



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:35 AM UTC

PDB ID : 8FNT / pdb_00008fnt
EMDB ID : EMD-29323
Title : Structure of RdrA from Escherichia coli RADAR defense system
Authors : Duncan-Lowey, B.; Johnson, A.G.; Rawson, S.; Mayer, M.L.; Kranzusch, P.J.
Deposited on : 2022-12-28
Resolution : 2.52 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

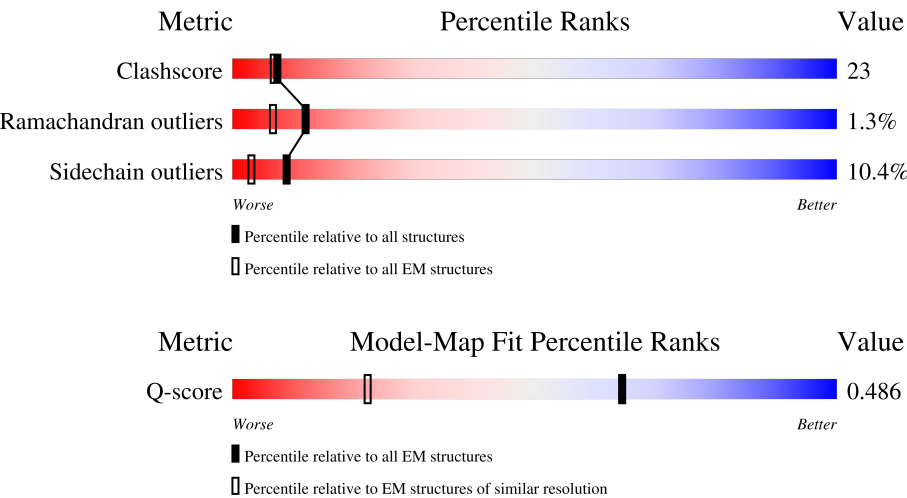
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.52 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

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

Mol	Chain	Length	Quality of chain
1	A	947	
1	B	947	
1	C	947	
1	D	947	

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Mol	Chain	Length	Quality of chain
1	E	947	53% 45% 31% 5% 18%
1	F	947	25% 45% 31% 5% 17%
1	G	947	9% 45% 32% 5% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 43868 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 Archaeal ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	785	Total	C	N	O	S	0	0
			6273	3980	1084	1178	31		
1	C	785	Total	C	N	O	S	0	0
			6273	3980	1084	1178	31		
1	D	784	Total	C	N	O	S	0	0
			6264	3974	1082	1177	31		
1	F	785	Total	C	N	O	S	0	0
			6273	3980	1084	1178	31		
1	G	785	Total	C	N	O	S	0	0
			6273	3980	1084	1178	31		
1	E	781	Total	C	N	O	S	0	0
			6239	3959	1076	1173	31		
1	A	785	Total	C	N	O	S	0	0
			6273	3980	1084	1178	31		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	LYS	GLU	conflict	UNP A0A8H9B1T2
B	24	SER	PRO	conflict	UNP A0A8H9B1T2
B	67	PRO	SER	conflict	UNP A0A8H9B1T2
B	335	SER	GLY	conflict	UNP A0A8H9B1T2
B	409	ASP	ASN	conflict	UNP A0A8H9B1T2
B	428	ASN	SER	conflict	UNP A0A8H9B1T2
B	583	ASN	HIS	conflict	UNP A0A8H9B1T2
B	586	GLU	GLY	conflict	UNP A0A8H9B1T2
B	636	ARG	LEU	conflict	UNP A0A8H9B1T2
B	858	ILE	VAL	conflict	UNP A0A8H9B1T2
C	11	LYS	GLU	conflict	UNP A0A8H9B1T2
C	24	SER	PRO	conflict	UNP A0A8H9B1T2
C	67	PRO	SER	conflict	UNP A0A8H9B1T2
C	335	SER	GLY	conflict	UNP A0A8H9B1T2
C	409	ASP	ASN	conflict	UNP A0A8H9B1T2
C	428	ASN	SER	conflict	UNP A0A8H9B1T2

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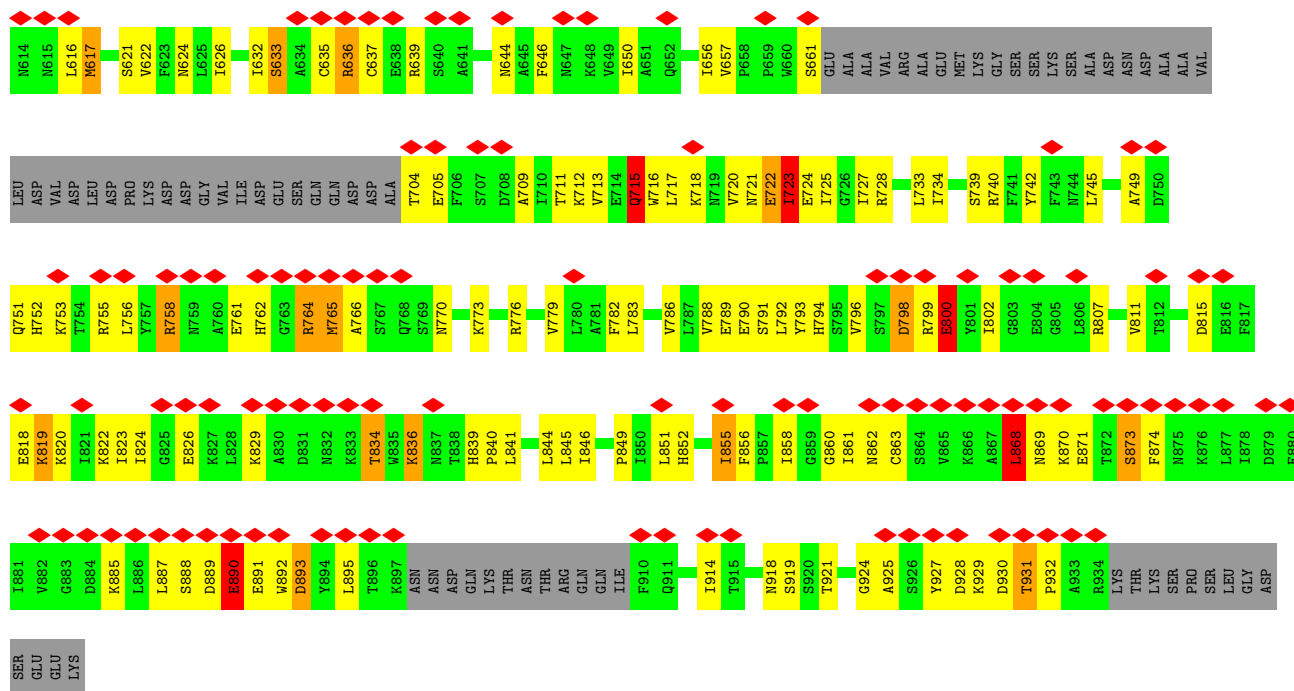
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C	586	GLU	GLY	conflict	UNP A0A8H9B1T2
C	636	ARG	LEU	conflict	UNP A0A8H9B1T2
C	858	ILE	VAL	conflict	UNP A0A8H9B1T2
D	11	LYS	GLU	conflict	UNP A0A8H9B1T2
D	24	SER	PRO	conflict	UNP A0A8H9B1T2
D	67	PRO	SER	conflict	UNP A0A8H9B1T2
D	335	SER	GLY	conflict	UNP A0A8H9B1T2
D	409	ASP	ASN	conflict	UNP A0A8H9B1T2
D	428	ASN	SER	conflict	UNP A0A8H9B1T2
D	583	ASN	HIS	conflict	UNP A0A8H9B1T2
D	586	GLU	GLY	conflict	UNP A0A8H9B1T2
D	636	ARG	LEU	conflict	UNP A0A8H9B1T2
D	858	ILE	VAL	conflict	UNP A0A8H9B1T2
F	11	LYS	GLU	conflict	UNP A0A8H9B1T2
F	24	SER	PRO	conflict	UNP A0A8H9B1T2
F	67	PRO	SER	conflict	UNP A0A8H9B1T2
F	335	SER	GLY	conflict	UNP A0A8H9B1T2
F	409	ASP	ASN	conflict	UNP A0A8H9B1T2
F	428	ASN	SER	conflict	UNP A0A8H9B1T2
F	583	ASN	HIS	conflict	UNP A0A8H9B1T2
F	586	GLU	GLY	conflict	UNP A0A8H9B1T2
F	636	ARG	LEU	conflict	UNP A0A8H9B1T2
F	858	ILE	VAL	conflict	UNP A0A8H9B1T2
G	11	LYS	GLU	conflict	UNP A0A8H9B1T2
G	24	SER	PRO	conflict	UNP A0A8H9B1T2
G	67	PRO	SER	conflict	UNP A0A8H9B1T2
G	335	SER	GLY	conflict	UNP A0A8H9B1T2
G	409	ASP	ASN	conflict	UNP A0A8H9B1T2
G	428	ASN	SER	conflict	UNP A0A8H9B1T2
G	583	ASN	HIS	conflict	UNP A0A8H9B1T2
G	586	GLU	GLY	conflict	UNP A0A8H9B1T2
G	636	ARG	LEU	conflict	UNP A0A8H9B1T2
G	858	ILE	VAL	conflict	UNP A0A8H9B1T2
E	11	LYS	GLU	conflict	UNP A0A8H9B1T2
E	24	SER	PRO	conflict	UNP A0A8H9B1T2
E	67	PRO	SER	conflict	UNP A0A8H9B1T2
E	335	SER	GLY	conflict	UNP A0A8H9B1T2
E	409	ASP	ASN	conflict	UNP A0A8H9B1T2
E	428	ASN	SER	conflict	UNP A0A8H9B1T2
E	583	ASN	HIS	conflict	UNP A0A8H9B1T2
E	586	GLU	GLY	conflict	UNP A0A8H9B1T2

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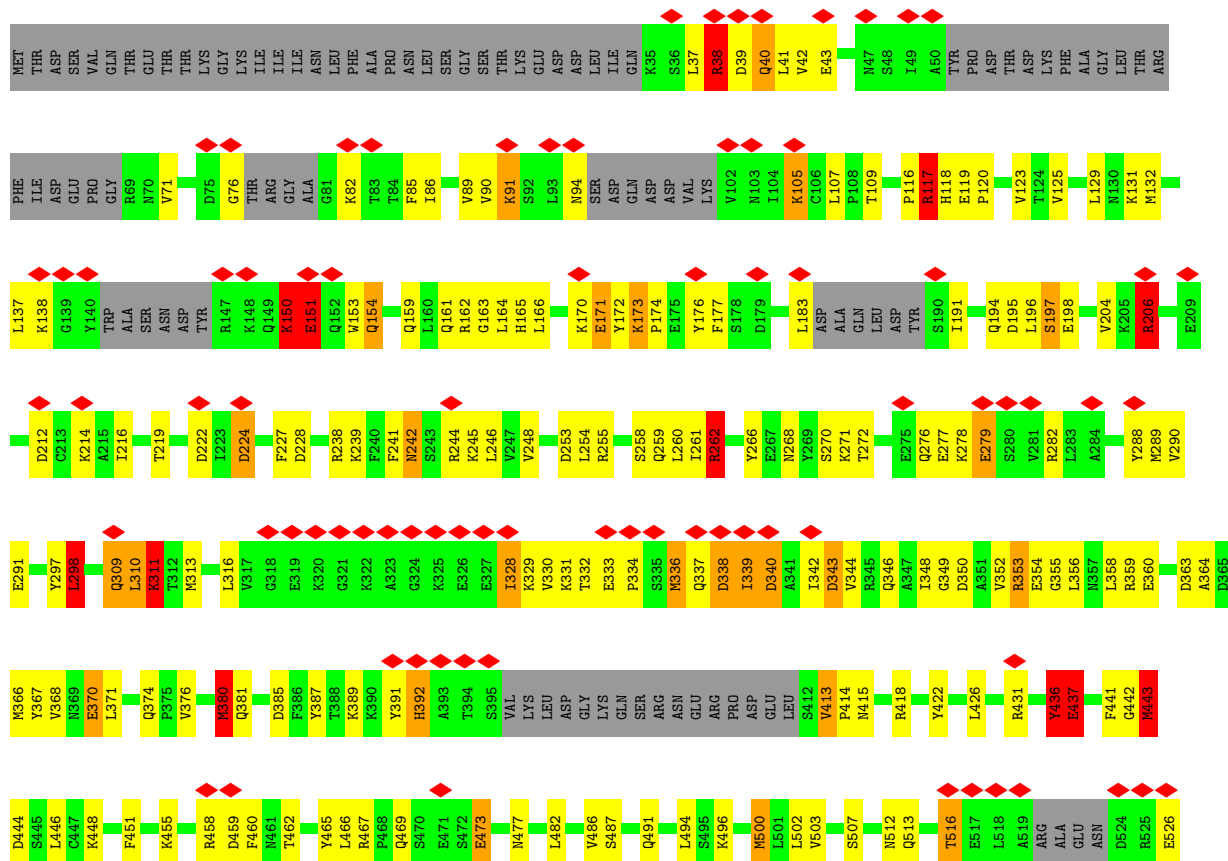
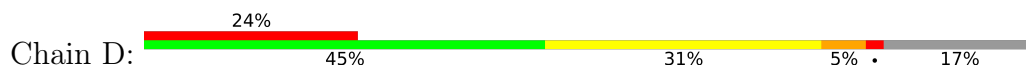
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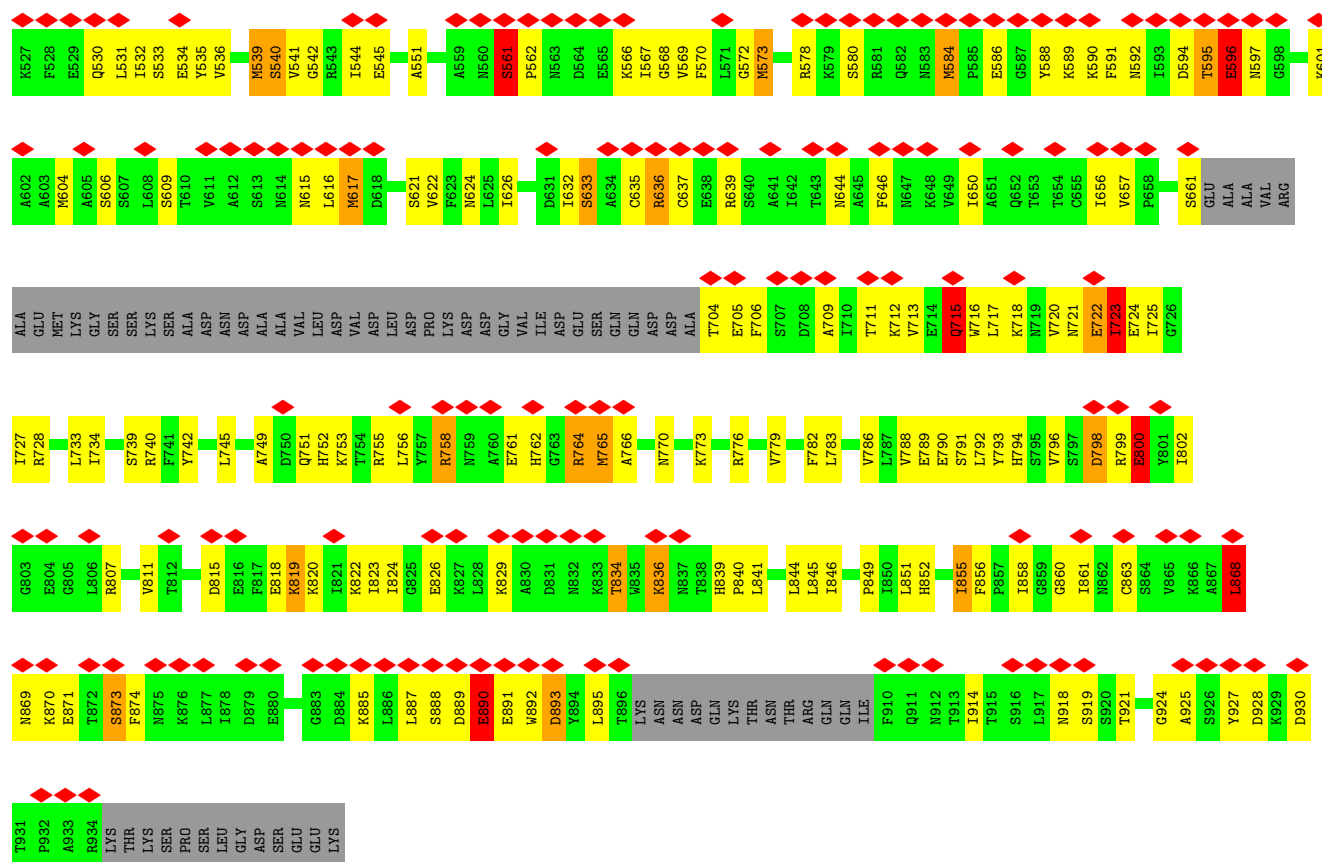
Chain	Residue	Modelled	Actual	Comment	Reference
E	636	ARG	LEU	conflict	UNP A0A8H9B1T2
E	858	ILE	VAL	conflict	UNP A0A8H9B1T2
A	11	LYS	GLU	conflict	UNP A0A8H9B1T2
A	24	SER	PRO	conflict	UNP A0A8H9B1T2
A	67	PRO	SER	conflict	UNP A0A8H9B1T2
A	335	SER	GLY	conflict	UNP A0A8H9B1T2
A	409	ASP	ASN	conflict	UNP A0A8H9B1T2
A	428	ASN	SER	conflict	UNP A0A8H9B1T2
A	583	ASN	HIS	conflict	UNP A0A8H9B1T2
A	586	GLU	GLY	conflict	UNP A0A8H9B1T2
A	636	ARG	LEU	conflict	UNP A0A8H9B1T2
A	858	ILE	VAL	conflict	UNP A0A8H9B1T2



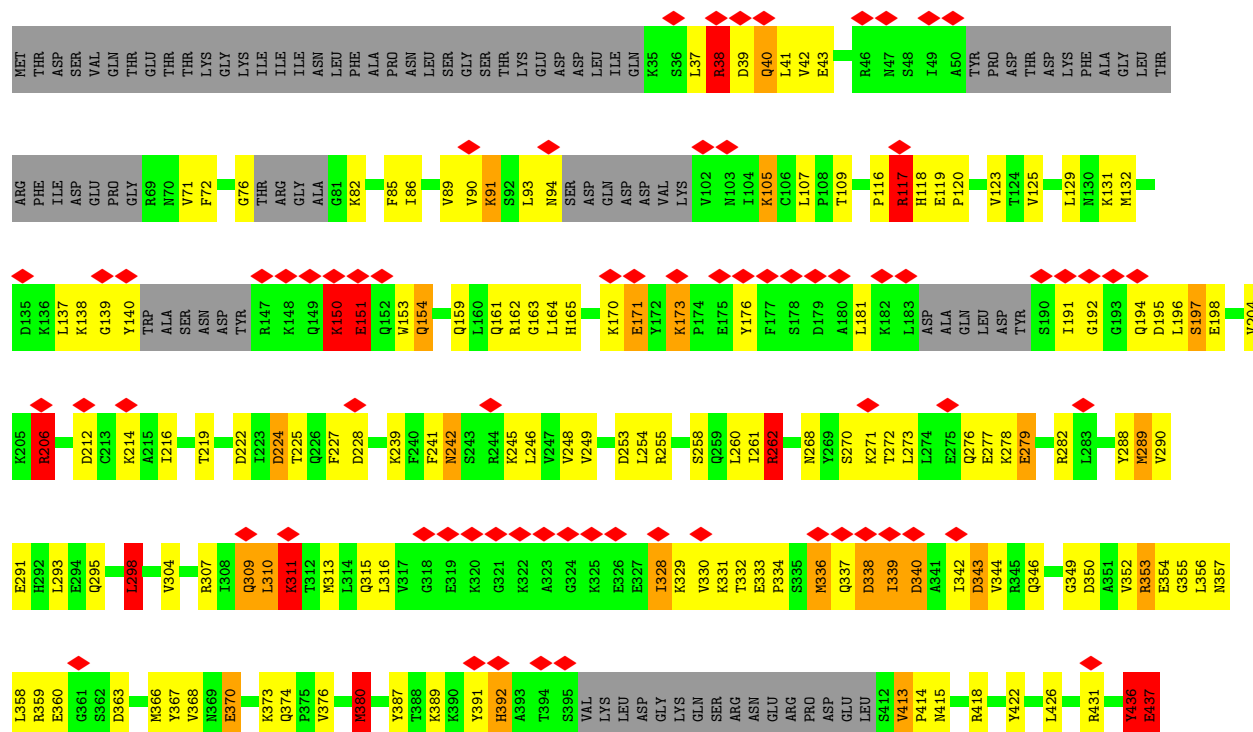
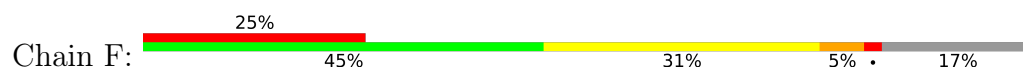


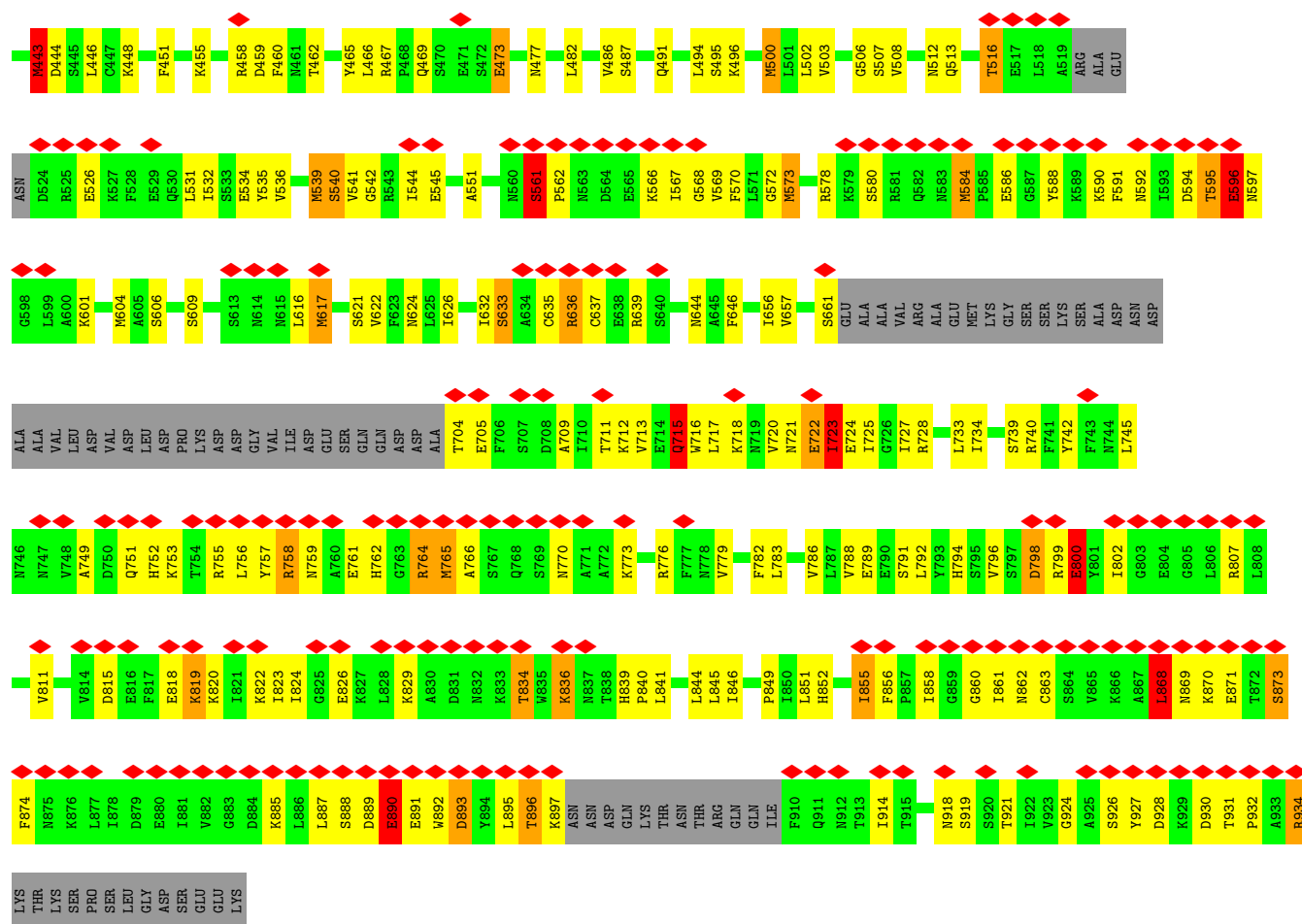
• Molecule 1: Archaeal ATPase



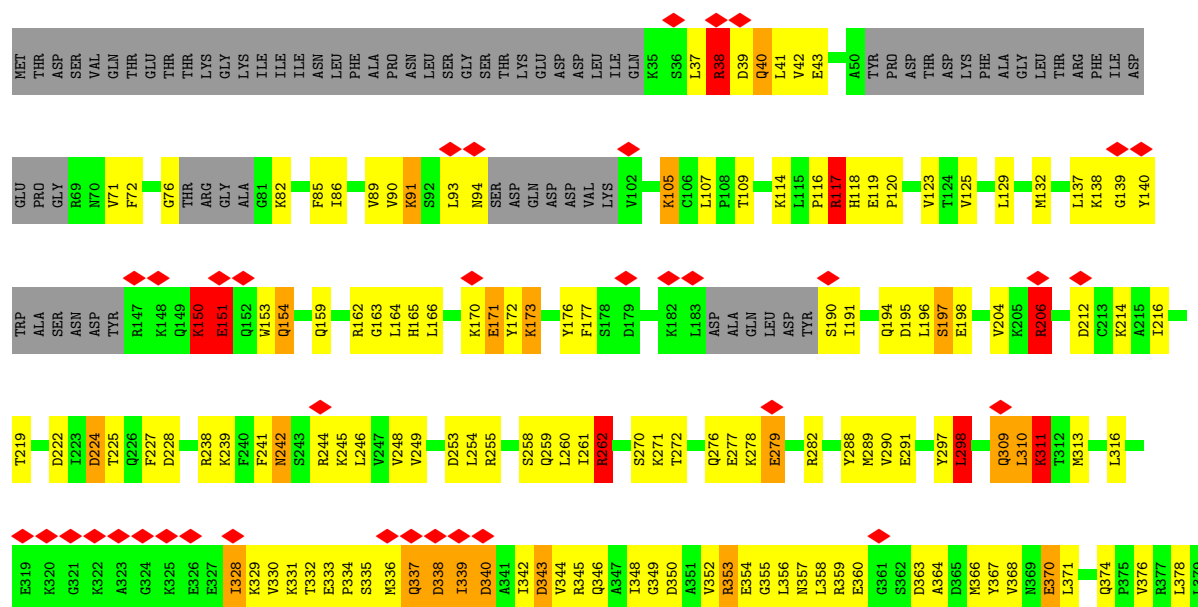
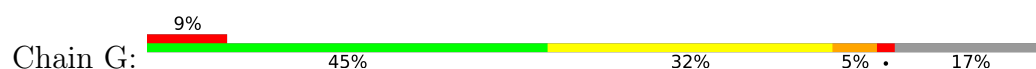


