



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 11:11 PM UTC

PDB ID : 1I84 / pdb_00001i84
Title : CRYO-EM STRUCTURE OF THE HEAVY MEROMYOSIN SUBFRAGMENT OF CHICKEN GIZZARD SMOOTH MUSCLE MYOSIN WITH REGULATORY LIGHT CHAIN IN THE DEPHOSPHORYLATED STATE. ONLY C ALPHAS PROVIDED FOR REGULATORY LIGHT CHAIN. ONLY BACKBONE ATOMS PROVIDED FOR S2 FRAGMENT.
Authors : Wendt, T.; Taylor, D.; Trybus, K.M.; Taylor, K.
Deposited on : 2001-03-12
Resolution : 20.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

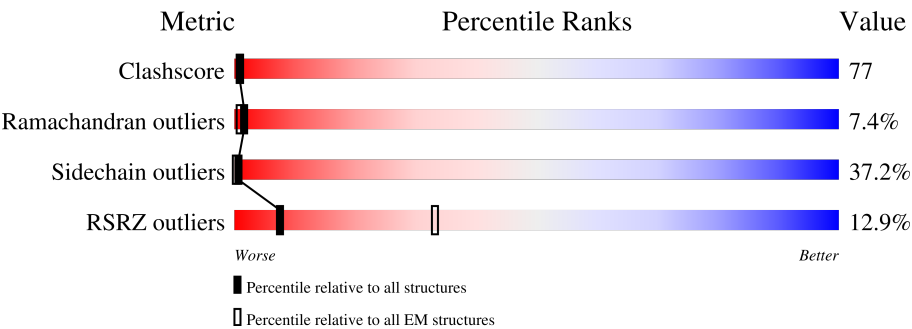
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 20.00 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

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

Mol	Chain	Length	Quality of chain
1	S	1184	11% 19% 35% 20% • 23%
1	V	1184	7% 20% 35% 20% • 23%
2	T	150	8% 12% 53% 33% ••
2	W	150	20% 14% 49% 35% ••
3	U	166	9% 82% • 17%
3	Z	166	8% 82% • 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SMOOTH MUSCLE MYOSIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	909	Total	C	N	O	S	0	0
			6992	4423	1226	1311	32		
1	V	909	Total	C	N	O	S	0	0
			6992	4423	1226	1311	32		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	ALA	SER	SEE REMARK 999	? P10587
S	820	GLU	THR	SEE REMARK 999	? P10587
S	821	SER	ALA	SEE REMARK 999	? P10587
S	822	ILE	MET	SEE REMARK 999	? P10587
S	823	PHE	LYS	SEE REMARK 999	? P10587
S	824	CYS	VAL	SEE REMARK 999	? P10587
S	827	TYR	ARG	SEE REMARK 999	? P10587
S	829	VAL	CYS	SEE REMARK 999	? P10587
S	830	ARG	ALA	SEE REMARK 999	? P10587
S	831	SER	ALA	SEE REMARK 999	? P10587
S	832	PHE	TYR	SEE REMARK 999	? P10587
S	833	MET	LEU	SEE REMARK 999	? P10587
S	834	ASN	LYS	SEE REMARK 999	? P10587
S	835	VAL	LEU	SEE REMARK 999	? P10587
S	836	MLY	ARG	SEE REMARK 999	? P10587
S	837	HIS	ASN	SEE REMARK 999	? P10587
S	839	PRO	GLN	SEE REMARK 999	? P10587
S	841	MET	TRP	SEE REMARK 999	? P10587
S	842	MLY	ARG	SEE REMARK 999	? P10587
S	845	PHE	THR	SEE REMARK 999	? P10587
S	846	MLY	LYS	SEE REMARK 999	? P10587
S	847	ILE	VAL	SEE REMARK 999	? P10587
S	848	MLY	LYS	SEE REMARK 999	? P10587
S	852	LYS	GLN	SEE REMARK 999	? P10587
S	1176	GLY	-	expression tag	? P10587
S	1177	SER	-	expression tag	? P10587

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1178	ASP	-	expression tag	? P10587
S	1179	TYR	-	expression tag	? P10587
S	1180	LYS	-	expression tag	? P10587
S	1181	ASP	-	expression tag	? P10587
S	1182	ASP	-	expression tag	? P10587
S	1183	ASP	-	expression tag	? P10587
S	1184	ASP	-	expression tag	? P10587
S	1185	LYS	-	expression tag	? P10587
V	2	ALA	SER	SEE REMARK 999	? P10587
V	820	GLU	THR	SEE REMARK 999	? P10587
V	821	SER	ALA	SEE REMARK 999	? P10587
V	822	ILE	MET	SEE REMARK 999	? P10587
V	823	PHE	LYS	SEE REMARK 999	? P10587
V	824	CYS	VAL	SEE REMARK 999	? P10587
V	827	TYR	ARG	SEE REMARK 999	? P10587
V	829	VAL	CYS	SEE REMARK 999	? P10587
V	830	ARG	ALA	SEE REMARK 999	? P10587
V	831	SER	ALA	SEE REMARK 999	? P10587
V	832	PHE	TYR	SEE REMARK 999	? P10587
V	833	MET	LEU	SEE REMARK 999	? P10587
V	834	ASN	LYS	SEE REMARK 999	? P10587
V	835	VAL	LEU	SEE REMARK 999	? P10587
V	836	MLY	ARG	SEE REMARK 999	? P10587
V	837	HIS	ASN	SEE REMARK 999	? P10587
V	839	PRO	GLN	SEE REMARK 999	? P10587
V	841	MET	TRP	SEE REMARK 999	? P10587
V	842	MLY	ARG	SEE REMARK 999	? P10587
V	845	PHE	THR	SEE REMARK 999	? P10587
V	846	MLY	LYS	SEE REMARK 999	? P10587
V	847	ILE	VAL	SEE REMARK 999	? P10587
V	848	MLY	LYS	SEE REMARK 999	? P10587
V	852	LYS	GLN	SEE REMARK 999	? P10587
V	1176	GLY	-	expression tag	? P10587
V	1177	SER	-	expression tag	? P10587
V	1178	ASP	-	expression tag	? P10587
V	1179	TYR	-	expression tag	? P10587
V	1180	LYS	-	expression tag	? P10587
V	1181	ASP	-	expression tag	? P10587
V	1182	ASP	-	expression tag	? P10587
V	1183	ASP	-	expression tag	? P10587
V	1184	ASP	-	expression tag	? P10587
V	1185	LYS	-	expression tag	? P10587

- Molecule 2 is a protein called SMOOTH MUSCLE MYOSIN ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	148	Total	C	N	O	S	0	0
			1160	722	193	234	11		
2	W	148	Total	C	N	O	S	0	0
			1160	722	193	234	11		

- Molecule 3 is a protein called SMOOTH MUSCLE MYOSIN REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	U	138	Total	C	0	138
			138	138		
3	Z	138	Total	C	0	138
			138	138		

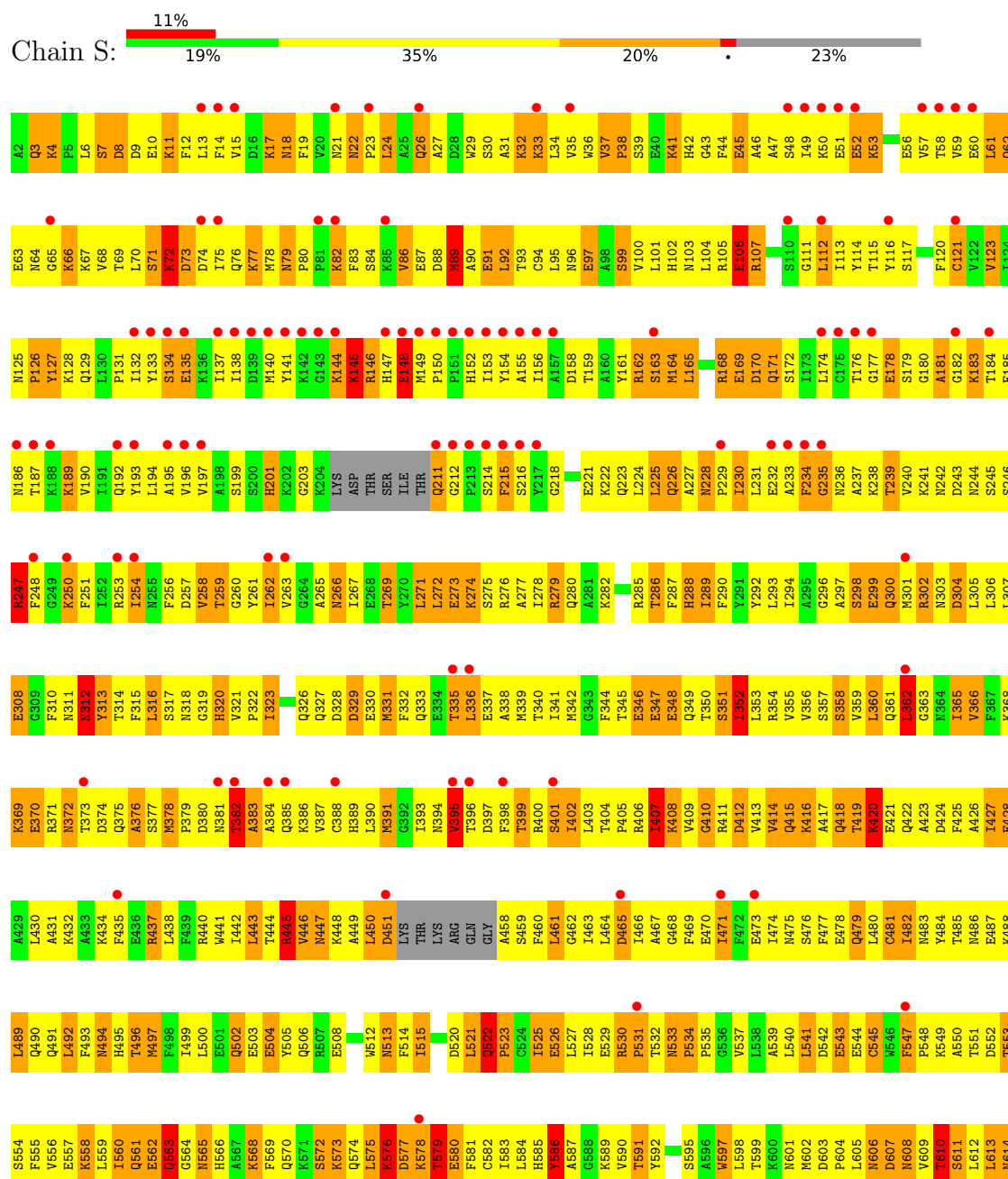
There are 18 discrepancies between the modelled and reference sequences:

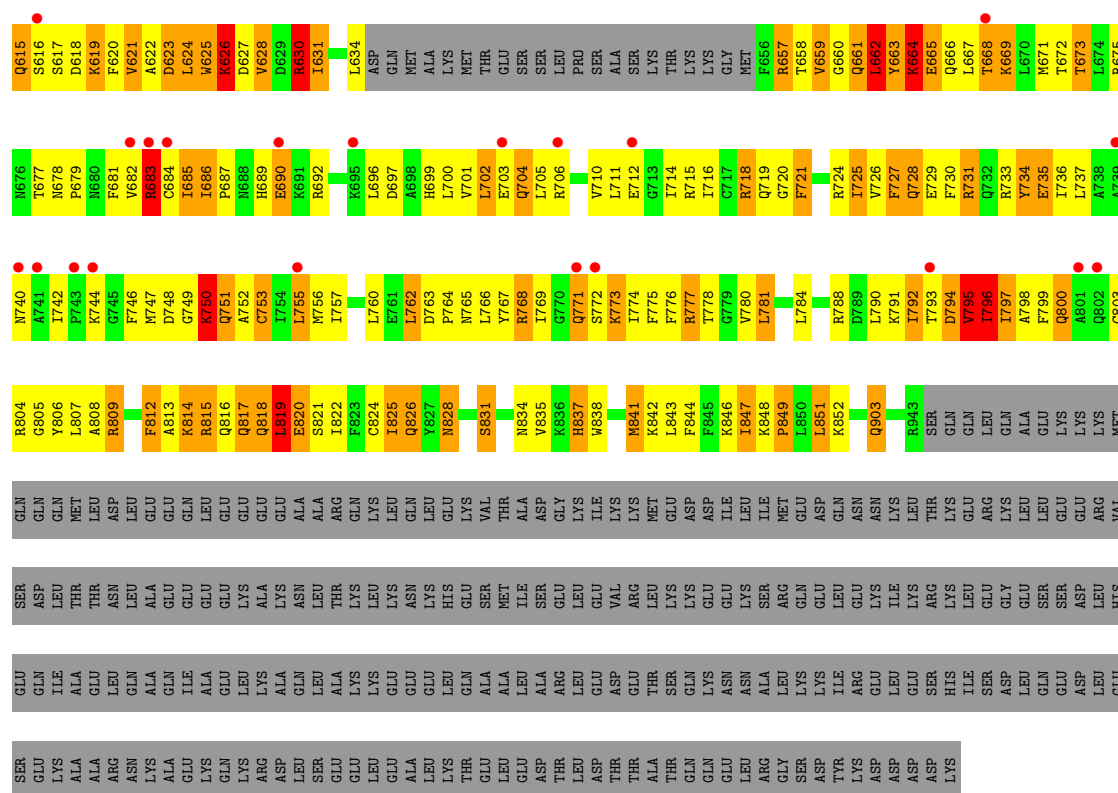
Chain	Residue	Modelled	Actual	Comment	Reference
Z	21	GLU	GLN	SEE REMARK 999	UNP P02609
Z	23	GLU	GLN	SEE REMARK 999	UNP P02609
Z	25	GLU	GLN	SEE REMARK 999	UNP P02609
Z	26	ASP	GLU	SEE REMARK 999	UNP P02609
Z	38	ALA	ARG	SEE REMARK 999	UNP P02609
Z	124	GLY	GLN	SEE REMARK 999	UNP P02609
Z	125	GLY	CYS	SEE REMARK 999	UNP P02609
Z	126	GLY	ASP	SEE REMARK 999	UNP P02609
Z	163	ALA	LYS	SEE REMARK 999	UNP P02609
U	21	GLU	GLN	SEE REMARK 999	UNP P02609
U	23	GLU	GLN	SEE REMARK 999	UNP P02609
U	25	GLU	GLN	SEE REMARK 999	UNP P02609
U	26	ASP	GLU	SEE REMARK 999	UNP P02609
U	38	ALA	ARG	SEE REMARK 999	UNP P02609
U	124	GLY	GLN	SEE REMARK 999	UNP P02609
U	125	GLY	CYS	SEE REMARK 999	UNP P02609
U	126	GLY	ASP	SEE REMARK 999	UNP P02609
U	163	ALA	LYS	SEE REMARK 999	UNP P02609

3 Residue-property plots

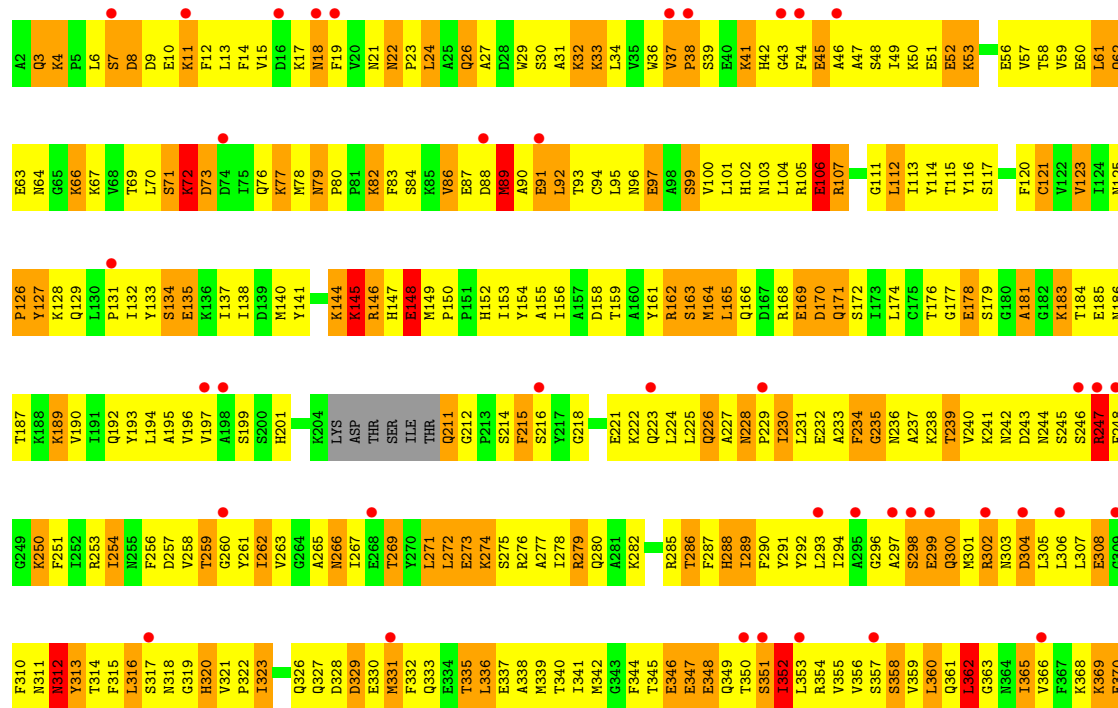
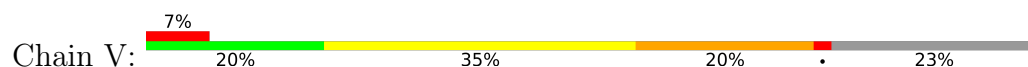
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

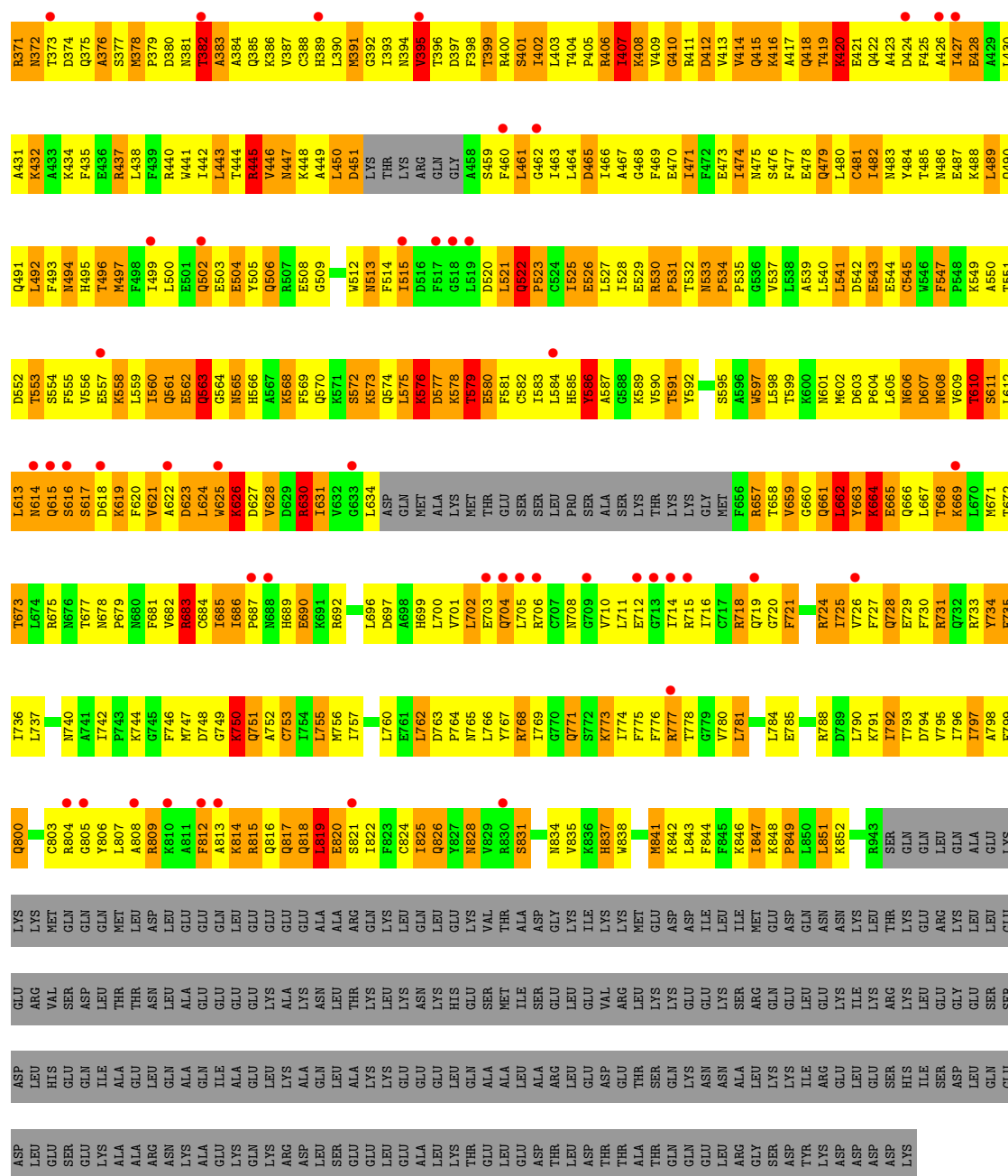
• Molecule 1: SMOOTH MUSCLE MYOSIN HEAVY CHAIN

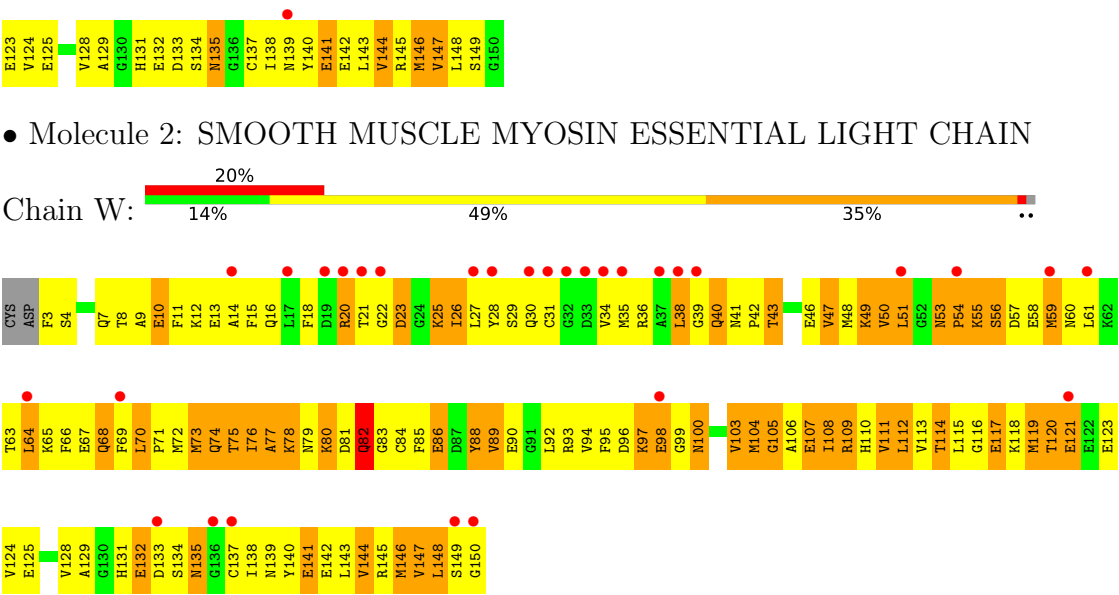




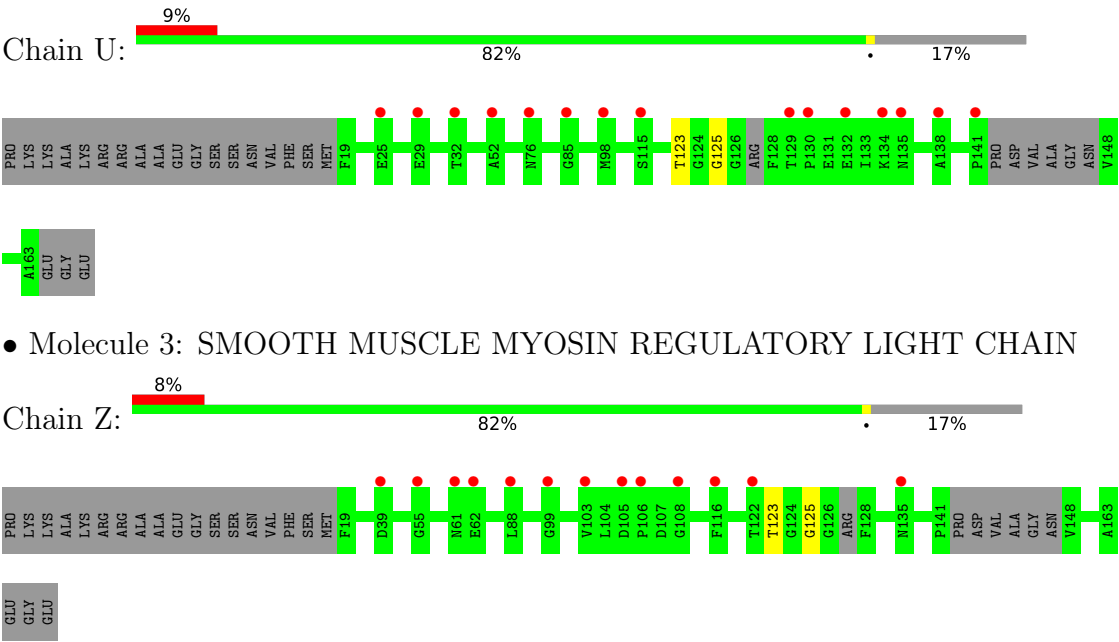
• Molecule 1: SMOOTH MUSCLE MYOSIN HEAVY CHAIN







• Molecule 3: SMOOTH MUSCLE MYOSIN REGULATORY LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	133.00Å 304.00Å 200.00Å 90.00° 90.00° 91.50°	Depositor
Resolution (Å)	(Not available) – 20.00 200.00 – 20.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00) 40.8 (200.00-20.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 100.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	16580	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

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	S	1.06	7/7076 (0.1%)	1.38	40/9501 (0.4%)
1	V	0.88	4/7076 (0.1%)	1.14	32/9501 (0.3%)
2	T	0.47	0/1175	0.89	0/1575
2	W	0.47	0/1175	0.89	0/1575
All	All	0.92	11/16502 (0.1%)	1.22	72/22152 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	819	LEU	C-N	44.19	1.95	1.33
1	S	819	LEU	C-N	44.15	1.95	1.33
1	S	903	GLN	C-N	37.89	1.86	1.33
1	S	796	ILE	C-N	28.82	1.72	1.33
1	S	795	VAL	C-N	12.73	1.50	1.33
1	S	597	TRP	NE1-CE2	-5.50	1.31	1.37
1	V	29	TRP	NE1-CE2	-5.38	1.31	1.37
1	V	625	TRP	NE1-CE2	-5.37	1.31	1.37
1	V	597	TRP	NE1-CE2	-5.35	1.31	1.37
1	S	29	TRP	NE1-CE2	-5.33	1.31	1.37
1	S	625	TRP	NE1-CE2	-5.28	1.31	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	796	ILE	O-C-N	-58.66	49.24	122.57
1	S	819	LEU	O-C-N	-41.46	67.45	122.59
1	V	819	LEU	O-C-N	-41.43	67.48	122.59
1	S	903	GLN	O-C-N	-39.45	70.11	122.59
1	S	903	GLN	CA-C-N	-14.78	95.85	122.46
1	S	903	GLN	C-N-CA	-14.78	95.85	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	796	ILE	CA-C-N	-12.22	99.98	121.97
1	S	796	ILE	C-N-CA	-12.22	99.98	121.97
1	S	817	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	V	817	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	S	669	LYS	N-CA-C	-9.14	100.88	111.03
1	V	669	LYS	N-CA-C	-9.09	100.94	111.03
1	S	668	THR	N-CA-C	-7.93	103.81	113.97
1	V	668	THR	N-CA-C	-7.93	103.82	113.97
1	V	312	ASN	N-CA-C	-7.49	103.99	113.72
1	S	312	ASN	N-CA-C	-7.48	104.00	113.72
1	V	97	GLU	N-CA-C	-7.38	103.54	112.54
1	S	97	GLU	N-CA-C	-7.35	103.58	112.54
1	S	795	VAL	CA-C-N	-6.89	109.57	121.97
1	S	795	VAL	C-N-CA	-6.89	109.57	121.97
1	S	819	LEU	CA-C-N	-6.78	108.59	121.54
1	S	819	LEU	C-N-CA	-6.78	108.59	121.54
1	V	819	LEU	CA-C-N	-6.78	108.59	121.54
1	V	819	LEU	C-N-CA	-6.78	108.59	121.54
1	S	817	GLN	CG-CD-NE2	6.75	126.52	116.40
1	V	817	GLN	CG-CD-NE2	6.70	126.45	116.40
1	V	445	ARG	N-CA-C	-6.65	103.21	112.45
1	S	445	ARG	N-CA-C	-6.63	103.24	112.45
1	S	464	LEU	N-CA-C	6.50	119.11	108.52
1	V	464	LEU	N-CA-C	6.44	119.01	108.52
1	S	336	LEU	N-CA-C	-6.37	104.25	111.07
1	V	336	LEU	N-CA-C	-6.33	104.30	111.07
1	V	558	LYS	N-CA-C	-6.31	104.41	111.28
1	S	558	LYS	N-CA-C	-6.28	104.44	111.28
1	V	578	LYS	N-CA-C	-6.23	105.51	113.23
1	S	578	LYS	N-CA-C	-6.20	105.54	113.23
1	V	505	TYR	N-CA-C	-6.00	104.75	111.28
1	S	505	TYR	N-CA-C	-5.99	104.75	111.28
1	V	662	LEU	N-CA-C	-5.97	104.69	111.14
1	S	662	LEU	N-CA-C	-5.92	104.75	111.14
1	S	757	ILE	N-CA-C	-5.88	104.06	112.35
1	V	757	ILE	N-CA-C	-5.86	104.08	112.35
1	S	434	LYS	N-CA-C	-5.85	105.03	111.82
1	V	434	LYS	N-CA-C	-5.77	105.13	111.82
1	V	837	HIS	CA-C-N	5.67	129.14	121.20
1	V	837	HIS	C-N-CA	5.67	129.14	121.20
1	S	837	HIS	CA-C-N	5.67	129.14	121.20
1	S	837	HIS	C-N-CA	5.67	129.14	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	3	GLN	N-CA-C	5.66	118.47	109.81
1	S	6	LEU	N-CA-C	5.64	118.16	109.07
1	V	6	LEU	N-CA-C	5.64	118.14	109.07
1	S	3	GLN	N-CA-C	5.60	118.38	109.81
1	V	285	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	V	279	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	S	630	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	S	285	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	S	247	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	V	630	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	V	247	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	S	279	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	V	522	GLN	N-CA-C	-5.26	106.82	113.77
1	S	734	TYR	N-CA-C	5.22	118.47	112.57
1	V	576	LYS	N-CA-C	-5.22	106.98	113.19
1	V	734	TYR	N-CA-C	5.21	118.46	112.57
1	S	522	GLN	N-CA-C	-5.18	106.93	113.77
1	S	576	LYS	N-CA-C	-5.18	107.02	113.19
1	S	586	TYR	N-CA-C	-5.14	106.17	112.90
1	V	586	TYR	N-CA-C	-5.10	106.21	112.90
1	S	547	PHE	CA-C-N	5.07	126.17	119.84
1	S	547	PHE	C-N-CA	5.07	126.17	119.84
1	V	547	PHE	CA-C-N	5.04	126.15	119.84
1	V	547	PHE	C-N-CA	5.04	126.15	119.84

There are no chirality outliers.

There are no planarity outliers.

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	S	6992	0	6742	1040	88
1	V	6992	0	6738	1135	0
2	T	1160	0	1117	304	0
2	W	1160	0	1126	170	4
3	U	138	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	138	0	0	3	0
All	All	16580	0	15723	2407	92

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 77.

