



Full wwPDB EM Validation Report (i)

Oct 5, 2024 – 11:46 PM JST

PDB ID : 5Y4O
EMDB ID : EMD-6805
Title : Cryo-EM structure of MscS channel, YnaI
Authors : Zhang, Y.; Yu, J.
Deposited on : 2017-08-04
Resolution : 3.80 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 (i) 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 \(i\)](#)) were used in the production of this report:

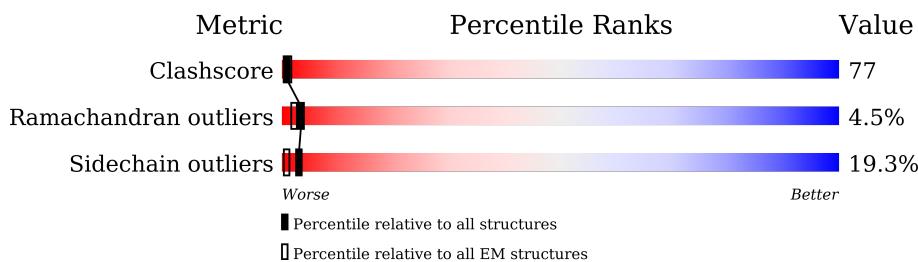
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12341 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 Low conductance mechanosensitive channel YnaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	223	1763	1138	296	320	9	0	0
1	B	223	1763	1138	296	320	9	0	0
1	C	223	1763	1138	296	320	9	0	0
1	D	223	1763	1138	296	320	9	0	0
1	E	223	1763	1138	296	320	9	0	0
1	F	223	1763	1138	296	320	9	0	0
1	G	223	1763	1138	296	320	9	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	HIS	-	expression tag	UNP P0AEB6
A	345	HIS	-	expression tag	UNP P0AEB6
A	346	HIS	-	expression tag	UNP P0AEB6
A	347	HIS	-	expression tag	UNP P0AEB6
A	348	HIS	-	expression tag	UNP P0AEB6
A	349	HIS	-	expression tag	UNP P0AEB6
B	344	HIS	-	expression tag	UNP P0AEB6
B	345	HIS	-	expression tag	UNP P0AEB6
B	346	HIS	-	expression tag	UNP P0AEB6
B	347	HIS	-	expression tag	UNP P0AEB6
B	348	HIS	-	expression tag	UNP P0AEB6
B	349	HIS	-	expression tag	UNP P0AEB6
C	344	HIS	-	expression tag	UNP P0AEB6
C	345	HIS	-	expression tag	UNP P0AEB6
C	346	HIS	-	expression tag	UNP P0AEB6
C	347	HIS	-	expression tag	UNP P0AEB6

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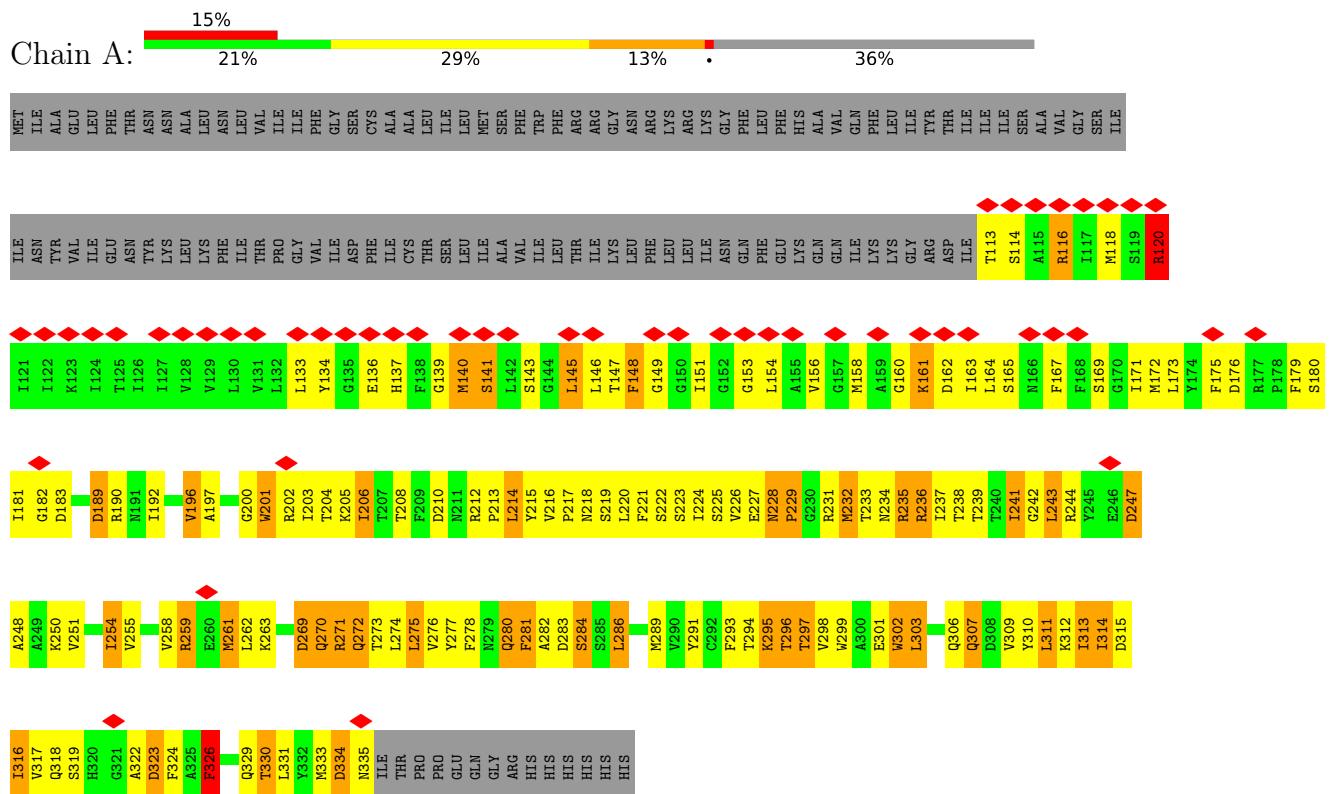
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Chain	Residue	Modelled	Actual	Comment	Reference
C	348	HIS	-	expression tag	UNP P0AEB6
C	349	HIS	-	expression tag	UNP P0AEB6
D	344	HIS	-	expression tag	UNP P0AEB6
D	345	HIS	-	expression tag	UNP P0AEB6
D	346	HIS	-	expression tag	UNP P0AEB6
D	347	HIS	-	expression tag	UNP P0AEB6
D	348	HIS	-	expression tag	UNP P0AEB6
D	349	HIS	-	expression tag	UNP P0AEB6
E	344	HIS	-	expression tag	UNP P0AEB6
E	345	HIS	-	expression tag	UNP P0AEB6
E	346	HIS	-	expression tag	UNP P0AEB6
E	347	HIS	-	expression tag	UNP P0AEB6
E	348	HIS	-	expression tag	UNP P0AEB6
E	349	HIS	-	expression tag	UNP P0AEB6
F	344	HIS	-	expression tag	UNP P0AEB6
F	345	HIS	-	expression tag	UNP P0AEB6
F	346	HIS	-	expression tag	UNP P0AEB6
F	347	HIS	-	expression tag	UNP P0AEB6
F	348	HIS	-	expression tag	UNP P0AEB6
F	349	HIS	-	expression tag	UNP P0AEB6
G	344	HIS	-	expression tag	UNP P0AEB6
G	345	HIS	-	expression tag	UNP P0AEB6
G	346	HIS	-	expression tag	UNP P0AEB6
G	347	HIS	-	expression tag	UNP P0AEB6
G	348	HIS	-	expression tag	UNP P0AEB6
G	349	HIS	-	expression tag	UNP P0AEB6

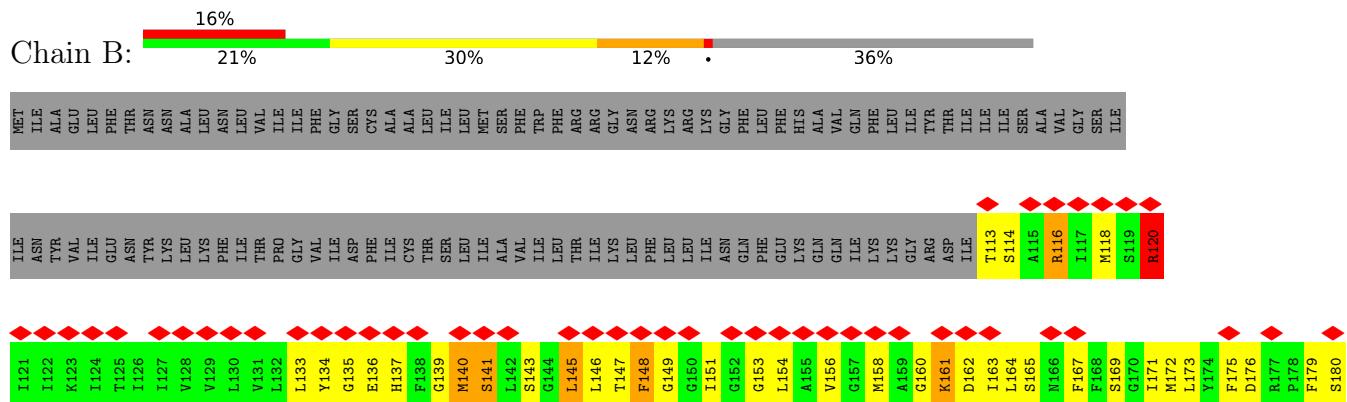
3 Residue-property plots

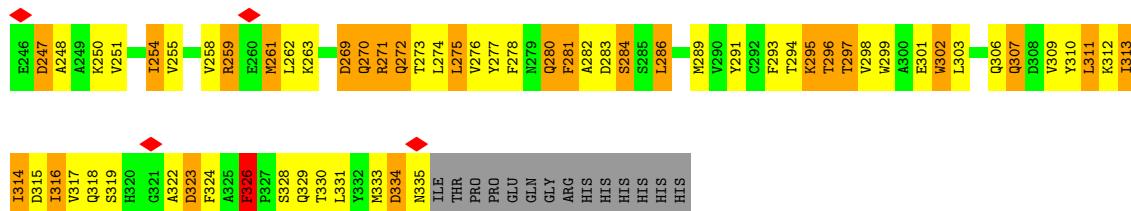
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Low conductance mechanosensitive channel YnaI

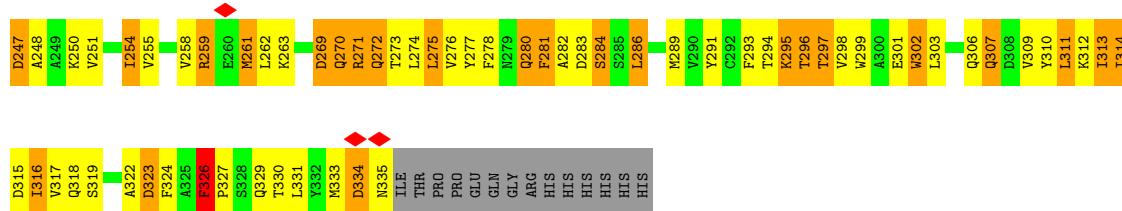
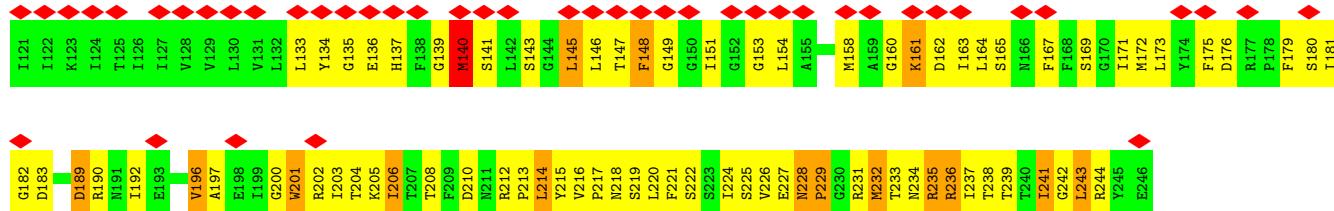
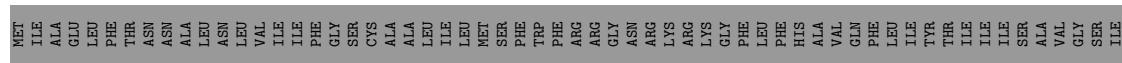
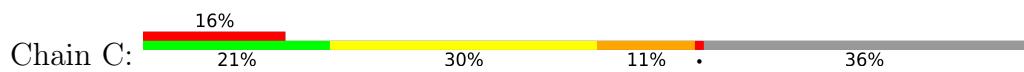


- Molecule 1: Low conductance mechanosensitive channel YnaI

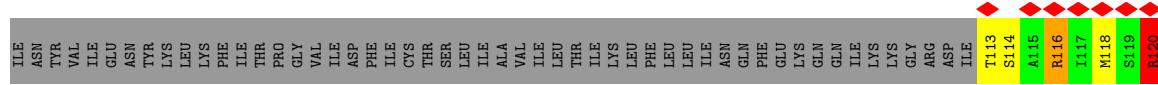
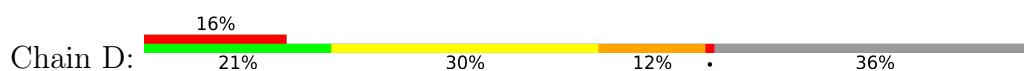


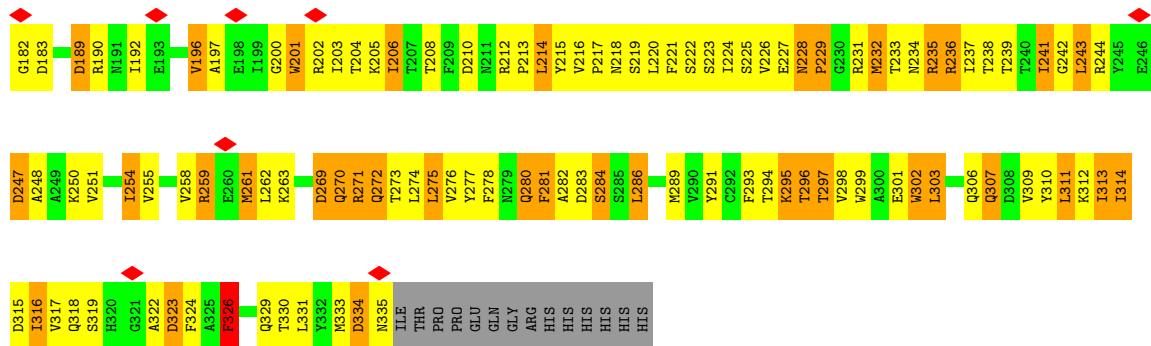


• Molecule 1: Low conductance mechanosensitive channel YnaI

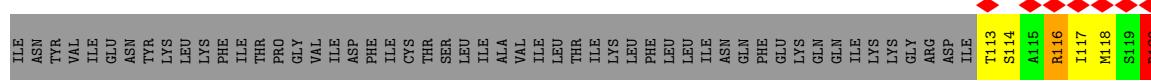


• Molecule 1: Low conductance mechanosensitive channel YnaI

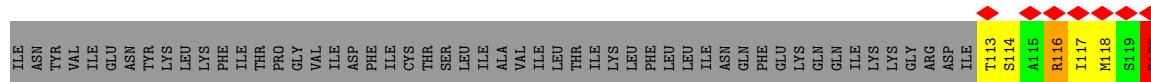
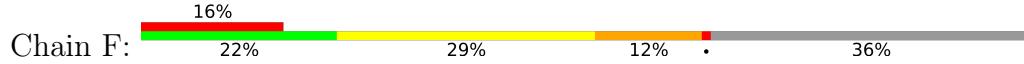




- Molecule 1: Low conductance mechanosensitive channel YnaI

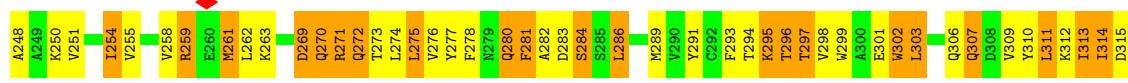
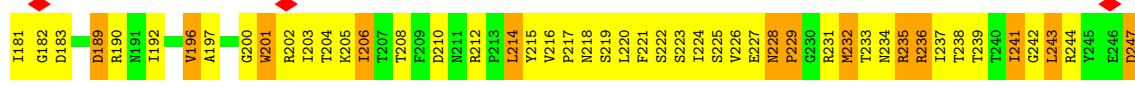
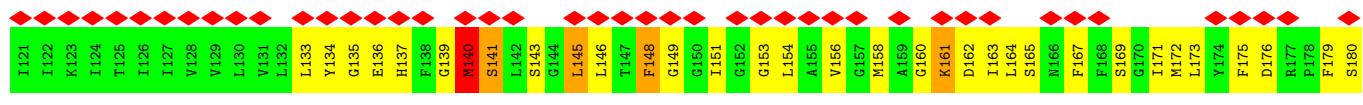
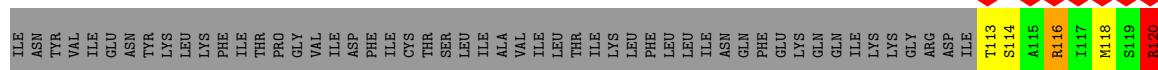
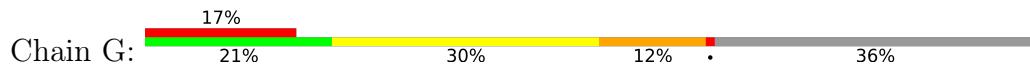


- Molecule 1: Low conductance mechanosensitive channel YnaI





- Molecule 1: Low conductance mechanosensitive channel YnaI



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	42000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.438	Depositor
Minimum map value	-0.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0745	Depositor
Map size (Å)	190.08, 190.08, 190.08	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.13	6/1801 (0.3%)	1.16	13/2443 (0.5%)
1	B	1.11	6/1801 (0.3%)	1.14	14/2443 (0.6%)
1	C	1.07	6/1801 (0.3%)	1.10	14/2443 (0.6%)
1	D	1.07	5/1801 (0.3%)	1.14	14/2443 (0.6%)
1	E	1.20	7/1801 (0.4%)	1.16	15/2443 (0.6%)
1	F	1.16	6/1801 (0.3%)	1.23	15/2443 (0.6%)
1	G	1.09	6/1801 (0.3%)	1.13	14/2443 (0.6%)
All	All	1.12	42/12607 (0.3%)	1.15	99/17101 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
All	All	0	21

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	148	PHE	C-N	27.53	1.82	1.33
1	F	148	PHE	C-N	27.50	1.82	1.33
1	B	148	PHE	C-N	27.49	1.82	1.33
1	A	148	PHE	C-N	27.48	1.82	1.33
1	D	148	PHE	C-N	27.47	1.82	1.33
1	G	148	PHE	C-N	27.46	1.82	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	PHE	C-N	27.43	1.82	1.33
1	E	140	MET	C-N	-23.22	0.80	1.34
1	F	140	MET	C-N	-19.40	0.89	1.34
1	A	140	MET	C-N	-14.59	1.00	1.34
1	B	140	MET	C-N	-11.78	1.06	1.34
1	G	140	MET	C-N	-8.99	1.13	1.34
1	A	113	THR	N-CA	5.84	1.58	1.46
1	B	113	THR	N-CA	5.83	1.58	1.46
1	G	113	THR	N-CA	5.83	1.57	1.46
1	D	113	THR	N-CA	5.81	1.57	1.46
1	F	113	THR	N-CA	5.79	1.57	1.46
1	E	113	THR	N-CA	5.79	1.57	1.46
1	C	113	THR	N-CA	5.78	1.57	1.46
1	D	143	SER	CA-CB	5.71	1.61	1.52
1	A	143	SER	CA-CB	5.69	1.61	1.52
1	C	143	SER	CA-CB	5.67	1.61	1.52
1	E	143	SER	CA-CB	5.65	1.61	1.52
1	F	143	SER	CA-CB	5.65	1.61	1.52
1	B	143	SER	CA-CB	5.64	1.61	1.52
1	G	143	SER	CA-CB	5.63	1.61	1.52
1	E	120	ARG	CD-NE	5.62	1.55	1.46
1	G	120	ARG	CD-NE	5.61	1.55	1.46
1	A	120	ARG	CD-NE	5.55	1.55	1.46
1	F	120	ARG	CD-NE	5.53	1.55	1.46
1	D	120	ARG	CD-NE	5.53	1.55	1.46
1	B	120	ARG	CD-NE	5.50	1.55	1.46
1	C	120	ARG	CD-NE	5.50	1.55	1.46
1	F	229	PRO	N-CD	5.13	1.55	1.47
1	A	229	PRO	N-CD	5.13	1.55	1.47
1	G	229	PRO	N-CD	5.10	1.54	1.47
1	E	229	PRO	N-CD	5.09	1.54	1.47
1	D	229	PRO	N-CD	5.08	1.54	1.47
1	B	229	PRO	N-CD	5.07	1.54	1.47
1	C	229	PRO	N-CD	5.06	1.54	1.47
1	E	327	PRO	N-CD	5.04	1.54	1.47
1	C	327	PRO	N-CD	5.03	1.54	1.47

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	140	MET	CA-C-N	-24.00	64.40	117.20
1	A	140	MET	CA-C-N	-23.51	65.47	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	MET	CA-C-N	-20.24	72.68	117.20
1	B	140	MET	CA-C-N	-20.01	73.17	117.20
1	D	140	MET	CA-C-N	-18.72	76.02	117.20
1	G	140	MET	CA-C-N	-17.84	77.96	117.20
1	F	140	MET	O-C-N	-17.14	95.28	122.70
1	E	148	PHE	CA-C-N	-14.45	87.30	116.20
1	G	148	PHE	CA-C-N	-14.44	87.33	116.20
1	D	148	PHE	CA-C-N	-14.43	87.35	116.20
1	A	148	PHE	CA-C-N	-14.43	87.35	116.20
1	B	148	PHE	CA-C-N	-14.43	87.35	116.20
1	C	148	PHE	CA-C-N	-14.43	87.35	116.20
1	F	148	PHE	CA-C-N	-14.42	87.35	116.20
1	D	148	PHE	O-C-N	13.64	146.39	123.20
1	G	148	PHE	O-C-N	13.63	146.38	123.20
1	F	148	PHE	O-C-N	13.63	146.37	123.20
1	A	148	PHE	O-C-N	13.63	146.37	123.20
1	C	148	PHE	O-C-N	13.63	146.36	123.20
1	E	148	PHE	O-C-N	13.62	146.35	123.20
1	B	148	PHE	O-C-N	13.61	146.34	123.20
1	C	140	MET	CA-C-N	-12.14	90.50	117.20
1	F	140	MET	C-N-CA	-11.92	91.90	121.70
1	E	140	MET	O-C-N	-11.51	104.28	122.70
1	C	140	MET	O-C-N	-10.37	106.11	122.70
1	E	148	PHE	C-N-CA	-9.57	102.21	122.30
1	B	148	PHE	C-N-CA	-9.55	102.25	122.30
1	F	148	PHE	C-N-CA	-9.55	102.25	122.30
1	G	148	PHE	C-N-CA	-9.54	102.26	122.30
1	A	148	PHE	C-N-CA	-9.54	102.26	122.30
1	D	148	PHE	C-N-CA	-9.54	102.27	122.30
1	C	148	PHE	C-N-CA	-9.53	102.28	122.30
1	D	140	MET	O-C-N	-9.09	108.16	122.70
1	C	118	MET	CG-SD-CE	-7.96	87.46	100.20
1	A	118	MET	CG-SD-CE	-7.96	87.46	100.20
1	F	118	MET	CG-SD-CE	-7.95	87.48	100.20
1	D	118	MET	CG-SD-CE	-7.95	87.48	100.20
1	G	118	MET	CG-SD-CE	-7.94	87.49	100.20
1	E	118	MET	CG-SD-CE	-7.92	87.52	100.20
1	B	118	MET	CG-SD-CE	-7.92	87.53	100.20
1	G	140	MET	O-C-N	-7.82	110.18	122.70
1	B	140	MET	O-C-N	-7.39	110.87	122.70
1	E	140	MET	C-N-CA	-6.92	104.40	121.70
1	G	133	LEU	CB-CG-CD2	6.08	121.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	LEU	CB-CG-CD2	6.06	121.31	111.00
1	B	133	LEU	CB-CG-CD2	6.05	121.29	111.00
1	D	133	LEU	CB-CG-CD2	6.05	121.29	111.00
1	E	133	LEU	CB-CG-CD2	6.05	121.29	111.00
1	A	133	LEU	CB-CG-CD2	6.05	121.28	111.00
1	F	133	LEU	CB-CG-CD2	6.03	121.25	111.00
1	B	137	HIS	CB-CA-C	-5.84	98.72	110.40
1	E	137	HIS	CB-CA-C	-5.83	98.73	110.40
1	F	137	HIS	CB-CA-C	-5.83	98.75	110.40
1	D	137	HIS	CB-CA-C	-5.82	98.75	110.40
1	G	116	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	137	HIS	CB-CA-C	-5.81	98.78	110.40
1	G	137	HIS	CB-CA-C	-5.80	98.80	110.40
1	A	137	HIS	CB-CA-C	-5.80	98.81	110.40
1	E	116	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	228	ASN	C-N-CD	5.73	140.43	128.40
1	B	228	ASN	C-N-CD	5.71	140.39	128.40
1	G	228	ASN	C-N-CD	5.71	140.38	128.40
1	A	116	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	228	ASN	C-N-CD	5.70	140.36	128.40
1	F	326	PHE	C-N-CD	5.69	140.35	128.40
1	A	134	TYR	CG-CD2-CE2	5.69	125.85	121.30
1	D	228	ASN	C-N-CD	5.69	140.35	128.40
1	E	228	ASN	C-N-CD	5.69	140.35	128.40
1	C	326	PHE	C-N-CD	5.68	140.33	128.40
1	E	134	TYR	CG-CD2-CE2	5.68	125.85	121.30
1	F	228	ASN	C-N-CD	5.68	140.32	128.40
1	A	326	PHE	C-N-CD	5.67	140.32	128.40
1	D	326	PHE	C-N-CD	5.67	140.31	128.40
1	G	326	PHE	C-N-CD	5.67	140.31	128.40
1	D	116	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	326	PHE	C-N-CD	5.67	140.30	128.40
1	G	134	TYR	CG-CD2-CE2	5.67	125.83	121.30
1	E	326	PHE	C-N-CD	5.66	140.29	128.40
1	D	134	TYR	CG-CD2-CE2	5.65	125.82	121.30
1	B	116	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	134	TYR	CG-CD2-CE2	5.64	125.81	121.30
1	F	116	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	116	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	134	TYR	CG-CD2-CE2	5.57	125.76	121.30
1	A	334	ASP	N-CA-C	5.57	126.05	111.00
1	F	334	ASP	N-CA-C	5.57	126.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	334	ASP	N-CA-C	5.57	126.05	111.00
1	F	134	TYR	CG-CD2-CE2	5.56	125.75	121.30
1	D	334	ASP	N-CA-C	5.55	126.00	111.00
1	B	334	ASP	N-CA-C	5.55	125.99	111.00
1	C	334	ASP	N-CA-C	5.55	125.99	111.00
1	E	334	ASP	N-CA-C	5.55	125.98	111.00
1	G	137	HIS	N-CA-CB	5.16	119.89	110.60
1	A	137	HIS	N-CA-CB	5.15	119.87	110.60
1	E	137	HIS	N-CA-CB	5.15	119.87	110.60
1	D	137	HIS	N-CA-CB	5.14	119.84	110.60
1	C	137	HIS	N-CA-CB	5.13	119.84	110.60
1	F	137	HIS	N-CA-CB	5.13	119.83	110.60
1	B	137	HIS	N-CA-CB	5.11	119.80	110.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ARG	Sidechain
1	A	140	MET	Peptide, Mainchain
1	B	120	ARG	Sidechain
1	B	140	MET	Peptide, Mainchain
1	C	120	ARG	Sidechain
1	C	140	MET	Peptide, Mainchain
1	D	120	ARG	Sidechain
1	D	140	MET	Peptide, Mainchain
1	E	120	ARG	Sidechain
1	E	140	MET	Peptide, Mainchain
1	F	120	ARG	Sidechain
1	F	140	MET	Peptide, Mainchain
1	G	120	ARG	Sidechain
1	G	140	MET	Peptide, Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1767	327	0
1	B	1763	0	1767	329	0
1	C	1763	0	1768	341	0
1	D	1763	0	1769	353	0
1	E	1763	0	1767	363	0
1	F	1763	0	1768	360	0
1	G	1763	0	1766	340	0
All	All	12341	0	12372	1910	0