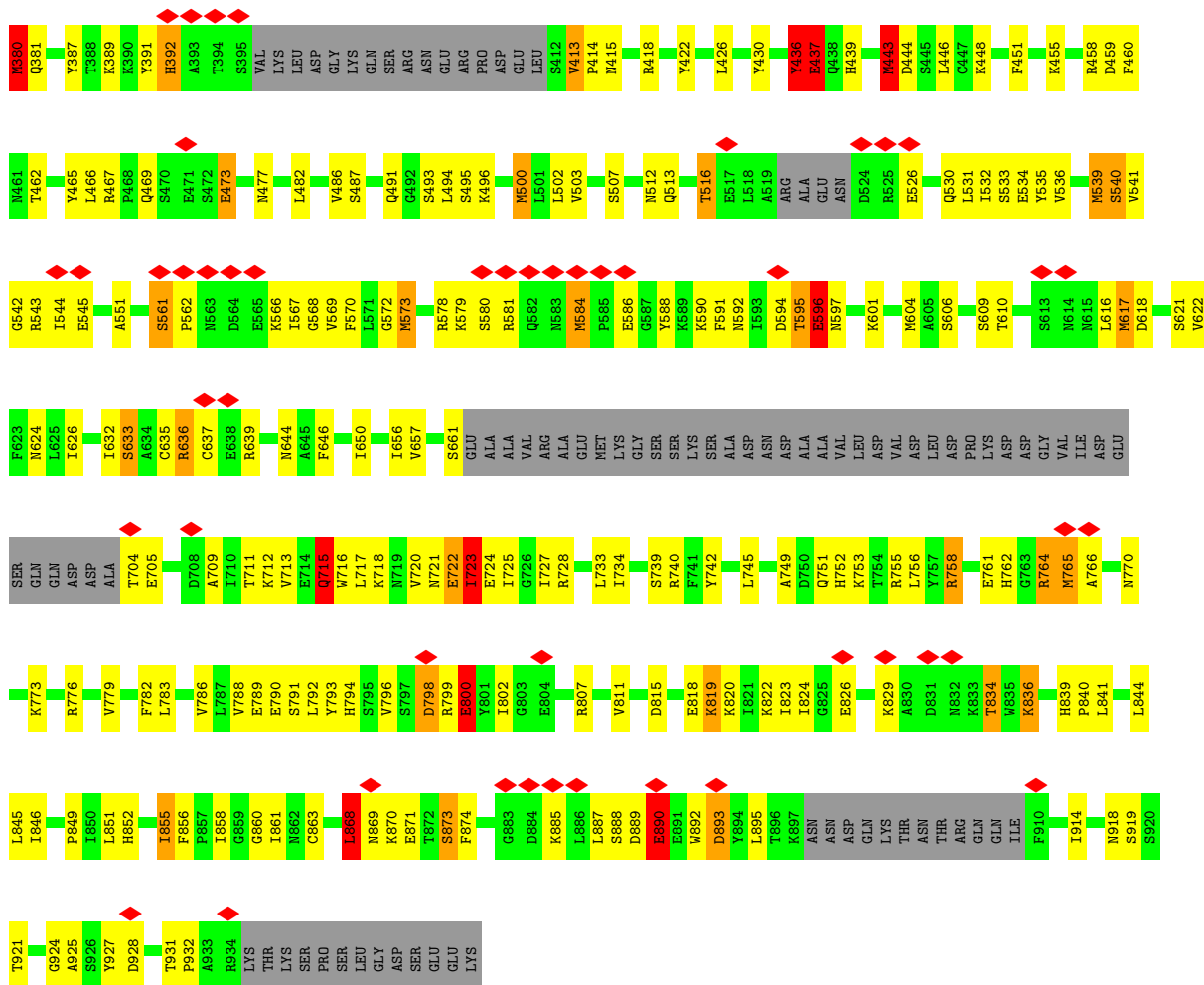
• Molecule 1: Archaeal ATPase



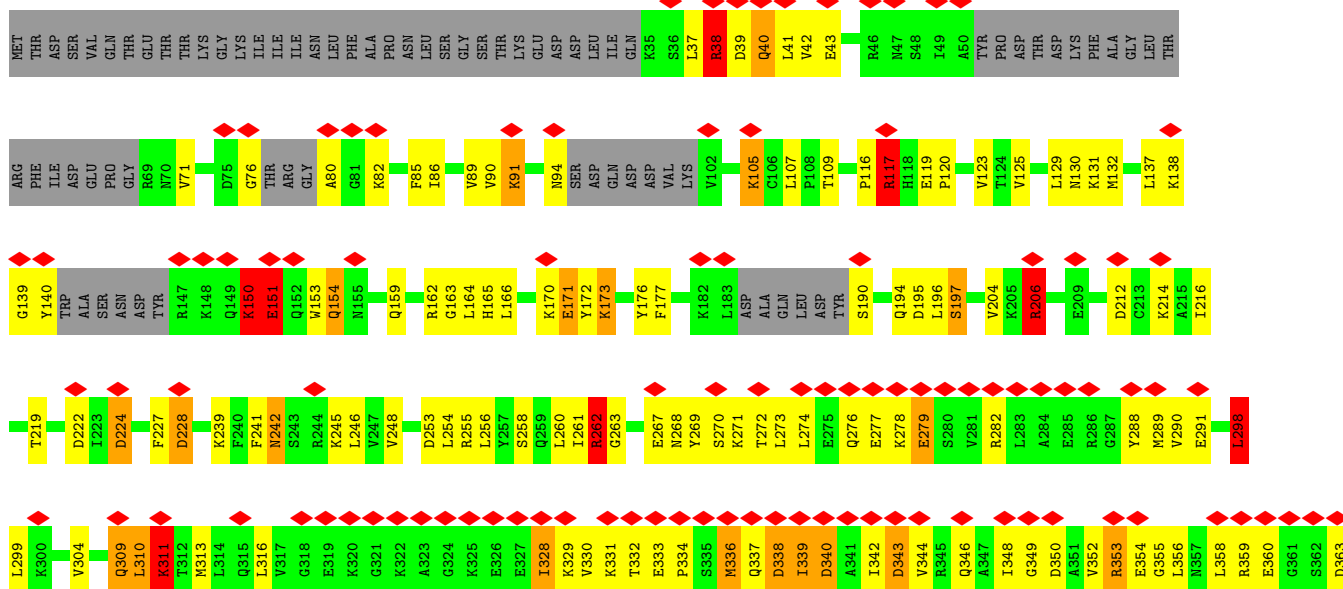
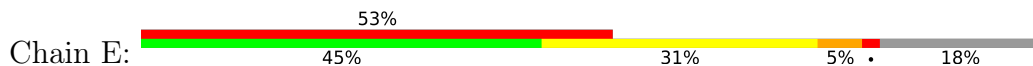


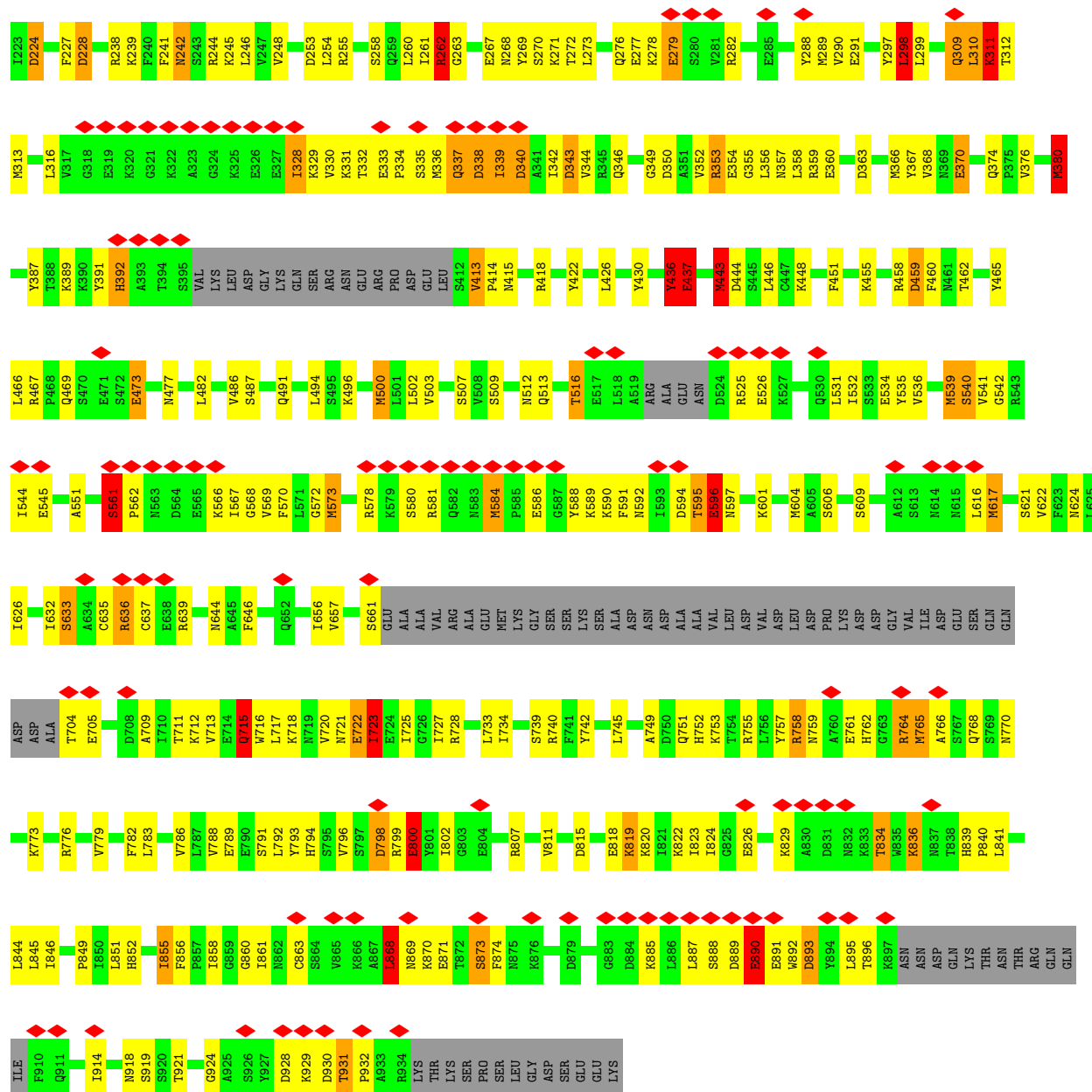
• Molecule 1: Archaeal ATPase





• Molecule 1: Archaeal ATPase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	472729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.641	Depositor
Minimum map value	-2.987	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.122	Depositor
Recommended contour level	0.65	Depositor
Map size ($\text{\AA}$)	343.19998, 343.19998, 343.19998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8249999, 0.8249999, 0.8249999	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	4/6375 (0.1%)	0.87	40/8586 (0.5%)
1	B	0.45	4/6375 (0.1%)	0.87	40/8586 (0.5%)
1	C	0.45	4/6375 (0.1%)	0.86	40/8586 (0.5%)
1	D	0.45	4/6366 (0.1%)	0.87	40/8575 (0.5%)
1	E	0.45	4/6340 (0.1%)	0.87	40/8539 (0.5%)
1	F	0.45	4/6375 (0.1%)	0.87	41/8586 (0.5%)
1	G	0.45	4/6375 (0.1%)	0.87	40/8586 (0.5%)
All	All	0.45	28/44581 (0.1%)	0.87	281/60044 (0.5%)

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	11
1	B	0	11
1	C	0	10
1	D	0	10
1	E	0	10
1	F	0	11
1	G	0	10
All	All	0	73

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	413	VAL	CA-CB	-9.49	1.49	1.54
1	E	413	VAL	CA-CB	-9.45	1.49	1.54
1	B	413	VAL	CA-CB	-9.37	1.49	1.54
1	F	413	VAL	CA-CB	-9.31	1.49	1.54
1	G	413	VAL	CA-CB	-9.28	1.49	1.54
1	C	413	VAL	CA-CB	-9.24	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	413	VAL	CA-CB	-9.22	1.49	1.54
1	A	310	LEU	C-N	8.79	1.46	1.33
1	F	310	LEU	C-N	8.75	1.46	1.33
1	G	310	LEU	C-N	8.74	1.46	1.33
1	E	310	LEU	C-N	8.73	1.46	1.33
1	B	310	LEU	C-N	8.71	1.45	1.33
1	D	310	LEU	C-N	8.71	1.45	1.33
1	C	310	LEU	C-N	8.70	1.45	1.33
1	C	91	LYS	CB-CG	-5.30	1.36	1.52
1	B	91	LYS	CB-CG	-5.29	1.36	1.52
1	E	91	LYS	CB-CG	-5.28	1.36	1.52
1	A	91	LYS	CB-CG	-5.28	1.36	1.52
1	G	91	LYS	CB-CG	-5.27	1.36	1.52
1	F	91	LYS	CB-CG	-5.27	1.36	1.52
1	D	91	LYS	CB-CG	-5.27	1.36	1.52
1	B	117	ARG	CG-CD	-5.16	1.36	1.52
1	A	117	ARG	CG-CD	-5.14	1.37	1.52
1	F	117	ARG	CG-CD	-5.14	1.37	1.52
1	E	117	ARG	CG-CD	-5.13	1.37	1.52
1	C	117	ARG	CG-CD	-5.13	1.37	1.52
1	G	117	ARG	CG-CD	-5.13	1.37	1.52
1	D	117	ARG	CG-CD	-5.12	1.37	1.52

