:HG13	2.00	0.44
2:S:93:TYR:HD1	2:S:107:THR:OG1	1.97	0.44
1:L:127:PHE:CZ	1:L:129:PRO:CB	3.00	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
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
2:S:68:GLY:O	2:S:169:PHE:CE2	2.71	0.44
2:S:165:PHE:HA	2:S:169:PHE:HE2	1.80	0.44
2:S:64:ALA:O	2:S:133:PHE:CD1	2.70	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
1:L:174:ASN:ND2	1:L:174:ASN:O	2.48	0.44
2:S:127:PRO:HD2	2:S:131:PHE:O	2.18	0.44
1:L:59:THR:CG2	1:L:60:VAL:N	2.80	0.44
1:L:107:ILE:HD12	1:L:149:THR:HG21	2.00	0.44
1:L:265:LEU:HD11	1:L:281:PHE:C	2.38	0.44
2:S:86:TRP:CZ2	2:S:112:GLN:O	2.70	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:95:ARG:CB	2:S:105:ALA:H	2.30	0.44
1:L:91:ALA:O	1:L:148:MET:CB	2.66	0.44
1:L:251:THR:HG1	1:L:294:LYS:HA	1.82	0.44
1:L:243:ARG:HH12	1:L:301:GLN:HG2	1.83	0.44
1:L:88:LEU:HD23	1:L:115:TRP:HZ2	1.76	0.44
2:S:177:MET:C	2:S:180:PHE:CZ	2.87	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
1:L:78:THR:HG23	1:L:79:ASN:H	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:L:26:ALA:C	1:L:54:GLN:OE1	2.56	0.43
1:L:284:ARG:CB	1:L:299:PHE:HZ	2.30	0.43
1:L:49:ASP:O	1:L:50:VAL:C	2.57	0.43
2:S:53:ASN:ND2	2:S:182:LEU:HB2	2.30	0.43
2:S:27:VAL:HG22	2:S:151:THR:C	2.38	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:280:SER:O	1:L:281:PHE:CD1	2.71	0.43
1:L:262:VAL:N	1:L:286:VAL:HG23	2.27	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
1:L:202:PHE:HB2	1:L:342:PHE:C	2.38	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:95:ARG:HG3	2:S:97:SER:H	1.82	0.43
1:L:244:GLY:CA	1:L:351:ILE:HD11	2.49	0.43
1:L:261:THR:HG1	1:L:287:GLN:HG3	1.81	0.43
1:L:367:ARG:C	1:L:369:LEU:N	2.71	0.43
1:L:91:ALA:O	1:L:92:ILE:HG12	2.18	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
2:S:65:TRP:HD1	2:S:173:GLY:N	2.17	0.43
2:S:39:ILE:H	2:S:39:ILE:HG13	1.61	0.43
1:L:75:THR:CG2	1:L:122:ASN:ND2	2.79	0.43
1:L:127:PHE:CZ	1:L:129:PRO:HD3	2.53	0.43
1:L:115:TRP:CH2	1:L:150:VAL:HG12	2.52	0.43
2:S:122:PHE:O	2:S:124:ILE:N	2.51	0.43
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
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:252:LYS:HZ2	1:L:256:PRO:HG3	1.78	0.43
1:L:314:PRO:HG3	1:L:365:GLY:HA2	1.94	0.43
2:S:62:THR:HG22	2:S:177:MET:CE	2.48	0.43
2:S:6:GLU:HG3	2:S:6:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:MET:HE3	1:L:104:VAL:CB	2.47	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:197:MET:SD	1:L:346:VAL:C	2.98	0.43
1:L:267:ALA:O	1:L:268:PHE:CG	2.72	0.43
1:L:73:LYS:CB	1:L:173:VAL:CG2	2.97	0.43
2:S:13:PRO:HB2	2:S:14:CYS:H	1.46	0.43
1:L:100:TYR:HA	2:S:178:PRO:CB	2.49	0.43
1:L:212:ARG:CA	1:L:327:TYR:HB2	2.49	0.42
1:L:79:ASN:O	1:L:80:ILE:HB	2.19	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:120:LYS:HG2	1:L:121:LYS:N	2.34	0.42
1:L:214:PRO:HB2	1:L:215:LEU:H	1.46	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:47:LEU:HD22	1:L:47:LEU:N	2.34	0.42
1:L:67:VAL:HG22	1:L:136:TRP:C	2.40	0.42
1:L:15:SER:CA	1:L:68:ILE:HA	2.49	0.42
1:L:59:THR:HG22	1:L:60:VAL:HG13	2.01	0.42
1:L:195:ARG:HB3	1:L:197:MET:CE	2.48	0.42
1:L:313:ASN:CB	1:L:363:ILE:HD13	2.50	0.42
2:S:128:ASN:O	2:S:129:SER:C	2.57	0.42
2:S:45:ASP:C	2:S:47:TRP:CD1	2.92	0.42
2:S:63:ALA:O	2:S:133:PHE:CE1	2.71	0.42
2:S:86:TRP:HZ2	2:S:112:GLN:O	2.02	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
2:S:83:ARG:HH11	2:S:83:ARG:CG	2.31	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:34:LYS:HG3	1:L:159:SER:OG	2.18	0.42
2:S:84:ALA:C	2:S:86:TRP:H	2.23	0.42
1:L:63:LEU:N	1:L:63:LEU:HD12	2.35	0.42
1:L:128:ASN:ND2	1:L:136:TRP:NE1	2.66	0.42
1:L:29:ARG:HB3	1:L:165:ILE:CG1	2.49	0.42
1:L:168:LEU:HD12	1:L:168:LEU:HA	1.27	0.42
1:L:263:THR:C	1:L:264:PHE:CD1	2.93	0.42
1:L:271:LEU:HD13	1:L:278:TYR:CE1	2.54	0.42
1:L:212:ARG:CZ	1:L:273:ASP:OD1	2.68	0.42
1:L:86:CYS:H	1:L:116:ASN:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:94:LEU:CA	2:S:146:LEU:HA	2.41	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:31:LEU:HD22	1:L:31:LEU:N	2.34	0.42
1:L:278:TYR:CD1	1:L:329:ILE:HG12	2.55	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:89:MET:HB3	1:L:104:VAL:HG12	2.02	0.42
1:L:17:ARG:HH21	1:L:19:SER:HA	1.85	0.42
1:L:265:LEU:HD22	1:L:283:HIS:CA	2.39	0.42
1:L:15:SER:HA	1:L:68:ILE:HG13	2.01	0.42
2:S:117:MET:HB2	2:S:118:LEU:H	1.64	0.42
2:S:68:GLY:HA2	2:S:169:PHE:HA	1.99	0.42