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 (1910) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PHE:HZ	1:D:120:ARG:CZ	1.07	1.59
1:D:167:PHE:CZ	1:E:120:ARG:NH1	1.68	1.57
1:F:167:PHE:CZ	1:G:120:ARG:NH1	1.70	1.57
1:C:167:PHE:CZ	1:D:120:ARG:CZ	1.89	1.55
1:D:167:PHE:HZ	1:E:120:ARG:CZ	1.11	1.54
1:F:167:PHE:HZ	1:G:120:ARG:CZ	1.14	1.54
1:D:167:PHE:CZ	1:E:120:ARG:CZ	1.84	1.54
1:E:167:PHE:CZ	1:F:120:ARG:CZ	1.92	1.51
1:C:167:PHE:CZ	1:D:120:ARG:NH1	1.73	1.51
1:B:236:ARG:HB2	1:B:293:PHE:CE1	1.47	1.49
1:A:236:ARG:HB2	1:A:293:PHE:CE1	1.47	1.48
1:C:236:ARG:HB2	1:C:293:PHE:CE1	1.47	1.48
1:F:236:ARG:HB2	1:F:293:PHE:CE1	1.47	1.48
1:D:236:ARG:HB2	1:D:293:PHE:CE1	1.47	1.46
1:G:236:ARG:HB2	1:G:293:PHE:CE1	1.47	1.46
1:E:236:ARG:HB2	1:E:293:PHE:CE1	1.47	1.46
1:F:167:PHE:CZ	1:G:120:ARG:CZ	1.94	1.43
1:E:167:PHE:HZ	1:F:120:ARG:CZ	1.27	1.43
1:F:269:ASP:OD1	1:F:272:GLN:CB	1.67	1.42
1:C:269:ASP:OD1	1:C:272:GLN:CB	1.67	1.40
1:D:269:ASP:OD1	1:D:272:GLN:CB	1.67	1.40
1:A:269:ASP:OD1	1:A:272:GLN:CB	1.67	1.40
1:B:269:ASP:OD1	1:B:272:GLN:CB	1.67	1.40
1:G:269:ASP:OD1	1:G:272:GLN:CB	1.67	1.40
1:E:269:ASP:OD1	1:E:272:GLN:CB	1.67	1.40
1:D:148:PHE:C	1:D:149:GLY:N	1.82	1.33
1:E:148:PHE:C	1:E:149:GLY:N	1.82	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PHE:C	1:F:149:GLY:N	1.82	1.33
1:F:278:PHE:HE1	1:F:286:LEU:CD2	1.42	1.32
1:B:278:PHE:HE1	1:B:286:LEU:CD2	1.42	1.32
1:G:148:PHE:C	1:G:149:GLY:N	1.82	1.32
1:D:278:PHE:HE1	1:D:286:LEU:CD2	1.42	1.32
1:B:261:MET:SD	1:B:262:LEU:HD23	1.68	1.32
1:C:148:PHE:C	1:C:149:GLY:N	1.82	1.32
1:C:278:PHE:HE1	1:C:286:LEU:CD2	1.42	1.32
1:E:261:MET:SD	1:E:262:LEU:HD23	1.69	1.32
1:G:278:PHE:HE1	1:G:286:LEU:CD2	1.42	1.32
1:C:261:MET:SD	1:C:262:LEU:HD23	1.69	1.31
1:D:176:ASP:OD2	1:E:202:ARG:HD2	1.21	1.31
1:D:261:MET:SD	1:D:262:LEU:HD23	1.69	1.31
1:A:261:MET:SD	1:A:262:LEU:HD23	1.69	1.31
1:E:278:PHE:HE1	1:E:286:LEU:CD2	1.42	1.31
1:G:261:MET:SD	1:G:262:LEU:HD23	1.68	1.31
1:A:235:ARG:NH1	1:A:297:THR:O	1.64	1.31
1:E:235:ARG:NH1	1:E:297:THR:O	1.64	1.31
1:B:148:PHE:C	1:B:149:GLY:N	1.82	1.30
1:D:167:PHE:CE2	1:E:120:ARG:NH1	1.97	1.30
1:F:235:ARG:NH1	1:F:297:THR:O	1.64	1.30
1:F:261:MET:SD	1:F:262:LEU:HD23	1.68	1.30
1:A:148:PHE:C	1:A:149:GLY:N	1.82	1.30
1:A:278:PHE:HE1	1:A:286:LEU:CD2	1.42	1.30
1:B:235:ARG:NH1	1:B:297:THR:O	1.64	1.30
1:E:176:ASP:OD2	1:F:202:ARG:HD2	1.22	1.29
1:G:235:ARG:NH1	1:G:297:THR:O	1.64	1.29
1:F:231:ARG:NH2	1:G:215:TYR:OH	1.61	1.28
1:D:235:ARG:NH1	1:D:297:THR:O	1.64	1.28
1:C:231:ARG:NH2	1:D:215:TYR:OH	1.64	1.27
1:D:278:PHE:HB2	1:E:307:GLN:OE1	1.34	1.27
1:E:278:PHE:HB2	1:F:307:GLN:OE1	1.31	1.27
1:C:176:ASP:OD2	1:D:202:ARG:HD2	1.13	1.27
1:C:235:ARG:NH1	1:C:297:THR:O	1.64	1.27
1:A:151:ILE:CD1	1:G:153:GLY:HA2	1.63	1.26
1:E:167:PHE:CE2	1:F:120:ARG:NH1	2.04	1.26
1:F:167:PHE:HZ	1:G:120:ARG:NH1	1.08	1.26
1:B:176:ASP:OD2	1:C:202:ARG:HD2	1.13	1.25
1:A:202:ARG:HD2	1:G:176:ASP:OD2	1.17	1.25
1:A:176:ASP:OD2	1:B:202:ARG:HD2	1.19	1.25
1:C:236:ARG:CB	1:C:293:PHE:HE1	1.50	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:PHE:CZ	1:F:120:ARG:NH1	2.01	1.25
1:A:236:ARG:CB	1:A:293:PHE:HE1	1.50	1.25
1:E:236:ARG:CB	1:E:293:PHE:HE1	1.50	1.25
1:G:236:ARG:CB	1:G:293:PHE:HE1	1.50	1.24
1:F:236:ARG:CB	1:F:293:PHE:HE1	1.50	1.24
1:D:236:ARG:CB	1:D:293:PHE:HE1	1.50	1.24
1:F:176:ASP:OD2	1:G:202:ARG:HD2	1.09	1.24
1:B:236:ARG:CB	1:B:293:PHE:HE1	1.50	1.22
1:E:278:PHE:CB	1:F:307:GLN:OE1	1.86	1.22
1:C:167:PHE:CE2	1:D:120:ARG:NH1	2.07	1.22
1:A:307:GLN:OE1	1:G:278:PHE:CB	1.89	1.21
1:B:231:ARG:NH2	1:C:215:TYR:OH	1.70	1.20
1:C:244:ARG:HD2	1:C:323:ASP:OD2	1.41	1.20
1:B:244:ARG:HD2	1:B:323:ASP:OD2	1.41	1.20
1:B:278:PHE:HB2	1:C:307:GLN:OE1	1.39	1.20
1:C:278:PHE:HB2	1:D:307:GLN:OE1	1.40	1.20
1:D:244:ARG:HD2	1:D:323:ASP:OD2	1.41	1.20
1:C:176:ASP:OD2	1:D:202:ARG:CD	1.91	1.19
1:D:153:GLY:HA2	1:E:151:ILE:CD1	1.72	1.19
1:D:278:PHE:CB	1:E:307:GLN:OE1	1.87	1.19
1:F:176:ASP:OD2	1:G:202:ARG:CD	1.89	1.19
1:A:307:GLN:OE1	1:G:278:PHE:HB2	1.39	1.19
1:A:231:ARG:NH2	1:B:215:TYR:OH	1.73	1.19
1:E:153:GLY:HA2	1:F:151:ILE:CD1	1.73	1.18
1:F:167:PHE:CE2	1:G:120:ARG:NH1	2.11	1.18
1:A:244:ARG:HD2	1:A:323:ASP:OD2	1.41	1.18
1:E:231:ARG:NH2	1:F:215:TYR:OH	1.76	1.18
1:A:278:PHE:HB2	1:B:307:GLN:OE1	1.40	1.18
1:E:244:ARG:HD2	1:E:323:ASP:OD2	1.41	1.17
1:B:278:PHE:CB	1:C:307:GLN:OE1	1.93	1.17
1:G:244:ARG:CD	1:G:323:ASP:OD2	1.93	1.16
1:A:244:ARG:CD	1:A:323:ASP:OD2	1.93	1.16
1:B:148:PHE:O	1:B:151:ILE:HG22	1.44	1.16
1:F:244:ARG:CD	1:F:323:ASP:OD2	1.93	1.16
1:C:309:VAL:O	1:C:313:ILE:HG22	1.46	1.15
1:E:148:PHE:O	1:E:151:ILE:HG22	1.44	1.15
1:G:244:ARG:HD2	1:G:323:ASP:OD2	1.41	1.15
1:A:278:PHE:CB	1:B:307:GLN:OE1	1.93	1.15
1:D:309:VAL:O	1:D:313:ILE:HG22	1.46	1.15
1:B:176:ASP:OD2	1:C:202:ARG:CD	1.94	1.15
1:B:309:VAL:O	1:B:313:ILE:HG22	1.46	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PHE:O	1:C:151:ILE:HG22	1.44	1.15
1:C:244:ARG:CD	1:C:323:ASP:OD2	1.93	1.15
1:F:148:PHE:O	1:F:151:ILE:HG22	1.44	1.15
1:D:231:ARG:NH2	1:E:215:TYR:OH	1.78	1.15
1:A:148:PHE:O	1:A:151:ILE:HG22	1.44	1.15
1:B:244:ARG:CD	1:B:323:ASP:OD2	1.93	1.15
1:C:278:PHE:CB	1:D:307:GLN:OE1	1.94	1.15
1:F:333:MET:CE	1:G:333:MET:SD	2.35	1.14
1:B:222:SER:OG	1:C:163:ILE:CD1	1.96	1.14
1:D:244:ARG:CD	1:D:323:ASP:OD2	1.93	1.14
1:E:244:ARG:CD	1:E:323:ASP:OD2	1.93	1.14
1:G:148:PHE:O	1:G:151:ILE:HG22	1.44	1.14
1:B:153:GLY:HA2	1:C:151:ILE:HD13	1.27	1.14
1:E:309:VAL:O	1:E:313:ILE:HG22	1.46	1.14
1:F:244:ARG:HD2	1:F:323:ASP:OD2	1.41	1.14
1:A:309:VAL:O	1:A:313:ILE:HG22	1.47	1.14
1:D:148:PHE:O	1:D:151:ILE:HG22	1.44	1.13
1:A:215:TYR:OH	1:G:231:ARG:NH2	1.81	1.13
1:C:248:ALA:O	1:C:251:VAL:HG13	1.48	1.13
1:E:248:ALA:O	1:E:251:VAL:HG13	1.48	1.13
1:F:309:VAL:O	1:F:313:ILE:HG22	1.46	1.12
1:A:153:GLY:HA2	1:B:151:ILE:CD1	1.79	1.12
1:A:248:ALA:O	1:A:251:VAL:HG13	1.48	1.12
1:D:248:ALA:O	1:D:251:VAL:HG13	1.48	1.12
1:G:309:VAL:O	1:G:313:ILE:HG22	1.47	1.12
1:C:153:GLY:HA2	1:D:151:ILE:HD13	1.25	1.11
1:G:248:ALA:O	1:G:251:VAL:HG13	1.48	1.11
1:D:278:PHE:CE1	1:D:286:LEU:CD2	2.34	1.11
1:F:248:ALA:O	1:F:251:VAL:HG13	1.48	1.11
1:G:251:VAL:O	1:G:255:VAL:HG23	1.51	1.11
1:B:248:ALA:O	1:B:251:VAL:HG13	1.48	1.11
1:C:167:PHE:CZ	1:D:120:ARG:NH2	2.19	1.11
1:D:153:GLY:HA2	1:E:151:ILE:HD13	1.14	1.11
1:F:278:PHE:CE1	1:F:286:LEU:CD2	2.34	1.11
1:B:251:VAL:O	1:B:255:VAL:HG23	1.51	1.10
1:C:167:PHE:HZ	1:D:120:ARG:NH1	1.16	1.10
1:C:278:PHE:CE1	1:C:286:LEU:CD2	2.34	1.10
1:E:278:PHE:CE1	1:E:286:LEU:CD2	2.34	1.10
1:A:278:PHE:CE1	1:A:286:LEU:CD2	2.34	1.10
1:A:153:GLY:HA2	1:B:151:ILE:HD13	1.23	1.09
1:B:278:PHE:CE1	1:B:286:LEU:CD2	2.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:VAL:O	1:E:255:VAL:HG23	1.51	1.09
1:F:222:SER:OG	1:G:163:ILE:CD1	2.00	1.09
1:G:278:PHE:CE1	1:G:286:LEU:CD2	2.34	1.09
1:A:176:ASP:OD2	1:B:202:ARG:CD	2.00	1.08
1:A:222:SER:OG	1:B:163:ILE:CD1	2.01	1.08
1:A:251:VAL:O	1:A:255:VAL:HG23	1.51	1.08
1:D:251:VAL:O	1:D:255:VAL:HG23	1.51	1.08
1:G:278:PHE:HE1	1:G:286:LEU:HD21	1.18	1.08
1:E:153:GLY:HA2	1:F:151:ILE:HD13	1.14	1.08
1:B:206:ILE:CG2	1:B:214:LEU:HD23	1.84	1.08
1:C:206:ILE:CG2	1:C:214:LEU:HD23	1.84	1.07
1:A:206:ILE:CG2	1:A:214:LEU:HD23	1.84	1.07
1:F:251:VAL:O	1:F:255:VAL:HG23	1.51	1.07
1:E:278:PHE:HE1	1:E:286:LEU:HD21	1.18	1.07
1:B:153:GLY:HA2	1:C:151:ILE:CD1	1.84	1.07
1:D:176:ASP:OD2	1:E:202:ARG:CD	2.03	1.07
1:D:206:ILE:CG2	1:D:214:LEU:HD23	1.84	1.07
1:A:278:PHE:HE1	1:A:286:LEU:HD21	1.17	1.06
1:D:278:PHE:HE1	1:D:286:LEU:HD21	1.17	1.06
1:A:202:ARG:CD	1:G:176:ASP:OD2	2.02	1.06
1:C:251:VAL:O	1:C:255:VAL:HG23	1.51	1.06
1:E:206:ILE:CG2	1:E:214:LEU:HD23	1.84	1.06
1:G:206:ILE:CG2	1:G:214:LEU:HD23	1.84	1.06
1:E:176:ASP:OD2	1:F:202:ARG:CD	2.03	1.06
1:F:206:ILE:CG2	1:F:214:LEU:HD23	1.84	1.06
1:F:153:GLY:HA2	1:G:151:ILE:HD13	1.34	1.05
1:B:206:ILE:HG23	1:B:214:LEU:HD23	1.06	1.05
1:C:206:ILE:HG23	1:C:214:LEU:HD23	1.06	1.05
1:D:206:ILE:HG23	1:D:214:LEU:HD23	1.06	1.05
1:D:247:ASP:OD1	1:D:322:ALA:HB2	1.56	1.05
1:E:247:ASP:OD1	1:E:322:ALA:HB2	1.56	1.05
1:F:278:PHE:HE1	1:F:286:LEU:HD21	1.17	1.05
1:D:222:SER:OG	1:E:163:ILE:CD1	2.06	1.04
1:B:278:PHE:HE1	1:B:286:LEU:HD21	1.17	1.04
1:C:278:PHE:HE1	1:C:286:LEU:HD21	1.18	1.04
1:E:261:MET:SD	1:E:262:LEU:CD2	2.46	1.04
1:F:261:MET:SD	1:F:262:LEU:CD2	2.46	1.04
1:C:261:MET:SD	1:C:262:LEU:CD2	2.46	1.03
1:E:206:ILE:HG23	1:E:214:LEU:HD23	1.06	1.03
1:A:206:ILE:HG23	1:A:214:LEU:HD23	1.06	1.03
1:D:261:MET:SD	1:D:262:LEU:CD2	2.46	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:MET:SD	1:A:262:LEU:CD2	2.46	1.03
1:B:222:SER:OG	1:C:163:ILE:HD12	1.57	1.03
1:G:261:MET:SD	1:G:262:LEU:CD2	2.46	1.03
1:B:236:ARG:HD2	1:C:210:ASP:OD1	1.59	1.03
1:B:275:LEU:H	1:B:275:LEU:HD12	1.24	1.03
1:B:333:MET:CE	1:C:333:MET:SD	2.47	1.03
1:C:153:GLY:HA2	1:D:151:ILE:CD1	1.88	1.03
1:C:222:SER:OG	1:D:163:ILE:CD1	2.07	1.03
1:C:269:ASP:OD1	1:C:272:GLN:HB2	0.85	1.03
1:D:269:ASP:OD1	1:D:272:GLN:HB2	0.85	1.03
1:F:278:PHE:HB2	1:G:307:GLN:OE1	1.59	1.02
1:A:151:ILE:HD13	1:G:153:GLY:HA2	1.05	1.02
1:B:261:MET:SD	1:B:262:LEU:CD2	2.46	1.02
1:E:269:ASP:OD1	1:E:272:GLN:HB2	0.85	1.02
1:F:206:ILE:HG23	1:F:214:LEU:HD23	1.06	1.02
1:B:247:ASP:OD1	1:B:322:ALA:HB2	1.56	1.02
1:B:269:ASP:OD1	1:B:272:GLN:HB2	0.85	1.02
1:E:222:SER:OG	1:F:163:ILE:CD1	2.07	1.02
1:D:275:LEU:H	1:D:275:LEU:HD12	1.24	1.02
1:G:206:ILE:HG23	1:G:214:LEU:HD23	1.06	1.02
1:A:269:ASP:OD1	1:A:272:GLN:HB2	0.85	1.01
1:C:247:ASP:OD1	1:C:322:ALA:HB2	1.56	1.01
1:F:139:GLY:O	1:F:141:SER:C	1.98	1.01
1:F:269:ASP:OD1	1:F:272:GLN:HB2	0.85	1.01
1:G:269:ASP:OD1	1:G:272:GLN:HB2	0.85	1.01
1:A:247:ASP:OD1	1:A:322:ALA:HB2	1.56	1.01
1:D:167:PHE:HZ	1:E:120:ARG:NH1	1.20	1.01
1:F:331:LEU:HD13	1:G:331:LEU:CD1	1.90	1.01
1:F:153:GLY:HA2	1:G:151:ILE:CD1	1.91	1.00
1:F:167:PHE:CZ	1:G:120:ARG:NH2	2.29	1.00
1:F:278:PHE:CB	1:G:307:GLN:OE1	2.09	1.00
1:F:247:ASP:OD1	1:F:322:ALA:HB2	1.56	1.00
1:G:247:ASP:OD1	1:G:322:ALA:HB2	1.56	1.00
1:B:222:SER:CB	1:C:163:ILE:CD1	2.39	0.99
1:G:275:LEU:H	1:G:275:LEU:HD12	1.24	0.99
1:C:275:LEU:H	1:C:275:LEU:HD12	1.24	0.99
1:A:236:ARG:HD2	1:B:210:ASP:OD1	1.63	0.99
1:B:222:SER:CB	1:C:163:ILE:HD11	1.91	0.99
1:E:236:ARG:HD2	1:F:210:ASP:OD1	1.62	0.99
1:A:236:ARG:CB	1:A:293:PHE:CE1	2.34	0.99
1:A:333:MET:SD	1:G:333:MET:CE	2.51	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:CB	1:B:293:PHE:CE1	2.34	0.98
1:F:275:LEU:H	1:F:275:LEU:HD12	1.24	0.98
1:G:236:ARG:CB	1:G:293:PHE:CE1	2.34	0.98
1:A:275:LEU:H	1:A:275:LEU:HD12	1.24	0.98
1:A:333:MET:CE	1:B:333:MET:SD	2.52	0.98
1:B:216:VAL:HG11	1:B:221:PHE:HE1	1.29	0.97
1:C:333:MET:CE	1:D:333:MET:SD	2.52	0.97
1:G:269:ASP:HB2	1:G:295:LYS:CE	1.95	0.97
1:E:275:LEU:HD12	1:E:275:LEU:H	1.24	0.97
1:C:236:ARG:HD2	1:D:210:ASP:OD1	1.63	0.97
1:D:333:MET:CE	1:E:333:MET:SD	2.53	0.97
1:F:333:MET:HE1	1:G:333:MET:SD	2.04	0.97
1:A:269:ASP:HB2	1:A:295:LYS:CE	1.95	0.97
1:A:222:SER:OG	1:B:163:ILE:HD12	1.62	0.97
1:F:269:ASP:HB2	1:F:295:LYS:CE	1.95	0.97
1:F:281:PHE:CZ	1:G:324:PHE:CE2	2.53	0.97
1:F:216:VAL:HG11	1:F:221:PHE:HE1	1.30	0.97
1:C:236:ARG:CB	1:C:293:PHE:CE1	2.33	0.96
1:D:216:VAL:HG11	1:D:221:PHE:HE1	1.30	0.96
1:D:222:SER:OG	1:E:163:ILE:HD12	1.64	0.96
1:G:216:VAL:HG11	1:G:221:PHE:HE1	1.30	0.96
1:A:222:SER:CB	1:B:163:ILE:CD1	2.44	0.96
1:E:228:ASN:ND2	1:E:231:ARG:HG3	1.80	0.96
1:F:228:ASN:ND2	1:F:231:ARG:HG3	1.80	0.96
1:B:269:ASP:HB2	1:B:295:LYS:CE	1.95	0.96
1:G:228:ASN:ND2	1:G:231:ARG:HG3	1.80	0.96
1:A:228:ASN:ND2	1:A:231:ARG:HG3	1.80	0.96
1:D:167:PHE:CZ	1:E:120:ARG:NH2	2.33	0.96
1:B:228:ASN:ND2	1:B:231:ARG:HG3	1.80	0.95
1:C:228:ASN:ND2	1:C:231:ARG:HG3	1.80	0.95
1:C:222:SER:CB	1:D:163:ILE:HD11	1.97	0.95
1:F:222:SER:CB	1:G:163:ILE:HD11	1.96	0.95
1:A:236:ARG:HA	1:A:293:PHE:HD1	1.31	0.95
1:D:236:ARG:HD2	1:E:210:ASP:OD1	1.65	0.95
1:D:269:ASP:HB2	1:D:295:LYS:CE	1.94	0.95
1:E:269:ASP:HB2	1:E:295:LYS:CE	1.95	0.95
1:A:216:VAL:HG11	1:A:221:PHE:HE1	1.30	0.95
1:A:222:SER:CB	1:B:163:ILE:HD11	1.95	0.95
1:B:236:ARG:CD	1:C:210:ASP:OD1	2.14	0.95
1:D:228:ASN:ND2	1:D:231:ARG:HG3	1.80	0.95
1:E:222:SER:OG	1:F:163:ILE:HD12	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:HB2	1:A:295:LYS:HE3	1.48	0.95
1:B:269:ASP:HB2	1:B:295:LYS:HE3	1.48	0.95
1:C:216:VAL:HG11	1:C:221:PHE:HE1	1.30	0.95
1:E:216:VAL:HG11	1:E:221:PHE:HE1	1.30	0.95
1:G:269:ASP:HB2	1:G:295:LYS:HE3	1.48	0.95
1:E:296:THR:O	1:E:298:VAL:N	2.00	0.95
1:C:269:ASP:HB2	1:C:295:LYS:CE	1.95	0.94
1:D:296:THR:O	1:D:298:VAL:N	1.99	0.94
1:B:236:ARG:HA	1:B:293:PHE:HD1	1.32	0.94
1:B:296:THR:O	1:B:298:VAL:N	2.00	0.94
1:D:222:SER:CB	1:E:163:ILE:HD11	1.98	0.94
1:D:236:ARG:CB	1:D:293:PHE:CE1	2.34	0.94
1:D:236:ARG:HA	1:D:293:PHE:HD1	1.31	0.94
1:F:296:THR:O	1:F:298:VAL:N	2.00	0.94
1:C:231:ARG:NH2	1:D:215:TYR:HH	1.61	0.94
1:C:269:ASP:OD2	1:C:271:ARG:HG2	1.68	0.94
1:C:296:THR:O	1:C:298:VAL:N	2.00	0.94
1:E:269:ASP:HB2	1:E:295:LYS:HE3	1.48	0.94
1:F:236:ARG:CB	1:F:293:PHE:CE1	2.34	0.94
1:F:269:ASP:OD2	1:F:271:ARG:HG2	1.68	0.94
1:D:222:SER:CB	1:E:163:ILE:CD1	2.46	0.94
1:D:269:ASP:HB2	1:D:295:LYS:HE3	1.48	0.94
1:C:247:ASP:OD1	1:C:322:ALA:CB	2.17	0.94
1:G:269:ASP:OD2	1:G:271:ARG:HG2	1.68	0.94
1:F:236:ARG:HD2	1:G:210:ASP:OD1	1.65	0.93
1:F:269:ASP:HB2	1:F:295:LYS:HE3	1.48	0.93
1:B:269:ASP:OD2	1:B:271:ARG:HG2	1.68	0.93
1:A:151:ILE:HD13	1:G:153:GLY:CA	1.96	0.93
1:C:236:ARG:HA	1:C:293:PHE:HD1	1.31	0.93
1:E:269:ASP:OD2	1:E:271:ARG:HG2	1.68	0.93
1:D:247:ASP:OD1	1:D:322:ALA:CB	2.17	0.93
1:A:296:THR:O	1:A:298:VAL:N	2.00	0.93
1:F:236:ARG:HA	1:F:293:PHE:HD1	1.32	0.93
1:A:269:ASP:OD2	1:A:271:ARG:HG2	1.68	0.93
1:C:148:PHE:CA	1:C:149:GLY:N	2.32	0.93
1:D:269:ASP:OD2	1:D:271:ARG:HG2	1.68	0.93
1:E:247:ASP:OD1	1:E:322:ALA:CB	2.17	0.93
1:G:296:THR:O	1:G:298:VAL:N	2.00	0.93
1:C:269:ASP:HB2	1:C:295:LYS:HE3	1.48	0.93
1:F:206:ILE:HG23	1:F:214:LEU:CD2	1.99	0.93
1:D:148:PHE:CA	1:D:149:GLY:N	2.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:CD1	1:G:222:SER:OG	2.17	0.92
1:B:148:PHE:CA	1:B:149:GLY:N	2.32	0.92
1:B:278:PHE:CE1	1:B:286:LEU:HD23	2.05	0.92
1:A:148:PHE:CA	1:A:149:GLY:N	2.32	0.92
1:C:243:LEU:HD21	1:C:254:ILE:HD11	1.50	0.92
1:D:243:LEU:HD21	1:D:254:ILE:HD11	1.50	0.92
1:E:236:ARG:CB	1:E:293:PHE:CE1	2.34	0.92
1:E:236:ARG:CD	1:F:210:ASP:OD1	2.18	0.92
1:E:222:SER:CB	1:F:163:ILE:CD1	2.48	0.92
1:F:247:ASP:OD1	1:F:322:ALA:CB	2.17	0.92
1:G:278:PHE:CE1	1:G:286:LEU:HD21	2.02	0.92
1:A:210:ASP:OD1	1:G:236:ARG:HD2	1.69	0.92
1:A:278:PHE:CE1	1:A:286:LEU:HD23	2.04	0.92
1:G:148:PHE:CA	1:G:149:GLY:N	2.32	0.92
1:E:222:SER:CB	1:F:163:ILE:HD11	1.99	0.92
1:E:148:PHE:CA	1:E:149:GLY:N	2.32	0.92
1:G:243:LEU:HD21	1:G:254:ILE:HD11	1.50	0.91
1:B:227:GLU:HB3	1:C:214:LEU:HB2	1.52	0.91
1:B:243:LEU:HD21	1:B:254:ILE:HD11	1.50	0.91
1:F:243:LEU:HD21	1:F:254:ILE:HD11	1.50	0.91
1:A:278:PHE:CE1	1:A:286:LEU:HD21	2.02	0.91
1:B:278:PHE:CE1	1:B:286:LEU:HD21	2.02	0.91
1:G:278:PHE:CE1	1:G:286:LEU:HD23	2.04	0.91
1:A:206:ILE:HG23	1:A:214:LEU:CD2	1.99	0.91
1:E:201:TRP:HH2	1:F:116:ARG:HE	1.07	0.91
1:D:236:ARG:CD	1:E:210:ASP:OD1	2.19	0.91
1:E:278:PHE:CE1	1:E:286:LEU:HD23	2.04	0.91
1:G:236:ARG:HA	1:G:293:PHE:HD1	1.31	0.91
1:F:222:SER:OG	1:G:163:ILE:HD12	1.68	0.91
1:G:247:ASP:OD1	1:G:322:ALA:CB	2.17	0.91
1:C:278:PHE:CE1	1:C:286:LEU:HD23	2.04	0.90
1:E:243:LEU:HD21	1:E:254:ILE:HD11	1.50	0.90
1:E:236:ARG:HA	1:E:293:PHE:HD1	1.32	0.90
1:F:148:PHE:CA	1:F:149:GLY:N	2.32	0.90
1:B:236:ARG:NE	1:C:210:ASP:OD1	2.03	0.90
1:D:236:ARG:NE	1:E:210:ASP:OD1	2.04	0.90
1:F:222:SER:CB	1:G:163:ILE:CD1	2.49	0.90
1:A:247:ASP:OD1	1:A:322:ALA:CB	2.17	0.90
1:E:206:ILE:HG23	1:E:214:LEU:CD2	1.99	0.90
1:C:236:ARG:CD	1:D:210:ASP:OD1	2.20	0.90
1:G:278:PHE:HE1	1:G:286:LEU:HD23	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ILE:HG23	1:C:214:LEU:CD2	1.99	0.90
1:D:278:PHE:CE1	1:D:286:LEU:HD23	2.04	0.90
1:F:278:PHE:CE1	1:F:286:LEU:HD21	2.02	0.90
1:A:243:LEU:HD21	1:A:254:ILE:HD11	1.50	0.90
1:D:206:ILE:HG23	1:D:214:LEU:CD2	1.99	0.90
1:A:236:ARG:CD	1:B:210:ASP:OD1	2.19	0.90
1:F:278:PHE:CE1	1:F:286:LEU:HD23	2.05	0.90
1:E:136:GLU:HG3	1:F:140:MET:C	1.89	0.89
1:B:247:ASP:OD1	1:B:322:ALA:CB	2.17	0.89
1:C:222:SER:CB	1:D:163:ILE:CD1	2.51	0.89
1:E:236:ARG:NE	1:F:210:ASP:OD1	2.05	0.89
1:C:278:PHE:CE1	1:C:286:LEU:HD21	2.02	0.89
1:F:333:MET:HE3	1:G:333:MET:SD	2.13	0.89
1:B:206:ILE:HG23	1:B:214:LEU:CD2	1.99	0.89
1:B:232:MET:HE3	1:C:212:ARG:HD3	1.53	0.89
1:A:270:GLN:OE1	1:A:271:ARG:N	2.06	0.89
1:B:278:PHE:HE1	1:B:286:LEU:HD23	1.36	0.89
1:E:171:ILE:HD11	1:F:120:ARG:HH22	1.35	0.88
1:F:281:PHE:CZ	1:G:324:PHE:HE2	1.90	0.88
1:F:222:SER:OG	1:G:163:ILE:HD11	1.69	0.88
1:E:270:GLN:OE1	1:E:271:ARG:N	2.06	0.88
1:E:278:PHE:CE1	1:E:286:LEU:HD21	2.02	0.88
1:F:270:GLN:OE1	1:F:271:ARG:N	2.06	0.88
1:D:139:GLY:O	1:D:141:SER:C	2.12	0.88
1:F:259:ARG:NH1	1:F:277:TYR:CE1	2.42	0.88
1:G:270:GLN:OE1	1:G:271:ARG:N	2.06	0.88
1:B:270:GLN:OE1	1:B:271:ARG:N	2.06	0.87
1:C:222:SER:OG	1:D:163:ILE:HD12	1.72	0.87
1:D:278:PHE:CE1	1:D:286:LEU:HD21	2.01	0.87
1:E:259:ARG:NH1	1:E:277:TYR:CE1	2.42	0.87
1:G:259:ARG:NH1	1:G:277:TYR:CE1	2.42	0.87
1:A:236:ARG:NE	1:B:210:ASP:OD1	2.08	0.87
1:G:206:ILE:HG23	1:G:214:LEU:CD2	1.99	0.87
1:D:270:GLN:OE1	1:D:271:ARG:N	2.06	0.87
1:A:259:ARG:NH1	1:A:277:TYR:CE1	2.42	0.87
1:E:236:ARG:HA	1:E:293:PHE:CD1	2.10	0.87
1:C:222:SER:OG	1:D:163:ILE:HD11	1.75	0.86
1:C:236:ARG:HA	1:C:293:PHE:CD1	2.10	0.86
1:C:270:GLN:OE1	1:C:271:ARG:N	2.06	0.86
1:D:259:ARG:NH1	1:D:277:TYR:CE1	2.42	0.86
1:D:236:ARG:HA	1:D:293:PHE:CD1	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:ILE:CD1	1:F:120:ARG:HH22	1.89	0.86
1:G:236:ARG:HA	1:G:293:PHE:CD1	2.10	0.86
1:E:139:GLY:O	1:E:141:SER:C	2.13	0.86
1:F:236:ARG:HA	1:F:293:PHE:CD1	2.10	0.86
1:C:236:ARG:NE	1:D:210:ASP:OD1	2.09	0.86
1:B:259:ARG:NH1	1:B:277:TYR:CE1	2.42	0.86
1:A:236:ARG:HA	1:A:293:PHE:CD1	2.10	0.86
1:B:222:SER:HB3	1:C:163:ILE:CD1	2.05	0.86
1:C:232:MET:HE3	1:D:212:ARG:HD3	1.58	0.86
1:B:236:ARG:HA	1:B:293:PHE:CD1	2.10	0.85
1:E:171:ILE:HD11	1:F:120:ARG:HH12	1.41	0.85
1:C:259:ARG:NH1	1:C:277:TYR:CE1	2.42	0.85
1:A:227:GLU:HB3	1:B:214:LEU:HB2	1.58	0.85
1:B:259:ARG:NH1	1:B:277:TYR:CZ	2.45	0.85
1:A:163:ILE:HD12	1:G:222:SER:OG	1.76	0.85
1:B:216:VAL:HG11	1:B:221:PHE:CE1	2.12	0.85
1:C:259:ARG:NH1	1:C:277:TYR:CZ	2.45	0.85
1:A:231:ARG:NH2	1:B:215:TYR:HH	1.68	0.85
1:A:216:VAL:HG11	1:A:221:PHE:CE1	2.12	0.85
1:A:310:TYR:HA	1:A:313:ILE:CG2	2.07	0.84
1:C:216:VAL:HG11	1:C:221:PHE:CE1	2.12	0.84
1:E:259:ARG:NH1	1:E:277:TYR:CZ	2.45	0.84
1:A:259:ARG:NH1	1:A:277:TYR:CZ	2.45	0.84
1:E:333:MET:CE	1:F:333:MET:SD	2.66	0.84
1:A:222:SER:HB3	1:B:163:ILE:CD1	2.08	0.84
1:B:139:GLY:O	1:B:141:SER:C	2.15	0.84
1:E:167:PHE:CZ	1:F:120:ARG:NH2	2.44	0.84
1:B:136:GLU:HA	1:C:141:SER:OG	1.76	0.84
1:F:236:ARG:CD	1:G:210:ASP:OD1	2.26	0.84
1:G:216:VAL:HG11	1:G:221:PHE:CE1	2.12	0.84
1:E:310:TYR:HA	1:E:313:ILE:CG2	2.08	0.84
1:D:216:VAL:HG11	1:D:221:PHE:CE1	2.12	0.84
1:F:259:ARG:NH1	1:F:277:TYR:CZ	2.45	0.84
1:B:310:TYR:HA	1:B:313:ILE:CG2	2.07	0.84
1:D:259:ARG:NH1	1:D:277:TYR:CZ	2.45	0.84
1:F:216:VAL:HG11	1:F:221:PHE:CE1	2.12	0.84
1:D:222:SER:HB3	1:E:163:ILE:CD1	2.08	0.83
1:F:278:PHE:HE1	1:F:286:LEU:HD23	1.36	0.83
1:G:259:ARG:NH1	1:G:277:TYR:CZ	2.45	0.83
1:A:210:ASP:OD1	1:G:236:ARG:CD	2.26	0.83
1:E:227:GLU:HB3	1:F:214:LEU:HB2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASP:OD1	1:G:236:ARG:NE	2.12	0.83
1:B:231:ARG:NH2	1:C:215:TYR:HH	1.69	0.83
1:E:171:ILE:HD11	1:F:120:ARG:NH2	1.93	0.83
1:F:310:TYR:HA	1:F:313:ILE:CG2	2.08	0.83
1:A:324:PHE:CE2	1:G:281:PHE:CZ	2.65	0.83
1:E:148:PHE:N	1:E:149:GLY:N	2.27	0.83
1:E:269:ASP:CG	1:E:272:GLN:HB2	1.98	0.83
1:B:331:LEU:HD13	1:C:331:LEU:CD1	2.08	0.83
1:C:310:TYR:HA	1:C:313:ILE:CG2	2.07	0.83
1:F:232:MET:HE1	1:G:212:ARG:HH11	1.43	0.83
1:A:331:LEU:HD13	1:B:331:LEU:CD1	2.07	0.83
1:E:216:VAL:HG11	1:E:221:PHE:CE1	2.12	0.83
1:G:148:PHE:N	1:G:149:GLY:N	2.27	0.83
1:E:231:ARG:NH2	1:F:215:TYR:HH	1.73	0.83
1:A:278:PHE:HE1	1:A:286:LEU:HD23	1.35	0.83
1:G:310:TYR:HA	1:G:313:ILE:CG2	2.08	0.83
1:A:148:PHE:N	1:A:149:GLY:N	2.27	0.83
1:B:148:PHE:N	1:B:149:GLY:N	2.27	0.83
1:D:148:PHE:N	1:D:149:GLY:N	2.27	0.83
1:D:227:GLU:HB3	1:E:214:LEU:HB2	1.59	0.83
1:D:310:TYR:HA	1:D:313:ILE:CG2	2.08	0.83
1:C:148:PHE:N	1:C:149:GLY:N	2.27	0.82
1:D:201:TRP:HH2	1:E:116:ARG:HE	1.27	0.82
1:F:148:PHE:N	1:F:149:GLY:N	2.27	0.82
1:D:231:ARG:NH2	1:E:215:TYR:HH	1.74	0.82
1:F:269:ASP:CG	1:F:272:GLN:HB2	1.98	0.82
1:E:222:SER:HB3	1:F:163:ILE:CD1	2.09	0.82
1:G:269:ASP:CG	1:G:272:GLN:HB2	1.98	0.82
1:A:215:TYR:HH	1:G:231:ARG:NH2	1.74	0.82
1:D:136:GLU:HA	1:E:141:SER:OG	1.80	0.82
1:E:171:ILE:CG1	1:F:120:ARG:HH22	1.93	0.82
1:A:163:ILE:HD11	1:G:222:SER:CB	2.10	0.82
1:F:227:GLU:HB3	1:G:214:LEU:HB2	1.61	0.82
1:B:222:SER:OG	1:C:163:ILE:HD11	1.73	0.81
1:C:227:GLU:HB3	1:D:214:LEU:HB2	1.62	0.81
1:G:243:LEU:HD21	1:G:254:ILE:CD1	2.10	0.81