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	311	LYS	CB-CG-CD	11.29	137.27	111.30
1	F	311	LYS	CB-CG-CD	11.28	137.24	111.30
1	C	311	LYS	CB-CG-CD	11.27	137.22	111.30
1	A	311	LYS	CB-CG-CD	11.27	137.22	111.30
1	E	311	LYS	CB-CG-CD	11.26	137.20	111.30
1	B	311	LYS	CB-CG-CD	11.26	137.19	111.30
1	D	311	LYS	CB-CG-CD	11.25	137.18	111.30
1	B	443	MET	CB-CG-SD	10.63	144.60	112.70
1	F	443	MET	CB-CG-SD	10.63	144.61	112.70
1	C	443	MET	CB-CG-SD	10.63	144.60	112.70
1	E	443	MET	CB-CG-SD	10.63	144.59	112.70
1	A	443	MET	CB-CG-SD	10.63	144.58	112.70
1	G	443	MET	CB-CG-SD	10.62	144.56	112.70
1	D	443	MET	CB-CG-SD	10.62	144.56	112.70
1	E	40	GLN	CB-CG-CD	9.79	129.25	112.60
1	B	40	GLN	CB-CG-CD	9.78	129.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	40	GLN	CB-CG-CD	9.77	129.20	112.60
1	A	40	GLN	CB-CG-CD	9.77	129.20	112.60
1	D	40	GLN	CB-CG-CD	9.76	129.19	112.60
1	G	40	GLN	CB-CG-CD	9.76	129.19	112.60
1	C	40	GLN	CB-CG-CD	9.74	129.16	112.60
1	F	890	GLU	CA-CB-CG	8.61	131.31	114.10
1	C	890	GLU	CA-CB-CG	8.61	131.31	114.10
1	B	890	GLU	CA-CB-CG	8.60	131.30	114.10
1	A	890	GLU	CA-CB-CG	8.60	131.29	114.10
1	D	890	GLU	CA-CB-CG	8.59	131.28	114.10
1	E	890	GLU	CA-CB-CG	8.59	131.27	114.10
1	G	890	GLU	CA-CB-CG	8.58	131.26	114.10
1	F	117	ARG	CA-CB-CG	-8.55	97.00	114.10
1	G	117	ARG	CA-CB-CG	-8.54	97.03	114.10
1	E	117	ARG	CA-CB-CG	-8.53	97.04	114.10
1	A	117	ARG	CA-CB-CG	-8.53	97.05	114.10
1	B	117	ARG	CA-CB-CG	-8.52	97.06	114.10
1	C	117	ARG	CA-CB-CG	-8.51	97.09	114.10
1	D	117	ARG	CA-CB-CG	-8.50	97.10	114.10
1	D	138	LYS	CG-CD-CE	8.50	130.84	111.30
1	B	138	LYS	CG-CD-CE	8.49	130.83	111.30
1	G	138	LYS	CG-CD-CE	8.49	130.82	111.30
1	E	138	LYS	CG-CD-CE	8.48	130.81	111.30
1	A	138	LYS	CG-CD-CE	8.48	130.81	111.30
1	C	138	LYS	CG-CD-CE	8.47	130.79	111.30
1	F	138	LYS	CG-CD-CE	8.47	130.79	111.30
1	F	43	GLU	CA-CB-CG	8.26	130.62	114.10
1	B	43	GLU	CA-CB-CG	8.25	130.60	114.10
1	G	43	GLU	CA-CB-CG	8.25	130.61	114.10
1	A	43	GLU	CA-CB-CG	8.24	130.58	114.10
1	D	43	GLU	CA-CB-CG	8.24	130.57	114.10
1	E	43	GLU	CA-CB-CG	8.23	130.57	114.10
1	C	43	GLU	CA-CB-CG	8.23	130.57	114.10
1	E	822	LYS	CD-CE-NZ	8.04	137.62	111.90
1	B	822	LYS	CD-CE-NZ	8.03	137.60	111.90
1	A	822	LYS	CD-CE-NZ	8.03	137.60	111.90
1	B	722	GLU	CA-CB-CG	8.03	130.16	114.10
1	D	722	GLU	CA-CB-CG	8.03	130.16	114.10
1	F	822	LYS	CD-CE-NZ	8.03	137.59	111.90
1	C	822	LYS	CD-CE-NZ	8.03	137.59	111.90
1	G	822	LYS	CD-CE-NZ	8.03	137.59	111.90
1	D	822	LYS	CD-CE-NZ	8.02	137.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	722	GLU	CA-CB-CG	8.02	130.14	114.10
1	F	722	GLU	CA-CB-CG	8.01	130.12	114.10
1	A	722	GLU	CA-CB-CG	8.01	130.12	114.10
1	G	722	GLU	CA-CB-CG	8.00	130.11	114.10
1	E	722	GLU	CA-CB-CG	8.00	130.10	114.10
1	B	584	MET	CA-CB-CG	-7.98	98.14	114.10
1	A	584	MET	CA-CB-CG	-7.98	98.14	114.10
1	E	584	MET	CA-CB-CG	-7.98	98.14	114.10
1	D	584	MET	CA-CB-CG	-7.97	98.15	114.10
1	F	584	MET	CA-CB-CG	-7.97	98.16	114.10
1	G	584	MET	CA-CB-CG	-7.97	98.16	114.10
1	C	584	MET	CA-CB-CG	-7.97	98.17	114.10
1	B	105	LYS	CB-CG-CD	7.61	128.81	111.30
1	C	105	LYS	CB-CG-CD	7.61	128.81	111.30
1	D	105	LYS	CB-CG-CD	7.61	128.80	111.30
1	A	105	LYS	CB-CG-CD	7.60	128.78	111.30
1	E	105	LYS	CB-CG-CD	7.60	128.78	111.30
1	F	105	LYS	CB-CG-CD	7.60	128.78	111.30
1	G	105	LYS	CB-CG-CD	7.59	128.76	111.30
1	A	502	LEU	CB-CG-CD1	7.57	133.42	110.70
1	B	502	LEU	CB-CG-CD1	7.57	133.41	110.70
1	E	502	LEU	CB-CG-CD1	7.57	133.41	110.70
1	D	502	LEU	CB-CG-CD1	7.57	133.41	110.70
1	F	502	LEU	CB-CG-CD1	7.57	133.41	110.70
1	G	502	LEU	CB-CG-CD1	7.57	133.41	110.70
1	C	502	LEU	CB-CG-CD1	7.56	133.38	110.70
1	A	740	ARG	CG-CD-NE	7.38	128.24	112.00
1	G	740	ARG	CG-CD-NE	7.38	128.24	112.00
1	C	740	ARG	CG-CD-NE	7.38	128.23	112.00
1	F	740	ARG	CG-CD-NE	7.37	128.22	112.00
1	D	740	ARG	CG-CD-NE	7.36	128.20	112.00
1	E	740	ARG	CG-CD-NE	7.36	128.19	112.00
1	B	740	ARG	CG-CD-NE	7.34	128.15	112.00
1	G	289	MET	CB-CG-SD	-7.05	91.55	112.70
1	F	289	MET	CB-CG-SD	-7.04	91.58	112.70
1	C	289	MET	CB-CG-SD	-7.04	91.58	112.70
1	A	289	MET	CB-CG-SD	-7.03	91.60	112.70
1	E	289	MET	CB-CG-SD	-7.03	91.61	112.70
1	B	289	MET	CB-CG-SD	-7.03	91.61	112.70
1	D	289	MET	CB-CG-SD	-7.02	91.63	112.70
1	F	617	MET	CB-CG-SD	-6.77	92.40	112.70
1	D	617	MET	CB-CG-SD	-6.76	92.43	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	617	MET	CB-CG-SD	-6.75	92.43	112.70
1	C	617	MET	CB-CG-SD	-6.75	92.44	112.70
1	A	617	MET	CB-CG-SD	-6.75	92.44	112.70
1	B	617	MET	CB-CG-SD	-6.75	92.47	112.70
1	E	617	MET	CB-CG-SD	-6.74	92.47	112.70
1	G	117	ARG	CG-CD-NE	6.57	126.45	112.00
1	E	117	ARG	CG-CD-NE	6.56	126.43	112.00
1	A	117	ARG	CG-CD-NE	6.56	126.42	112.00
1	F	117	ARG	CG-CD-NE	6.55	126.42	112.00
1	C	117	ARG	CG-CD-NE	6.55	126.41	112.00
1	B	117	ARG	CG-CD-NE	6.54	126.39	112.00
1	D	117	ARG	CG-CD-NE	6.53	126.36	112.00
1	C	117	ARG	CB-CG-CD	6.26	125.69	111.30
1	E	117	ARG	CB-CG-CD	6.25	125.68	111.30
1	B	117	ARG	CB-CG-CD	6.25	125.67	111.30
1	F	117	ARG	CB-CG-CD	6.24	125.66	111.30
1	D	117	ARG	CB-CG-CD	6.24	125.66	111.30
1	G	117	ARG	CB-CG-CD	6.24	125.65	111.30
1	A	117	ARG	CB-CG-CD	6.22	125.60	111.30
1	G	138	LYS	CB-CG-CD	6.16	125.48	111.30
1	C	138	LYS	CB-CG-CD	6.16	125.47	111.30
1	E	138	LYS	CB-CG-CD	6.16	125.46	111.30
1	D	138	LYS	CB-CG-CD	6.15	125.45	111.30
1	F	138	LYS	CB-CG-CD	6.15	125.45	111.30
1	B	138	LYS	CB-CG-CD	6.15	125.45	111.30
1	A	138	LYS	CB-CG-CD	6.15	125.44	111.30
1	B	298	LEU	CB-CG-CD1	6.12	129.07	110.70
1	C	298	LEU	CB-CG-CD1	6.12	129.06	110.70
1	G	298	LEU	CB-CG-CD1	6.12	129.05	110.70
1	A	298	LEU	CB-CG-CD1	6.12	129.04	110.70
1	D	298	LEU	CB-CG-CD1	6.11	129.03	110.70
1	E	298	LEU	CB-CG-CD1	6.11	129.02	110.70
1	F	298	LEU	CB-CG-CD1	6.10	129.01	110.70
1	E	455	LYS	CD-CE-NZ	6.07	131.33	111.90
1	C	455	LYS	CD-CE-NZ	6.07	131.33	111.90
1	A	455	LYS	CD-CE-NZ	6.07	131.32	111.90
1	D	455	LYS	CD-CE-NZ	6.07	131.31	111.90
1	F	455	LYS	CD-CE-NZ	6.07	131.31	111.90
1	B	455	LYS	CD-CE-NZ	6.06	131.31	111.90
1	G	455	LYS	CD-CE-NZ	6.06	131.29	111.90
1	B	151	GLU	CA-CB-CG	5.98	126.05	114.10
1	F	151	GLU	CA-CB-CG	5.97	126.05	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	868	LEU	CB-CG-CD2	5.97	128.61	110.70
1	F	868	LEU	CB-CG-CD2	5.96	128.59	110.70
1	E	151	GLU	CA-CB-CG	5.96	126.03	114.10
1	B	868	LEU	CB-CG-CD2	5.96	128.58	110.70
1	A	868	LEU	CB-CG-CD2	5.96	128.58	110.70
1	A	151	GLU	CA-CB-CG	5.96	126.02	114.10
1	C	868	LEU	CB-CG-CD2	5.95	128.56	110.70
1	G	151	GLU	CA-CB-CG	5.95	126.01	114.10
1	G	868	LEU	CB-CG-CD2	5.95	128.56	110.70
1	E	868	LEU	CB-CG-CD2	5.95	128.55	110.70
1	C	151	GLU	CA-CB-CG	5.95	125.99	114.10
1	D	151	GLU	CA-CB-CG	5.94	125.97	114.10
1	D	150	LYS	CB-CG-CD	5.83	124.71	111.30
1	F	150	LYS	CB-CG-CD	5.82	124.69	111.30
1	G	150	LYS	CB-CG-CD	5.82	124.69	111.30
1	C	150	LYS	CB-CG-CD	5.82	124.67	111.30
1	A	150	LYS	CB-CG-CD	5.81	124.67	111.30
1	E	150	LYS	CB-CG-CD	5.81	124.66	111.30
1	B	150	LYS	CB-CG-CD	5.80	124.65	111.30
1	E	500	MET	CB-CG-SD	5.78	130.03	112.70
1	A	500	MET	CB-CG-SD	5.77	130.02	112.70
1	B	500	MET	CB-CG-SD	5.77	130.02	112.70
1	F	500	MET	CB-CG-SD	5.76	129.99	112.70
1	C	500	MET	CB-CG-SD	5.76	129.97	112.70
1	D	500	MET	CB-CG-SD	5.76	129.97	112.70
1	G	500	MET	CB-CG-SD	5.75	129.95	112.70
1	C	586	GLU	CB-CA-C	-5.64	109.07	115.79
1	F	819	LYS	CB-CG-CD	5.64	124.27	111.30
1	B	819	LYS	CB-CG-CD	5.64	124.26	111.30
1	A	819	LYS	CB-CG-CD	5.63	124.26	111.30
1	C	819	LYS	CB-CG-CD	5.63	124.24	111.30
1	B	586	GLU	CB-CA-C	-5.62	109.10	115.79
1	E	819	LYS	CB-CG-CD	5.62	124.23	111.30
1	F	586	GLU	CB-CA-C	-5.62	109.10	115.79
1	D	819	LYS	CB-CG-CD	5.62	124.22	111.30
1	G	819	LYS	CB-CG-CD	5.62	124.22	111.30
1	F	91	LYS	CA-CB-CG	-5.61	102.88	114.10
1	B	91	LYS	CA-CB-CG	-5.60	102.89	114.10
1	G	586	GLU	CB-CA-C	-5.60	109.13	115.79
1	E	586	GLU	CB-CA-C	-5.60	109.13	115.79
1	A	91	LYS	CA-CB-CG	-5.60	102.91	114.10
1	G	91	LYS	CA-CB-CG	-5.59	102.92	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	91	LYS	CA-CB-CG	-5.59	102.92	114.10
1	A	586	GLU	CB-CA-C	-5.59	109.14	115.79
1	C	91	LYS	CA-CB-CG	-5.58	102.94	114.10
1	D	91	LYS	CA-CB-CG	-5.58	102.95	114.10
1	C	715	GLN	CA-CB-CG	5.53	125.16	114.10
1	D	715	GLN	CA-CB-CG	5.51	125.12	114.10
1	F	715	GLN	CA-CB-CG	5.51	125.11	114.10
1	E	715	GLN	CA-CB-CG	5.51	125.11	114.10
1	A	715	GLN	CA-CB-CG	5.51	125.11	114.10
1	G	715	GLN	CA-CB-CG	5.50	125.11	114.10
1	B	715	GLN	CA-CB-CG	5.49	125.07	114.10
1	G	40	GLN	CA-CB-CG	5.47	125.04	114.10
1	A	40	GLN	CA-CB-CG	5.47	125.04	114.10
1	C	40	GLN	CA-CB-CG	5.46	125.03	114.10
1	F	40	GLN	CA-CB-CG	5.46	125.03	114.10
1	D	40	GLN	CA-CB-CG	5.45	125.00	114.10
1	E	40	GLN	CA-CB-CG	5.44	124.99	114.10
1	B	40	GLN	CA-CB-CG	5.44	124.98	114.10
1	B	566	LYS	CD-CE-NZ	5.39	129.16	111.90
1	C	566	LYS	CD-CE-NZ	5.39	129.16	111.90
1	D	566	LYS	CD-CE-NZ	5.38	129.13	111.90
1	A	566	LYS	CD-CE-NZ	5.38	129.12	111.90
1	B	715	GLN	CB-CG-CD	5.38	121.74	112.60
1	G	715	GLN	CB-CG-CD	5.38	121.74	112.60
1	E	566	LYS	CD-CE-NZ	5.38	129.10	111.90
1	G	566	LYS	CD-CE-NZ	5.37	129.09	111.90
1	E	715	GLN	CB-CG-CD	5.37	121.73	112.60
1	F	566	LYS	CD-CE-NZ	5.37	129.09	111.90
1	F	715	GLN	CB-CG-CD	5.37	121.72	112.60
1	A	715	GLN	CB-CG-CD	5.36	121.71	112.60
1	D	715	GLN	CB-CG-CD	5.35	121.70	112.60
1	C	715	GLN	CB-CG-CD	5.33	121.66	112.60
1	E	91	LYS	CD-CE-NZ	5.26	128.73	111.90
1	D	91	LYS	CD-CE-NZ	5.25	128.70	111.90
1	B	91	LYS	CD-CE-NZ	5.24	128.68	111.90
1	G	91	LYS	CD-CE-NZ	5.24	128.67	111.90
1	A	91	LYS	CD-CE-NZ	5.24	128.67	111.90
1	C	91	LYS	CD-CE-NZ	5.24	128.66	111.90
1	F	91	LYS	CD-CE-NZ	5.23	128.64	111.90
1	B	309	GLN	CA-CB-CG	5.19	124.48	114.10
1	A	309	GLN	CA-CB-CG	5.19	124.48	114.10
1	F	896	THR	O-C-N	-5.19	115.50	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	GLN	CA-CB-CG	5.18	124.47	114.10
1	G	723	ILE	CA-CB-CG1	5.18	119.21	110.40
1	C	309	GLN	CA-CB-CG	5.18	124.46	114.10
1	F	309	GLN	CA-CB-CG	5.18	124.45	114.10
1	E	309	GLN	CA-CB-CG	5.18	124.45	114.10
1	B	723	ILE	CA-CB-CG1	5.17	119.19	110.40
1	G	309	GLN	CA-CB-CG	5.17	124.45	114.10
1	C	723	ILE	CA-CB-CG1	5.17	119.19	110.40
1	D	723	ILE	CA-CB-CG1	5.16	119.17	110.40
1	A	723	ILE	CA-CB-CG1	5.15	119.16	110.40
1	F	723	ILE	CA-CB-CG1	5.15	119.15	110.40
1	E	723	ILE	CA-CB-CG1	5.13	119.13	110.40
1	D	586	GLU	CB-CA-C	-5.11	109.14	115.89
1	E	138	LYS	CA-CB-CG	-5.11	103.88	114.10
1	A	138	LYS	CA-CB-CG	-5.11	103.89	114.10
1	B	138	LYS	CA-CB-CG	-5.10	103.90	114.10
1	D	138	LYS	CA-CB-CG	-5.10	103.90	114.10
1	A	309	GLN	CB-CG-CD	5.10	121.27	112.60
1	C	138	LYS	CA-CB-CG	-5.09	103.92	114.10
1	F	138	LYS	CA-CB-CG	-5.09	103.92	114.10
1	G	138	LYS	CA-CB-CG	-5.09	103.92	114.10
1	E	309	GLN	CB-CG-CD	5.09	121.26	112.60
1	B	601	LYS	CD-CE-NZ	5.09	128.18	111.90
1	E	601	LYS	CD-CE-NZ	5.09	128.18	111.90
1	D	601	LYS	CD-CE-NZ	5.08	128.17	111.90
1	C	601	LYS	CD-CE-NZ	5.08	128.16	111.90
1	A	601	LYS	CD-CE-NZ	5.08	128.16	111.90
1	D	309	GLN	CB-CG-CD	5.08	121.23	112.60
1	G	309	GLN	CB-CG-CD	5.08	121.23	112.60
1	G	601	LYS	CD-CE-NZ	5.08	128.15	111.90
1	F	601	LYS	CD-CE-NZ	5.07	128.14	111.90
1	F	309	GLN	CB-CG-CD	5.07	121.22	112.60
1	C	309	GLN	CB-CG-CD	5.07	121.21	112.60
1	B	380	MET	CB-CG-SD	5.07	127.90	112.70
1	C	380	MET	CB-CG-SD	5.07	127.90	112.70
1	D	380	MET	CB-CG-SD	5.07	127.89	112.70
1	B	309	GLN	CB-CG-CD	5.06	121.21	112.60
1	G	380	MET	CB-CG-SD	5.06	127.88	112.70
1	E	380	MET	CB-CG-SD	5.06	127.88	112.70
1	A	380	MET	CB-CG-SD	5.06	127.87	112.70
1	F	380	MET	CB-CG-SD	5.05	127.85	112.70
1	B	800	GLU	CB-CG-CD	5.05	121.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	CB-CG-CD	5.04	121.16	112.60
1	E	437	GLU	CB-CG-CD	5.04	121.16	112.60
1	B	437	GLU	CB-CG-CD	5.03	121.16	112.60
1	D	437	GLU	CB-CG-CD	5.03	121.15	112.60
1	F	800	GLU	CB-CG-CD	5.03	121.15	112.60
1	E	800	GLU	CB-CG-CD	5.03	121.15	112.60
1	C	437	GLU	CB-CG-CD	5.03	121.15	112.60
1	F	437	GLU	CB-CG-CD	5.03	121.15	112.60
1	G	800	GLU	CB-CG-CD	5.02	121.14	112.60
1	C	800	GLU	CB-CG-CD	5.02	121.14	112.60
1	G	437	GLU	CB-CG-CD	5.01	121.12	112.60
1	A	800	GLU	CB-CG-CD	5.01	121.11	112.60
1	D	800	GLU	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	206	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	353	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	436	TYR	Sidechain
1	A	596	GLU	Peptide
1	A	758	ARG	Sidechain
1	A	764	ARG	Sidechain
1	A	807	ARG	Sidechain
1	A	896	THR	Mainchain
1	B	117	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	262	ARG	Sidechain
1	B	353	ARG	Sidechain
1	B	38	ARG	Sidechain
1	B	436	TYR	Sidechain
1	B	596	GLU	Peptide
1	B	758	ARG	Sidechain
1	B	764	ARG	Sidechain
1	B	807	ARG	Sidechain
1	B	896	THR	Mainchain
1	C	117	ARG	Sidechain
1	C	206	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	262	ARG	Sidechain
1	C	353	ARG	Sidechain
1	C	38	ARG	Sidechain
1	C	436	TYR	Sidechain
1	C	596	GLU	Peptide
1	C	758	ARG	Sidechain
1	C	764	ARG	Sidechain
1	C	807	ARG	Sidechain
1	D	117	ARG	Sidechain
1	D	206	ARG	Sidechain
1	D	262	ARG	Sidechain
1	D	353	ARG	Sidechain
1	D	38	ARG	Sidechain
1	D	436	TYR	Sidechain
1	D	596	GLU	Peptide
1	D	758	ARG	Sidechain
1	D	764	ARG	Sidechain
1	D	807	ARG	Sidechain
1	E	117	ARG	Sidechain
1	E	206	ARG	Sidechain
1	E	262	ARG	Sidechain
1	E	353	ARG	Sidechain
1	E	38	ARG	Sidechain
1	E	436	TYR	Sidechain
1	E	596	GLU	Peptide
1	E	758	ARG	Sidechain
1	E	764	ARG	Sidechain
1	E	807	ARG	Sidechain
1	F	117	ARG	Sidechain
1	F	206	ARG	Sidechain
1	F	262	ARG	Sidechain
1	F	353	ARG	Sidechain
1	F	38	ARG	Sidechain
1	F	436	TYR	Sidechain
1	F	596	GLU	Peptide
1	F	758	ARG	Sidechain
1	F	764	ARG	Sidechain
1	F	807	ARG	Sidechain
1	F	896	THR	Mainchain
1	G	117	ARG	Sidechain
1	G	206	ARG	Sidechain
1	G	262	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	353	ARG	Sidechain
1	G	38	ARG	Sidechain
1	G	436	TYR	Sidechain
1	G	596	GLU	Peptide
1	G	758	ARG	Sidechain
1	G	764	ARG	Sidechain
1	G	807	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6273	0	6322	298	0
1	B	6273	0	6322	307	0
1	C	6273	0	6322	310	0
1	D	6264	0	6309	317	0
1	E	6239	0	6282	339	0
1	F	6273	0	6321	325	0
1	G	6273	0	6322	303	0
All	All	43868	0	44200	2046	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 23.