All (2407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:102:THR:CG2	1:V:617:SER:H	1.12	1.60
1:S:258:VAL:CG1	1:V:406:ARG:HH12	1.06	1.59
2:T:94:VAL:HA	1:V:396:THR:CG2	1.26	1.56
2:T:94:VAL:CA	1:V:396:THR:HG21	1.42	1.49
1:S:258:VAL:HG13	1:V:406:ARG:NH1	1.30	1.46
2:T:94:VAL:HA	1:V:396:THR:CB	1.47	1.45
2:T:102:THR:CG2	1:V:617:SER:N	1.72	1.45
2:T:140:TYR:OH	1:V:394:ASN:CA	1.66	1.43
2:T:141:GLU:OE1	1:V:389:HIS:CG	1.76	1.39
2:T:100:ASN:OD1	1:V:612:LEU:CA	1.75	1.33
2:T:102:THR:HG21	1:V:617:SER:N	1.06	1.33
1:S:458:ALA:O	1:V:413:VAL:CG1	1.74	1.33
1:S:168:ARG:O	1:V:415:GLN:HG2	1.24	1.32
2:T:94:VAL:CB	1:V:396:THR:HG21	1.57	1.32
1:S:168:ARG:NH2	1:V:406:ARG:HB2	1.42	1.31
1:S:259:THR:CG2	2:T:104:MET:SD	2.21	1.29
1:S:168:ARG:NE	1:V:400:ARG:HD3	1.44	1.29
2:T:94:VAL:CA	1:V:396:THR:CG2	2.02	1.27
2:T:102:THR:HG21	1:V:616:SER:C	1.60	1.27
1:S:819:LEU:C	1:S:820:GLU:N	1.95	1.24
1:V:819:LEU:C	1:V:820:GLU:N	1.95	1.22
2:T:100:ASN:OD1	1:V:612:LEU:CG	1.89	1.21
1:S:259:THR:HG21	2:T:104:MET:SD	1.79	1.20
1:V:818:GLN:O	1:V:822:ILE:HG13	1.42	1.20
2:T:100:ASN:OD1	1:V:612:LEU:CB	1.89	1.20
1:S:818:GLN:O	1:S:822:ILE:HG13	1.42	1.19
1:S:258:VAL:CG1	1:V:406:ARG:NH1	1.88	1.18
1:S:168:ARG:NH1	1:V:404:THR:O	1.76	1.17
1:S:818:GLN:O	1:S:822:ILE:CG1	1.93	1.16
2:T:100:ASN:OD1	1:V:612:LEU:HA	1.33	1.16
1:S:168:ARG:NH1	1:V:404:THR:OG1	1.75	1.15
1:S:458:ALA:O	1:V:413:VAL:HG11	0.97	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:818:GLN:O	1:V:822:ILE:CG1	1.93	1.15
1:S:168:ARG:NE	1:V:406:ARG:HG3	1.62	1.14
1:S:168:ARG:CB	1:V:415:GLN:HE21	1.59	1.14
2:T:94:VAL:CG2	1:V:396:THR:HG21	1.78	1.13
1:S:819:LEU:CA	1:S:822:ILE:HG13	1.81	1.11
1:V:818:GLN:C	1:V:822:ILE:HG13	1.76	1.11
2:T:140:TYR:HE2	1:V:394:ASN:HB2	1.07	1.11
1:V:8:ASP:HA	1:V:11:LYS:HD2	1.32	1.11
1:S:168:ARG:HB2	1:V:415:GLN:HE21	1.12	1.10
1:S:458:ALA:C	1:V:413:VAL:HG11	1.76	1.10
1:S:795:VAL:O	1:S:798:ALA:HB3	1.52	1.10
1:V:819:LEU:O	1:V:820:GLU:CA	1.99	1.10
1:S:8:ASP:HA	1:S:11:LYS:HD2	1.32	1.10
1:S:818:GLN:C	1:S:822:ILE:HG13	1.76	1.10
1:V:819:LEU:CA	1:V:822:ILE:HG13	1.81	1.10
1:S:795:VAL:O	1:S:798:ALA:CB	1.98	1.09
1:S:819:LEU:O	1:S:820:GLU:CA	1.99	1.09
1:V:819:LEU:HA	1:V:822:ILE:HG13	1.30	1.09
1:V:819:LEU:HA	1:V:822:ILE:CG1	1.82	1.08
1:S:168:ARG:CZ	1:V:400:ARG:HD3	1.83	1.08
1:S:819:LEU:HA	1:S:822:ILE:CG1	1.82	1.08
2:T:94:VAL:HG22	1:V:396:THR:CG2	1.82	1.08
1:S:168:ARG:HB2	1:V:415:GLN:NE2	1.67	1.07
1:S:727:PHE:HB2	1:V:370:GLU:CD	1.72	1.07
1:S:819:LEU:HA	1:S:822:ILE:HG13	1.30	1.07
2:T:140:TYR:CE2	1:V:394:ASN:HB2	1.89	1.07
1:V:819:LEU:O	1:V:820:GLU:N	1.87	1.06
1:S:819:LEU:O	1:S:820:GLU:N	1.87	1.06
1:V:819:LEU:O	1:V:820:GLU:C	1.97	1.05
1:S:168:ARG:NH2	1:V:406:ARG:CB	2.18	1.05
1:S:771:GLN:O	1:V:371:ARG:O	1.73	1.05
2:T:98:GLU:HB2	1:V:612:LEU:HB2	1.34	1.05
2:T:101:GLY:C	1:V:393:ILE:C	1.77	1.05
1:S:819:LEU:O	1:S:820:GLU:C	1.97	1.05
1:S:258:VAL:HG12	1:V:406:ARG:HH12	1.21	1.03
2:T:102:THR:HG22	1:V:617:SER:H	1.16	1.03
2:T:140:TYR:CZ	1:V:394:ASN:HA	1.93	1.03
1:S:259:THR:CG2	2:T:104:MET:CE	2.36	1.03
2:T:94:VAL:HA	1:V:396:THR:OG1	1.57	1.02
2:T:94:VAL:CA	1:V:396:THR:OG1	2.08	1.01
1:V:419:THR:H	1:V:422:GLN:HE21	1.06	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:610:THR:HG21	1:V:631:ILE:HG13	1.42	1.01
1:V:49:ILE:HA	1:V:59:VAL:HG22	1.40	1.00
2:W:89:VAL:HG12	2:W:144:VAL:HG21	1.43	1.00
1:S:610:THR:HG21	1:S:631:ILE:HG13	1.42	1.00
1:S:49:ILE:HA	1:S:59:VAL:HG22	1.40	1.00
1:S:796:ILE:C	1:S:798:ALA:H	1.69	0.99
2:T:99:GLY:HA3	1:V:398:PHE:CA	1.92	0.99
2:T:100:ASN:CG	1:V:612:LEU:HG	1.76	0.99
1:V:541:LEU:HD23	1:V:601:ASN:HD22	1.25	0.99
1:V:628:VAL:HG13	1:V:631:ILE:HG13	1.45	0.99
1:S:259:THR:CG2	2:T:104:MET:HE1	1.91	0.99
1:S:419:THR:H	1:S:422:GLN:HE21	1.06	0.99
1:S:259:THR:HG23	2:T:104:MET:CE	1.91	0.99
1:S:82:LYS:HG2	1:S:82:LYS:O	1.62	0.99
1:S:541:LEU:HD23	1:S:601:ASN:HD22	1.25	0.98
1:S:79:ASN:HD22	1:S:80:PRO:HD2	1.28	0.98
2:T:89:VAL:HG12	2:T:144:VAL:HG21	1.43	0.98
1:V:805:GLY:HA2	2:W:36:ARG:HG2	1.42	0.98
1:S:805:GLY:HA2	2:T:36:ARG:HG2	1.42	0.97
1:S:168:ARG:HE	1:V:406:ARG:HG3	1.17	0.97
1:S:628:VAL:HG13	1:S:631:ILE:CG1	1.95	0.97
1:V:82:LYS:HG2	1:V:82:LYS:O	1.62	0.97
1:S:269:THR:HG21	1:S:443:LEU:HD13	1.46	0.96
1:V:628:VAL:HG13	1:V:631:ILE:CG1	1.95	0.96
2:T:141:GLU:OE1	1:V:389:HIS:CD2	2.18	0.96
2:T:99:GLY:HA3	1:V:398:PHE:HA	1.47	0.96
1:V:79:ASN:HD22	1:V:80:PRO:HD2	1.29	0.95
1:V:269:THR:HG21	1:V:443:LEU:HD13	1.46	0.95
2:T:93:ARG:O	1:V:396:THR:OG1	1.84	0.95
1:S:796:ILE:O	1:S:798:ALA:N	1.99	0.95
2:T:102:THR:HG23	1:V:392:GLY:O	1.66	0.95
2:T:102:THR:CG2	1:V:392:GLY:O	2.16	0.94
1:S:628:VAL:HG13	1:S:631:ILE:HG13	1.44	0.94
1:V:527:LEU:O	1:V:527:LEU:HD23	1.68	0.94
2:T:102:THR:HG22	1:V:617:SER:HB3	1.50	0.93
1:V:13:LEU:HD11	1:V:132:ILE:HB	1.49	0.93
1:S:458:ALA:C	1:V:413:VAL:HG21	1.94	0.93
1:S:678:ASN:HD22	1:S:679:PRO:HD2	1.32	0.93
1:S:527:LEU:O	1:S:527:LEU:HD23	1.68	0.93
2:T:94:VAL:CG2	1:V:396:THR:CG2	2.43	0.93
1:S:168:ARG:HH12	1:V:404:THR:C	1.76	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:259:THR:HG22	2:T:104:MET:HE1	1.51	0.92
2:T:99:GLY:CA	1:V:398:PHE:CA	2.47	0.92
1:V:678:ASN:HD22	1:V:679:PRO:HD2	1.32	0.91
1:S:13:LEU:HD11	1:S:132:ILE:HB	1.49	0.91
1:S:458:ALA:O	1:V:413:VAL:CB	2.17	0.91
2:T:141:GLU:OE1	1:V:389:HIS:CB	2.17	0.91
2:T:99:GLY:CA	1:V:398:PHE:HB2	1.99	0.91
1:V:628:VAL:O	1:V:631:ILE:HG12	1.71	0.91
1:S:36:TRP:NE1	1:S:78:MET:HG3	1.86	0.90
1:S:401:SER:HB3	1:S:608:ASN:HB3	1.53	0.90
1:S:135:GLU:HB2	1:S:212:GLY:O	1.71	0.90
1:V:401:SER:HB3	1:V:608:ASN:HB3	1.53	0.90
1:S:576:LYS:HA	1:S:579:THR:HA	1.54	0.89
1:S:471:ILE:O	1:S:471:ILE:HG12	1.70	0.89
1:V:135:GLU:HB2	1:V:212:GLY:O	1.71	0.89
1:V:36:TRP:NE1	1:V:78:MET:HG3	1.86	0.89
2:W:26:ILE:HG23	2:W:30:GLN:HB2	1.54	0.89
1:S:628:VAL:O	1:S:631:ILE:HG12	1.71	0.89
2:T:26:ILE:HG23	2:T:30:GLN:HB2	1.54	0.89
2:T:98:GLU:N	1:V:397:ASP:HB3	1.86	0.89
1:V:607:ASP:HA	1:V:610:THR:HB	1.55	0.89
1:V:345:THR:HB	1:V:348:GLU:HB2	1.53	0.88
1:S:258:VAL:HG12	1:V:406:ARG:NH1	1.79	0.88
1:S:345:THR:HB	1:S:348:GLU:HB2	1.54	0.88
2:T:140:TYR:OH	1:V:394:ASN:HA	0.71	0.88
1:S:259:THR:HG23	2:T:104:MET:SD	2.14	0.88
1:V:471:ILE:HG12	1:V:471:ILE:O	1.70	0.87
1:V:576:LYS:HA	1:V:579:THR:HA	1.54	0.87
1:S:818:GLN:O	1:S:822:ILE:HG12	1.74	0.87
2:T:99:GLY:HA2	1:V:398:PHE:HB2	1.57	0.86
2:T:100:ASN:OD1	1:V:612:LEU:CD1	2.22	0.86
1:V:818:GLN:O	1:V:822:ILE:HG12	1.74	0.86
2:T:101:GLY:C	1:V:393:ILE:O	2.04	0.86
1:S:168:ARG:HH21	1:V:406:ARG:HB2	1.06	0.86
1:S:419:THR:N	1:S:422:GLN:HE21	1.73	0.86
1:S:607:ASP:HA	1:S:610:THR:HB	1.55	0.86
1:V:819:LEU:N	1:V:822:ILE:HG13	1.90	0.86
1:S:187:THR:HG23	1:S:463:ILE:HG21	1.56	0.85
1:V:419:THR:N	1:V:422:GLN:HE21	1.73	0.85
2:T:94:VAL:CA	1:V:396:THR:CB	2.41	0.85
1:S:168:ARG:CZ	1:V:400:ARG:CD	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:ILE:HG22	1:S:231:LEU:HD23	1.58	0.85
2:T:99:GLY:HA3	1:V:398:PHE:CB	2.07	0.85
1:V:230:ILE:HG22	1:V:231:LEU:HD23	1.58	0.84
1:V:187:THR:HG23	1:V:463:ILE:HG21	1.56	0.84
2:T:141:GLU:CD	1:V:389:HIS:HA	2.03	0.84
1:V:236:ASN:ND2	1:V:246:SER:HA	1.93	0.84
1:V:747:MET:HE3	1:V:752:ALA:HA	1.60	0.84
1:S:471:ILE:O	1:S:471:ILE:CG1	2.26	0.84
1:S:819:LEU:N	1:S:822:ILE:HG13	1.90	0.84
1:S:236:ASN:ND2	1:S:246:SER:HA	1.93	0.84
1:S:625:TRP:O	1:S:627:ASP:N	2.10	0.84
1:S:772:SER:HB2	1:V:373:THR:CA	2.08	0.83
1:V:232:GLU:HA	1:V:236:ASN:OD1	1.79	0.83
1:V:625:TRP:O	1:V:627:ASP:N	2.10	0.83
1:S:747:MET:HE3	1:S:752:ALA:HA	1.60	0.82
1:V:377:SER:O	1:V:379:PRO:HD3	1.79	0.82
1:V:37:VAL:HG12	1:V:38:PRO:HD2	1.61	0.82
1:S:795:VAL:O	1:S:798:ALA:HB2	1.80	0.82
1:V:164:MET:HE1	1:V:256:PHE:HE2	1.44	0.82
1:S:576:LYS:O	1:S:579:THR:HG23	1.78	0.82
2:T:99:GLY:N	1:V:398:PHE:N	2.28	0.82
1:S:377:SER:O	1:S:379:PRO:HD3	1.79	0.81
2:T:100:ASN:CG	1:V:612:LEU:CG	2.44	0.81
1:V:576:LYS:O	1:V:579:THR:HG23	1.78	0.81
1:S:232:GLU:HA	1:S:236:ASN:OD1	1.79	0.81
1:V:62:GLN:O	1:V:62:GLN:HG3	1.79	0.81
1:V:806:TYR:CD2	2:W:147:VAL:HA	2.16	0.81
1:S:806:TYR:CD2	2:T:147:VAL:HA	2.16	0.81
2:T:99:GLY:H	1:V:398:PHE:N	1.78	0.81
1:S:62:GLN:O	1:S:62:GLN:HG3	1.79	0.81
1:V:405:PRO:HB2	1:V:407:ILE:CG2	2.11	0.81
1:V:471:ILE:O	1:V:471:ILE:CG1	2.26	0.81
2:T:58:GLU:HA	2:T:61:LEU:HD12	1.63	0.81
1:S:405:PRO:HB2	1:S:407:ILE:CG2	2.11	0.80
1:S:168:ARG:O	1:V:415:GLN:CG	2.20	0.80
1:S:420:LYS:O	1:S:423:ALA:HB3	1.82	0.80
1:V:420:LYS:O	1:V:423:ALA:HB3	1.82	0.80
1:S:258:VAL:HG13	1:V:406:ARG:HH12	0.64	0.80
1:S:796:ILE:C	1:S:798:ALA:N	2.39	0.80
1:V:331:MET:O	1:V:335:THR:HG23	1.82	0.80
1:V:558:LYS:O	1:V:561:GLN:HB3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:99:GLY:HA2	1:V:394:ASN:O	1.82	0.80
2:T:140:TYR:CE2	1:V:394:ASN:CB	2.64	0.80
1:V:540:LEU:HD12	1:V:559:LEU:HD12	1.63	0.80
1:S:37:VAL:HG12	1:S:38:PRO:HD2	1.61	0.80
2:T:99:GLY:CA	1:V:398:PHE:N	2.45	0.80
1:S:628:VAL:O	1:S:628:VAL:CG1	2.30	0.80
2:T:100:ASN:OD1	1:V:612:LEU:HD12	1.80	0.79
1:S:83:PHE:HB3	1:S:92:LEU:HD23	1.64	0.79
2:T:102:THR:CG2	1:V:616:SER:HA	2.12	0.79
1:V:83:PHE:HB3	1:V:92:LEU:HD23	1.64	0.79
2:W:58:GLU:HA	2:W:61:LEU:HD12	1.63	0.79
1:S:164:MET:HE1	1:S:256:PHE:HE2	1.43	0.79
1:S:168:ARG:HH21	1:V:406:ARG:CB	1.91	0.79
1:S:558:LYS:O	1:S:561:GLN:HB3	1.82	0.79
2:T:101:GLY:O	1:V:393:ILE:O	2.00	0.79
1:V:164:MET:HE1	1:V:256:PHE:CE2	2.17	0.79
1:V:628:VAL:O	1:V:628:VAL:CG1	2.30	0.79
1:S:148:GLU:O	1:S:149:MET:HG2	1.83	0.79
1:S:352:ILE:HG21	1:S:442:ILE:HD11	1.64	0.79
1:S:493:PHE:O	1:S:497:MET:HB2	1.82	0.79
1:S:540:LEU:HD12	1:S:559:LEU:HD12	1.63	0.79
1:S:690:GLU:HB3	1:S:692:ARG:HG3	1.65	0.79
2:T:140:TYR:HE2	1:V:394:ASN:CB	1.90	0.79
1:V:814:LYS:HE3	1:V:818:GLN:HE22	1.48	0.79
1:S:437:ARG:HE	1:S:625:TRP:HA	1.47	0.79
1:V:376:ALA:HB2	1:V:420:LYS:HB2	1.65	0.79
1:V:690:GLU:HB3	1:V:692:ARG:HG3	1.65	0.79
1:S:331:MET:O	1:S:335:THR:HG23	1.82	0.79
1:V:148:GLU:O	1:V:149:MET:HG2	1.83	0.79
1:V:804:ARG:HG2	1:V:804:ARG:HH11	1.48	0.79
2:T:98:GLU:HB2	1:V:612:LEU:CB	2.13	0.78
1:V:493:PHE:O	1:V:497:MET:HB2	1.82	0.78
2:T:65:LYS:HD2	2:T:68:GLN:HE21	1.49	0.78
1:S:168:ARG:NE	1:V:406:ARG:CG	2.44	0.78
1:S:164:MET:HE1	1:S:256:PHE:CE2	2.17	0.78
1:S:259:THR:HB	1:S:261:TYR:CE1	2.18	0.78
1:S:424:ASP:HA	1:S:427:ILE:HG22	1.64	0.78
2:W:65:LYS:HD2	2:W:68:GLN:HE21	1.49	0.78
1:S:376:ALA:HB2	1:S:420:LYS:HB2	1.65	0.78
2:T:99:GLY:CA	1:V:398:PHE:CB	2.60	0.78
1:V:244:ASN:O	1:V:244:ASN:ND2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:582:CYS:SG	1:S:591:THR:HG23	2.24	0.78
1:S:814:LYS:HE3	1:S:818:GLN:HE22	1.47	0.78
1:V:582:CYS:SG	1:V:591:THR:HG23	2.23	0.78
1:S:804:ARG:HG2	1:S:804:ARG:HH11	1.48	0.77
1:S:502:GLN:HG2	1:S:512:TRP:HE1	1.49	0.77
1:S:418:GLN:HB3	1:S:422:GLN:HB2	1.65	0.77
1:V:424:ASP:HA	1:V:427:ILE:HG22	1.64	0.77
1:S:244:ASN:O	1:S:244:ASN:ND2	2.17	0.77
1:V:323:ILE:HG23	1:V:326:GLN:HB3	1.65	0.77
1:V:418:GLN:HB3	1:V:422:GLN:HB2	1.65	0.77
2:W:10:GLU:HA	2:W:13:GLU:HG3	1.66	0.77
1:S:168:ARG:CZ	1:V:406:ARG:HG3	2.15	0.77
1:S:323:ILE:HG23	1:S:326:GLN:HB3	1.65	0.77
1:V:259:THR:HB	1:V:261:TYR:CE1	2.18	0.77
1:V:437:ARG:HE	1:V:625:TRP:HA	1.47	0.77
1:S:818:GLN:C	1:S:822:ILE:CG1	2.52	0.77
1:S:79:ASN:HD22	1:S:80:PRO:CD	1.98	0.76
1:V:659:VAL:HG12	1:V:660:GLY:N	2.00	0.76
1:V:114:TYR:CE2	1:V:153:ILE:HB	2.21	0.76
1:S:168:ARG:CB	1:V:415:GLN:NE2	2.37	0.76
1:V:502:GLN:HG2	1:V:512:TRP:HE1	1.49	0.76
1:V:352:ILE:HG21	1:V:442:ILE:HD11	1.65	0.76
1:S:114:TYR:CE2	1:S:153:ILE:HB	2.21	0.76
1:S:814:LYS:O	1:S:817:GLN:HG2	1.86	0.76
1:S:520:ASP:C	1:S:521:LEU:HD23	2.11	0.76
2:T:94:VAL:C	1:V:396:THR:OG1	2.28	0.76
1:V:814:LYS:O	1:V:817:GLN:HG2	1.85	0.76
2:T:102:THR:HG21	1:V:616:SER:CA	2.16	0.75
1:V:79:ASN:HD22	1:V:80:PRO:CD	1.98	0.75
1:V:610:THR:HG22	1:V:611:SER:N	2.00	0.75
1:V:293:LEU:HD11	1:V:301:MET:HE1	1.67	0.75
2:T:10:GLU:HA	2:T:13:GLU:HG3	1.66	0.75
1:V:135:GLU:CD	1:V:215:PHE:HB2	2.11	0.75
1:V:272:LEU:C	1:V:272:LEU:HD12	2.11	0.75
1:S:135:GLU:CD	1:S:215:PHE:HB2	2.11	0.75
1:S:293:LEU:HD11	1:S:301:MET:HE1	1.67	0.75
1:S:458:ALA:HA	1:V:413:VAL:CG2	2.15	0.75
2:W:114:THR:C	2:W:115:LEU:HD12	2.11	0.75
1:S:168:ARG:HD3	1:V:415:GLN:NE2	2.01	0.75
1:S:458:ALA:HA	1:V:413:VAL:HG22	1.68	0.75
1:S:610:THR:HG22	1:S:611:SER:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:659:VAL:HG12	1:S:660:GLY:N	2.00	0.75
1:S:771:GLN:HE21	1:S:771:GLN:C	1.95	0.75
1:V:30:SER:C	1:V:32:LYS:H	1.94	0.75
1:V:520:ASP:C	1:V:521:LEU:HD23	2.11	0.75
1:V:663:TYR:O	1:V:665:GLU:N	2.20	0.74
1:S:168:ARG:HE	1:V:400:ARG:HD3	1.52	0.74
1:S:663:TYR:O	1:S:665:GLU:N	2.20	0.74
2:T:102:THR:HG23	1:V:617:SER:H	1.44	0.74
2:T:114:THR:C	2:T:115:LEU:HD12	2.11	0.74
1:V:771:GLN:HE21	1:V:771:GLN:C	1.95	0.74
1:S:272:LEU:C	1:S:272:LEU:HD12	2.12	0.74
2:T:100:ASN:CG	1:V:612:LEU:CA	2.60	0.74
2:T:139:ASN:N	1:V:617:SER:HB2	2.02	0.74
1:V:407:ILE:HG13	1:V:414:VAL:O	1.88	0.74
2:W:141:GLU:O	2:W:145:ARG:HG3	1.88	0.73
1:S:22:ASN:OD1	1:S:24:LEU:HB2	1.88	0.73
1:S:30:SER:C	1:S:32:LYS:H	1.94	0.73
1:S:772:SER:OG	1:V:373:THR:HA	1.87	0.73
1:S:727:PHE:H	1:V:372:ASN:HB2	1.52	0.73
2:T:141:GLU:O	2:T:145:ARG:HG3	1.88	0.73
1:V:22:ASN:OD1	1:V:24:LEU:HB2	1.88	0.73
1:V:792:ILE:O	1:V:796:ILE:HG12	1.89	0.73
2:T:102:THR:CG2	1:V:616:SER:CA	2.66	0.73
1:S:302:ARG:O	1:S:307:LEU:HD12	1.89	0.73
1:S:407:ILE:HG13	1:S:414:VAL:O	1.88	0.73
1:V:13:LEU:CD1	1:V:132:ILE:HB	2.19	0.73
1:V:33:LYS:HB3	1:V:49:ILE:HB	1.70	0.73
1:S:168:ARG:HD3	1:V:415:GLN:HE22	1.52	0.72
1:S:33:LYS:HB3	1:S:49:ILE:HB	1.70	0.72
1:S:715:ARG:O	1:S:719:GLN:HG2	1.89	0.72
1:S:168:ARG:HB3	1:V:415:GLN:HE21	1.51	0.72
1:S:407:ILE:HD12	1:S:408:LYS:N	2.05	0.72
1:V:50:LYS:HE3	1:V:60:GLU:HB3	1.72	0.72
2:T:99:GLY:H	1:V:397:ASP:CB	2.03	0.72
1:V:10:GLU:O	1:V:14:PHE:HB2	1.90	0.72
1:S:721:PHE:N	1:S:721:PHE:CD1	2.57	0.72
2:T:98:GLU:CB	1:V:612:LEU:HB2	2.18	0.72
1:V:302:ARG:O	1:V:307:LEU:HD12	1.90	0.72
1:S:18:ASN:O	1:S:19:PHE:CD1	2.42	0.72
1:S:700:LEU:HD23	1:S:704:GLN:HE22	1.55	0.72
1:V:715:ARG:O	1:V:719:GLN:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:13:LEU:CD1	1:S:132:ILE:HB	2.19	0.72
1:V:18:ASN:O	1:V:19:PHE:CD1	2.42	0.72
1:V:48:SER:C	1:V:59:VAL:HG13	2.15	0.72
1:V:61:LEU:C	1:V:63:GLU:H	1.96	0.72
1:V:407:ILE:HD12	1:V:408:LYS:N	2.04	0.72
2:W:86:GLU:CD	2:W:86:GLU:H	1.98	0.72
1:S:377:SER:C	1:S:379:PRO:HD3	2.14	0.71
1:V:700:LEU:HD23	1:V:704:GLN:HE22	1.55	0.71
1:V:721:PHE:N	1:V:721:PHE:CD1	2.57	0.71
2:T:93:ARG:C	1:V:396:THR:HG1	1.95	0.71
2:T:102:THR:HG22	1:V:617:SER:N	1.85	0.71
1:S:48:SER:C	1:S:59:VAL:HG13	2.15	0.71
2:T:94:VAL:HA	1:V:396:THR:HG21	1.07	0.71
1:S:10:GLU:O	1:S:14:PHE:HB2	1.90	0.71
1:S:61:LEU:C	1:S:63:GLU:H	1.96	0.71
2:T:86:GLU:CD	2:T:86:GLU:H	1.98	0.71
1:V:377:SER:C	1:V:379:PRO:HD3	2.14	0.71
2:T:4:SER:N	2:T:7:GLN:HE21	1.89	0.71
2:W:65:LYS:O	2:W:68:GLN:HG3	1.90	0.71
2:T:102:THR:HG22	1:V:392:GLY:O	1.91	0.71
1:S:399:THR:HG22	1:S:403:LEU:HD11	1.73	0.71
2:T:65:LYS:O	2:T:68:GLN:HG3	1.90	0.71
1:V:243:ASP:HB3	1:V:323:ILE:HD11	1.73	0.71
1:S:727:PHE:CB	1:V:370:GLU:CD	2.51	0.71
1:V:747:MET:HB3	1:V:752:ALA:HB2	1.73	0.71
2:W:4:SER:N	2:W:7:GLN:HE21	1.89	0.71
1:S:568:LYS:HD3	1:S:584:LEU:HB2	1.72	0.70
1:V:619:LYS:O	1:V:622:ALA:HB3	1.91	0.70
1:S:365:ILE:HD13	1:S:427:ILE:HD11	1.72	0.70
2:T:97:LYS:C	1:V:397:ASP:HB3	2.16	0.70
1:V:814:LYS:HG3	1:V:815:ARG:N	2.06	0.70
1:S:747:MET:HB3	1:S:752:ALA:HB2	1.73	0.70
1:V:361:GLN:C	1:V:363:GLY:H	1.99	0.70
1:V:399:THR:HG22	1:V:403:LEU:HD11	1.73	0.70
1:S:814:LYS:HG3	1:S:815:ARG:N	2.06	0.70
1:V:242:ASN:OD1	1:V:244:ASN:N	2.24	0.70
1:V:736:ILE:HG23	1:V:737:LEU:HD23	1.72	0.70
1:S:361:GLN:C	1:S:363:GLY:H	1.99	0.70
1:S:168:ARG:CZ	1:V:406:ARG:CG	2.70	0.70
1:S:494:ASN:HD22	1:S:494:ASN:H	1.40	0.70
1:V:293:LEU:HD22	1:V:353:LEU:HD23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:302:ARG:HH21	1:V:307:LEU:N	1.90	0.70
1:S:134:SER:HB2	1:S:212:GLY:HA2	1.74	0.70
1:S:628:VAL:HG13	1:S:631:ILE:HG12	1.74	0.70
1:V:494:ASN:H	1:V:494:ASN:HD22	1.39	0.70
1:V:541:LEU:HD23	1:V:601:ASN:ND2	2.05	0.70
1:S:50:LYS:HE3	1:S:60:GLU:HB3	1.72	0.70
1:S:736:ILE:HG23	1:S:737:LEU:HD23	1.72	0.70
1:S:619:LYS:O	1:S:622:ALA:HB3	1.91	0.70
1:V:568:LYS:HD3	1:V:584:LEU:HB2	1.72	0.70
1:S:243:ASP:HB3	1:S:323:ILE:HD11	1.73	0.70
1:S:306:LEU:HD12	1:S:390:LEU:HD21	1.74	0.69
2:T:102:THR:HG22	1:V:617:SER:CB	2.22	0.69
1:V:365:ILE:HD13	1:V:427:ILE:HD11	1.72	0.69
1:V:320:HIS:C	1:V:320:HIS:HD1	1.99	0.69
2:T:83:GLY:HA3	2:T:88:TYR:CZ	2.28	0.69
1:S:242:ASN:OD1	1:S:244:ASN:N	2.24	0.69
1:S:293:LEU:HD22	1:S:353:LEU:HD23	1.73	0.69
1:S:320:HIS:C	1:S:320:HIS:HD1	1.99	0.69
1:S:344:PHE:CE1	1:S:445:ARG:HB3	2.27	0.69
1:S:552:ASP:O	1:S:556:VAL:HG23	1.92	0.69
2:T:140:TYR:CZ	1:V:393:ILE:O	2.46	0.69
1:V:161:TYR:O	1:V:165:LEU:HD12	1.92	0.69
1:V:344:PHE:CE1	1:V:445:ARG:HB3	2.27	0.69
2:T:94:VAL:HG22	1:V:396:THR:HG22	1.75	0.69
1:V:552:ASP:O	1:V:556:VAL:HG23	1.92	0.69
2:W:83:GLY:HA3	2:W:88:TYR:CZ	2.28	0.69
2:W:113:VAL:HG13	2:W:119:MET:O	1.93	0.69
1:V:134:SER:HB2	1:V:212:GLY:HA2	1.74	0.69
2:T:25:LYS:HB3	2:T:63:THR:HB	1.74	0.69
2:T:112:LEU:HD13	2:T:119:MET:HE3	1.74	0.69
1:V:306:LEU:HD12	1:V:390:LEU:HD21	1.74	0.69
1:V:313:TYR:HB2	1:V:316:LEU:CD1	2.23	0.69
1:V:407:ILE:HD11	1:V:414:VAL:HB	1.75	0.69
2:W:112:LEU:HD13	2:W:119:MET:HE3	1.74	0.69
1:V:419:THR:H	1:V:422:GLN:NE2	1.87	0.69
1:V:678:ASN:HD22	1:V:679:PRO:CD	2.05	0.69
1:S:199:SER:HB2	1:S:221:GLU:HG2	1.75	0.68
1:S:824:CYS:O	1:S:828:ASN:HB2	1.93	0.68
1:V:269:THR:CG2	1:V:443:LEU:HD13	2.21	0.68
1:V:407:ILE:HD12	1:V:409:VAL:N	2.09	0.68
1:S:313:TYR:HB2	1:S:316:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:376:ALA:HB3	1:V:420:LYS:HA	1.75	0.68
2:W:25:LYS:HB3	2:W:63:THR:HB	1.74	0.68
2:W:43:THR:O	2:W:47:VAL:HG23	1.93	0.68
1:S:258:VAL:HG12	1:V:406:ARG:CZ	2.23	0.68
1:S:302:ARG:HH21	1:S:307:LEU:N	1.90	0.68
1:S:407:ILE:HD12	1:S:409:VAL:N	2.09	0.68
1:S:450:LEU:N	1:S:450:LEU:HD23	2.08	0.68
1:S:678:ASN:HD22	1:S:679:PRO:CD	2.05	0.68
1:S:161:TYR:O	1:S:165:LEU:HD12	1.92	0.68
1:S:301:MET:HA	1:S:304:ASP:HB2	1.75	0.68
2:T:4:SER:O	2:T:7:GLN:HG2	1.92	0.68
1:V:689:HIS:CE1	1:V:700:LEU:HD11	2.29	0.68
2:W:4:SER:O	2:W:7:GLN:HG2	1.92	0.68
1:V:301:MET:HA	1:V:304:ASP:HB2	1.75	0.68
1:V:628:VAL:HG13	1:V:631:ILE:HG12	1.74	0.68
1:S:689:HIS:CE1	1:S:700:LEU:HD11	2.29	0.68
2:T:36:ARG:HA	2:T:40:GLN:O	1.94	0.68
1:V:33:LYS:HD3	1:V:49:ILE:HD12	1.75	0.68
1:V:824:CYS:O	1:V:828:ASN:HB2	1.93	0.68
1:S:376:ALA:HB3	1:S:420:LYS:HA	1.75	0.68
2:T:43:THR:O	2:T:47:VAL:HG23	1.93	0.68
1:V:13:LEU:HD21	1:V:132:ILE:CD1	2.24	0.68
1:V:407:ILE:HD13	1:V:409:VAL:HG23	1.76	0.68
1:S:320:HIS:C	1:S:320:HIS:ND1	2.52	0.68
2:W:36:ARG:HA	2:W:40:GLN:O	1.93	0.68
1:S:13:LEU:HD21	1:S:132:ILE:CD1	2.24	0.68
1:S:407:ILE:HD13	1:S:409:VAL:HG23	1.76	0.68
1:S:627:ASP:CG	1:S:627:ASP:O	2.38	0.68
1:V:320:HIS:C	1:V:320:HIS:ND1	2.52	0.68
1:S:407:ILE:CD1	1:S:409:VAL:HG23	2.24	0.67
2:T:113:VAL:HG13	2:T:119:MET:O	1.93	0.67
1:V:169:GLU:O	1:V:169:GLU:HG2	1.93	0.67
1:V:189:LYS:HD3	1:V:192:GLN:OE1	1.94	0.67
1:S:57:VAL:O	1:S:69:THR:HG23	1.94	0.67
1:S:169:GLU:O	1:S:169:GLU:HG2	1.93	0.67
1:V:496:THR:HA	1:V:500:LEU:HD12	1.76	0.67
1:S:47:ALA:HA	1:S:62:GLN:H	1.59	0.67
1:S:145:LYS:HG3	1:S:146:ARG:HE	1.59	0.67
1:S:189:LYS:HD3	1:S:192:GLN:OE1	1.94	0.67
1:S:419:THR:H	1:S:422:GLN:NE2	1.87	0.67
1:V:407:ILE:CD1	1:V:409:VAL:HG23	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:269:THR:CG2	1:S:443:LEU:HD13	2.21	0.67
1:S:407:ILE:HD11	1:S:414:VAL:HB	1.75	0.67
1:V:47:ALA:HA	1:V:62:GLN:H	1.59	0.67
1:V:57:VAL:O	1:V:69:THR:HG23	1.94	0.67
2:W:43:THR:HG23	2:W:46:GLU:CD	2.19	0.67
1:S:533:ASN:HB3	1:S:534:PRO:HD2	1.75	0.67
1:S:728:GLN:CA	1:S:728:GLN:HE21	2.08	0.67
1:V:199:SER:HB2	1:V:221:GLU:HG2	1.75	0.67
1:V:527:LEU:O	1:V:537:VAL:HG23	1.95	0.67
2:T:94:VAL:CG1	1:V:396:THR:HG21	2.24	0.67
1:V:494:ASN:HD22	1:V:494:ASN:N	1.92	0.67
2:T:25:LYS:HA	2:T:64:LEU:O	1.95	0.67
1:V:450:LEU:N	1:V:450:LEU:HD23	2.08	0.67
1:S:227:ALA:C	1:S:229:PRO:HD2	2.20	0.67
1:S:362:LEU:HD23	1:S:427:ILE:HG13	1.76	0.67
1:V:145:LYS:HG3	1:V:146:ARG:HE	1.59	0.67
2:T:31:CYS:O	2:T:35:MET:HG3	1.95	0.67
1:S:234:PHE:HD1	1:S:289:ILE:HG21	1.59	0.67
1:S:796:ILE:C	1:S:797:ILE:HB	2.19	0.67
2:T:43:THR:HG23	2:T:46:GLU:CD	2.19	0.67
1:V:362:LEU:HD23	1:V:427:ILE:HG13	1.76	0.67
1:S:33:LYS:HD3	1:S:49:ILE:HD12	1.75	0.66
1:V:242:ASN:OD1	1:V:242:ASN:C	2.38	0.66
1:V:533:ASN:HB3	1:V:534:PRO:HD2	1.76	0.66
1:V:556:VAL:HG12	1:V:560:ILE:HD11	1.77	0.66
1:S:168:ARG:HH22	1:V:406:ARG:H	1.41	0.66
1:S:259:THR:HG23	2:T:104:MET:HE1	1.63	0.66
1:S:494:ASN:HD22	1:S:494:ASN:N	1.92	0.66
2:T:98:GLU:OE1	1:V:612:LEU:HA	1.95	0.66
1:V:627:ASP:CG	1:V:627:ASP:O	2.38	0.66
2:W:31:CYS:O	2:W:35:MET:HG3	1.95	0.66
1:S:527:LEU:HD12	1:S:566:HIS:CG	2.31	0.66
1:V:700:LEU:HD23	1:V:704:GLN:NE2	2.10	0.66
1:S:458:ALA:C	1:V:413:VAL:CG2	2.68	0.66
1:S:527:LEU:O	1:S:537:VAL:HG23	1.95	0.66
1:V:227:ALA:C	1:V:229:PRO:HD2	2.20	0.66
1:V:234:PHE:HD1	1:V:289:ILE:HG21	1.60	0.66
1:V:686:ILE:HD13	1:V:687:PRO:HD2	1.78	0.66
1:S:556:VAL:HG12	1:S:560:ILE:HD11	1.77	0.66
1:S:279:ARG:NH2	1:S:428:GLU:HG3	2.11	0.66
1:S:496:THR:HA	1:S:500:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:57:VAL:C	1:V:69:THR:HG23	2.21	0.66
1:V:527:LEU:HD12	1:V:566:HIS:CG	2.31	0.66
1:V:728:GLN:CA	1:V:728:GLN:HE21	2.08	0.66
1:S:370:GLU:O	1:S:374:ASP:N	2.29	0.66
2:W:93:ARG:HG3	2:W:93:ARG:O	1.94	0.66
1:S:242:ASN:OD1	1:S:242:ASN:C	2.38	0.66
1:V:747:MET:HE1	1:V:755:LEU:HD22	1.78	0.66
1:S:727:PHE:HB2	1:V:370:GLU:OE1	1.94	0.65
1:S:747:MET:HE1	1:S:755:LEU:HD22	1.78	0.65
1:V:279:ARG:NH2	1:V:428:GLU:HG3	2.11	0.65
1:V:313:TYR:HB2	1:V:316:LEU:HD11	1.77	0.65
1:V:818:GLN:C	1:V:822:ILE:CG1	2.52	0.65
1:V:502:GLN:HG2	1:V:512:TRP:NE1	2.12	0.65
1:S:700:LEU:HD23	1:S:704:GLN:NE2	2.10	0.65
1:V:522:GLN:N	1:V:523:PRO:HD2	2.11	0.65
1:S:541:LEU:HD23	1:S:601:ASN:ND2	2.05	0.65
2:T:93:ARG:O	2:T:93:ARG:HG3	1.94	0.65
1:V:230:ILE:HG22	1:V:231:LEU:N	2.11	0.65
1:V:535:PRO:HB2	1:V:540:LEU:HD21	1.78	0.65
1:S:57:VAL:C	1:S:69:THR:HG23	2.21	0.65
1:S:627:ASP:O	1:S:627:ASP:OD1	2.15	0.65
2:W:97:LYS:C	2:W:98:GLU:HG3	2.22	0.65
1:S:362:LEU:HD22	1:S:431:ALA:HB2	1.79	0.65
1:S:419:THR:O	1:S:420:LYS:C	2.40	0.65
1:S:481:CYS:O	1:S:484:TYR:HB3	1.97	0.65
1:V:419:THR:O	1:V:420:LYS:C	2.40	0.65
1:S:313:TYR:HB2	1:S:316:LEU:HD11	1.77	0.65
1:S:630:ARG:HH22	1:S:657:ARG:CB	2.10	0.65
1:V:97:GLU:OE2	1:V:702:LEU:HG	1.96	0.65
1:V:700:LEU:CD2	1:V:704:GLN:HE22	2.10	0.65
1:S:97:GLU:OE2	1:S:702:LEU:HG	1.96	0.65
1:S:120:PHE:HD1	1:S:120:PHE:H	1.43	0.65
1:S:661:GLN:O	1:S:665:GLU:HB2	1.97	0.65
1:V:187:THR:HG23	1:V:463:ILE:CG2	2.26	0.65
1:V:400:ARG:HG2	1:V:404:THR:OG1	1.97	0.65
1:S:555:PHE:CZ	1:S:559:LEU:HD13	2.32	0.65
1:S:259:THR:HB	1:S:261:TYR:HE1	1.61	0.64
1:S:400:ARG:HG2	1:S:404:THR:OG1	1.97	0.64
1:S:772:SER:CB	1:V:373:THR:CA	2.71	0.64
1:V:630:ARG:HH22	1:V:657:ARG:CB	2.10	0.64
1:V:555:PHE:CZ	1:V:559:LEU:HD13	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:25:LYS:HA	2:W:64:LEU:O	1.95	0.64
1:S:606:ASN:OD1	1:S:609:VAL:HG12	1.97	0.64
2:T:99:GLY:HA2	1:V:398:PHE:H	1.62	0.64
1:V:418:GLN:HB3	1:V:422:GLN:CB	2.28	0.64
1:V:661:GLN:O	1:V:665:GLU:HB2	1.97	0.64
1:S:181:ALA:O	1:S:684:CYS:HB3	1.98	0.64
1:S:535:PRO:HB2	1:S:540:LEU:HD21	1.78	0.64
1:S:552:ASP:O	1:S:555:PHE:HB3	1.97	0.64
1:S:700:LEU:CD2	1:S:704:GLN:HE22	2.10	0.64
1:V:552:ASP:O	1:V:555:PHE:HB3	1.97	0.64
1:V:586:TYR:HD1	1:V:586:TYR:H	1.45	0.64
1:S:187:THR:HG23	1:S:463:ILE:CG2	2.26	0.64
1:S:230:ILE:HG22	1:S:231:LEU:N	2.11	0.64
2:T:38:LEU:HD12	2:T:73:MET:HE2	1.78	0.64
1:V:481:CYS:O	1:V:484:TYR:HB3	1.97	0.64
1:S:44:PHE:CE2	1:S:702:LEU:HD21	2.33	0.64
1:S:391:MET:HE2	1:S:613:LEU:HD21	1.80	0.64
1:S:686:ILE:HD13	1:S:687:PRO:HD2	1.77	0.64
1:S:831:SER:O	1:S:834:ASN:HB2	1.97	0.64
2:T:55:LYS:HB2	2:T:58:GLU:OE2	1.97	0.64
2:T:100:ASN:CG	1:V:612:LEU:HA	2.19	0.64
1:V:120:PHE:HD1	1:V:120:PHE:H	1.43	0.64
1:V:181:ALA:O	1:V:684:CYS:HB3	1.98	0.64
1:V:391:MET:HE2	1:V:613:LEU:HD21	1.80	0.64
1:V:613:LEU:O	1:V:615:GLN:N	2.31	0.64
1:S:79:ASN:ND2	1:S:80:PRO:HD2	2.08	0.64
1:S:522:GLN:N	1:S:523:PRO:HD2	2.11	0.64
1:S:812:PHE:C	1:S:814:LYS:H	2.06	0.64
1:V:44:PHE:CE2	1:V:702:LEU:HD21	2.33	0.64
1:V:370:GLU:O	1:V:374:ASP:N	2.29	0.64
1:V:606:ASN:OD1	1:V:609:VAL:HG12	1.98	0.64
1:S:502:GLN:HG2	1:S:512:TRP:NE1	2.11	0.64
1:S:796:ILE:C	1:S:797:ILE:CB	2.67	0.64
1:V:345:THR:HB	1:V:348:GLU:CB	2.27	0.64
2:W:35:MET:O	2:W:40:GLN:HB2	1.98	0.64
2:T:97:LYS:C	2:T:98:GLU:HG3	2.22	0.64
1:V:259:THR:HB	1:V:261:TYR:HE1	1.61	0.64
1:S:399:THR:HG22	1:S:403:LEU:CD1	2.28	0.63
1:S:686:ILE:HG22	1:S:700:LEU:HD21	1.80	0.63
1:V:369:LYS:HZ2	1:V:420:LYS:HB3	1.61	0.63
1:V:753:CYS:O	1:V:756:MET:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:831:SER:O	1:V:834:ASN:HB2	1.97	0.63
1:S:613:LEU:O	1:S:615:GLN:N	2.31	0.63
1:S:673:THR:O	1:S:677:THR:HG23	1.98	0.63
1:V:627:ASP:O	1:V:627:ASP:OD1	2.15	0.63
1:S:342:MET:HE1	1:S:449:ALA:HB3	1.80	0.63
1:S:409:VAL:HG22	1:S:634:LEU:HD12	1.80	0.63
1:S:561:GLN:OE1	1:S:562:GLU:HG2	1.99	0.63
1:V:158:ASP:HB2	1:V:193:TYR:OH	1.99	0.63
1:V:551:THR:N	1:V:554:SER:OG	2.29	0.63
2:T:102:THR:HG23	1:V:616:SER:HA	1.79	0.63
1:V:323:ILE:CG2	1:V:326:GLN:HB3	2.28	0.63
1:V:362:LEU:HD22	1:V:431:ALA:HB2	1.79	0.63
1:S:530:ARG:HG2	1:S:534:PRO:O	1.98	0.63
1:V:79:ASN:ND2	1:V:80:PRO:HD2	2.08	0.63
1:V:399:THR:HG22	1:V:403:LEU:CD1	2.28	0.63
1:V:405:PRO:HB2	1:V:407:ILE:HG23	1.79	0.63
1:V:409:VAL:HG22	1:V:634:LEU:HD12	1.80	0.63
1:V:530:ARG:HG2	1:V:534:PRO:O	1.98	0.63
2:W:38:LEU:HD12	2:W:73:MET:HE2	1.78	0.63
1:S:772:SER:HB2	1:V:373:THR:C	2.24	0.63
1:S:794:ASP:O	1:S:797:ILE:HG22	1.98	0.63
1:S:158:ASP:HB2	1:S:193:TYR:OH	1.99	0.63
1:S:369:LYS:HZ2	1:S:420:LYS:HB3	1.63	0.63
1:S:628:VAL:O	1:S:628:VAL:HG12	1.99	0.63
1:S:753:CYS:O	1:S:756:MET:HG3	1.98	0.63
1:S:803:CYS:CB	2:T:119:MET:HE1	2.29	0.63
1:V:497:MET:HA	1:V:497:MET:HE3	1.81	0.63
2:T:99:GLY:HA3	1:V:398:PHE:HB2	1.70	0.63