1:C:243:LEU:HD21	1:C:254:ILE:CD1	2.11	0.81
1:C:281:PHE:CZ	1:D:324:PHE:CE2	2.68	0.81
1:E:243:LEU:HD21	1:E:254:ILE:CD1	2.11	0.81
1:B:243:LEU:HD21	1:B:254:ILE:CD1	2.10	0.81
1:D:153:GLY:CA	1:E:151:ILE:HD13	2.07	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:CZ	1:B:324:PHE:CE2	2.68	0.81
1:F:228:ASN:HD21	1:F:231:ARG:HG3	1.46	0.81
1:F:232:MET:HE3	1:G:212:ARG:HD3	1.62	0.81
1:G:228:ASN:HD21	1:G:231:ARG:HG3	1.46	0.81
1:A:269:ASP:CG	1:A:272:GLN:HB2	1.98	0.81
1:B:241:ILE:HD11	1:B:313:ILE:HD11	1.63	0.81
1:A:243:LEU:HD21	1:A:254:ILE:CD1	2.10	0.81
1:A:163:ILE:CD1	1:G:222:SER:CB	2.58	0.81
1:A:333:MET:SD	1:G:333:MET:HE3	2.21	0.80
1:A:241:ILE:HD11	1:A:313:ILE:HD11	1.63	0.80
1:B:269:ASP:CG	1:B:272:GLN:HB2	1.98	0.80
1:C:241:ILE:HD11	1:C:313:ILE:HD11	1.63	0.80
1:D:241:ILE:HD11	1:D:313:ILE:HD11	1.63	0.80
1:E:228:ASN:HD21	1:E:231:ARG:HG3	1.46	0.80
1:E:241:ILE:HD11	1:E:313:ILE:HD11	1.63	0.80
1:F:139:GLY:O	1:F:141:SER:O	1.99	0.80
1:F:243:LEU:HD21	1:F:254:ILE:CD1	2.10	0.80
1:D:243:LEU:HD21	1:D:254:ILE:CD1	2.10	0.80
1:E:167:PHE:HE2	1:F:120:ARG:NH1	1.69	0.80
1:E:275:LEU:CD1	1:E:291:TYR:HD2	1.94	0.80
1:B:275:LEU:CD1	1:B:291:TYR:HD2	1.94	0.80
1:A:214:LEU:HB2	1:G:227:GLU:HB3	1.64	0.80
1:A:222:SER:OG	1:B:163:ILE:HD11	1.77	0.80
1:A:228:ASN:HD21	1:A:231:ARG:HG3	1.46	0.80
1:B:236:ARG:HB2	1:B:293:PHE:HE1	0.67	0.80
1:F:241:ILE:HD11	1:F:313:ILE:HD11	1.63	0.80
1:A:244:ARG:NE	1:A:323:ASP:OD2	2.15	0.80
1:B:281:PHE:CZ	1:C:324:PHE:CE2	2.70	0.80
1:E:167:PHE:HZ	1:F:120:ARG:NE	1.79	0.80
1:B:244:ARG:NE	1:B:323:ASP:OD2	2.15	0.80
1:C:172:MET:HE3	1:D:163:ILE:HG22	1.63	0.80
1:G:272:GLN:HE21	1:G:273:THR:H	1.28	0.80
1:B:167:PHE:CE1	1:C:120:ARG:NH2	2.37	0.80
1:C:275:LEU:CD1	1:C:291:TYR:HD2	1.94	0.80
1:G:241:ILE:HD11	1:G:313:ILE:HD11	1.63	0.80
1:A:275:LEU:CD1	1:A:291:TYR:HD2	1.94	0.79
1:F:272:GLN:HE21	1:F:273:THR:H	1.28	0.79
1:D:272:GLN:HE21	1:D:273:THR:H	1.29	0.79
1:E:153:GLY:CA	1:F:151:ILE:HD13	2.07	0.79
1:F:236:ARG:HB2	1:F:293:PHE:HE1	0.67	0.79
1:F:275:LEU:CD1	1:F:291:TYR:HD2	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:PHE:HE2	1:D:120:ARG:HH12	1.24	0.79
1:C:272:GLN:HE21	1:C:273:THR:H	1.28	0.79
1:D:333:MET:HE3	1:E:333:MET:SD	2.21	0.79
1:C:244:ARG:NE	1:C:323:ASP:OD2	2.15	0.79
1:E:171:ILE:HD11	1:F:120:ARG:NH1	1.98	0.79
1:G:244:ARG:NE	1:G:323:ASP:OD2	2.15	0.79
1:C:269:ASP:CG	1:C:272:GLN:HB2	1.98	0.79
1:C:222:SER:HB3	1:D:163:ILE:CD1	2.13	0.79
1:G:139:GLY:O	1:G:141:SER:C	2.21	0.79
1:G:275:LEU:CD1	1:G:291:TYR:HD2	1.94	0.79
1:E:236:ARG:HB2	1:E:293:PHE:HE1	0.67	0.79
1:D:275:LEU:CD1	1:D:291:TYR:HD2	1.94	0.79
1:C:278:PHE:HE1	1:C:286:LEU:HD23	1.35	0.79
1:C:331:LEU:HD13	1:D:331:LEU:CD1	2.13	0.79
1:B:272:GLN:HE21	1:B:273:THR:H	1.28	0.78
1:A:272:GLN:HE21	1:A:273:THR:H	1.28	0.78
1:D:228:ASN:HD21	1:D:231:ARG:HG3	1.46	0.78
1:F:244:ARG:NE	1:F:323:ASP:OD2	2.15	0.78
1:C:333:MET:HE3	1:D:333:MET:SD	2.23	0.78
1:B:333:MET:HE3	1:C:333:MET:SD	2.22	0.78
1:D:244:ARG:NE	1:D:323:ASP:OD2	2.15	0.78
1:A:269:ASP:OD1	1:A:272:GLN:N	2.17	0.78
1:B:333:MET:HE1	1:C:333:MET:SD	2.22	0.78
1:E:244:ARG:NE	1:E:323:ASP:OD2	2.15	0.78
1:E:272:GLN:HE21	1:E:273:THR:H	1.28	0.78
1:A:139:GLY:O	1:A:141:SER:C	2.22	0.78
1:B:228:ASN:HD21	1:B:231:ARG:HG3	1.46	0.78
1:D:139:GLY:C	1:D:141:SER:N	2.35	0.78
1:B:269:ASP:OD1	1:B:272:GLN:N	2.17	0.77
1:D:269:ASP:CG	1:D:272:GLN:HB2	1.98	0.77
1:G:236:ARG:HB2	1:G:293:PHE:HE1	0.67	0.77
1:D:232:MET:HE3	1:E:212:ARG:HD3	1.65	0.77
1:G:269:ASP:OD1	1:G:272:GLN:N	2.17	0.77
1:C:167:PHE:CE1	1:D:120:ARG:NH2	2.52	0.77
1:D:167:PHE:CE1	1:E:120:ARG:CZ	2.65	0.77
1:F:206:ILE:CG2	1:F:214:LEU:CD2	2.61	0.77
1:C:236:ARG:HB2	1:C:293:PHE:HE1	0.67	0.77
1:D:269:ASP:OD1	1:D:272:GLN:N	2.17	0.77
1:E:281:PHE:CZ	1:F:324:PHE:CE2	2.73	0.77
1:C:206:ILE:CG2	1:C:214:LEU:CD2	2.61	0.76
1:C:269:ASP:OD1	1:C:272:GLN:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:SER:HB3	1:G:163:ILE:CD1	2.15	0.76
1:A:333:MET:HE1	1:B:333:MET:SD	2.23	0.76
1:D:281:PHE:CZ	1:E:324:PHE:CE2	2.73	0.76
1:E:201:TRP:HH2	1:F:116:ARG:NE	1.83	0.76
1:E:206:ILE:CG2	1:E:214:LEU:CD2	2.61	0.76
1:E:269:ASP:OD1	1:E:272:GLN:N	2.17	0.76
1:A:206:ILE:CG2	1:A:214:LEU:CD2	2.61	0.76
1:A:232:MET:HE3	1:B:212:ARG:HD3	1.66	0.76
1:A:307:GLN:OE1	1:G:278:PHE:N	2.19	0.76
1:B:232:MET:CE	1:C:212:ARG:HD3	2.16	0.75
1:C:228:ASN:HD21	1:C:231:ARG:HG3	1.46	0.75
1:C:200:GLY:O	1:C:218:ASN:ND2	2.18	0.75
1:F:269:ASP:OD1	1:F:272:GLN:N	2.17	0.75
1:B:200:GLY:O	1:B:218:ASN:ND2	2.18	0.75
1:F:200:GLY:O	1:F:218:ASN:ND2	2.18	0.75
1:F:248:ALA:O	1:F:251:VAL:CG1	2.34	0.75
1:D:331:LEU:HD13	1:E:331:LEU:CD1	2.15	0.75
1:A:160:GLY:HA2	1:A:164:LEU:HD13	1.69	0.75
1:B:248:ALA:O	1:B:251:VAL:CG1	2.34	0.75
1:E:160:GLY:HA2	1:E:164:LEU:HD13	1.69	0.75
1:D:200:GLY:O	1:D:218:ASN:ND2	2.18	0.75
1:E:278:PHE:HE1	1:E:286:LEU:HD23	1.35	0.75
1:B:160:GLY:HA2	1:B:164:LEU:HD13	1.69	0.74
1:B:254:ILE:O	1:B:258:VAL:HG23	1.87	0.74
1:F:160:GLY:HA2	1:F:164:LEU:HD13	1.69	0.74
1:A:200:GLY:O	1:A:218:ASN:ND2	2.18	0.74
1:A:254:ILE:O	1:A:258:VAL:HG23	1.87	0.74
1:D:254:ILE:O	1:D:258:VAL:HG23	1.87	0.74
1:G:200:GLY:O	1:G:218:ASN:ND2	2.18	0.74
1:G:160:GLY:HA2	1:G:164:LEU:HD13	1.69	0.74
1:G:254:ILE:O	1:G:258:VAL:HG23	1.87	0.74
1:C:254:ILE:O	1:C:258:VAL:HG23	1.87	0.74
1:D:160:GLY:HA2	1:D:164:LEU:HD13	1.69	0.74
1:C:148:PHE:C	1:C:149:GLY:CA	2.56	0.74
1:C:269:ASP:OD1	1:C:272:GLN:CA	2.36	0.74
1:F:236:ARG:NE	1:G:210:ASP:OD1	2.19	0.74
1:G:248:ALA:O	1:G:251:VAL:CG1	2.34	0.74
1:C:136:GLU:HA	1:D:141:SER:OG	1.88	0.74
1:C:160:GLY:HA2	1:C:164:LEU:HD13	1.69	0.74
1:E:232:MET:HE1	1:F:212:ARG:HH11	1.53	0.74
1:A:148:PHE:C	1:A:149:GLY:CA	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HE1	1:B:212:ARG:HH11	1.52	0.74
1:A:281:PHE:CZ	1:B:324:PHE:HE2	2.05	0.74
1:D:316:ILE:HD13	1:D:316:ILE:N	2.03	0.74
1:E:148:PHE:C	1:E:149:GLY:CA	2.56	0.74
1:E:316:ILE:HD13	1:E:316:ILE:N	2.03	0.73
1:F:254:ILE:O	1:F:258:VAL:HG23	1.87	0.73
1:F:272:GLN:HE21	1:F:273:THR:N	1.86	0.73
1:A:275:LEU:HD12	1:A:275:LEU:N	2.03	0.73
1:B:241:ILE:CD1	1:B:313:ILE:HD11	2.19	0.73
1:D:269:ASP:OD1	1:D:272:GLN:CA	2.36	0.73
1:F:148:PHE:C	1:F:149:GLY:CA	2.56	0.73
1:B:316:ILE:HD13	1:B:316:ILE:N	2.03	0.73
1:C:241:ILE:CD1	1:C:313:ILE:HD11	2.18	0.73
1:G:241:ILE:CD1	1:G:313:ILE:HD11	2.19	0.73
1:A:241:ILE:CD1	1:A:313:ILE:HD11	2.18	0.73
1:B:148:PHE:C	1:B:149:GLY:CA	2.56	0.73
1:F:272:GLN:NE2	1:F:273:THR:H	1.86	0.73
1:G:275:LEU:HD12	1:G:275:LEU:N	2.03	0.73
1:B:269:ASP:OD1	1:B:272:GLN:CA	2.36	0.73
1:B:272:GLN:HE21	1:B:273:THR:N	1.86	0.73
1:C:281:PHE:CZ	1:D:324:PHE:HE2	2.05	0.73
1:C:316:ILE:HD13	1:C:316:ILE:N	2.03	0.73
1:E:222:SER:OG	1:F:163:ILE:HD11	1.83	0.73
1:F:241:ILE:CD1	1:F:313:ILE:HD11	2.18	0.73
1:D:139:GLY:O	1:D:141:SER:N	2.21	0.73
1:D:139:GLY:C	1:D:141:SER:H	1.92	0.73
1:D:148:PHE:C	1:D:149:GLY:CA	2.56	0.73
1:D:241:ILE:CD1	1:D:313:ILE:HD11	2.18	0.73
1:E:200:GLY:O	1:E:218:ASN:ND2	2.18	0.73
1:E:272:GLN:HE21	1:E:273:THR:N	1.86	0.73
1:G:272:GLN:HE21	1:G:273:THR:N	1.86	0.73
1:A:163:ILE:CD1	1:G:222:SER:HB3	2.19	0.73
1:F:269:ASP:OD1	1:F:272:GLN:CA	2.36	0.73
1:B:160:GLY:O	1:B:161:LYS:O	2.07	0.73
1:E:254:ILE:O	1:E:258:VAL:HG23	1.87	0.73
1:G:272:GLN:NE2	1:G:273:THR:H	1.86	0.73
1:B:206:ILE:CG2	1:B:214:LEU:CD2	2.61	0.73
1:F:232:MET:CE	1:G:212:ARG:HD3	2.18	0.73
1:F:275:LEU:HD12	1:F:275:LEU:N	2.03	0.73
1:A:236:ARG:HB2	1:A:293:PHE:HE1	0.67	0.73
1:A:316:ILE:HD13	1:A:316:ILE:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ASP:OD1	1:E:272:GLN:CA	2.36	0.73
1:E:272:GLN:NE2	1:E:273:THR:H	1.86	0.73
1:E:275:LEU:HD12	1:E:275:LEU:N	2.03	0.73
1:B:272:GLN:NE2	1:B:273:THR:H	1.86	0.72
1:C:272:GLN:HE21	1:C:273:THR:N	1.86	0.72
1:D:206:ILE:CG2	1:D:214:LEU:CD2	2.61	0.72
1:E:251:VAL:HG21	1:F:311:LEU:HD21	1.70	0.72
1:D:153:GLY:HA2	1:E:151:ILE:HD12	1.70	0.72
1:E:274:LEU:HD23	1:E:274:LEU:O	1.89	0.72
1:F:172:MET:HE3	1:G:163:ILE:HG22	1.70	0.72
1:G:148:PHE:C	1:G:149:GLY:CA	2.56	0.72
1:A:139:GLY:O	1:A:141:SER:O	2.06	0.72
1:A:160:GLY:O	1:A:161:LYS:O	2.07	0.72
1:A:272:GLN:HE21	1:A:273:THR:N	1.86	0.72
1:B:236:ARG:HD2	1:C:210:ASP:CG	2.10	0.72
1:C:272:GLN:NE2	1:C:273:THR:H	1.86	0.72
1:D:251:VAL:O	1:D:255:VAL:CG2	2.36	0.72
1:E:241:ILE:CD1	1:E:313:ILE:HD11	2.18	0.72
1:G:269:ASP:OD1	1:G:272:GLN:CA	2.36	0.72
1:C:160:GLY:O	1:C:161:LYS:O	2.07	0.72
1:D:275:LEU:HD12	1:D:275:LEU:N	2.03	0.72
1:E:139:GLY:O	1:E:141:SER:O	2.07	0.72
1:F:316:ILE:HD13	1:F:316:ILE:N	2.03	0.72
1:G:316:ILE:HD13	1:G:316:ILE:N	2.03	0.72
1:A:274:LEU:O	1:A:274:LEU:HD23	1.89	0.72
1:D:236:ARG:HB2	1:D:293:PHE:HE1	0.67	0.72
1:A:333:MET:HE3	1:B:333:MET:SD	2.26	0.72
1:B:274:LEU:O	1:B:274:LEU:HD23	1.89	0.72
1:D:274:LEU:O	1:D:274:LEU:HD23	1.89	0.72
1:F:274:LEU:HD23	1:F:274:LEU:O	1.89	0.72
1:A:324:PHE:HE2	1:G:281:PHE:CZ	2.05	0.72
1:A:331:LEU:CD1	1:G:331:LEU:HD13	2.19	0.72
1:C:248:ALA:O	1:C:251:VAL:CG1	2.34	0.72
1:D:272:GLN:HE21	1:D:273:THR:N	1.86	0.72
1:E:251:VAL:O	1:E:255:VAL:CG2	2.36	0.72
1:E:278:PHE:HB3	1:F:307:GLN:OE1	1.89	0.72
1:E:160:GLY:O	1:E:161:LYS:O	2.07	0.72
1:F:167:PHE:CE1	1:G:120:ARG:NH2	2.57	0.72
1:A:272:GLN:NE2	1:A:273:THR:H	1.86	0.72
1:D:278:PHE:HB3	1:E:307:GLN:OE1	1.86	0.72
1:A:269:ASP:OD1	1:A:272:GLN:CA	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLN:HE21	1:C:272:GLN:CA	2.03	0.72
1:C:314:ILE:O	1:C:314:ILE:HD13	1.90	0.72
1:E:153:GLY:HA2	1:F:151:ILE:HD12	1.72	0.72
1:F:231:ARG:CZ	1:G:215:TYR:OH	2.37	0.72
1:A:232:MET:CE	1:B:212:ARG:HD3	2.20	0.71
1:D:160:GLY:O	1:D:161:LYS:O	2.07	0.71
1:C:274:LEU:HD23	1:C:274:LEU:O	1.89	0.71
1:G:206:ILE:CG2	1:G:214:LEU:CD2	2.61	0.71
1:G:160:GLY:O	1:G:161:LYS:O	2.07	0.71
1:G:314:ILE:HD13	1:G:314:ILE:O	1.90	0.71
1:B:231:ARG:CZ	1:C:215:TYR:OH	2.39	0.71
1:F:160:GLY:O	1:F:161:LYS:O	2.07	0.71
1:F:314:ILE:O	1:F:314:ILE:HD13	1.90	0.71
1:C:232:MET:CE	1:D:212:ARG:HD3	2.20	0.71
1:D:314:ILE:O	1:D:314:ILE:HD13	1.90	0.71
1:E:251:VAL:CG2	1:F:311:LEU:HD21	2.20	0.71
1:B:281:PHE:CZ	1:C:324:PHE:HE2	2.07	0.71
1:D:272:GLN:HE21	1:D:272:GLN:CA	2.03	0.71
1:E:318:GLN:OE1	1:E:318:GLN:HA	1.91	0.71
1:G:274:LEU:O	1:G:274:LEU:HD23	1.89	0.71
1:A:153:GLY:HA2	1:B:151:ILE:HD12	1.72	0.70
1:B:272:GLN:HE21	1:B:272:GLN:CA	2.03	0.70
1:C:275:LEU:HD12	1:C:275:LEU:N	2.03	0.70
1:E:331:LEU:HD13	1:F:331:LEU:CD1	2.21	0.70
1:B:314:ILE:HD13	1:B:314:ILE:O	1.90	0.70
1:D:272:GLN:NE2	1:D:273:THR:H	1.86	0.70
1:A:248:ALA:O	1:A:251:VAL:CG1	2.34	0.70
1:F:318:GLN:OE1	1:F:318:GLN:HA	1.91	0.70
1:D:222:SER:OG	1:E:163:ILE:HD11	1.83	0.70
1:F:331:LEU:HD13	1:G:331:LEU:HD11	1.74	0.70
1:D:200:GLY:O	1:D:203:ILE:O	2.10	0.70
1:E:314:ILE:O	1:E:314:ILE:HD13	1.90	0.70
1:C:231:ARG:CZ	1:D:215:TYR:OH	2.40	0.70
1:D:167:PHE:HE2	1:E:120:ARG:NH1	1.80	0.70
1:E:272:GLN:HE21	1:E:272:GLN:CA	2.03	0.70
1:A:272:GLN:HE21	1:A:272:GLN:CA	2.03	0.70
1:E:200:GLY:O	1:E:203:ILE:O	2.10	0.70
1:A:151:ILE:HD12	1:G:153:GLY:HA2	1.66	0.70
1:A:311:LEU:HD21	1:G:251:VAL:HG21	1.73	0.70
1:F:200:GLY:O	1:F:203:ILE:O	2.10	0.69
1:G:318:GLN:OE1	1:G:318:GLN:HA	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:O	1:A:314:ILE:HD13	1.90	0.69
1:D:248:ALA:O	1:D:251:VAL:CG1	2.34	0.69
1:D:318:GLN:HA	1:D:318:GLN:OE1	1.91	0.69
1:A:200:GLY:O	1:A:203:ILE:O	2.10	0.69
1:B:318:GLN:OE1	1:B:318:GLN:HA	1.91	0.69
1:C:333:MET:HE1	1:D:333:MET:SD	2.31	0.69
1:F:167:PHE:CE1	1:G:120:ARG:CZ	2.72	0.69
1:A:116:ARG:HE	1:G:201:TRP:HH2	1.41	0.69
1:B:200:GLY:O	1:B:203:ILE:O	2.10	0.69
1:E:232:MET:CE	1:F:212:ARG:HD3	2.23	0.69
1:F:272:GLN:HE21	1:F:272:GLN:CA	2.03	0.69
1:D:139:GLY:O	1:D:141:SER:CA	2.41	0.69
1:F:136:GLU:HA	1:G:141:SER:OG	1.93	0.69
1:B:278:PHE:HB3	1:C:307:GLN:OE1	1.91	0.69
1:C:318:GLN:OE1	1:C:318:GLN:HA	1.91	0.69
1:A:236:ARG:HG2	1:A:238:THR:HG23	1.75	0.69
1:C:251:VAL:O	1:C:255:VAL:CG2	2.36	0.69
1:G:200:GLY:O	1:G:203:ILE:O	2.10	0.69
1:A:167:PHE:CE1	1:B:120:ARG:NH2	2.54	0.69
1:A:217:PRO:HG2	1:A:220:LEU:HD13	1.75	0.69
1:B:222:SER:HB3	1:C:163:ILE:HD13	1.73	0.69
1:B:236:ARG:HG2	1:B:238:THR:HG23	1.75	0.69
1:D:167:PHE:CE1	1:E:120:ARG:NH2	2.61	0.69
1:E:236:ARG:HG2	1:E:238:THR:HG23	1.75	0.69
1:F:331:LEU:HD13	1:G:331:LEU:CG	2.23	0.69
1:G:272:GLN:HE21	1:G:272:GLN:CA	2.03	0.69
1:G:217:PRO:HG2	1:G:220:LEU:HD13	1.75	0.69
1:A:236:ARG:HD2	1:B:210:ASP:CG	2.14	0.69
1:A:307:GLN:OE1	1:G:278:PHE:HB3	1.88	0.69
1:A:318:GLN:HA	1:A:318:GLN:OE1	1.91	0.69
1:C:200:GLY:O	1:C:203:ILE:O	2.10	0.69
1:C:236:ARG:HD2	1:D:210:ASP:CG	2.13	0.69
1:E:261:MET:CE	1:E:262:LEU:HD23	2.23	0.69
1:E:275:LEU:HD11	1:E:291:TYR:HD2	1.58	0.69
1:D:236:ARG:HG2	1:D:238:THR:HG23	1.75	0.68
1:B:139:GLY:O	1:B:141:SER:O	2.11	0.68
1:C:236:ARG:HG2	1:C:238:THR:HG23	1.75	0.68
1:C:261:MET:CE	1:C:262:LEU:HD23	2.24	0.68
1:B:227:GLU:HB3	1:C:214:LEU:CB	2.24	0.68
1:E:248:ALA:O	1:E:251:VAL:CG1	2.34	0.68
1:F:331:LEU:HD13	1:G:331:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:MET:CE	1:G:262:LEU:HD23	2.24	0.68
1:E:281:PHE:CZ	1:F:324:PHE:HE2	2.11	0.68
1:G:236:ARG:HG2	1:G:238:THR:HG23	1.75	0.68
1:A:278:PHE:HB3	1:B:307:GLN:OE1	1.91	0.68
1:B:217:PRO:HG2	1:B:220:LEU:HD13	1.75	0.68
1:D:217:PRO:HG2	1:D:220:LEU:HD13	1.75	0.68
1:F:236:ARG:HD2	1:G:210:ASP:CG	2.14	0.68
1:F:236:ARG:HG2	1:F:238:THR:HG23	1.75	0.68
1:F:251:VAL:O	1:F:255:VAL:CG2	2.36	0.68
1:C:275:LEU:HD11	1:C:291:TYR:HD2	1.58	0.68
1:A:251:VAL:O	1:A:255:VAL:CG2	2.36	0.68
1:E:232:MET:HE3	1:F:212:ARG:HD3	1.76	0.68
1:G:251:VAL:O	1:G:255:VAL:CG2	2.36	0.68
1:G:275:LEU:HD11	1:G:291:TYR:HD2	1.58	0.67
1:D:236:ARG:HB2	1:D:293:PHE:CD1	2.26	0.67
1:F:217:PRO:HG2	1:F:220:LEU:HD13	1.75	0.67
1:D:232:MET:CE	1:E:212:ARG:HD3	2.24	0.67
1:D:261:MET:CE	1:D:262:LEU:HD23	2.23	0.67
1:F:261:MET:CE	1:F:262:LEU:HD23	2.24	0.67
1:A:311:LEU:HD21	1:G:251:VAL:CG2	2.23	0.67
1:D:275:LEU:HD11	1:D:291:TYR:HD2	1.59	0.67
1:E:278:PHE:N	1:F:307:GLN:OE1	2.26	0.67
1:A:311:LEU:O	1:A:314:ILE:HG22	1.95	0.67
1:E:217:PRO:HG2	1:E:220:LEU:HD13	1.75	0.67
1:E:311:LEU:O	1:E:314:ILE:HG22	1.95	0.67
1:E:333:MET:HE1	1:F:333:MET:SD	2.33	0.67
1:A:261:MET:CE	1:A:262:LEU:HD23	2.24	0.67
1:B:261:MET:CE	1:B:262:LEU:HD23	2.23	0.67
1:C:139:GLY:O	1:C:141:SER:C	2.33	0.67
1:C:217:PRO:HG2	1:C:220:LEU:HD13	1.75	0.67
1:D:311:LEU:O	1:D:314:ILE:HG22	1.95	0.67
1:G:243:LEU:CD2	1:G:254:ILE:CD1	2.73	0.67
1:G:311:LEU:O	1:G:314:ILE:HG22	1.95	0.67
1:B:275:LEU:HD11	1:B:291:TYR:HD2	1.58	0.67
1:B:311:LEU:O	1:B:314:ILE:HG22	1.95	0.67
1:F:311:LEU:O	1:F:314:ILE:HG22	1.95	0.67
1:F:331:LEU:CD1	1:G:331:LEU:CD1	2.70	0.67
1:D:243:LEU:CD2	1:D:254:ILE:CD1	2.73	0.66
1:F:243:LEU:CD2	1:F:254:ILE:CD1	2.73	0.66
1:F:197:ALA:HB3	1:F:205:LYS:HB3	1.78	0.66
1:F:275:LEU:CD1	1:F:291:TYR:CD2	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:LEU:HD11	1:F:291:TYR:HD2	1.58	0.66
1:G:197:ALA:HB3	1:G:205:LYS:HB3	1.78	0.66
1:A:307:GLN:OE1	1:G:278:PHE:CA	2.44	0.66
1:C:243:LEU:CD2	1:C:254:ILE:CD1	2.73	0.66
1:D:275:LEU:CD1	1:D:291:TYR:CD2	2.79	0.66
1:E:197:ALA:HB3	1:E:205:LYS:HB3	1.78	0.66
1:G:312:LYS:O	1:G:316:ILE:HD11	1.96	0.66
1:A:151:ILE:CD1	1:G:153:GLY:CA	2.58	0.66
1:B:243:LEU:CD2	1:B:254:ILE:CD1	2.73	0.66
1:D:281:PHE:CZ	1:E:324:PHE:HE2	2.11	0.66
1:F:312:LYS:O	1:F:316:ILE:CD1	2.44	0.66
1:G:204:THR:OG1	1:G:218:ASN:OD1	2.13	0.66
1:C:311:LEU:O	1:C:314:ILE:HG22	1.95	0.66
1:C:312:LYS:O	1:C:316:ILE:CD1	2.44	0.66
1:D:197:ALA:HB3	1:D:205:LYS:HB3	1.78	0.66
1:A:212:ARG:HH11	1:G:232:MET:HE1	1.61	0.66
1:C:312:LYS:O	1:C:316:ILE:HD11	1.96	0.66
1:A:197:ALA:HB3	1:A:205:LYS:HB3	1.78	0.66
1:A:243:LEU:CD2	1:A:254:ILE:CD1	2.73	0.66
1:A:275:LEU:HD11	1:A:291:TYR:HD2	1.58	0.66
1:B:275:LEU:CD1	1:B:291:TYR:CD2	2.79	0.66
1:B:312:LYS:O	1:B:316:ILE:CD1	2.44	0.66
1:E:243:LEU:CD2	1:E:254:ILE:CD1	2.73	0.66
1:F:204:THR:OG1	1:F:218:ASN:OD1	2.13	0.66
1:G:312:LYS:O	1:G:316:ILE:CD1	2.44	0.66
1:D:312:LYS:O	1:D:316:ILE:HD11	1.96	0.66
1:D:312:LYS:O	1:D:316:ILE:CD1	2.44	0.65
1:E:312:LYS:O	1:E:316:ILE:CD1	2.44	0.65
1:A:222:SER:HB3	1:B:163:ILE:HD13	1.77	0.65
1:A:231:ARG:CZ	1:B:215:TYR:OH	2.44	0.65
1:A:312:LYS:O	1:A:316:ILE:HD11	1.96	0.65
1:C:232:MET:HE1	1:D:212:ARG:HH11	1.59	0.65
1:D:278:PHE:N	1:E:307:GLN:OE1	2.29	0.65
1:F:312:LYS:O	1:F:316:ILE:HD11	1.96	0.65
1:B:251:VAL:O	1:B:255:VAL:CG2	2.36	0.65
1:A:312:LYS:O	1:A:316:ILE:CD1	2.44	0.65
1:C:204:THR:OG1	1:C:218:ASN:OD1	2.13	0.65
1:F:331:LEU:CD1	1:G:331:LEU:HD11	2.26	0.65
1:A:212:ARG:HD2	1:G:229:PRO:CB	2.25	0.65
1:C:261:MET:SD	1:C:262:LEU:N	2.70	0.65
1:A:314:ILE:HD13	1:A:314:ILE:C	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LYS:O	1:B:316:ILE:HD11	1.96	0.65
1:E:236:ARG:HB2	1:E:293:PHE:CD1	2.26	0.65
1:E:236:ARG:HD2	1:F:210:ASP:CG	2.16	0.65
1:E:314:ILE:HD13	1:E:314:ILE:C	2.17	0.65
1:A:275:LEU:CD1	1:A:291:TYR:CD2	2.79	0.65
1:D:298:VAL:HG13	1:D:301:GLU:HB2	1.79	0.65
1:F:261:MET:SD	1:F:262:LEU:N	2.70	0.65
1:B:232:MET:HE1	1:C:212:ARG:HH11	1.61	0.65
1:C:197:ALA:HB3	1:C:205:LYS:HB3	1.78	0.65
1:F:298:VAL:HG13	1:F:301:GLU:HB2	1.79	0.65
1:B:261:MET:SD	1:B:262:LEU:N	2.70	0.65
1:C:314:ILE:HD13	1:C:314:ILE:C	2.17	0.65
1:D:261:MET:SD	1:D:262:LEU:N	2.70	0.65
1:G:261:MET:SD	1:G:262:LEU:N	2.70	0.65
1:B:197:ALA:HB3	1:B:205:LYS:HB3	1.78	0.65
1:B:216:VAL:CG1	1:B:221:PHE:HE1	2.09	0.65
1:E:261:MET:SD	1:E:262:LEU:N	2.70	0.65
1:F:314:ILE:HD13	1:F:314:ILE:C	2.17	0.65
1:A:204:THR:OG1	1:A:218:ASN:OD1	2.13	0.64
1:F:261:MET:CE	1:F:262:LEU:CD2	2.76	0.64
1:D:236:ARG:HD2	1:E:210:ASP:CG	2.16	0.64
1:A:163:ILE:HD11	1:G:222:SER:OG	1.92	0.64
1:A:278:PHE:N	1:B:307:GLN:OE1	2.30	0.64
1:B:227:GLU:HA	1:C:214:LEU:HA	1.78	0.64
1:C:275:LEU:CD1	1:C:291:TYR:CD2	2.79	0.64
1:F:176:ASP:CG	1:G:202:ARG:CD	2.66	0.64
1:G:298:VAL:HG13	1:G:301:GLU:HB2	1.79	0.64
1:A:261:MET:CE	1:A:262:LEU:CD2	2.76	0.64
1:C:261:MET:CE	1:C:262:LEU:CD2	2.76	0.64
1:C:298:VAL:HG13	1:C:301:GLU:HB2	1.79	0.64
1:D:333:MET:HE1	1:E:333:MET:SD	2.37	0.64
1:G:139:GLY:C	1:G:141:SER:N	2.48	0.64
1:G:261:MET:CE	1:G:262:LEU:CD2	2.76	0.64
1:A:201:TRP:HH2	1:B:116:ARG:HE	1.45	0.64
1:A:261:MET:SD	1:A:262:LEU:N	2.70	0.64
1:D:269:ASP:OD1	1:D:272:GLN:CG	2.46	0.64
1:E:275:LEU:CD1	1:E:291:TYR:CD2	2.79	0.64
1:A:136:GLU:HA	1:B:141:SER:OG	1.97	0.64
1:D:314:ILE:HD13	1:D:314:ILE:C	2.18	0.64
1:A:251:VAL:CG2	1:B:311:LEU:HD21	2.28	0.64
1:B:153:GLY:HA2	1:C:151:ILE:HD12	1.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:MET:CE	1:D:262:LEU:CD2	2.75	0.64
1:E:312:LYS:O	1:E:316:ILE:HD11	1.96	0.64
1:A:269:ASP:OD1	1:A:272:GLN:CG	2.46	0.64
1:C:222:SER:HB3	1:D:163:ILE:HD11	1.74	0.64
1:D:222:SER:HB3	1:E:163:ILE:HD13	1.79	0.64
1:E:261:MET:CE	1:E:262:LEU:CD2	2.76	0.64
1:E:278:PHE:CA	1:F:307:GLN:OE1	2.45	0.64
1:F:278:PHE:N	1:G:307:GLN:OE1	2.31	0.64
1:A:251:VAL:HG21	1:B:311:LEU:HD21	1.80	0.64
1:B:176:ASP:CG	1:C:202:ARG:CD	2.67	0.64
1:E:204:THR:OG1	1:E:218:ASN:OD1	2.13	0.64
1:F:331:LEU:HD13	1:G:331:LEU:HG	1.80	0.64
1:E:171:ILE:HD11	1:F:120:ARG:CZ	2.27	0.64
1:G:216:VAL:CG1	1:G:221:PHE:HE1	2.09	0.64
1:G:275:LEU:CD1	1:G:291:TYR:CD2	2.79	0.64
1:E:231:ARG:CZ	1:F:215:TYR:OH	2.47	0.63
1:G:314:ILE:HD13	1:G:314:ILE:C	2.17	0.63
1:A:216:VAL:CG1	1:A:221:PHE:HE1	2.09	0.63
1:A:236:ARG:CA	1:A:293:PHE:CD1	2.82	0.63
1:B:269:ASP:OD1	1:B:272:GLN:CG	2.45	0.63
1:B:314:ILE:HD13	1:B:314:ILE:C	2.17	0.63
1:B:236:ARG:CA	1:B:293:PHE:CD1	2.82	0.63
1:B:261:MET:CE	1:B:262:LEU:CD2	2.76	0.63
1:B:275:LEU:HD12	1:B:275:LEU:N	2.03	0.63
1:C:278:PHE:HB3	1:D:307:GLN:OE1	1.92	0.63
1:A:214:LEU:HA	1:G:227:GLU:HA	1.81	0.63
1:B:298:VAL:HG13	1:B:301:GLU:HB2	1.79	0.63
1:E:227:GLU:HB3	1:F:214:LEU:CB	2.28	0.63
1:E:298:VAL:HG13	1:E:301:GLU:HB2	1.79	0.63
1:A:120:ARG:NH2	1:G:167:PHE:CE1	2.57	0.63
1:A:298:VAL:HG13	1:A:301:GLU:HB2	1.79	0.63
1:C:236:ARG:CA	1:C:293:PHE:CD1	2.82	0.63
1:C:278:PHE:N	1:D:307:GLN:OE1	2.31	0.63
1:G:306:GLN:HG2	1:G:310:TYR:HE2	1.64	0.63
1:D:139:GLY:O	1:D:141:SER:O	2.16	0.63
1:F:236:ARG:HB2	1:F:293:PHE:CD1	2.26	0.63
1:F:232:MET:CE	1:G:212:ARG:HH11	2.11	0.62
1:G:236:ARG:CA	1:G:293:PHE:CD1	2.82	0.62
1:D:231:ARG:CZ	1:E:215:TYR:OH	2.47	0.62
1:F:269:ASP:OD1	1:F:272:GLN:CG	2.46	0.62
1:B:204:THR:OG1	1:B:218:ASN:OD1	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:VAL:CG1	1:C:221:PHE:HE1	2.09	0.62
1:D:251:VAL:HG21	1:E:311:LEU:HD21	1.80	0.62
1:A:333:MET:SD	1:G:333:MET:HE1	2.37	0.62
1:B:278:PHE:N	1:C:307:GLN:OE1	2.32	0.62
1:C:251:VAL:CG2	1:D:311:LEU:HD21	2.29	0.62
1:E:306:GLN:HG2	1:E:310:TYR:HE2	1.64	0.62
1:D:216:VAL:CG1	1:D:221:PHE:HE1	2.09	0.62
1:A:215:TYR:OH	1:G:231:ARG:CZ	2.45	0.62
1:B:306:GLN:HG2	1:B:310:TYR:HE2	1.64	0.62
1:E:136:GLU:HA	1:F:141:SER:OG	2.00	0.62
1:A:163:ILE:HG22	1:G:172:MET:HE3	1.82	0.62
1:D:236:ARG:CA	1:D:293:PHE:CD1	2.82	0.62
1:D:204:THR:OG1	1:D:218:ASN:OD1	2.13	0.62
1:E:269:ASP:OD1	1:E:272:GLN:CG	2.46	0.62
1:F:216:VAL:CG1	1:F:221:PHE:HE1	2.09	0.62
1:G:269:ASP:OD1	1:G:272:GLN:CG	2.46	0.62
1:C:251:VAL:HG21	1:D:311:LEU:HD21	1.81	0.62
1:D:306:GLN:HG2	1:D:310:TYR:HE2	1.64	0.62
1:F:306:GLN:HG2	1:F:310:TYR:HE2	1.64	0.62
1:A:306:GLN:HG2	1:A:310:TYR:HE2	1.64	0.61
1:B:251:VAL:CG2	1:C:311:LEU:HD21	2.30	0.61