2:S:49:THR:O	2:S:51:ILE:HG13	2.20	0.42
1:L:75:THR:OG1	1:L:122:ASN:ND2	2.43	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:284:ARG:HH22	1:L:298:VAL:CG1	2.33	0.42
1:L:262:VAL:N	1:L:286:VAL:CG2	2.76	0.42
2:S:120:PHE:CG	2:S:121:SER:N	2.88	0.42
2:S:28:THR:O	2:S:29:ALA:CB	2.65	0.42
1:L:183:HIS:CE1	1:L:185:ALA:CB	3.02	0.42
1:L:73:LYS:HE3	1:L:172:ILE:O	2.20	0.42
1:L:189:ASN:N	1:L:189:ASN:HD22	2.17	0.42
1:L:21:LEU:HA	1:L:24:LYS:HB2	2.02	0.42
1:L:275:PHE:HE1	1:L:277:PHE:HD2	1.67	0.42
2:S:122:PHE:CD2	2:S:144:TRP:CZ2	3.08	0.42
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
1:L:183:HIS:CE1	1:L:185:ALA:HB3	2.53	0.42
1:L:67:VAL:HA	1:L:136:TRP:O	2.20	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:91:ALA:HB2	1:L:149:THR:OG1	2.19	0.41
1:L:59:THR:HG22	1:L:60:VAL:N	2.35	0.41
1:L:165:ILE:O	1:L:166:ALA:O	2.37	0.41
1:L:191:LEU:HG	1:L:193:LEU:CD1	2.48	0.41
1:L:197:MET:HE2	1:L:248:PHE:CE2	2.55	0.41
1:L:301:GLN:HG3	1:L:305:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:ASN:HB3	1:L:353:ASP:OD1	2.20	0.41
1:L:71:LYS:O	1:L:73:LYS:N	2.53	0.41
2:S:53:ASN:C	2:S:61:ARG:HH22	2.23	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
1:L:190:TRP:C	1:L:351:ILE:HG22	2.41	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
1:L:256:PRO:HB3	1:L:290:GLU:HG2	2.01	0.41
1:L:170:TRP:O	1:L:171:SER:HB3	2.21	0.41
1:L:136:TRP:CH2	1:L:172:ILE:HG12	2.55	0.41
1:L:245:GLU:CG	1:L:352:LYS:CB	2.98	0.41
1:L:31:LEU:HA	1:L:165:ILE:CB	2.50	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:97:ARG:N	2:S:176:LEU:O	2.54	0.41
1:L:84:SER:HB3	1:L:158:LEU:HD12	2.03	0.41
1:L:191:LEU:HA	1:L:192:PRO:HD3	1.56	0.41
1:L:325:TYR:HE1	1:L:327:TYR:CG	2.39	0.41
1:L:194:ASN:O	1:L:347:LYS:HE2	2.21	0.41
1:L:189:ASN:HA	1:L:353:ASP:CA	2.51	0.41
2:S:125:ILE:CG1	2:S:126:GLY:N	2.83	0.41
2:S:133:PHE:O	2:S:134:ALA:C	2.59	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
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:119:ASN:N	2:S:119:ASN:ND2	2.69	0.41
2:S:138:TRP:HE3	2:S:138:TRP:C	2.23	0.41
1:L:136:TRP:CH2	1:L:172:ILE:CD1	3.04	0.41
1:L:20:LEU:HD11	1:L:173:VAL:HA	2.03	0.41
1:L:366:SER:O	1:L:367:ARG:C	2.59	0.41
2:S:148:CYS:O	2:S:149:VAL:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:21:PRO:O	2:S:24:PHE:CB	2.68	0.41
2:S:34:LEU:CB	2:S:145:TYR:HA	2.45	0.41
1:L:256:PRO:C	1:L:259:LYS:HZ1	2.23	0.40
1:L:297:LEU:CD1	1:L:299:PHE:CE1	2.95	0.40
1:L:313:ASN:C	1:L:313:ASN:OD1	2.59	0.40
1:L:313:ASN:OD1	1:L:315:ARG:HB2	2.21	0.40
1:L:90:LEU:CD1	1:L:148:MET:SD	3.09	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
2:S:56:ILE:HD12	2:S:56:ILE:C	2.41	0.40
2:S:34:LEU:CD2	2:S:94:LEU:HD13	2.52	0.40
1:L:22:ASP:HA	1:L:57:ARG:CB	2.51	0.40
1:L:235:TRP:C	1:L:237:SER:H	2.24	0.40
1:L:217:ILE:CD1	1:L:242:PHE:CD1	3.04	0.40
1:L:364:ASP:OD1	1:L:365:GLY:N	2.55	0.40
1:L:91:ALA:HB1	1:L:107:ILE:CB	2.47	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:105:TYR:OH	1:L:220:GLY:HA2	2.21	0.40
1:L:200:LEU:H	1:L:343:ASN:CG	2.25	0.40
1:L:45:GLU:OE1	1:L:50:VAL:HG22	2.20	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:86:CYS:SG	1:L:156:TRP:CD2	3.07	0.40
1:L:195:ARG:HH21	1:L:217:ILE:H	1.69	0.40
1:L:32:LEU:HB2	1:L:164:VAL:C	2.42	0.40
1:L:363:ILE:CG2	1:L:364:ASP:H	2.31	0.40
1:L:313:ASN:HB3	1:L:363:ILE:HD13	2.04	0.40
1:L:74:VAL:HG22	1:L:170:TRP:CG	2.56	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
2:S:143:THR:O	2:S:145:TYR:CE1	2.74	0.40
1:L:119:CYS:SG	1:L:293:GLU:CD	2.99	0.40
1:L:235:TRP:HA	1:L:238:MET:SD	2.62	0.40
1:L:304:PHE:CD2	1:L:304:PHE:O	2.75	0.40
1:L:264:PHE:CZ	1:L:344:LEU:HD21	2.56	0.40
1:L:355:CYS:SG	1:L:355:CYS:O	2.77	0.40
1:L:88:LEU:HB3	1:L:115:TRP:CD2	2.54	0.40
2:S:86:TRP:CD2	2:S:113:PRO:HA	2.56	0.40
2:S:12:SER:CB	2:S:56:ILE:HD11	2.42	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:14:SER:OG	1:L:57:ARG:HH2[2_555]	1.27	0.33
1:L:1:MET:N	1:L:124:SER:CA[2_555]	1.87	0.33
1:L:1:MET:O	1:L:122:ASN:HD2[2_555]	1.30	0.30
1:L:55:ASP:OD2	1:L:64:ARG:HH1[2_555]	1.32	0.28
1:L:12:ASP:CG	1:L:57:ARG:HE[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
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:HD2[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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	209 (66%)	109 (34%)	0	2
2	S	163/163 (100%)	109 (67%)	54 (33%)	0	3
All	All	481/481 (100%)	318 (66%)	163 (34%)	0	2