1:V:305:LEU:HD22	1:V:354:ARG:HB3	1.81	0.63
2:W:3:PHE:HA	2:W:7:GLN:HE21	1.63	0.63
1:S:418:GLN:HB3	1:S:422:GLN:CB	2.28	0.63
2:T:35:MET:O	2:T:40:GLN:HB2	1.98	0.63
1:V:145:LYS:CG	1:V:146:ARG:H	2.12	0.63
1:V:271:LEU:HD21	1:V:663:TYR:CE1	2.34	0.63
1:V:671:MET:O	1:V:675:ARG:HD2	1.99	0.63
1:S:305:LEU:HD22	1:S:354:ARG:HB3	1.81	0.62
1:S:405:PRO:HB2	1:S:407:ILE:HG23	1.79	0.62
1:S:469:PHE:CE2	1:S:587:ALA:HB3	2.34	0.62
1:S:747:MET:HE1	1:S:755:LEU:CD2	2.29	0.62
1:V:607:ASP:CA	1:V:610:THR:HB	2.28	0.62
1:V:609:VAL:O	1:V:612:LEU:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:803:CYS:CB	2:W:119:MET:HE1	2.29	0.62
2:T:3:PHE:HA	2:T:7:GLN:HE21	1.63	0.62
1:S:586:TYR:HD1	1:S:586:TYR:H	1.45	0.62
1:V:267:ILE:HD11	1:V:450:LEU:HD12	1.81	0.62
1:V:480:LEU:HD22	1:V:597:TRP:CH2	2.34	0.62
1:V:561:GLN:OE1	1:V:562:GLU:HG2	1.99	0.62
1:V:788:ARG:HG2	1:V:788:ARG:HH11	1.64	0.62
1:V:678:ASN:ND2	1:V:679:PRO:HD2	2.10	0.62
2:W:55:LYS:HB2	2:W:58:GLU:OE2	1.97	0.62
1:S:497:MET:HA	1:S:497:MET:HE3	1.81	0.62
1:S:788:ARG:HG2	1:S:788:ARG:HH11	1.64	0.62
1:V:342:MET:HE1	1:V:449:ALA:HB3	1.80	0.62
1:V:686:ILE:HG22	1:V:700:LEU:HD21	1.80	0.62
1:S:609:VAL:O	1:S:612:LEU:HB3	1.99	0.62
1:V:747:MET:HE1	1:V:755:LEU:CD2	2.29	0.62
1:V:812:PHE:C	1:V:814:LYS:H	2.06	0.62
1:S:267:ILE:HD11	1:S:450:LEU:HD12	1.81	0.62
1:S:328:ASP:HA	1:S:331:MET:HB2	1.82	0.62
1:V:60:GLU:HG3	1:V:66:LYS:O	2.00	0.62
1:S:145:LYS:CG	1:S:146:ARG:H	2.12	0.62
1:S:551:THR:N	1:S:554:SER:OG	2.29	0.62
2:T:97:LYS:O	1:V:400:ARG:NH1	2.30	0.62
1:V:815:ARG:HA	1:V:818:GLN:CD	2.25	0.62
1:S:60:GLU:HG3	1:S:66:LYS:O	2.00	0.62
1:V:302:ARG:NH2	1:V:303:ASN:HA	2.14	0.62
1:V:819:LEU:HA	1:V:822:ILE:CD1	2.30	0.62
2:W:70:LEU:N	2:W:71:PRO:HD2	2.15	0.62
1:S:302:ARG:NH2	1:S:303:ASN:HA	2.14	0.62
1:S:313:TYR:HD2	1:S:360:LEU:HB3	1.65	0.62
1:S:480:LEU:HD22	1:S:597:TRP:CH2	2.34	0.62
1:S:804:ARG:HG2	1:S:804:ARG:NH1	2.15	0.62
2:T:65:LYS:HD2	2:T:68:GLN:NE2	2.15	0.62
1:V:469:PHE:CE2	1:V:587:ALA:HB3	2.34	0.62
1:V:527:LEU:HD23	1:V:537:VAL:HG23	1.82	0.62
1:V:628:VAL:O	1:V:628:VAL:HG12	1.99	0.62
2:W:72:MET:HA	2:W:75:THR:OG1	2.00	0.62
1:S:271:LEU:HD21	1:S:663:TYR:CE1	2.34	0.61
2:W:65:LYS:HD2	2:W:68:GLN:NE2	2.15	0.61
1:S:527:LEU:HD23	1:S:537:VAL:HG23	1.82	0.61
1:S:796:ILE:HG22	1:S:797:ILE:N	2.16	0.61
1:V:405:PRO:HD2	1:V:417:ALA:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:409:VAL:HB	1:V:414:VAL:HG21	1.82	0.61
1:V:673:THR:O	1:V:677:THR:HG23	1.98	0.61
1:V:819:LEU:HA	1:V:822:ILE:CB	2.30	0.61
2:T:70:LEU:N	2:T:71:PRO:HD2	2.14	0.61
2:T:72:MET:HA	2:T:75:THR:OG1	2.00	0.61
1:V:804:ARG:HG2	1:V:804:ARG:NH1	2.15	0.61
1:S:458:ALA:O	1:V:413:VAL:CG2	2.47	0.61
1:S:527:LEU:HD11	1:S:569:PHE:HB2	1.82	0.61
1:S:667:LEU:O	1:S:667:LEU:HG	2.00	0.61
1:S:728:GLN:HB2	1:V:370:GLU:HG3	1.83	0.61
1:V:328:ASP:HA	1:V:331:MET:HB2	1.82	0.61
1:S:345:THR:HB	1:S:348:GLU:CB	2.27	0.61
1:S:819:LEU:HA	1:S:822:ILE:CB	2.30	0.61
1:S:819:LEU:HA	1:S:822:ILE:CD1	2.30	0.61
1:V:382:THR:O	1:V:385:GLN:HB3	2.01	0.61
1:S:323:ILE:CG2	1:S:326:GLN:HB3	2.29	0.61
1:S:671:MET:O	1:S:675:ARG:HD2	1.99	0.61
2:W:84:CYS:O	2:W:85:PHE:C	2.42	0.61
1:S:243:ASP:HB3	1:S:323:ILE:CD1	2.31	0.61
2:T:84:CYS:O	2:T:85:PHE:C	2.43	0.61
1:S:527:LEU:HG	1:S:563:GLN:HG3	1.82	0.61
2:T:93:ARG:HG3	1:V:396:THR:N	2.16	0.61
2:T:102:THR:N	1:V:393:ILE:HA	1.75	0.61
1:V:822:ILE:O	1:V:826:GLN:N	2.30	0.61
1:S:7:SER:HB3	1:S:10:GLU:OE1	2.00	0.61
1:V:7:SER:HB3	1:V:10:GLU:OE1	2.01	0.61
1:V:243:ASP:HB3	1:V:323:ILE:CD1	2.31	0.61
1:V:266:ASN:HA	1:V:447:ASN:OD1	2.00	0.61
1:V:362:LEU:HD21	1:V:430:LEU:HD23	1.83	0.61
1:S:56:GLU:HG3	1:S:71:SER:HA	1.83	0.61
2:T:55:LYS:O	2:T:58:GLU:HG2	2.01	0.61
1:V:186:ASN:O	1:V:190:VAL:HG23	2.01	0.61
1:V:391:MET:HG2	1:V:613:LEU:CD2	2.31	0.61
1:V:731:ARG:HG2	1:V:731:ARG:HH11	1.66	0.61
1:S:382:THR:O	1:S:385:GLN:HB3	2.01	0.60
1:S:391:MET:HG2	1:S:613:LEU:CD2	2.31	0.60
1:V:89:MET:C	1:V:91:GLU:H	2.09	0.60
2:W:55:LYS:O	2:W:58:GLU:HG2	2.01	0.60
1:S:409:VAL:HB	1:S:414:VAL:HG21	1.82	0.60
1:S:815:ARG:HA	1:S:818:GLN:CD	2.25	0.60
1:V:527:LEU:HD11	1:V:569:PHE:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:667:LEU:O	1:V:667:LEU:HG	2.00	0.60
1:S:266:ASN:HA	1:S:447:ASN:OD1	2.00	0.60
1:V:56:GLU:HG3	1:V:71:SER:HA	1.84	0.60
1:V:313:TYR:HD2	1:V:360:LEU:HB3	1.65	0.60
1:S:186:ASN:O	1:S:190:VAL:HG23	2.01	0.60
1:S:362:LEU:HD21	1:S:430:LEU:HD23	1.83	0.60
1:S:728:GLN:HE21	1:S:728:GLN:HA	1.66	0.60
1:V:541:LEU:HD21	1:V:597:TRP:HB3	1.83	0.60
1:S:50:LYS:HE3	1:S:60:GLU:CB	2.32	0.60
1:S:405:PRO:HD2	1:S:417:ALA:HA	1.83	0.60
1:S:380:ASP:OD1	1:S:382:THR:HG23	2.02	0.60
2:T:4:SER:H	2:T:7:GLN:HE21	1.48	0.60
1:V:89:MET:HE1	1:V:104:LEU:HG	1.84	0.60
1:S:846:MLY:O	1:S:849:PRO:HD2	2.02	0.60
1:V:663:TYR:OH	1:V:667:LEU:HD13	2.02	0.60
1:V:846:MLY:O	1:V:849:PRO:HD2	2.02	0.60
1:S:8:ASP:CA	1:S:11:LYS:HD2	2.20	0.60
1:S:89:MET:C	1:S:91:GLU:H	2.09	0.60
1:S:458:ALA:O	1:V:413:VAL:HG21	2.01	0.60
1:S:541:LEU:HD21	1:S:597:TRP:HB3	1.83	0.60
1:S:731:ARG:HG2	1:S:731:ARG:HH11	1.66	0.60
2:T:140:TYR:CD1	2:T:141:GLU:HG2	2.37	0.60
1:S:23:PRO:HA	1:S:26:GLN:HB3	1.84	0.60
1:S:258:VAL:HG12	1:V:406:ARG:NH2	2.15	0.60
2:T:99:GLY:HA2	1:V:398:PHE:CB	2.27	0.60
1:V:103:ASN:O	1:V:107:ARG:HG3	2.02	0.60
2:W:140:TYR:CD1	2:W:141:GLU:HG2	2.37	0.60
2:T:99:GLY:H	1:V:397:ASP:C	2.10	0.60
1:V:568:LYS:CD	1:V:584:LEU:HB2	2.32	0.60
1:V:361:GLN:C	1:V:363:GLY:N	2.58	0.59
2:W:85:PHE:HE1	2:W:145:ARG:HG2	1.67	0.59
1:S:33:LYS:HB3	1:S:49:ILE:CB	2.32	0.59
1:S:607:ASP:CA	1:S:610:THR:HB	2.28	0.59
1:S:678:ASN:ND2	1:S:679:PRO:HD2	2.10	0.59
1:S:703:GLU:O	1:S:706:ARG:HB2	2.02	0.59
1:V:50:LYS:HE3	1:V:60:GLU:CB	2.32	0.59
1:V:527:LEU:HG	1:V:563:GLN:HG3	1.83	0.59
1:V:728:GLN:HE21	1:V:728:GLN:HA	1.66	0.59
2:T:40:GLN:HB3	2:T:42:PRO:HD3	1.85	0.59
2:T:99:GLY:H	1:V:397:ASP:HB2	1.66	0.59
1:V:443:LEU:O	1:V:447:ASN:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:490:GLN:O	1:S:494:ASN:ND2	2.36	0.59
1:V:703:GLU:O	1:V:706:ARG:HB2	2.02	0.59
1:V:712:GLU:CD	1:V:712:GLU:H	2.10	0.59
1:S:630:ARG:HH22	1:S:657:ARG:HB3	1.67	0.59
1:S:663:TYR:OH	1:S:667:LEU:HD13	2.02	0.59
1:S:705:LEU:HD22	1:S:710:VAL:HG21	1.85	0.59
1:V:36:TRP:HE1	1:V:78:MET:HG3	1.65	0.59
1:V:380:ASP:OD1	1:V:382:THR:HG23	2.02	0.59
1:S:378:MET:HA	1:S:378:MET:HE3	1.84	0.59
1:S:726:VAL:HG22	1:V:370:GLU:OE1	2.03	0.59
1:V:437:ARG:HB3	1:V:624:LEU:HD23	1.85	0.59
2:W:40:GLN:HB3	2:W:42:PRO:HD3	1.84	0.59
2:W:140:TYR:CD1	2:W:141:GLU:N	2.70	0.59
1:S:568:LYS:CD	1:S:584:LEU:HB2	2.32	0.59
1:S:702:LEU:O	1:S:706:ARG:HG3	2.02	0.59
2:T:85:PHE:CZ	2:T:145:ARG:CZ	2.85	0.59
1:V:630:ARG:HH22	1:V:657:ARG:HB3	1.67	0.59
2:W:131:HIS:CE1	2:W:146:MET:HE3	2.38	0.59
1:S:36:TRP:HE1	1:S:78:MET:HG3	1.65	0.59
1:S:478:GLU:OE1	1:S:478:GLU:N	2.24	0.59
1:S:763:ASP:HB3	1:S:766:LEU:HD11	1.84	0.59
2:T:140:TYR:CD1	2:T:141:GLU:N	2.70	0.59
1:V:378:MET:HA	1:V:378:MET:HE3	1.84	0.59
1:S:100:VAL:O	1:S:104:LEU:HG	2.03	0.59
1:S:721:PHE:N	1:S:721:PHE:HD1	2.00	0.59
1:V:766:LEU:HB3	1:V:780:VAL:HG21	1.85	0.59
1:S:52:GLU:HA	1:S:57:VAL:HG13	1.84	0.59
1:S:89:MET:HE1	1:S:104:LEU:HG	1.84	0.59
1:S:458:ALA:HB1	1:V:413:VAL:CG1	2.33	0.59
1:S:533:ASN:O	1:S:534:PRO:C	2.45	0.59
1:S:712:GLU:CD	1:S:712:GLU:H	2.10	0.59
2:T:125:GLU:O	2:T:129:ALA:HB2	2.03	0.59
1:V:33:LYS:HB3	1:V:49:ILE:CB	2.32	0.59
1:V:88:ASP:HB3	1:V:91:GLU:OE1	2.03	0.59
1:V:302:ARG:HH21	1:V:307:LEU:H	1.49	0.59
1:V:702:LEU:O	1:V:706:ARG:HG3	2.02	0.59
1:S:302:ARG:HH21	1:S:307:LEU:H	1.50	0.58
1:S:766:LEU:HB3	1:S:780:VAL:HG21	1.85	0.58
2:T:85:PHE:CE1	2:T:145:ARG:HG2	2.38	0.58
2:T:131:HIS:CE1	2:T:146:MET:HE3	2.38	0.58
1:V:247:ARG:HA	1:V:247:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:568:LYS:HA	1:V:568:LYS:HE3	1.85	0.58
1:S:125:ASN:OD1	1:S:126:PRO:HD2	2.04	0.58
1:S:428:GLU:C	1:S:430:LEU:H	2.11	0.58
1:S:469:PHE:CZ	1:S:587:ALA:HB3	2.38	0.58
1:S:533:ASN:CB	1:S:534:PRO:HD2	2.33	0.58
1:S:610:THR:HG23	1:S:628:VAL:CG2	2.33	0.58
2:T:85:PHE:HE1	2:T:145:ARG:HG2	1.67	0.58
1:V:469:PHE:CZ	1:V:587:ALA:HB3	2.38	0.58
2:W:85:PHE:CZ	2:W:145:ARG:CZ	2.85	0.58
1:S:347:GLU:C	1:S:349:GLN:H	2.11	0.58
1:S:568:LYS:HA	1:S:568:LYS:HE3	1.85	0.58
2:T:100:ASN:OD1	1:V:612:LEU:HG	1.72	0.58
2:T:140:TYR:CE2	1:V:394:ASN:ND2	2.68	0.58
1:V:125:ASN:OD1	1:V:126:PRO:HD2	2.04	0.58
1:V:361:GLN:O	1:V:363:GLY:N	2.36	0.58
2:W:64:LEU:HD23	2:W:68:GLN:OE1	2.04	0.58
2:W:140:TYR:O	2:W:141:GLU:C	2.45	0.58
1:S:310:PHE:CD2	1:S:320:HIS:HB2	2.38	0.58
1:S:443:LEU:O	1:S:447:ASN:HB2	2.03	0.58
1:S:477:PHE:O	1:S:480:LEU:HB3	2.04	0.58
1:S:663:TYR:C	1:S:665:GLU:H	2.11	0.58
2:T:104:MET:C	2:T:106:ALA:H	2.12	0.58
2:T:140:TYR:O	2:T:141:GLU:C	2.45	0.58
1:V:23:PRO:HA	1:V:26:GLN:HB3	1.84	0.58
1:V:52:GLU:HA	1:V:57:VAL:HG13	1.84	0.58
1:S:88:ASP:HB3	1:S:91:GLU:OE1	2.03	0.58
1:S:103:ASN:O	1:S:107:ARG:HG3	2.02	0.58
1:S:247:ARG:HA	1:S:247:ARG:HH11	1.68	0.58
1:S:361:GLN:O	1:S:363:GLY:N	2.36	0.58
1:V:533:ASN:O	1:V:534:PRO:C	2.45	0.58
1:V:663:TYR:C	1:V:665:GLU:H	2.11	0.58
2:W:104:MET:C	2:W:106:ALA:H	2.11	0.58
1:V:477:PHE:O	1:V:480:LEU:HB3	2.04	0.58
1:V:800:GLN:HA	2:W:119:MET:HE2	1.85	0.58
2:T:64:LEU:HD23	2:T:68:GLN:OE1	2.04	0.58
1:V:293:LEU:HD11	1:V:301:MET:CE	2.34	0.58
1:V:763:ASP:HB3	1:V:766:LEU:HD11	1.84	0.58
1:S:399:THR:O	1:S:403:LEU:HD12	2.03	0.58
1:S:553:THR:O	1:S:557:GLU:HG2	2.04	0.58
1:S:742:ILE:HD11	1:S:756:MET:HG2	1.86	0.58
1:V:100:VAL:O	1:V:104:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:399:THR:O	1:V:403:LEU:HD12	2.03	0.58
1:V:428:GLU:C	1:V:430:LEU:H	2.12	0.58
1:V:490:GLN:O	1:V:494:ASN:ND2	2.36	0.58
1:V:533:ASN:CB	1:V:534:PRO:HD2	2.33	0.58
1:V:610:THR:HG23	1:V:628:VAL:CG2	2.33	0.58
2:W:85:PHE:CE1	2:W:145:ARG:HG2	2.38	0.58
1:S:659:VAL:CG1	1:S:660:GLY:N	2.67	0.58
1:V:480:LEU:HD11	1:V:528:ILE:HD12	1.86	0.58
1:S:123:VAL:HG12	1:S:123:VAL:O	2.04	0.57
1:S:168:ARG:NH2	1:V:406:ARG:CG	2.66	0.57
1:S:293:LEU:HD11	1:S:301:MET:CE	2.34	0.57
1:S:570:GLN:OE1	1:S:589:LYS:HE2	2.04	0.57
1:V:570:GLN:OE1	1:V:589:LYS:HE2	2.04	0.57
1:V:711:LEU:HD22	1:V:711:LEU:N	2.19	0.57
1:V:721:PHE:N	1:V:721:PHE:HD1	1.99	0.57
1:V:818:GLN:O	1:V:822:ILE:N	2.37	0.57
2:W:125:GLU:O	2:W:129:ALA:HB2	2.03	0.57
1:S:513:ASN:HD22	1:S:513:ASN:C	2.12	0.57
2:T:140:TYR:HD1	2:T:141:GLU:H	1.51	0.57
1:V:138:ILE:HD13	1:V:154:TYR:CE2	2.39	0.57
1:V:310:PHE:CD2	1:V:320:HIS:HB2	2.39	0.57
1:V:347:GLU:C	1:V:349:GLN:N	2.60	0.57
1:V:742:ILE:HD11	1:V:756:MET:HG2	1.86	0.57
1:S:458:ALA:CA	1:V:413:VAL:CG2	2.82	0.57
1:S:750:LYS:HB2	1:V:372:ASN:OD1	2.04	0.57
1:S:772:SER:CB	1:V:373:THR:HA	2.34	0.57
1:S:788:ARG:HG2	1:S:788:ARG:NH1	2.19	0.57
1:S:797:ILE:HG22	1:S:798:ALA:N	2.19	0.57
1:V:89:MET:HE3	1:V:100:VAL:HG13	1.86	0.57
1:V:347:GLU:C	1:V:349:GLN:H	2.11	0.57
1:V:788:ARG:HG2	1:V:788:ARG:NH1	2.20	0.57
1:S:437:ARG:HB3	1:S:624:LEU:HD23	1.85	0.57
2:T:101:GLY:C	1:V:392:GLY:C	2.71	0.57
1:V:267:ILE:HB	1:V:447:ASN:ND2	2.20	0.57
1:V:628:VAL:HG13	1:V:628:VAL:O	2.04	0.57
1:V:796:ILE:HG22	1:V:800:GLN:OE1	2.04	0.57
2:W:4:SER:H	2:W:7:GLN:HE21	1.49	0.57
1:S:611:SER:O	1:S:615:GLN:NE2	2.37	0.57
1:S:818:GLN:O	1:S:822:ILE:N	2.37	0.57
1:S:822:ILE:O	1:S:825:ILE:N	2.37	0.57
1:S:104:LEU:HD12	1:S:705:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:480:LEU:HD11	1:S:528:ILE:HD12	1.86	0.57
1:S:568:LYS:CE	1:S:584:LEU:HB2	2.35	0.57
1:S:628:VAL:HG13	1:S:628:VAL:O	2.04	0.57
1:S:89:MET:HE2	1:S:104:LEU:HD21	1.86	0.57
1:S:273:GLU:HG2	1:S:273:GLU:O	2.05	0.57
1:V:405:PRO:C	1:V:407:ILE:H	2.13	0.57
1:V:705:LEU:HD22	1:V:710:VAL:HG21	1.85	0.57
2:W:80:LYS:H	2:W:80:LYS:HD2	1.70	0.57
1:S:361:GLN:C	1:S:363:GLY:N	2.58	0.57
2:T:14:ALA:CB	2:T:38:LEU:HD21	2.35	0.57
2:T:85:PHE:HE1	2:T:145:ARG:CG	2.18	0.57
1:V:568:LYS:CE	1:V:584:LEU:HB2	2.35	0.57
1:V:711:LEU:H	1:V:711:LEU:CD2	2.18	0.57
1:V:822:ILE:O	1:V:825:ILE:N	2.37	0.57
2:W:14:ALA:CB	2:W:38:LEU:HD21	2.35	0.57
1:S:13:LEU:HD21	1:S:132:ILE:HD12	1.86	0.57
1:S:226:GLN:C	1:S:229:PRO:HD2	2.30	0.57
1:S:267:ILE:HB	1:S:447:ASN:ND2	2.20	0.57
1:S:420:LYS:HD2	1:S:421:GLU:CD	2.30	0.57
1:S:727:PHE:N	1:V:373:THR:HG23	2.19	0.57
1:S:747:MET:CE	1:S:755:LEU:HD22	2.35	0.57
1:V:89:MET:HE2	1:V:104:LEU:HD21	1.86	0.57
2:T:99:GLY:C	1:V:393:ILE:HB	2.24	0.57
1:V:13:LEU:HD21	1:V:132:ILE:HD12	1.86	0.57
1:V:123:VAL:O	1:V:123:VAL:HG12	2.04	0.57
1:V:308:GLU:N	1:V:313:TYR:OH	2.38	0.57
1:V:769:ILE:HD13	1:V:774:ILE:HG23	1.87	0.57
1:S:482:ILE:HG22	1:S:483:ASN:N	2.20	0.56
1:V:161:TYR:CZ	1:V:165:LEU:HD11	2.40	0.56
1:V:369:LYS:NZ	1:V:420:LYS:HB3	2.20	0.56
1:V:420:LYS:HD2	1:V:421:GLU:CD	2.30	0.56
1:S:278:ILE:HA	1:S:315:PHE:CD1	2.40	0.56
1:S:347:GLU:C	1:S:349:GLN:N	2.60	0.56
1:S:711:LEU:N	1:S:711:LEU:HD22	2.19	0.56
2:T:93:ARG:O	1:V:396:THR:N	2.38	0.56
1:V:36:TRP:CE2	1:V:78:MET:HG3	2.40	0.56
1:V:44:PHE:HE2	1:V:702:LEU:HD21	1.69	0.56
1:V:273:GLU:HG2	1:V:273:GLU:O	2.05	0.56
1:S:242:ASN:ND2	1:S:245:SER:HA	2.21	0.56
1:S:382:THR:HA	1:S:385:GLN:OE1	2.06	0.56
2:T:80:LYS:H	2:T:80:LYS:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:98:GLU:CA	1:V:397:ASP:HB3	2.35	0.56
2:T:140:TYR:HD1	2:T:141:GLU:N	2.02	0.56
1:V:8:ASP:CA	1:V:11:LYS:HD2	2.20	0.56
1:V:71:SER:C	1:V:73:ASP:H	2.13	0.56
1:V:226:GLN:C	1:V:229:PRO:HD2	2.30	0.56
1:V:278:ILE:HA	1:V:315:PHE:CD1	2.40	0.56
1:V:553:THR:O	1:V:557:GLU:HG2	2.04	0.56
1:V:747:MET:CE	1:V:755:LEU:HD22	2.35	0.56
2:W:85:PHE:HE1	2:W:145:ARG:CG	2.18	0.56
1:S:13:LEU:HD21	1:S:132:ILE:HD13	1.86	0.56
1:S:138:ILE:HD13	1:S:154:TYR:CE2	2.39	0.56
1:V:13:LEU:HD21	1:V:132:ILE:HD13	1.86	0.56
1:S:50:LYS:HG3	1:S:67:LYS:HE3	1.87	0.56
1:S:51:GLU:HG2	1:S:53:LYS:HE3	1.87	0.56
1:S:293:LEU:HA	1:S:332:PHE:CE1	2.41	0.56
1:S:308:GLU:N	1:S:313:TYR:OH	2.38	0.56
1:S:572:SER:HB3	1:S:580:GLU:O	2.06	0.56
1:S:711:LEU:H	1:S:711:LEU:CD2	2.18	0.56
1:V:513:ASN:C	1:V:513:ASN:HD22	2.12	0.56
1:S:36:TRP:CE2	1:S:78:MET:HG3	2.40	0.56
1:S:89:MET:HE3	1:S:100:VAL:HG13	1.86	0.56
1:S:800:GLN:HA	2:T:119:MET:HE2	1.85	0.56
1:V:104:LEU:HD12	1:V:705:LEU:HD11	1.85	0.56
1:V:165:LEU:HD21	1:V:260:GLY:HA2	1.88	0.56
1:V:226:GLN:O	1:V:229:PRO:HG2	2.06	0.56
1:V:611:SER:O	1:V:615:GLN:NE2	2.37	0.56
1:S:161:TYR:CZ	1:S:165:LEU:HD11	2.40	0.56
1:S:259:THR:HB	1:S:261:TYR:CD1	2.41	0.56
1:V:42:HIS:C	1:V:44:PHE:H	2.13	0.56
1:V:61:LEU:HD12	1:V:64:ASN:HB3	1.88	0.56
1:S:64:ASN:C	1:S:66:LYS:H	2.14	0.56
1:S:278:ILE:HG13	1:S:279:ARG:N	2.21	0.56
2:T:93:ARG:NH2	1:V:398:PHE:HB3	2.20	0.56
2:W:40:GLN:C	2:W:42:PRO:HD3	2.31	0.56
1:S:44:PHE:HE2	1:S:702:LEU:HD21	1.69	0.56
1:S:258:VAL:HG12	1:V:406:ARG:HH22	1.70	0.56
1:S:272:LEU:O	1:S:274:LYS:N	2.38	0.56
1:S:458:ALA:C	1:V:413:VAL:CG1	2.55	0.56
2:T:94:VAL:CA	1:V:396:THR:HG23	2.25	0.56
1:V:51:GLU:HG2	1:V:53:LYS:HE3	1.87	0.56
1:V:66:LYS:HD3	1:V:67:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:170:ASP:C	1:V:171:GLN:HG2	2.31	0.56
1:V:278:ILE:HG13	1:V:279:ARG:N	2.21	0.56
1:V:293:LEU:HA	1:V:332:PHE:CE1	2.41	0.56
1:V:572:SER:HB3	1:V:580:GLU:O	2.06	0.56
1:V:803:CYS:O	1:V:807:LEU:HB2	2.06	0.56
2:W:55:LYS:HB2	2:W:58:GLU:CD	2.31	0.56
1:S:165:LEU:HD21	1:S:260:GLY:HA2	1.88	0.56
1:S:275:SER:O	1:S:277:ALA:N	2.39	0.56
1:S:369:LYS:NZ	1:S:420:LYS:HB3	2.20	0.56
1:S:771:GLN:HE21	1:S:771:GLN:CA	2.18	0.56
2:T:48:MET:HG3	2:T:53:ASN:HA	1.88	0.56
2:T:55:LYS:HB2	2:T:58:GLU:CD	2.31	0.56
1:V:242:ASN:ND2	1:V:245:SER:HA	2.21	0.56
1:V:275:SER:O	1:V:277:ALA:N	2.39	0.56
1:V:478:GLU:OE1	1:V:478:GLU:N	2.24	0.56
1:V:815:ARG:O	1:V:818:GLN:HG2	2.06	0.56
1:S:405:PRO:C	1:S:407:ILE:H	2.13	0.55
1:S:822:ILE:O	1:S:826:GLN:N	2.30	0.55
2:T:99:GLY:HA2	1:V:398:PHE:N	2.17	0.55
1:V:267:ILE:HB	1:V:447:ASN:HD21	1.72	0.55
1:V:482:ILE:HG22	1:V:483:ASN:N	2.20	0.55
2:W:35:MET:HE1	2:W:76:ILE:HG13	1.88	0.55
1:S:32:LYS:C	1:S:34:LEU:H	2.14	0.55
1:S:48:SER:O	1:S:59:VAL:HG13	2.07	0.55
2:T:20:ARG:HA	3:U:123:THR:CA	2.37	0.55
2:W:140:TYR:HD1	2:W:141:GLU:N	2.02	0.55
1:S:107:ARG:HB3	1:S:112:LEU:HD12	1.89	0.55
1:S:168:ARG:CD	1:V:415:GLN:NE2	2.69	0.55
1:S:553:THR:O	1:S:554:SER:C	2.49	0.55
1:V:107:ARG:CA	1:V:112:LEU:HD12	2.37	0.55
1:V:382:THR:HA	1:V:385:GLN:OE1	2.06	0.55
1:V:731:ARG:HG2	1:V:731:ARG:NH1	2.21	0.55
1:S:610:THR:CG2	1:S:631:ILE:HG13	2.28	0.55
1:S:769:ILE:HD13	1:S:774:ILE:HG23	1.87	0.55
1:S:807:LEU:HD23	1:S:807:LEU:O	2.07	0.55
1:S:815:ARG:O	1:S:818:GLN:HG2	2.06	0.55
2:T:40:GLN:C	2:T:42:PRO:HD3	2.31	0.55
1:V:50:LYS:HG3	1:V:67:LYS:HE3	1.87	0.55
1:V:292:TYR:CE2	1:V:331:MET:HB3	2.42	0.55
1:V:712:GLU:OE1	1:V:712:GLU:N	2.35	0.55
2:W:3:PHE:HA	2:W:7:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:20:ARG:HA	3:Z:123:THR:CA	2.37	0.55
1:S:267:ILE:HB	1:S:447:ASN:HD21	1.72	0.55
1:S:458:ALA:CA	1:V:413:VAL:HG21	2.37	0.55
2:T:3:PHE:HA	2:T:7:GLN:NE2	2.22	0.55
2:T:35:MET:HE1	2:T:76:ILE:HG13	1.88	0.55
1:V:272:LEU:O	1:V:274:LYS:N	2.38	0.55
1:V:352:ILE:CG2	1:V:442:ILE:HD11	2.35	0.55
1:V:807:LEU:O	1:V:807:LEU:HD23	2.07	0.55
1:S:66:LYS:HD3	1:S:67:LYS:H	1.71	0.55
1:S:71:SER:C	1:S:73:ASP:H	2.13	0.55
1:S:712:GLU:OE1	1:S:712:GLU:N	2.35	0.55
1:V:797:ILE:HG22	1:V:798:ALA:N	2.19	0.55
2:W:4:SER:H	2:W:7:GLN:NE2	2.05	0.55
1:S:103:ASN:ND2	1:S:107:ARG:HD2	2.22	0.55
1:S:107:ARG:CA	1:S:112:LEU:HD12	2.37	0.55
1:S:539:ALA:O	1:S:542:ASP:HB2	2.07	0.55
2:T:94:VAL:N	1:V:396:THR:CG2	2.66	0.55
2:T:101:GLY:C	1:V:392:GLY:O	2.49	0.55
1:V:32:LYS:C	1:V:34:LEU:H	2.14	0.55
1:V:259:THR:HB	1:V:261:TYR:CD1	2.41	0.55
1:V:543:GLU:C	1:V:545:CYS:H	2.15	0.55
1:V:622:ALA:O	1:V:626:LYS:N	2.40	0.55
1:S:33:LYS:HB3	1:S:49:ILE:N	2.22	0.55
1:S:33:LYS:CB	1:S:49:ILE:HB	2.37	0.55
1:S:42:HIS:C	1:S:44:PHE:H	2.13	0.55
1:S:170:ASP:C	1:S:171:GLN:HG2	2.31	0.55
1:S:458:ALA:CA	1:V:413:VAL:CG1	2.85	0.55
1:S:525:ILE:O	1:S:529:GLU:N	2.40	0.55
1:V:37:VAL:CG1	1:V:38:PRO:HD2	2.35	0.55
1:V:771:GLN:HE21	1:V:771:GLN:CA	2.17	0.55
1:S:107:ARG:HA	1:S:112:LEU:HD12	1.89	0.55
1:S:731:ARG:HG2	1:S:731:ARG:NH1	2.21	0.55
2:T:28:TYR:CD2	2:T:51:LEU:HD13	2.41	0.55
1:V:416:LYS:HE2	1:V:417:ALA:H	1.72	0.55
1:V:529:GLU:O	1:V:664:LYS:NZ	2.40	0.55
1:V:669:LYS:O	1:V:672:THR:HB	2.07	0.55
1:S:126:PRO:O	1:S:127:TYR:HB2	2.07	0.55
1:S:168:ARG:NH1	1:V:404:THR:CB	2.70	0.55
1:S:226:GLN:O	1:S:229:PRO:HG2	2.06	0.55
1:S:265:ALA:HB3	1:S:450:LEU:HB3	1.88	0.55
1:S:312:ASN:HD22	1:S:312:ASN:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:416:LYS:HE2	1:S:417:ALA:H	1.72	0.55
1:V:103:ASN:ND2	1:V:107:ARG:HD2	2.22	0.55
1:V:250:LYS:HG2	1:V:465:ASP:OD2	2.07	0.55
1:S:292:TYR:CE2	1:S:331:MET:HB3	2.42	0.54
1:S:540:LEU:O	1:S:542:ASP:N	2.40	0.54
1:V:33:LYS:CB	1:V:49:ILE:HB	2.37	0.54
1:V:48:SER:O	1:V:59:VAL:HG13	2.07	0.54
1:V:107:ARG:HB3	1:V:112:LEU:HD12	1.89	0.54
1:V:344:PHE:HE1	1:V:445:ARG:HB3	1.72	0.54
1:V:370:GLU:O	1:V:374:ASP:HA	2.08	0.54
1:V:521:LEU:O	1:V:525:ILE:HG13	2.07	0.54
1:V:553:THR:O	1:V:554:SER:C	2.49	0.54
1:V:607:ASP:HA	1:V:610:THR:CB	2.32	0.54
1:S:803:CYS:O	1:S:807:LEU:HB2	2.06	0.54
2:T:4:SER:H	2:T:7:GLN:NE2	2.05	0.54
1:V:126:PRO:O	1:V:127:TYR:HB2	2.06	0.54
2:W:28:TYR:CD2	2:W:51:LEU:HD13	2.41	0.54
1:S:352:ILE:CG2	1:S:442:ILE:HD11	2.35	0.54
1:S:521:LEU:O	1:S:525:ILE:HG13	2.07	0.54
1:S:727:PHE:N	1:V:372:ASN:HB2	2.22	0.54
2:T:102:THR:HG23	1:V:616:SER:CA	2.37	0.54
1:V:147:HIS:C	1:V:149:MET:H	2.15	0.54
1:V:218:GLY:HA3	1:V:221:GLU:OE1	2.08	0.54
1:S:61:LEU:HD12	1:S:64:ASN:HB3	1.88	0.54
1:S:228:ASN:N	1:S:229:PRO:HD2	2.23	0.54
1:S:669:LYS:O	1:S:672:THR:HB	2.07	0.54
1:S:797:ILE:HG13	2:T:117:GLU:H	1.72	0.54
2:T:102:THR:CG2	1:V:617:SER:CA	2.77	0.54
1:V:228:ASN:N	1:V:229:PRO:HD2	2.23	0.54
1:V:298:SER:O	1:V:302:ARG:N	2.40	0.54
1:V:539:ALA:O	1:V:542:ASP:HB2	2.07	0.54
1:S:298:SER:O	1:S:302:ARG:N	2.40	0.54
1:S:489:LEU:O	1:S:492:LEU:HB3	2.07	0.54
1:V:64:ASN:C	1:V:66:LYS:H	2.14	0.54
1:V:312:ASN:HD22	1:V:312:ASN:N	2.05	0.54
1:V:347:GLU:O	1:V:349:GLN:N	2.40	0.54
1:S:623:ASP:HA	1:S:626:LYS:HB3	1.88	0.54
1:S:711:LEU:HD22	1:S:711:LEU:H	1.73	0.54
1:V:254:ILE:O	1:V:460:PHE:HA	2.08	0.54
1:S:134:SER:CB	1:S:212:GLY:HA2	2.37	0.54
1:S:239:THR:C	1:S:241:LYS:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:100:ASN:CG	1:V:612:LEU:CD1	2.79	0.54
1:V:114:TYR:HE2	1:V:153:ILE:HB	1.70	0.54
1:V:265:ALA:HB3	1:V:450:LEU:HB3	1.88	0.54
1:V:418:GLN:CB	1:V:422:GLN:HB2	2.35	0.54
1:S:61:LEU:C	1:S:63:GLU:N	2.64	0.54
1:S:86:VAL:HG12	1:S:103:ASN:ND2	2.23	0.54
1:S:114:TYR:HE2	1:S:153:ILE:HB	1.70	0.54
1:V:107:ARG:HA	1:V:112:LEU:HD12	1.89	0.54
1:S:168:ARG:NH2	1:V:406:ARG:H	2.05	0.54
1:S:250:LYS:HG2	1:S:465:ASP:OD2	2.07	0.54
1:S:370:GLU:O	1:S:374:ASP:HA	2.07	0.54
1:S:413:VAL:HG12	1:S:413:VAL:O	2.08	0.54
1:S:424:ASP:C	1:S:426:ALA:N	2.63	0.54
1:S:490:GLN:NE2	1:S:494:ASN:HD21	2.06	0.54
2:T:55:LYS:O	2:T:56:SER:C	2.51	0.54
2:T:99:GLY:CA	1:V:398:PHE:HA	2.20	0.54
2:T:140:TYR:OH	1:V:393:ILE:O	2.25	0.54
1:V:134:SER:CB	1:V:212:GLY:HA2	2.37	0.54
1:V:305:LEU:HD12	1:V:307:LEU:HD11	1.90	0.54
1:V:610:THR:HG23	1:V:628:VAL:HG21	1.90	0.54
1:V:623:ASP:HA	1:V:626:LYS:HB3	1.88	0.54
1:S:218:GLY:HA3	1:S:221:GLU:OE1	2.07	0.54
1:V:96:ASN:HB2	1:V:99:SER:OG	2.08	0.54
1:V:703:GLU:O	1:V:706:ARG:N	2.38	0.54
1:S:147:HIS:C	1:S:149:MET:H	2.15	0.53
1:S:347:GLU:O	1:S:349:GLN:N	2.40	0.53
1:S:405:PRO:HD2	1:S:416:LYS:O	2.07	0.53
1:S:543:GLU:C	1:S:545:CYS:H	2.15	0.53
2:T:23:ASP:HB2	2:T:25:LYS:HD3	1.90	0.53
2:T:96:ASP:CG	1:V:397:ASP:HB2	2.33	0.53
1:V:132:ILE:HD12	1:V:152:HIS:CD2	2.43	0.53
1:V:144:LYS:HG3	1:V:148:GLU:HB2	1.90	0.53
1:V:405:PRO:HD2	1:V:416:LYS:O	2.07	0.53
1:V:490:GLN:NE2	1:V:494:ASN:HD21	2.06	0.53
1:S:30:SER:C	1:S:32:LYS:N	2.64	0.53
1:S:96:ASN:HB2	1:S:99:SER:OG	2.07	0.53
1:S:168:ARG:NH2	1:V:406:ARG:N	2.57	0.53
1:S:254:ILE:O	1:S:460:PHE:HA	2.08	0.53
1:S:553:THR:CG2	1:S:579:THR:HG21	2.38	0.53
1:S:766:LEU:O	1:S:777:ARG:HB2	2.08	0.53
1:V:553:THR:CG2	1:V:579:THR:HG21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:259:THR:HG22	2:T:104:MET:SD	2.37	0.53
1:S:298:SER:O	1:S:302:ARG:HB2	2.08	0.53
1:S:527:LEU:HB2	1:S:566:HIS:NE2	2.23	0.53
1:V:7:SER:O	1:V:11:LYS:HG3	2.09	0.53
1:V:18:ASN:O	1:V:19:PHE:HD1	1.88	0.53
1:V:400:ARG:O	1:V:404:THR:N	2.40	0.53
1:V:418:GLN:HA	1:V:422:GLN:NE2	2.23	0.53
1:V:449:ALA:C	1:V:451:ASP:H	2.17	0.53
1:V:766:LEU:O	1:V:777:ARG:HB2	2.08	0.53
1:S:259:THR:HG22	2:T:104:MET:CE	2.16	0.53
1:V:33:LYS:HB3	1:V:49:ILE:N	2.22	0.53
1:V:267:ILE:N	1:V:447:ASN:HD21	2.07	0.53
1:V:416:LYS:HE2	1:V:417:ALA:N	2.23	0.53
1:V:437:ARG:NH2	1:V:625:TRP:HE3	2.06	0.53
1:V:489:LEU:O	1:V:492:LEU:HB3	2.07	0.53
1:V:540:LEU:O	1:V:542:ASP:N	2.40	0.53
2:W:48:MET:HG3	2:W:53:ASN:HA	1.88	0.53
2:W:116:GLY:O	2:W:118:LYS:N	2.42	0.53
1:S:18:ASN:O	1:S:19:PHE:HD1	1.88	0.53
1:V:239:THR:C	1:V:241:LYS:H	2.16	0.53
1:V:298:SER:O	1:V:302:ARG:HB2	2.08	0.53
2:W:144:VAL:HG12	2:W:145:ARG:N	2.22	0.53
1:S:388:CYS:SG	1:S:393:ILE:HD11	2.49	0.53
1:S:437:ARG:NH2	1:S:625:TRP:HE3	2.07	0.53
1:S:610:THR:CG2	1:S:628:VAL:HG11	2.39	0.53
2:T:144:VAL:HG12	2:T:145:ARG:N	2.22	0.53
1:V:424:ASP:C	1:V:426:ALA:N	2.63	0.53
1:S:36:TRP:HB2	1:S:76:GLN:HB2	1.91	0.53
1:S:132:ILE:HD12	1:S:152:HIS:CD2	2.43	0.53
1:S:267:ILE:N	1:S:447:ASN:HD21	2.07	0.53
1:S:553:THR:HG23	1:S:579:THR:HG21	1.91	0.53
1:V:271:LEU:HD21	1:V:663:TYR:CD1	2.44	0.53
1:V:797:ILE:HG13	2:W:117:GLU:H	1.72	0.53
1:V:721:PHE:CZ	1:V:768:ARG:HG2	2.44	0.53
1:V:814:LYS:HD2	1:V:818:GLN:OE1	2.09	0.53
1:S:721:PHE:CZ	1:S:768:ARG:HG2	2.44	0.53
1:V:86:VAL:HG12	1:V:103:ASN:ND2	2.23	0.53
1:V:527:LEU:HB2	1:V:566:HIS:NE2	2.23	0.53
1:S:140:MET:HE2	1:S:149:MET:HE1	1.91	0.53
1:S:416:LYS:HE2	1:S:417:ALA:N	2.23	0.53
1:S:847:ILE:C	1:S:849:PRO:HD2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:112:LEU:CD1	2:T:119:MET:HE3	2.39	0.53
1:V:145:LYS:HB3	1:V:148:GLU:HG3	1.90	0.53
1:V:248:PHE:CD1	1:V:248:PHE:O	2.62	0.53
1:S:271:LEU:HD21	1:S:663:TYR:CD1	2.44	0.52
1:S:418:GLN:CB	1:S:422:GLN:HB2	2.35	0.52
1:S:542:ASP:O	1:S:545:CYS:HB3	2.09	0.52
1:V:140:MET:HE2	1:V:149:MET:HE1	1.91	0.52
1:V:193:TYR:CE1	1:V:197:VAL:HG21	2.44	0.52
2:W:30:GLN:O	2:W:31:CYS:C	2.52	0.52
2:W:76:ILE:O	2:W:79:ASN:ND2	2.42	0.52
1:S:7:SER:O	1:S:11:LYS:HG3	2.09	0.52
1:S:37:VAL:CG1	1:S:38:PRO:HD2	2.35	0.52
1:S:144:LYS:HG3	1:S:148:GLU:HB2	1.91	0.52
1:S:258:VAL:HB	2:T:97:LYS:HD2	1.90	0.52
1:S:349:GLN:O	1:S:350:THR:C	2.52	0.52
1:S:369:LYS:HG3	1:S:370:GLU:N	2.23	0.52
1:S:418:GLN:HA	1:S:422:GLN:NE2	2.23	0.52
1:S:607:ASP:HA	1:S:610:THR:CB	2.32	0.52
1:S:610:THR:CG2	1:S:611:SER:N	2.70	0.52
2:T:99:GLY:CA	1:V:398:PHE:H	2.17	0.52
2:W:140:TYR:HD1	2:W:141:GLU:H	1.51	0.52
1:S:193:TYR:CE1	1:S:197:VAL:HG21	2.44	0.52
1:S:278:ILE:O	1:S:279:ARG:HG3	2.09	0.52
1:S:541:LEU:CD2	1:S:601:ASN:HD22	2.10	0.52
1:S:747:MET:CG	1:S:751:GLN:HE22	2.22	0.52
1:S:812:PHE:C	1:S:814:LYS:N	2.68	0.52
2:T:76:ILE:O	2:T:79:ASN:ND2	2.42	0.52
1:V:351:SER:O	1:V:354:ARG:HG2	2.09	0.52
1:V:413:VAL:O	1:V:413:VAL:HG12	2.08	0.52
1:V:542:ASP:O	1:V:545:CYS:HB3	2.09	0.52
2:W:23:ASP:HB2	2:W:25:LYS:HD3	1.90	0.52
1:S:248:PHE:CD1	1:S:248:PHE:O	2.63	0.52
1:S:382:THR:C	1:S:385:GLN:HB3	2.35	0.52
1:S:449:ALA:C	1:S:451:ASP:H	2.17	0.52
1:V:359:VAL:HG12	1:V:359:VAL:O	2.10	0.52
1:V:382:THR:C	1:V:385:GLN:HB3	2.35	0.52
1:V:525:ILE:O	1:V:529:GLU:N	2.40	0.52
1:V:610:THR:CG2	1:V:628:VAL:HG11	2.39	0.52
1:V:711:LEU:HD22	1:V:711:LEU:H	1.73	0.52
2:W:55:LYS:O	2:W:56:SER:C	2.51	0.52
1:S:145:LYS:HB3	1:S:148:GLU:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:351:SER:O	1:S:354:ARG:HG2	2.09	0.52
1:V:290:PHE:CD1	1:V:360:LEU:HD11	2.44	0.52
1:V:369:LYS:HG3	1:V:370:GLU:N	2.24	0.52
1:S:176:THR:O	1:S:183:LYS:CD	2.57	0.52
1:S:290:PHE:CD1	1:S:360:LEU:HD11	2.44	0.52
1:S:305:LEU:HD12	1:S:307:LEU:HD11	1.90	0.52
1:S:586:TYR:CD1	1:S:587:ALA:N	2.78	0.52
2:T:30:GLN:O	2:T:31:CYS:C	2.52	0.52
1:V:269:THR:HG23	1:V:440:ARG:NH1	2.24	0.52
1:V:572:SER:CB	1:V:580:GLU:HG3	2.40	0.52
1:V:586:TYR:CD1	1:V:587:ALA:N	2.78	0.52
1:S:437:ARG:NH2	1:S:625:TRP:CE3	2.78	0.52
1:S:480:LEU:HD11	1:S:528:ILE:CD1	2.40	0.52
1:S:529:GLU:O	1:S:664:LYS:NZ	2.40	0.52
2:T:8:THR:O	2:T:12:LYS:HG3	2.10	0.52