1:B:251:VAL:HG21	1:C:311:LEU:HD21	1.82	0.61
1:D:227:GLU:HB3	1:E:214:LEU:CB	2.28	0.61
1:D:251:VAL:CG2	1:E:311:LEU:HD21	2.29	0.61
1:C:269:ASP:OD1	1:C:272:GLN:CG	2.46	0.61
1:D:227:GLU:HA	1:E:214:LEU:HA	1.83	0.61
1:E:222:SER:HB3	1:F:163:ILE:HD13	1.81	0.61
1:F:236:ARG:CA	1:F:293:PHE:CD1	2.82	0.61
1:B:229:PRO:HB3	1:C:212:ARG:HD2	1.81	0.61
1:G:236:ARG:HB2	1:G:293:PHE:CD1	2.26	0.61
1:A:236:ARG:HB2	1:A:293:PHE:CD1	2.26	0.61
1:C:167:PHE:CE1	1:D:120:ARG:CZ	2.72	0.61
1:E:227:GLU:HA	1:F:214:LEU:HA	1.83	0.61
1:A:212:ARG:NE	1:G:229:PRO:HG3	2.14	0.61
1:C:306:GLN:HG2	1:C:310:TYR:HE2	1.64	0.61
1:E:216:VAL:CG1	1:E:221:PHE:HE1	2.09	0.61
1:F:206:ILE:HG22	1:F:214:LEU:O	2.01	0.61
1:A:212:ARG:HD2	1:G:229:PRO:HB3	1.82	0.61
1:A:212:ARG:CD	1:G:229:PRO:HB3	2.30	0.61
1:A:294:THR:HG22	1:A:295:LYS:N	2.16	0.61
1:E:206:ILE:HG22	1:E:214:LEU:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:ARG:CA	1:E:293:PHE:CD1	2.82	0.61
1:D:192:ILE:HG22	1:D:214:LEU:HD11	1.82	0.61
1:F:229:PRO:HA	1:G:212:ARG:HD2	1.81	0.61
1:G:206:ILE:HG22	1:G:214:LEU:O	2.01	0.61
1:A:192:ILE:HG22	1:A:214:LEU:HD11	1.83	0.61
1:B:229:PRO:CB	1:C:212:ARG:HD2	2.31	0.61
1:D:232:MET:HE1	1:E:212:ARG:HH11	1.65	0.61
1:E:229:PRO:CB	1:F:212:ARG:HD2	2.31	0.61
1:G:192:ILE:HG22	1:G:214:LEU:HD11	1.82	0.61
1:G:294:THR:HG22	1:G:295:LYS:N	2.16	0.61
1:A:214:LEU:CB	1:G:227:GLU:HB3	2.30	0.60
1:A:212:ARG:HD3	1:G:232:MET:CE	2.31	0.60
1:A:172:MET:HE3	1:B:163:ILE:HG22	1.83	0.60
1:E:192:ILE:HG22	1:E:214:LEU:HD11	1.82	0.60
1:A:227:GLU:HB3	1:B:214:LEU:CB	2.29	0.60
1:F:243:LEU:CD2	1:F:254:ILE:HD13	2.32	0.60
1:B:331:LEU:HD13	1:C:331:LEU:HD11	1.83	0.60
1:F:222:SER:HB3	1:G:163:ILE:HD11	1.79	0.60
1:B:192:ILE:HG22	1:B:214:LEU:HD11	1.82	0.60
1:C:192:ILE:HG22	1:C:214:LEU:HD11	1.82	0.60
1:D:294:THR:HG22	1:D:295:LYS:N	2.16	0.60
1:F:251:VAL:CG2	1:G:311:LEU:HD21	2.31	0.60
1:F:272:GLN:HE21	1:F:272:GLN:HA	1.67	0.60
1:D:206:ILE:HG22	1:D:214:LEU:O	2.01	0.60
1:E:172:MET:HE3	1:F:163:ILE:HG22	1.84	0.60
1:D:243:LEU:CD2	1:D:254:ILE:HD13	2.32	0.60
1:F:160:GLY:O	1:F:161:LYS:C	2.40	0.60
1:A:243:LEU:CD2	1:A:254:ILE:HD13	2.32	0.60
1:B:226:VAL:O	1:B:226:VAL:HG12	2.02	0.60
1:C:294:THR:HG22	1:C:295:LYS:N	2.16	0.60
1:F:294:THR:HG22	1:F:295:LYS:N	2.16	0.60
1:G:226:VAL:O	1:G:226:VAL:HG12	2.02	0.60
1:G:243:LEU:CD2	1:G:254:ILE:HD13	2.32	0.60
1:A:206:ILE:HG22	1:A:214:LEU:O	2.01	0.60
1:B:236:ARG:HB2	1:B:293:PHE:CD1	2.26	0.60
1:B:294:THR:HG22	1:B:295:LYS:N	2.16	0.60
1:F:139:GLY:O	1:F:141:SER:CA	2.50	0.60
1:A:227:GLU:HA	1:B:214:LEU:HA	1.83	0.59
1:D:272:GLN:HE21	1:D:272:GLN:HA	1.66	0.59
1:E:243:LEU:CD2	1:E:254:ILE:HD13	2.32	0.59
1:E:294:THR:HG22	1:E:295:LYS:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ILE:HG22	1:F:214:LEU:HD11	1.82	0.59
1:A:226:VAL:O	1:A:226:VAL:HG12	2.02	0.59
1:D:160:GLY:O	1:D:161:LYS:C	2.40	0.59
1:G:272:GLN:HE21	1:G:272:GLN:HA	1.67	0.59
1:C:226:VAL:O	1:C:226:VAL:HG12	2.02	0.59
1:G:139:GLY:O	1:G:141:SER:N	2.35	0.59
1:A:331:LEU:HD13	1:B:331:LEU:HG	1.84	0.59
1:C:206:ILE:HG22	1:C:214:LEU:O	2.01	0.59
1:D:222:SER:HB3	1:E:163:ILE:HD11	1.77	0.59
1:G:139:GLY:O	1:G:141:SER:O	2.20	0.59
1:A:250:LYS:O	1:A:254:ILE:CG2	2.51	0.59
1:A:272:GLN:HE21	1:A:272:GLN:HA	1.67	0.59
1:B:206:ILE:HG22	1:B:214:LEU:O	2.01	0.59
1:C:243:LEU:CD2	1:C:254:ILE:HD13	2.32	0.59
1:C:272:GLN:HE21	1:C:272:GLN:HA	1.66	0.59
1:G:160:GLY:O	1:G:161:LYS:C	2.40	0.59
1:B:250:LYS:O	1:B:254:ILE:CG2	2.51	0.59
1:E:250:LYS:O	1:E:254:ILE:CG2	2.51	0.59
1:E:272:GLN:HE21	1:E:272:GLN:HA	1.67	0.59
1:F:153:GLY:HA2	1:G:151:ILE:HD12	1.82	0.59
1:B:229:PRO:HB3	1:C:212:ARG:CD	2.33	0.59
1:D:229:PRO:CB	1:E:212:ARG:HD2	2.32	0.59
1:B:172:MET:HE3	1:C:163:ILE:HG22	1.85	0.58
1:B:183:ASP:O	1:B:196:VAL:HG23	2.03	0.58
1:C:183:ASP:O	1:C:196:VAL:HG23	2.03	0.58
1:E:226:VAL:O	1:E:226:VAL:HG12	2.02	0.58
1:E:229:PRO:HB3	1:F:212:ARG:HD2	1.84	0.58
1:B:160:GLY:O	1:B:161:LYS:C	2.40	0.58
1:B:272:GLN:HE21	1:B:272:GLN:HA	1.67	0.58
1:D:250:LYS:O	1:D:254:ILE:CG2	2.51	0.58
1:G:250:LYS:O	1:G:254:ILE:CG2	2.51	0.58
1:C:176:ASP:CG	1:D:202:ARG:CD	2.70	0.58
1:D:183:ASP:O	1:D:196:VAL:HG23	2.03	0.58
1:E:221:PHE:N	1:E:221:PHE:HD1	2.01	0.58
1:D:221:PHE:N	1:D:221:PHE:HD1	2.01	0.58
1:F:226:VAL:HG12	1:F:226:VAL:O	2.02	0.58
1:A:183:ASP:O	1:A:196:VAL:HG23	2.03	0.58
1:A:221:PHE:N	1:A:221:PHE:HD1	2.01	0.58
1:B:139:GLY:O	1:B:141:SER:N	2.36	0.58
1:C:221:PHE:N	1:C:221:PHE:HD1	2.01	0.58
1:D:226:VAL:O	1:D:226:VAL:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:CD2	1:B:254:ILE:HD13	2.32	0.58
1:C:236:ARG:HB2	1:C:293:PHE:CD1	2.26	0.58
1:E:160:GLY:O	1:E:161:LYS:C	2.40	0.58
1:F:221:PHE:N	1:F:221:PHE:HD1	2.01	0.58
1:A:331:LEU:HD13	1:B:331:LEU:CG	2.33	0.58
1:B:278:PHE:HE1	1:B:286:LEU:CG	2.15	0.58
1:D:135:GLY:HA3	1:D:145:LEU:HD11	1.86	0.58
1:F:222:SER:HB3	1:G:163:ILE:HD13	1.85	0.58
1:F:250:LYS:O	1:F:254:ILE:CG2	2.51	0.58
1:A:160:GLY:O	1:A:161:LYS:C	2.40	0.58
1:F:183:ASP:O	1:F:196:VAL:HG23	2.03	0.58
1:A:229:PRO:CB	1:B:212:ARG:HD2	2.34	0.58
1:B:221:PHE:N	1:B:221:PHE:HD1	2.01	0.58
1:C:250:LYS:O	1:C:254:ILE:CG2	2.51	0.58
1:D:278:PHE:CA	1:E:307:GLN:OE1	2.49	0.58
1:E:333:MET:HE3	1:F:333:MET:SD	2.44	0.58
1:B:156:VAL:HB	1:C:151:ILE:HD11	1.85	0.57
1:C:224:ILE:O	1:C:226:VAL:HG23	2.05	0.57
1:D:278:PHE:HE1	1:D:286:LEU:CG	2.15	0.57
1:C:238:THR:HG22	1:C:291:TYR:CD1	2.40	0.57
1:C:269:ASP:HB2	1:C:295:LYS:HE2	1.85	0.57
1:E:229:PRO:HB3	1:F:212:ARG:CD	2.33	0.57
1:A:153:GLY:CA	1:B:151:ILE:HD13	2.15	0.57
1:A:238:THR:HG22	1:A:291:TYR:CD1	2.40	0.57
1:D:224:ILE:O	1:D:226:VAL:HG23	2.04	0.57
1:E:183:ASP:O	1:E:196:VAL:HG23	2.03	0.57
1:G:221:PHE:N	1:G:221:PHE:CD1	2.73	0.57
1:G:238:THR:HG22	1:G:291:TYR:CD1	2.40	0.57
1:A:156:VAL:HB	1:B:151:ILE:HD11	1.86	0.57
1:A:202:ARG:CD	1:G:176:ASP:CG	2.72	0.57
1:A:326:PHE:N	1:A:326:PHE:CD1	2.73	0.57
1:B:238:THR:HG22	1:B:291:TYR:CD1	2.40	0.57
1:D:238:THR:HG22	1:D:291:TYR:CD1	2.40	0.57
1:G:326:PHE:N	1:G:326:PHE:CD1	2.73	0.57
1:A:306:GLN:HG2	1:A:310:TYR:CE2	2.40	0.57
1:A:331:LEU:HD13	1:B:331:LEU:HD11	1.87	0.57
1:B:224:ILE:O	1:B:226:VAL:HG23	2.05	0.57
1:D:171:ILE:HD11	1:E:120:ARG:NH1	2.20	0.57
1:D:269:ASP:HB2	1:D:295:LYS:HE2	1.85	0.57
1:G:221:PHE:N	1:G:221:PHE:HD1	2.01	0.57
1:G:306:GLN:HG2	1:G:310:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TRP:N	1:C:201:TRP:CD1	2.73	0.57
1:D:201:TRP:N	1:D:201:TRP:CD1	2.73	0.57
1:D:229:PRO:HB3	1:E:212:ARG:HD2	1.85	0.57
1:E:238:THR:HG22	1:E:291:TYR:CD1	2.40	0.57
1:G:180:SER:O	1:G:182:GLY:N	2.38	0.57
1:A:221:PHE:N	1:A:221:PHE:CD1	2.73	0.57
1:F:278:PHE:HB3	1:G:307:GLN:OE1	2.01	0.57
1:F:306:GLN:HG2	1:F:310:TYR:CE2	2.40	0.57
1:D:306:GLN:HG2	1:D:310:TYR:CE2	2.40	0.57
1:F:180:SER:O	1:F:182:GLY:N	2.38	0.57
1:F:278:PHE:HE1	1:F:286:LEU:CG	2.15	0.57
1:A:180:SER:O	1:A:182:GLY:N	2.38	0.56
1:B:201:TRP:CD1	1:B:201:TRP:N	2.73	0.56
1:B:326:PHE:N	1:B:326:PHE:CD1	2.73	0.56
1:C:160:GLY:O	1:C:161:LYS:C	2.40	0.56
1:C:326:PHE:CD1	1:C:326:PHE:N	2.73	0.56
1:G:183:ASP:O	1:G:196:VAL:HG23	2.03	0.56
1:B:306:GLN:HG2	1:B:310:TYR:CE2	2.40	0.56
1:E:201:TRP:CD1	1:E:201:TRP:N	2.73	0.56
1:F:224:ILE:O	1:F:226:VAL:HG23	2.04	0.56
1:F:238:THR:HG22	1:F:291:TYR:CD1	2.40	0.56
1:G:224:ILE:O	1:G:226:VAL:HG23	2.04	0.56
1:A:176:ASP:CG	1:B:202:ARG:CD	2.74	0.56
1:A:229:PRO:HB3	1:B:212:ARG:HD2	1.86	0.56
1:A:275:LEU:H	1:A:275:LEU:CD1	2.07	0.56
1:D:180:SER:O	1:D:182:GLY:N	2.38	0.56
1:D:326:PHE:N	1:D:326:PHE:CD1	2.73	0.56
1:E:221:PHE:N	1:E:221:PHE:CD1	2.73	0.56
1:E:269:ASP:HB2	1:E:295:LYS:HE2	1.85	0.56
1:C:306:GLN:HG2	1:C:310:TYR:CE2	2.40	0.56
1:E:306:GLN:HG2	1:E:310:TYR:CE2	2.40	0.56
1:E:326:PHE:N	1:E:326:PHE:CD1	2.73	0.56
1:G:334:ASP:OD1	1:G:335:ASN:N	2.39	0.56
1:A:222:SER:HB3	1:B:163:ILE:HD11	1.77	0.56
1:A:334:ASP:OD1	1:A:335:ASN:N	2.39	0.56
1:C:180:SER:O	1:C:182:GLY:N	2.38	0.56
1:C:221:PHE:N	1:C:221:PHE:CD1	2.73	0.56
1:C:334:ASP:OD1	1:C:335:ASN:N	2.39	0.56
1:F:298:VAL:HG11	1:F:301:GLU:OE2	2.06	0.56
1:A:229:PRO:HB3	1:B:212:ARG:CD	2.36	0.56
1:B:180:SER:O	1:B:182:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:ILE:O	1:E:226:VAL:HG23	2.04	0.56
1:F:326:PHE:CD1	1:F:326:PHE:N	2.73	0.56
1:B:236:ARG:CG	1:B:238:THR:HG23	2.36	0.56
1:A:212:ARG:HD2	1:G:229:PRO:HA	1.86	0.56
1:G:145:LEU:O	1:G:149:GLY:N	2.39	0.56
1:G:269:ASP:HB2	1:G:295:LYS:HE2	1.85	0.56
1:D:298:VAL:HG11	1:D:301:GLU:OE2	2.06	0.56
1:E:145:LEU:O	1:E:149:GLY:N	2.39	0.56
1:F:269:ASP:HB2	1:F:295:LYS:HE2	1.85	0.56
1:A:201:TRP:N	1:A:201:TRP:CD1	2.73	0.55
1:A:224:ILE:O	1:A:226:VAL:HG23	2.04	0.55
1:B:317:VAL:HG11	1:B:324:PHE:CD1	2.42	0.55
1:B:334:ASP:OD1	1:B:335:ASN:N	2.39	0.55
1:D:317:VAL:HG11	1:D:324:PHE:CD1	2.42	0.55
1:F:317:VAL:HG11	1:F:324:PHE:CD1	2.42	0.55
1:A:317:VAL:HG11	1:A:324:PHE:CD1	2.42	0.55
1:D:145:LEU:O	1:D:149:GLY:N	2.39	0.55
1:D:334:ASP:OD1	1:D:335:ASN:N	2.39	0.55
1:E:317:VAL:HG11	1:E:324:PHE:CD1	2.42	0.55
1:F:334:ASP:OD1	1:F:335:ASN:N	2.39	0.55
1:G:278:PHE:HE1	1:G:286:LEU:CG	2.15	0.55
1:A:145:LEU:O	1:A:149:GLY:N	2.39	0.55
1:B:298:VAL:HG11	1:B:301:GLU:OE2	2.06	0.55
1:C:236:ARG:CG	1:C:238:THR:HG23	2.36	0.55
1:C:278:PHE:HE1	1:C:286:LEU:CG	2.15	0.55
1:C:317:VAL:HG11	1:C:324:PHE:CD1	2.42	0.55
1:G:317:VAL:HG11	1:G:324:PHE:CD1	2.42	0.55
1:A:278:PHE:CA	1:B:307:GLN:OE1	2.53	0.55
1:A:298:VAL:HG11	1:A:301:GLU:OE2	2.06	0.55
1:B:278:PHE:CA	1:C:307:GLN:OE1	2.54	0.55
1:E:180:SER:O	1:E:182:GLY:N	2.38	0.55
1:E:236:ARG:CG	1:E:238:THR:HG23	2.36	0.55
1:A:236:ARG:CG	1:A:238:THR:HG23	2.36	0.55
1:C:227:GLU:HB3	1:D:214:LEU:CB	2.35	0.55
1:E:298:VAL:HG11	1:E:301:GLU:OE2	2.06	0.55
1:F:227:GLU:HB3	1:G:214:LEU:CB	2.35	0.55
1:G:298:VAL:HG11	1:G:301:GLU:OE2	2.06	0.55
1:C:298:VAL:HG11	1:C:301:GLU:OE2	2.06	0.55
1:D:236:ARG:CG	1:D:238:THR:HG23	2.36	0.55
1:B:243:LEU:HD23	1:B:254:ILE:HD13	1.89	0.55
1:C:222:SER:HB3	1:D:163:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:ASP:OD1	1:E:335:ASN:N	2.39	0.55
1:F:221:PHE:N	1:F:221:PHE:CD1	2.73	0.55
1:B:139:GLY:O	1:B:141:SER:CA	2.54	0.55
1:C:145:LEU:O	1:C:149:GLY:N	2.39	0.55
1:D:156:VAL:HB	1:E:151:ILE:HD11	1.88	0.55
1:D:172:MET:HE3	1:E:163:ILE:HG22	1.89	0.55
1:E:229:PRO:HG3	1:F:212:ARG:NE	2.22	0.55
1:F:201:TRP:N	1:F:201:TRP:CD1	2.73	0.55
1:F:251:VAL:HG21	1:G:311:LEU:HD21	1.88	0.55
1:A:210:ASP:CG	1:G:236:ARG:HD2	2.26	0.55
1:B:145:LEU:O	1:B:149:GLY:N	2.39	0.55
1:B:221:PHE:N	1:B:221:PHE:CD1	2.73	0.55
1:C:167:PHE:HE2	1:D:120:ARG:NH1	1.87	0.54
1:D:229:PRO:HB3	1:E:212:ARG:CD	2.36	0.54
1:D:243:LEU:HD23	1:D:254:ILE:HD13	1.89	0.54
1:F:145:LEU:O	1:F:149:GLY:N	2.39	0.54
1:F:227:GLU:HA	1:G:214:LEU:HA	1.89	0.54
1:A:314:ILE:HG23	1:A:315:ASP:N	2.22	0.54
1:B:314:ILE:HG23	1:B:315:ASP:N	2.22	0.54
1:C:227:GLU:HA	1:D:214:LEU:HA	1.89	0.54
1:C:243:LEU:HD23	1:C:254:ILE:HD13	1.89	0.54
1:C:314:ILE:HG23	1:C:315:ASP:N	2.22	0.54
1:D:314:ILE:HG23	1:D:315:ASP:N	2.22	0.54
1:E:314:ILE:HG23	1:E:315:ASP:N	2.22	0.54
1:G:139:GLY:O	1:G:141:SER:CA	2.55	0.54
1:A:212:ARG:HD2	1:G:229:PRO:CA	2.36	0.54
1:A:243:LEU:HD23	1:A:254:ILE:HD13	1.89	0.54
1:D:221:PHE:N	1:D:221:PHE:CD1	2.73	0.54
1:E:229:PRO:HA	1:F:212:ARG:HD2	1.89	0.54
1:E:278:PHE:HE1	1:E:286:LEU:CG	2.16	0.54
1:F:243:LEU:HD23	1:F:254:ILE:HD13	1.89	0.54
1:F:167:PHE:HE2	1:G:120:ARG:NH1	1.96	0.54
1:F:236:ARG:CG	1:F:238:THR:HG23	2.36	0.54
1:C:229:PRO:HB3	1:D:212:ARG:HD2	1.88	0.54
1:E:243:LEU:HD23	1:E:254:ILE:HD13	1.89	0.54
1:B:216:VAL:CG1	1:B:221:PHE:CE1	2.88	0.54
1:F:229:PRO:HB3	1:G:212:ARG:CD	2.37	0.54
1:G:201:TRP:N	1:G:201:TRP:CD1	2.73	0.54
1:A:216:VAL:CG1	1:A:221:PHE:CE1	2.89	0.54
1:E:250:LYS:O	1:E:254:ILE:HG23	2.08	0.54
1:A:154:LEU:CD2	1:G:154:LEU:HD12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LYS:O	1:A:254:ILE:HG23	2.08	0.53
1:D:236:ARG:CA	1:D:293:PHE:HD1	2.14	0.53
1:G:250:LYS:O	1:G:254:ILE:HG23	2.08	0.53
1:C:229:PRO:HA	1:D:212:ARG:HD2	1.89	0.53
1:G:216:VAL:CG1	1:G:221:PHE:CE1	2.88	0.53
1:G:314:ILE:HG23	1:G:315:ASP:N	2.22	0.53
1:C:229:PRO:HB3	1:D:212:ARG:CD	2.38	0.53
1:G:236:ARG:CB	1:G:293:PHE:CD1	2.90	0.53
1:A:154:LEU:HD12	1:B:154:LEU:CD2	2.38	0.53
1:C:250:LYS:O	1:C:254:ILE:HG23	2.08	0.53
1:D:311:LEU:O	1:D:311:LEU:HD13	2.09	0.53
1:G:243:LEU:HD23	1:G:254:ILE:HD13	1.89	0.53
1:A:229:PRO:HA	1:B:212:ARG:HD2	1.89	0.53
1:B:269:ASP:HB2	1:B:295:LYS:HE2	1.85	0.53
1:C:275:LEU:H	1:C:275:LEU:CD1	2.07	0.53
1:D:331:LEU:HD13	1:E:331:LEU:HD11	1.89	0.53
1:E:311:LEU:O	1:E:311:LEU:HD13	2.09	0.53
1:A:278:PHE:HE1	1:A:286:LEU:CG	2.16	0.53
1:B:250:LYS:O	1:B:254:ILE:HG23	2.09	0.53
1:B:272:GLN:NE2	1:B:272:GLN:HA	2.24	0.53
1:C:216:VAL:CG1	1:C:221:PHE:CE1	2.88	0.53
1:C:231:ARG:HH21	1:D:215:TYR:HH	1.54	0.53
1:C:311:LEU:O	1:C:311:LEU:HD13	2.09	0.53
1:D:154:LEU:HD12	1:E:154:LEU:CD2	2.38	0.53
1:F:250:LYS:O	1:F:254:ILE:HG23	2.08	0.53
1:G:236:ARG:CG	1:G:238:THR:HG23	2.36	0.53
1:E:331:LEU:HD13	1:F:331:LEU:HG	1.91	0.53
1:F:314:ILE:HG23	1:F:315:ASP:N	2.22	0.53
1:G:278:PHE:CE1	1:G:286:LEU:CG	2.92	0.53
1:C:229:PRO:CB	1:D:212:ARG:HD2	2.37	0.53
1:D:243:LEU:N	1:D:243:LEU:CD1	2.72	0.53
1:D:272:GLN:NE2	1:D:272:GLN:HA	2.24	0.53
1:F:201:TRP:HH2	1:G:116:ARG:HE	1.57	0.53
1:F:236:ARG:CB	1:F:293:PHE:CD1	2.90	0.53
1:F:311:LEU:O	1:F:311:LEU:HD13	2.09	0.53
1:A:212:ARG:HD3	1:G:232:MET:HE3	1.91	0.53
1:G:311:LEU:O	1:G:311:LEU:HD13	2.09	0.53
1:A:139:GLY:O	1:A:141:SER:N	2.42	0.53
1:A:272:GLN:NE2	1:A:272:GLN:HA	2.24	0.53
1:C:244:ARG:CG	1:C:323:ASP:OD2	2.57	0.53
1:A:183:ASP:OD1	1:A:196:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:N	1:A:243:LEU:CD1	2.72	0.52
1:C:331:LEU:HD13	1:D:331:LEU:HD11	1.90	0.52
1:F:229:PRO:CB	1:G:212:ARG:HD2	2.38	0.52
1:B:183:ASP:OD1	1:B:196:VAL:HG23	2.10	0.52
1:C:278:PHE:CA	1:D:307:GLN:OE1	2.54	0.52
1:C:296:THR:HB	1:C:298:VAL:HG12	1.92	0.52
1:D:250:LYS:O	1:D:254:ILE:HG23	2.09	0.52
1:F:160:GLY:C	1:F:161:LYS:O	2.48	0.52
1:G:272:GLN:NE2	1:G:272:GLN:HA	2.24	0.52
1:C:183:ASP:OD1	1:C:196:VAL:HG23	2.10	0.52
1:C:243:LEU:N	1:C:243:LEU:CD1	2.72	0.52
1:D:296:THR:HB	1:D:298:VAL:HG12	1.92	0.52
1:E:296:THR:HB	1:E:298:VAL:HG12	1.92	0.52
1:F:272:GLN:NE2	1:F:272:GLN:HA	2.24	0.52
1:C:272:GLN:NE2	1:C:272:GLN:HA	2.24	0.52
1:D:272:GLN:CA	1:D:272:GLN:NE2	2.73	0.52
1:E:272:GLN:NE2	1:E:272:GLN:HA	2.24	0.52
1:F:296:THR:HB	1:F:298:VAL:HG12	1.92	0.52
1:A:311:LEU:O	1:A:311:LEU:HD13	2.09	0.52
1:B:296:THR:HB	1:B:298:VAL:HG12	1.92	0.52
1:C:272:GLN:CA	1:C:272:GLN:NE2	2.73	0.52
1:D:294:THR:CG2	1:D:295:LYS:N	2.73	0.52
1:E:243:LEU:N	1:E:243:LEU:CD1	2.72	0.52
1:E:281:PHE:CD2	1:F:310:TYR:CD1	2.98	0.52
1:F:229:PRO:CA	1:G:212:ARG:HD2	2.40	0.52
1:F:278:PHE:CE1	1:F:286:LEU:CG	2.92	0.52
1:F:294:THR:CG2	1:F:295:LYS:N	2.73	0.52
1:C:232:MET:CE	1:D:212:ARG:HH11	2.23	0.52
1:E:160:GLY:C	1:E:161:LYS:O	2.48	0.52
1:E:236:ARG:CB	1:E:293:PHE:CD1	2.90	0.52
1:E:294:THR:CG2	1:E:295:LYS:N	2.73	0.52
1:G:248:ALA:C	1:G:251:VAL:HG13	2.28	0.52
1:G:294:THR:CG2	1:G:295:LYS:N	2.73	0.52
1:G:296:THR:HB	1:G:298:VAL:HG12	1.92	0.52
1:C:139:GLY:O	1:C:141:SER:N	2.43	0.52
1:F:216:VAL:CG1	1:F:221:PHE:CE1	2.88	0.52
1:G:183:ASP:OD1	1:G:196:VAL:HG23	2.10	0.52
1:G:236:ARG:CA	1:G:293:PHE:HD1	2.14	0.52
1:G:243:LEU:N	1:G:243:LEU:CD1	2.72	0.52
1:A:296:THR:HB	1:A:298:VAL:HG12	1.91	0.52
1:B:243:LEU:N	1:B:243:LEU:CD1	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:VAL:CG1	1:D:221:PHE:CE1	2.88	0.52
1:B:244:ARG:CG	1:B:323:ASP:OD2	2.57	0.52
1:E:272:GLN:CA	1:E:272:GLN:NE2	2.73	0.52
1:A:269:ASP:HB2	1:A:295:LYS:HE2	1.86	0.52
1:C:275:LEU:HD11	1:C:291:TYR:CD2	2.44	0.52
1:C:294:THR:CG2	1:C:295:LYS:N	2.73	0.52
1:D:183:ASP:OD1	1:D:196:VAL:HG23	2.10	0.52
1:D:229:PRO:HG3	1:E:212:ARG:NE	2.25	0.52
1:E:244:ARG:CG	1:E:323:ASP:OD2	2.57	0.52
1:E:310:TYR:HA	1:E:313:ILE:HG21	1.90	0.52
1:B:311:LEU:O	1:B:311:LEU:HD13	2.09	0.51
1:D:223:SER:O	1:E:217:PRO:HG3	2.10	0.51
1:A:160:GLY:C	1:A:161:LYS:O	2.48	0.51
1:B:272:GLN:CA	1:B:272:GLN:NE2	2.73	0.51
1:C:139:GLY:C	1:C:141:SER:N	2.64	0.51
1:D:244:ARG:CG	1:D:323:ASP:OD2	2.57	0.51
1:D:310:TYR:HA	1:D:313:ILE:HG21	1.90	0.51
1:E:278:PHE:CE1	1:E:286:LEU:CG	2.92	0.51
1:F:243:LEU:N	1:F:243:LEU:CD1	2.72	0.51
1:G:190:ARG:NH2	1:G:220:LEU:HD21	2.26	0.51
1:C:310:TYR:HA	1:C:313:ILE:HG21	1.90	0.51
1:E:190:ARG:NH2	1:E:220:LEU:HD21	2.26	0.51
1:F:229:PRO:HB3	1:G:212:ARG:HD2	1.91	0.51
1:A:294:THR:CG2	1:A:295:LYS:N	2.73	0.51
1:B:190:ARG:NH2	1:B:220:LEU:HD21	2.26	0.51
1:B:248:ALA:C	1:B:251:VAL:HG13	2.28	0.51
1:D:190:ARG:NH2	1:D:220:LEU:HD21	2.26	0.51
1:E:248:ALA:C	1:E:251:VAL:HG13	2.28	0.51
1:E:317:VAL:HG21	1:E:324:PHE:HE1	1.76	0.51
1:F:310:TYR:HA	1:F:313:ILE:HG21	1.90	0.51
1:A:190:ARG:NH2	1:A:220:LEU:HD21	2.26	0.51
1:C:153:GLY:CA	1:D:151:ILE:HD13	2.19	0.51
1:D:278:PHE:CE1	1:D:286:LEU:CG	2.92	0.51
1:D:317:VAL:HG21	1:D:324:PHE:HE1	1.75	0.51
1:A:208:THR:HG23	1:A:210:ASP:H	1.76	0.51
1:A:232:MET:CE	1:B:212:ARG:HH11	2.23	0.51
1:A:302:TRP:C	1:A:302:TRP:CD1	2.84	0.51
1:E:176:ASP:CG	1:F:202:ARG:CD	2.77	0.51
1:E:208:THR:HG23	1:E:210:ASP:H	1.76	0.51
1:E:216:VAL:CG1	1:E:221:PHE:CE1	2.88	0.51
1:F:229:PRO:HG3	1:G:212:ARG:NE	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ARG:CG	1:F:323:ASP:OD2	2.57	0.51
1:F:317:VAL:HG21	1:F:324:PHE:HE1	1.76	0.51
1:A:244:ARG:CG	1:A:323:ASP:OD2	2.57	0.51
1:A:317:VAL:HG21	1:A:324:PHE:HE1	1.76	0.51
1:A:331:LEU:CD1	1:B:331:LEU:CD1	2.86	0.51
1:C:160:GLY:C	1:C:161:LYS:O	2.48	0.51
1:C:190:ARG:NH2	1:C:220:LEU:HD21	2.26	0.51
1:F:183:ASP:OD1	1:F:196:VAL:HG23	2.10	0.51
1:F:190:ARG:NH2	1:F:220:LEU:HD21	2.26	0.51
1:F:272:GLN:NE2	1:F:272:GLN:CA	2.73	0.51
1:F:302:TRP:C	1:F:302:TRP:CD1	2.85	0.51
1:D:176:ASP:CG	1:E:202:ARG:CD	2.76	0.51
1:D:179:PHE:CD2	1:D:196:VAL:HG11	2.46	0.51
1:D:229:PRO:HA	1:E:212:ARG:HD2	1.93	0.51
1:E:179:PHE:CD2	1:E:196:VAL:HG11	2.46	0.51
1:A:189:ASP:OD2	1:A:224:ILE:CG2	2.59	0.51
1:B:208:THR:HG23	1:B:210:ASP:H	1.76	0.51
1:D:189:ASP:OD2	1:D:224:ILE:CG2	2.59	0.51
1:G:160:GLY:C	1:G:161:LYS:O	2.48	0.51
1:B:189:ASP:OD2	1:B:224:ILE:CG2	2.59	0.50
1:D:183:ASP:OD1	1:D:183:ASP:N	2.44	0.50
1:E:154:LEU:HD12	1:F:154:LEU:CD2	2.40	0.50
1:E:183:ASP:OD1	1:E:196:VAL:HG23	2.10	0.50
1:A:141:SER:OG	1:G:136:GLU:HA	2.12	0.50
1:B:223:SER:O	1:C:217:PRO:HG3	2.11	0.50
1:B:229:PRO:HG3	1:C:212:ARG:NE	2.26	0.50
1:C:208:THR:HG23	1:C:210:ASP:H	1.76	0.50
1:E:229:PRO:CA	1:F:212:ARG:HD2	2.42	0.50
1:E:313:ILE:HA	1:E:316:ILE:HG12	1.93	0.50
1:F:172:MET:HE1	1:G:163:ILE:O	2.11	0.50
1:G:189:ASP:OD2	1:G:224:ILE:CG2	2.60	0.50
1:A:280:GLN:HG2	1:A:282:ALA:HB2	1.94	0.50
1:B:160:GLY:C	1:B:161:LYS:O	2.48	0.50
1:B:302:TRP:CD1	1:B:302:TRP:C	2.84	0.50
1:B:331:LEU:HD13	1:C:331:LEU:CG	2.42	0.50
1:C:183:ASP:OD1	1:C:183:ASP:N	2.44	0.50
1:D:236:ARG:CB	1:D:293:PHE:CD1	2.90	0.50
1:E:171:ILE:CD1	1:F:120:ARG:NH2	2.60	0.50
1:E:189:ASP:OD2	1:E:224:ILE:CG2	2.59	0.50
1:E:223:SER:O	1:F:217:PRO:HG3	2.11	0.50
1:F:172:MET:CE	1:G:163:ILE:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:THR:HG23	1:F:210:ASP:H	1.76	0.50
1:A:229:PRO:HG3	1:B:212:ARG:NE	2.25	0.50
1:B:294:THR:CG2	1:B:295:LYS:N	2.73	0.50
1:B:310:TYR:HA	1:B:313:ILE:HG21	1.90	0.50
1:E:302:TRP:CD1	1:E:302:TRP:C	2.84	0.50
1:G:208:THR:HG23	1:G:210:ASP:H	1.76	0.50
1:G:244:ARG:CG	1:G:323:ASP:OD2	2.57	0.50
1:A:313:ILE:HA	1:A:316:ILE:HG12	1.93	0.50
1:B:179:PHE:CD2	1:B:196:VAL:HG11	2.46	0.50
1:B:280:GLN:HG2	1:B:282:ALA:HB2	1.94	0.50
1:C:179:PHE:CD2	1:C:196:VAL:HG11	2.46	0.50
1:C:280:GLN:HG2	1:C:282:ALA:HB2	1.94	0.50
1:C:317:VAL:HG21	1:C:324:PHE:HE1	1.76	0.50
1:D:275:LEU:HD11	1:D:291:TYR:CD2	2.44	0.50
1:E:156:VAL:HB	1:F:151:ILE:HD11	1.94	0.50
1:D:269:ASP:CB	1:D:295:LYS:HE3	2.32	0.50
1:F:313:ILE:HA	1:F:316:ILE:HG12	1.93	0.50
1:G:179:PHE:CD2	1:G:196:VAL:HG11	2.46	0.50
1:A:278:PHE:CE1	1:A:286:LEU:CG	2.92	0.50
1:B:259:ARG:NH1	1:B:277:TYR:OH	2.45	0.50
1:D:302:TRP:C	1:D:302:TRP:CD1	2.84	0.50
1:F:179:PHE:CD2	1:F:196:VAL:HG11	2.46	0.50
1:F:189:ASP:OD2	1:F:224:ILE:CG2	2.59	0.50
1:G:280:GLN:HG2	1:G:282:ALA:HB2	1.94	0.50
1:G:302:TRP:CD1	1:G:302:TRP:C	2.84	0.50
1:G:310:TYR:HA	1:G:313:ILE:HG21	1.90	0.50
1:D:313:ILE:HA	1:D:316:ILE:HG12	1.93	0.50
1:G:183:ASP:OD1	1:G:183:ASP:N	2.44	0.50
1:G:259:ARG:NH1	1:G:277:TYR:OH	2.45	0.50
1:G:317:VAL:HG21	1:G:324:PHE:HE1	1.76	0.50
1:A:223:SER:O	1:B:217:PRO:HG3	2.12	0.50
1:A:331:LEU:HD13	1:B:331:LEU:HD12	1.94	0.50
1:B:222:SER:HB3	1:C:163:ILE:HD11	1.76	0.50
1:B:229:PRO:HA	1:C:212:ARG:HD2	1.92	0.50
1:B:278:PHE:CE1	1:B:286:LEU:CG	2.92	0.50
1:D:280:GLN:HG2	1:D:282:ALA:HB2	1.94	0.50
1:G:313:ILE:HA	1:G:316:ILE:HG12	1.93	0.49
1:A:310:TYR:HA	1:A:313:ILE:HG21	1.90	0.49
1:C:189:ASP:OD2	1:C:224:ILE:CG2	2.59	0.49
1:B:154:LEU:HD12	1:C:154:LEU:CD2	2.42	0.49
1:B:313:ILE:HA	1:B:316:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLY:O	1:C:141:SER:CA	2.61	0.49
1:D:160:GLY:C	1:D:161:LYS:O	2.48	0.49
1:D:259:ARG:NH1	1:D:277:TYR:OH	2.45	0.49
1:E:171:ILE:HG12	1:F:120:ARG:NH2	2.28	0.49
1:A:202:ARG:HD2	1:G:176:ASP:CG	2.16	0.49
1:A:331:LEU:CD1	1:B:331:LEU:HD11	2.42	0.49
1:C:229:PRO:HG3	1:D:212:ARG:NE	2.27	0.49
1:A:270:GLN:CD	1:A:270:GLN:H	2.16	0.49