All (163) 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	11	ASP
1	L	17	ARG
1	L	20	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
1	L	50	VAL
1	L	54	GLN
1	L	57	ARG
1	L	59	THR
1	L	62	PHE
1	L	63	LEU
1	L	65	THR
1	L	66	HIS
1	L	74	VAL
1	L	75	THR
1	L	86	CYS
1	L	90	LEU
1	L	96	VAL
1	L	102	THR
1	L	106	THR
1	L	108	CYS
1	L	111	ASP
1	L	112	SER
1	L	120	LYS
1	L	136	TRP
1	L	139	GLU
1	L	144	SER
1	L	148	MET
1	L	150	VAL
1	L	151	ILE
1	L	156	TRP
1	L	158	LEU
1	L	160	PRO
1	L	163	ASP

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Mol	Chain	Res	Type
1	L	165	ILE
1	L	170	TRP
1	L	173	VAL
1	L	176	LYS
1	L	177	CYS
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	248	PHE
1	L	253	MET
1	L	254	SER
1	L	257	TYR
1	L	259	LYS
1	L	263	THR
1	L	265	LEU
1	L	270	ASN
1	L	271	LEU
1	L	277	PHE
1	L	278	TYR
1	L	281	PHE
1	L	283	HIS
1	L	287	GLN