All (2046) 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:E:751:GLN:OE1	1:E:811:VAL:CG1	1.72	1.37
1:F:751:GLN:OE1	1:F:811:VAL:CG1	1.73	1.36
1:G:751:GLN:OE1	1:G:811:VAL:CG1	1.73	1.36
1:C:751:GLN:OE1	1:C:811:VAL:CG1	1.72	1.35
1:D:751:GLN:OE1	1:D:811:VAL:CG1	1.73	1.35
1:B:751:GLN:OE1	1:B:811:VAL:CG1	1.73	1.35
1:A:751:GLN:OE1	1:A:811:VAL:CG1	1.72	1.35
1:E:756:LEU:HB3	1:E:927:TYR:CE1	1.68	1.27
1:F:759:ASN:N	1:F:930:ASP:OD2	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ASN:HB3	1:E:228:ASP:OD2	1.38	1.20
1:D:751:GLN:OE1	1:D:811:VAL:HG11	1.43	1.16
1:A:931:THR:HG22	1:A:932:PRO:HD2	1.16	1.15
1:B:931:THR:HG22	1:B:932:PRO:HD2	1.29	1.15
1:C:751:GLN:OE1	1:C:811:VAL:HG11	1.42	1.12
1:F:751:GLN:OE1	1:F:811:VAL:HG11	1.43	1.12
1:E:758:ARG:NH1	1:E:928:ASP:O	1.80	1.11
1:B:751:GLN:OE1	1:B:811:VAL:HG11	1.43	1.10
1:E:751:GLN:OE1	1:E:811:VAL:HG11	1.42	1.09
1:F:751:GLN:OE1	1:F:811:VAL:HG12	1.53	1.08
1:A:751:GLN:OE1	1:A:811:VAL:HG11	1.42	1.08
1:G:751:GLN:OE1	1:G:811:VAL:HG12	1.53	1.08
1:G:751:GLN:OE1	1:G:811:VAL:HG11	1.43	1.08
1:E:751:GLN:OE1	1:E:811:VAL:HG12	1.53	1.06
1:D:751:GLN:OE1	1:D:811:VAL:HG12	1.53	1.04
1:E:756:LEU:HB3	1:E:927:TYR:HE1	1.00	1.04
1:B:751:GLN:OE1	1:B:811:VAL:HG12	1.53	1.03
1:D:758:ARG:NH1	1:D:928:ASP:O	1.90	1.03
1:A:751:GLN:OE1	1:A:811:VAL:HG12	1.53	1.03
1:C:751:GLN:OE1	1:C:811:VAL:HG12	1.53	1.02
1:B:724:GLU:O	1:B:727:ILE:HG12	1.57	1.02
1:G:758:ARG:NH1	1:G:928:ASP:O	1.92	1.01
1:C:724:GLU:O	1:C:727:ILE:HG12	1.61	1.00
1:F:268:ASN:CB	1:E:228:ASP:OD2	2.09	1.00
1:G:724:GLU:O	1:G:727:ILE:HG12	1.61	0.99
1:D:436:TYR:CE2	1:E:255:ARG:HG3	1.98	0.99
1:G:578:ARG:NH1	1:G:616:LEU:O	1.96	0.99
1:E:578:ARG:NH1	1:E:616:LEU:O	1.96	0.98
1:C:578:ARG:NH1	1:C:616:LEU:O	1.96	0.98
1:D:578:ARG:NH1	1:D:616:LEU:O	1.96	0.98
1:B:578:ARG:NH1	1:B:616:LEU:O	1.96	0.98
1:A:578:ARG:NH1	1:A:616:LEU:O	1.96	0.97
1:F:578:ARG:NH1	1:F:616:LEU:O	1.96	0.97
1:F:765:MET:O	1:F:773:LYS:NZ	2.00	0.95
1:D:765:MET:O	1:D:773:LYS:NZ	2.00	0.95
1:B:758:ARG:HD3	1:B:928:ASP:HA	1.48	0.95
1:B:765:MET:O	1:B:773:LYS:NZ	2.00	0.95
1:A:765:MET:O	1:A:773:LYS:NZ	2.00	0.95
1:C:765:MET:O	1:C:773:LYS:NZ	2.00	0.95
1:F:724:GLU:O	1:F:727:ILE:HG12	1.65	0.94
1:G:765:MET:O	1:G:773:LYS:NZ	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:756:LEU:CB	1:E:927:TYR:HE1	1.80	0.94
1:E:765:MET:O	1:E:773:LYS:NZ	2.00	0.93
1:E:758:ARG:CZ	1:E:928:ASP:O	2.15	0.93
1:A:758:ARG:NH1	1:A:928:ASP:O	2.01	0.93
1:F:291:GLU:OE1	1:E:431:ARG:HD3	1.67	0.93
1:E:858:ILE:HD13	1:E:895:LEU:HD23	1.51	0.92
1:C:426:LEU:HD11	1:C:436:TYR:CE1	2.05	0.92
1:B:426:LEU:HD11	1:B:436:TYR:CE1	2.05	0.92
1:E:426:LEU:HD11	1:E:436:TYR:CE1	2.05	0.92
1:B:858:ILE:HD13	1:B:895:LEU:HD23	1.51	0.92
1:A:858:ILE:HD13	1:A:895:LEU:HD23	1.51	0.92
1:G:858:ILE:HD13	1:G:895:LEU:HD23	1.51	0.92
1:A:426:LEU:HD11	1:A:436:TYR:CE1	2.05	0.92
1:D:426:LEU:HD11	1:D:436:TYR:CE1	2.05	0.91
1:D:259:GLN:OE1	1:E:273:LEU:HD21	1.69	0.91
1:C:858:ILE:HD13	1:C:895:LEU:HD23	1.51	0.91
1:C:758:ARG:NH1	1:C:928:ASP:O	2.03	0.91
1:G:426:LEU:HD11	1:G:436:TYR:CE1	2.05	0.91
1:B:931:THR:CG2	1:B:932:PRO:HD2	2.00	0.91
1:F:426:LEU:HD11	1:F:436:TYR:CE1	2.05	0.91
1:F:858:ILE:HD13	1:F:895:LEU:HD23	1.51	0.90
1:D:858:ILE:HD13	1:D:895:LEU:HD23	1.52	0.90
1:G:512:ASN:O	1:G:516:THR:OG1	1.90	0.90
1:A:931:THR:CG2	1:A:932:PRO:HD2	2.02	0.90
1:F:512:ASN:O	1:F:516:THR:OG1	1.90	0.90
1:A:512:ASN:O	1:A:516:THR:OG1	1.90	0.90
1:B:512:ASN:O	1:B:516:THR:OG1	1.90	0.90
1:F:338:ASP:O	1:F:339:ILE:HD13	1.73	0.89
1:C:512:ASN:O	1:C:516:THR:OG1	1.90	0.89
1:E:437:GLU:OE1	1:E:437:GLU:N	2.06	0.89
1:E:512:ASN:O	1:E:516:THR:OG1	1.90	0.89
1:D:437:GLU:OE1	1:D:437:GLU:N	2.06	0.89
1:D:512:ASN:O	1:D:516:THR:OG1	1.90	0.88
1:B:338:ASP:O	1:B:339:ILE:HD13	1.73	0.88
1:A:437:GLU:N	1:A:437:GLU:OE1	2.06	0.88
1:G:437:GLU:OE1	1:G:437:GLU:N	2.06	0.88
1:A:931:THR:HG22	1:A:932:PRO:CD	2.03	0.88
1:B:437:GLU:OE1	1:B:437:GLU:N	2.06	0.88
1:E:338:ASP:O	1:E:339:ILE:HD13	1.73	0.88
1:F:437:GLU:N	1:F:437:GLU:OE1	2.06	0.87
1:F:291:GLU:OE1	1:E:431:ARG:CD	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLU:OE1	1:C:437:GLU:N	2.06	0.87
1:D:338:ASP:O	1:D:339:ILE:HD13	1.73	0.87
1:C:338:ASP:O	1:C:339:ILE:HD13	1.73	0.87
1:E:758:ARG:HG2	1:E:927:TYR:O	1.76	0.86
1:C:751:GLN:CD	1:C:811:VAL:HG11	2.02	0.84
1:F:646:PHE:HZ	1:F:713:VAL:HG21	1.42	0.84
1:E:756:LEU:CB	1:E:927:TYR:CE1	2.56	0.84
1:A:758:ARG:HD3	1:A:928:ASP:HA	1.59	0.84
1:A:751:GLN:CD	1:A:811:VAL:HG11	2.02	0.84
1:G:338:ASP:O	1:G:339:ILE:HD13	1.77	0.84
1:D:751:GLN:CD	1:D:811:VAL:HG11	2.03	0.84
1:E:646:PHE:HZ	1:E:713:VAL:HG21	1.42	0.84
1:G:646:PHE:HZ	1:G:713:VAL:HG21	1.42	0.84
1:B:751:GLN:CD	1:B:811:VAL:HG11	2.02	0.84
1:D:646:PHE:HZ	1:D:713:VAL:HG21	1.42	0.84
1:F:758:ARG:HD3	1:F:928:ASP:C	2.02	0.84
1:G:751:GLN:CD	1:G:811:VAL:HG11	2.02	0.84
1:B:646:PHE:HZ	1:B:713:VAL:HG21	1.42	0.84
1:C:646:PHE:HZ	1:C:713:VAL:HG21	1.42	0.83
1:A:646:PHE:HZ	1:A:713:VAL:HG21	1.42	0.83
1:E:751:GLN:CD	1:E:811:VAL:HG11	2.02	0.83
1:B:277:GLU:OE1	1:A:262:ARG:HD2	1.79	0.83
1:B:513:GLN:OE1	1:B:742:TYR:OH	1.97	0.82
1:C:116:PRO:HG3	1:D:166:LEU:HD13	1.60	0.82
1:F:751:GLN:CD	1:F:811:VAL:HG11	2.02	0.82
1:A:513:GLN:OE1	1:A:742:TYR:OH	1.97	0.82
1:C:513:GLN:OE1	1:C:742:TYR:OH	1.97	0.82
1:F:513:GLN:OE1	1:F:742:TYR:OH	1.97	0.81
1:E:513:GLN:OE1	1:E:742:TYR:OH	1.97	0.81
1:D:513:GLN:OE1	1:D:742:TYR:OH	1.97	0.81
1:G:513:GLN:OE1	1:G:742:TYR:OH	1.97	0.81
1:G:414:PRO:HG2	1:G:491:GLN:OE1	1.81	0.81
1:D:414:PRO:HG2	1:D:491:GLN:OE1	1.81	0.81
1:A:414:PRO:HG2	1:A:491:GLN:OE1	1.81	0.80
1:F:414:PRO:HG2	1:F:491:GLN:OE1	1.81	0.80
1:F:757:TYR:HB3	1:F:930:ASP:HA	1.61	0.80
1:G:262:ARG:HD2	1:A:277:GLU:OE1	1.82	0.80
1:F:304:VAL:HG13	1:E:423:GLY:HA3	1.64	0.80
1:E:414:PRO:HG2	1:E:491:GLN:OE1	1.81	0.80
1:B:414:PRO:HG2	1:B:491:GLN:OE1	1.81	0.79
1:C:414:PRO:HG2	1:C:491:GLN:OE1	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASP:OD1	1:G:340:ASP:N	2.13	0.79
1:F:340:ASP:OD1	1:F:340:ASP:N	2.14	0.79
1:F:295:GLN:HE21	1:E:427:SER:HB2	1.47	0.79
1:C:338:ASP:O	1:C:339:ILE:CD1	2.31	0.79
1:E:340:ASP:OD1	1:E:340:ASP:N	2.14	0.79
1:E:578:ARG:O	1:E:590:LYS:NZ	2.14	0.79
1:D:338:ASP:O	1:D:339:ILE:CD1	2.31	0.79
1:E:338:ASP:O	1:E:339:ILE:CD1	2.31	0.79
1:F:338:ASP:O	1:F:339:ILE:CD1	2.30	0.78
1:F:276:GLN:NE2	1:E:274:LEU:HB3	1.98	0.78
1:B:338:ASP:O	1:B:339:ILE:CD1	2.31	0.78
1:C:931:THR:HG22	1:C:932:PRO:HD2	1.65	0.78
1:G:338:ASP:O	1:G:339:ILE:CD1	2.32	0.77
1:G:578:ARG:O	1:G:590:LYS:NZ	2.14	0.77
1:D:530:GLN:NE2	1:E:525:ARG:HD2	1.99	0.77
1:F:304:VAL:CG1	1:E:423:GLY:HA3	2.15	0.77
1:F:758:ARG:HD3	1:F:928:ASP:O	1.85	0.77
1:D:728:ARG:HH11	1:D:728:ARG:HG3	1.50	0.77
1:B:340:ASP:OD1	1:B:340:ASP:N	2.15	0.77
1:B:578:ARG:O	1:B:590:LYS:NZ	2.14	0.77
1:C:116:PRO:HB3	1:D:166:LEU:HB3	1.66	0.77
1:E:724:GLU:O	1:E:727:ILE:HG12	1.85	0.77
1:D:262:ARG:HD2	1:E:277:GLU:OE1	1.85	0.77
1:F:315:GLN:NE2	1:E:439:HIS:HA	2.00	0.76
1:F:756:LEU:HB3	1:F:927:TYR:HE1	1.50	0.76
1:F:758:ARG:HD3	1:F:928:ASP:CA	2.15	0.76
1:E:728:ARG:HH11	1:E:728:ARG:HG3	1.51	0.76
1:F:578:ARG:O	1:F:590:LYS:NZ	2.14	0.76
1:D:340:ASP:OD1	1:D:340:ASP:N	2.14	0.76
1:F:728:ARG:HH11	1:F:728:ARG:HG3	1.51	0.75
1:D:578:ARG:O	1:D:590:LYS:NZ	2.14	0.75
1:D:724:GLU:O	1:D:727:ILE:HG12	1.86	0.74
1:F:758:ARG:HD3	1:F:928:ASP:HA	1.69	0.74
1:F:758:ARG:CD	1:F:928:ASP:O	2.35	0.74
1:G:436:TYR:CE2	1:A:255:ARG:HG3	2.23	0.74
1:C:578:ARG:O	1:C:590:LYS:NZ	2.14	0.74
1:B:41:LEU:HD23	1:B:89:VAL:HG21	1.70	0.73
1:E:41:LEU:HD23	1:E:89:VAL:HG21	1.70	0.73
1:A:41:LEU:HD23	1:A:89:VAL:HG21	1.70	0.73
1:A:578:ARG:O	1:A:590:LYS:NZ	2.14	0.73
1:G:41:LEU:HD23	1:G:89:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:764:ARG:CZ	1:F:897:LYS:C	2.61	0.73
1:F:41:LEU:HD23	1:F:89:VAL:HG21	1.70	0.73
1:C:41:LEU:HD23	1:C:89:VAL:HG21	1.70	0.72
1:E:863:CYS:HA	1:E:868:LEU:HD11	1.71	0.72
1:D:863:CYS:HA	1:D:868:LEU:HD11	1.71	0.72
1:B:931:THR:HG22	1:B:932:PRO:CD	2.16	0.72
1:D:41:LEU:HD23	1:D:89:VAL:HG21	1.70	0.72
1:F:863:CYS:HA	1:F:868:LEU:HD11	1.71	0.72
1:C:931:THR:CG2	1:C:932:PRO:HD2	2.19	0.72
1:G:863:CYS:HA	1:G:868:LEU:HD11	1.71	0.72
1:F:268:ASN:CA	1:E:228:ASP:OD2	2.38	0.71
1:A:863:CYS:HA	1:A:868:LEU:HD11	1.71	0.71
1:B:759:ASN:ND2	1:B:930:ASP:OD1	2.24	0.71
1:D:646:PHE:CZ	1:D:713:VAL:HG21	2.26	0.71
1:E:870:LYS:O	1:E:874:PHE:N	2.24	0.71
1:B:870:LYS:O	1:B:874:PHE:N	2.24	0.71
1:D:473:GLU:OE1	1:D:477:ASN:ND2	2.24	0.71
1:A:870:LYS:O	1:A:874:PHE:N	2.24	0.71
1:B:863:CYS:HA	1:B:868:LEU:HD11	1.71	0.71
1:C:494:LEU:HD12	1:C:633:SER:OG	1.91	0.71
1:C:870:LYS:O	1:C:874:PHE:N	2.24	0.70
1:E:473:GLU:OE1	1:E:477:ASN:ND2	2.24	0.70
1:G:224:ASP:OD2	1:G:224:ASP:N	2.25	0.70
1:A:224:ASP:OD2	1:A:224:ASP:N	2.25	0.70
1:C:503:VAL:O	1:C:507:SER:HB2	1.92	0.70
1:D:503:VAL:O	1:D:507:SER:HB2	1.92	0.70
1:D:870:LYS:O	1:D:874:PHE:N	2.24	0.70
1:E:503:VAL:O	1:E:507:SER:HB2	1.92	0.70
1:B:473:GLU:OE1	1:B:477:ASN:ND2	2.24	0.70
1:C:340:ASP:OD1	1:C:340:ASP:N	2.21	0.70
1:C:863:CYS:HA	1:C:868:LEU:HD11	1.71	0.70
1:A:473:GLU:OE1	1:A:477:ASN:ND2	2.24	0.70
1:C:473:GLU:OE1	1:C:477:ASN:ND2	2.24	0.70
1:D:261:ILE:CD1	1:D:298:LEU:HD12	2.22	0.70
1:F:870:LYS:O	1:F:874:PHE:N	2.24	0.70
1:G:870:LYS:O	1:G:874:PHE:N	2.24	0.70
1:E:494:LEU:HD12	1:E:633:SER:OG	1.91	0.70
1:B:224:ASP:OD2	1:B:224:ASP:N	2.25	0.70
1:B:261:ILE:CD1	1:B:298:LEU:HD12	2.22	0.70
1:B:494:LEU:HD12	1:B:633:SER:OG	1.91	0.70
1:B:503:VAL:O	1:B:507:SER:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:ARG:HG3	1:B:728:ARG:HH11	1.56	0.70
1:C:224:ASP:OD2	1:C:224:ASP:N	2.25	0.70
1:F:503:VAL:O	1:F:507:SER:HB2	1.91	0.70
1:C:165:HIS:HA	1:D:174:PRO:HG3	1.74	0.69
1:F:261:ILE:CD1	1:F:298:LEU:HD12	2.22	0.69
1:F:646:PHE:CZ	1:F:713:VAL:HG21	2.26	0.69
1:G:473:GLU:OE1	1:G:477:ASN:ND2	2.24	0.69
1:E:261:ILE:CD1	1:E:298:LEU:HD12	2.22	0.69
1:E:646:PHE:CZ	1:E:713:VAL:HG21	2.26	0.69
1:D:494:LEU:HD12	1:D:633:SER:OG	1.91	0.69
1:F:473:GLU:OE1	1:F:477:ASN:ND2	2.24	0.69
1:F:494:LEU:HD12	1:F:633:SER:OG	1.91	0.69
1:G:261:ILE:CD1	1:G:298:LEU:HD12	2.22	0.69
1:C:758:ARG:HD3	1:C:928:ASP:HA	1.74	0.69
1:G:494:LEU:HD12	1:G:633:SER:OG	1.91	0.69
1:A:503:VAL:O	1:A:507:SER:HB2	1.91	0.69
1:C:261:ILE:CD1	1:C:298:LEU:HD12	2.22	0.69
1:A:261:ILE:CD1	1:A:298:LEU:HD12	2.22	0.69
1:C:443:MET:HG3	1:C:446:LEU:HD23	1.75	0.69
1:C:225:THR:HG21	1:D:238:ARG:CZ	2.23	0.69
1:C:755:ARG:NH1	1:C:766:ALA:O	2.26	0.69
1:G:931:THR:CG2	1:G:932:PRO:HD2	2.23	0.69
1:E:224:ASP:OD2	1:E:224:ASP:N	2.25	0.69
1:A:758:ARG:CZ	1:A:928:ASP:O	2.40	0.69
1:B:443:MET:HG3	1:B:446:LEU:HD23	1.75	0.69
1:F:755:ARG:NH1	1:F:766:ALA:O	2.26	0.69
1:A:755:ARG:NH1	1:A:766:ALA:O	2.26	0.69
1:A:443:MET:HG3	1:A:446:LEU:HD23	1.75	0.69
1:B:426:LEU:HD11	1:B:436:TYR:HE1	1.56	0.68
1:D:443:MET:HG3	1:D:446:LEU:HD23	1.75	0.68
1:G:503:VAL:O	1:G:507:SER:HB2	1.92	0.68
1:E:426:LEU:HD11	1:E:436:TYR:HE1	1.56	0.68
1:A:357:ASN:CG	1:A:728:ARG:HB3	2.18	0.68
1:A:494:LEU:HD12	1:A:633:SER:OG	1.91	0.68
1:A:727:ILE:HG13	1:A:727:ILE:O	1.92	0.68
1:B:755:ARG:NH1	1:B:766:ALA:O	2.26	0.68
1:C:749:ALA:O	1:C:753:LYS:HE2	1.94	0.68
1:G:646:PHE:CZ	1:G:713:VAL:HG21	2.26	0.68
1:A:426:LEU:HD11	1:A:436:TYR:HE1	1.56	0.68
1:B:646:PHE:CZ	1:B:713:VAL:HG21	2.26	0.68
1:G:755:ARG:NH1	1:G:766:ALA:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD11	1:A:216:ILE:HD13	1.76	0.68
1:D:129:LEU:HD11	1:D:216:ILE:HD13	1.76	0.68
1:G:129:LEU:HD11	1:G:216:ILE:HD13	1.76	0.68
1:G:749:ALA:O	1:G:753:LYS:HE2	1.94	0.68
1:C:646:PHE:CZ	1:C:713:VAL:HG21	2.26	0.68
1:G:712:LYS:O	1:G:715:GLN:HB2	1.94	0.68
1:D:749:ALA:O	1:D:753:LYS:HE2	1.94	0.68
1:G:443:MET:HG3	1:G:446:LEU:HD23	1.75	0.68
1:B:129:LEU:HD11	1:B:216:ILE:HD13	1.76	0.68
1:D:755:ARG:NH1	1:D:766:ALA:O	2.26	0.68
1:F:712:LYS:O	1:F:715:GLN:HB2	1.94	0.68
1:G:118:HIS:O	1:A:172:TYR:HB2	1.93	0.68
1:G:197:SER:OG	1:G:239:LYS:O	2.12	0.68
1:A:646:PHE:CZ	1:A:713:VAL:HG21	2.26	0.68
1:A:712:LYS:O	1:A:715:GLN:HB2	1.94	0.68
1:F:224:ASP:OD2	1:F:224:ASP:N	2.25	0.68
1:A:197:SER:OG	1:A:239:LYS:O	2.12	0.68
1:F:451:PHE:HE2	1:F:507:SER:O	1.75	0.68
1:G:426:LEU:HD11	1:G:436:TYR:HE1	1.56	0.68
1:C:129:LEU:HD11	1:C:216:ILE:HD13	1.76	0.68
1:F:129:LEU:HD11	1:F:216:ILE:HD13	1.76	0.68
1:F:197:SER:OG	1:F:239:LYS:O	2.12	0.68
1:F:749:ALA:O	1:F:753:LYS:HE2	1.94	0.68
1:A:749:ALA:O	1:A:753:LYS:HE2	1.94	0.68
1:B:177:PHE:HD2	1:A:161:GLN:HG3	1.59	0.67
1:B:749:ALA:O	1:B:753:LYS:HE2	1.94	0.67
1:C:426:LEU:HD11	1:C:436:TYR:HE1	1.56	0.67
1:A:798:ASP:OD2	1:A:798:ASP:N	2.28	0.67
1:B:712:LYS:O	1:B:715:GLN:HB2	1.94	0.67
1:G:798:ASP:OD2	1:G:798:ASP:N	2.27	0.67
1:E:197:SER:OG	1:E:239:LYS:O	2.12	0.67
1:E:755:ARG:NH1	1:E:766:ALA:O	2.26	0.67
1:C:798:ASP:OD2	1:C:798:ASP:N	2.28	0.67
1:G:357:ASN:CG	1:G:728:ARG:HB3	2.20	0.67
1:B:197:SER:OG	1:B:239:LYS:O	2.12	0.67
1:F:759:ASN:CA	1:F:930:ASP:OD2	2.19	0.67
1:G:722:GLU:HB2	1:G:723:ILE:CG2	2.25	0.67
1:D:712:LYS:O	1:D:715:GLN:HB2	1.94	0.67
1:C:357:ASN:CG	1:C:728:ARG:HB3	2.20	0.67
1:D:380:MET:HA	1:D:380:MET:HE3	1.77	0.67
1:E:443:MET:HG3	1:E:446:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:GLU:HB2	1:E:723:ILE:CG2	2.25	0.67
1:E:749:ALA:O	1:E:753:LYS:HE2	1.94	0.67
1:C:197:SER:OG	1:C:239:LYS:O	2.12	0.67
1:C:712:LYS:O	1:C:715:GLN:HB2	1.94	0.67
1:D:426:LEU:HD11	1:D:436:TYR:HE1	1.56	0.67
1:F:380:MET:HA	1:F:380:MET:HE3	1.77	0.67
1:F:295:GLN:NE2	1:E:427:SER:HB2	2.10	0.66
1:F:443:MET:HG3	1:F:446:LEU:HD23	1.75	0.66
1:F:798:ASP:OD2	1:F:798:ASP:N	2.27	0.66
1:B:431:ARG:HG2	1:C:291:GLU:OE1	1.96	0.66
1:D:727:ILE:HG13	1:D:727:ILE:O	1.95	0.66
1:G:380:MET:HA	1:G:380:MET:HE3	1.77	0.66
1:E:712:LYS:O	1:E:715:GLN:HB2	1.94	0.66
1:A:722:GLU:HB2	1:A:723:ILE:CG2	2.25	0.66
1:C:722:GLU:HB2	1:C:723:ILE:CG2	2.25	0.66
1:D:197:SER:OG	1:D:239:LYS:O	2.12	0.66
1:A:380:MET:HA	1:A:380:MET:HE3	1.77	0.66
1:E:129:LEU:HD11	1:E:216:ILE:HD13	1.76	0.66
1:B:722:GLU:HB2	1:B:723:ILE:CG2	2.25	0.66
1:C:431:ARG:HH12	1:E:277:GLU:CD	2.04	0.66
1:F:291:GLU:OE1	1:E:431:ARG:CG	2.43	0.66
1:B:380:MET:HA	1:B:380:MET:HE3	1.77	0.66
1:B:798:ASP:OD2	1:B:798:ASP:N	2.28	0.66
1:F:722:GLU:HB2	1:F:723:ILE:CG2	2.25	0.66
1:E:380:MET:HA	1:E:380:MET:HE3	1.77	0.66
1:E:798:ASP:OD2	1:E:798:ASP:N	2.28	0.66
1:C:116:PRO:CG	1:D:166:LEU:HD13	2.24	0.65
1:C:380:MET:HA	1:C:380:MET:HE3	1.77	0.65
1:D:722:GLU:HB2	1:D:723:ILE:CG2	2.25	0.65
1:F:426:LEU:HD11	1:F:436:TYR:HE1	1.56	0.65
1:D:173:LYS:HD2	1:D:176:TYR:CE1	2.32	0.65
1:D:333:GLU:N	1:D:336:MET:HE3	2.11	0.65
1:G:173:LYS:HD2	1:G:176:TYR:CE1	2.32	0.65
1:D:436:TYR:CZ	1:E:255:ARG:HG3	2.31	0.65
1:C:888:SER:O	1:C:892:TRP:N	2.29	0.65
1:G:764:ARG:O	1:G:863:CYS:N	2.22	0.65
1:E:173:LYS:HD2	1:E:176:TYR:CE1	2.32	0.65
1:B:764:ARG:O	1:B:863:CYS:N	2.22	0.65
1:D:118:HIS:O	1:E:172:TYR:HB2	1.97	0.65
1:D:367:TYR:OH	1:D:466:LEU:O	2.15	0.65
1:D:798:ASP:OD2	1:D:798:ASP:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:727:ILE:O	1:E:727:ILE:HG13	1.95	0.65
1:B:424:SER:HA	1:C:304:VAL:HG21	1.79	0.65
1:C:173:LYS:HD2	1:C:176:TYR:CE1	2.32	0.65
1:D:888:SER:O	1:D:892:TRP:N	2.29	0.65
1:F:173:LYS:HD2	1:F:176:TYR:CE1	2.32	0.65
1:E:367:TYR:OH	1:E:466:LEU:O	2.15	0.65
1:A:436:TYR:HB3	1:A:437:GLU:OE1	1.97	0.65