1:B:317:VAL:HG21	1:B:324:PHE:HE1	1.76	0.49
1:D:208:THR:HG23	1:D:210:ASP:H	1.76	0.49
1:E:280:GLN:HG2	1:E:282:ALA:HB2	1.94	0.49
1:F:280:GLN:HG2	1:F:282:ALA:HB2	1.94	0.49
1:A:163:ILE:HD13	1:G:222:SER:HB3	1.91	0.49
1:C:270:GLN:CD	1:C:270:GLN:H	2.16	0.49
1:A:179:PHE:CD2	1:A:196:VAL:HG11	2.46	0.49
1:B:331:LEU:CD1	1:C:331:LEU:HD11	2.42	0.49
1:E:171:ILE:HG12	1:F:120:ARG:HH22	1.72	0.49
1:A:259:ARG:NH1	1:A:277:TYR:OH	2.45	0.49
1:B:331:LEU:HD13	1:C:331:LEU:HD12	1.94	0.49
1:C:162:ASP:HA	1:C:165:SER:OG	2.13	0.49
1:C:259:ARG:NH1	1:C:277:TYR:OH	2.45	0.49
1:C:302:TRP:CD1	1:C:302:TRP:C	2.84	0.49
1:B:183:ASP:OD1	1:B:183:ASP:N	2.44	0.49
1:C:278:PHE:CE1	1:C:286:LEU:CG	2.92	0.49
1:F:242:GLY:C	1:F:243:LEU:HD12	2.33	0.49
1:A:183:ASP:OD1	1:A:183:ASP:N	2.44	0.49
1:A:242:GLY:C	1:A:243:LEU:HD12	2.34	0.49
1:B:162:ASP:HA	1:B:165:SER:OG	2.13	0.49
1:C:206:ILE:CG2	1:C:214:LEU:O	2.61	0.48
1:E:242:GLY:C	1:E:243:LEU:HD12	2.34	0.48
1:E:275:LEU:HD11	1:E:291:TYR:CD2	2.44	0.48
1:G:206:ILE:CG2	1:G:214:LEU:O	2.61	0.48
1:B:331:LEU:HD13	1:C:331:LEU:HG	1.95	0.48
1:C:228:ASN:HD21	1:C:231:ARG:CG	2.23	0.48
1:D:162:ASP:HA	1:D:165:SER:OG	2.13	0.48
1:D:206:ILE:CG2	1:D:214:LEU:O	2.61	0.48
1:E:162:ASP:HA	1:E:165:SER:OG	2.13	0.48
1:E:236:ARG:CA	1:E:293:PHE:HD1	2.14	0.48
1:F:206:ILE:CG2	1:F:214:LEU:O	2.61	0.48
1:A:162:ASP:HA	1:A:165:SER:OG	2.13	0.48
1:A:237:ILE:HG13	1:A:237:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:HA	1:C:316:ILE:HG12	1.93	0.48
1:D:242:GLY:C	1:D:243:LEU:HD12	2.34	0.48
1:E:174:TYR:CZ	1:F:117:ILE:HG21	2.47	0.48
1:F:162:ASP:HA	1:F:165:SER:OG	2.13	0.48
1:F:232:MET:HE1	1:G:212:ARG:NH1	2.21	0.48
1:G:237:ILE:O	1:G:237:ILE:HG13	2.13	0.48
1:E:270:GLN:H	1:E:270:GLN:CD	2.16	0.48
1:F:237:ILE:HG13	1:F:237:ILE:O	2.13	0.48
1:F:270:GLN:CD	1:F:270:GLN:H	2.16	0.48
1:B:237:ILE:O	1:B:237:ILE:HG13	2.13	0.48
1:C:269:ASP:CB	1:C:295:LYS:HE3	2.32	0.48
1:D:237:ILE:HG13	1:D:237:ILE:O	2.13	0.48
1:D:270:GLN:CD	1:D:270:GLN:H	2.16	0.48
1:F:259:ARG:NH1	1:F:277:TYR:OH	2.45	0.48
1:G:242:GLY:C	1:G:243:LEU:HD12	2.34	0.48
1:C:236:ARG:CB	1:C:293:PHE:CD1	2.90	0.48
1:D:171:ILE:HD11	1:E:120:ARG:HH22	1.77	0.48
1:D:310:TYR:CA	1:D:313:ILE:CG2	2.88	0.48
1:F:248:ALA:C	1:F:251:VAL:HG13	2.28	0.48
1:B:206:ILE:CG2	1:B:214:LEU:O	2.61	0.48
1:G:162:ASP:HA	1:G:165:SER:OG	2.13	0.48
1:A:229:PRO:CA	1:B:212:ARG:HD2	2.43	0.48
1:E:173:LEU:HD11	1:E:179:PHE:CZ	2.49	0.48
1:F:206:ILE:HG21	1:F:214:LEU:CD2	2.44	0.48
1:F:275:LEU:HD11	1:F:291:TYR:CD2	2.44	0.48
1:G:241:ILE:CG2	1:G:243:LEU:HD11	2.44	0.48
1:A:331:LEU:HD11	1:G:331:LEU:HD13	1.93	0.48
1:C:242:GLY:C	1:C:243:LEU:HD12	2.34	0.48
1:C:269:ASP:HA	1:C:295:LYS:HZ1	1.78	0.48
1:D:241:ILE:CG2	1:D:243:LEU:HD11	2.44	0.48
1:C:172:MET:CE	1:D:163:ILE:O	2.62	0.47
1:A:275:LEU:HD11	1:A:291:TYR:CD2	2.44	0.47
1:B:173:LEU:HD11	1:B:179:PHE:CZ	2.49	0.47
1:B:261:MET:CE	1:B:262:LEU:HD21	2.45	0.47
1:C:229:PRO:CA	1:D:212:ARG:HD2	2.44	0.47
1:E:206:ILE:CG2	1:E:214:LEU:O	2.61	0.47
1:E:237:ILE:O	1:E:237:ILE:HG13	2.13	0.47
1:G:270:GLN:H	1:G:270:GLN:CD	2.16	0.47
1:A:206:ILE:CG2	1:A:214:LEU:O	2.61	0.47
1:B:242:GLY:C	1:B:243:LEU:HD12	2.33	0.47
1:B:275:LEU:HD11	1:B:291:TYR:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HA	1:C:141:SER:HA	1.36	0.47
1:E:206:ILE:HG21	1:E:214:LEU:CD2	2.44	0.47
1:F:261:MET:SD	1:F:261:MET:C	2.93	0.47
1:A:261:MET:CE	1:A:262:LEU:HD21	2.45	0.47
1:B:270:GLN:H	1:B:270:GLN:CD	2.16	0.47
1:B:311:LEU:HD22	1:B:311:LEU:HA	1.74	0.47
1:C:173:LEU:HD11	1:C:179:PHE:CZ	2.49	0.47
1:C:311:LEU:HD22	1:C:311:LEU:HA	1.74	0.47
1:D:161:LYS:HB3	1:D:162:ASP:H	1.57	0.47
1:D:173:LEU:HD11	1:D:179:PHE:CZ	2.49	0.47
1:E:183:ASP:OD1	1:E:183:ASP:N	2.45	0.47
1:E:222:SER:HB3	1:F:163:ILE:HD11	1.77	0.47
1:E:261:MET:SD	1:E:261:MET:C	2.93	0.47
1:F:183:ASP:OD1	1:F:183:ASP:N	2.44	0.47
1:D:228:ASN:HD21	1:D:231:ARG:CG	2.23	0.47
1:E:241:ILE:CG2	1:E:243:LEU:HD11	2.44	0.47
1:F:173:LEU:HD11	1:F:179:PHE:CZ	2.49	0.47
1:F:241:ILE:CG2	1:F:243:LEU:HD11	2.44	0.47
1:A:248:ALA:C	1:A:251:VAL:HG13	2.28	0.47
1:B:241:ILE:CG2	1:B:243:LEU:HD11	2.44	0.47
1:C:237:ILE:HG13	1:C:237:ILE:O	2.13	0.47
1:C:241:ILE:CG2	1:C:243:LEU:HD11	2.44	0.47
1:D:229:PRO:CA	1:E:212:ARG:HD2	2.45	0.47
1:G:261:MET:SD	1:G:261:MET:C	2.93	0.47
1:B:161:LYS:HB3	1:B:162:ASP:H	1.57	0.47
1:C:261:MET:CE	1:C:262:LEU:HD21	2.45	0.47
1:C:331:LEU:HD13	1:D:331:LEU:HD12	1.93	0.47
1:D:206:ILE:HG21	1:D:214:LEU:CD2	2.44	0.47
1:F:228:ASN:HD21	1:F:231:ARG:CG	2.23	0.47
1:A:241:ILE:CG2	1:A:243:LEU:HD11	2.44	0.47
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.76	0.47
1:B:232:MET:CE	1:C:212:ARG:HH11	2.26	0.47
1:B:261:MET:SD	1:B:261:MET:C	2.93	0.47
1:D:248:ALA:C	1:D:251:VAL:HG13	2.28	0.47
1:G:169:SER:HG	1:G:222:SER:HG	1.58	0.47
1:G:272:GLN:NE2	1:G:272:GLN:CA	2.73	0.47
1:G:310:TYR:CA	1:G:313:ILE:CG2	2.88	0.47
1:A:173:LEU:HD11	1:A:179:PHE:CZ	2.49	0.47
1:B:206:ILE:HG21	1:B:214:LEU:CD2	2.44	0.47
1:D:261:MET:SD	1:D:261:MET:C	2.93	0.47
1:G:261:MET:CE	1:G:262:LEU:HD21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:LEU:HD11	1:G:291:TYR:CD2	2.44	0.47
1:A:161:LYS:HB3	1:A:162:ASP:H	1.57	0.46
1:A:261:MET:SD	1:A:261:MET:C	2.93	0.46
1:C:206:ILE:HG21	1:C:214:LEU:CD2	2.44	0.46
1:F:261:MET:CE	1:F:262:LEU:HD21	2.45	0.46
1:G:173:LEU:HD11	1:G:179:PHE:CZ	2.49	0.46
1:B:228:ASN:HD21	1:B:231:ARG:CG	2.23	0.46
1:D:311:LEU:HD22	1:D:311:LEU:HA	1.74	0.46
1:G:269:ASP:CB	1:G:295:LYS:HE3	2.32	0.46
1:D:261:MET:CE	1:D:262:LEU:HD21	2.45	0.46
1:F:139:GLY:O	1:F:141:SER:N	2.47	0.46
1:G:289:MET:O	1:G:289:MET:HG2	2.16	0.46
1:A:323:ASP:OD1	1:A:323:ASP:N	2.49	0.46
1:B:236:ARG:CB	1:B:293:PHE:CD1	2.90	0.46
1:C:153:GLY:HA2	1:D:151:ILE:HD12	1.88	0.46
1:E:261:MET:CE	1:E:262:LEU:HD21	2.45	0.46
1:A:217:PRO:HG3	1:G:223:SER:O	2.15	0.46
1:C:261:MET:SD	1:C:261:MET:C	2.93	0.46
1:E:289:MET:HG2	1:E:289:MET:O	2.16	0.46
1:E:323:ASP:N	1:E:323:ASP:OD1	2.49	0.46
1:F:323:ASP:OD1	1:F:323:ASP:N	2.49	0.46
1:B:323:ASP:N	1:B:323:ASP:OD1	2.49	0.46
1:F:311:LEU:HD22	1:F:311:LEU:HA	1.74	0.46
1:A:236:ARG:CA	1:A:293:PHE:CE1	2.99	0.46
1:B:229:PRO:CA	1:C:212:ARG:HD2	2.44	0.46
1:C:201:TRP:HH2	1:D:116:ARG:HE	1.64	0.46
1:C:317:VAL:HG11	1:C:324:PHE:CE1	2.51	0.46
1:D:317:VAL:HG11	1:D:324:PHE:CE1	2.51	0.46
1:E:281:PHE:CD2	1:F:310:TYR:HD1	2.33	0.46
1:E:331:LEU:HD13	1:F:331:LEU:CG	2.44	0.46
1:G:323:ASP:N	1:G:323:ASP:OD1	2.49	0.46
1:E:269:ASP:HA	1:E:295:LYS:HZ1	1.81	0.46
1:E:317:VAL:HG11	1:E:324:PHE:CE1	2.51	0.46
1:F:317:VAL:HG11	1:F:324:PHE:CE1	2.51	0.46
1:E:259:ARG:NH1	1:E:277:TYR:OH	2.45	0.46
1:A:317:VAL:HG11	1:A:324:PHE:CE1	2.51	0.46
1:B:269:ASP:CB	1:B:295:LYS:HE3	2.32	0.46
1:F:156:VAL:HB	1:G:151:ILE:HD11	1.97	0.46
1:B:317:VAL:HG11	1:B:324:PHE:CE1	2.51	0.45
1:E:315:ASP:O	1:E:319:SER:N	2.48	0.45
1:F:269:ASP:CB	1:F:295:LYS:HE3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HG	1:C:163:ILE:HD12	1.82	0.45
1:B:179:PHE:CE1	1:B:221:PHE:HD2	2.35	0.45
1:C:179:PHE:CE1	1:C:221:PHE:HD2	2.35	0.45
1:D:281:PHE:CD2	1:E:310:TYR:CD1	3.04	0.45
1:A:147:THR:HG23	1:G:149:GLY:HA3	1.98	0.45
1:D:179:PHE:CE1	1:D:221:PHE:HD2	2.35	0.45
1:D:323:ASP:OD1	1:D:323:ASP:N	2.49	0.45
1:A:289:MET:O	1:A:289:MET:HG2	2.16	0.45
1:B:289:MET:O	1:B:289:MET:HG2	2.16	0.45
1:C:189:ASP:OD2	1:C:224:ILE:HG21	2.17	0.45
1:E:250:LYS:O	1:E:254:ILE:HG22	2.17	0.45
1:E:311:LEU:C	1:E:314:ILE:HG22	2.36	0.45
1:F:250:LYS:O	1:F:254:ILE:HG22	2.17	0.45
1:G:311:LEU:C	1:G:314:ILE:HG22	2.36	0.45
1:A:179:PHE:CE1	1:A:221:PHE:HD2	2.35	0.45
1:A:189:ASP:OD2	1:A:224:ILE:HG21	2.17	0.45
1:A:201:TRP:O	1:A:218:ASN:ND2	2.50	0.45
1:C:323:ASP:OD1	1:C:323:ASP:N	2.49	0.45
1:D:331:LEU:HD13	1:E:331:LEU:HD12	1.98	0.45
1:E:189:ASP:OD2	1:E:224:ILE:HG21	2.17	0.45
1:E:311:LEU:O	1:E:314:ILE:CG2	2.64	0.45
1:F:201:TRP:O	1:F:218:ASN:ND2	2.50	0.45
1:F:275:LEU:HD13	1:F:291:TYR:CD2	2.51	0.45
1:A:269:ASP:HA	1:A:295:LYS:HZ1	1.82	0.45
1:A:333:MET:SD	1:G:333:MET:HE2	2.53	0.45
1:D:149:GLY:HA3	1:E:147:THR:HG23	1.97	0.45
1:G:201:TRP:O	1:G:218:ASN:ND2	2.50	0.45
1:G:317:VAL:HG11	1:G:324:PHE:CE1	2.51	0.45
1:A:311:LEU:HD22	1:A:311:LEU:HA	1.74	0.45
1:A:311:LEU:C	1:A:314:ILE:HG22	2.36	0.45
1:B:275:LEU:HD13	1:B:291:TYR:CD2	2.51	0.45
1:D:135:GLY:CA	1:D:145:LEU:HD11	2.46	0.45
1:E:275:LEU:HD13	1:E:291:TYR:CD2	2.51	0.45
1:E:276:VAL:O	1:E:277:TYR:CG	2.70	0.45
1:F:276:VAL:O	1:F:277:TYR:CG	2.70	0.45
1:F:311:LEU:O	1:F:314:ILE:CG2	2.64	0.45
1:A:269:ASP:CB	1:A:295:LYS:HE3	2.32	0.45
1:A:295:LYS:HD3	1:A:295:LYS:HA	1.72	0.45
1:B:201:TRP:O	1:B:218:ASN:ND2	2.50	0.45
1:B:276:VAL:O	1:B:277:TYR:CG	2.70	0.45
1:C:311:LEU:C	1:C:314:ILE:HG22	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:TYR:CZ	1:E:117:ILE:HG21	2.52	0.45
1:D:189:ASP:OD2	1:D:224:ILE:HG21	2.17	0.45
1:D:201:TRP:O	1:D:218:ASN:ND2	2.50	0.45
1:D:250:LYS:O	1:D:254:ILE:HG22	2.17	0.45
1:E:241:ILE:HG23	1:E:324:PHE:CZ	2.52	0.45
1:E:310:TYR:CA	1:E:313:ILE:CG2	2.88	0.45
1:F:289:MET:O	1:F:289:MET:HG2	2.16	0.45
1:F:311:LEU:C	1:F:314:ILE:HG22	2.36	0.45
1:A:149:GLY:HA3	1:B:147:THR:HG23	1.98	0.45
1:A:276:VAL:O	1:A:277:TYR:CG	2.70	0.45
1:C:201:TRP:O	1:C:218:ASN:ND2	2.50	0.45
1:C:275:LEU:CD1	1:C:275:LEU:N	2.73	0.45
1:D:303:LEU:HD12	1:D:303:LEU:HA	1.76	0.45
1:F:189:ASP:OD2	1:F:224:ILE:HG21	2.17	0.45
1:G:275:LEU:HD13	1:G:291:TYR:CD2	2.51	0.45
1:A:281:PHE:CD1	1:A:281:PHE:O	2.70	0.45
1:A:310:TYR:CA	1:A:313:ILE:CG2	2.88	0.45
1:A:331:LEU:HD12	1:G:331:LEU:HD13	1.96	0.45
1:B:241:ILE:HG23	1:B:324:PHE:CZ	2.52	0.45
1:C:281:PHE:CD1	1:C:281:PHE:O	2.70	0.45
1:C:289:MET:HG2	1:C:289:MET:O	2.16	0.45
1:D:276:VAL:O	1:D:277:TYR:CG	2.70	0.45
1:D:311:LEU:C	1:D:314:ILE:HG22	2.36	0.45
1:E:281:PHE:O	1:E:281:PHE:CD1	2.70	0.45
1:F:281:PHE:HZ	1:G:324:PHE:CE2	2.28	0.45
1:G:241:ILE:HG23	1:G:324:PHE:CZ	2.52	0.45
1:E:179:PHE:CE1	1:E:221:PHE:HD2	2.35	0.44
1:E:251:VAL:HG21	1:F:311:LEU:CD2	2.42	0.44
1:F:241:ILE:HG23	1:F:324:PHE:CZ	2.52	0.44
1:G:189:ASP:OD2	1:G:224:ILE:HG21	2.17	0.44
1:G:250:LYS:O	1:G:254:ILE:HG22	2.17	0.44
1:A:311:LEU:O	1:A:314:ILE:CG2	2.64	0.44
1:A:315:ASP:O	1:A:319:SER:N	2.48	0.44
1:B:189:ASP:OD2	1:B:224:ILE:HG21	2.17	0.44
1:C:250:LYS:O	1:C:254:ILE:HG22	2.17	0.44
1:C:276:VAL:O	1:C:277:TYR:CG	2.70	0.44
1:D:241:ILE:HG23	1:D:324:PHE:CZ	2.52	0.44
1:E:161:LYS:O	1:E:163:ILE:N	2.51	0.44
1:G:311:LEU:O	1:G:314:ILE:CG2	2.64	0.44
1:G:315:ASP:O	1:G:319:SER:N	2.48	0.44
1:A:241:ILE:HG22	1:A:243:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HG22	1:B:243:LEU:CD1	2.48	0.44
1:B:311:LEU:C	1:B:314:ILE:HG22	2.37	0.44
1:F:241:ILE:HG22	1:F:243:LEU:CD1	2.48	0.44
1:B:135:GLY:HA3	1:B:145:LEU:HD11	1.99	0.44
1:B:261:MET:SD	1:B:262:LEU:CG	3.06	0.44
1:C:161:LYS:O	1:C:163:ILE:N	2.51	0.44
1:C:219:SER:O	1:C:222:SER:HB2	2.18	0.44
1:D:219:SER:O	1:D:222:SER:HB2	2.18	0.44
1:D:315:ASP:O	1:D:319:SER:N	2.48	0.44
1:F:154:LEU:HD12	1:G:154:LEU:CD2	2.47	0.44
1:F:281:PHE:CD1	1:F:281:PHE:O	2.70	0.44
1:G:179:PHE:CE1	1:G:221:PHE:HD2	2.35	0.44
1:G:276:VAL:O	1:G:277:TYR:CG	2.70	0.44
1:A:241:ILE:HG23	1:A:324:PHE:CZ	2.52	0.44
1:B:161:LYS:O	1:B:163:ILE:N	2.51	0.44
1:C:161:LYS:HB3	1:C:162:ASP:H	1.57	0.44
1:C:241:ILE:HG23	1:C:324:PHE:CZ	2.52	0.44
1:D:275:LEU:HD13	1:D:291:TYR:CD2	2.51	0.44
1:D:289:MET:O	1:D:289:MET:HG2	2.16	0.44
1:F:236:ARG:CA	1:F:293:PHE:CE1	2.99	0.44
1:F:303:LEU:HD12	1:F:303:LEU:HA	1.76	0.44
1:F:315:ASP:O	1:F:319:SER:N	2.48	0.44
1:A:275:LEU:HD13	1:A:291:TYR:CD2	2.51	0.44
1:B:241:ILE:HD12	1:B:313:ILE:HD11	1.99	0.44
1:B:269:ASP:HA	1:B:295:LYS:HZ1	1.82	0.44
1:C:208:THR:HG22	1:C:212:ARG:H	1.83	0.44
1:D:135:GLY:HA3	1:D:145:LEU:CD1	2.46	0.44
1:D:283:ASP:HB3	1:D:284:SER:H	1.62	0.44
1:E:201:TRP:O	1:E:218:ASN:ND2	2.50	0.44
1:E:219:SER:O	1:E:222:SER:HB2	2.18	0.44
1:F:161:LYS:O	1:F:163:ILE:N	2.51	0.44
1:F:278:PHE:CE1	1:F:286:LEU:HG	2.53	0.44
1:G:219:SER:O	1:G:222:SER:HB2	2.18	0.44
1:B:281:PHE:O	1:B:281:PHE:CD1	2.71	0.44
1:C:275:LEU:HD13	1:C:291:TYR:CD2	2.51	0.44
1:C:281:PHE:O	1:C:281:PHE:HD1	2.01	0.44
1:E:208:THR:HG22	1:E:212:ARG:H	1.83	0.44
1:G:161:LYS:O	1:G:163:ILE:N	2.51	0.44
1:A:161:LYS:O	1:A:163:ILE:N	2.51	0.44
1:A:250:LYS:O	1:A:254:ILE:HG22	2.17	0.44
1:A:281:PHE:O	1:A:281:PHE:HD1	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:O	1:B:281:PHE:HD1	2.01	0.44
1:B:295:LYS:HD3	1:B:295:LYS:HA	1.72	0.44
1:C:241:ILE:HD12	1:C:313:ILE:HD11	1.99	0.44
1:D:208:THR:HG22	1:D:212:ARG:H	1.83	0.44
1:E:278:PHE:CE1	1:E:286:LEU:HG	2.53	0.44
1:G:241:ILE:HG22	1:G:243:LEU:CD1	2.48	0.44
1:G:281:PHE:O	1:G:281:PHE:HD1	2.01	0.44
1:A:219:SER:O	1:A:222:SER:HB2	2.18	0.44
1:D:281:PHE:O	1:D:281:PHE:HD1	2.01	0.44
1:D:311:LEU:O	1:D:314:ILE:CG2	2.64	0.44
1:E:171:ILE:CD1	1:F:120:ARG:HH12	2.22	0.44
1:F:236:ARG:CA	1:F:293:PHE:HD1	2.14	0.44
1:F:269:ASP:HA	1:F:295:LYS:HZ1	1.83	0.44
1:A:278:PHE:CE1	1:A:286:LEU:HG	2.53	0.43
1:B:250:LYS:O	1:B:254:ILE:HG22	2.17	0.43
1:E:281:PHE:O	1:E:281:PHE:HD1	2.01	0.43
1:F:179:PHE:CE1	1:F:221:PHE:HD2	2.35	0.43
1:G:295:LYS:HD3	1:G:295:LYS:HA	1.71	0.43
1:B:278:PHE:CE1	1:B:286:LEU:HG	2.53	0.43
1:D:281:PHE:O	1:D:281:PHE:CD1	2.71	0.43
1:E:169:SER:HG	1:E:222:SER:HG	1.67	0.43
1:F:281:PHE:O	1:F:281:PHE:HD1	2.01	0.43
1:G:281:PHE:O	1:G:281:PHE:CD1	2.70	0.43
1:B:208:THR:HG22	1:B:212:ARG:H	1.83	0.43
1:B:315:ASP:O	1:B:319:SER:N	2.48	0.43
1:C:241:ILE:HG22	1:C:243:LEU:CD1	2.48	0.43
1:C:261:MET:SD	1:C:262:LEU:CG	3.06	0.43
1:D:161:LYS:O	1:D:163:ILE:N	2.51	0.43
1:D:241:ILE:HG22	1:D:243:LEU:CD1	2.48	0.43
1:E:311:LEU:HD22	1:E:311:LEU:HA	1.74	0.43
1:F:208:THR:HG22	1:F:212:ARG:H	1.83	0.43
1:A:281:PHE:CD2	1:B:310:TYR:CD1	3.06	0.43
1:B:172:MET:CE	1:C:163:ILE:O	2.65	0.43
1:C:169:SER:OG	1:C:222:SER:OG	2.36	0.43
1:C:248:ALA:C	1:C:251:VAL:HG13	2.28	0.43
1:D:331:LEU:HD13	1:E:331:LEU:CG	2.48	0.43
1:E:139:GLY:O	1:E:141:SER:CA	2.66	0.43
1:E:149:GLY:HA3	1:F:147:THR:HG23	2.00	0.43
1:E:231:ARG:CZ	1:F:215:TYR:HH	2.28	0.43
1:E:241:ILE:HG22	1:E:243:LEU:CD1	2.48	0.43
1:F:219:SER:O	1:F:222:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:O	1:B:314:ILE:CG2	2.64	0.43
1:A:228:ASN:HD21	1:A:231:ARG:CG	2.23	0.43
1:C:278:PHE:CE1	1:C:286:LEU:HG	2.53	0.43
1:B:331:LEU:CD1	1:C:331:LEU:CD1	2.90	0.43
1:C:212:ARG:HA	1:C:213:PRO:HD3	1.80	0.43
1:C:315:ASP:O	1:C:319:SER:N	2.48	0.43
1:G:269:ASP:HA	1:G:295:LYS:HZ1	1.83	0.43
1:G:161:LYS:HB3	1:G:162:ASP:H	1.56	0.43
1:G:208:THR:HG22	1:G:212:ARG:H	1.83	0.43
1:A:208:THR:HG22	1:A:212:ARG:H	1.83	0.43
1:B:219:SER:O	1:B:222:SER:HB2	2.18	0.43
1:B:310:TYR:CA	1:B:313:ILE:CG2	2.88	0.43
1:D:278:PHE:CE1	1:D:286:LEU:HG	2.53	0.43
1:B:231:ARG:CZ	1:C:215:TYR:HH	2.27	0.42
1:B:281:PHE:CD2	1:C:310:TYR:CD1	3.07	0.42
1:C:171:ILE:HD11	1:D:120:ARG:HH22	1.84	0.42
1:C:310:TYR:CA	1:C:313:ILE:CG2	2.88	0.42
1:D:171:ILE:CG1	1:E:120:ARG:HH22	2.32	0.42
1:A:314:ILE:C	1:A:314:ILE:CD1	2.85	0.42
1:C:135:GLY:HA3	1:C:145:LEU:HD11	2.00	0.42
1:E:331:LEU:HD13	1:F:331:LEU:HD11	2.00	0.42
1:A:205:LYS:NZ	1:G:231:ARG:HH22	2.17	0.42
1:C:283:ASP:HB3	1:C:284:SER:H	1.62	0.42
1:D:149:GLY:HA3	1:E:147:THR:CG2	2.50	0.42
1:D:172:MET:HA	1:D:175:PHE:HD2	1.85	0.42
1:D:269:ASP:HA	1:D:295:LYS:HZ1	1.83	0.42
1:E:228:ASN:HD21	1:E:231:ARG:CG	2.23	0.42
1:F:233:THR:O	1:F:234:ASN:ND2	2.53	0.42
1:F:330:THR:HB	1:G:328:SER:HB2	2.00	0.42
1:G:243:LEU:CD2	1:G:254:ILE:HD11	2.34	0.42
1:C:270:GLN:CD	1:C:270:GLN:N	2.73	0.42
1:D:261:MET:SD	1:D:262:LEU:CG	3.06	0.42
1:F:247:ASP:OD1	1:F:322:ALA:HB1	2.07	0.42
1:F:278:PHE:CA	1:G:307:GLN:OE1	2.65	0.42
1:G:206:ILE:HG21	1:G:214:LEU:CD2	2.44	0.42
1:G:278:PHE:CE1	1:G:286:LEU:HG	2.53	0.42
1:A:206:ILE:HG21	1:A:214:LEU:CD2	2.44	0.42
1:B:233:THR:O	1:B:234:ASN:ND2	2.53	0.42
1:B:270:GLN:CD	1:B:270:GLN:N	2.73	0.42
1:D:233:THR:O	1:D:234:ASN:ND2	2.53	0.42
1:G:172:MET:HA	1:G:175:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASP:OD2	1:D:202:ARG:NE	2.51	0.42
1:F:172:MET:HA	1:F:175:PHE:HD2	1.85	0.42
1:F:314:ILE:CG2	1:F:315:ASP:N	2.83	0.42
1:G:283:ASP:HB3	1:G:284:SER:H	1.62	0.42
1:C:331:LEU:CD1	1:D:331:LEU:HD11	2.50	0.42
1:D:140:MET:HA	1:D:141:SER:HA	1.14	0.42
1:E:233:THR:O	1:E:234:ASN:ND2	2.53	0.42
1:E:239:THR:HG22	1:E:310:TYR:OH	2.20	0.42
1:E:269:ASP:CB	1:E:295:LYS:HE3	2.32	0.42
1:E:314:ILE:CG2	1:E:315:ASP:N	2.83	0.42
1:F:239:THR:HG22	1:F:310:TYR:OH	2.20	0.42
1:A:154:LEU:HD12	1:B:154:LEU:HD21	2.01	0.42
1:A:239:THR:HG22	1:A:310:TYR:OH	2.20	0.42
1:B:172:MET:HA	1:B:175:PHE:HD2	1.85	0.42
1:C:311:LEU:O	1:C:314:ILE:CG2	2.64	0.42
1:F:243:LEU:CD2	1:F:254:ILE:HD11	2.34	0.42
1:G:233:THR:O	1:G:234:ASN:ND2	2.53	0.42
1:G:241:ILE:HD12	1:G:313:ILE:HD11	1.99	0.42
1:A:139:GLY:O	1:A:141:SER:CA	2.67	0.42
1:B:239:THR:HG22	1:B:310:TYR:OH	2.20	0.42
1:D:331:LEU:CD1	1:E:331:LEU:HD11	2.49	0.42
1:E:140:MET:C	1:E:141:SER:CB	2.54	0.42
1:F:283:ASP:HB3	1:F:284:SER:H	1.62	0.42
1:G:311:LEU:HD22	1:G:311:LEU:HA	1.74	0.42
1:A:215:TYR:HH	1:G:231:ARG:CZ	2.27	0.42
1:A:261:MET:SD	1:A:262:LEU:CG	3.06	0.42
1:B:172:MET:HE1	1:C:163:ILE:O	2.20	0.42
1:C:233:THR:O	1:C:234:ASN:ND2	2.53	0.42
1:D:167:PHE:CE2	1:D:171:ILE:HD11	2.55	0.42
1:D:331:LEU:HD13	1:E:331:LEU:HG	2.00	0.42
1:G:135:GLY:HA3	1:G:145:LEU:HD11	2.01	0.42
1:G:140:MET:HA	1:G:141:SER:HA	1.16	0.42
1:G:270:GLN:CD	1:G:270:GLN:N	2.73	0.42
1:A:169:SER:HG	1:B:163:ILE:HD12	1.85	0.41
1:A:233:THR:O	1:A:234:ASN:ND2	2.53	0.41
1:C:167:PHE:CE2	1:C:171:ILE:HD11	2.55	0.41
1:C:298:VAL:CG1	1:C:301:GLU:HB2	2.49	0.41
1:D:296:THR:C	1:D:298:VAL:N	2.72	0.41
1:G:314:ILE:CG2	1:G:315:ASP:N	2.83	0.41
1:A:120:ARG:NH1	1:G:171:ILE:HD11	2.35	0.41
1:A:151:ILE:HD11	1:G:156:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ILE:CG2	1:C:315:ASP:N	2.83	0.41
1:D:295:LYS:HA	1:D:295:LYS:HD3	1.71	0.41
1:E:303:LEU:HD12	1:E:303:LEU:HA	1.76	0.41
1:G:239:THR:HG22	1:G:310:TYR:OH	2.20	0.41
1:A:167:PHE:CE2	1:A:171:ILE:HD11	2.55	0.41
1:C:229:PRO:O	1:C:232:MET:SD	2.79	0.41
1:C:247:ASP:OD1	1:C:322:ALA:HB1	2.07	0.41
1:D:239:THR:HG22	1:D:310:TYR:OH	2.20	0.41
1:E:212:ARG:HA	1:E:213:PRO:HD3	1.80	0.41
1:E:261:MET:SD	1:E:262:LEU:CG	3.06	0.41
1:E:270:GLN:CD	1:E:270:GLN:N	2.73	0.41
1:E:295:LYS:HD3	1:E:295:LYS:HA	1.72	0.41
1:G:229:PRO:O	1:G:232:MET:SD	2.79	0.41
1:G:314:ILE:C	1:G:314:ILE:CD1	2.85	0.41
1:A:283:ASP:HB3	1:A:284:SER:H	1.62	0.41
1:B:167:PHE:CE2	1:B:171:ILE:HD11	2.55	0.41
1:D:171:ILE:HD11	1:E:120:ARG:NH2	2.35	0.41
1:D:270:GLN:CD	1:D:270:GLN:N	2.73	0.41
1:F:310:TYR:CA	1:F:313:ILE:CG2	2.88	0.41
1:A:172:MET:HA	1:A:175:PHE:HD2	1.85	0.41
1:A:229:PRO:O	1:A:232:MET:SD	2.79	0.41
1:D:314:ILE:CG2	1:D:315:ASP:N	2.83	0.41
1:E:167:PHE:CE2	1:E:171:ILE:HD11	2.55	0.41
1:F:229:PRO:O	1:F:232:MET:SD	2.79	0.41
1:G:298:VAL:CG1	1:G:301:GLU:HB2	2.49	0.41
1:C:314:ILE:C	1:C:314:ILE:CD1	2.85	0.41
1:F:261:MET:SD	1:F:262:LEU:CG	3.06	0.41
1:G:296:THR:C	1:G:298:VAL:N	2.72	0.41
1:A:314:ILE:CG2	1:A:315:ASP:N	2.83	0.41
1:B:283:ASP:HB3	1:B:284:SER:H	1.62	0.41
1:C:239:THR:HG22	1:C:310:TYR:OH	2.20	0.41
1:G:261:MET:SD	1:G:262:LEU:CG	3.06	0.41
1:A:163:ILE:HD11	1:G:222:SER:HB3	1.86	0.41
1:E:172:MET:HA	1:E:175:PHE:HD2	1.85	0.41
1:E:229:PRO:O	1:E:232:MET:SD	2.79	0.41
1:E:241:ILE:HD12	1:E:313:ILE:HD11	1.99	0.41
1:F:140:MET:C	1:F:141:SER:OG	2.52	0.41
1:F:167:PHE:CE2	1:F:171:ILE:HD11	2.55	0.41
1:F:232:MET:HG2	1:F:234:ASN:O	2.21	0.41
1:G:167:PHE:CE2	1:G:171:ILE:HD11	2.55	0.41
1:A:232:MET:HG2	1:A:234:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLN:CD	1:A:270:GLN:N	2.73	0.41
1:B:149:GLY:HA3	1:C:147:THR:HG23	2.03	0.41
1:B:176:ASP:OD2	1:C:202:ARG:NE	2.49	0.41
1:B:212:ARG:HA	1:B:213:PRO:HD3	1.80	0.41
1:B:229:PRO:O	1:B:232:MET:SD	2.79	0.41
1:B:314:ILE:CG2	1:B:315:ASP:N	2.83	0.41
1:C:172:MET:HE1	1:D:163:ILE:O	2.20	0.41
1:C:295:LYS:HD3	1:C:295:LYS:HA	1.71	0.41
1:D:232:MET:CE	1:E:212:ARG:HH11	2.33	0.41
1:F:275:LEU:H	1:F:275:LEU:CD1	2.07	0.41
1:A:212:ARG:HA	1:A:213:PRO:HD3	1.80	0.40
1:B:232:MET:HG2	1:B:234:ASN:O	2.21	0.40
1:C:172:MET:HA	1:C:175:PHE:HD2	1.85	0.40
1:C:331:LEU:HD13	1:D:331:LEU:CG	2.51	0.40
1:D:212:ARG:HA	1:D:213:PRO:HD3	1.80	0.40
1:D:232:MET:HG2	1:D:234:ASN:O	2.21	0.40
1:E:283:ASP:HB3	1:E:284:SER:H	1.62	0.40
1:F:314:ILE:C	1:F:314:ILE:CD1	2.85	0.40
1:G:228:ASN:HD21	1:G:231:ARG:CG	2.23	0.40
1:A:147:THR:CG2	1:G:149:GLY:HA3	2.51	0.40
1:C:171:ILE:HD11	1:D:120:ARG:HH12	1.86	0.40
1:D:229:PRO:O	1:D:232:MET:SD	2.79	0.40
1:F:241:ILE:HD12	1:F:313:ILE:HD11	1.99	0.40
1:D:172:MET:HE1	1:E:163:ILE:O	2.21	0.40
1:E:167:PHE:HZ	1:F:120:ARG:CD	2.32	0.40
1:F:272:GLN:HE21	1:F:272:GLN:C	2.25	0.40
1:A:330:THR:HB	1:B:328:SER:HB2	2.04	0.40
1:C:232:MET:HG2	1:C:234:ASN:O	2.21	0.40
1:E:167:PHE:CE1	1:F:120:ARG:NH2	2.89	0.40
1:E:171:ILE:CG1	1:F:120:ARG:NH2	2.71	0.40
1:E:174:TYR:CE2	1:F:117:ILE:HG21	2.57	0.40
1:E:232:MET:CE	1:F:212:ARG:HH11	2.30	0.40
1:E:269:ASP:OD2	1:E:271:ARG:CG	2.56	0.40
1:F:270:GLN:CD	1:F:270:GLN:N	2.73	0.40
1:G:232:MET:HG2	1:G:234:ASN:O	2.21	0.40
1:G:303:LEU:HA	1:G:303:LEU:HD12	1.76	0.40
1:D:272:GLN:HE21	1:D:272:GLN:C	2.25	0.40
1:D:281:PHE:CD2	1:E:310:TYR:HD1	2.40	0.40