1:V:100:VAL:HG21	1:V:711:LEU:CD1	2.40	0.52
1:V:145:LYS:HB3	1:V:148:GLU:CG	2.40	0.52
1:V:480:LEU:HD11	1:V:528:ILE:CD1	2.40	0.52
1:V:847:ILE:C	1:V:849:PRO:HD2	2.34	0.52
2:W:8:THR:O	2:W:12:LYS:HG3	2.10	0.52
1:S:100:VAL:HG21	1:S:711:LEU:CD1	2.40	0.52
1:S:145:LYS:HB3	1:S:148:GLU:CG	2.40	0.52
1:S:164:MET:SD	1:S:256:PHE:CD2	3.03	0.52
1:S:416:LYS:NZ	1:S:417:ALA:O	2.40	0.52
1:V:388:CYS:SG	1:V:393:ILE:HD11	2.49	0.52
2:W:128:VAL:HB	2:W:138:ILE:HD11	1.92	0.52
1:S:153:ILE:HG23	1:S:154:TYR:N	2.25	0.52
1:S:199:SER:HB2	1:S:221:GLU:CG	2.40	0.52
1:S:604:PRO:O	1:S:605:LEU:HB2	2.09	0.52
1:V:164:MET:SD	1:V:256:PHE:CD2	3.03	0.52
1:V:562:GLU:OE1	1:V:562:GLU:HA	2.09	0.52
1:V:604:PRO:O	1:V:605:LEU:HB2	2.09	0.52
2:W:15:PHE:O	2:W:18:PHE:HB2	2.10	0.52
2:W:112:LEU:CD1	2:W:119:MET:HE3	2.39	0.52
1:S:269:THR:HG23	1:S:440:ARG:NH1	2.24	0.52
1:S:359:VAL:O	1:S:359:VAL:HG12	2.10	0.52
1:S:610:THR:HG23	1:S:628:VAL:HG21	1.90	0.52
2:T:94:VAL:O	2:T:94:VAL:HG12	2.10	0.52
2:T:120:THR:HG23	2:T:123:GLU:CD	2.35	0.52
1:V:36:TRP:HB2	1:V:76:GLN:HB2	1.91	0.52
1:V:176:THR:O	1:V:183:LYS:CD	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:278:ILE:O	1:V:279:ARG:HG3	2.09	0.52
1:V:307:LEU:HA	1:V:313:TYR:OH	2.10	0.52
2:W:64:LEU:HD21	2:W:72:MET:HE1	1.92	0.52
1:S:495:HIS:ND1	1:S:499:ILE:HD12	2.25	0.51
2:T:93:ARG:CG	1:V:396:THR:H	2.24	0.51
2:T:140:TYR:OH	1:V:394:ASN:CB	2.53	0.51
1:V:437:ARG:NH2	1:V:625:TRP:CE3	2.78	0.51
1:V:553:THR:HG23	1:V:579:THR:HG21	1.91	0.51
1:V:747:MET:CG	1:V:751:GLN:HE22	2.23	0.51
1:V:815:ARG:NE	1:V:818:GLN:NE2	2.58	0.51
2:W:120:THR:HG23	2:W:123:GLU:CD	2.35	0.51
1:S:33:LYS:HB2	1:S:48:SER:OG	2.11	0.51
1:S:269:THR:CG2	1:S:443:LEU:CD1	2.88	0.51
1:S:337:GLU:O	1:S:340:THR:OG1	2.28	0.51
1:S:562:GLU:OE1	1:S:562:GLU:HA	2.09	0.51
1:V:700:LEU:HD23	1:V:700:LEU:C	2.35	0.51
2:W:94:VAL:O	2:W:94:VAL:HG12	2.10	0.51
1:S:152:HIS:CE1	1:S:154:TYR:CD2	2.99	0.51
1:S:572:SER:CB	1:S:580:GLU:HG3	2.40	0.51
1:S:625:TRP:C	1:S:627:ASP:N	2.68	0.51
1:S:700:LEU:HD23	1:S:700:LEU:C	2.35	0.51
1:S:815:ARG:NE	1:S:818:GLN:NE2	2.58	0.51
2:T:66:PHE:CE1	2:T:70:LEU:HB2	2.46	0.51
1:V:30:SER:C	1:V:32:LYS:N	2.64	0.51
1:V:235:GLY:O	1:V:247:ARG:HB2	2.10	0.51
1:V:361:GLN:HB3	1:V:387:VAL:HG22	1.92	0.51
1:V:409:VAL:HG13	1:V:634:LEU:CD1	2.40	0.51
1:V:435:PHE:O	1:V:438:LEU:N	2.31	0.51
1:S:145:LYS:CB	1:S:148:GLU:HG3	2.41	0.51
1:S:168:ARG:CZ	1:V:404:THR:O	2.56	0.51
1:S:184:THR:O	1:S:185:GLU:C	2.53	0.51
1:S:193:TYR:CZ	1:S:197:VAL:HG21	2.46	0.51
1:S:514:PHE:CD1	1:S:515:ILE:N	2.78	0.51
2:T:3:PHE:CA	2:T:7:GLN:HE21	2.23	0.51
2:T:128:VAL:HB	2:T:138:ILE:HD11	1.92	0.51
1:V:193:TYR:CZ	1:V:197:VAL:HG21	2.46	0.51
1:V:250:LYS:HG2	1:V:465:ASP:HB3	1.93	0.51
1:V:351:SER:C	1:V:353:LEU:H	2.19	0.51
1:V:495:HIS:ND1	1:V:499:ILE:HD12	2.25	0.51
1:V:658:THR:HG23	1:V:661:GLN:HB3	1.91	0.51
2:W:3:PHE:CA	2:W:7:GLN:HE21	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:258:VAL:HB	2:T:97:LYS:CD	2.05	0.51
1:S:495:HIS:CD2	1:S:500:LEU:HG	2.46	0.51
1:S:544:GLU:OE1	1:S:550:ALA:HB1	2.11	0.51
1:S:556:VAL:O	1:S:559:LEU:HB3	2.11	0.51
1:S:721:PHE:HB3	1:S:776:PHE:O	2.10	0.51
2:T:15:PHE:O	2:T:18:PHE:HB2	2.10	0.51
1:V:351:SER:C	1:V:353:LEU:N	2.68	0.51
1:V:556:VAL:O	1:V:559:LEU:HB3	2.11	0.51
1:V:803:CYS:HB2	2:W:119:MET:HE1	1.91	0.51
1:S:235:GLY:O	1:S:247:ARG:HB2	2.10	0.51
1:S:658:THR:HG23	1:S:661:GLN:HB3	1.91	0.51
2:T:35:MET:HE3	2:T:73:MET:HA	1.93	0.51
2:T:116:GLY:O	2:T:118:LYS:N	2.41	0.51
1:V:184:THR:O	1:V:185:GLU:C	2.53	0.51
1:V:199:SER:HB2	1:V:221:GLU:CG	2.40	0.51
1:V:359:VAL:O	1:V:359:VAL:CG1	2.59	0.51
1:V:514:PHE:CD1	1:V:515:ILE:N	2.78	0.51
1:V:812:PHE:C	1:V:814:LYS:N	2.68	0.51
2:W:85:PHE:O	2:W:86:GLU:C	2.54	0.51
1:S:120:PHE:CD1	1:S:120:PHE:N	2.75	0.51
1:S:409:VAL:HG13	1:S:634:LEU:CD1	2.40	0.51
1:S:803:CYS:HB2	2:T:119:MET:HE1	1.91	0.51
1:S:819:LEU:O	1:S:821:SER:N	2.43	0.51
2:W:66:PHE:CE1	2:W:70:LEU:HB2	2.45	0.51
1:S:551:THR:H	1:S:554:SER:CB	2.22	0.51
1:S:814:LYS:HD2	1:S:818:GLN:OE1	2.09	0.51
2:T:74:GLN:O	2:T:75:THR:C	2.53	0.51
1:V:145:LYS:CB	1:V:148:GLU:HG3	2.41	0.51
1:S:307:LEU:HA	1:S:313:TYR:OH	2.10	0.51
1:V:541:LEU:CD2	1:V:601:ASN:HD22	2.11	0.51
1:V:657:ARG:HB2	1:V:657:ARG:HH11	1.76	0.51
1:V:721:PHE:HB3	1:V:776:PHE:O	2.10	0.51
1:S:313:TYR:CD2	1:S:360:LEU:HB3	2.45	0.51
1:S:344:PHE:HE1	1:S:445:ARG:HB3	1.72	0.51
1:S:351:SER:C	1:S:353:LEU:H	2.19	0.51
1:V:495:HIS:CD2	1:V:500:LEU:HG	2.46	0.51
1:V:663:TYR:C	1:V:665:GLU:N	2.69	0.51
1:V:719:GLN:HA	1:V:719:GLN:NE2	2.26	0.51
1:S:168:ARG:CD	1:V:400:ARG:HD3	2.37	0.50
1:S:293:LEU:HD13	1:S:353:LEU:HD22	1.92	0.50
1:S:361:GLN:HB3	1:S:387:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:419:THR:O	1:S:421:GLU:N	2.44	0.50
1:S:574:GLN:C	1:S:576:LYS:HE3	2.37	0.50
1:V:250:LYS:HE2	1:V:465:ASP:OD2	2.11	0.50
2:W:35:MET:HE3	2:W:73:MET:HA	1.93	0.50
1:S:253:ARG:O	1:S:265:ALA:HA	2.11	0.50
1:S:359:VAL:O	1:S:359:VAL:CG1	2.59	0.50
1:S:657:ARG:HH11	1:S:657:ARG:HB2	1.76	0.50
2:T:83:GLY:HA3	2:T:88:TYR:CE2	2.47	0.50
1:V:584:LEU:N	1:V:584:LEU:HD23	2.25	0.50
1:S:286:THR:HB	1:S:290:PHE:HD2	1.77	0.50
1:S:326:GLN:HG3	1:S:331:MET:HE3	1.93	0.50
1:S:521:LEU:HD23	1:S:521:LEU:N	2.26	0.50
1:S:551:THR:O	1:S:552:ASP:C	2.55	0.50
1:S:719:GLN:HA	1:S:719:GLN:NE2	2.26	0.50
1:V:33:LYS:HB2	1:V:48:SER:OG	2.11	0.50
1:V:521:LEU:HD23	1:V:521:LEU:N	2.26	0.50
1:V:610:THR:CG2	1:V:628:VAL:CG1	2.90	0.50
1:S:36:TRP:HE1	1:S:78:MET:HA	1.77	0.50
1:S:458:ALA:CA	1:V:413:VAL:HG11	2.41	0.50
1:S:575:LEU:C	1:S:577:ASP:H	2.19	0.50
1:S:733:ARG:HG2	1:S:734:TYR:CE1	2.47	0.50
1:V:89:MET:C	1:V:91:GLU:N	2.70	0.50
1:V:327:GLN:HG2	1:V:330:GLU:HG2	1.93	0.50
1:V:419:THR:O	1:V:421:GLU:N	2.44	0.50
1:V:551:THR:H	1:V:554:SER:CB	2.22	0.50
1:S:250:LYS:HE2	1:S:465:ASP:OD2	2.11	0.50
1:S:490:GLN:HE21	1:S:494:ASN:HD21	1.59	0.50
1:S:581:PHE:HZ	1:S:597:TRP:CH2	2.30	0.50
2:T:85:PHE:O	2:T:86:GLU:C	2.54	0.50
1:V:145:LYS:HG3	1:V:146:ARG:H	1.76	0.50
1:V:152:HIS:CE1	1:V:154:TYR:CD2	2.99	0.50
1:V:349:GLN:O	1:V:350:THR:C	2.53	0.50
1:V:815:ARG:NE	1:V:818:GLN:HE21	2.09	0.50
1:S:625:TRP:C	1:S:627:ASP:H	2.19	0.50
2:T:64:LEU:HD21	2:T:72:MET:HE1	1.92	0.50
2:T:140:TYR:CZ	1:V:394:ASN:CA	2.71	0.50
1:V:120:PHE:CD1	1:V:120:PHE:N	2.75	0.50
1:V:320:HIS:ND1	1:V:320:HIS:O	2.39	0.50
1:V:326:GLN:HG3	1:V:331:MET:HE3	1.93	0.50
1:V:623:ASP:OD1	1:V:623:ASP:N	2.45	0.50
1:V:733:ARG:HG2	1:V:734:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:381:ASN:O	1:S:382:THR:C	2.55	0.50
1:S:815:ARG:NE	1:S:818:GLN:HE21	2.09	0.50
1:V:232:GLU:O	1:V:236:ASN:HB2	2.12	0.50
1:V:490:GLN:HE21	1:V:494:ASN:HD21	1.59	0.50
1:V:630:ARG:HH22	1:V:657:ARG:HB2	1.76	0.50
1:V:763:ASP:HB3	1:V:766:LEU:CD1	2.42	0.50
2:W:48:MET:HE1	2:W:59:MET:HE1	1.94	0.50
2:W:68:GLN:O	2:W:71:PRO:HG2	2.12	0.50
1:S:435:PHE:O	1:S:438:LEU:N	2.31	0.50
1:S:610:THR:CG2	1:S:628:VAL:CG1	2.90	0.50
1:V:61:LEU:C	1:V:63:GLU:N	2.64	0.50
1:V:153:ILE:HG23	1:V:154:TYR:N	2.25	0.50
1:S:128:LYS:HG2	1:S:129:GLN:N	2.27	0.50
1:S:449:ALA:C	1:S:451:ASP:N	2.69	0.50
1:S:458:ALA:HB1	1:V:413:VAL:HG13	1.93	0.50
1:S:584:LEU:N	1:S:584:LEU:HD23	2.25	0.50
1:V:36:TRP:HE1	1:V:78:MET:HA	1.77	0.50
1:V:134:SER:O	1:V:135:GLU:C	2.55	0.50
1:V:269:THR:CG2	1:V:443:LEU:CD1	2.88	0.50
1:V:478:GLU:HB2	1:V:479:GLN:OE1	2.12	0.50
1:V:545:CYS:HA	1:V:598:LEU:HD22	1.94	0.50
2:W:74:GLN:O	2:W:75:THR:C	2.53	0.50
2:W:83:GLY:HA3	2:W:88:TYR:CE2	2.47	0.50
2:W:98:GLU:O	2:W:100:ASN:N	2.45	0.50
1:S:199:SER:CB	1:S:221:GLU:HG2	2.42	0.49
1:S:250:LYS:HG2	1:S:465:ASP:HB3	1.92	0.49
1:S:327:GLN:HG2	1:S:330:GLU:HG2	1.93	0.49
1:S:478:GLU:HB2	1:S:479:GLN:OE1	2.12	0.49
1:S:630:ARG:HH22	1:S:657:ARG:HB2	1.76	0.49
1:S:795:VAL:O	1:S:796:ILE:C	2.55	0.49
2:T:20:ARG:HG3	3:U:123:THR:CA	2.42	0.49
1:V:145:LYS:HG3	1:V:146:ARG:NE	2.26	0.49
1:V:253:ARG:O	1:V:265:ALA:HA	2.11	0.49
1:V:286:THR:HB	1:V:290:PHE:HD2	1.77	0.49
1:V:533:ASN:O	1:V:535:PRO:N	2.45	0.49
1:V:551:THR:O	1:V:552:ASP:C	2.55	0.49
1:S:89:MET:C	1:S:91:GLU:N	2.70	0.49
1:S:224:LEU:HD12	1:S:224:LEU:O	2.12	0.49
1:S:287:PHE:O	1:S:288:HIS:C	2.54	0.49
1:S:299:GLU:O	1:S:302:ARG:CB	2.60	0.49
1:S:545:CYS:HA	1:S:598:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:630:ARG:HH12	1:S:657:ARG:HB3	1.77	0.49
2:T:64:LEU:HD21	2:T:72:MET:CE	2.43	0.49
1:V:199:SER:HB2	1:V:221:GLU:CD	2.37	0.49
1:V:224:LEU:HD12	1:V:224:LEU:O	2.12	0.49
1:V:293:LEU:HD13	1:V:353:LEU:HD22	1.92	0.49
1:V:416:LYS:NZ	1:V:417:ALA:O	2.40	0.49
1:V:625:TRP:C	1:V:627:ASP:H	2.19	0.49
1:V:819:LEU:O	1:V:821:SER:N	2.43	0.49
1:V:826:GLN:HE22	3:Z:125:GLY:CA	2.26	0.49
2:W:20:ARG:HG3	3:Z:123:THR:CA	2.42	0.49
1:S:280:GLN:NE2	1:S:315:PHE:O	2.43	0.49
1:S:293:LEU:O	1:S:297:ALA:HB2	2.12	0.49
2:T:135:ASN:HB2	2:T:137:CYS:SG	2.52	0.49
1:V:299:GLU:O	1:V:302:ARG:CB	2.61	0.49
1:V:351:SER:O	1:V:353:LEU:N	2.46	0.49
1:V:362:LEU:CD2	1:V:427:ILE:HG13	2.43	0.49
1:V:610:THR:CG2	1:V:631:ILE:HG13	2.28	0.49
1:V:767:TYR:O	1:V:768:ARG:HD3	2.12	0.49
2:W:35:MET:SD	2:W:76:ILE:HD12	2.51	0.49
1:S:168:ARG:HH22	1:V:406:ARG:N	2.10	0.49
1:S:345:THR:HG22	1:S:346:GLU:HG2	1.94	0.49
2:T:35:MET:SD	2:T:76:ILE:HD12	2.52	0.49
2:T:95:PHE:O	2:T:103:VAL:HG13	2.13	0.49
1:V:166:GLN:HE22	2:W:107:GLU:HG2	1.76	0.49
1:V:287:PHE:O	1:V:288:HIS:C	2.54	0.49
1:V:430:LEU:HB2	1:V:605:LEU:HD11	1.94	0.49
1:V:575:LEU:C	1:V:577:ASP:H	2.19	0.49
1:V:725:ILE:HD13	1:V:730:PHE:HB2	1.94	0.49
1:S:145:LYS:HG3	1:S:146:ARG:NE	2.26	0.49
1:S:296:GLY:HA3	1:S:332:PHE:CG	2.48	0.49
1:S:351:SER:O	1:S:353:LEU:N	2.46	0.49
1:S:533:ASN:O	1:S:535:PRO:N	2.45	0.49
1:S:545:CYS:O	1:S:602:MET:HE1	2.13	0.49
1:S:623:ASP:OD1	1:S:623:ASP:N	2.45	0.49
1:S:725:ILE:HD13	1:S:730:PHE:HB2	1.94	0.49
2:T:68:GLN:O	2:T:71:PRO:HG2	2.12	0.49
1:V:58:THR:HA	1:V:69:THR:OG1	2.13	0.49
1:V:581:PHE:HZ	1:V:597:TRP:CH2	2.30	0.49
2:W:143:LEU:O	2:W:147:VAL:HG22	2.13	0.49
1:S:622:ALA:O	1:S:626:LYS:N	2.40	0.49
1:S:797:ILE:HG12	2:T:117:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:848:MLY:HB2	1:S:849:PRO:HD3	1.94	0.49
1:V:407:ILE:CD1	1:V:409:VAL:N	2.76	0.49
1:S:134:SER:O	1:S:135:GLU:C	2.55	0.49
1:S:199:SER:HB2	1:S:221:GLU:CD	2.37	0.49
1:S:405:PRO:O	1:S:407:ILE:HG23	2.12	0.49
2:T:55:LYS:H	2:T:58:GLU:CG	2.26	0.49
2:T:93:ARG:C	1:V:396:THR:OG1	2.50	0.49
2:T:143:LEU:O	2:T:147:VAL:HG22	2.13	0.49
1:V:288:HIS:HB3	1:V:292:TYR:CE1	2.48	0.49
1:V:381:ASN:O	1:V:382:THR:C	2.55	0.49
1:V:405:PRO:O	1:V:407:ILE:HG23	2.12	0.49
1:V:544:GLU:OE1	1:V:550:ALA:HB1	2.11	0.49
1:V:553:THR:HG22	1:V:557:GLU:OE2	2.13	0.49
2:W:55:LYS:H	2:W:58:GLU:CG	2.26	0.49
2:W:95:PHE:O	2:W:103:VAL:HG13	2.13	0.49
2:W:104:MET:O	2:W:106:ALA:N	2.46	0.49
2:W:135:ASN:HB2	2:W:137:CYS:SG	2.52	0.49
1:S:232:GLU:O	1:S:236:ASN:HB2	2.12	0.49
1:S:313:TYR:HB2	1:S:316:LEU:HD12	1.93	0.49
1:S:504:GLU:OE2	1:S:508:GLU:HG2	2.12	0.49
1:V:174:LEU:HD12	1:V:681:PHE:CE1	2.47	0.49
1:V:543:GLU:C	1:V:545:CYS:N	2.69	0.49
1:V:574:GLN:C	1:V:576:LYS:HE3	2.37	0.49
2:W:36:ARG:O	2:W:39:GLY:N	2.44	0.49
1:S:80:PRO:HD2	1:S:83:PHE:CD2	2.48	0.49
1:S:145:LYS:HG3	1:S:146:ARG:H	1.76	0.49
1:S:288:HIS:HB3	1:S:292:TYR:CE1	2.48	0.49
1:S:553:THR:HG22	1:S:557:GLU:OE2	2.13	0.49
1:S:556:VAL:HG21	1:S:579:THR:HB	1.95	0.49
2:T:48:MET:HE1	2:T:59:MET:HE1	1.94	0.49
1:V:313:TYR:CD1	1:V:313:TYR:N	2.81	0.49
1:V:697:ASP:C	1:V:697:ASP:OD1	2.55	0.49
1:V:797:ILE:HG12	2:W:117:GLU:HG2	1.94	0.49
2:W:64:LEU:HD21	2:W:72:MET:CE	2.42	0.49
1:S:401:SER:O	1:S:606:ASN:ND2	2.46	0.49
1:S:819:LEU:O	1:S:820:GLU:HA	2.06	0.49
1:V:362:LEU:HD12	1:V:387:VAL:HG13	1.95	0.49
1:V:504:GLU:OE2	1:V:508:GLU:HG2	2.12	0.49
1:V:625:TRP:C	1:V:627:ASP:N	2.68	0.49
1:V:848:MLY:N	1:V:849:PRO:CD	2.75	0.49
2:W:76:ILE:O	2:W:78:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:174:LEU:HD12	1:S:681:PHE:CE1	2.47	0.48
1:S:267:ILE:H	1:S:447:ASN:HD21	1.60	0.48
1:S:313:TYR:N	1:S:313:TYR:CD1	2.81	0.48
1:S:370:GLU:O	1:S:374:ASP:CA	2.61	0.48
1:S:763:ASP:HB3	1:S:766:LEU:CD1	2.42	0.48
1:S:826:GLN:HE22	3:U:125:GLY:CA	2.26	0.48
1:S:848:MLY:N	1:S:849:PRO:CD	2.75	0.48
2:T:41:ASN:N	2:T:42:PRO:HD3	2.28	0.48
1:V:293:LEU:O	1:V:297:ALA:HB2	2.12	0.48
1:V:545:CYS:O	1:V:602:MET:HE1	2.13	0.48
1:V:563:GLN:O	1:V:565:ASN:N	2.46	0.48
1:V:618:ASP:CG	1:V:621:VAL:HG23	2.38	0.48
1:V:848:MLY:HB2	1:V:849:PRO:HD3	1.94	0.48
1:S:575:LEU:C	1:S:577:ASP:N	2.71	0.48
1:S:767:TYR:O	1:S:768:ARG:HD3	2.13	0.48
2:T:108:ILE:HG22	2:T:109:ARG:N	2.27	0.48
1:V:128:LYS:HG2	1:V:129:GLN:N	2.27	0.48
1:V:280:GLN:NE2	1:V:315:PHE:O	2.43	0.48
1:V:313:TYR:CD2	1:V:360:LEU:HB3	2.45	0.48
1:V:449:ALA:C	1:V:451:ASP:N	2.69	0.48
1:V:819:LEU:O	1:V:820:GLU:HA	2.06	0.48
1:V:247:ARG:HH22	1:V:470:GLU:CD	2.22	0.48
1:V:513:ASN:O	1:V:515:ILE:HD12	2.14	0.48
2:W:41:ASN:N	2:W:42:PRO:HD3	2.29	0.48
1:S:430:LEU:HB2	1:S:605:LEU:HD11	1.94	0.48
1:S:513:ASN:O	1:S:513:ASN:ND2	2.41	0.48
1:S:513:ASN:O	1:S:515:ILE:HD12	2.13	0.48
1:S:703:GLU:O	1:S:706:ARG:N	2.38	0.48
2:T:124:VAL:O	2:T:128:VAL:HG22	2.13	0.48
1:V:80:PRO:HD2	1:V:83:PHE:CD2	2.48	0.48
1:V:152:HIS:CE1	1:V:154:TYR:CG	3.01	0.48
1:V:313:TYR:HB2	1:V:316:LEU:HD12	1.93	0.48
1:V:345:THR:HG22	1:V:346:GLU:HG2	1.94	0.48
1:V:401:SER:O	1:V:606:ASN:ND2	2.46	0.48
1:V:556:VAL:HG21	1:V:579:THR:HB	1.95	0.48
1:V:630:ARG:HH12	1:V:657:ARG:HB3	1.77	0.48
1:S:39:SER:C	1:S:41:LYS:H	2.22	0.48
1:S:183:LYS:HE2	1:S:183:LYS:HB2	1.61	0.48
1:S:742:ILE:CD1	1:S:756:MET:HE3	2.44	0.48
2:T:104:MET:O	2:T:106:ALA:N	2.46	0.48
1:S:351:SER:C	1:S:353:LEU:N	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:397:ASP:O	1:S:398:PHE:C	2.57	0.48
1:S:556:VAL:O	1:S:560:ILE:HG12	2.13	0.48
1:S:563:GLN:O	1:S:565:ASN:N	2.46	0.48
1:V:296:GLY:HA3	1:V:332:PHE:CG	2.48	0.48
1:V:370:GLU:O	1:V:374:ASP:CA	2.61	0.48
1:V:389:HIS:C	1:V:389:HIS:HD1	2.22	0.48
1:V:479:GLN:OE1	1:V:479:GLN:N	2.47	0.48
1:S:405:PRO:HG2	1:S:416:LYS:HG3	1.95	0.48
1:V:100:VAL:HG21	1:V:711:LEU:HD11	1.96	0.48
1:V:236:ASN:ND2	1:V:246:SER:CA	2.73	0.48
1:V:382:THR:OG1	1:V:383:ALA:N	2.47	0.48
1:S:697:ASP:C	1:S:697:ASP:OD1	2.55	0.48
1:S:819:LEU:HA	1:S:822:ILE:HB	1.96	0.48
2:T:104:MET:C	2:T:106:ALA:N	2.72	0.48
1:V:404:THR:O	1:V:404:THR:OG1	2.31	0.48
1:S:31:ALA:O	1:S:33:LYS:N	2.46	0.48
1:S:64:ASN:C	1:S:66:LYS:N	2.72	0.48
1:S:271:LEU:HD21	1:S:663:TYR:CZ	2.49	0.48
1:S:389:HIS:HD1	1:S:389:HIS:C	2.22	0.48
1:S:479:GLN:OE1	1:S:479:GLN:N	2.47	0.48
1:V:39:SER:C	1:V:41:LYS:H	2.22	0.48
1:V:64:ASN:C	1:V:66:LYS:N	2.72	0.48
1:V:742:ILE:CD1	1:V:756:MET:HE3	2.44	0.48
1:S:407:ILE:CD1	1:S:409:VAL:N	2.76	0.48
2:T:36:ARG:O	2:T:39:GLY:N	2.44	0.48
1:V:397:ASP:O	1:V:398:PHE:C	2.57	0.48
1:V:575:LEU:C	1:V:577:ASP:N	2.71	0.48
1:V:814:LYS:O	1:V:818:GLN:OE1	2.32	0.48
2:W:105:GLY:O	2:W:109:ARG:HB2	2.13	0.48
2:W:108:ILE:HG22	2:W:109:ARG:N	2.27	0.48
1:S:152:HIS:CE1	1:S:154:TYR:CG	3.01	0.47
1:S:355:VAL:HG21	1:S:620:PHE:CE2	2.49	0.47
1:S:424:ASP:C	1:S:426:ALA:H	2.22	0.47
1:S:469:PHE:N	1:S:486:ASN:OD1	2.45	0.47
2:T:76:ILE:O	2:T:78:LYS:N	2.46	0.47
1:V:355:VAL:HG21	1:V:620:PHE:CE2	2.49	0.47
2:W:105:GLY:O	2:W:109:ARG:NH1	2.47	0.47
1:S:311:ASN:HD22	1:S:311:ASN:N	2.12	0.47
1:S:569:PHE:CD2	1:S:570:GLN:N	2.82	0.47
1:S:814:LYS:C	1:S:816:GLN:N	2.72	0.47
2:T:93:ARG:HG3	1:V:396:THR:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:105:GLY:O	2:T:109:ARG:HB2	2.13	0.47
1:V:31:ALA:O	1:V:33:LYS:N	2.46	0.47
1:V:728:GLN:NE2	1:V:728:GLN:O	2.47	0.47
2:W:124:VAL:O	2:W:128:VAL:HG22	2.13	0.47
1:S:618:ASP:CG	1:S:621:VAL:HG23	2.38	0.47
2:T:139:ASN:HD21	2:T:141:GLU:HG3	1.78	0.47
1:V:106:GLU:O	1:V:107:ARG:C	2.57	0.47
1:V:551:THR:H	1:V:554:SER:HG	1.57	0.47
2:W:76:ILE:O	2:W:77:ALA:C	2.57	0.47
1:S:247:ARG:HH22	1:S:470:GLU:CD	2.22	0.47
1:S:621:VAL:HG12	1:S:625:TRP:CD1	2.49	0.47
1:V:77:LYS:H	1:V:77:LYS:HD2	1.79	0.47
1:V:261:TYR:CD1	1:V:261:TYR:N	2.82	0.47
1:V:330:GLU:O	1:V:331:MET:C	2.58	0.47
1:V:428:GLU:C	1:V:430:LEU:N	2.72	0.47
1:V:569:PHE:CD2	1:V:570:GLN:N	2.82	0.47
1:V:769:ILE:CD1	1:V:774:ILE:HG12	2.45	0.47
1:S:58:THR:HA	1:S:69:THR:OG1	2.13	0.47
1:S:333:GLN:O	1:S:337:GLU:HG3	2.15	0.47
1:S:382:THR:OG1	1:S:383:ALA:N	2.47	0.47
1:V:79:ASN:OD1	1:V:94:CYS:HB2	2.15	0.47
1:V:226:GLN:HG2	1:V:341:ILE:HB	1.97	0.47
1:V:267:ILE:H	1:V:447:ASN:HD21	1.60	0.47
1:V:311:ASN:HD22	1:V:311:ASN:N	2.12	0.47
1:V:446:VAL:HG12	1:V:447:ASN:N	2.29	0.47
1:V:520:ASP:OD1	1:V:523:PRO:HD2	2.14	0.47
1:V:556:VAL:O	1:V:560:ILE:HG12	2.13	0.47
2:W:54:PRO:HB2	2:W:59:MET:HG2	1.95	0.47
2:W:139:ASN:HD21	2:W:141:GLU:HG3	1.79	0.47
1:S:36:TRP:NE1	1:S:78:MET:HA	2.30	0.47
1:S:294:ILE:HB	1:S:310:PHE:CZ	2.50	0.47
1:S:756:MET:O	1:S:760:LEU:HG	2.15	0.47
2:T:94:VAL:N	1:V:396:THR:HG23	2.29	0.47
2:T:105:GLY:O	2:T:109:ARG:NH1	2.47	0.47
1:V:337:GLU:O	1:V:340:THR:OG1	2.28	0.47
1:V:405:PRO:HG2	1:V:416:LYS:HG3	1.95	0.47
1:V:424:ASP:O	1:V:426:ALA:N	2.48	0.47
1:V:768:ARG:HD3	1:V:768:ARG:HA	1.63	0.47
1:S:13:LEU:HG	1:S:132:ILE:HG21	1.96	0.47
1:S:161:TYR:O	1:S:161:TYR:CG	2.67	0.47
1:S:199:SER:HB2	1:S:221:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:237:ALA:HA	1:S:288:HIS:CD2	2.50	0.47
1:S:321:VAL:HG13	1:S:322:PRO:HD2	1.96	0.47
1:S:329:ASP:OD1	1:S:329:ASP:N	2.43	0.47
1:S:362:LEU:HD12	1:S:387:VAL:HG13	1.95	0.47
1:S:428:GLU:C	1:S:430:LEU:N	2.72	0.47
1:S:489:LEU:C	1:S:489:LEU:HD12	2.40	0.47
1:S:520:ASP:OD1	1:S:523:PRO:HD2	2.14	0.47
1:S:551:THR:O	1:S:554:SER:N	2.48	0.47
1:S:621:VAL:HG12	1:S:625:TRP:HD1	1.80	0.47
1:S:721:PHE:CE2	1:S:768:ARG:HG2	2.50	0.47
1:S:769:ILE:CD1	1:S:774:ILE:HG12	2.45	0.47
2:T:131:HIS:NE2	2:T:146:MET:HE3	2.29	0.47
1:V:7:SER:N	1:V:10:GLU:OE1	2.43	0.47
1:V:36:TRP:NE1	1:V:78:MET:HA	2.30	0.47
1:V:79:ASN:OD1	1:V:92:LEU:HB3	2.15	0.47
1:V:89:MET:HA	1:V:92:LEU:HD12	1.95	0.47
1:V:161:TYR:O	1:V:161:TYR:CG	2.67	0.47
1:V:199:SER:HB2	1:V:221:GLU:OE2	2.15	0.47
1:V:294:ILE:HB	1:V:310:PHE:CZ	2.50	0.47
1:V:407:ILE:HD12	1:V:409:VAL:H	1.80	0.47
1:V:424:ASP:C	1:V:426:ALA:H	2.22	0.47
1:V:489:LEU:C	1:V:489:LEU:HD12	2.40	0.47
1:V:573:LYS:N	1:V:573:LYS:HD2	2.30	0.47
1:V:621:VAL:HG12	1:V:625:TRP:HD1	1.80	0.47
1:V:806:TYR:CB	2:W:147:VAL:HG12	2.45	0.47
2:W:131:HIS:NE2	2:W:146:MET:HE3	2.29	0.47
1:S:100:VAL:HG21	1:S:711:LEU:HD11	1.96	0.47
1:S:107:ARG:HH11	1:S:115:THR:HG23	1.79	0.47
1:S:280:GLN:OE1	1:S:316:LEU:HA	2.15	0.47
1:S:573:LYS:N	1:S:573:LYS:HD2	2.30	0.47
1:S:718:ARG:HG3	1:S:719:GLN:N	2.30	0.47
2:T:69:PHE:HA	2:T:72:MET:HE3	1.97	0.47
2:T:76:ILE:O	2:T:77:ALA:C	2.57	0.47
1:V:235:GLY:HA3	1:V:248:PHE:HE2	1.79	0.47
1:V:271:LEU:HD21	1:V:663:TYR:CZ	2.49	0.47
1:V:613:LEU:C	1:V:615:GLN:N	2.72	0.47
1:S:420:LYS:HD2	1:S:421:GLU:OE2	2.15	0.47
1:S:814:LYS:O	1:S:818:GLN:OE1	2.32	0.47
2:T:54:PRO:HB2	2:T:59:MET:HG2	1.95	0.47
2:T:140:TYR:CZ	1:V:394:ASN:CB	2.98	0.47
1:V:280:GLN:OE1	1:V:316:LEU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:551:THR:O	1:V:554:SER:N	2.48	0.47
1:V:726:VAL:HA	1:V:773:LYS:HA	1.97	0.47
2:W:69:PHE:CZ	2:W:73:MET:HG2	2.49	0.47
1:S:711:LEU:N	1:S:711:LEU:CD2	2.77	0.47
1:S:763:ASP:OD1	1:S:765:ASN:N	2.48	0.47
1:V:13:LEU:HG	1:V:132:ILE:HG21	1.96	0.47
1:V:211:GLN:HG3	1:V:214:SER:HB2	1.96	0.47
1:V:272:LEU:C	1:V:272:LEU:CD1	2.82	0.47
1:V:508:GLU:HG3	1:V:775:PHE:HE1	1.80	0.47
1:V:621:VAL:HG12	1:V:625:TRP:CD1	2.49	0.47
2:W:70:LEU:HG	2:W:74:GLN:HE21	1.80	0.47
1:S:278:ILE:C	1:S:279:ARG:HG3	2.40	0.46
1:S:442:ILE:O	1:S:445:ARG:N	2.43	0.46
1:S:607:ASP:OD1	1:S:607:ASP:N	2.34	0.46
1:S:726:VAL:HA	1:S:773:LYS:HA	1.97	0.46
1:V:107:ARG:HH11	1:V:115:THR:HG23	1.79	0.46
1:V:145:LYS:CG	1:V:146:ARG:N	2.78	0.46
1:V:199:SER:CB	1:V:221:GLU:HG2	2.42	0.46
1:V:257:ASP:C	1:V:257:ASP:OD1	2.57	0.46
1:V:267:ILE:CD1	1:V:450:LEU:HD12	2.45	0.46
1:V:354:ARG:HG3	1:V:355:VAL:N	2.31	0.46
1:S:77:LYS:H	1:S:77:LYS:HD2	1.79	0.46
1:S:79:ASN:OD1	1:S:94:CYS:HB2	2.15	0.46
1:V:278:ILE:C	1:V:279:ARG:HG3	2.40	0.46
2:W:132:GLU:H	2:W:132:GLU:HG2	1.46	0.46
1:S:89:MET:HA	1:S:92:LEU:HD12	1.96	0.46
1:S:177:GLY:O	1:S:183:LYS:NZ	2.49	0.46
1:S:211:GLN:HG3	1:S:214:SER:HB2	1.96	0.46
1:S:543:GLU:C	1:S:545:CYS:N	2.69	0.46
1:V:80:PRO:HD2	1:V:83:PHE:HD2	1.81	0.46
1:V:342:MET:O	1:V:342:MET:HE3	2.16	0.46
1:V:763:ASP:OD1	1:V:765:ASN:N	2.48	0.46
2:W:43:THR:HG23	2:W:46:GLU:OE1	2.16	0.46
2:W:69:PHE:HA	2:W:72:MET:HE3	1.97	0.46
1:S:226:GLN:HG2	1:S:341:ILE:HB	1.96	0.46
1:S:261:TYR:CD1	1:S:261:TYR:N	2.82	0.46
1:S:728:GLN:NE2	1:S:728:GLN:O	2.47	0.46
2:T:69:PHE:CZ	2:T:73:MET:HG2	2.49	0.46
1:V:566:HIS:CE1	1:V:568:LYS:HB2	2.50	0.46
2:W:104:MET:C	2:W:106:ALA:N	2.72	0.46
1:S:106:GLU:O	1:S:107:ARG:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:235:GLY:HA3	1:S:248:PHE:HE2	1.79	0.46
1:S:540:LEU:C	1:S:542:ASP:H	2.24	0.46
2:T:100:ASN:OD1	1:V:612:LEU:C	2.45	0.46
2:T:100:ASN:CG	1:V:612:LEU:HD12	2.40	0.46
2:T:133:ASP:OD1	2:T:135:ASN:N	2.48	0.46
1:V:308:GLU:OE1	1:V:312:ASN:HB3	2.16	0.46
1:V:310:PHE:O	1:V:311:ASN:HB2	2.15	0.46
1:V:469:PHE:N	1:V:486:ASN:OD1	2.46	0.46
1:V:756:MET:O	1:V:760:LEU:HG	2.15	0.46
1:S:80:PRO:HD2	1:S:83:PHE:HD2	1.81	0.46
1:S:236:ASN:ND2	1:S:246:SER:CA	2.73	0.46
1:S:236:ASN:HD22	1:S:245:SER:C	2.24	0.46
1:S:272:LEU:C	1:S:272:LEU:CD1	2.82	0.46
1:S:400:ARG:O	1:S:404:THR:N	2.40	0.46
1:S:409:VAL:HB	1:S:414:VAL:CG2	2.46	0.46
1:S:551:THR:H	1:S:554:SER:HG	1.60	0.46
1:S:611:SER:HA	1:S:614:ASN:HB2	1.98	0.46
1:S:719:GLN:HA	1:S:719:GLN:HE21	1.81	0.46
1:S:806:TYR:CB	2:T:147:VAL:HG12	2.45	0.46
1:V:611:SER:HA	1:V:614:ASN:HB2	1.98	0.46
1:S:79:ASN:OD1	1:S:92:LEU:HB3	2.15	0.46
1:S:310:PHE:O	1:S:311:ASN:HB2	2.15	0.46
1:S:424:ASP:O	1:S:426:ALA:N	2.48	0.46
2:T:43:THR:HG23	2:T:46:GLU:OE1	2.15	0.46
1:V:152:HIS:ND1	1:V:154:TYR:N	2.63	0.46
1:V:321:VAL:HG13	1:V:322:PRO:HD2	1.96	0.46
1:V:504:GLU:O	1:V:504:GLU:HG3	2.15	0.46
1:V:719:GLN:HA	1:V:719:GLN:HE21	1.81	0.46
2:W:81:ASP:HB3	2:W:82:GLN:H	1.58	0.46
1:S:43:GLY:HA2	1:S:699:HIS:CE1	2.51	0.46
1:S:267:ILE:CD1	1:S:450:LEU:HD12	2.45	0.46
1:S:330:GLU:O	1:S:331:MET:C	2.58	0.46
1:S:795:VAL:C	1:S:798:ALA:HB2	2.40	0.46
1:V:88:ASP:HB3	1:V:91:GLU:CD	2.41	0.46
1:V:133:TYR:HB3	1:V:154:TYR:OH	2.15	0.46
1:V:145:LYS:HB2	1:V:145:LYS:HE3	1.56	0.46
1:V:465:ASP:CG	1:V:465:ASP:O	2.59	0.46
1:V:806:TYR:CG	2:W:147:VAL:HG12	2.51	0.46
2:W:10:GLU:HG3	2:W:13:GLU:CD	2.41	0.46
1:S:613:LEU:C	1:S:615:GLN:N	2.72	0.46
2:T:10:GLU:HG3	2:T:13:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:98:GLU:OE1	1:V:612:LEU:CA	2.63	0.46
1:V:420:LYS:HD2	1:V:421:GLU:OE2	2.15	0.46
1:V:721:PHE:CE2	1:V:768:ARG:HG2	2.50	0.46
1:S:168:ARG:HH11	1:V:404:THR:CB	2.28	0.46
1:S:308:GLU:OE1	1:S:312:ASN:HB3	2.16	0.46
1:S:508:GLU:HG3	1:S:775:PHE:HE1	1.80	0.46
1:S:508:GLU:HG3	1:S:775:PHE:CE1	2.51	0.46
1:S:806:TYR:CG	2:T:147:VAL:HG12	2.51	0.46
1:S:844:PHE:O	1:S:848:MLY:N	2.49	0.46
2:T:110:HIS:O	2:T:111:VAL:C	2.59	0.46
1:V:236:ASN:HD22	1:V:245:SER:C	2.24	0.46
1:V:244:ASN:O	1:V:244:ASN:CG	2.58	0.46
1:V:275:SER:C	1:V:277:ALA:H	2.24	0.46
1:V:508:GLU:HG3	1:V:775:PHE:CE1	2.51	0.46
1:V:513:ASN:O	1:V:513:ASN:ND2	2.41	0.46
1:V:540:LEU:C	1:V:542:ASP:H	2.24	0.46
1:V:540:LEU:C	1:V:542:ASP:N	2.74	0.46
2:W:110:HIS:O	2:W:111:VAL:C	2.58	0.46
2:W:140:TYR:CE1	2:W:141:GLU:HG2	2.51	0.46
1:S:133:TYR:HB3	1:S:154:TYR:OH	2.15	0.45
1:S:168:ARG:CZ	1:V:406:ARG:CB	2.87	0.45
1:S:275:SER:C	1:S:277:ALA:H	2.24	0.45
1:S:504:GLU:O	1:S:504:GLU:HG3	2.15	0.45
1:S:607:ASP:O	1:S:610:THR:HB	2.16	0.45
1:S:702:LEU:HD12	1:S:702:LEU:HA	1.81	0.45
2:T:10:GLU:HA	2:T:13:GLU:CG	2.42	0.45
2:T:20:ARG:HE	2:T:20:ARG:HB2	1.46	0.45
2:T:140:TYR:CE1	2:T:141:GLU:HG2	2.51	0.45
1:V:31:ALA:C	1:V:33:LYS:N	2.73	0.45
1:V:141:TYR:CE1	1:V:149:MET:HB3	2.51	0.45
1:V:409:VAL:HB	1:V:414:VAL:CG2	2.46	0.45
1:V:491:GLN:OE1	1:V:521:LEU:HG	2.16	0.45
1:V:530:ARG:HA	1:V:531:PRO:HD3	1.79	0.45
1:V:625:TRP:O	1:V:626:LYS:C	2.60	0.45
1:V:718:ARG:HG3	1:V:719:GLN:N	2.30	0.45
1:S:146:ARG:NH1	1:S:159:THR:HG23	2.32	0.45
1:S:280:GLN:CD	1:S:286:THR:HG23	2.42	0.45
1:S:342:MET:O	1:S:342:MET:HE3	2.16	0.45
1:S:407:ILE:HD12	1:S:409:VAL:H	1.80	0.45
1:S:540:LEU:C	1:S:542:ASP:N	2.74	0.45
1:S:566:HIS:CE1	1:S:568:LYS:HB2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:735:GLU:HA	1:S:756:MET:HE1	1.98	0.45
2:T:97:LYS:HG2	2:T:98:GLU:HG3	1.97	0.45
1:V:223:GLN:C	1:V:225:LEU:N	2.73	0.45
1:V:306:LEU:HD22	1:V:386:LYS:HD3	1.98	0.45
1:V:425:PHE:CD1	1:V:425:PHE:O	2.70	0.45
1:V:711:LEU:N	1:V:711:LEU:CD2	2.78	0.45
1:V:776:PHE:CD2	1:V:781:LEU:HD22	2.51	0.45
1:S:354:ARG:HG3	1:S:355:VAL:N	2.31	0.45
1:S:491:GLN:OE1	1:S:521:LEU:HG	2.17	0.45
1:S:776:PHE:CD2	1:S:781:LEU:HD22	2.51	0.45
2:T:141:GLU:CD	1:V:389:HIS:CA	2.82	0.45
1:V:265:ALA:N	1:V:450:LEU:O	2.49	0.45
1:V:333:GLN:O	1:V:337:GLU:HG3	2.15	0.45
1:V:347:GLU:H	1:V:347:GLU:HG3	1.55	0.45
1:V:527:LEU:HD12	1:V:566:HIS:CD2	2.51	0.45
1:V:690:GLU:HB3	1:V:692:ARG:CG	2.43	0.45
2:W:74:GLN:O	2:W:78:LYS:HD2	2.16	0.45
1:S:141:TYR:CE1	1:S:149:MET:HB3	2.51	0.45
1:S:226:GLN:O	1:S:230:ILE:HD12	2.17	0.45
1:S:228:ASN:N	1:S:229:PRO:CD	2.80	0.45
1:S:269:THR:HG21	1:S:443:LEU:CD1	2.32	0.45
1:S:521:LEU:O	1:S:522:GLN:C	2.58	0.45
1:S:728:GLN:CB	1:V:370:GLU:HG3	2.46	0.45
1:S:747:MET:CG	1:S:751:GLN:NE2	2.79	0.45
2:T:71:PRO:HA	2:T:74:GLN:NE2	2.32	0.45
2:T:89:VAL:HG12	2:T:144:VAL:CG2	2.32	0.45
2:T:93:ARG:O	1:V:396:THR:CB	2.64	0.45
1:V:32:LYS:C	1:V:34:LEU:N	2.75	0.45
1:V:43:GLY:HA2	1:V:699:HIS:CE1	2.51	0.45
1:V:88:ASP:O	1:V:91:GLU:N	2.50	0.45
1:V:237:ALA:HA	1:V:288:HIS:CD2	2.50	0.45
1:V:318:ASN:O	1:V:319:GLY:C	2.59	0.45
2:W:26:ILE:HG22	2:W:26:ILE:O	2.17	0.45
1:S:362:LEU:CD2	1:S:427:ILE:HG13	2.43	0.45
1:S:425:PHE:CD1	1:S:425:PHE:O	2.70	0.45
1:S:532:THR:C	1:S:533:ASN:O	2.57	0.45
1:S:699:HIS:HA	1:S:702:LEU:HB2	1.98	0.45
2:T:70:LEU:HG	2:T:74:GLN:HE21	1.80	0.45
2:T:74:GLN:O	2:T:78:LYS:HD2	2.16	0.45
2:T:81:ASP:HB3	2:T:82:GLN:H	1.58	0.45
2:T:141:GLU:OE1	1:V:389:HIS:HB2	2.11	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:239:THR:C	1:V:241:LYS:N	2.75	0.45
1:V:407:ILE:CG1	1:V:414:VAL:O	2.63	0.45
1:V:437:ARG:NE	1:V:625:TRP:HA	2.25	0.45