1:A:173:LYS:HD2	1:A:176:TYR:CE1	2.32	0.65
1:B:173:LYS:HD2	1:B:176:TYR:CE1	2.32	0.65
1:C:436:TYR:HB3	1:C:437:GLU:OE1	1.97	0.65
1:F:436:TYR:HB3	1:F:437:GLU:OE1	1.97	0.65
1:B:333:GLU:N	1:B:336:MET:HE3	2.12	0.64
1:B:758:ARG:HD3	1:B:928:ASP:CA	2.25	0.64
1:F:273:LEU:HD13	1:E:263:GLY:HA2	1.78	0.64
1:B:357:ASN:CG	1:B:728:ARG:HB3	2.22	0.64
1:B:436:TYR:HB3	1:B:437:GLU:OE1	1.97	0.64
1:E:436:TYR:HB3	1:E:437:GLU:OE1	1.97	0.64
1:F:436:TYR:CE2	1:G:255:ARG:HG3	2.32	0.64
1:G:367:TYR:OH	1:G:466:LEU:O	2.15	0.64
1:E:888:SER:O	1:E:892:TRP:N	2.29	0.64
1:G:888:SER:O	1:G:892:TRP:N	2.29	0.64
1:D:333:GLU:H	1:D:336:MET:HE3	1.62	0.64
1:D:436:TYR:HB3	1:D:437:GLU:OE1	1.97	0.64
1:F:333:GLU:N	1:F:336:MET:HE3	2.12	0.64
1:F:367:TYR:OH	1:F:466:LEU:O	2.15	0.64
1:E:758:ARG:NE	1:E:928:ASP:O	2.30	0.64
1:F:333:GLU:H	1:F:336:MET:HE3	1.63	0.64
1:F:764:ARG:O	1:F:863:CYS:N	2.22	0.64
1:B:118:HIS:O	1:C:172:TYR:HB2	1.97	0.64
1:D:530:GLN:NE2	1:E:525:ARG:CD	2.61	0.64
1:F:758:ARG:CD	1:F:928:ASP:C	2.70	0.64
1:A:367:TYR:OH	1:A:466:LEU:O	2.15	0.64
1:B:888:SER:O	1:B:892:TRP:N	2.29	0.63
1:G:436:TYR:HB3	1:G:437:GLU:OE1	1.97	0.63
1:B:861:ILE:HG23	1:B:871:GLU:OE2	1.99	0.63
1:C:861:ILE:HG23	1:C:871:GLU:OE2	1.99	0.63
1:F:458:ARG:HH12	1:E:530:GLN:HE22	1.46	0.63
1:F:861:ILE:HG23	1:F:871:GLU:OE2	1.99	0.63
1:A:888:SER:O	1:A:892:TRP:N	2.29	0.63
1:D:861:ILE:HG23	1:D:871:GLU:OE2	1.99	0.63
1:E:333:GLU:N	1:E:336:MET:HE3	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:TYR:O	1:E:539:MET:HB2	1.98	0.63
1:E:333:GLU:H	1:E:336:MET:HE3	1.62	0.63
1:B:333:GLU:H	1:B:336:MET:HE3	1.63	0.63
1:D:535:TYR:O	1:D:539:MET:HB2	1.99	0.63
1:F:535:TYR:O	1:F:539:MET:HB2	1.99	0.63
1:F:888:SER:O	1:F:892:TRP:N	2.29	0.63
1:G:535:TYR:O	1:G:539:MET:HB2	1.98	0.63
1:E:38:ARG:O	1:E:42:VAL:HG23	1.99	0.63
1:A:861:ILE:HG23	1:A:871:GLU:OE2	1.98	0.63
1:G:38:ARG:O	1:G:42:VAL:HG23	1.99	0.63
1:A:535:TYR:O	1:A:539:MET:HB2	1.98	0.63
1:C:279:GLU:N	1:C:279:GLU:OE1	2.32	0.63
1:G:758:ARG:HG2	1:G:927:TYR:O	1.99	0.63
1:C:551:ALA:CB	1:C:624:ASN:OD1	2.47	0.63
1:E:279:GLU:OE1	1:E:279:GLU:N	2.32	0.63
1:E:861:ILE:HG23	1:E:871:GLU:OE2	1.98	0.63
1:A:38:ARG:O	1:A:42:VAL:HG23	1.99	0.63
1:A:722:GLU:HB2	1:A:723:ILE:HG22	1.81	0.63
1:G:861:ILE:HG23	1:G:871:GLU:OE2	1.98	0.62
1:E:254:LEU:HD22	1:E:298:LEU:HD21	1.81	0.62
1:B:367:TYR:OH	1:B:466:LEU:O	2.15	0.62
1:B:722:GLU:HB2	1:B:723:ILE:HG22	1.81	0.62
1:F:38:ARG:O	1:F:42:VAL:HG23	1.99	0.62
1:D:551:ALA:CB	1:D:624:ASN:OD1	2.47	0.62
1:D:722:GLU:HB2	1:D:723:ILE:HG22	1.82	0.62
1:E:802:ILE:HD11	1:E:820:LYS:HD3	1.82	0.62
1:B:279:GLU:OE1	1:B:279:GLU:N	2.32	0.62
1:B:431:ARG:CG	1:C:291:GLU:OE1	2.47	0.62
1:B:535:TYR:O	1:B:539:MET:HB2	1.98	0.62
1:B:551:ALA:CB	1:B:624:ASN:OD1	2.47	0.62
1:E:137:LEU:HD13	1:E:150:LYS:HG3	1.82	0.62
1:C:722:GLU:HB2	1:C:723:ILE:HG22	1.81	0.62
1:F:192:GLY:CA	1:E:131:LYS:HD3	2.29	0.62
1:F:802:ILE:HD11	1:F:820:LYS:HD3	1.82	0.62
1:F:887:LEU:HD22	1:F:895:LEU:HD11	1.81	0.62
1:G:887:LEU:HD22	1:G:895:LEU:HD11	1.81	0.62
1:B:38:ARG:O	1:B:42:VAL:HG23	1.99	0.62
1:C:535:TYR:O	1:C:539:MET:HB2	1.98	0.62
1:G:551:ALA:CB	1:G:624:ASN:OD1	2.47	0.62
1:G:722:GLU:HB2	1:G:723:ILE:HG22	1.81	0.62
1:G:931:THR:HG22	1:G:932:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:887:LEU:HD22	1:E:895:LEU:HD11	1.81	0.62
1:C:137:LEU:HD13	1:C:150:LYS:HG3	1.82	0.62
1:D:137:LEU:HD13	1:D:150:LYS:HG3	1.82	0.62
1:E:751:GLN:OE1	1:E:811:VAL:CB	2.48	0.62
1:C:38:ARG:O	1:C:42:VAL:HG23	1.99	0.62
1:C:436:TYR:CE2	1:D:255:ARG:HG3	2.34	0.62
1:D:38:ARG:O	1:D:42:VAL:HG23	1.99	0.62
1:F:279:GLU:OE1	1:F:279:GLU:N	2.32	0.62
1:A:704:THR:OG1	1:A:705:GLU:N	2.33	0.62
1:A:887:LEU:HD22	1:A:895:LEU:HD11	1.81	0.62
1:A:551:ALA:CB	1:A:624:ASN:OD1	2.47	0.62
1:B:704:THR:OG1	1:B:705:GLU:N	2.33	0.62
1:D:254:LEU:HD22	1:D:298:LEU:HD21	1.81	0.62
1:B:357:ASN:HB3	1:B:728:ARG:O	2.00	0.61
1:F:551:ALA:CB	1:F:624:ASN:OD1	2.47	0.61
1:E:704:THR:OG1	1:E:705:GLU:N	2.33	0.61
1:A:764:ARG:O	1:A:863:CYS:N	2.22	0.61
1:B:887:LEU:HD22	1:B:895:LEU:HD11	1.81	0.61
1:C:254:LEU:HD22	1:C:298:LEU:HD21	1.81	0.61
1:D:758:ARG:CZ	1:D:928:ASP:O	2.47	0.61
1:D:764:ARG:O	1:D:863:CYS:N	2.22	0.61
1:G:802:ILE:HD11	1:G:820:LYS:HD3	1.82	0.61
1:G:863:CYS:HA	1:G:868:LEU:CD1	2.31	0.61
1:A:863:CYS:HA	1:A:868:LEU:CD1	2.31	0.61
1:B:863:CYS:HA	1:B:868:LEU:CD1	2.31	0.61
1:D:279:GLU:OE1	1:D:279:GLU:N	2.32	0.61
1:F:254:LEU:HD22	1:F:298:LEU:HD21	1.81	0.61
1:F:863:CYS:HA	1:F:868:LEU:CD1	2.31	0.61
1:G:254:LEU:HD22	1:G:298:LEU:HD21	1.81	0.61
1:D:802:ILE:HD11	1:D:820:LYS:HD3	1.82	0.61
1:F:722:GLU:HB2	1:F:723:ILE:HG22	1.81	0.61
1:E:551:ALA:CB	1:E:624:ASN:OD1	2.47	0.61
1:B:137:LEU:HD13	1:B:150:LYS:HG3	1.82	0.61
1:B:357:ASN:ND2	1:B:728:ARG:HB3	2.15	0.61
1:B:724:GLU:O	1:B:727:ILE:CG1	2.41	0.61
1:G:279:GLU:OE1	1:G:279:GLU:N	2.32	0.61
1:A:254:LEU:HD22	1:A:298:LEU:HD21	1.81	0.61
1:A:340:ASP:OD1	1:A:340:ASP:N	2.21	0.61
1:C:863:CYS:HA	1:C:868:LEU:CD1	2.31	0.61
1:C:887:LEU:HD22	1:C:895:LEU:HD11	1.81	0.61
1:C:802:ILE:HD11	1:C:820:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:GLU:HB2	1:E:723:ILE:HG22	1.81	0.61
1:E:863:CYS:HA	1:E:868:LEU:CD1	2.31	0.61
1:B:254:LEU:HD22	1:B:298:LEU:HD21	1.81	0.60
1:B:852:HIS:HA	1:B:855:ILE:HG13	1.83	0.60
1:F:727:ILE:HG13	1:F:727:ILE:O	1.99	0.60
1:C:852:HIS:HA	1:C:855:ILE:HG13	1.84	0.60
1:D:852:HIS:HA	1:D:855:ILE:HG13	1.84	0.60
1:A:137:LEU:HD13	1:A:150:LYS:HG3	1.82	0.60
1:B:802:ILE:HD11	1:B:820:LYS:HD3	1.82	0.60
1:C:764:ARG:O	1:C:863:CYS:N	2.22	0.60
1:D:751:GLN:OE1	1:D:811:VAL:CB	2.48	0.60
1:F:304:VAL:HG21	1:E:424:SER:HA	1.81	0.60
1:A:758:ARG:HD3	1:A:928:ASP:CA	2.30	0.60
1:A:279:GLU:OE1	1:A:279:GLU:N	2.32	0.60
1:A:751:GLN:OE1	1:A:811:VAL:CB	2.48	0.60
1:A:852:HIS:HA	1:A:855:ILE:HG13	1.83	0.60
1:G:259:GLN:HG3	1:A:269:TYR:HE2	1.67	0.60
1:E:562:PRO:HG2	1:E:570:PHE:CD2	2.37	0.60
1:G:116:PRO:HG3	1:A:166:LEU:HD13	1.82	0.60
1:G:704:THR:OG1	1:G:705:GLU:N	2.33	0.60
1:E:852:HIS:HA	1:E:855:ILE:HG13	1.83	0.60
1:B:430:TYR:CE1	1:C:255:ARG:HG2	2.36	0.60
1:B:757:TYR:HE1	1:A:581:ARG:HH22	1.48	0.60
1:D:863:CYS:HA	1:D:868:LEU:CD1	2.31	0.60
1:F:311:LYS:HD3	1:F:316:LEU:HD21	1.84	0.60
1:F:562:PRO:HG2	1:F:570:PHE:CD2	2.37	0.60
1:C:367:TYR:OH	1:C:466:LEU:O	2.15	0.60
1:D:887:LEU:HD22	1:D:895:LEU:HD11	1.81	0.60
1:G:562:PRO:HG2	1:G:570:PHE:CD2	2.37	0.60
1:G:751:GLN:OE1	1:G:811:VAL:CB	2.48	0.60
1:A:802:ILE:HD11	1:A:820:LYS:HD3	1.82	0.60
1:C:311:LYS:HD3	1:C:316:LEU:HD21	1.84	0.60
1:D:311:LYS:HD3	1:D:316:LEU:HD21	1.84	0.60
1:D:858:ILE:CD1	1:D:895:LEU:HD23	2.30	0.60
1:F:137:LEU:HD13	1:F:150:LYS:HG3	1.82	0.60
1:G:137:LEU:HD13	1:G:150:LYS:HG3	1.82	0.60
1:G:852:HIS:HA	1:G:855:ILE:HG13	1.83	0.60
1:A:759:ASN:ND2	1:A:931:THR:OG1	2.34	0.60
1:G:311:LYS:HD3	1:G:316:LEU:HD21	1.84	0.59
1:G:858:ILE:CD1	1:G:895:LEU:HD23	2.30	0.59
1:B:562:PRO:HG2	1:B:570:PHE:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:OD2	1:D:224:ASP:N	2.25	0.59
1:D:704:THR:OG1	1:D:705:GLU:N	2.33	0.59
1:E:758:ARG:HD3	1:E:928:ASP:HA	1.83	0.59
1:A:562:PRO:HG2	1:A:570:PHE:CD2	2.37	0.59
1:E:580:SER:HB3	1:E:590:LYS:HD2	1.85	0.59
1:D:562:PRO:HG2	1:D:570:PHE:CD2	2.37	0.59
1:F:852:HIS:HA	1:F:855:ILE:HG13	1.83	0.59
1:E:311:LYS:HD3	1:E:316:LEU:HD21	1.84	0.59
1:A:311:LYS:HD3	1:A:316:LEU:HD21	1.83	0.59
1:B:858:ILE:CD1	1:B:895:LEU:HD23	2.30	0.59
1:C:562:PRO:HG2	1:C:570:PHE:CD2	2.37	0.59
1:F:751:GLN:OE1	1:F:811:VAL:CB	2.48	0.59
1:B:311:LYS:HD3	1:B:316:LEU:HD21	1.84	0.59
1:C:431:ARG:HB2	1:D:291:GLU:OE1	2.02	0.59
1:F:704:THR:OG1	1:F:705:GLU:N	2.33	0.58
1:B:751:GLN:OE1	1:B:811:VAL:CB	2.48	0.58
1:D:580:SER:HB3	1:D:590:LYS:HD2	1.85	0.58
1:C:580:SER:HB3	1:C:590:LYS:HD2	1.85	0.58
1:G:259:GLN:OE1	1:A:273:LEU:HD21	2.03	0.58
1:F:764:ARG:NH1	1:F:897:LYS:C	2.62	0.58
1:G:242:ASN:OD1	1:G:242:ASN:O	2.22	0.58
1:G:570:PHE:HB2	1:G:573:MET:CG	2.33	0.58
1:A:242:ASN:OD1	1:A:242:ASN:O	2.22	0.58
1:C:206:ARG:HA	1:C:206:ARG:HE	1.68	0.58
1:F:242:ASN:O	1:F:242:ASN:OD1	2.22	0.58
1:A:580:SER:HB3	1:A:590:LYS:HD2	1.85	0.58
1:B:242:ASN:OD1	1:B:242:ASN:O	2.22	0.58
1:B:570:PHE:HB2	1:B:573:MET:CG	2.33	0.58
1:B:580:SER:HB3	1:B:590:LYS:HD2	1.85	0.58
1:G:530:GLN:NE2	1:A:525:ARG:HD2	2.18	0.58
1:E:206:ARG:HA	1:E:206:ARG:HE	1.68	0.58
1:A:570:PHE:HB2	1:A:573:MET:CG	2.33	0.58
1:E:242:ASN:OD1	1:E:242:ASN:O	2.22	0.58
1:F:315:GLN:HE21	1:E:439:HIS:HA	1.65	0.58
1:F:580:SER:HB3	1:F:590:LYS:HD2	1.85	0.58
1:E:764:ARG:O	1:E:863:CYS:N	2.22	0.58
1:D:206:ARG:HA	1:D:206:ARG:HE	1.68	0.58
1:F:570:PHE:HB2	1:F:573:MET:CG	2.34	0.58
1:F:262:ARG:HD2	1:G:277:GLU:OE1	2.04	0.57
1:A:720:VAL:HG22	1:A:844:LEU:HD22	1.86	0.57
1:D:570:PHE:HB2	1:D:573:MET:CG	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:ASP:O	1:G:339:ILE:CG1	2.51	0.57
1:G:580:SER:HB3	1:G:590:LYS:HD2	1.85	0.57
1:E:720:VAL:HG22	1:E:844:LEU:HD22	1.86	0.57
1:B:255:ARG:HG2	1:A:430:TYR:CE1	2.38	0.57
1:C:751:GLN:OE1	1:C:811:VAL:CB	2.48	0.57
1:D:530:GLN:HE22	1:E:525:ARG:HD2	1.70	0.57
1:F:756:LEU:HB3	1:F:927:TYR:CE1	2.38	0.57
1:B:720:VAL:HG22	1:B:844:LEU:HD22	1.86	0.57
1:C:704:THR:OG1	1:C:705:GLU:N	2.33	0.57
1:G:381:GLN:NE2	1:A:299:LEU:O	2.37	0.57
1:G:720:VAL:HG22	1:G:844:LEU:HD22	1.86	0.57
1:E:570:PHE:HB2	1:E:573:MET:CG	2.33	0.57
1:B:451:PHE:HE2	1:B:507:SER:O	1.88	0.57
1:C:242:ASN:O	1:C:242:ASN:OD1	2.22	0.57
1:C:570:PHE:HB2	1:C:573:MET:CG	2.33	0.57
1:A:354:GLU:HB3	1:A:413:VAL:HG11	1.87	0.57
1:C:720:VAL:HG22	1:C:844:LEU:HD22	1.86	0.57
1:F:206:ARG:HA	1:F:206:ARG:HE	1.68	0.57
1:D:570:PHE:HB2	1:D:573:MET:HG3	1.87	0.57
1:A:206:ARG:HA	1:A:206:ARG:HE	1.68	0.57
1:A:918:ASN:OD1	1:A:919:SER:N	2.38	0.57
1:C:451:PHE:HE2	1:C:507:SER:O	1.88	0.57
1:D:242:ASN:OD1	1:D:242:ASN:O	2.22	0.57
1:F:570:PHE:HB2	1:F:573:MET:HG3	1.87	0.57
1:G:206:ARG:HA	1:G:206:ARG:HE	1.68	0.57
1:G:354:GLU:HB3	1:G:413:VAL:HG11	1.87	0.57
1:G:570:PHE:HB2	1:G:573:MET:HG3	1.87	0.57
1:G:918:ASN:OD1	1:G:919:SER:N	2.38	0.57
1:B:354:GLU:HB3	1:B:413:VAL:HG11	1.87	0.56
1:B:458:ARG:O	1:B:460:PHE:N	2.38	0.56
1:C:338:ASP:O	1:C:339:ILE:CG1	2.53	0.56
1:F:764:ARG:CZ	1:F:897:LYS:O	2.53	0.56
1:B:338:ASP:O	1:B:339:ILE:CG1	2.53	0.56
1:B:918:ASN:OD1	1:B:919:SER:N	2.38	0.56
1:C:503:VAL:O	1:C:507:SER:CB	2.53	0.56
1:F:262:ARG:HG3	1:F:290:VAL:CG1	2.36	0.56
1:F:458:ARG:O	1:F:460:PHE:N	2.38	0.56
1:F:918:ASN:OD1	1:F:919:SER:N	2.38	0.56
1:E:338:ASP:N	1:E:338:ASP:OD1	2.39	0.56
1:E:503:VAL:O	1:E:507:SER:CB	2.53	0.56
1:C:570:PHE:HB2	1:C:573:MET:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:PHE:CE2	1:E:268:ASN:HB2	2.39	0.56
1:D:338:ASP:O	1:D:339:ILE:CG1	2.53	0.56
1:D:338:ASP:OD1	1:D:338:ASP:N	2.39	0.56
1:D:436:TYR:CD2	1:E:255:ARG:CD	2.89	0.56
1:D:503:VAL:O	1:D:507:SER:CB	2.53	0.56
1:F:720:VAL:HG22	1:F:844:LEU:HD22	1.86	0.56
1:G:262:ARG:HG3	1:G:290:VAL:CG1	2.36	0.56
1:G:451:PHE:HE2	1:G:507:SER:O	1.88	0.56
1:E:570:PHE:HB2	1:E:573:MET:HG3	1.87	0.56
1:B:206:ARG:HA	1:B:206:ARG:HE	1.68	0.56
1:D:458:ARG:O	1:D:460:PHE:N	2.38	0.56
1:D:720:VAL:HG22	1:D:844:LEU:HD22	1.86	0.56
1:F:451:PHE:CE2	1:F:507:SER:O	2.57	0.56
1:F:503:VAL:O	1:F:507:SER:CB	2.53	0.56
1:E:458:ARG:O	1:E:460:PHE:N	2.38	0.56
1:F:116:PRO:HG3	1:G:166:LEU:HD13	1.85	0.56
1:E:758:ARG:CG	1:E:927:TYR:O	2.52	0.56
1:D:758:ARG:HD3	1:D:928:ASP:HA	1.86	0.56
1:F:116:PRO:HB3	1:G:166:LEU:HB3	1.88	0.56
1:F:431:ARG:HH12	1:A:277:GLU:CD	2.13	0.56
1:F:448:LYS:HE3	1:F:536:VAL:HG11	1.88	0.56
1:G:338:ASP:O	1:G:339:ILE:HG12	2.06	0.56
1:G:458:ARG:O	1:G:460:PHE:N	2.38	0.56
1:E:338:ASP:O	1:E:339:ILE:CG1	2.53	0.56
1:A:458:ARG:O	1:A:460:PHE:N	2.38	0.56
1:G:448:LYS:HE3	1:G:536:VAL:HG11	1.88	0.56
1:A:503:VAL:O	1:A:507:SER:CB	2.53	0.56
1:A:570:PHE:HB2	1:A:573:MET:HG3	1.87	0.56
1:C:354:GLU:HB3	1:C:413:VAL:HG11	1.87	0.56
1:D:262:ARG:HG3	1:D:290:VAL:CG1	2.36	0.56
1:D:431:ARG:NH1	1:F:282:ARG:CZ	2.69	0.56
1:D:436:TYR:CD2	1:E:255:ARG:HD3	2.41	0.56
1:F:338:ASP:O	1:F:339:ILE:CG1	2.53	0.56
1:F:357:ASN:CG	1:F:728:ARG:HB3	2.30	0.56
1:G:503:VAL:O	1:G:507:SER:CB	2.53	0.56
1:A:262:ARG:HG3	1:A:290:VAL:CG1	2.36	0.56
1:A:885:LYS:HZ2	1:A:888:SER:HA	1.70	0.56
1:D:354:GLU:HB3	1:D:413:VAL:HG11	1.87	0.56
1:F:289:MET:HE2	1:E:256:LEU:HD23	1.88	0.56
1:F:858:ILE:CD1	1:F:895:LEU:HD23	2.30	0.56
1:E:539:MET:HB3	1:E:541:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:PHE:HB2	1:B:573:MET:HG3	1.87	0.56
1:D:448:LYS:HE3	1:D:536:VAL:HG11	1.88	0.56
1:C:458:ARG:O	1:C:460:PHE:N	2.38	0.55
1:B:503:VAL:O	1:B:507:SER:CB	2.53	0.55
1:E:451:PHE:HE2	1:E:507:SER:O	1.88	0.55
1:B:431:ARG:HB2	1:C:291:GLU:OE1	2.06	0.55
1:B:448:LYS:HE3	1:B:536:VAL:HG11	1.88	0.55
1:C:448:LYS:HE3	1:C:536:VAL:HG11	1.88	0.55
1:C:918:ASN:OD1	1:C:919:SER:N	2.38	0.55
1:D:436:TYR:CE2	1:E:255:ARG:CG	2.84	0.55
1:F:770:ASN:OD1	1:F:773:LYS:HB2	2.07	0.55
1:E:354:GLU:HB3	1:E:413:VAL:HG11	1.87	0.55
1:E:770:ASN:OD1	1:E:773:LYS:HB2	2.07	0.55
1:A:448:LYS:HE3	1:A:536:VAL:HG11	1.88	0.55
1:B:349:GLY:HA2	1:B:368:VAL:HG21	1.89	0.55
1:C:349:GLY:HA2	1:C:368:VAL:HG21	1.89	0.55
1:C:770:ASN:OD1	1:C:773:LYS:HB2	2.07	0.55
1:D:131:LYS:HE2	1:E:190:SER:C	2.32	0.55
1:D:349:GLY:HA2	1:D:368:VAL:HG21	1.89	0.55
1:F:91:LYS:O	1:F:94:ASN:N	2.36	0.55
1:A:551:ALA:HB3	1:A:624:ASN:OD1	2.07	0.55
1:B:539:MET:HB3	1:B:541:VAL:HG23	1.88	0.55
1:B:567:ILE:CG2	1:B:569:VAL:HG23	2.37	0.55
1:F:338:ASP:OD1	1:F:338:ASP:N	2.38	0.55
1:G:770:ASN:OD1	1:G:773:LYS:HB2	2.07	0.55
1:E:262:ARG:HG3	1:E:290:VAL:CG1	2.36	0.55
1:D:91:LYS:O	1:D:94:ASN:N	2.36	0.55
1:F:354:GLU:HB3	1:F:413:VAL:HG11	1.87	0.55
1:E:349:GLY:HA2	1:E:368:VAL:HG21	1.89	0.55
1:B:757:TYR:HE1	1:A:581:ARG:NH2	2.04	0.55
1:C:262:ARG:HG3	1:C:290:VAL:CG1	2.36	0.55
1:D:539:MET:HB3	1:D:541:VAL:HG23	1.88	0.55
1:D:885:LYS:HZ2	1:D:888:SER:HA	1.71	0.55
1:E:448:LYS:HE3	1:E:536:VAL:HG11	1.88	0.55
1:B:330:VAL:HB	1:B:344:VAL:HG23	1.89	0.55
1:C:551:ALA:HB3	1:C:624:ASN:OD1	2.07	0.55
1:D:820:LYS:O	1:D:824:ILE:HD12	2.07	0.55
1:E:330:VAL:HB	1:E:344:VAL:HG23	1.89	0.55
1:E:918:ASN:OD1	1:E:919:SER:N	2.38	0.55
1:A:349:GLY:HA2	1:A:368:VAL:HG21	1.89	0.55
1:A:539:MET:HB3	1:A:541:VAL:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:LYS:O	1:A:824:ILE:HD12	2.07	0.55
1:B:262:ARG:HG3	1:B:290:VAL:CG1	2.36	0.55
1:C:539:MET:HB3	1:C:541:VAL:HG23	1.88	0.55
1:D:272:THR:O	1:D:276:GLN:HG2	2.07	0.55
1:D:551:ALA:HB3	1:D:624:ASN:OD1	2.07	0.55
1:D:918:ASN:OD1	1:D:919:SER:N	2.38	0.55
1:F:192:GLY:HA2	1:E:131:LYS:HD3	1.88	0.55
1:F:551:ALA:HB3	1:F:624:ASN:OD1	2.07	0.55
1:A:330:VAL:HB	1:A:344:VAL:HG23	1.89	0.55
1:A:770:ASN:OD1	1:A:773:LYS:HB2	2.07	0.55
1:C:288:TYR:O	1:C:291:GLU:HB2	2.08	0.54
1:D:355:GLY:O	1:D:487:SER:OG	2.24	0.54
1:D:567:ILE:CG2	1:D:569:VAL:HG23	2.37	0.54
1:G:436:TYR:CZ	1:A:255:ARG:HG3	2.42	0.54
1:G:567:ILE:CG2	1:G:569:VAL:HG23	2.37	0.54
1:G:820:LYS:O	1:G:824:ILE:HD12	2.07	0.54
1:B:338:ASP:N	1:B:338:ASP:OD1	2.39	0.54
1:C:858:ILE:CD1	1:C:895:LEU:HD23	2.30	0.54
1:D:451:PHE:HE2	1:D:507:SER:O	1.88	0.54
1:D:770:ASN:OD1	1:D:773:LYS:HB2	2.07	0.54
1:F:163:GLY:HA2	1:F:194:GLN:OE1	2.08	0.54
1:G:539:MET:HB3	1:G:541:VAL:HG23	1.88	0.54
1:B:770:ASN:OD1	1:B:773:LYS:HB2	2.07	0.54
1:C:272:THR:O	1:C:276:GLN:HG2	2.07	0.54