There are no symmetry-related clashes.

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	A	221/349 (63%)	194 (88%)	17 (8%)	10 (4%)	2 19
1	B	221/349 (63%)	194 (88%)	17 (8%)	10 (4%)	2 19
1	C	221/349 (63%)	195 (88%)	17 (8%)	9 (4%)	2 20
1	D	221/349 (63%)	194 (88%)	17 (8%)	10 (4%)	2 19
1	E	221/349 (63%)	194 (88%)	17 (8%)	10 (4%)	2 19
1	F	221/349 (63%)	193 (87%)	18 (8%)	10 (4%)	2 19
1	G	221/349 (63%)	194 (88%)	17 (8%)	10 (4%)	2 19
All	All	1547/2443 (63%)	1358 (88%)	120 (8%)	69 (4%)	3 19

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	B	161	LYS
1	C	161	LYS
1	D	161	LYS
1	E	161	LYS
1	F	141	SER
1	F	161	LYS
1	G	161	LYS
1	A	141	SER
1	A	146	LEU
1	A	297	THR
1	B	146	LEU
1	B	297	THR
1	C	146	LEU
1	C	297	THR
1	D	146	LEU
1	D	297	THR
1	E	141	SER

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Mol	Chain	Res	Type
1	E	146	LEU
1	E	297	THR
1	F	146	LEU
1	F	297	THR
1	G	146	LEU
1	G	297	THR
1	B	141	SER
1	A	145	LEU
1	A	181	ILE
1	A	189	ASP
1	B	145	LEU
1	B	181	ILE
1	B	189	ASP
1	C	145	LEU
1	C	181	ILE
1	C	189	ASP
1	D	141	SER
1	D	145	LEU
1	D	181	ILE
1	D	189	ASP
1	E	145	LEU
1	E	181	ILE
1	E	189	ASP
1	F	145	LEU
1	F	181	ILE
1	F	189	ASP
1	G	145	LEU
1	G	181	ILE
1	G	189	ASP
1	A	114	SER
1	B	114	SER
1	C	114	SER
1	D	114	SER
1	E	114	SER
1	F	114	SER
1	G	114	SER
1	G	141	SER
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	E	206	ILE