1:V:607:ASP:O	1:V:610:THR:HB	2.16	0.45
1:V:735:GLU:HA	1:V:756:MET:HE1	1.98	0.45
1:V:747:MET:CG	1:V:751:GLN:NE2	2.79	0.45
2:W:133:ASP:C	2:W:133:ASP:OD1	2.59	0.45
1:S:318:ASN:O	1:S:319:GLY:C	2.59	0.45
1:S:395:VAL:O	1:S:396:THR:C	2.59	0.45
1:S:446:VAL:HG12	1:S:447:ASN:N	2.29	0.45
1:S:477:PHE:O	1:S:480:LEU:N	2.46	0.45
1:S:663:TYR:CZ	1:S:667:LEU:HD13	2.52	0.45
1:S:763:ASP:C	1:S:765:ASN:H	2.24	0.45
1:S:838:TRP:O	1:S:841:MET:N	2.50	0.45
2:T:66:PHE:CD1	2:T:66:PHE:C	2.95	0.45
1:V:147:HIS:C	1:V:149:MET:N	2.74	0.45
1:V:402:ILE:HG22	1:V:403:LEU:HG	1.99	0.45
1:V:494:ASN:N	1:V:494:ASN:ND2	2.61	0.45
1:V:547:PHE:CD1	1:V:547:PHE:C	2.94	0.45
2:W:66:PHE:CD1	2:W:66:PHE:C	2.95	0.45
2:W:133:ASP:OD1	2:W:135:ASN:N	2.49	0.45
1:S:31:ALA:C	1:S:33:LYS:N	2.73	0.45
1:S:265:ALA:N	1:S:450:LEU:O	2.49	0.45
1:S:293:LEU:HA	1:S:332:PHE:HE1	1.81	0.45
1:S:306:LEU:HD22	1:S:386:LYS:HD3	1.98	0.45
1:S:352:ILE:HG21	1:S:442:ILE:CD1	2.41	0.45
2:T:85:PHE:CD1	2:T:144:VAL:HG11	2.51	0.45
2:T:110:HIS:O	2:T:113:VAL:N	2.37	0.45
1:V:659:VAL:CG1	1:V:660:GLY:N	2.67	0.45
1:V:763:ASP:N	1:V:766:LEU:HD12	2.32	0.45
1:S:42:HIS:C	1:S:44:PHE:N	2.75	0.45
1:S:88:ASP:HB3	1:S:91:GLU:CD	2.41	0.45
1:S:116:TYR:HD1	1:S:121:CYS:HB2	1.82	0.45
1:S:145:LYS:CG	1:S:146:ARG:N	2.78	0.45
1:S:748:ASP:O	1:S:749:GLY:C	2.59	0.45
1:S:763:ASP:N	1:S:766:LEU:HD12	2.32	0.45
2:T:26:ILE:O	2:T:26:ILE:HG22	2.16	0.45
2:T:140:TYR:O	2:T:142:GLU:N	2.50	0.45
1:V:103:ASN:HD21	1:V:107:ARG:HD2	1.82	0.45
1:V:280:GLN:CD	1:V:286:THR:HG23	2.41	0.45
1:V:408:LYS:HG2	1:V:412:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:762:LEU:HD13	1:V:766:LEU:CD1	2.47	0.45
1:V:819:LEU:HA	1:V:822:ILE:HB	1.95	0.45
2:W:16:GLN:C	2:W:18:PHE:H	2.25	0.45
2:W:85:PHE:CD1	2:W:144:VAL:HG11	2.51	0.45
1:S:32:LYS:C	1:S:34:LEU:N	2.75	0.45
1:S:103:ASN:HD21	1:S:107:ARG:HD2	1.82	0.45
1:S:466:ILE:HD12	1:S:467:ALA:O	2.17	0.45
1:S:527:LEU:HD12	1:S:566:HIS:CD2	2.51	0.45
1:S:619:LYS:HA	1:S:622:ALA:HB3	1.99	0.45
1:S:769:ILE:HD13	1:S:769:ILE:HA	1.79	0.45
1:V:60:GLU:OE1	1:V:67:LYS:HD2	2.17	0.45
1:V:266:ASN:HD22	1:V:267:ILE:H	1.65	0.45
1:V:663:TYR:CZ	1:V:667:LEU:HD13	2.52	0.45
1:S:172:SER:HA	1:S:462:GLY:O	2.17	0.45
1:S:189:LYS:O	1:S:192:GLN:HB3	2.17	0.45
1:S:402:ILE:HG22	1:S:403:LEU:HG	1.99	0.45
1:S:404:THR:OG1	1:S:404:THR:O	2.31	0.45
1:S:565:ASN:O	1:S:565:ASN:CG	2.60	0.45
1:V:352:ILE:HG21	1:V:442:ILE:CD1	2.41	0.45
1:V:532:THR:C	1:V:533:ASN:O	2.57	0.45
2:W:140:TYR:O	2:W:142:GLU:N	2.50	0.45
1:S:168:ARG:NH2	1:V:400:ARG:CD	2.80	0.44
1:S:239:THR:C	1:S:241:LYS:N	2.75	0.44
1:S:320:HIS:ND1	1:S:320:HIS:O	2.39	0.44
1:S:326:GLN:CG	1:S:331:MET:HE3	2.48	0.44
1:S:742:ILE:HG23	1:S:747:MET:HE2	1.99	0.44
2:T:133:ASP:OD1	2:T:133:ASP:C	2.59	0.44
1:V:83:PHE:CB	1:V:92:LEU:HD23	2.43	0.44
1:V:369:LYS:HG3	1:V:370:GLU:H	1.81	0.44
1:V:699:HIS:HA	1:V:702:LEU:HB2	1.98	0.44
2:W:92:LEU:HD13	2:W:108:ILE:HD11	1.98	0.44
2:W:97:LYS:HG2	2:W:98:GLU:HG3	1.97	0.44
1:S:342:MET:HE3	1:S:342:MET:C	2.42	0.44
1:S:399:THR:C	1:S:403:LEU:HD12	2.42	0.44
2:T:9:ALA:HA	2:T:12:LYS:CE	2.47	0.44
2:T:55:LYS:H	2:T:58:GLU:HG2	1.83	0.44
1:V:146:ARG:NH1	1:V:159:THR:HG23	2.31	0.44
1:V:682:VAL:HG12	1:V:682:VAL:O	2.16	0.44
1:V:763:ASP:C	1:V:765:ASN:H	2.24	0.44
1:V:844:PHE:O	1:V:848:MLY:N	2.49	0.44
2:W:35:MET:CE	2:W:73:MET:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:88:ASP:O	1:S:91:GLU:N	2.50	0.44
1:S:288:HIS:O	1:S:289:ILE:C	2.61	0.44
1:S:408:LYS:HG2	1:S:412:ASP:O	2.17	0.44
1:S:409:VAL:HG13	1:S:634:LEU:HD11	1.99	0.44
1:V:149:MET:HB3	1:V:150:PRO:HD2	1.99	0.44
1:V:153:ILE:C	1:V:155:ALA:N	2.74	0.44
1:V:183:LYS:HE2	1:V:183:LYS:HB2	1.61	0.44
1:V:189:LYS:O	1:V:192:GLN:HB3	2.17	0.44
1:V:228:ASN:N	1:V:229:PRO:CD	2.80	0.44
1:V:293:LEU:HA	1:V:332:PHE:HE1	1.81	0.44
1:V:407:ILE:CD1	1:V:409:VAL:H	2.30	0.44
2:W:98:GLU:O	2:W:100:ASN:OD1	2.36	0.44
1:S:465:ASP:O	1:S:465:ASP:CG	2.59	0.44
1:S:610:THR:HG22	1:S:628:VAL:HG11	2.00	0.44
1:S:762:LEU:HD13	1:S:766:LEU:CD1	2.47	0.44
1:S:771:GLN:O	1:V:372:ASN:HA	2.17	0.44
1:V:22:ASN:ND2	1:V:22:ASN:O	2.51	0.44
1:V:256:PHE:CE1	1:V:262:ILE:HG13	2.52	0.44
1:V:395:VAL:O	1:V:396:THR:C	2.59	0.44
1:V:409:VAL:HG13	1:V:634:LEU:HD11	1.99	0.44
1:V:475:ASN:HB2	1:V:592:TYR:HA	1.99	0.44
1:V:522:GLN:N	1:V:523:PRO:CD	2.79	0.44
1:V:565:ASN:O	1:V:565:ASN:CG	2.60	0.44
1:V:662:LEU:HD12	1:V:662:LEU:HA	1.74	0.44
1:S:60:GLU:OE1	1:S:67:LYS:HD2	2.17	0.44
1:S:345:THR:O	1:S:346:GLU:C	2.61	0.44
1:S:407:ILE:CD1	1:S:409:VAL:H	2.30	0.44
1:S:547:PHE:HA	1:S:548:PRO:HD2	1.77	0.44
1:S:607:ASP:C	1:S:610:THR:HB	2.42	0.44
1:S:682:VAL:O	1:S:682:VAL:HG12	2.16	0.44
1:V:234:PHE:CE1	1:V:289:ILE:HG12	2.52	0.44
1:V:323:ILE:HG23	1:V:323:ILE:O	2.18	0.44
1:V:345:THR:O	1:V:346:GLU:C	2.61	0.44
1:V:466:ILE:HD12	1:V:467:ALA:O	2.17	0.44
1:V:610:THR:HG22	1:V:628:VAL:HG11	2.00	0.44
1:V:742:ILE:HG23	1:V:747:MET:HE2	1.99	0.44
1:S:22:ASN:ND2	1:S:22:ASN:O	2.51	0.44
1:S:149:MET:HB3	1:S:150:PRO:HD2	1.99	0.44
1:S:547:PHE:CD1	1:S:547:PHE:C	2.94	0.44
1:S:575:LEU:HD23	1:S:577:ASP:OD1	2.17	0.44
1:S:661:GLN:HE21	1:S:661:GLN:HB2	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:23:PRO:O	1:V:27:ALA:CB	2.66	0.44
1:V:116:TYR:HD1	1:V:121:CYS:HB2	1.81	0.44
1:V:226:GLN:O	1:V:230:ILE:HD12	2.17	0.44
1:V:250:LYS:CE	1:V:465:ASP:OD2	2.66	0.44
1:V:288:HIS:O	1:V:289:ILE:C	2.61	0.44
1:V:326:GLN:CG	1:V:331:MET:HE3	2.48	0.44
1:V:399:THR:C	1:V:403:LEU:HD12	2.42	0.44
1:V:575:LEU:HD23	1:V:577:ASP:OD1	2.17	0.44
1:S:196:VAL:CG1	1:S:197:VAL:N	2.81	0.44
1:S:250:LYS:CE	1:S:465:ASP:OD2	2.66	0.44
1:S:251:PHE:O	1:S:251:PHE:CD1	2.71	0.44
1:S:720:GLY:C	1:S:721:PHE:CD1	2.95	0.44
1:S:799:PHE:O	1:S:800:GLN:C	2.60	0.44
2:T:16:GLN:C	2:T:18:PHE:H	2.25	0.44
1:V:487:GLU:OE1	1:V:585:HIS:HA	2.18	0.44
1:V:720:GLY:C	1:V:721:PHE:CD1	2.95	0.44
2:W:71:PRO:HA	2:W:74:GLN:NE2	2.32	0.44
2:W:121:GLU:H	2:W:121:GLU:CD	2.24	0.44
1:S:53:LYS:HD2	1:S:58:THR:HG23	1.99	0.44
1:S:121:CYS:SG	1:S:156:ILE:HD11	2.58	0.44
1:S:257:ASP:C	1:S:257:ASP:OD1	2.57	0.44
1:S:413:VAL:O	1:S:415:GLN:N	2.51	0.44
1:S:468:GLY:O	1:S:469:PHE:C	2.61	0.44
1:S:625:TRP:O	1:S:626:LYS:C	2.60	0.44
1:S:663:TYR:C	1:S:665:GLU:N	2.69	0.44
2:T:92:LEU:HD13	2:T:108:ILE:HD11	1.98	0.44
2:T:99:GLY:N	1:V:397:ASP:HB2	2.31	0.44
1:V:53:LYS:HD2	1:V:58:THR:HG23	1.99	0.44
2:W:25:LYS:HE3	2:W:65:LYS:HE2	2.00	0.44
2:W:55:LYS:H	2:W:58:GLU:HG2	1.83	0.44
1:S:104:LEU:CD1	1:S:705:LEU:HD11	2.48	0.44
1:S:152:HIS:CE1	1:S:153:ILE:HG22	2.53	0.44
1:S:171:GLN:HA	1:S:678:ASN:H	1.83	0.44
2:T:85:PHE:CZ	2:T:145:ARG:NH1	2.86	0.44
1:V:33:LYS:O	1:V:49:ILE:HG13	2.18	0.44
1:V:251:PHE:O	1:V:251:PHE:CD1	2.71	0.44
1:V:521:LEU:O	1:V:522:GLN:C	2.58	0.44
1:V:607:ASP:C	1:V:610:THR:HB	2.42	0.44
1:V:619:LYS:HA	1:V:622:ALA:HB3	1.99	0.44
2:W:50:VAL:O	2:W:51:LEU:HD23	2.18	0.44
1:S:12:PHE:CD1	1:S:111:GLY:HA3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:23:PRO:O	1:S:27:ALA:CB	2.66	0.43
1:S:223:GLN:C	1:S:225:LEU:N	2.73	0.43
1:S:256:PHE:CE1	1:S:262:ILE:HG13	2.52	0.43
1:S:375:GLN:HG3	1:S:418:GLN:O	2.18	0.43
1:S:475:ASN:HB2	1:S:592:TYR:HA	1.99	0.43
1:S:541:LEU:HD11	1:S:597:TRP:HB3	2.00	0.43
2:T:99:GLY:N	1:V:397:ASP:CB	2.77	0.43
1:V:9:ASP:O	1:V:12:PHE:HB2	2.18	0.43
1:V:132:ILE:HD12	1:V:152:HIS:HD2	1.82	0.43
1:V:152:HIS:CE1	1:V:153:ILE:HG22	2.52	0.43
1:V:342:MET:HE3	1:V:342:MET:C	2.42	0.43
1:V:747:MET:HE3	1:V:752:ALA:CA	2.42	0.43
1:S:132:ILE:HD12	1:S:152:HIS:HD2	1.82	0.43
1:S:266:ASN:HD22	1:S:267:ILE:H	1.65	0.43
1:S:525:ILE:O	1:S:529:GLU:HB3	2.18	0.43
1:S:742:ILE:HD13	1:S:756:MET:HE3	2.00	0.43
2:T:35:MET:CE	2:T:73:MET:HA	2.47	0.43
1:V:3:GLN:O	1:V:4:LYS:O	2.36	0.43
1:V:33:LYS:CG	1:V:49:ILE:HB	2.48	0.43
1:V:425:PHE:CD1	1:V:425:PHE:C	2.96	0.43
1:V:541:LEU:HD11	1:V:597:TRP:HB3	2.00	0.43
1:V:771:GLN:CA	1:V:771:GLN:NE2	2.81	0.43
1:S:145:LYS:HB2	1:S:145:LYS:HE3	1.56	0.43
1:S:234:PHE:CE1	1:S:289:ILE:HG12	2.52	0.43
1:S:300:GLN:C	1:S:302:ARG:N	2.75	0.43
1:S:369:LYS:HG3	1:S:370:GLU:H	1.81	0.43
1:S:391:MET:HB3	1:S:393:ILE:HG12	2.00	0.43
1:S:405:PRO:HB2	1:S:407:ILE:HG22	1.97	0.43
1:S:419:THR:O	1:S:422:GLN:N	2.51	0.43
1:S:487:GLU:OE1	1:S:585:HIS:HA	2.18	0.43
1:S:530:ARG:HA	1:S:531:PRO:HD3	1.78	0.43
1:S:769:ILE:HD13	1:S:774:ILE:HG12	2.00	0.43
2:T:50:VAL:O	2:T:51:LEU:HD23	2.18	0.43
1:V:196:VAL:CG1	1:V:197:VAL:N	2.81	0.43
1:V:376:ALA:CB	1:V:420:LYS:HB2	2.44	0.43
1:V:468:GLY:O	1:V:469:PHE:C	2.61	0.43
1:V:742:ILE:HD13	1:V:756:MET:HE3	2.00	0.43
1:V:750:LYS:O	1:V:751:GLN:C	2.61	0.43
1:V:767:TYR:CD1	1:V:767:TYR:C	2.96	0.43
1:S:33:LYS:CG	1:S:49:ILE:HB	2.48	0.43
1:S:767:TYR:CD1	1:S:767:TYR:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:768:ARG:HD3	1:S:768:ARG:HA	1.63	0.43
1:S:792:ILE:O	1:S:796:ILE:HG12	2.17	0.43
2:T:18:PHE:CD2	2:T:34:VAL:HG22	2.54	0.43
1:V:300:GLN:C	1:V:302:ARG:N	2.75	0.43
1:V:375:GLN:O	1:V:376:ALA:C	2.61	0.43
1:V:419:THR:O	1:V:422:GLN:N	2.51	0.43
1:V:525:ILE:O	1:V:529:GLU:HB3	2.18	0.43
1:V:606:ASN:OD1	1:V:608:ASN:HB2	2.18	0.43
1:S:9:ASP:O	1:S:12:PHE:HB2	2.18	0.43
1:S:606:ASN:OD1	1:S:608:ASN:HB2	2.18	0.43
1:V:12:PHE:CD1	1:V:111:GLY:HA3	2.52	0.43
1:V:172:SER:HA	1:V:462:GLY:O	2.17	0.43
1:V:477:PHE:O	1:V:480:LEU:N	2.46	0.43
1:V:527:LEU:HD23	1:V:527:LEU:C	2.42	0.43
1:V:748:ASP:O	1:V:749:GLY:C	2.59	0.43
2:W:96:ASP:O	2:W:98:GLU:N	2.52	0.43
1:S:3:GLN:O	1:S:4:LYS:O	2.36	0.43
1:S:87:GLU:OE1	1:S:107:ARG:NH2	2.51	0.43
1:S:244:ASN:O	1:S:244:ASN:CG	2.58	0.43
1:S:347:GLU:H	1:S:347:GLU:HG3	1.55	0.43
1:S:522:GLN:OE1	1:S:525:ILE:HD12	2.19	0.43
1:S:806:TYR:HB3	2:T:147:VAL:HG12	2.01	0.43
2:T:3:PHE:C	2:T:7:GLN:HE21	2.27	0.43
1:V:26:GLN:HE21	1:V:26:GLN:C	2.27	0.43
1:V:349:GLN:HA	1:V:352:ILE:HG13	2.01	0.43
1:V:375:GLN:HG3	1:V:418:GLN:O	2.18	0.43
1:V:391:MET:HB3	1:V:393:ILE:HG12	2.00	0.43
1:S:45:GLU:OE2	1:S:61:LEU:HB3	2.19	0.43
1:S:153:ILE:C	1:S:155:ALA:N	2.75	0.43
1:S:162:ARG:O	1:S:163:SER:C	2.62	0.43
1:S:520:ASP:OD1	1:S:522:GLN:N	2.49	0.43
1:S:613:LEU:C	1:S:615:GLN:H	2.27	0.43
2:T:10:GLU:O	2:T:11:PHE:C	2.62	0.43
2:T:124:VAL:HG23	2:T:125:GLU:N	2.33	0.43
1:V:104:LEU:CD1	1:V:705:LEU:HD11	2.48	0.43
1:V:107:ARG:CB	1:V:112:LEU:HD12	2.48	0.43
1:V:121:CYS:SG	1:V:156:ILE:HD11	2.58	0.43
1:V:442:ILE:O	1:V:445:ARG:N	2.43	0.43
1:V:838:TRP:O	1:V:841:MET:N	2.50	0.43
2:W:9:ALA:HA	2:W:12:LYS:CE	2.47	0.43
2:W:10:GLU:O	2:W:11:PHE:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:124:VAL:HG23	2:W:125:GLU:N	2.33	0.43
1:S:298:SER:O	1:S:299:GLU:C	2.62	0.43
1:S:323:ILE:HG23	1:S:323:ILE:O	2.18	0.43
1:S:373:THR:O	1:S:374:ASP:HB2	2.19	0.43
1:S:395:VAL:O	1:S:398:PHE:N	2.52	0.43
1:S:425:PHE:CD1	1:S:425:PHE:C	2.96	0.43
1:S:572:SER:HB2	1:S:580:GLU:HG3	2.00	0.43
2:T:14:ALA:HB3	2:T:38:LEU:HD21	2.00	0.43
1:V:46:ALA:HB1	1:V:62:GLN:HG2	2.00	0.43
1:V:153:ILE:CG2	1:V:154:TYR:N	2.82	0.43
1:V:413:VAL:O	1:V:415:GLN:N	2.51	0.43
1:V:607:ASP:OD1	1:V:607:ASP:N	2.34	0.43
1:V:686:ILE:HG22	1:V:686:ILE:O	2.17	0.43
2:W:85:PHE:CZ	2:W:145:ARG:NH1	2.86	0.43
1:S:33:LYS:O	1:S:49:ILE:HG13	2.18	0.43
1:S:619:LYS:HA	1:S:622:ALA:CB	2.49	0.43
1:S:686:ILE:HG22	1:S:686:ILE:O	2.17	0.43
1:V:13:LEU:HG	1:V:132:ILE:CG2	2.49	0.43
1:V:71:SER:HB3	1:V:73:ASP:OD2	2.19	0.43
1:V:171:GLN:HA	1:V:678:ASN:H	1.83	0.43
1:V:373:THR:O	1:V:374:ASP:HB2	2.19	0.43
1:S:344:PHE:N	1:S:344:PHE:CD1	2.86	0.43
1:S:576:LYS:C	1:S:579:THR:H	2.27	0.43
2:T:41:ASN:N	2:T:42:PRO:CD	2.82	0.43
2:T:121:GLU:CD	2:T:121:GLU:H	2.24	0.43
1:V:172:SER:OG	1:V:679:PRO:HA	2.18	0.43
1:V:817:GLN:HG2	1:V:818:GLN:OE1	2.19	0.43
1:S:102:HIS:O	1:S:105:ARG:N	2.52	0.42
1:S:107:ARG:CB	1:S:112:LEU:HD12	2.49	0.42
1:S:361:GLN:CG	1:S:387:VAL:HG23	2.49	0.42
1:S:405:PRO:C	1:S:407:ILE:N	2.76	0.42
1:S:492:LEU:O	1:S:496:THR:OG1	2.37	0.42
1:S:715:ARG:HH21	1:S:719:GLN:CD	2.27	0.42
1:S:819:LEU:CA	1:S:822:ILE:CG1	2.59	0.42
1:V:24:LEU:HD23	1:V:24:LEU:N	2.34	0.42
1:V:87:GLU:OE1	1:V:107:ARG:NH2	2.51	0.42
1:V:102:HIS:O	1:V:105:ARG:N	2.52	0.42
1:V:275:SER:O	1:V:278:ILE:HG12	2.19	0.42
1:V:395:VAL:O	1:V:398:PHE:N	2.52	0.42
1:V:522:GLN:OE1	1:V:525:ILE:HD12	2.19	0.42
1:V:576:LYS:C	1:V:579:THR:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:799:PHE:O	1:V:800:GLN:C	2.60	0.42
1:V:806:TYR:HB3	2:W:147:VAL:HG12	2.01	0.42
2:W:14:ALA:HB3	2:W:38:LEU:HD21	2.00	0.42
2:W:27:LEU:C	2:W:29:SER:N	2.76	0.42
1:S:33:LYS:O	1:S:48:SER:HA	2.19	0.42
1:S:39:SER:OG	1:S:42:HIS:HB2	2.19	0.42
1:S:147:HIS:C	1:S:149:MET:N	2.74	0.42
1:S:172:SER:OG	1:S:679:PRO:HA	2.18	0.42
1:S:356:VAL:O	1:S:360:LEU:HD12	2.19	0.42
1:S:445:ARG:HD2	1:S:445:ARG:HA	1.65	0.42
1:S:540:LEU:H	1:S:540:LEU:HG	1.58	0.42
1:S:797:ILE:CG1	2:T:117:GLU:HG2	2.49	0.42
2:T:81:ASP:O	2:T:82:GLN:HB2	2.20	0.42
2:T:96:ASP:O	2:T:98:GLU:N	2.52	0.42
1:V:274:LYS:HD2	1:V:274:LYS:C	2.44	0.42
1:V:526:GLU:C	1:V:528:ILE:N	2.77	0.42
1:V:613:LEU:C	1:V:615:GLN:H	2.27	0.42
2:W:18:PHE:CD2	2:W:34:VAL:HG22	2.54	0.42
1:S:13:LEU:HG	1:S:132:ILE:CG2	2.49	0.42
1:S:26:GLN:HE21	1:S:26:GLN:C	2.27	0.42
1:S:36:TRP:C	1:S:37:VAL:HG22	2.45	0.42
1:S:349:GLN:HA	1:S:352:ILE:HG13	2.01	0.42
1:S:662:LEU:HD12	1:S:662:LEU:HA	1.74	0.42
1:S:817:GLN:HG2	1:S:818:GLN:OE1	2.18	0.42
1:S:848:MLY:N	1:S:849:PRO:HD2	2.35	0.42
2:T:25:LYS:HE3	2:T:65:LYS:HE2	2.00	0.42
1:V:39:SER:OG	1:V:42:HIS:HB2	2.19	0.42
1:V:769:ILE:HD13	1:V:774:ILE:HG12	2.00	0.42
1:V:814:LYS:C	1:V:816:GLN:N	2.72	0.42
1:V:848:MLY:N	1:V:849:PRO:HD2	2.35	0.42
2:W:111:VAL:HA	2:W:115:LEU:HD13	2.01	0.42
1:S:71:SER:HB3	1:S:73:ASP:OD2	2.19	0.42
1:S:178:GLU:O	1:S:183:LYS:NZ	2.53	0.42
1:S:527:LEU:HD23	1:S:527:LEU:C	2.42	0.42
1:S:619:LYS:O	1:S:622:ALA:N	2.52	0.42
1:S:771:GLN:CA	1:S:771:GLN:NE2	2.81	0.42
2:T:38:LEU:CD1	2:T:73:MET:HE2	2.48	0.42
1:V:22:ASN:HA	1:V:23:PRO:HD3	1.82	0.42
1:V:294:ILE:HG22	1:V:294:ILE:O	2.19	0.42
1:V:361:GLN:CG	1:V:387:VAL:HG23	2.49	0.42
1:V:582:CYS:HA	1:V:590:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:685:ILE:HD11	1:V:705:LEU:HD23	2.02	0.42
2:W:95:PHE:CZ	2:W:111:VAL:HG21	2.55	0.42
1:S:415:GLN:O	1:S:415:GLN:HG3	2.19	0.42
1:V:619:LYS:HA	1:V:622:ALA:CB	2.49	0.42
2:W:3:PHE:C	2:W:7:GLN:HE21	2.27	0.42
2:W:35:MET:HE2	2:W:35:MET:HB3	1.93	0.42
1:S:384:ALA:HA	1:S:387:VAL:HB	2.02	0.42
1:S:407:ILE:CG1	1:S:414:VAL:O	2.63	0.42
2:T:92:LEU:C	2:T:94:VAL:H	2.26	0.42
2:T:95:PHE:CZ	2:T:111:VAL:HG21	2.55	0.42
1:V:178:GLU:O	1:V:183:LYS:NZ	2.53	0.42
1:V:256:PHE:HA	1:V:261:TYR:O	2.19	0.42
1:V:345:THR:N	1:V:348:GLU:HB3	2.35	0.42
1:V:356:VAL:O	1:V:360:LEU:HD12	2.19	0.42
1:V:835:VAL:O	1:V:837:HIS:N	2.53	0.42
2:W:71:PRO:HA	2:W:74:GLN:OE1	2.20	0.42
1:S:153:ILE:CG2	1:S:154:TYR:N	2.82	0.42
1:S:235:GLY:HA3	1:S:248:PHE:CE2	2.55	0.42
1:S:256:PHE:HA	1:S:261:TYR:O	2.19	0.42
1:S:306:LEU:HD22	1:S:386:LYS:CD	2.50	0.42
1:S:586:TYR:CD1	1:S:586:TYR:N	2.87	0.42
1:S:690:GLU:HB3	1:S:692:ARG:CG	2.43	0.42
1:S:750:LYS:O	1:S:751:GLN:C	2.61	0.42
1:S:800:GLN:O	1:S:803:CYS:HB2	2.20	0.42
2:T:111:VAL:HA	2:T:115:LEU:HD13	2.01	0.42
1:V:352:ILE:O	1:V:356:VAL:HG23	2.20	0.42
1:V:480:LEU:HA	1:V:592:TYR:CE1	2.54	0.42
1:V:619:LYS:O	1:V:622:ALA:N	2.52	0.42
1:V:751:GLN:HE21	1:V:751:GLN:HB3	1.74	0.42
1:V:800:GLN:O	1:V:803:CYS:HB2	2.20	0.42
1:S:46:ALA:HB1	1:S:62:GLN:HG2	2.00	0.42
1:S:275:SER:O	1:S:278:ILE:HG12	2.19	0.42
1:S:526:GLU:C	1:S:528:ILE:N	2.77	0.42
1:V:51:GLU:CG	1:V:53:LYS:HE3	2.50	0.42
1:V:358:SER:C	1:V:360:LEU:H	2.28	0.42
1:V:407:ILE:HD12	1:V:408:LYS:C	2.45	0.42
1:V:797:ILE:CG1	2:W:117:GLU:HG2	2.49	0.42
2:W:139:ASN:OD1	2:W:142:GLU:HG2	2.20	0.42
1:S:345:THR:N	1:S:348:GLU:HB3	2.35	0.42
2:T:71:PRO:HA	2:T:74:GLN:OE1	2.20	0.42
2:T:96:ASP:C	2:T:96:ASP:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:38:PRO:HG2	1:V:70:LEU:HD13	2.02	0.42
1:V:43:GLY:HA2	1:V:699:HIS:NE2	2.34	0.42
1:V:45:GLU:OE2	1:V:61:LEU:HB3	2.19	0.42
1:V:156:ILE:HD13	1:V:682:VAL:HG22	2.02	0.42
1:V:298:SER:O	1:V:299:GLU:C	2.62	0.42
1:V:329:ASP:OD1	1:V:329:ASP:N	2.43	0.42
1:V:445:ARG:HD2	1:V:445:ARG:HA	1.65	0.42
1:V:474:ILE:H	1:V:474:ILE:HG13	1.48	0.42
1:V:716:ILE:HA	1:V:719:GLN:HB2	2.02	0.42
2:W:76:ILE:O	2:W:79:ASN:CG	2.63	0.42
2:W:128:VAL:O	2:W:129:ALA:C	2.63	0.42
1:S:195:ALA:O	1:S:199:SER:HB3	2.19	0.42
1:S:265:ALA:O	1:S:450:LEU:HB2	2.20	0.42
1:S:348:GLU:O	1:S:352:ILE:HG13	2.20	0.42
1:S:375:GLN:O	1:S:376:ALA:C	2.61	0.42
1:S:480:LEU:HA	1:S:592:TYR:CE1	2.54	0.42
1:S:514:PHE:CG	1:S:515:ILE:N	2.88	0.42
1:S:551:THR:C	1:S:553:THR:N	2.77	0.42
1:S:610:THR:HG23	1:S:628:VAL:HG22	2.02	0.42
2:T:76:ILE:O	2:T:79:ASN:CG	2.62	0.42
1:V:33:LYS:O	1:V:48:SER:HA	2.19	0.42
1:V:176:THR:O	1:V:183:LYS:HD2	2.20	0.42
1:V:235:GLY:HA3	1:V:248:PHE:CE2	2.54	0.42
1:V:348:GLU:O	1:V:352:ILE:HG13	2.20	0.42
1:V:405:PRO:CD	1:V:416:LYS:O	2.68	0.42
1:V:663:TYR:O	1:V:666:GLN:N	2.53	0.42
1:V:724:ARG:HE	1:V:724:ARG:HB3	1.63	0.42
1:V:851:LEU:N	1:V:851:LEU:CD1	2.82	0.42
2:W:41:ASN:N	2:W:42:PRO:CD	2.82	0.42
1:S:7:SER:N	1:S:10:GLU:OE1	2.43	0.41
1:S:24:LEU:HD23	1:S:24:LEU:N	2.34	0.41
1:S:168:ARG:NH2	1:V:406:ARG:CA	2.82	0.41
1:S:582:CYS:HA	1:S:590:VAL:O	2.19	0.41
2:T:128:VAL:HG23	2:T:129:ALA:N	2.35	0.41
2:T:140:TYR:HE1	2:T:141:GLU:OE2	2.03	0.41
1:V:87:GLU:OE1	1:V:87:GLU:HA	2.20	0.41
1:V:177:GLY:O	1:V:183:LYS:NZ	2.49	0.41
1:V:586:TYR:CD1	1:V:586:TYR:N	2.87	0.41
1:V:610:THR:HG23	1:V:628:VAL:HG22	2.02	0.41
1:V:683:ARG:HE	1:V:683:ARG:HB3	1.50	0.41
1:V:746:PHE:O	1:V:747:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:46:GLU:O	2:W:50:VAL:HG23	2.20	0.41
1:S:49:ILE:HG23	1:S:57:VAL:CG1	2.49	0.41
1:S:51:GLU:CG	1:S:53:LYS:HE3	2.50	0.41
1:S:330:GLU:HG2	1:S:330:GLU:H	1.63	0.41
1:S:610:THR:HG21	1:S:628:VAL:HG13	2.02	0.41
1:S:772:SER:HA	1:V:371:ARG:O	2.20	0.41
2:T:46:GLU:O	2:T:50:VAL:HG23	2.21	0.41
2:T:100:ASN:O	1:V:616:SER:HB2	2.20	0.41
1:V:8:ASP:OD1	1:V:8:ASP:N	2.53	0.41
1:V:23:PRO:O	1:V:27:ALA:HB2	2.21	0.41
1:V:36:TRP:C	1:V:37:VAL:HG22	2.45	0.41
1:V:140:MET:HB3	1:V:149:MET:CE	2.50	0.41
1:V:162:ARG:O	1:V:163:SER:C	2.62	0.41
1:V:195:ALA:O	1:V:199:SER:HB3	2.19	0.41
1:V:265:ALA:O	1:V:450:LEU:HB2	2.20	0.41
1:V:352:ILE:HG23	1:V:438:LEU:HD11	2.01	0.41
1:V:378:MET:HA	1:V:378:MET:CE	2.45	0.41
1:V:432:LYS:HE2	1:V:432:LYS:HB2	1.75	0.41
1:V:551:THR:C	1:V:553:THR:N	2.77	0.41
2:W:92:LEU:C	2:W:94:VAL:H	2.26	0.41
1:S:33:LYS:N	1:S:33:LYS:HE2	2.35	0.41
1:S:274:LYS:HD2	1:S:274:LYS:C	2.44	0.41
1:S:294:ILE:O	1:S:294:ILE:HG22	2.19	0.41
1:S:352:ILE:O	1:S:356:VAL:HG23	2.20	0.41
1:S:407:ILE:HD12	1:S:408:LYS:C	2.45	0.41
1:S:437:ARG:NE	1:S:625:TRP:HA	2.25	0.41
1:S:716:ILE:HA	1:S:719:GLN:HB2	2.02	0.41
2:T:104:MET:H	2:T:104:MET:HG3	1.47	0.41
1:V:225:LEU:HD12	1:V:225:LEU:HA	1.89	0.41
1:V:299:GLU:O	1:V:302:ARG:HB3	2.21	0.41
1:V:384:ALA:HA	1:V:387:VAL:HB	2.02	0.41
1:V:514:PHE:CG	1:V:515:ILE:N	2.88	0.41
1:V:683:ARG:H	1:V:683:ARG:HG2	1.34	0.41
1:V:696:LEU:C	1:V:696:LEU:HD12	2.46	0.41
2:W:125:GLU:O	2:W:129:ALA:CB	2.68	0.41
1:S:43:GLY:HA2	1:S:699:HIS:NE2	2.34	0.41
1:S:140:MET:C	1:S:149:MET:HE3	2.46	0.41
1:S:358:SER:C	1:S:360:LEU:H	2.28	0.41
1:S:378:MET:HA	1:S:378:MET:CE	2.45	0.41
1:S:545:CYS:SG	1:S:602:MET:SD	3.19	0.41
1:S:703:GLU:O	1:S:704:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:27:LEU:C	2:T:29:SER:N	2.76	0.41
2:T:102:THR:HG22	1:V:617:SER:CA	2.46	0.41
1:V:138:ILE:HG21	1:V:196:VAL:HG11	2.01	0.41
1:V:165:LEU:HD21	1:V:260:GLY:CA	2.51	0.41
1:V:572:SER:HB2	1:V:580:GLU:HG3	2.01	0.41
1:S:140:MET:HB3	1:S:149:MET:CE	2.50	0.41
1:S:305:LEU:HB2	1:S:307:LEU:HG	2.01	0.41
1:S:558:LYS:O	1:S:561:GLN:N	2.53	0.41
1:S:685:ILE:HD11	1:S:705:LEU:HD23	2.02	0.41
1:S:746:PHE:O	1:S:747:MET:HB2	2.20	0.41
1:S:747:MET:HG2	1:S:751:GLN:NE2	2.36	0.41
2:T:128:VAL:O	2:T:129:ALA:C	2.63	0.41
2:T:141:GLU:OE1	1:V:389:HIS:CA	2.66	0.41
1:V:409:VAL:O	1:V:410:GLY:C	2.63	0.41
1:V:438:LEU:O	1:V:441:TRP:HB3	2.21	0.41
1:V:545:CYS:SG	1:V:602:MET:SD	3.19	0.41
1:V:606:ASN:OD1	1:V:606:ASN:C	2.63	0.41
1:S:72:LYS:O	1:S:72:LYS:HG2	2.20	0.41
1:S:164:MET:HE3	1:S:461:LEU:HD12	2.03	0.41
1:S:311:ASN:C	1:S:312:ASN:HD22	2.28	0.41
1:S:352:ILE:HG23	1:S:438:LEU:HD11	2.01	0.41
1:S:494:ASN:N	1:S:494:ASN:ND2	2.61	0.41
1:S:728:GLN:CA	1:S:728:GLN:NE2	2.79	0.41
2:T:139:ASN:OD1	2:T:142:GLU:HG2	2.20	0.41
2:T:142:GLU:O	2:T:143:LEU:C	2.63	0.41
1:V:49:ILE:HG23	1:V:57:VAL:CG1	2.49	0.41
1:V:362:LEU:HD12	1:V:387:VAL:CG1	2.51	0.41
1:V:715:ARG:HH21	1:V:719:GLN:CD	2.28	0.41
2:W:81:ASP:O	2:W:82:GLN:HB2	2.20	0.41
2:W:96:ASP:OD1	2:W:96:ASP:C	2.62	0.41
2:W:128:VAL:HG23	2:W:129:ALA:N	2.35	0.41
1:S:8:ASP:OD1	1:S:8:ASP:N	2.53	0.41
1:S:156:ILE:HD13	1:S:682:VAL:HG22	2.02	0.41
1:S:179:SER:HA	1:S:183:LYS:HZ1	1.86	0.41
1:S:302:ARG:CZ	1:S:303:ASN:HA	2.50	0.41
1:S:337:GLU:O	1:S:341:ILE:HG12	2.21	0.41
1:S:362:LEU:HD12	1:S:387:VAL:CG1	2.51	0.41
1:S:526:GLU:C	1:S:528:ILE:H	2.29	0.41
1:V:558:LYS:O	1:V:561:GLN:N	2.53	0.41
1:V:809:ARG:HD2	2:W:36:ARG:O	2.21	0.41
1:S:38:PRO:HG2	1:S:70:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:71:SER:C	1:S:73:ASP:N	2.78	0.41
1:S:87:GLU:OE1	1:S:87:GLU:HA	2.20	0.41
1:S:152:HIS:ND1	1:S:154:TYR:N	2.62	0.41
1:S:176:THR:O	1:S:183:LYS:HD2	2.20	0.41
1:S:382:THR:CA	1:S:385:GLN:HB3	2.51	0.41
1:S:522:GLN:N	1:S:523:PRO:CD	2.79	0.41
1:S:618:ASP:HB3	1:S:621:VAL:HG23	2.03	0.41
1:S:712:GLU:C	1:S:714:ILE:N	2.78	0.41
1:S:719:GLN:HE21	1:S:719:GLN:CA	2.33	0.41
1:S:806:TYR:C	1:S:808:ALA:N	2.78	0.41
1:V:33:LYS:N	1:V:33:LYS:HE2	2.35	0.41
1:V:42:HIS:C	1:V:44:PHE:N	2.75	0.41
1:V:306:LEU:HD22	1:V:386:LYS:CD	2.50	0.41
1:V:703:GLU:O	1:V:704:GLN:C	2.63	0.41
1:S:180:GLY:C	1:S:182:GLY:H	2.29	0.41
1:S:225:LEU:HD12	1:S:225:LEU:HA	1.89	0.41
1:S:234:PHE:HD1	1:S:289:ILE:CG2	2.32	0.41
1:S:438:LEU:O	1:S:441:TRP:HB3	2.21	0.41
1:S:613:LEU:O	1:S:614:ASN:C	2.64	0.41
1:S:696:LEU:C	1:S:696:LEU:HD12	2.45	0.41
1:S:835:VAL:O	1:S:837:HIS:N	2.53	0.41
2:T:87:ASP:O	2:T:88:TYR:C	2.64	0.41
2:T:93:ARG:C	1:V:396:THR:HG23	2.46	0.41
2:T:144:VAL:O	2:T:147:VAL:HG23	2.21	0.41
1:V:31:ALA:O	1:V:32:LYS:C	2.64	0.41
1:V:71:SER:C	1:V:73:ASP:N	2.78	0.41
1:V:302:ARG:CZ	1:V:303:ASN:HA	2.50	0.41
1:V:305:LEU:HB2	1:V:307:LEU:HG	2.01	0.41
1:V:337:GLU:O	1:V:341:ILE:HG12	2.21	0.41
1:V:405:PRO:HB2	1:V:407:ILE:HG22	1.97	0.41
1:V:465:ASP:OD1	1:V:465:ASP:C	2.64	0.41
1:V:526:GLU:C	1:V:528:ILE:H	2.29	0.41
1:V:771:GLN:NE2	1:V:771:GLN:O	2.53	0.41
2:W:80:LYS:H	2:W:80:LYS:CD	2.30	0.41
2:W:110:HIS:HB3	2:W:111:VAL:H	1.78	0.41
2:W:142:GLU:O	2:W:143:LEU:C	2.63	0.41
1:S:201:HIS:C	1:S:203:GLY:H	2.29	0.41
1:S:409:VAL:O	1:S:410:GLY:C	2.63	0.41
1:S:568:LYS:HA	1:S:568:LYS:CE	2.51	0.41
1:S:630:ARG:O	1:S:631:ILE:C	2.64	0.41
1:S:683:ARG:HE	1:S:683:ARG:HB3	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:140:MET:C	1:V:149:MET:HE3	2.46	0.41
1:V:179:SER:HA	1:V:183:LYS:HZ1	1.85	0.41
1:V:506:GLN:O	1:V:509:GLY:N	2.53	0.41
1:V:522:GLN:O	1:V:523:PRO:C	2.64	0.41
1:V:821:SER:O	1:V:825:ILE:HG13	2.21	0.41
1:V:849:PRO:C	1:V:851:LEU:N	2.79	0.41
2:W:120:THR:HG23	2:W:123:GLU:OE1	2.21	0.41
1:S:23:PRO:O	1:S:27:ALA:HB2	2.21	0.40
1:S:37:VAL:CB	1:S:38:PRO:HD2	2.50	0.40
1:S:51:GLU:HB3	1:S:53:LYS:HD2	2.03	0.40
1:S:338:ALA:O	1:S:339:MET:C	2.64	0.40
1:S:409:VAL:HG13	1:S:634:LEU:HD12	2.03	0.40
1:S:543:GLU:HG2	1:S:544:GLU:N	2.32	0.40
1:S:606:ASN:OD1	1:S:606:ASN:C	2.63	0.40
1:S:812:PHE:CD2	1:S:813:ALA:N	2.89	0.40
2:T:4:SER:N	2:T:7:GLN:NE2	2.61	0.40
2:T:10:GLU:O	2:T:13:GLU:N	2.55	0.40
1:V:338:ALA:O	1:V:339:MET:C	2.64	0.40
1:V:492:LEU:O	1:V:496:THR:OG1	2.37	0.40
1:V:606:ASN:OD1	1:V:606:ASN:O	2.39	0.40
1:V:630:ARG:O	1:V:631:ILE:C	2.64	0.40
1:V:704:GLN:O	1:V:708:ASN:HB2	2.21	0.40
1:V:719:GLN:HE21	1:V:719:GLN:CA	2.33	0.40
2:W:71:PRO:HA	2:W:74:GLN:CD	2.46	0.40
2:W:112:LEU:HD22	2:W:112:LEU:HA	1.91	0.40
1:S:394:ASN:OD1	1:S:397:ASP:OD1	2.39	0.40
1:S:450:LEU:HD23	1:S:450:LEU:H	1.84	0.40
1:S:458:ALA:CB	1:V:413:VAL:CG1	2.99	0.40
1:S:819:LEU:HA	1:S:822:ILE:HD12	2.03	0.40
1:S:851:LEU:N	1:S:851:LEU:CD1	2.82	0.40
2:T:80:LYS:H	2:T:80:LYS:CD	2.30	0.40
1:V:72:LYS:O	1:V:72:LYS:HG2	2.20	0.40
1:V:269:THR:HG21	1:V:443:LEU:CD1	2.32	0.40
1:V:291:TYR:O	1:V:292:TYR:C	2.65	0.40
1:V:415:GLN:OE1	1:V:416:LYS:N	2.54	0.40
1:V:619:LYS:O	1:V:622:ALA:CB	2.66	0.40
1:V:804:ARG:O	1:V:808:ALA:HB2	2.21	0.40
2:W:10:GLU:O	2:W:13:GLU:N	2.54	0.40
1:S:63:GLU:CD	1:S:63:GLU:C	2.88	0.40
1:S:370:GLU:OE1	1:S:372:ASN:HB2	2.21	0.40
1:S:849:PRO:C	1:S:851:LEU:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:35:MET:HE2	2:T:35:MET:HB3	1.94	0.40
2:T:122:GLU:O	2:T:123:GLU:C	2.65	0.40
1:V:164:MET:HE3	1:V:461:LEU:HD12	2.03	0.40
1:V:231:LEU:HD23	1:V:231:LEU:N	2.37	0.40
1:V:438:LEU:HD12	1:V:438:LEU:HA	1.80	0.40
1:V:712:GLU:C	1:V:714:ILE:N	2.78	0.40
1:V:769:ILE:HD13	1:V:769:ILE:HA	1.79	0.40
1:V:785:GLU:CD	1:V:788:ARG:HH21	2.28	0.40
1:S:17:LYS:HE2	1:S:17:LYS:HB3	1.66	0.40
1:S:102:HIS:O	1:S:103:ASN:C	2.65	0.40
1:S:275:SER:C	1:S:277:ALA:N	2.80	0.40
1:V:152:HIS:O	1:V:155:ALA:HB3	2.22	0.40
1:V:365:ILE:HD11	1:V:384:ALA:HB2	2.03	0.40
1:V:409:VAL:HG13	1:V:634:LEU:HD12	2.02	0.40
1:V:415:GLN:O	1:V:415:GLN:HG3	2.19	0.40
1:V:530:ARG:HG3	1:V:531:PRO:N	2.34	0.40
1:V:618:ASP:HB3	1:V:621:VAL:HG23	2.03	0.40
1:V:849:PRO:C	1:V:851:LEU:H	2.30	0.40
2:W:148:LEU:C	2:W:150:GLY:N	2.78	0.40
1:S:9:ASP:C	1:S:11:LYS:N	2.79	0.40
1:S:31:ALA:O	1:S:32:LYS:C	2.64	0.40
1:S:138:ILE:HG21	1:S:196:VAL:HG11	2.01	0.40
1:S:231:LEU:HD23	1:S:231:LEU:N	2.37	0.40
1:S:349:GLN:C	1:S:351:SER:N	2.78	0.40
1:S:366:VAL:O	1:S:378:MET:HE1	2.22	0.40
1:S:426:ALA:C	1:S:428:GLU:N	2.78	0.40
1:S:500:LEU:HD23	1:S:500:LEU:HA	1.91	0.40
1:S:606:ASN:OD1	1:S:606:ASN:O	2.39	0.40
1:S:663:TYR:O	1:S:666:GLN:N	2.53	0.40
1:S:809:ARG:HD2	2:T:36:ARG:O	2.21	0.40
2:T:71:PRO:HA	2:T:74:GLN:CD	2.46	0.40
1:V:37:VAL:CB	1:V:38:PRO:HD2	2.50	0.40
1:V:63:GLU:CD	1:V:63:GLU:C	2.88	0.40
1:V:735:GLU:C	1:V:737:LEU:N	2.79	0.40
1:V:747:MET:HG2	1:V:751:GLN:NE2	2.36	0.40
1:V:812:PHE:CD2	1:V:813:ALA:N	2.89	0.40
2:W:65:LYS:O	2:W:66:PHE:C	2.64	0.40
2:W:70:LEU:N	2:W:71:PRO:CD	2.84	0.40