1:F:539:MET:HB3	1:F:541:VAL:HG23	1.88	0.54
1:E:288:TYR:O	1:E:291:GLU:HB2	2.08	0.54
1:E:572:GLY:HA2	1:E:745:LEU:HD22	1.89	0.54
1:A:163:GLY:HA2	1:A:194:GLN:OE1	2.07	0.54
1:A:858:ILE:CD1	1:A:895:LEU:HD23	2.30	0.54
1:B:820:LYS:O	1:B:824:ILE:HD12	2.07	0.54
1:E:272:THR:O	1:E:276:GLN:HG2	2.07	0.54
1:E:567:ILE:CG2	1:E:569:VAL:HG23	2.37	0.54
1:E:820:LYS:O	1:E:824:ILE:HD12	2.07	0.54
1:A:567:ILE:CG2	1:A:569:VAL:HG23	2.37	0.54
1:B:163:GLY:HA2	1:B:194:GLN:OE1	2.07	0.54
1:C:330:VAL:HB	1:C:344:VAL:HG23	1.89	0.54
1:C:890:GLU:OE2	1:C:890:GLU:O	2.26	0.54
1:D:242:ASN:OD1	1:D:242:ASN:C	2.51	0.54
1:F:242:ASN:OD1	1:F:242:ASN:C	2.51	0.54
1:G:163:GLY:HA2	1:G:194:GLN:OE1	2.07	0.54
1:G:330:VAL:HB	1:G:344:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:GLY:HA2	1:G:368:VAL:HG21	1.89	0.54
1:G:551:ALA:HB3	1:G:624:ASN:OD1	2.07	0.54
1:B:131:LYS:HG3	1:C:183:LEU:HD13	1.89	0.54
1:B:288:TYR:O	1:B:291:GLU:HB2	2.08	0.54
1:D:443:MET:O	1:D:443:MET:HG2	2.08	0.54
1:F:820:LYS:O	1:F:824:ILE:HD12	2.07	0.54
1:F:885:LYS:HZ2	1:F:888:SER:HA	1.73	0.54
1:F:890:GLU:OE2	1:F:890:GLU:O	2.26	0.54
1:E:551:ALA:HB3	1:E:624:ASN:OD1	2.07	0.54
1:C:567:ILE:CG2	1:C:569:VAL:HG23	2.37	0.54
1:C:572:GLY:HA2	1:C:745:LEU:HD22	1.89	0.54
1:D:890:GLU:O	1:D:890:GLU:OE2	2.26	0.54
1:F:288:TYR:O	1:F:291:GLU:HB2	2.08	0.54
1:F:567:ILE:CG2	1:F:569:VAL:HG23	2.37	0.54
1:G:288:TYR:O	1:G:291:GLU:HB2	2.08	0.54
1:E:311:LYS:HD3	1:E:316:LEU:CD2	2.38	0.54
1:D:288:TYR:O	1:D:291:GLU:HB2	2.08	0.54
1:F:349:GLY:HA2	1:F:368:VAL:HG21	1.89	0.54
1:F:572:GLY:HA2	1:F:745:LEU:HD22	1.89	0.54
1:G:272:THR:O	1:G:276:GLN:HG2	2.07	0.54
1:G:500:MET:HG3	1:G:734:ILE:HG21	1.90	0.54
1:G:885:LYS:HZ2	1:G:888:SER:HA	1.73	0.54
1:B:272:THR:O	1:B:276:GLN:HG2	2.07	0.54
1:B:890:GLU:O	1:B:890:GLU:OE2	2.26	0.54
1:C:820:LYS:O	1:C:824:ILE:HD12	2.07	0.54
1:F:330:VAL:HB	1:F:344:VAL:HG23	1.89	0.54
1:E:262:ARG:HG3	1:E:290:VAL:HG11	1.90	0.54
1:A:242:ASN:OD1	1:A:242:ASN:C	2.51	0.54
1:A:288:TYR:O	1:A:291:GLU:HB2	2.08	0.54
1:B:131:LYS:HG3	1:C:183:LEU:CD1	2.38	0.53
1:D:262:ARG:HG3	1:D:290:VAL:HG11	1.90	0.53
1:F:150:LYS:O	1:F:153:TRP:N	2.41	0.53
1:F:272:THR:O	1:F:276:GLN:HG2	2.07	0.53
1:G:890:GLU:O	1:G:890:GLU:OE2	2.26	0.53
1:B:500:MET:HG3	1:B:734:ILE:HG21	1.90	0.53
1:D:500:MET:HG3	1:D:734:ILE:HG21	1.90	0.53
1:F:826:GLU:HA	1:F:829:LYS:HD2	1.91	0.53
1:G:370:GLU:OE2	1:G:370:GLU:O	2.27	0.53
1:A:272:THR:O	1:A:276:GLN:HG2	2.07	0.53
1:A:370:GLU:O	1:A:370:GLU:OE2	2.27	0.53
1:A:500:MET:HG3	1:A:734:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASN:OD1	1:C:242:ASN:C	2.51	0.53
1:C:370:GLU:O	1:C:370:GLU:OE2	2.27	0.53
1:D:116:PRO:HB3	1:E:166:LEU:HB3	1.90	0.53
1:D:163:GLY:HA2	1:D:194:GLN:OE1	2.07	0.53
1:D:259:GLN:HG3	1:E:269:TYR:HE2	1.72	0.53
1:G:533:SER:HB3	1:A:458:ARG:HH12	1.72	0.53
1:E:163:GLY:HA2	1:E:194:GLN:OE1	2.07	0.53
1:F:315:GLN:NE2	1:E:439:HIS:CA	2.71	0.53
1:G:363:ASP:O	1:G:366:MET:HB3	2.09	0.53
1:B:242:ASN:OD1	1:B:242:ASN:C	2.51	0.53
1:C:163:GLY:HA2	1:C:194:GLN:OE1	2.07	0.53
1:C:262:ARG:HG3	1:C:290:VAL:HG11	1.90	0.53
1:C:500:MET:HG3	1:C:734:ILE:HG21	1.90	0.53
1:D:330:VAL:HB	1:D:344:VAL:HG23	1.89	0.53
1:D:885:LYS:NZ	1:D:888:SER:HA	2.24	0.53
1:F:500:MET:HG3	1:F:734:ILE:HG21	1.90	0.53
1:G:116:PRO:HB3	1:A:166:LEU:HB3	1.91	0.53
1:G:242:ASN:OD1	1:G:242:ASN:C	2.51	0.53
1:G:826:GLU:HA	1:G:829:LYS:HD2	1.91	0.53
1:G:885:LYS:NZ	1:G:888:SER:HA	2.24	0.53
1:E:355:GLY:O	1:E:487:SER:OG	2.24	0.53
1:E:890:GLU:O	1:E:890:GLU:OE2	2.26	0.53
1:A:363:ASP:O	1:A:366:MET:HB3	2.09	0.53
1:A:826:GLU:HA	1:A:829:LYS:HD2	1.91	0.53
1:B:311:LYS:HD3	1:B:316:LEU:CD2	2.38	0.53
1:B:370:GLU:OE2	1:B:370:GLU:O	2.27	0.53
1:C:311:LYS:HD3	1:C:316:LEU:CD2	2.38	0.53
1:F:262:ARG:HG3	1:F:290:VAL:HG11	1.90	0.53
1:F:363:ASP:O	1:F:366:MET:HB3	2.09	0.53
1:F:443:MET:O	1:F:443:MET:HG2	2.08	0.53
1:G:262:ARG:HG3	1:G:290:VAL:HG11	1.90	0.53
1:A:311:LYS:HD3	1:A:316:LEU:CD2	2.38	0.53
1:A:890:GLU:O	1:A:890:GLU:OE2	2.26	0.53
1:B:572:GLY:HA2	1:B:745:LEU:HD22	1.89	0.53
1:D:572:GLY:HA2	1:D:745:LEU:HD22	1.89	0.53
1:G:727:ILE:O	1:G:727:ILE:HG13	2.09	0.53
1:E:370:GLU:O	1:E:370:GLU:OE2	2.27	0.53
1:E:826:GLU:HA	1:E:829:LYS:HD2	1.91	0.53
1:G:338:ASP:C	1:G:339:ILE:HG12	2.33	0.53
1:E:567:ILE:HG22	1:E:569:VAL:H	1.74	0.53
1:B:826:GLU:HA	1:B:829:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:LYS:NZ	1:B:888:SER:HA	2.24	0.53
1:C:720:VAL:HG13	1:C:844:LEU:HD13	1.91	0.53
1:C:727:ILE:HG13	1:C:727:ILE:O	2.08	0.53
1:F:370:GLU:O	1:F:370:GLU:OE2	2.27	0.53
1:F:885:LYS:NZ	1:F:888:SER:HA	2.24	0.53
1:E:443:MET:HG2	1:E:443:MET:O	2.08	0.53
1:B:150:LYS:O	1:B:153:TRP:N	2.41	0.53
1:D:311:LYS:HD3	1:D:316:LEU:CD2	2.38	0.53
1:G:443:MET:O	1:G:443:MET:HG2	2.08	0.53
1:E:242:ASN:OD1	1:E:242:ASN:C	2.51	0.53
1:A:262:ARG:HG3	1:A:290:VAL:HG11	1.90	0.53
1:B:91:LYS:O	1:B:94:ASN:N	2.37	0.52
1:G:572:GLY:HA2	1:G:745:LEU:HD22	1.89	0.52
1:E:858:ILE:CD1	1:E:895:LEU:HD23	2.30	0.52
1:E:885:LYS:NZ	1:E:888:SER:HA	2.24	0.52
1:A:206:ARG:HA	1:A:206:ARG:NE	2.24	0.52
1:A:572:GLY:HA2	1:A:745:LEU:HD22	1.89	0.52
1:B:268:ASN:HA	1:A:228:ASP:OD2	2.09	0.52
1:B:720:VAL:HG13	1:B:844:LEU:HD13	1.91	0.52
1:C:443:MET:HG2	1:C:443:MET:O	2.08	0.52
1:D:370:GLU:OE2	1:D:370:GLU:O	2.27	0.52
1:F:311:LYS:HD3	1:F:316:LEU:CD2	2.38	0.52
1:F:431:ARG:NH1	1:A:277:GLU:OE2	2.42	0.52
1:G:91:LYS:O	1:G:94:ASN:N	2.37	0.52
1:G:311:LYS:HD3	1:G:316:LEU:CD2	2.38	0.52
1:E:206:ARG:HA	1:E:206:ARG:NE	2.24	0.52
1:E:261:ILE:HD13	1:E:298:LEU:HD12	1.91	0.52
1:E:363:ASP:O	1:E:366:MET:HB3	2.09	0.52
1:A:716:TRP:O	1:A:720:VAL:HG23	2.10	0.52
1:B:206:ARG:HA	1:B:206:ARG:NE	2.24	0.52
1:B:551:ALA:HB3	1:B:624:ASN:OD1	2.07	0.52
1:C:206:ARG:HA	1:C:206:ARG:NE	2.24	0.52
1:C:567:ILE:HG22	1:C:569:VAL:H	1.74	0.52
1:F:206:ARG:HA	1:F:206:ARG:NE	2.24	0.52
1:E:500:MET:HG3	1:E:734:ILE:HG21	1.90	0.52
1:E:720:VAL:HG13	1:E:844:LEU:HD13	1.91	0.52
1:B:255:ARG:HG2	1:A:430:TYR:CZ	2.45	0.52
1:B:262:ARG:HG3	1:B:290:VAL:HG11	1.90	0.52
1:B:363:ASP:O	1:B:366:MET:HB3	2.09	0.52
1:D:116:PRO:HG3	1:E:166:LEU:HD13	1.92	0.52
1:D:716:TRP:O	1:D:720:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:439:HIS:HB3	1:A:312:THR:HG21	1.90	0.52
1:B:716:TRP:O	1:B:720:VAL:HG23	2.10	0.52
1:C:150:LYS:O	1:C:153:TRP:N	2.41	0.52
1:D:206:ARG:HA	1:D:206:ARG:NE	2.24	0.52
1:D:728:ARG:HG3	1:D:728:ARG:NH1	2.21	0.52
1:F:728:ARG:HG3	1:F:728:ARG:NH1	2.22	0.52
1:E:91:LYS:O	1:E:94:ASN:N	2.37	0.52
1:F:720:VAL:HG13	1:F:844:LEU:HD13	1.91	0.52
1:G:261:ILE:HD13	1:G:298:LEU:HD12	1.91	0.52
1:E:214:LYS:O	1:E:245:LYS:HD3	2.10	0.52
1:E:462:THR:HG22	1:E:465:TYR:CE1	2.45	0.52
1:E:885:LYS:HZ2	1:E:888:SER:HA	1.74	0.52
1:A:76:GLY:HA3	1:A:82:LYS:HD3	1.92	0.52
1:A:443:MET:O	1:A:443:MET:HG2	2.08	0.52
1:B:261:ILE:HD13	1:B:298:LEU:HD12	1.91	0.52
1:B:567:ILE:HG22	1:B:569:VAL:H	1.74	0.52
1:C:709:ALA:O	1:C:713:VAL:HG23	2.10	0.52
1:C:885:LYS:NZ	1:C:888:SER:HA	2.24	0.52
1:D:214:LYS:O	1:D:245:LYS:HD3	2.10	0.52
1:D:709:ALA:O	1:D:713:VAL:HG23	2.10	0.52
1:F:357:ASN:ND2	1:F:728:ARG:HB3	2.24	0.52
1:A:261:ILE:HD13	1:A:298:LEU:HD12	1.91	0.52
1:B:76:GLY:HA3	1:B:82:LYS:HD3	1.92	0.52
1:B:338:ASP:C	1:B:339:ILE:HG12	2.35	0.52
1:D:253:ASP:OD2	1:D:255:ARG:HB2	2.10	0.52
1:G:567:ILE:HG22	1:G:569:VAL:H	1.74	0.52
1:G:716:TRP:O	1:G:720:VAL:HG23	2.10	0.52
1:A:720:VAL:HG13	1:A:844:LEU:HD13	1.91	0.52
1:B:443:MET:HG2	1:B:443:MET:O	2.08	0.52
1:C:153:TRP:HE3	1:C:206:ARG:HB3	1.75	0.52
1:C:338:ASP:C	1:C:339:ILE:HG12	2.35	0.52
1:C:462:THR:HG22	1:C:465:TYR:CE1	2.45	0.52
1:D:338:ASP:C	1:D:339:ILE:HG12	2.35	0.52
1:D:826:GLU:HA	1:D:829:LYS:HD2	1.91	0.52
1:G:76:GLY:HA3	1:G:82:LYS:HD3	1.92	0.52
1:A:91:LYS:O	1:A:94:ASN:N	2.37	0.52
1:A:709:ALA:O	1:A:713:VAL:HG23	2.10	0.52
1:A:845:LEU:O	1:A:851:LEU:HD12	2.10	0.52
1:D:462:THR:HG22	1:D:465:TYR:CE1	2.45	0.52
1:G:227:PHE:CE2	1:A:268:ASN:HB2	2.45	0.52
1:E:716:TRP:O	1:E:720:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:758:ARG:HD3	1:E:928:ASP:O	2.09	0.52
1:E:845:LEU:O	1:E:851:LEU:HD12	2.10	0.52
1:A:253:ASP:OD2	1:A:255:ARG:HB2	2.10	0.52
1:B:253:ASP:OD2	1:B:255:ARG:HB2	2.10	0.51
1:B:462:THR:HG22	1:B:465:TYR:CE1	2.45	0.51
1:B:717:LEU:O	1:B:721:ASN:ND2	2.30	0.51
1:C:214:LYS:O	1:C:245:LYS:HD3	2.10	0.51
1:C:277:GLU:OE2	1:C:282:ARG:HD2	2.11	0.51
1:C:363:ASP:O	1:C:366:MET:HB3	2.09	0.51
1:C:826:GLU:HA	1:C:829:LYS:HD2	1.91	0.51
1:D:261:ILE:HD13	1:D:298:LEU:HD12	1.91	0.51
1:D:363:ASP:O	1:D:366:MET:HB3	2.09	0.51
1:D:431:ARG:CZ	1:F:282:ARG:NH2	2.73	0.51
1:F:567:ILE:HG22	1:F:569:VAL:H	1.74	0.51
1:G:709:ALA:O	1:G:713:VAL:HG23	2.10	0.51
1:G:720:VAL:HG13	1:G:844:LEU:HD13	1.91	0.51
1:E:709:ALA:O	1:E:713:VAL:HG23	2.10	0.51
1:A:153:TRP:HE3	1:A:206:ARG:HB3	1.75	0.51
1:A:462:THR:O	1:A:465:TYR:HB2	2.10	0.51
1:A:567:ILE:HG22	1:A:569:VAL:H	1.74	0.51
1:B:225:THR:HG21	1:C:238:ARG:CZ	2.41	0.51
1:B:462:THR:O	1:B:465:TYR:HB2	2.10	0.51
1:C:716:TRP:O	1:C:720:VAL:HG23	2.10	0.51
1:F:253:ASP:OD2	1:F:255:ARG:HB2	2.10	0.51
1:F:462:THR:O	1:F:465:TYR:HB2	2.11	0.51
1:F:716:TRP:O	1:F:720:VAL:HG23	2.10	0.51
1:F:722:GLU:HB2	1:F:723:ILE:HG23	1.93	0.51
1:F:845:LEU:O	1:F:851:LEU:HD12	2.10	0.51
1:E:338:ASP:O	1:E:339:ILE:HG12	2.10	0.51
1:B:153:TRP:HE3	1:B:206:ARG:HB3	1.75	0.51
1:B:277:GLU:OE2	1:B:282:ARG:HD2	2.10	0.51
1:C:195:ASP:OD1	1:C:197:SER:HB2	2.11	0.51
1:C:462:THR:O	1:C:465:TYR:HB2	2.11	0.51
1:G:277:GLU:OE2	1:G:282:ARG:HD2	2.11	0.51
1:G:462:THR:O	1:G:465:TYR:HB2	2.11	0.51
1:A:277:GLU:OE2	1:A:282:ARG:HD2	2.11	0.51
1:A:885:LYS:NZ	1:A:888:SER:HA	2.24	0.51
1:C:253:ASP:OD2	1:C:255:ARG:HB2	2.10	0.51
1:C:261:ILE:HD13	1:C:298:LEU:HD12	1.91	0.51
1:D:720:VAL:HG13	1:D:844:LEU:HD13	1.91	0.51
1:F:261:ILE:HD13	1:F:298:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:ASP:OD1	1:E:197:SER:HB2	2.11	0.51
1:E:253:ASP:OD2	1:E:255:ARG:HB2	2.10	0.51
1:D:195:ASP:OD1	1:D:197:SER:HB2	2.11	0.51
1:D:338:ASP:O	1:D:339:ILE:HG12	2.10	0.51
1:D:845:LEU:O	1:D:851:LEU:HD12	2.10	0.51
1:F:214:LYS:O	1:F:245:LYS:HD3	2.10	0.51
1:G:206:ARG:HA	1:G:206:ARG:NE	2.24	0.51
1:E:338:ASP:C	1:E:339:ILE:HG12	2.35	0.51
1:C:845:LEU:O	1:C:851:LEU:HD12	2.10	0.51
1:D:462:THR:O	1:D:465:TYR:HB2	2.10	0.51
1:F:462:THR:HG22	1:F:465:TYR:CE1	2.45	0.51
1:G:153:TRP:HE3	1:G:206:ARG:HB3	1.75	0.51
1:G:462:THR:HG22	1:G:465:TYR:CE1	2.45	0.51
1:B:845:LEU:O	1:B:851:LEU:HD12	2.10	0.51
1:D:153:TRP:HE3	1:D:206:ARG:HB3	1.75	0.51
1:D:266:TYR:CE1	1:E:276:GLN:HG3	2.46	0.51
1:D:567:ILE:HG22	1:D:569:VAL:H	1.74	0.51
1:E:277:GLU:OE2	1:E:282:ARG:HD2	2.11	0.51
1:A:722:GLU:HB2	1:A:723:ILE:HG23	1.93	0.51
1:A:788:VAL:O	1:A:791:SER:OG	2.24	0.51
1:B:214:LYS:O	1:B:245:LYS:HD3	2.10	0.51
1:C:76:GLY:HA3	1:C:82:LYS:HD3	1.92	0.51
1:F:161:GLN:HG3	1:G:177:PHE:HB3	1.93	0.51
1:F:277:GLU:OE2	1:F:282:ARG:HD2	2.11	0.51
1:G:195:ASP:OD1	1:G:197:SER:HB2	2.11	0.51
1:G:788:VAL:O	1:G:791:SER:OG	2.24	0.51
1:E:462:THR:O	1:E:465:TYR:HB2	2.10	0.51
1:E:758:ARG:CD	1:E:928:ASP:O	2.59	0.51
1:A:37:LEU:HD21	1:A:310:LEU:H	1.76	0.51
1:A:462:THR:HG22	1:A:465:TYR:CE1	2.45	0.51
1:C:37:LEU:HD21	1:C:310:LEU:H	1.76	0.51
1:C:717:LEU:O	1:C:721:ASN:ND2	2.30	0.51
1:D:76:GLY:HA3	1:D:82:LYS:HD3	1.92	0.51
1:F:37:LEU:HD21	1:F:310:LEU:H	1.76	0.51
1:F:255:ARG:HG2	1:E:430:TYR:CZ	2.46	0.51
1:F:338:ASP:C	1:F:339:ILE:HG12	2.35	0.51
1:F:788:VAL:O	1:F:791:SER:OG	2.24	0.51
1:B:195:ASP:OD1	1:B:197:SER:HB2	2.11	0.51
1:B:709:ALA:O	1:B:713:VAL:HG23	2.10	0.51
1:D:858:ILE:HG22	1:D:918:ASN:HD22	1.76	0.51
1:F:76:GLY:HA3	1:F:82:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LYS:O	1:E:153:TRP:N	2.41	0.51
1:E:722:GLU:HB2	1:E:723:ILE:HG23	1.93	0.51
1:D:596:GLU:OE1	1:D:914:ILE:HG23	2.12	0.50
1:F:338:ASP:O	1:F:339:ILE:HG12	2.11	0.50
1:F:709:ALA:O	1:F:713:VAL:HG23	2.10	0.50
1:A:195:ASP:OD1	1:A:197:SER:HB2	2.11	0.50
1:A:596:GLU:OE1	1:A:914:ILE:HG23	2.12	0.50
1:B:858:ILE:HG22	1:B:918:ASN:HD22	1.76	0.50
1:C:756:LEU:HB3	1:C:927:TYR:CE1	2.46	0.50
1:G:214:LYS:O	1:G:245:LYS:HD3	2.10	0.50
1:G:845:LEU:O	1:G:851:LEU:HD12	2.10	0.50
1:B:173:LYS:HG2	1:B:176:TYR:CD1	2.47	0.50
1:F:153:TRP:HE3	1:F:206:ARG:HB3	1.75	0.50
1:F:195:ASP:OD1	1:F:197:SER:HB2	2.11	0.50
1:G:596:GLU:OE1	1:G:914:ILE:HG23	2.12	0.50
1:E:153:TRP:HE3	1:E:206:ARG:HB3	1.75	0.50
1:E:173:LYS:HG2	1:E:176:TYR:CD1	2.46	0.50
1:B:596:GLU:OE1	1:B:914:ILE:HG23	2.12	0.50
1:G:173:LYS:HG2	1:G:176:TYR:CD1	2.46	0.50
1:G:253:ASP:OD2	1:G:255:ARG:HB2	2.10	0.50
1:E:37:LEU:HD21	1:E:310:LEU:H	1.76	0.50
1:E:76:GLY:HA3	1:E:82:LYS:HD3	1.92	0.50
1:A:357:ASN:HB3	1:A:728:ARG:O	2.11	0.50
1:B:352:VAL:HG13	1:B:356:LEU:HD12	1.94	0.50
1:C:131:LYS:HG3	1:D:183:LEU:HD13	1.94	0.50
1:A:352:VAL:HG13	1:A:356:LEU:HD12	1.94	0.50
1:C:352:VAL:HG13	1:C:356:LEU:HD12	1.94	0.50
1:C:885:LYS:HZ2	1:C:888:SER:HA	1.77	0.50
1:D:277:GLU:OE2	1:D:282:ARG:HD2	2.11	0.50
1:F:276:GLN:HE22	1:E:274:LEU:HB3	1.72	0.50
1:E:858:ILE:HG22	1:E:918:ASN:HD22	1.76	0.50
1:A:173:LYS:HG2	1:A:176:TYR:CD1	2.46	0.50
1:A:214:LYS:O	1:A:245:LYS:HD3	2.10	0.50
1:C:596:GLU:OE1	1:C:914:ILE:HG23	2.12	0.50
1:C:722:GLU:HB2	1:C:723:ILE:HG23	1.93	0.50
1:D:37:LEU:HD21	1:D:310:LEU:H	1.76	0.50
1:F:858:ILE:HG22	1:F:918:ASN:HD22	1.76	0.50
1:C:338:ASP:O	1:C:339:ILE:HG12	2.11	0.50
1:G:37:LEU:HD21	1:G:310:LEU:H	1.76	0.50
1:G:352:VAL:HG13	1:G:356:LEU:HD12	1.94	0.50
1:A:150:LYS:O	1:A:153:TRP:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:O	1:B:339:ILE:HG12	2.11	0.50
1:B:728:ARG:HG3	1:B:728:ARG:NH1	2.25	0.50
1:C:173:LYS:HG2	1:C:176:TYR:CD1	2.46	0.50
1:G:756:LEU:HB3	1:G:927:TYR:CE1	2.47	0.50
1:A:889:ASP:O	1:A:893:ASP:N	2.41	0.50
1:D:756:LEU:HB3	1:D:927:TYR:CE1	2.47	0.49
1:G:858:ILE:HG22	1:G:918:ASN:HD22	1.76	0.49
1:E:758:ARG:HD3	1:E:928:ASP:C	2.37	0.49
1:D:173:LYS:HG2	1:D:176:TYR:CD1	2.46	0.49
1:F:596:GLU:OE1	1:F:914:ILE:HG23	2.12	0.49
1:B:172:TYR:HB2	1:A:118:HIS:O	2.12	0.49
1:D:567:ILE:HG22	1:D:569:VAL:HG23	1.94	0.49
1:F:131:LYS:HE2	1:G:190:SER:C	2.37	0.49
1:F:717:LEU:O	1:F:721:ASN:ND2	2.30	0.49
1:E:756:LEU:HB3	1:E:927:TYR:CZ	2.37	0.49
1:C:858:ILE:HG22	1:C:918:ASN:HD22	1.76	0.49
1:F:173:LYS:HG2	1:F:176:TYR:CD1	2.46	0.49
1:A:334:PRO:HG2	1:A:391:TYR:CE2	2.47	0.49
1:B:37:LEU:HD21	1:B:310:LEU:H	1.76	0.49
1:B:334:PRO:HG2	1:B:391:TYR:CE2	2.47	0.49
1:C:758:ARG:HD3	1:C:928:ASP:CA	2.39	0.49
1:D:644:ASN:OD1	1:D:644:ASN:N	2.45	0.49
1:D:722:GLU:HB2	1:D:723:ILE:HG23	1.93	0.49
1:F:644:ASN:OD1	1:F:644:ASN:N	2.45	0.49
1:G:770:ASN:OD1	1:G:770:ASN:N	2.46	0.49
1:E:644:ASN:OD1	1:E:644:ASN:N	2.45	0.49
1:A:570:PHE:HB2	1:A:573:MET:SD	2.52	0.49
1:A:770:ASN:OD1	1:A:770:ASN:N	2.46	0.49
1:A:858:ILE:HG22	1:A:918:ASN:HD22	1.76	0.49
1:B:788:VAL:O	1:B:791:SER:OG	2.24	0.49
1:F:109:THR:HA	1:F:219:THR:HG23	1.95	0.49
1:F:570:PHE:HB2	1:F:573:MET:SD	2.53	0.49
1:G:109:THR:HA	1:G:219:THR:HG23	1.95	0.49
1:G:334:PRO:HG2	1:G:391:TYR:CE2	2.47	0.49
1:E:567:ILE:HG22	1:E:569:VAL:HG23	1.94	0.49
1:E:596:GLU:OE1	1:E:914:ILE:HG23	2.12	0.49
1:B:770:ASN:OD1	1:B:770:ASN:N	2.46	0.49
1:C:925:ALA:HB3	1:C:927:TYR:CE2	2.48	0.49
1:D:334:PRO:HG2	1:D:391:TYR:CE2	2.47	0.49
1:F:352:VAL:HG13	1:F:356:LEU:HD12	1.94	0.49
1:B:343:ASP:HB3	1:B:346:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ILE:O	1:D:90:VAL:HG23	2.13	0.49