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Mol	Chain	Res	Type
1	F	206	ILE
1	G	206	ILE
1	A	241	ILE
1	B	241	ILE
1	C	241	ILE
1	D	241	ILE
1	E	241	ILE
1	F	241	ILE
1	G	241	ILE

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	B	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	C	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	D	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	E	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	F	192/304 (63%)	155 (81%)	37 (19%)	1 7
1	G	192/304 (63%)	155 (81%)	37 (19%)	1 7
All	All	1344/2128 (63%)	1085 (81%)	259 (19%)	3 7

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	MET
1	A	196	VAL
1	A	201	TRP
1	A	214	LEU
1	A	225	SER
1	A	232	MET
1	A	235	ARG
1	A	236	ARG

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	247	ASP
1	A	254	ILE
1	A	259	ARG
1	A	261	MET
1	A	263	LYS
1	A	269	ASP
1	A	270	GLN
1	A	271	ARG
1	A	272	GLN
1	A	275	LEU
1	A	280	GLN
1	A	281	PHE
1	A	284	SER
1	A	286	LEU
1	A	295	LYS
1	A	296	THR
1	A	299	TRP
1	A	302	TRP
1	A	303	LEU
1	A	307	GLN
1	A	311	LEU
1	A	313	ILE
1	A	314	ILE
1	A	316	ILE
1	A	323	ASP
1	A	326	PHE
1	A	329	GLN
1	A	330	THR
1	B	158	MET
1	B	196	VAL
1	B	201	TRP
1	B	214	LEU
1	B	225	SER
1	B	232	MET
1	B	235	ARG
1	B	236	ARG
1	B	243	LEU
1	B	247	ASP
1	B	254	ILE
1	B	259	ARG
1	B	261	MET

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Mol	Chain	Res	Type
1	B	263	LYS
1	B	269	ASP
1	B	270	GLN
1	B	271	ARG
1	B	272	GLN
1	B	275	LEU
1	B	280	GLN
1	B	281	PHE
1	B	284	SER
1	B	286	LEU
1	B	295	LYS
1	B	296	THR
1	B	299	TRP
1	B	302	TRP
1	B	303	LEU
1	B	307	GLN
1	B	311	LEU
1	B	313	ILE
1	B	314	ILE
1	B	316	ILE
1	B	323	ASP
1	B	326	PHE
1	B	329	GLN
1	B	330	THR
1	C	158	MET
1	C	196	VAL
1	C	201	TRP
1	C	214	LEU
1	C	225	SER
1	C	232	MET
1	C	235	ARG
1	C	236	ARG
1	C	243	LEU
1	C	247	ASP
1	C	254	ILE
1	C	259	ARG
1	C	261	MET
1	C	263	LYS
1	C	269	ASP
1	C	270	GLN
1	C	271	ARG
1	C	272	GLN

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Mol	Chain	Res	Type
1	C	275	LEU
1	C	280	GLN
1	C	281	PHE
1	C	284	SER
1	C	286	LEU
1	C	295	LYS
1	C	296	THR
1	C	299	TRP
1	C	302	TRP
1	C	303	LEU
1	C	307	GLN
1	C	311	LEU
1	C	313	ILE
1	C	314	ILE
1	C	316	ILE
1	C	323	ASP
1	C	326	PHE
1	C	329	GLN
1	C	330	THR
1	D	158	MET
1	D	196	VAL
1	D	201	TRP
1	D	214	LEU
1	D	225	SER
1	D	232	MET
1	D	235	ARG
1	D	236	ARG
1	D	243	LEU
1	D	247	ASP
1	D	254	ILE
1	D	259	ARG
1	D	261	MET
1	D	263	LYS
1	D	269	ASP
1	D	270	GLN
1	D	271	ARG
1	D	272	GLN
1	D	275	LEU
1	D	280	GLN
1	D	281	PHE
1	D	284	SER
1	D	286	LEU

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Mol	Chain	Res	Type
1	D	295	LYS
1	D	296	THR
1	D	299	TRP
1	D	302	TRP
1	D	303	LEU
1	D	307	GLN
1	D	311	LEU
1	D	313	ILE
1	D	314	ILE
1	D	316	ILE
1	D	323	ASP
1	D	326	PHE
1	D	329	GLN
1	D	330	THR
1	E	158	MET
1	E	196	VAL
1	E	201	TRP
1	E	214	LEU
1	E	225	SER
1	E	232	MET
1	E	235	ARG
1	E	236	ARG
1	E	243	LEU
1	E	247	ASP
1	E	254	ILE
1	E	259	ARG
1	E	261	MET
1	E	263	LYS
1	E	269	ASP
1	E	270	GLN
1	E	271	ARG
1	E	272	GLN
1	E	275	LEU
1	E	280	GLN
1	E	281	PHE
1	E	284	SER
1	E	286	LEU
1	E	295	LYS
1	E	296	THR
1	E	299	TRP
1	E	302	TRP
1	E	303	LEU

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Mol	Chain	Res	Type
1	E	307	GLN
1	E	311	LEU
1	E	313	ILE
1	E	314	ILE
1	E	316	ILE
1	E	323	ASP
1	E	326	PHE
1	E	329	GLN
1	E	330	THR
1	F	158	MET
1	F	196	VAL
1	F	201	TRP
1	F	214	LEU
1	F	225	SER
1	F	232	MET
1	F	235	ARG
1	F	236	ARG
1	F	243	LEU
1	F	247	ASP
1	F	254	ILE
1	F	259	ARG
1	F	261	MET
1	F	263	LYS
1	F	269	ASP
1	F	270	GLN
1	F	271	ARG
1	F	272	GLN
1	F	275	LEU
1	F	280	GLN
1	F	281	PHE
1	F	284	SER
1	F	286	LEU
1	F	295	LYS
1	F	296	THR
1	F	299	TRP
1	F	302	TRP
1	F	303	LEU
1	F	307	GLN
1	F	311	LEU
1	F	313	ILE
1	F	314	ILE
1	F	316	ILE

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Mol	Chain	Res	Type
1	F	323	ASP
1	F	326	PHE
1	F	329	GLN
1	F	330	THR
1	G	158	MET
1	G	196	VAL
1	G	201	TRP
1	G	214	LEU
1	G	225	SER
1	G	232	MET
1	G	235	ARG
1	G	236	ARG
1	G	243	LEU
1	G	247	ASP
1	G	254	ILE
1	G	259	ARG
1	G	261	MET
1	G	263	LYS
1	G	269	ASP
1	G	270	GLN
1	G	271	ARG
1	G	272	GLN
1	G	275	LEU
1	G	280	GLN
1	G	281	PHE
1	G	284	SER
1	G	286	LEU
1	G	295	LYS
1	G	296	THR
1	G	299	TRP
1	G	302	TRP
1	G	303	LEU
1	G	307	GLN
1	G	311	LEU
1	G	313	ILE
1	G	314	ILE
1	G	316	ILE
1	G	323	ASP
1	G	326	PHE
1	G	329	GLN
1	G	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	272	GLN
1	B	234	ASN
1	B	265	HIS
1	B	272	GLN
1	C	234	ASN
1	C	272	GLN
1	D	234	ASN
1	D	265	HIS
1	D	272	GLN
1	E	234	ASN
1	E	272	GLN
1	F	234	ASN
1	F	272	GLN
1	G	234	ASN
1	G	265	HIS
1	G	272	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no 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	A	2
1	B	2
1	E	2
1	F	2
1	G	2
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	148:PHE	C	149:GLY	N	1.82
1	B	148:PHE	C	149:GLY	N	1.82
1	C	148:PHE	C	149:GLY	N	1.82
1	D	148:PHE	C	149:GLY	N	1.82
1	E	148:PHE	C	149:GLY	N	1.82
1	F	148:PHE	C	149:GLY	N	1.82
1	G	148:PHE	C	149:GLY	N	1.82
1	G	140:MET	C	141:SER	N	1.13
1	B	140:MET	C	141:SER	N	1.07
1	A	140:MET	C	141:SER	N	1.00
1	F	140:MET	C	141:SER	N	0.89
1	E	140:MET	C	141:SER	N	0.80

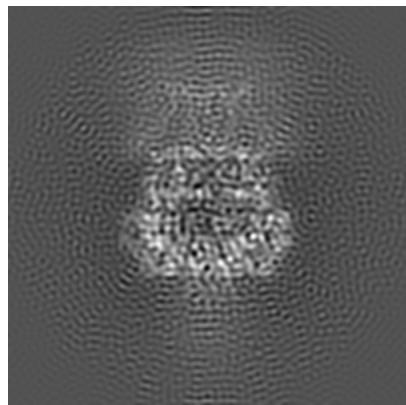
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6805. These allow visual inspection of the internal detail of the map and identification of artifacts.