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Mol	Chain	Res	Type
1	L	294	LYS
1	L	297	LEU
1	L	302	GLN
1	L	304	PHE
1	L	306	THR
1	L	309	SER
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	331	HIS
1	L	334	THR
1	L	335	THR
1	L	337	THR
1	L	341	ASP
1	L	342	PHE
1	L	348	LEU
1	L	357	ILE
1	L	359	SER
1	L	369	LEU
2	S	3	VAL
2	S	11	TYR
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	36	ASN
2	S	40	THR
2	S	46	ASN
2	S	50	HIS
2	S	53	ASN
2	S	57	MET
2	S	65	TRP
2	S	67	SER

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Mol	Chain	Res	Type
2	S	69	THR
2	S	73	GLN
2	S	74	LEU
2	S	76	VAL
2	S	87	ASP
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	160	GLU
2	S	164	ARG
2	S	169	PHE
2	S	171	VAL
2	S	174	ASN
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

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

Mol	Chain	Res	Type
1	L	83	ASN

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Mol	Chain	Res	Type
1	L	116	ASN
1	L	128	ASN
1	L	188	GLN
1	L	189	ASN
1	L	204	GLN
1	L	230	ASN
1	L	233	ASN
1	L	247	HIS
1	L	311	GLN
1	L	331	HIS
1	L	360	ASN
2	S	36	ASN
2	S	48	ASN
2	S	119	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	L	369/369 (100%)	0.58	27 (7%)	18 13	15, 15, 15, 15	0
2	S	189/189 (100%)	0.68	16 (8%)	13 10	15, 15, 15, 15	0
All	All	558/558 (100%)	0.62	43 (7%)	16 11	15, 15, 15, 15	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	189	LEU	4.3
1	L	129	PRO	4.2
2	S	186	THR	4.1
1	L	293	GLU	4.0
1	L	368	LEU	3.8
2	S	111	SER	3.6
1	L	364	ASP	3.6
1	L	14	SER	3.5
1	L	365	GLY	3.3
1	L	13	THR	3.2
1	L	37	ALA	3.0
2	S	137	PRO	3.0
2	S	179	PRO	3.0
1	L	12	ASP	2.9
1	L	127	PHE	2.8
1	L	369	LEU	2.8
1	L	367	ARG	2.8
2	S	68	GLY	2.7
1	L	281	PHE	2.7
2	S	1	GLY	2.6
2	S	116	ALA	2.5
1	L	219	GLY	2.5
1	L	80	ILE	2.4
1	L	107	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	S	39	ILE	2.4
1	L	312	VAL	2.4
1	L	276	GLY	2.4
2	S	187	PRO	2.3
1	L	57	ARG	2.3
1	L	145	ARG	2.3
2	S	66	LYS	2.3
2	S	88	GLY	2.2
1	L	229	ALA	2.2
1	L	294	LYS	2.2
2	S	89	GLN	2.2
2	S	25	SER	2.1
1	L	305	VAL	2.1
1	L	313	ASN	2.1
1	L	95	GLY	2.1
1	L	175	GLU	2.0
2	S	69	THR	2.0
2	S	64	ALA	2.0
1	L	366	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.