1:F:153:TRP:HD1	1:F:154:GLN:OE1	1.96	0.49
1:G:567:ILE:HG22	1:G:569:VAL:HG23	1.95	0.49
1:G:570:PHE:HB2	1:G:573:MET:SD	2.53	0.49
1:C:153:TRP:HD1	1:C:154:GLN:OE1	1.96	0.49
1:D:570:PHE:HB2	1:D:573:MET:SD	2.53	0.49
1:D:758:ARG:HG2	1:D:927:TYR:O	2.13	0.49
1:F:334:PRO:HG2	1:F:391:TYR:CE2	2.47	0.49
1:G:722:GLU:HB2	1:G:723:ILE:HG23	1.93	0.49
1:E:352:VAL:HG13	1:E:356:LEU:HD12	1.94	0.49
1:A:109:THR:HA	1:A:219:THR:HG23	1.95	0.49
1:A:153:TRP:HD1	1:A:154:GLN:OE1	1.96	0.49
1:B:86:ILE:O	1:B:90:VAL:HG23	2.13	0.49
1:B:431:ARG:CB	1:C:291:GLU:OE1	2.60	0.49
1:C:342:ILE:HD12	1:C:342:ILE:O	2.13	0.49
1:C:570:PHE:HB2	1:C:573:MET:SD	2.53	0.49
1:D:109:THR:HA	1:D:219:THR:HG23	1.95	0.49
1:D:343:ASP:HB3	1:D:346:GLN:HB2	1.95	0.49
1:G:150:LYS:O	1:G:153:TRP:N	2.41	0.49
1:A:343:ASP:HB3	1:A:346:GLN:HB2	1.95	0.49
1:A:567:ILE:HG22	1:A:569:VAL:HG23	1.95	0.49
1:A:728:ARG:HH11	1:A:728:ARG:HG3	1.78	0.49
1:C:334:PRO:HG2	1:C:391:TYR:CE2	2.47	0.48
1:D:342:ILE:HD12	1:D:342:ILE:O	2.13	0.48
1:D:352:VAL:HG13	1:D:356:LEU:HD12	1.94	0.48
1:E:86:ILE:O	1:E:90:VAL:HG23	2.13	0.48
1:E:889:ASP:O	1:E:893:ASP:N	2.41	0.48
1:A:355:GLY:O	1:A:487:SER:OG	2.24	0.48
1:B:722:GLU:HB2	1:B:723:ILE:HG23	1.93	0.48
1:F:567:ILE:HG22	1:F:569:VAL:HG23	1.95	0.48
1:G:543:ARG:HB2	1:A:469:GLN:HB3	1.94	0.48
1:G:644:ASN:OD1	1:G:644:ASN:N	2.45	0.48
1:E:109:THR:HA	1:E:219:THR:HG23	1.95	0.48
1:B:153:TRP:HD1	1:B:154:GLN:OE1	1.96	0.48
1:B:355:GLY:O	1:B:487:SER:OG	2.24	0.48
1:B:570:PHE:HB2	1:B:573:MET:SD	2.53	0.48
1:C:161:GLN:HG3	1:D:177:PHE:HB3	1.95	0.48
1:C:343:ASP:HB3	1:C:346:GLN:HB2	1.95	0.48
1:D:422:TYR:OH	1:D:436:TYR:O	2.29	0.48
1:A:342:ILE:HD12	1:A:342:ILE:O	2.13	0.48
1:A:768:GLN:NE2	1:A:931:THR:OG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HD12	1:B:342:ILE:O	2.13	0.48
1:B:424:SER:CA	1:C:304:VAL:HG21	2.43	0.48
1:D:153:TRP:HD1	1:D:154:GLN:OE1	1.96	0.48
1:F:342:ILE:HD12	1:F:342:ILE:O	2.13	0.48
1:E:922:ILE:HD12	1:E:927:TYR:OH	2.13	0.48
1:A:86:ILE:O	1:A:90:VAL:HG23	2.13	0.48
1:B:885:LYS:HZ2	1:B:888:SER:HA	1.78	0.48
1:F:86:ILE:O	1:F:90:VAL:HG23	2.13	0.48
1:F:494:LEU:HD23	1:F:841:LEU:HD23	1.96	0.48
1:G:153:TRP:HD1	1:G:154:GLN:OE1	1.96	0.48
1:G:225:THR:HG23	1:A:297:TYR:HE2	1.78	0.48
1:G:343:ASP:HB3	1:G:346:GLN:HB2	1.95	0.48
1:E:343:ASP:HB3	1:E:346:GLN:HB2	1.95	0.48
1:E:422:TYR:OH	1:E:436:TYR:O	2.29	0.48
1:E:494:LEU:HD23	1:E:841:LEU:HD23	1.96	0.48
1:E:570:PHE:HB2	1:E:573:MET:SD	2.53	0.48
1:E:758:ARG:HD3	1:E:928:ASP:CA	2.43	0.48
1:B:443:MET:SD	1:B:446:LEU:HD23	2.54	0.48
1:C:788:VAL:O	1:C:791:SER:OG	2.24	0.48
1:D:150:LYS:O	1:D:153:TRP:N	2.41	0.48
1:D:443:MET:SD	1:D:446:LEU:HD23	2.54	0.48
1:F:856:PHE:HB3	1:F:861:ILE:HD11	1.96	0.48
1:G:579:LYS:NZ	1:A:751:GLN:HA	2.29	0.48
1:E:334:PRO:HG2	1:E:391:TYR:CE2	2.47	0.48
1:E:426:LEU:HD21	1:E:436:TYR:OH	2.14	0.48
1:B:109:THR:HA	1:B:219:THR:HG23	1.95	0.48
1:C:86:ILE:O	1:C:90:VAL:HG23	2.13	0.48
1:C:815:ASP:O	1:C:819:LYS:HD3	2.14	0.48
1:G:856:PHE:HB3	1:G:861:ILE:HD11	1.96	0.48
1:B:443:MET:HE1	1:B:496:LYS:O	2.14	0.48
1:B:567:ILE:HG22	1:B:569:VAL:HG23	1.94	0.48
1:B:815:ASP:O	1:B:819:LYS:HD3	2.14	0.48
1:C:443:MET:HE1	1:C:496:LYS:O	2.14	0.48
1:C:567:ILE:HG22	1:C:569:VAL:HG23	1.94	0.48
1:D:815:ASP:O	1:D:819:LYS:HD3	2.14	0.48
1:G:494:LEU:HD23	1:G:841:LEU:HD23	1.96	0.48
1:A:443:MET:HE1	1:A:496:LYS:O	2.14	0.48
1:C:109:THR:HA	1:C:219:THR:HG23	1.95	0.48
1:C:332:THR:HG23	1:C:387:TYR:CD1	2.49	0.48
1:D:332:THR:HG23	1:D:387:TYR:CD1	2.49	0.48
1:D:443:MET:HE1	1:D:496:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:889:ASP:O	1:D:893:ASP:N	2.41	0.48
1:D:925:ALA:HB3	1:D:927:TYR:CE2	2.49	0.48
1:F:343:ASP:HB3	1:F:346:GLN:HB2	1.95	0.48
1:F:764:ARG:NH2	1:F:897:LYS:O	2.47	0.48
1:G:342:ILE:HD12	1:G:342:ILE:O	2.13	0.48
1:G:443:MET:SD	1:G:446:LEU:HD23	2.54	0.48
1:E:153:TRP:HD1	1:E:154:GLN:OE1	1.96	0.48
1:B:426:LEU:HD21	1:B:436:TYR:OH	2.14	0.48
1:C:426:LEU:HD21	1:C:436:TYR:OH	2.14	0.48
1:C:443:MET:SD	1:C:446:LEU:HD23	2.54	0.48
1:D:381:GLN:NE2	1:E:299:LEU:O	2.36	0.48
1:D:839:HIS:N	1:D:840:PRO:CD	2.77	0.48
1:F:431:ARG:HB2	1:G:291:GLU:OE1	2.13	0.48
1:E:342:ILE:HD12	1:E:342:ILE:O	2.13	0.48
1:B:173:LYS:CG	1:B:176:TYR:CE1	2.97	0.47
1:B:776:ARG:NH1	1:B:860:GLY:O	2.47	0.47
1:B:789:GLU:HA	1:B:789:GLU:OE2	2.14	0.47
1:C:91:LYS:O	1:C:94:ASN:N	2.36	0.47
1:C:770:ASN:OD1	1:C:770:ASN:N	2.46	0.47
1:F:118:HIS:O	1:G:172:TYR:HB2	2.13	0.47
1:F:173:LYS:CG	1:F:176:TYR:CE1	2.97	0.47
1:G:85:PHE:O	1:G:89:VAL:HG23	2.15	0.47
1:E:752:HIS:NE2	1:E:811:VAL:O	2.37	0.47
1:A:332:THR:HG23	1:A:387:TYR:CD1	2.49	0.47
1:B:71:VAL:HG22	1:B:248:VAL:HB	1.96	0.47
1:D:776:ARG:NH1	1:D:860:GLY:O	2.47	0.47
1:F:443:MET:HE1	1:F:496:LYS:O	2.14	0.47
1:F:443:MET:SD	1:F:446:LEU:HD23	2.54	0.47
1:G:173:LYS:CG	1:G:176:TYR:CE1	2.97	0.47
1:G:422:TYR:OH	1:G:436:TYR:O	2.29	0.47
1:G:426:LEU:HD21	1:G:436:TYR:OH	2.14	0.47
1:E:173:LYS:CG	1:E:176:TYR:CE1	2.97	0.47
1:E:789:GLU:HA	1:E:789:GLU:OE2	2.15	0.47
1:A:71:VAL:HG22	1:A:248:VAL:HB	1.96	0.47
1:A:494:LEU:HD23	1:A:841:LEU:HD23	1.96	0.47
1:A:591:PHE:CE1	1:A:604:MET:HE2	2.50	0.47
1:A:839:HIS:N	1:A:840:PRO:CD	2.77	0.47
1:B:273:LEU:HB2	1:A:263:GLY:HA2	1.96	0.47
1:D:789:GLU:HA	1:D:789:GLU:OE2	2.15	0.47
1:G:86:ILE:O	1:G:90:VAL:HG23	2.13	0.47
1:G:332:THR:HG23	1:G:387:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:591:PHE:CE1	1:G:604:MET:HE2	2.50	0.47
1:G:839:HIS:N	1:G:840:PRO:CD	2.77	0.47
1:E:815:ASP:O	1:E:819:LYS:HD3	2.14	0.47
1:A:173:LYS:CG	1:A:176:TYR:CE1	2.97	0.47
1:A:443:MET:SD	1:A:446:LEU:HD23	2.54	0.47
1:A:776:ARG:NH1	1:A:860:GLY:O	2.48	0.47
1:A:815:ASP:O	1:A:819:LYS:HD3	2.14	0.47
1:A:856:PHE:HB3	1:A:861:ILE:HD11	1.96	0.47
1:B:177:PHE:CD2	1:A:161:GLN:HG3	2.46	0.47
1:B:567:ILE:HG22	1:B:569:VAL:N	2.30	0.47
1:B:856:PHE:HB3	1:B:861:ILE:HD11	1.96	0.47
1:C:173:LYS:CG	1:C:176:TYR:CE1	2.97	0.47
1:D:591:PHE:CE1	1:D:604:MET:HE2	2.50	0.47
1:D:856:PHE:HB3	1:D:861:ILE:HD11	1.96	0.47
1:F:71:VAL:HG22	1:F:248:VAL:HB	1.96	0.47
1:F:815:ASP:O	1:F:819:LYS:HD3	2.14	0.47
1:F:839:HIS:N	1:F:840:PRO:CD	2.77	0.47
1:G:71:VAL:HG22	1:G:248:VAL:HB	1.96	0.47
1:G:378:LEU:HD12	1:A:299:LEU:HD11	1.96	0.47
1:G:717:LEU:O	1:G:721:ASN:ND2	2.30	0.47
1:E:71:VAL:HG22	1:E:248:VAL:HB	1.96	0.47
1:E:443:MET:SD	1:E:446:LEU:HD23	2.54	0.47
1:A:644:ASN:OD1	1:A:644:ASN:N	2.45	0.47
1:B:839:HIS:N	1:B:840:PRO:CD	2.77	0.47
1:C:71:VAL:HG22	1:C:248:VAL:HB	1.96	0.47
1:C:789:GLU:OE2	1:C:789:GLU:HA	2.15	0.47
1:D:788:VAL:O	1:D:791:SER:OG	2.24	0.47
1:D:885:LYS:NZ	1:D:887:LEU:O	2.48	0.47
1:F:85:PHE:O	1:F:89:VAL:HG23	2.15	0.47
1:F:332:THR:HG23	1:F:387:TYR:CD1	2.49	0.47
1:F:426:LEU:HD21	1:F:436:TYR:OH	2.14	0.47
1:F:776:ARG:NH1	1:F:860:GLY:O	2.48	0.47
1:G:195:ASP:OD1	1:G:195:ASP:C	2.58	0.47
1:G:733:LEU:HD22	1:G:794:HIS:HD2	1.80	0.47
1:A:85:PHE:O	1:A:89:VAL:HG23	2.15	0.47
1:A:426:LEU:HD21	1:A:436:TYR:OH	2.14	0.47
1:B:332:THR:HG23	1:B:387:TYR:CD1	2.49	0.47
1:C:430:TYR:CE1	1:D:255:ARG:HG2	2.49	0.47
1:D:494:LEU:HD23	1:D:841:LEU:HD23	1.96	0.47
1:D:723:ILE:HD13	1:D:836:LYS:HG2	1.97	0.47
1:D:728:ARG:HH11	1:D:728:ARG:CG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:728:ARG:HG3	1:E:728:ARG:NH1	2.22	0.47
1:E:839:HIS:N	1:E:840:PRO:CD	2.77	0.47
1:E:885:LYS:NZ	1:E:887:LEU:O	2.48	0.47
1:B:195:ASP:OD1	1:B:195:ASP:C	2.58	0.47
1:B:378:LEU:HD12	1:C:299:LEU:HD11	1.96	0.47
1:B:494:LEU:HD23	1:B:841:LEU:HD23	1.96	0.47
1:B:591:PHE:CE1	1:B:604:MET:HE2	2.50	0.47
1:C:195:ASP:OD1	1:C:195:ASP:C	2.58	0.47
1:C:431:ARG:CB	1:D:291:GLU:OE1	2.63	0.47
1:C:591:PHE:CE1	1:C:604:MET:HE2	2.50	0.47
1:C:776:ARG:NH1	1:C:860:GLY:O	2.48	0.47
1:C:839:HIS:N	1:C:840:PRO:CD	2.77	0.47
1:D:426:LEU:HD21	1:D:436:TYR:OH	2.14	0.47
1:F:567:ILE:HG22	1:F:569:VAL:N	2.30	0.47
1:F:591:PHE:CE1	1:F:604:MET:HE2	2.50	0.47
1:F:724:GLU:O	1:F:727:ILE:CG1	2.52	0.47
1:G:443:MET:HE1	1:G:496:LYS:O	2.14	0.47
1:E:567:ILE:HG22	1:E:569:VAL:N	2.30	0.47
1:E:770:ASN:OD1	1:E:770:ASN:N	2.46	0.47
1:E:799:ARG:NE	1:E:800:GLU:O	2.48	0.47
1:E:856:PHE:HB3	1:E:861:ILE:HD11	1.96	0.47
1:A:567:ILE:HG22	1:A:569:VAL:N	2.30	0.47
1:A:931:THR:CG2	1:A:932:PRO:CD	2.78	0.47
1:B:733:LEU:HD22	1:B:794:HIS:HD2	1.80	0.47
1:D:71:VAL:HG22	1:D:248:VAL:HB	1.96	0.47
1:D:195:ASP:OD1	1:D:195:ASP:C	2.58	0.47
1:D:567:ILE:HG22	1:D:569:VAL:N	2.30	0.47
1:F:723:ILE:HD13	1:F:836:LYS:HG2	1.97	0.47
1:G:925:ALA:HB3	1:G:927:TYR:CE2	2.49	0.47
1:B:85:PHE:O	1:B:89:VAL:HG23	2.15	0.47
1:C:885:LYS:NZ	1:C:887:LEU:O	2.48	0.47
1:F:733:LEU:HD22	1:F:794:HIS:HD2	1.80	0.47
1:E:38:ARG:HB2	1:E:85:PHE:CE1	2.50	0.47
1:E:85:PHE:O	1:E:89:VAL:HG23	2.15	0.47
1:D:770:ASN:OD1	1:D:770:ASN:N	2.46	0.47
1:F:789:GLU:HA	1:F:789:GLU:OE2	2.15	0.47
1:F:889:ASP:O	1:F:893:ASP:N	2.41	0.47
1:G:776:ARG:NH1	1:G:860:GLY:O	2.47	0.47
1:G:931:THR:HG23	1:G:932:PRO:HD2	1.97	0.47
1:E:443:MET:HE1	1:E:496:LYS:O	2.14	0.47
1:A:752:HIS:NE2	1:A:811:VAL:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:TYR:CZ	1:C:255:ARG:HG2	2.51	0.46
1:C:206:ARG:HE	1:C:206:ARG:CA	2.28	0.46
1:C:494:LEU:HD23	1:C:841:LEU:HD23	1.96	0.46
1:C:723:ILE:HD13	1:C:836:LYS:HG2	1.97	0.46
1:C:856:PHE:HB3	1:C:861:ILE:HD11	1.96	0.46
1:D:85:PHE:O	1:D:89:VAL:HG23	2.15	0.46
1:D:615:ASN:ND2	1:E:564:ASP:OD2	2.43	0.46
1:F:195:ASP:OD1	1:F:195:ASP:C	2.58	0.46
1:F:443:MET:HE1	1:F:500:MET:H	1.80	0.46
1:E:349:GLY:HA2	1:E:368:VAL:CG2	2.45	0.46
1:E:591:PHE:CE1	1:E:604:MET:HE2	2.50	0.46
1:E:723:ILE:HD13	1:E:836:LYS:HG2	1.97	0.46
1:A:789:GLU:HA	1:A:789:GLU:OE2	2.15	0.46
1:D:173:LYS:CG	1:D:176:TYR:CE1	2.97	0.46
1:A:885:LYS:NZ	1:A:887:LEU:O	2.48	0.46
1:B:889:ASP:O	1:B:893:ASP:N	2.41	0.46
1:C:567:ILE:HG22	1:C:569:VAL:N	2.30	0.46
1:C:637:CYS:HA	1:C:718:LYS:NZ	2.31	0.46
1:F:422:TYR:OH	1:F:436:TYR:O	2.29	0.46
1:G:758:ARG:HD3	1:G:928:ASP:C	2.40	0.46
1:G:815:ASP:O	1:G:819:LYS:HD3	2.14	0.46
1:E:332:THR:HG23	1:E:387:TYR:CD1	2.49	0.46
1:E:776:ARG:NH1	1:E:860:GLY:O	2.47	0.46
1:A:38:ARG:HE	1:A:38:ARG:HB3	1.54	0.46
1:B:885:LYS:NZ	1:B:887:LEU:O	2.48	0.46
1:D:426:LEU:CD1	1:D:436:TYR:HE1	2.27	0.46
1:F:770:ASN:OD1	1:F:770:ASN:N	2.46	0.46
1:G:567:ILE:HG22	1:G:569:VAL:N	2.30	0.46
1:G:723:ILE:HD13	1:G:836:LYS:HG2	1.97	0.46
1:G:885:LYS:NZ	1:G:887:LEU:O	2.48	0.46
1:E:206:ARG:HE	1:E:206:ARG:CA	2.28	0.46
1:A:637:CYS:HA	1:A:718:LYS:NZ	2.31	0.46
1:B:206:ARG:HE	1:B:206:ARG:CA	2.28	0.46
1:B:349:GLY:HA2	1:B:368:VAL:CG2	2.45	0.46
1:B:723:ILE:HD13	1:B:836:LYS:HG2	1.97	0.46
1:C:85:PHE:O	1:C:89:VAL:HG23	2.15	0.46
1:C:752:HIS:NE2	1:C:811:VAL:O	2.37	0.46
1:D:206:ARG:HE	1:D:206:ARG:CA	2.28	0.46
1:F:934:ARG:CZ	1:F:934:ARG:HB3	2.42	0.46
1:G:562:PRO:HG2	1:G:570:PHE:CE2	2.51	0.46
1:G:799:ARG:NE	1:G:800:GLU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HB2	1:A:85:PHE:CE1	2.50	0.46
1:A:195:ASP:OD1	1:A:195:ASP:C	2.58	0.46
1:A:349:GLY:HA2	1:A:368:VAL:CG2	2.45	0.46
1:A:562:PRO:HG2	1:A:570:PHE:CE2	2.51	0.46
1:B:491:GLN:NE2	1:B:728:ARG:HG2	2.30	0.46
1:F:562:PRO:HG2	1:F:570:PHE:CE2	2.51	0.46
1:E:195:ASP:OD1	1:E:195:ASP:C	2.58	0.46
1:B:562:PRO:HG2	1:B:570:PHE:CE2	2.51	0.46
1:B:752:HIS:NE2	1:B:811:VAL:O	2.37	0.46
1:C:415:ASN:OD1	1:C:418:ARG:NH2	2.49	0.46
1:D:38:ARG:HB2	1:D:85:PHE:CE1	2.50	0.46
1:D:436:TYR:CG	1:E:255:ARG:HD3	2.51	0.46
1:G:225:THR:HG21	1:A:238:ARG:CZ	2.45	0.46
1:G:349:GLY:HA2	1:G:368:VAL:CG2	2.45	0.46
1:G:789:GLU:HA	1:G:789:GLU:OE2	2.15	0.46
1:E:80:ALA:HB1	1:E:376:VAL:HG11	1.97	0.46
1:A:723:ILE:HD13	1:A:836:LYS:HG2	1.97	0.46
1:B:423:GLY:HA3	1:C:304:VAL:HG13	1.97	0.46
1:B:644:ASN:OD1	1:B:644:ASN:N	2.45	0.46
1:B:727:ILE:O	1:B:727:ILE:HG13	2.16	0.46
1:C:38:ARG:HB2	1:C:85:PHE:CE1	2.50	0.46
1:D:165:HIS:CE1	1:D:176:TYR:CD2	3.04	0.46
1:F:291:GLU:OE1	1:E:431:ARG:HG2	2.15	0.46
1:G:38:ARG:HB2	1:G:85:PHE:CE1	2.50	0.46
1:G:335:SER:O	1:G:336:MET:C	2.59	0.46
1:G:752:HIS:NE2	1:G:811:VAL:O	2.37	0.46
1:B:38:ARG:HB2	1:B:85:PHE:CE1	2.50	0.46
1:C:443:MET:HE1	1:C:500:MET:H	1.80	0.46
1:D:118:HIS:CG	1:E:171:GLU:HA	2.50	0.46
1:D:349:GLY:HA2	1:D:368:VAL:CG2	2.45	0.46
1:D:385:ASP:OD2	1:E:304:VAL:HG12	2.16	0.46
1:D:706:PHE:HE2	1:E:806:LEU:HD22	1.81	0.46
1:E:562:PRO:HG2	1:E:570:PHE:CE2	2.51	0.46
1:C:335:SER:O	1:C:336:MET:C	2.58	0.46
1:D:562:PRO:HG2	1:D:570:PHE:CE2	2.51	0.46
1:F:38:ARG:HB2	1:F:85:PHE:CE1	2.50	0.46
1:F:268:ASN:HA	1:E:228:ASP:OD2	2.15	0.46
1:G:637:CYS:HA	1:G:718:LYS:NZ	2.31	0.46
1:G:889:ASP:O	1:G:893:ASP:N	2.41	0.46
1:A:733:LEU:HD22	1:A:794:HIS:HD2	1.80	0.46
1:B:799:ARG:NE	1:B:800:GLU:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:ARG:HE	1:F:206:ARG:CA	2.28	0.45
1:G:389:LYS:HA	1:G:392:HIS:HB2	1.99	0.45
1:E:733:LEU:HD22	1:E:794:HIS:HD2	1.80	0.45
1:A:389:LYS:HA	1:A:392:HIS:HB2	1.99	0.45
1:B:165:HIS:CE1	1:B:176:TYR:CD2	3.04	0.45
1:B:374:GLN:OE1	1:B:374:GLN:HA	2.17	0.45
1:B:415:ASN:OD1	1:B:418:ARG:NH2	2.49	0.45
1:C:118:HIS:O	1:D:172:TYR:HD2	1.99	0.45
1:C:562:PRO:HG2	1:C:570:PHE:CE2	2.51	0.45
1:D:637:CYS:HA	1:D:718:LYS:NZ	2.31	0.45
1:E:637:CYS:HA	1:E:718:LYS:NZ	2.31	0.45
1:A:165:HIS:CE1	1:A:176:TYR:CD2	3.04	0.45
1:C:349:GLY:HA2	1:C:368:VAL:CG2	2.45	0.45
1:C:374:GLN:OE1	1:C:374:GLN:HA	2.17	0.45
1:C:733:LEU:HD22	1:C:794:HIS:HD2	1.80	0.45
1:D:38:ARG:HE	1:D:38:ARG:HB3	1.54	0.45
1:F:349:GLY:HA2	1:F:368:VAL:CG2	2.45	0.45
1:F:885:LYS:NZ	1:F:887:LEU:O	2.48	0.45
1:E:165:HIS:CE1	1:E:176:TYR:CD2	3.04	0.45
1:E:773:LYS:NZ	1:E:862:ASN:OD1	2.34	0.45
1:C:357:ASN:HB3	1:C:728:ARG:O	2.17	0.45
1:C:799:ARG:NE	1:C:800:GLU:O	2.48	0.45
1:D:161:GLN:HG3	1:E:177:PHE:HB3	1.97	0.45
1:D:443:MET:HE1	1:D:500:MET:H	1.80	0.45
1:D:733:LEU:HD22	1:D:794:HIS:HD2	1.80	0.45
1:F:125:VAL:HG21	1:F:241:PHE:CZ	2.52	0.45
1:F:165:HIS:CE1	1:F:176:TYR:CD2	3.04	0.45
1:F:374:GLN:OE1	1:F:374:GLN:HA	2.17	0.45
1:F:637:CYS:HA	1:F:718:LYS:NZ	2.31	0.45
1:G:165:HIS:CE1	1:G:176:TYR:CD2	3.04	0.45
1:G:783:LEU:HD13	1:G:846:ILE:HD12	1.99	0.45
1:E:125:VAL:HG21	1:E:241:PHE:CZ	2.52	0.45
1:E:443:MET:HE1	1:E:500:MET:H	1.81	0.45
1:A:443:MET:HE1	1:A:500:MET:H	1.80	0.45
1:A:572:GLY:O	1:A:622:VAL:HG12	2.17	0.45
1:A:783:LEU:HD13	1:A:846:ILE:HD12	1.99	0.45
1:C:125:VAL:HG21	1:C:241:PHE:CZ	2.52	0.45
1:F:389:LYS:HA	1:F:392:HIS:HB2	1.99	0.45
1:F:572:GLY:O	1:F:622:VAL:HG12	2.17	0.45
1:F:773:LYS:NZ	1:F:862:ASN:OD1	2.34	0.45
1:A:335:SER:O	1:A:336:MET:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLN:HA	1:A:374:GLN:OE1	2.17	0.45
1:A:451:PHE:HE1	1:A:532:ILE:HG23	1.82	0.45
1:B:389:LYS:HA	1:B:392:HIS:HB2	1.99	0.45
1:B:782:PHE:HE1	1:B:786:VAL:HG21	1.82	0.45
1:B:783:LEU:HD13	1:B:846:ILE:HD12	1.99	0.45
1:C:783:LEU:HD13	1:C:846:ILE:HD12	1.99	0.45
1:D:415:ASN:OD1	1:D:418:ARG:NH2	2.49	0.45
1:F:374:GLN:NE2	1:F:477:ASN:OD1	2.44	0.45
1:F:451:PHE:HE1	1:F:532:ILE:HG23	1.82	0.45
1:F:783:LEU:HD13	1:F:846:ILE:HD12	1.99	0.45
1:G:206:ARG:HE	1:G:206:ARG:CA	2.28	0.45
1:G:357:ASN:HB3	1:G:728:ARG:O	2.17	0.45
1:G:415:ASN:OD1	1:G:418:ARG:NH2	2.49	0.45
1:G:789:GLU:O	1:G:793:TYR:N	2.46	0.45
1:A:338:ASP:OD1	1:A:338:ASP:N	2.49	0.45
1:B:637:CYS:HA	1:B:718:LYS:NZ	2.31	0.45
1:B:893:ASP:O	1:B:897:LYS:HB2	2.17	0.45
1:C:165:HIS:CE1	1:C:176:TYR:CD2	3.04	0.45
1:C:572:GLY:O	1:C:622:VAL:HG12	2.17	0.45