All (92) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:61:LEU:O	1:S:70:LEU:CD1[2_665]	0.35	1.85
1:S:47:ALA:C	1:S:68:VAL:C[2_665]	0.39	1.81
1:S:38:PRO:CA	1:S:64:ASN:CB[2_665]	0.41	1.79
1:S:38:PRO:CB	1:S:64:ASN:CA[2_665]	0.60	1.60
1:S:37:VAL:CA	1:S:66:LYS:CB[2_665]	0.72	1.48
1:S:62:GLN:CA	1:S:70:LEU:CD2[2_665]	0.73	1.47
1:S:38:PRO:CG	1:S:64:ASN:C[2_665]	0.76	1.44
1:S:47:ALA:N	1:S:68:VAL:CB[2_665]	0.76	1.44
1:S:60:GLU:OE1	1:S:75:ILE:CG2[2_665]	0.82	1.38
1:S:41:LYS:CE	1:S:41:LYS:CE[2_665]	0.85	1.35
1:S:48:SER:CB	1:S:69:THR:CB[2_665]	0.97	1.23
1:S:59:VAL:C	1:S:59:VAL:CB[2_665]	0.98	1.22
1:S:33:LYS:CB	1:S:58:THR:CG2[2_665]	1.05	1.15
1:S:47:ALA:N	1:S:68:VAL:CG1[2_665]	1.06	1.14
1:S:35:VAL:CG2	1:S:67:LYS:CB[2_665]	1.18	1.02
1:S:59:VAL:C	1:S:59:VAL:CG1[2_665]	1.23	0.97
1:S:59:VAL:O	1:S:59:VAL:CG1[2_665]	1.24	0.96
1:S:48:SER:O	1:S:59:VAL:N[2_665]	1.26	0.94
1:S:59:VAL:CA	1:S:59:VAL:CA[2_665]	1.28	0.92
1:S:60:GLU:OE1	1:S:75:ILE:CB[2_665]	1.30	0.90
1:S:61:LEU:C	1:S:70:LEU:CD1[2_665]	1.33	0.87
1:S:37:VAL:N	1:S:66:LYS:CD[2_665]	1.34	0.86
2:W:78:LYS:O	2:W:80:LYS:CG[2_655]	1.35	0.85
1:S:37:VAL:CG1	1:S:66:LYS:C[2_665]	1.36	0.84
1:S:35:VAL:C	1:S:67:LYS:O[2_665]	1.40	0.80
1:S:65:GLY:C	1:S:74:ASP:O[2_665]	1.43	0.77
1:S:59:VAL:CB	1:S:60:GLU:N[2_665]	1.44	0.76
1:S:60:GLU:CD	1:S:75:ILE:CG2[2_665]	1.48	0.72
1:S:38:PRO:CB	1:S:64:ASN:CB[2_665]	1.49	0.71
2:W:49:LYS:CD	2:W:49:LYS:CD[2_655]	1.49	0.71
1:S:38:PRO:CD	1:S:64:ASN:C[2_665]	1.50	0.70
1:S:65:GLY:O	1:S:74:ASP:C[2_665]	1.50	0.70
1:S:37:VAL:N	1:S:66:LYS:CB[2_665]	1.51	0.69
1:S:37:VAL:CG1	1:S:66:LYS:O[2_665]	1.52	0.68
1:S:48:SER:N	1:S:68:VAL:O[2_665]	1.52	0.68
1:S:47:ALA:C	1:S:69:THR:N[2_665]	1.55	0.65
1:S:47:ALA:O	1:S:68:VAL:C[2_665]	1.55	0.65
1:S:48:SER:N	1:S:69:THR:N[2_665]	1.57	0.63
1:S:48:SER:CB	1:S:69:THR:OG1[2_665]	1.59	0.61
1:S:49:ILE:CB	1:S:58:THR:OG1[2_665]	1.61	0.59
1:S:37:VAL:CB	1:S:66:LYS:CA[2_665]	1.62	0.58
1:S:48:SER:C	1:S:59:VAL:N[2_665]	1.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:62:GLN:N	1:S:70:LEU:CD2[2_665]	1.67	0.53
1:S:48:SER:OG	1:S:69:THR:OG1[2_665]	1.68	0.52
1:S:38:PRO:CD	1:S:64:ASN:O[2_665]	1.74	0.46
1:S:38:PRO:CA	1:S:64:ASN:CG[2_665]	1.74	0.46
1:S:65:GLY:O	1:S:74:ASP:O[2_665]	1.75	0.45
1:S:35:VAL:CB	1:S:67:LYS:CB[2_665]	1.76	0.44
1:S:38:PRO:CB	1:S:64:ASN:N[2_665]	1.76	0.44
1:S:49:ILE:O	1:S:58:THR:OG1[2_665]	1.76	0.44
1:S:47:ALA:O	1:S:69:THR:N[2_665]	1.77	0.43
1:S:47:ALA:C	1:S:68:VAL:O[2_665]	1.78	0.42
1:S:46:ALA:C	1:S:68:VAL:CG2[2_665]	1.81	0.39
1:S:59:VAL:CA	1:S:59:VAL:CB[2_665]	1.83	0.37
1:S:50:LYS:N	1:S:50:LYS:N[2_665]	1.84	0.36
2:W:49:LYS:CE	2:W:49:LYS:CE[2_655]	1.85	0.35
1:S:49:ILE:C	1:S:58:THR:OG1[2_665]	1.88	0.32
1:S:37:VAL:N	1:S:66:LYS:CG[2_665]	1.89	0.31
1:S:47:ALA:CA	1:S:68:VAL:CA[2_665]	1.89	0.31
1:S:49:ILE:N	1:S:58:THR:C[2_665]	1.90	0.30
1:S:50:LYS:CD	1:S:57:VAL:CB[2_665]	1.91	0.29
1:S:48:SER:N	1:S:69:THR:CA[2_665]	1.95	0.25
1:S:36:TRP:O	1:S:67:LYS:N[2_665]	1.97	0.23
1:S:38:PRO:CG	1:S:64:ASN:O[2_665]	1.98	0.22
2:W:78:LYS:C	2:W:80:LYS:CB[2_655]	1.98	0.22
1:S:48:SER:N	1:S:68:VAL:C[2_665]	2.01	0.19
1:S:36:TRP:O	1:S:66:LYS:C[2_665]	2.03	0.17
1:S:45:GLU:O	1:S:66:LYS:NZ[2_665]	2.05	0.15
1:S:49:ILE:CA	1:S:58:THR:O[2_665]	2.05	0.15
1:S:62:GLN:N	1:S:70:LEU:CG[2_665]	2.05	0.15
1:S:38:PRO:CA	1:S:64:ASN:CA[2_665]	2.06	0.14
1:S:49:ILE:N	1:S:58:THR:CA[2_665]	2.06	0.14
1:S:49:ILE:C	1:S:58:THR:O[2_665]	2.06	0.14
1:S:38:PRO:CA	1:S:64:ASN:OD1[2_665]	2.07	0.13
1:S:47:ALA:CB	1:S:68:VAL:CB[2_665]	2.07	0.13
1:S:38:PRO:C	1:S:64:ASN:CG[2_665]	2.09	0.11
1:S:59:VAL:CB	1:S:59:VAL:CB[2_665]	2.09	0.11
1:S:38:PRO:C	1:S:64:ASN:CB[2_665]	2.11	0.09
1:S:49:ILE:CA	1:S:58:THR:CB[2_665]	2.11	0.09
1:S:37:VAL:CB	1:S:66:LYS:N[2_665]	2.13	0.07
1:S:47:ALA:CA	1:S:68:VAL:CB[2_665]	2.13	0.07
1:S:48:SER:CB	1:S:69:THR:CG2[2_665]	2.13	0.07
1:S:59:VAL:CA	1:S:59:VAL:CG2[2_665]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:61:LEU:C	1:S:70:LEU:CG[2_665]	2.13	0.07
1:S:41:LYS:CD	1:S:41:LYS:CE[2_665]	2.15	0.05
1:S:62:GLN:CA	1:S:70:LEU:CG[2_665]	2.15	0.05
1:S:61:LEU:O	1:S:70:LEU:CG[2_665]	2.16	0.04
1:S:67:LYS:CD	1:S:75:ILE:CD1[2_665]	2.16	0.04
1:S:36:TRP:CE3	1:S:66:LYS:NZ[2_665]	2.17	0.03
1:S:37:VAL:CA	1:S:66:LYS:CA[2_665]	2.18	0.02
1:S:41:LYS:CG	1:S:41:LYS:CG[2_665]	2.18	0.02
1:S:48:SER:OG	1:S:69:THR:CG2[2_665]	2.18	0.02