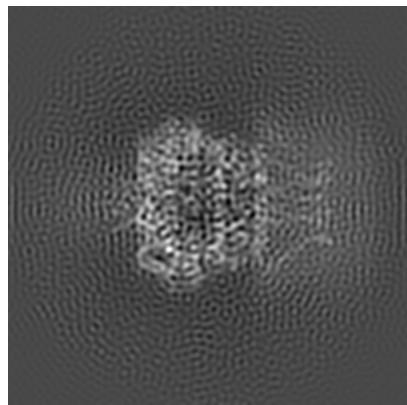
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

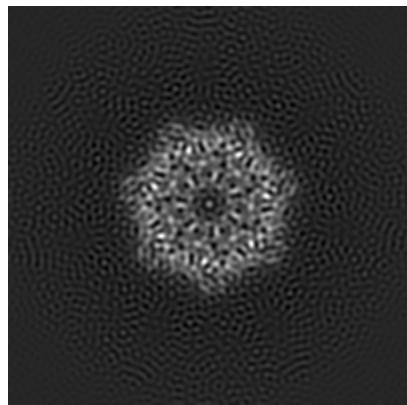
6.1.1 Primary map



X



Y

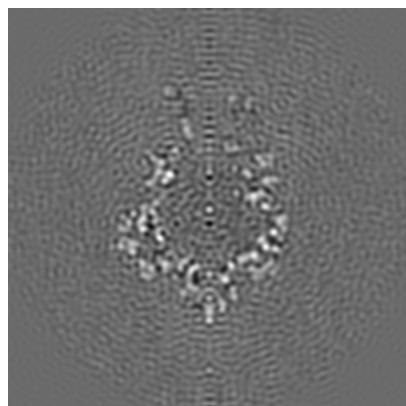


Z

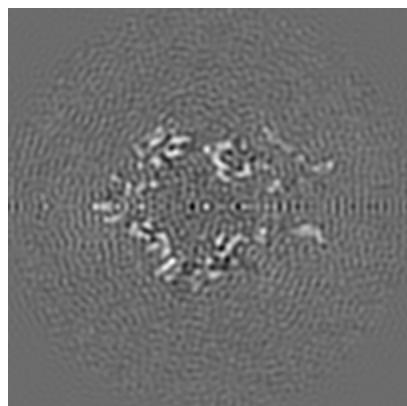
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

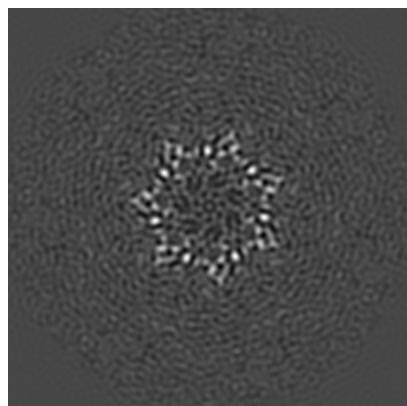
6.2.1 Primary map



X Index: 72



Y Index: 72

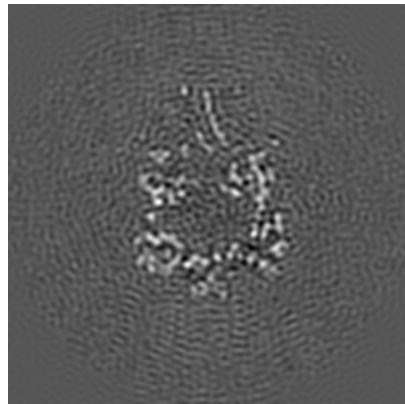


Z Index: 72

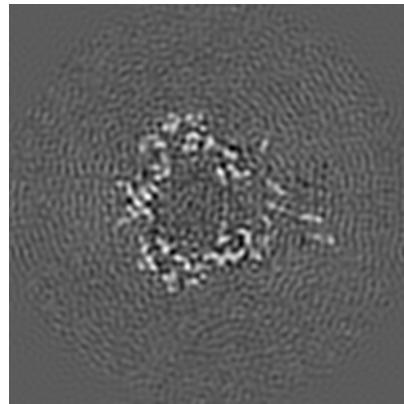
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

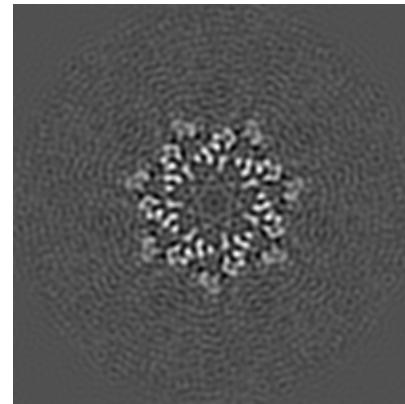
6.3.1 Primary map



X Index: 64



Y Index: 78

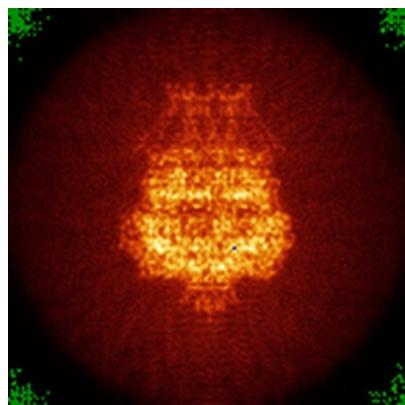


Z Index: 57

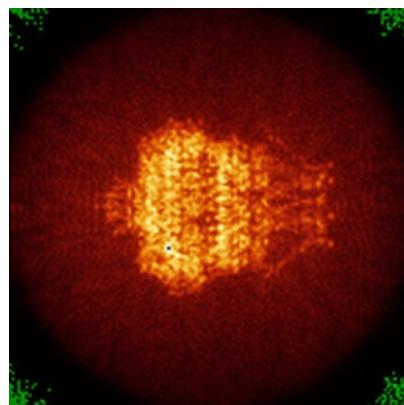
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

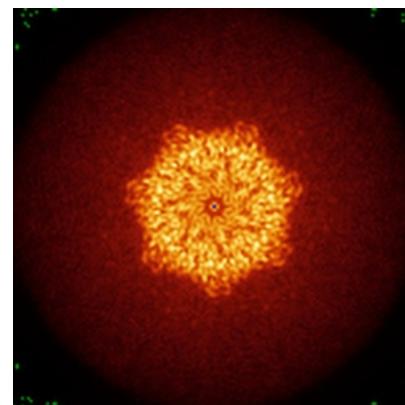
6.4.1 Primary map



X



Y

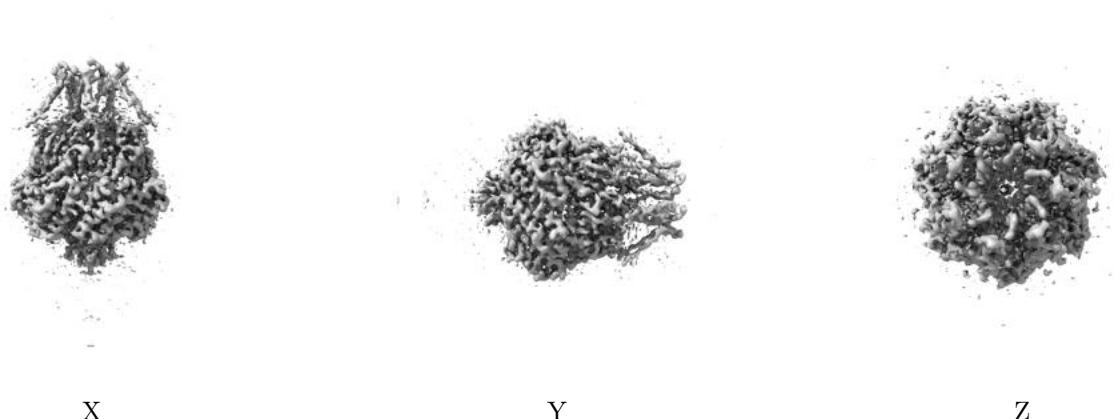


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [\(i\)](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0745. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

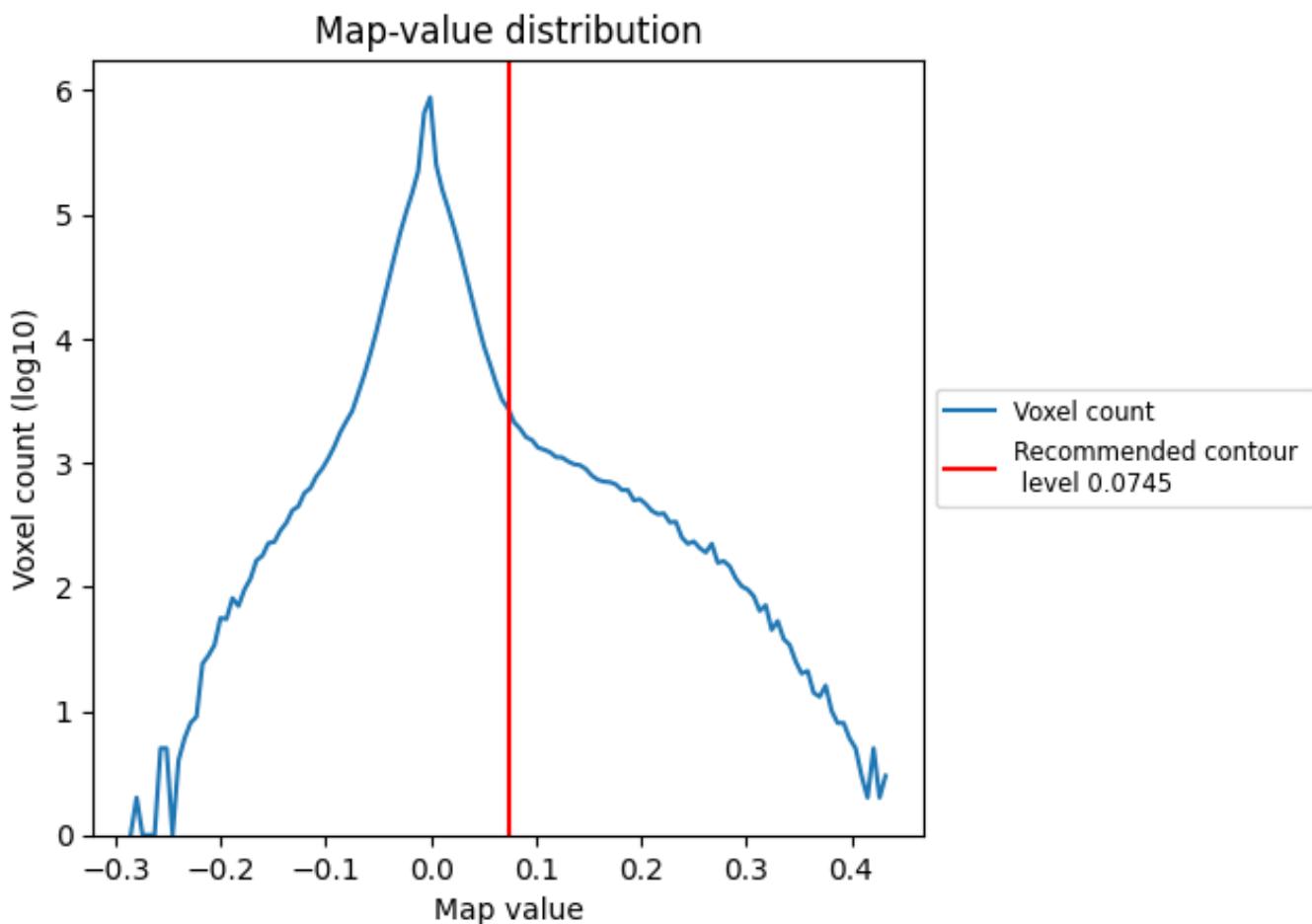
6.6 Mask visualisation [\(i\)](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

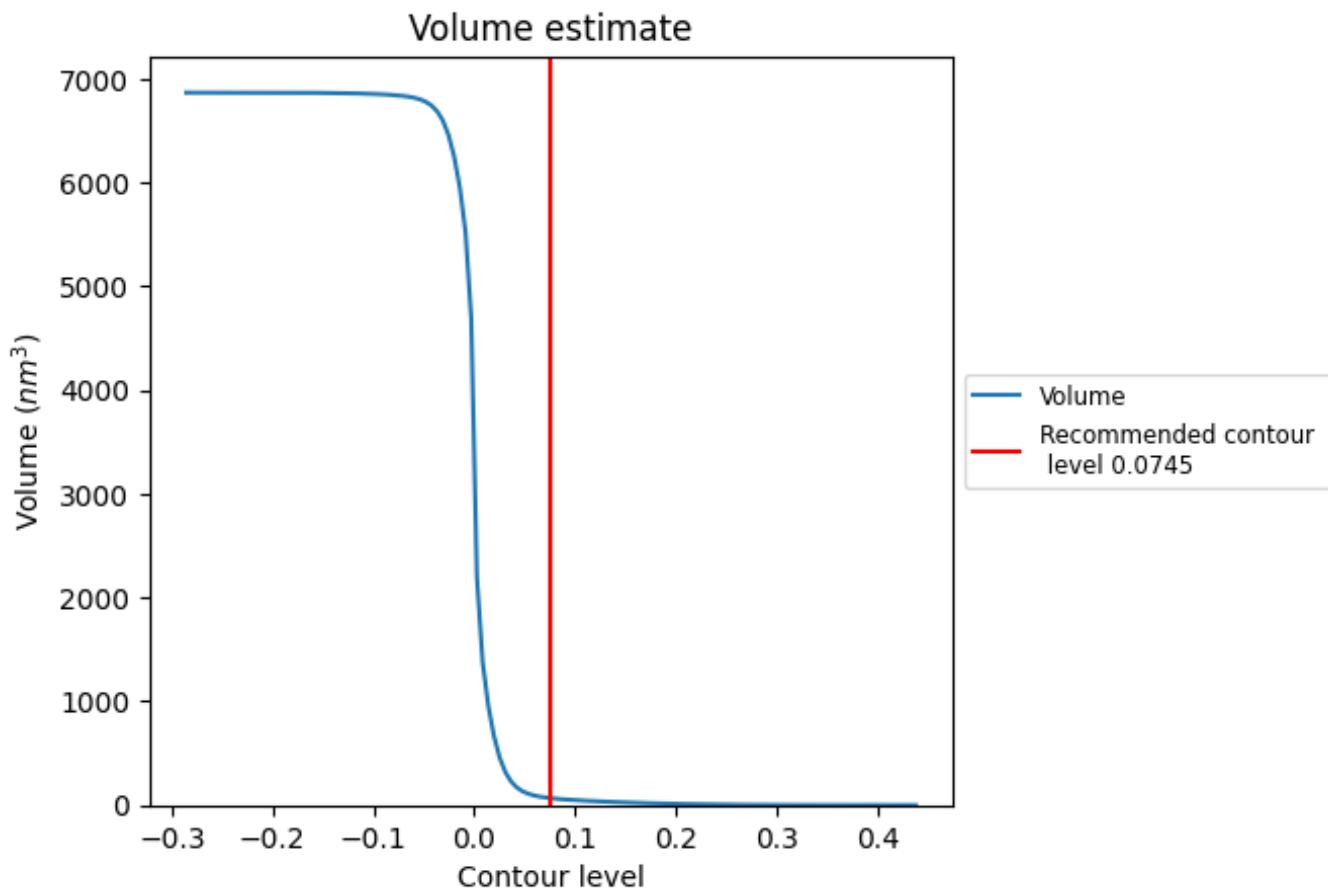
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

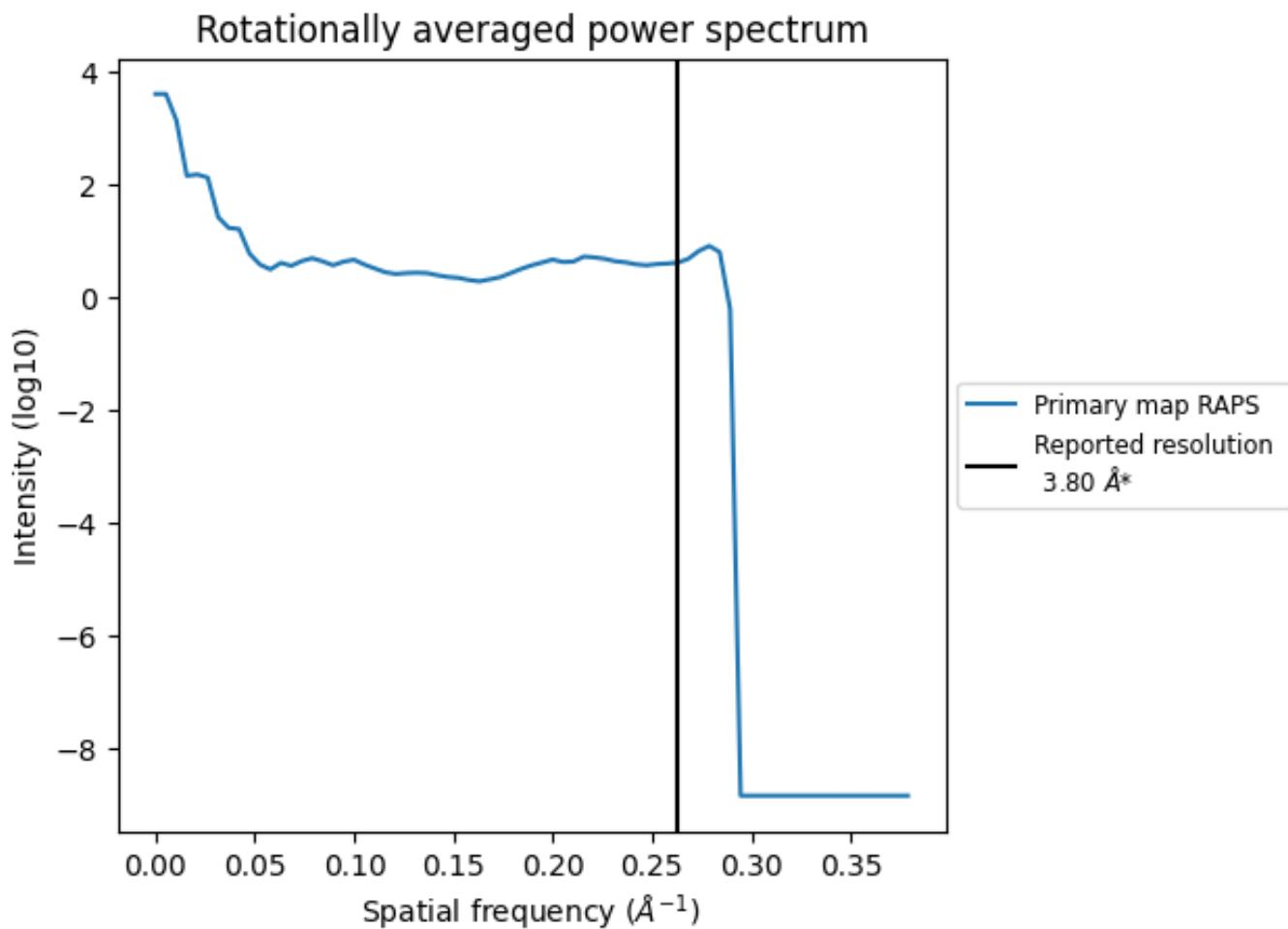
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 69 nm³; this corresponds to an approximate mass of 62 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

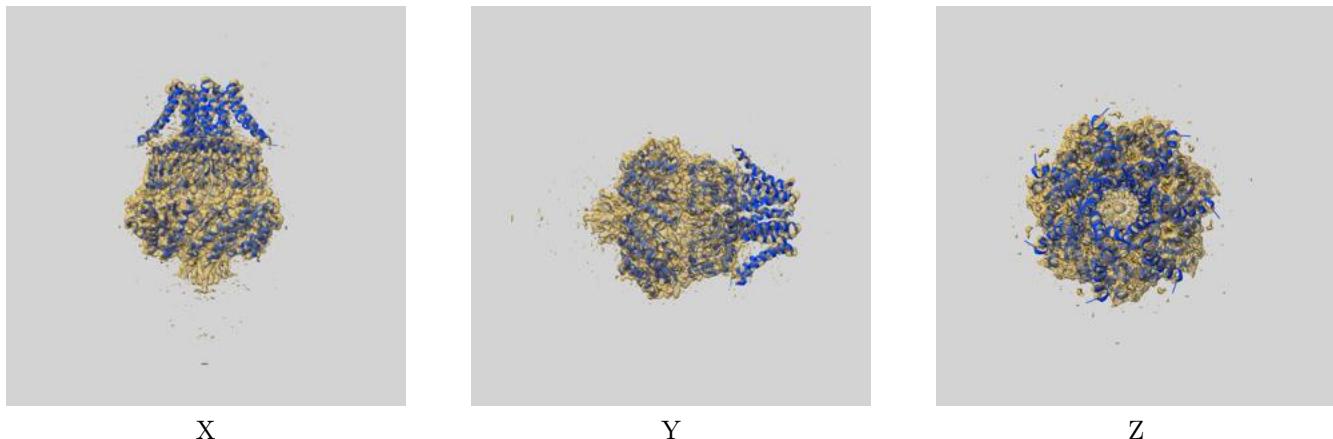
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit i

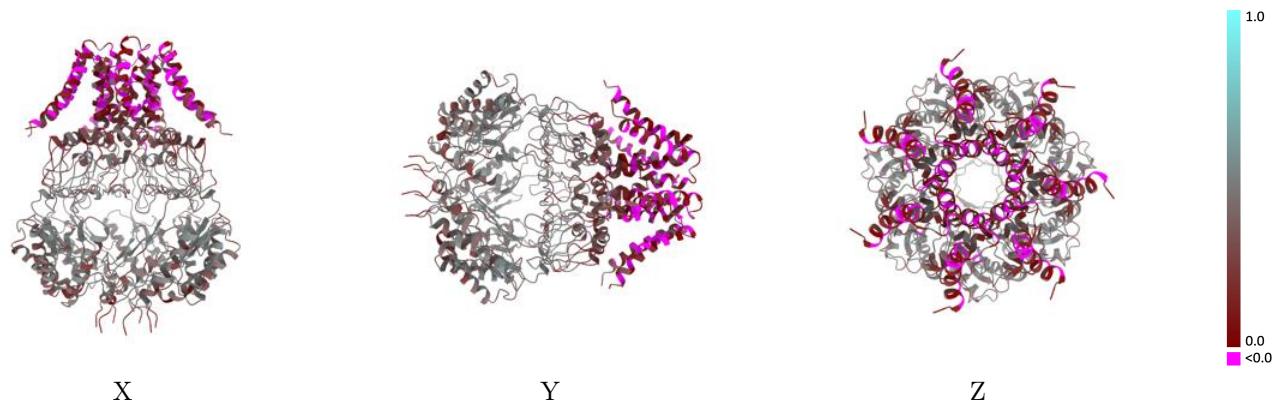
This section contains information regarding the fit between EMDB map EMD-6805 and PDB model 5Y4O. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay i



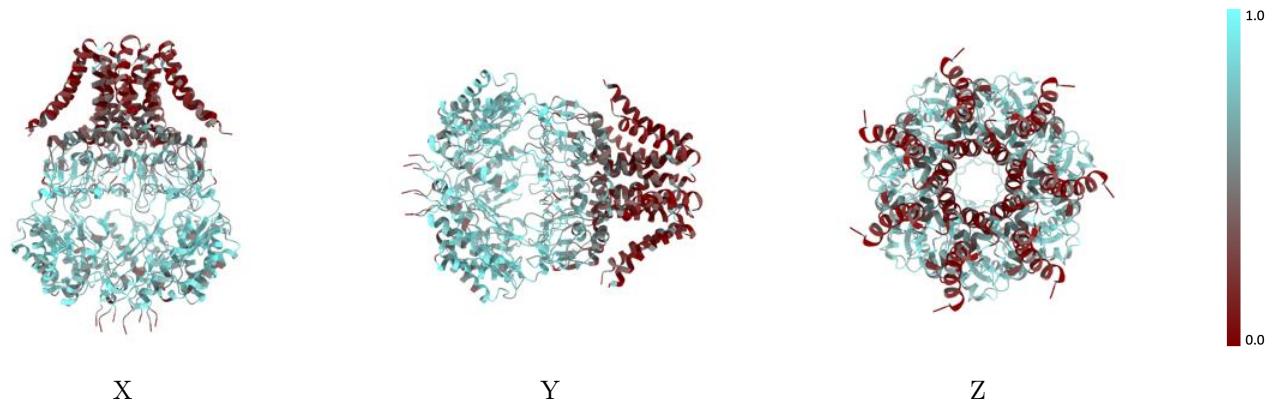
The images above show the 3D surface view of the map at the recommended contour level 0.0745 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



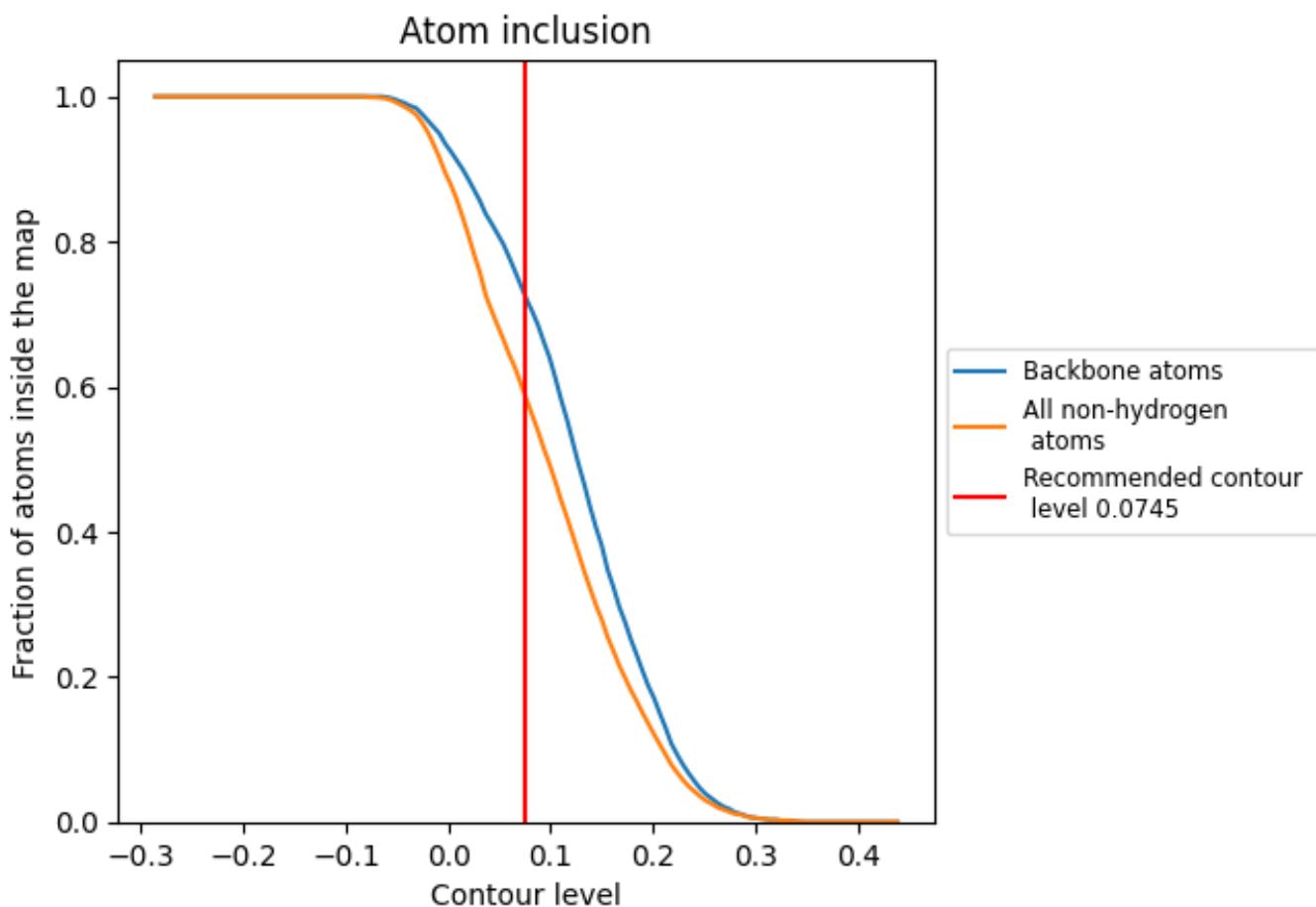
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0745).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 73% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0745) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.3310
A	0.5990	0.3390
B	0.5900	0.3290
C	0.5890	0.3290
D	0.5900	0.3300
E	0.5950	0.3320
F	0.5860	0.3280
G	0.5850	0.3280