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 PDB entries followed by that with respect to all EM entries.

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	S	891/1184 (75%)	649 (73%)	178 (20%)	64 (7%)	1	11
1	V	891/1184 (75%)	651 (73%)	178 (20%)	62 (7%)	1	11
2	T	146/150 (97%)	101 (69%)	31 (21%)	14 (10%)	0	7
2	W	146/150 (97%)	101 (69%)	31 (21%)	14 (10%)	0	7
All	All	2074/2668 (78%)	1502 (72%)	418 (20%)	154 (7%)	1	10

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	145	LYS
1	S	170	ASP
1	S	383	ALA
1	S	395	VAL
1	S	414	VAL
1	S	531	PRO
1	S	614	ASN
1	S	626	LYS

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Mol	Chain	Res	Type
1	S	664	LYS
1	S	683	ARG
1	S	796	ILE
1	S	903	GLN
2	T	97	LYS
1	V	145	LYS
1	V	170	ASP
1	V	383	ALA
1	V	395	VAL
1	V	414	VAL
1	V	531	PRO
1	V	614	ASN
1	V	626	LYS
1	V	664	LYS
1	V	683	ARG
2	W	97	LYS
1	S	32	LYS
1	S	38	PRO
1	S	123	VAL
1	S	181	ALA
1	S	273	GLU
1	S	276	ARG
1	S	288	HIS
1	S	362	LEU
1	S	376	ALA
1	S	420	LYS
1	S	541	LEU
1	S	564	GLY
1	S	572	SER
1	S	606	ASN
1	S	750	LYS
2	T	56	SER
2	T	77	ALA
2	T	99	GLY
2	T	105	GLY
2	T	117	GLU
1	V	32	LYS
1	V	38	PRO
1	V	123	VAL
1	V	181	ALA
1	V	273	GLU
1	V	276	ARG

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Mol	Chain	Res	Type
1	V	288	HIS
1	V	362	LEU
1	V	376	ALA
1	V	420	LYS
1	V	541	LEU
1	V	564	GLY
1	V	572	SER
1	V	606	ASN
1	V	750	LYS
2	W	56	SER
2	W	77	ALA
2	W	99	GLY
2	W	105	GLY
2	W	117	GLU
1	S	131	PRO
1	S	304	ASP
1	S	348	GLU
1	S	533	ASN
1	S	562	GLU
1	S	727	PHE
1	S	819	LEU
1	S	820	GLU
2	T	82	GLN
2	T	148	LEU
1	V	131	PRO
1	V	304	ASP
1	V	348	GLU
1	V	533	ASN
1	V	562	GLU
1	V	727	PHE
1	V	819	LEU
1	V	820	GLU
2	W	82	GLN
2	W	148	LEU
1	S	90	ALA
1	S	106	GLU
1	S	382	THR
1	S	407	ILE
1	S	476	SER
1	S	563	GLN
1	S	579	THR
1	S	610	THR

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Mol	Chain	Res	Type
1	S	631	ILE
1	S	826	GLN
2	T	22	GLY
2	T	86	GLU
2	T	141	GLU
1	V	72	LYS
1	V	90	ALA
1	V	106	GLU
1	V	382	THR
1	V	407	ILE
1	V	476	SER
1	V	563	GLN
1	V	579	THR
1	V	610	THR
1	V	826	GLN
2	W	22	GLY
2	W	86	GLU
2	W	141	GLU
1	S	4	LYS
1	S	72	LYS
1	S	89	MET
1	S	168	ARG
1	S	233	ALA
1	S	300	GLN
1	S	534	PRO
2	T	149	SER
1	V	4	LYS
1	V	89	MET
1	V	168	ARG
1	V	233	ALA
1	V	300	GLN
1	V	534	PRO
1	V	631	ILE
2	W	149	SER
1	S	126	PRO
1	S	148	GLU
1	S	215	PHE
1	S	289	ILE
1	S	663	TYR
1	S	764	PRO
2	T	54	PRO
1	V	126	PRO

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Mol	Chain	Res	Type
1	V	148	GLU
1	V	215	PHE
1	V	289	ILE
1	V	663	TYR
1	V	764	PRO
2	W	54	PRO
1	S	240	VAL
1	S	352	ILE
1	S	849	PRO
2	T	111	VAL
1	V	240	VAL
1	V	352	ILE
1	V	849	PRO
2	W	111	VAL
1	S	410	GLY
1	S	523	PRO
1	V	410	GLY
1	V	523	PRO
1	S	235	GLY
1	V	235	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	S	717/1047 (68%)	452 (63%)	265 (37%)	0	1
1	V	717/1047 (68%)	453 (63%)	264 (37%)	0	1
2	T	127/129 (98%)	78 (61%)	49 (39%)	0	1
2	W	127/129 (98%)	77 (61%)	50 (39%)	0	1
All	All	1688/2352 (72%)	1060 (63%)	628 (37%)	1	1

All (628) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	7	SER

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Mol	Chain	Res	Type
1	S	8	ASP
1	S	11	LYS
1	S	15	VAL
1	S	17	LYS
1	S	18	ASN
1	S	21	ASN
1	S	22	ASN
1	S	24	LEU
1	S	26	GLN
1	S	33	LYS
1	S	37	VAL
1	S	41	LYS
1	S	45	GLU
1	S	52	GLU
1	S	53	LYS
1	S	61	LEU
1	S	62	GLN
1	S	66	LYS
1	S	71	SER
1	S	72	LYS
1	S	73	ASP
1	S	77	LYS
1	S	79	ASN
1	S	82	LYS
1	S	84	SER
1	S	86	VAL
1	S	89	MET
1	S	91	GLU
1	S	92	LEU
1	S	93	THR
1	S	95	LEU
1	S	99	SER
1	S	101	LEU
1	S	106	GLU
1	S	107	ARG
1	S	112	LEU
1	S	113	ILE
1	S	117	SER
1	S	121	CYS
1	S	127	TYR
1	S	134	SER
1	S	135	GLU

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Mol	Chain	Res	Type
1	S	137	ILE
1	S	144	LYS
1	S	145	LYS
1	S	146	ARG
1	S	148	GLU
1	S	162	ARG
1	S	163	SER
1	S	164	MET
1	S	165	LEU
1	S	169	GLU
1	S	171	GLN
1	S	178	GLU
1	S	183	LYS
1	S	189	LYS
1	S	194	LEU
1	S	201	HIS
1	S	211	GLN
1	S	216	SER
1	S	222	LYS
1	S	225	LEU
1	S	226	GLN
1	S	228	ASN
1	S	230	ILE
1	S	234	PHE
1	S	238	LYS
1	S	239	THR
1	S	247	ARG
1	S	250	LYS
1	S	254	ILE
1	S	258	VAL
1	S	259	THR
1	S	262	ILE
1	S	263	VAL
1	S	266	ASN
1	S	269	THR
1	S	271	LEU
1	S	272	LEU
1	S	274	LYS
1	S	282	LYS
1	S	286	THR
1	S	298	SER
1	S	299	GLU

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Mol	Chain	Res	Type
1	S	302	ARG
1	S	308	GLU
1	S	312	ASN
1	S	313	TYR
1	S	314	THR
1	S	316	LEU
1	S	317	SER
1	S	320	HIS
1	S	323	ILE
1	S	329	ASP
1	S	331	MET
1	S	335	THR
1	S	336	LEU
1	S	346	GLU
1	S	347	GLU
1	S	351	SER
1	S	352	ILE
1	S	357	SER
1	S	358	SER
1	S	360	LEU
1	S	362	LEU
1	S	365	ILE
1	S	366	VAL
1	S	368	LYS
1	S	369	LYS
1	S	370	GLU
1	S	371	ARG
1	S	372	ASN
1	S	378	MET
1	S	382	THR
1	S	391	MET
1	S	395	VAL
1	S	399	THR
1	S	401	SER
1	S	402	ILE
1	S	406	ARG
1	S	407	ILE
1	S	408	LYS
1	S	411	ARG
1	S	412	ASP
1	S	415	GLN
1	S	416	LYS

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Mol	Chain	Res	Type
1	S	418	GLN
1	S	419	THR
1	S	420	LYS
1	S	427	ILE
1	S	428	GLU
1	S	432	LYS
1	S	437	ARG
1	S	443	LEU
1	S	444	THR
1	S	445	ARG
1	S	446	VAL
1	S	447	ASN
1	S	448	LYS
1	S	450	LEU
1	S	451	ASP
1	S	459	SER
1	S	461	LEU
1	S	465	ASP
1	S	471	ILE
1	S	473	GLU
1	S	474	ILE
1	S	479	GLN
1	S	481	CYS
1	S	482	ILE
1	S	485	THR
1	S	488	LYS
1	S	489	LEU
1	S	492	LEU
1	S	494	ASN
1	S	496	THR
1	S	497	MET
1	S	502	GLN
1	S	503	GLU
1	S	504	GLU
1	S	506	GLN
1	S	513	ASN
1	S	515	ILE
1	S	521	LEU
1	S	522	GLN
1	S	525	ILE
1	S	526	GLU
1	S	530	ARG

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Mol	Chain	Res	Type
1	S	543	GLU
1	S	545	CYS
1	S	549	LYS
1	S	553	THR
1	S	560	ILE
1	S	561	GLN
1	S	563	GLN
1	S	565	ASN
1	S	568	LYS
1	S	573	LYS
1	S	575	LEU
1	S	576	LYS
1	S	577	ASP
1	S	578	LYS
1	S	579	THR
1	S	580	GLU
1	S	583	ILE
1	S	586	TYR
1	S	591	THR
1	S	595	SER
1	S	599	THR
1	S	603	ASP
1	S	607	ASP
1	S	608	ASN
1	S	610	THR
1	S	611	SER
1	S	613	LEU
1	S	615	GLN
1	S	616	SER
1	S	617	SER
1	S	619	LYS
1	S	621	VAL
1	S	623	ASP
1	S	624	LEU
1	S	626	LYS
1	S	628	VAL
1	S	630	ARG
1	S	657	ARG
1	S	659	VAL
1	S	661	GLN
1	S	662	LEU
1	S	664	LYS

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Mol	Chain	Res	Type
1	S	665	GLU
1	S	668	THR
1	S	673	THR
1	S	683	ARG
1	S	685	ILE
1	S	686	ILE
1	S	690	GLU
1	S	701	VAL
1	S	702	LEU
1	S	704	GLN
1	S	718	ARG
1	S	721	PHE
1	S	724	ARG
1	S	725	ILE
1	S	728	GLN
1	S	729	GLU
1	S	731	ARG
1	S	735	GLU
1	S	740	ASN
1	S	744	LYS
1	S	750	LYS
1	S	751	GLN
1	S	753	CYS
1	S	755	LEU
1	S	762	LEU
1	S	768	ARG
1	S	771	GLN
1	S	773	LYS
1	S	777	ARG
1	S	778	THR
1	S	781	LEU
1	S	784	LEU
1	S	790	LEU
1	S	791	LYS
1	S	792	ILE
1	S	793	THR
1	S	794	ASP
1	S	795	VAL
1	S	797	ILE
1	S	800	GLN
1	S	809	ARG
1	S	812	PHE

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Mol	Chain	Res	Type
1	S	814	LYS
1	S	815	ARG
1	S	818	GLN
1	S	819	LEU
1	S	825	ILE
1	S	828	ASN
1	S	831	SER
1	S	841	MET
1	S	843	LEU
1	S	847	ILE
1	S	851	LEU
1	S	852	LYS
2	T	10	GLU
2	T	20	ARG
2	T	21	THR
2	T	23	ASP
2	T	25	LYS
2	T	26	ILE
2	T	38	LEU
2	T	40	GLN
2	T	43	THR
2	T	47	VAL
2	T	49	LYS
2	T	50	VAL
2	T	51	LEU
2	T	53	ASN
2	T	55	LYS
2	T	57	ASP
2	T	59	MET
2	T	60	ASN
2	T	67	GLU
2	T	68	GLN
2	T	70	LEU
2	T	73	MET
2	T	74	GLN
2	T	75	THR
2	T	76	ILE
2	T	78	LYS
2	T	80	LYS
2	T	82	GLN
2	T	88	TYR
2	T	89	VAL

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Mol	Chain	Res	Type
2	T	90	GLU
2	T	98	GLU
2	T	100	ASN
2	T	103	VAL
2	T	104	MET
2	T	107	GLU
2	T	108	ILE
2	T	109	ARG
2	T	112	LEU
2	T	114	THR
2	T	119	MET
2	T	120	THR
2	T	121	GLU
2	T	132	GLU
2	T	134	SER
2	T	135	ASN
2	T	144	VAL
2	T	146	MET
2	T	147	VAL
1	V	7	SER
1	V	8	ASP
1	V	11	LYS
1	V	15	VAL
1	V	17	LYS
1	V	18	ASN
1	V	21	ASN
1	V	22	ASN
1	V	24	LEU
1	V	26	GLN
1	V	33	LYS
1	V	37	VAL
1	V	41	LYS
1	V	45	GLU
1	V	52	GLU
1	V	53	LYS
1	V	61	LEU
1	V	62	GLN
1	V	66	LYS
1	V	71	SER
1	V	72	LYS
1	V	73	ASP
1	V	77	LYS

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Mol	Chain	Res	Type
1	V	79	ASN
1	V	82	LYS
1	V	84	SER
1	V	86	VAL
1	V	89	MET
1	V	91	GLU
1	V	92	LEU
1	V	93	THR
1	V	95	LEU
1	V	99	SER
1	V	101	LEU
1	V	106	GLU
1	V	107	ARG
1	V	112	LEU
1	V	113	ILE
1	V	117	SER
1	V	121	CYS
1	V	127	TYR
1	V	134	SER
1	V	135	GLU
1	V	137	ILE
1	V	144	LYS
1	V	145	LYS
1	V	146	ARG
1	V	148	GLU
1	V	162	ARG
1	V	163	SER
1	V	164	MET
1	V	165	LEU
1	V	169	GLU
1	V	171	GLN
1	V	178	GLU
1	V	183	LYS
1	V	189	LYS
1	V	194	LEU
1	V	201	HIS
1	V	211	GLN
1	V	216	SER
1	V	222	LYS
1	V	226	GLN
1	V	228	ASN
1	V	230	ILE

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Mol	Chain	Res	Type
1	V	234	PHE
1	V	238	LYS
1	V	239	THR
1	V	247	ARG
1	V	250	LYS
1	V	254	ILE
1	V	258	VAL
1	V	259	THR
1	V	262	ILE
1	V	263	VAL
1	V	266	ASN
1	V	269	THR
1	V	271	LEU
1	V	272	LEU
1	V	274	LYS
1	V	282	LYS
1	V	286	THR
1	V	298	SER
1	V	299	GLU
1	V	302	ARG
1	V	308	GLU
1	V	312	ASN
1	V	313	TYR
1	V	314	THR
1	V	316	LEU
1	V	317	SER
1	V	320	HIS
1	V	323	ILE
1	V	329	ASP
1	V	331	MET
1	V	335	THR
1	V	336	LEU
1	V	346	GLU
1	V	347	GLU
1	V	351	SER
1	V	352	ILE
1	V	357	SER
1	V	358	SER
1	V	360	LEU
1	V	362	LEU
1	V	365	ILE
1	V	366	VAL

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Mol	Chain	Res	Type
1	V	368	LYS
1	V	369	LYS
1	V	370	GLU
1	V	371	ARG
1	V	372	ASN
1	V	378	MET
1	V	382	THR
1	V	391	MET
1	V	395	VAL
1	V	399	THR
1	V	401	SER
1	V	402	ILE
1	V	406	ARG
1	V	407	ILE
1	V	408	LYS
1	V	411	ARG
1	V	412	ASP
1	V	415	GLN
1	V	416	LYS
1	V	418	GLN
1	V	419	THR
1	V	420	LYS
1	V	427	ILE
1	V	428	GLU
1	V	432	LYS
1	V	437	ARG
1	V	443	LEU
1	V	444	THR
1	V	445	ARG
1	V	446	VAL
1	V	447	ASN
1	V	448	LYS
1	V	450	LEU
1	V	451	ASP
1	V	459	SER
1	V	461	LEU
1	V	465	ASP
1	V	471	ILE
1	V	473	GLU
1	V	474	ILE
1	V	479	GLN
1	V	481	CYS

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Mol	Chain	Res	Type
1	V	482	ILE
1	V	485	THR
1	V	488	LYS
1	V	489	LEU
1	V	492	LEU
1	V	494	ASN
1	V	496	THR
1	V	497	MET
1	V	502	GLN
1	V	503	GLU
1	V	504	GLU
1	V	506	GLN
1	V	513	ASN
1	V	515	ILE
1	V	521	LEU
1	V	522	GLN
1	V	525	ILE
1	V	526	GLU
1	V	530	ARG
1	V	543	GLU
1	V	545	CYS
1	V	549	LYS
1	V	553	THR
1	V	560	ILE
1	V	561	GLN
1	V	563	GLN
1	V	565	ASN
1	V	568	LYS
1	V	573	LYS
1	V	575	LEU
1	V	576	LYS
1	V	577	ASP
1	V	578	LYS
1	V	579	THR
1	V	580	GLU
1	V	583	ILE
1	V	586	TYR
1	V	591	THR
1	V	595	SER
1	V	599	THR
1	V	603	ASP
1	V	607	ASP

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Mol	Chain	Res	Type
1	V	608	ASN
1	V	610	THR
1	V	611	SER
1	V	613	LEU
1	V	615	GLN
1	V	616	SER
1	V	617	SER
1	V	619	LYS
1	V	621	VAL
1	V	623	ASP
1	V	624	LEU
1	V	626	LYS
1	V	628	VAL
1	V	630	ARG
1	V	657	ARG
1	V	659	VAL
1	V	661	GLN
1	V	662	LEU
1	V	664	LYS
1	V	665	GLU
1	V	668	THR
1	V	673	THR
1	V	683	ARG
1	V	685	ILE
1	V	686	ILE
1	V	690	GLU
1	V	701	VAL
1	V	702	LEU
1	V	704	GLN
1	V	718	ARG
1	V	721	PHE
1	V	724	ARG
1	V	725	ILE
1	V	728	GLN
1	V	729	GLU
1	V	731	ARG
1	V	735	GLU
1	V	740	ASN
1	V	744	LYS
1	V	750	LYS
1	V	751	GLN
1	V	753	CYS

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Mol	Chain	Res	Type
1	V	755	LEU
1	V	762	LEU
1	V	768	ARG
1	V	771	GLN
1	V	773	LYS
1	V	777	ARG
1	V	778	THR
1	V	781	LEU
1	V	784	LEU
1	V	790	LEU
1	V	791	LYS
1	V	792	ILE
1	V	793	THR
1	V	794	ASP
1	V	795	VAL
1	V	797	ILE
1	V	800	GLN
1	V	809	ARG
1	V	812	PHE
1	V	814	LYS
1	V	815	ARG
1	V	818	GLN
1	V	819	LEU
1	V	825	ILE
1	V	828	ASN
1	V	831	SER
1	V	841	MET
1	V	843	LEU
1	V	847	ILE
1	V	851	LEU
1	V	852	LYS
2	W	10	GLU
2	W	20	ARG
2	W	21	THR
2	W	23	ASP
2	W	25	LYS
2	W	26	ILE
2	W	38	LEU
2	W	40	GLN
2	W	43	THR
2	W	47	VAL
2	W	49	LYS

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Mol	Chain	Res	Type
2	W	50	VAL
2	W	51	LEU
2	W	53	ASN
2	W	55	LYS
2	W	57	ASP
2	W	59	MET
2	W	60	ASN
2	W	64	LEU
2	W	67	GLU
2	W	68	GLN
2	W	70	LEU
2	W	73	MET
2	W	74	GLN
2	W	75	THR
2	W	76	ILE
2	W	78	LYS
2	W	80	LYS
2	W	82	GLN
2	W	88	TYR
2	W	89	VAL
2	W	90	GLU
2	W	98	GLU
2	W	100	ASN
2	W	103	VAL
2	W	104	MET
2	W	107	GLU
2	W	108	ILE
2	W	109	ARG
2	W	112	LEU
2	W	114	THR
2	W	119	MET
2	W	120	THR
2	W	121	GLU
2	W	132	GLU
2	W	134	SER
2	W	135	ASN
2	W	144	VAL
2	W	146	MET
2	W	147	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	3	GLN
1	S	26	GLN
1	S	96	ASN
1	S	186	ASN
1	S	226	GLN
1	S	266	ASN
1	S	288	HIS
1	S	311	ASN
1	S	312	ASN
1	S	326	GLN
1	S	361	GLN
1	S	375	GLN
1	S	422	GLN
1	S	494	ASN
1	S	495	HIS
1	S	533	ASN
1	S	565	ASN
1	S	601	ASN
1	S	661	GLN
1	S	678	ASN
1	S	728	GLN
1	S	751	GLN
1	S	771	GLN
1	S	783	HIS
1	S	834	ASN
2	T	7	GLN
2	T	30	GLN
2	T	60	ASN
2	T	139	ASN
1	V	3	GLN
1	V	26	GLN
1	V	96	ASN
1	V	102	HIS
1	V	166	GLN
1	V	186	ASN
1	V	201	HIS
1	V	244	ASN
1	V	266	ASN
1	V	288	HIS
1	V	311	ASN
1	V	312	ASN
1	V	326	GLN
1	V	361	GLN

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Mol	Chain	Res	Type
1	V	415	GLN
1	V	422	GLN
1	V	447	ASN
1	V	494	ASN
1	V	495	HIS
1	V	533	ASN
1	V	601	ASN
1	V	661	GLN
1	V	678	ASN
1	V	728	GLN
1	V	751	GLN
1	V	771	GLN
1	V	783	HIS
1	V	834	ASN
2	W	7	GLN
2	W	30	GLN
2	W	60	ASN
2	W	79	ASN
2	W	110	HIS
2	W	135	ASN
2	W	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	S	836	1	9,10,11	0.68	0	6,11,13	0.47	0
1	MLY	S	846	1	9,10,11	0.58	0	6,11,13	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	S	842	1	9,10,11	1.13	2 (22%)	6,11,13	0.30	0
1	MLY	S	848	1	9,10,11	0.68	0	6,11,13	0.79	0
1	MLY	V	836	1	9,10,11	0.67	0	6,11,13	0.47	0
1	MLY	V	842	1	9,10,11	1.13	2 (22%)	6,11,13	0.31	0
1	MLY	V	848	1	9,10,11	0.67	0	6,11,13	0.78	0
1	MLY	V	846	1	9,10,11	0.60	0	6,11,13	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	S	836	1	-	1/8/9/11	-
1	MLY	S	846	1	-	6/8/9/11	-
1	MLY	S	842	1	-	6/8/9/11	-
1	MLY	S	848	1	-	3/8/9/11	-
1	MLY	V	836	1	-	1/8/9/11	-
1	MLY	V	842	1	-	6/8/9/11	-
1	MLY	V	848	1	-	3/8/9/11	-
1	MLY	V	846	1	-	6/8/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	842	MLY	CA-N	-2.09	1.42	1.48
1	V	842	MLY	CA-N	-2.08	1.42	1.48
1	V	842	MLY	CB-CA	-2.05	1.50	1.53
1	S	842	MLY	CB-CA	-2.04	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S	842	MLY	CD-CE-NZ-CH1
1	S	842	MLY	CD-CE-NZ-CH2
1	S	846	MLY	CD-CE-NZ-CH2
1	V	842	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	V	842	MLY	CD-CE-NZ-CH2
1	V	846	MLY	CD-CE-NZ-CH2
1	S	846	MLY	CD-CE-NZ-CH1
1	S	848	MLY	CD-CE-NZ-CH2
1	V	846	MLY	CD-CE-NZ-CH1
1	V	848	MLY	CD-CE-NZ-CH2
1	S	848	MLY	CD-CE-NZ-CH1
1	V	848	MLY	CD-CE-NZ-CH1
1	V	842	MLY	CE-CD-CG-CB
1	S	842	MLY	CE-CD-CG-CB
1	S	846	MLY	CA-CB-CG-CD
1	V	846	MLY	CA-CB-CG-CD
1	S	842	MLY	CA-CB-CG-CD
1	V	842	MLY	CA-CB-CG-CD
1	S	848	MLY	CE-CD-CG-CB
1	V	848	MLY	CE-CD-CG-CB
1	S	836	MLY	C-CA-CB-CG
1	S	842	MLY	C-CA-CB-CG
1	V	836	MLY	C-CA-CB-CG
1	V	842	MLY	C-CA-CB-CG
1	S	842	MLY	N-CA-CB-CG
1	S	846	MLY	N-CA-CB-CG
1	V	842	MLY	N-CA-CB-CG
1	V	846	MLY	N-CA-CB-CG
1	V	846	MLY	CE-CD-CG-CB
1	S	846	MLY	CE-CD-CG-CB
1	S	846	MLY	C-CA-CB-CG
1	V	846	MLY	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S	846	MLY	1	0
1	S	848	MLY	4	0
1	V	848	MLY	4	0
1	V	846	MLY	1	0

5.5 Carbohydrates

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S	6
1	V	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	852:LYS	C	853:VAL	N	5.40
1	V	903:GLN	C	904:ALA	N	3.37
1	S	860:MET	C	861:GLN	N	2.66
1	V	852:LYS	C	853:VAL	N	2.29
1	S	854:THR	C	855:ARG	N	2.18
1	V	860:MET	C	861:GLN	N	2.16
1	S	819:LEU	C	820:GLU	N	1.95
1	V	819:LEU	C	820:GLU	N	1.95
1	S	903:GLN	C	904:ALA	N	1.86
1	S	796:ILE	C	797:ILE	N	1.72