1:D:125:VAL:HG21	1:D:241:PHE:CZ	2.51	0.45
1:D:728:ARG:NH1	1:D:728:ARG:CG	2.79	0.45
1:F:279:GLU:H	1:F:279:GLU:CD	2.25	0.45
1:F:373:LYS:HZ3	1:E:440:ARG:NH2	2.15	0.45
1:F:415:ASN:OD1	1:F:418:ARG:NH2	2.49	0.45
1:F:799:ARG:NE	1:F:800:GLU:O	2.48	0.45
1:G:374:GLN:OE1	1:G:374:GLN:HA	2.17	0.45
1:G:782:PHE:HE1	1:G:786:VAL:HG21	1.82	0.45
1:E:374:GLN:OE1	1:E:374:GLN:HA	2.17	0.45
1:E:451:PHE:HE1	1:E:532:ILE:HG23	1.82	0.45
1:B:125:VAL:HG21	1:B:241:PHE:CZ	2.52	0.45
1:B:451:PHE:HE1	1:B:532:ILE:HG23	1.82	0.45
1:B:711:THR:O	1:B:715:GLN:N	2.42	0.45
1:D:374:GLN:HA	1:D:374:GLN:OE1	2.17	0.45
1:E:465:TYR:HB3	1:E:467:ARG:HG3	1.99	0.45
1:C:225:THR:HG21	1:D:238:ARG:NE	2.31	0.45
1:C:451:PHE:HE1	1:C:532:ILE:HG23	1.82	0.45
1:C:782:PHE:HE1	1:C:786:VAL:HG21	1.82	0.45
1:D:588:TYR:HB3	1:D:921:THR:HG22	1.99	0.45
1:F:225:THR:HG23	1:G:297:TYR:HE2	1.82	0.45
1:F:225:THR:HG21	1:G:238:ARG:CZ	2.46	0.45
1:F:350:ASP:OD1	1:F:353:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:VAL:HG21	1:G:241:PHE:CZ	2.52	0.45
1:E:415:ASN:OD1	1:E:418:ARG:NH2	2.49	0.45
1:A:279:GLU:H	1:A:279:GLU:CD	2.25	0.45
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.49	0.45
1:B:594:ASP:N	1:B:594:ASP:OD1	2.50	0.45
1:C:594:ASP:N	1:C:594:ASP:OD1	2.50	0.45
1:G:443:MET:HE1	1:G:500:MET:H	1.81	0.45
1:A:206:ARG:HE	1:A:206:ARG:CA	2.28	0.45
1:A:350:ASP:OD1	1:A:353:ARG:NH1	2.50	0.45
1:A:718:LYS:HE2	1:A:718:LYS:N	2.32	0.45
1:A:789:GLU:O	1:A:793:TYR:N	2.46	0.45
1:B:279:GLU:H	1:B:279:GLU:CD	2.25	0.44
1:C:350:ASP:OD1	1:C:353:ARG:NH1	2.50	0.44
1:C:644:ASN:N	1:C:644:ASN:OD1	2.45	0.44
1:C:718:LYS:N	1:C:718:LYS:HE2	2.32	0.44
1:B:443:MET:HE1	1:B:500:MET:H	1.81	0.44
1:B:718:LYS:HE2	1:B:718:LYS:N	2.32	0.44
1:C:328:ILE:HG13	1:C:329:LYS:N	2.31	0.44
1:F:373:LYS:NZ	1:E:440:ARG:NH2	2.65	0.44
1:F:426:LEU:CD1	1:F:436:TYR:HE1	2.27	0.44
1:F:819:LYS:O	1:F:823:ILE:HG13	2.18	0.44
1:G:718:LYS:HE2	1:G:718:LYS:N	2.32	0.44
1:E:159:GLN:HA	1:E:162:ARG:HG2	2.00	0.44
1:A:422:TYR:OH	1:A:436:TYR:O	2.29	0.44
1:B:439:HIS:HB3	1:C:312:THR:HG21	2.00	0.44
1:C:107:LEU:HD23	1:C:132:MET:SD	2.58	0.44
1:C:389:LYS:HA	1:C:392:HIS:HB2	1.98	0.44
1:D:259:GLN:OE1	1:E:273:LEU:CD2	2.54	0.44
1:D:328:ILE:HG13	1:D:329:LYS:N	2.31	0.44
1:D:594:ASP:OD1	1:D:594:ASP:N	2.50	0.44
1:D:819:LYS:O	1:D:823:ILE:HG13	2.18	0.44
1:F:465:TYR:HB3	1:F:467:ARG:HG3	1.99	0.44
1:G:350:ASP:OD1	1:G:353:ARG:NH1	2.50	0.44
1:G:451:PHE:HE1	1:G:532:ILE:HG23	1.82	0.44
1:G:819:LYS:O	1:G:823:ILE:HG13	2.18	0.44
1:E:588:TYR:HB3	1:E:921:THR:HG22	1.99	0.44
1:A:333:GLU:HB2	1:A:336:MET:HE2	1.99	0.44
1:A:782:PHE:HE1	1:A:786:VAL:HG21	1.82	0.44
1:B:114:LYS:HE3	1:C:239:LYS:HA	2.00	0.44
1:B:467:ARG:HD3	1:B:469:GLN:OE1	2.18	0.44
1:B:572:GLY:O	1:B:622:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:GLY:O	1:D:622:VAL:HG12	2.17	0.44
1:D:783:LEU:HD13	1:D:846:ILE:HD12	1.99	0.44
1:E:389:LYS:HA	1:E:392:HIS:HB2	1.99	0.44
1:A:819:LYS:O	1:A:823:ILE:HG13	2.18	0.44
1:B:328:ILE:HG13	1:B:329:LYS:N	2.31	0.44
1:B:757:TYR:CE1	1:A:581:ARG:NH2	2.84	0.44
1:C:338:ASP:N	1:C:338:ASP:OD1	2.48	0.44
1:D:451:PHE:HE1	1:D:532:ILE:HG23	1.82	0.44
1:D:718:LYS:HE2	1:D:718:LYS:N	2.32	0.44
1:F:506:GLY:C	1:F:508:VAL:H	2.25	0.44
1:G:279:GLU:H	1:G:279:GLU:CD	2.25	0.44
1:G:572:GLY:O	1:G:622:VAL:HG12	2.17	0.44
1:E:350:ASP:OD1	1:E:353:ARG:NH1	2.50	0.44
1:E:727:ILE:HG22	1:E:840:PRO:HB2	1.99	0.44
1:E:819:LYS:O	1:E:823:ILE:HG13	2.18	0.44
1:A:107:LEU:HD23	1:A:132:MET:SD	2.58	0.44
1:A:328:ILE:HG13	1:A:329:LYS:N	2.31	0.44
1:A:467:ARG:HD3	1:A:469:GLN:OE1	2.18	0.44
1:A:799:ARG:NE	1:A:800:GLU:O	2.48	0.44
1:B:82:LYS:HE3	1:B:222:ASP:CB	2.48	0.44
1:B:759:ASN:CG	1:B:930:ASP:OD1	2.60	0.44
1:D:350:ASP:OD1	1:D:353:ARG:NH1	2.50	0.44
1:D:782:PHE:HE1	1:D:786:VAL:HG21	1.82	0.44
1:G:259:GLN:HG3	1:A:269:TYR:CE2	2.48	0.44
1:G:426:LEU:CD1	1:G:436:TYR:HE1	2.27	0.44
1:G:610:THR:OG1	1:G:618:ASP:OD2	2.28	0.44
1:E:572:GLY:O	1:E:622:VAL:HG12	2.17	0.44
1:C:728:ARG:HH11	1:C:728:ARG:HG3	1.83	0.44
1:C:931:THR:HG22	1:C:932:PRO:CD	2.42	0.44
1:F:304:VAL:HG11	1:E:423:GLY:HA3	1.94	0.44
1:F:307:ARG:NH1	1:E:426:LEU:CD2	2.81	0.44
1:G:467:ARG:HD3	1:G:469:GLN:OE1	2.18	0.44
1:E:82:LYS:HE3	1:E:222:ASP:CB	2.48	0.44
1:E:717:LEU:C	1:E:721:ASN:HD22	2.21	0.44
1:E:783:LEU:HD13	1:E:846:ILE:HD12	1.99	0.44
1:A:82:LYS:HE3	1:A:222:ASP:CB	2.48	0.44
1:A:594:ASP:OD1	1:A:594:ASP:N	2.50	0.44
1:C:467:ARG:HD3	1:C:469:GLN:OE1	2.18	0.44
1:D:107:LEU:HD23	1:D:132:MET:SD	2.58	0.44
1:D:159:GLN:HA	1:D:162:ARG:HG2	2.00	0.44
1:D:534:GLU:OE1	1:D:534:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:782:PHE:HE1	1:F:786:VAL:HG21	1.82	0.44
1:F:889:ASP:HA	1:F:892:TRP:HB3	2.00	0.44
1:G:333:GLU:HB2	1:G:336:MET:HE2	1.99	0.44
1:G:465:TYR:HB3	1:G:467:ARG:HG3	1.99	0.44
1:G:889:ASP:HA	1:G:892:TRP:HB3	2.00	0.44
1:A:609:SER:HB2	1:A:624:ASN:HD22	1.83	0.44
1:B:107:LEU:HD23	1:B:132:MET:SD	2.58	0.44
1:C:164:LEU:HA	1:C:196:LEU:HD11	2.00	0.44
1:C:204:VAL:HG21	1:C:246:LEU:HD11	2.00	0.44
1:D:727:ILE:HG22	1:D:840:PRO:HB2	1.98	0.44
1:F:159:GLN:HA	1:F:162:ARG:HG2	2.00	0.44
1:F:328:ILE:HG13	1:F:329:LYS:N	2.31	0.44
1:F:588:TYR:HB3	1:F:921:THR:HG22	1.99	0.44
1:B:350:ASP:OD1	1:B:353:ARG:NH1	2.50	0.43
1:B:789:GLU:O	1:B:793:TYR:N	2.46	0.43
1:C:534:GLU:HA	1:C:534:GLU:OE1	2.18	0.43
1:D:279:GLU:H	1:D:279:GLU:CD	2.25	0.43
1:D:467:ARG:HD3	1:D:469:GLN:OE1	2.18	0.43
1:F:107:LEU:HD23	1:F:132:MET:SD	2.58	0.43
1:F:467:ARG:HD3	1:F:469:GLN:OE1	2.18	0.43
1:F:609:SER:HB2	1:F:624:ASN:HD22	1.83	0.43
1:G:328:ILE:HG13	1:G:329:LYS:N	2.31	0.43
1:G:588:TYR:HB3	1:G:921:THR:HG22	1.99	0.43
1:A:125:VAL:HG21	1:A:241:PHE:CZ	2.52	0.43
1:B:426:LEU:CD1	1:B:436:TYR:HE1	2.27	0.43
1:B:756:LEU:HB3	1:B:927:TYR:CE1	2.53	0.43
1:C:82:LYS:HE3	1:C:222:ASP:CB	2.48	0.43
1:C:588:TYR:HB3	1:C:921:THR:HG22	1.99	0.43
1:D:389:LYS:HA	1:D:392:HIS:HB2	1.98	0.43
1:D:758:ARG:HD3	1:D:928:ASP:CA	2.48	0.43
1:F:635:CYS:O	1:F:636:ARG:HG3	2.18	0.43
1:F:718:LYS:HE2	1:F:718:LYS:N	2.32	0.43
1:F:888:SER:O	1:F:891:GLU:N	2.51	0.43
1:E:328:ILE:HG13	1:E:329:LYS:N	2.31	0.43
1:E:374:GLN:NE2	1:E:477:ASN:OD1	2.44	0.43
1:E:635:CYS:O	1:E:636:ARG:HG3	2.18	0.43
1:E:717:LEU:O	1:E:721:ASN:ND2	2.30	0.43
1:A:261:ILE:CD1	1:A:298:LEU:CD1	2.96	0.43
1:B:116:PRO:HG3	1:C:166:LEU:HD13	1.98	0.43
1:B:609:SER:HB2	1:B:624:ASN:HD22	1.83	0.43
1:D:164:LEU:HA	1:D:196:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:SER:HB2	1:D:624:ASN:HD22	1.83	0.43
1:F:656:ILE:HG22	1:F:657:VAL:O	2.19	0.43
1:E:107:LEU:HD23	1:E:132:MET:SD	2.58	0.43
1:E:467:ARG:HD3	1:E:469:GLN:OE1	2.18	0.43
1:B:176:TYR:CD1	1:B:176:TYR:N	2.86	0.43
1:B:426:LEU:HD23	1:C:254:LEU:HD13	2.00	0.43
1:B:819:LYS:O	1:B:823:ILE:HG13	2.17	0.43
1:B:888:SER:O	1:B:891:GLU:N	2.51	0.43
1:C:176:TYR:CD1	1:C:176:TYR:N	2.87	0.43
1:F:204:VAL:HG21	1:F:246:LEU:HD11	2.00	0.43
1:F:272:THR:CG2	1:E:267:GLU:HG2	2.48	0.43
1:F:534:GLU:OE1	1:F:534:GLU:HA	2.18	0.43
1:G:635:CYS:O	1:G:636:ARG:HG3	2.18	0.43
1:E:120:PRO:HG2	1:E:123:VAL:HG23	2.01	0.43
1:E:176:TYR:CD1	1:E:176:TYR:N	2.87	0.43
1:E:609:SER:HB2	1:E:624:ASN:HD22	1.83	0.43
1:E:656:ILE:HG22	1:E:657:VAL:O	2.19	0.43
1:E:756:LEU:O	1:E:927:TYR:HD1	2.01	0.43
1:A:889:ASP:HA	1:A:892:TRP:HB3	2.00	0.43
1:B:534:GLU:OE1	1:B:534:GLU:HA	2.18	0.43
1:B:889:ASP:HA	1:B:892:TRP:HB3	2.00	0.43
1:C:333:GLU:HB2	1:C:336:MET:HE2	1.99	0.43
1:C:635:CYS:O	1:C:636:ARG:HG3	2.18	0.43
1:C:789:GLU:O	1:C:793:TYR:N	2.46	0.43
1:C:819:LYS:O	1:C:823:ILE:HG13	2.18	0.43
1:D:465:TYR:HB3	1:D:467:ARG:HG3	1.99	0.43
1:F:355:GLY:O	1:F:487:SER:OG	2.24	0.43
1:A:465:TYR:HB3	1:A:467:ARG:HG3	1.99	0.43
1:G:82:LYS:HE3	1:G:222:ASP:CB	2.48	0.43
1:G:107:LEU:HD23	1:G:132:MET:SD	2.58	0.43
1:E:718:LYS:N	1:E:718:LYS:HE2	2.32	0.43
1:E:728:ARG:NH1	1:E:728:ARG:CG	2.80	0.43
1:A:159:GLN:HA	1:A:162:ARG:HG2	2.00	0.43
1:A:374:GLN:NE2	1:A:477:ASN:OD1	2.44	0.43
1:A:426:LEU:CD1	1:A:436:TYR:HE1	2.27	0.43
1:A:451:PHE:HE2	1:A:507:SER:O	2.01	0.43
1:B:159:GLN:HA	1:B:162:ARG:HG2	2.00	0.43
1:B:161:GLN:HG3	1:C:177:PHE:HD2	1.84	0.43
1:B:580:SER:O	1:B:580:SER:OG	2.35	0.43
1:B:588:TYR:HB3	1:B:921:THR:HG22	1.99	0.43
1:C:159:GLN:HA	1:C:162:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ILE:HG22	1:C:657:VAL:O	2.19	0.43
1:D:711:THR:O	1:D:715:GLN:N	2.42	0.43
1:F:165:HIS:ND1	1:F:176:TYR:CE2	2.87	0.43
1:G:717:LEU:C	1:G:721:ASN:HD22	2.21	0.43
1:A:635:CYS:O	1:A:636:ARG:HG3	2.18	0.43
1:B:164:LEU:HA	1:B:196:LEU:HD11	2.00	0.43
1:C:465:TYR:HB3	1:C:467:ARG:HG3	1.99	0.43
1:F:161:GLN:HG3	1:G:177:PHE:HD2	1.84	0.43
1:G:165:HIS:ND1	1:G:176:TYR:CE2	2.87	0.43
1:E:164:LEU:HA	1:E:196:LEU:HD11	2.00	0.43
1:A:204:VAL:HG21	1:A:246:LEU:HD11	2.00	0.43
1:B:500:MET:HG3	1:B:734:ILE:HD13	2.01	0.43
1:D:82:LYS:HE3	1:D:222:ASP:CB	2.48	0.43
1:D:227:PHE:CD1	1:D:260:LEU:HD13	2.54	0.43
1:F:596:GLU:C	1:F:597:ASN:OD1	2.62	0.43
1:G:114:LYS:HE3	1:A:239:LYS:HA	2.00	0.43
1:G:159:GLN:HA	1:G:162:ARG:HG2	2.00	0.43
1:G:164:LEU:HA	1:G:196:LEU:HD11	2.00	0.43
1:G:594:ASP:OD1	1:G:594:ASP:N	2.50	0.43
1:E:279:GLU:H	1:E:279:GLU:CD	2.25	0.43
1:E:342:ILE:HD13	1:E:346:GLN:OE1	2.19	0.43
1:E:534:GLU:OE1	1:E:534:GLU:HA	2.18	0.43
1:E:782:PHE:HE1	1:E:786:VAL:HG21	1.82	0.43
1:A:500:MET:HG3	1:A:734:ILE:HD13	2.01	0.43
1:A:588:TYR:HB3	1:A:921:THR:HG22	1.99	0.43
1:B:165:HIS:ND1	1:B:176:TYR:CE2	2.87	0.43
1:B:204:VAL:HG21	1:B:246:LEU:HD11	2.00	0.43
1:C:332:THR:HB	1:C:336:MET:HE3	2.00	0.43
1:D:120:PRO:HG2	1:D:123:VAL:HG23	2.01	0.43
1:D:635:CYS:O	1:D:636:ARG:HG3	2.19	0.43
1:D:888:SER:O	1:D:891:GLU:N	2.51	0.43
1:F:82:LYS:HE3	1:F:222:ASP:CB	2.48	0.43
1:F:500:MET:HG3	1:F:734:ILE:HD13	2.01	0.43
1:A:165:HIS:ND1	1:A:176:TYR:CE2	2.87	0.43
1:A:534:GLU:OE1	1:A:534:GLU:HA	2.18	0.43
1:A:717:LEU:C	1:A:721:ASN:HD22	2.21	0.43
1:B:120:PRO:HG2	1:B:123:VAL:HG23	2.01	0.42
1:B:465:TYR:HB3	1:B:467:ARG:HG3	1.99	0.42
1:B:596:GLU:C	1:B:597:ASN:OD1	2.62	0.42
1:B:656:ILE:HG22	1:B:657:VAL:O	2.19	0.42
1:C:227:PHE:CD1	1:C:260:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:TYR:CD1	1:D:176:TYR:N	2.86	0.42
1:D:444:ASP:O	1:D:542:GLY:HA2	2.19	0.42
1:D:869:ASN:O	1:D:873:SER:HB3	2.19	0.42
1:F:164:LEU:HA	1:F:196:LEU:HD11	2.00	0.42
1:F:482:LEU:O	1:F:486:VAL:HG23	2.19	0.42
1:F:717:LEU:C	1:F:721:ASN:HD22	2.21	0.42
1:G:338:ASP:C	1:G:339:ILE:CG1	2.92	0.42
1:G:355:GLY:O	1:G:487:SER:OG	2.24	0.42
1:G:436:TYR:CD2	1:A:255:ARG:NE	2.87	0.42
1:G:534:GLU:OE1	1:G:534:GLU:HA	2.18	0.42
1:G:656:ILE:HG22	1:G:657:VAL:O	2.19	0.42
1:E:756:LEU:O	1:E:927:TYR:CD1	2.71	0.42
1:A:120:PRO:HG2	1:A:123:VAL:HG23	2.01	0.42
1:A:869:ASN:O	1:A:873:SER:HB3	2.19	0.42
1:C:82:LYS:HE3	1:C:222:ASP:HB2	2.02	0.42
1:C:165:HIS:ND1	1:C:176:TYR:CE2	2.87	0.42
1:C:225:THR:HG23	1:D:297:TYR:HE2	1.84	0.42
1:C:227:PHE:CE2	1:D:268:ASN:HB2	2.53	0.42
1:C:500:MET:HG3	1:C:734:ILE:HD13	2.01	0.42
1:C:889:ASP:HA	1:C:892:TRP:HB3	2.00	0.42
1:A:164:LEU:HA	1:A:196:LEU:HD11	2.00	0.42
1:A:342:ILE:HD13	1:A:346:GLN:OE1	2.19	0.42
1:A:444:ASP:O	1:A:542:GLY:HA2	2.19	0.42
1:B:225:THR:HG23	1:C:297:TYR:HE2	1.85	0.42
1:B:328:ILE:O	1:B:329:LYS:HB2	2.20	0.42
1:B:342:ILE:HD13	1:B:346:GLN:OE1	2.19	0.42
1:B:444:ASP:O	1:B:542:GLY:HA2	2.19	0.42
1:C:120:PRO:HG2	1:C:123:VAL:HG23	2.01	0.42
1:D:656:ILE:HG22	1:D:657:VAL:O	2.19	0.42
1:F:82:LYS:HE3	1:F:222:ASP:HB2	2.02	0.42
1:F:358:LEU:O	1:F:359:ARG:HB2	2.19	0.42
1:F:594:ASP:OD1	1:F:594:ASP:N	2.50	0.42
1:F:779:VAL:HG13	1:F:851:LEU:HD22	2.02	0.42
1:G:120:PRO:HG2	1:G:123:VAL:HG23	2.01	0.42
1:G:176:TYR:CD1	1:G:176:TYR:N	2.86	0.42
1:G:358:LEU:O	1:G:359:ARG:HB2	2.19	0.42
1:G:500:MET:HG3	1:G:734:ILE:HD13	2.01	0.42
1:G:581:ARG:NH2	1:A:757:TYR:HE1	2.17	0.42
1:G:596:GLU:C	1:G:597:ASN:OD1	2.62	0.42
1:G:869:ASN:O	1:G:873:SER:HB3	2.19	0.42
1:E:165:HIS:ND1	1:E:176:TYR:CE2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:788:VAL:O	1:E:791:SER:OG	2.24	0.42
1:B:869:ASN:O	1:B:873:SER:HB3	2.20	0.42
1:C:118:HIS:O	1:D:172:TYR:CD2	2.72	0.42
1:C:422:TYR:OH	1:C:436:TYR:O	2.29	0.42
1:C:609:SER:HB2	1:C:624:ASN:HD22	1.83	0.42
1:D:165:HIS:ND1	1:D:176:TYR:CE2	2.87	0.42
1:D:717:LEU:O	1:D:721:ASN:ND2	2.30	0.42
1:F:227:PHE:CD1	1:F:260:LEU:HD13	2.54	0.42
1:F:567:ILE:HA	1:F:924:GLY:HA3	2.01	0.42
1:F:752:HIS:NE2	1:F:811:VAL:O	2.37	0.42
1:G:82:LYS:O	1:G:86:ILE:HG12	2.20	0.42
1:G:261:ILE:CD1	1:G:298:LEU:CD1	2.96	0.42
1:G:444:ASP:O	1:G:542:GLY:HA2	2.19	0.42
1:G:609:SER:HB2	1:G:624:ASN:HD22	1.83	0.42
1:E:227:PHE:CD1	1:E:260:LEU:HD13	2.54	0.42
1:E:779:VAL:HG13	1:E:851:LEU:HD22	2.02	0.42
1:C:204:VAL:HG12	1:C:245:LYS:HB3	2.02	0.42
1:C:342:ILE:HD13	1:C:346:GLN:OE1	2.19	0.42
1:C:426:LEU:CD1	1:C:436:TYR:HE1	2.27	0.42
1:C:444:ASP:O	1:C:542:GLY:HA2	2.19	0.42
1:C:758:ARG:HG2	1:C:927:TYR:O	2.20	0.42
1:C:888:SER:O	1:C:891:GLU:N	2.51	0.42
1:D:259:GLN:HG3	1:E:269:TYR:CE2	2.52	0.42
1:D:889:ASP:HA	1:D:892:TRP:HB3	2.00	0.42
1:F:82:LYS:O	1:F:86:ILE:HG12	2.20	0.42
1:F:869:ASN:O	1:F:873:SER:HB3	2.20	0.42
1:G:779:VAL:HG13	1:G:851:LEU:HD22	2.02	0.42
1:G:794:HIS:ND1	1:G:796:VAL:HG22	2.35	0.42
1:E:444:ASP:O	1:E:542:GLY:HA2	2.19	0.42
1:E:482:LEU:O	1:E:486:VAL:HG23	2.20	0.42
1:E:567:ILE:HA	1:E:924:GLY:HA3	2.02	0.42
1:E:596:GLU:C	1:E:597:ASN:OD1	2.62	0.42
1:E:869:ASN:O	1:E:873:SER:HB3	2.20	0.42
1:B:482:LEU:O	1:B:486:VAL:HG23	2.20	0.42
1:B:794:HIS:ND1	1:B:796:VAL:HG22	2.35	0.42
1:D:82:LYS:O	1:D:86:ILE:HG12	2.20	0.42
1:D:391:TYR:CD1	1:D:391:TYR:C	2.98	0.42
1:D:482:LEU:O	1:D:486:VAL:HG23	2.20	0.42
1:D:551:ALA:HB1	1:D:624:ASN:OD1	2.20	0.42
1:F:794:HIS:ND1	1:F:796:VAL:HG22	2.35	0.42
1:G:82:LYS:HE3	1:G:222:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:PHE:CD1	1:G:260:LEU:HD13	2.54	0.42
1:G:328:ILE:O	1:G:329:LYS:HB2	2.20	0.42
1:G:332:THR:HB	1:G:336:MET:HE3	2.00	0.42
1:E:204:VAL:HG21	1:E:246:LEU:HD11	2.00	0.42
1:E:354:GLU:OE1	1:E:413:VAL:HG11	2.20	0.42
1:E:358:LEU:O	1:E:359:ARG:HB2	2.19	0.42
1:A:328:ILE:O	1:A:329:LYS:HB2	2.20	0.42
1:A:354:GLU:OE1	1:A:413:VAL:HG11	2.20	0.42
1:A:391:TYR:CD1	1:A:391:TYR:C	2.98	0.42
1:A:794:HIS:ND1	1:A:796:VAL:HG22	2.35	0.42
1:B:82:LYS:HE3	1:B:222:ASP:HB2	2.02	0.42
1:B:635:CYS:O	1:B:636:ARG:HG3	2.18	0.42
1:C:116:PRO:HD2	1:C:119:GLU:OE2	2.20	0.42
1:C:118:HIS:O	1:D:172:TYR:HB2	2.19	0.42
1:C:338:ASP:C	1:C:339:ILE:CG1	2.93	0.42
1:C:355:GLY:O	1:C:487:SER:OG	2.24	0.42
1:C:358:LEU:O	1:C:359:ARG:HB2	2.19	0.42
1:D:358:LEU:O	1:D:359:ARG:HB2	2.19	0.42
1:D:849:PRO:HA	1:D:852:HIS:ND1	2.35	0.42
1:F:373:LYS:HD2	1:E:440:ARG:HH21	1.84	0.42
1:E:139:GLY:O	1:E:140:TYR:C	2.63	0.42
1:E:889:ASP:HA	1:E:892:TRP:HB3	2.00	0.42
1:A:176:TYR:CD1	1:A:176:TYR:N	2.87	0.42
1:A:551:ALA:HB1	1:A:624:ASN:OD1	2.20	0.42
1:A:596:GLU:C	1:A:597:ASN:OD1	2.62	0.42
1:B:204:VAL:HG12	1:B:245:LYS:HB3	2.02	0.42
1:B:354:GLU:OE1	1:B:413:VAL:HG11	2.20	0.42
1:C:82:LYS:O	1:C:86:ILE:HG12	2.20	0.42
1:C:139:GLY:O	1:C:140:TYR:C	2.63	0.42
1:C:758:ARG:HD3	1:C:928:ASP:C	2.44	0.42
1:D:204:VAL:HG21	1:D:246:LEU:HD11	2.00	0.42
1:D:533:SER:HB3	1:E:458:ARG:HH12	1.84	0.42
1:D:567:ILE:HA	1:D:924:GLY:HA3	2.02	0.42
1:D:596:GLU:C	1:D:597:ASN:OD1	2.62	0.42
1:F:176:TYR:CD1	1:F:176:TYR:N	2.87	0.42
1:F:728:ARG:NH1	1:F:728:ARG:CG	2.80	0.42
1:G:482:LEU:O	1:G:486:VAL:HG23	2.19	0.42
1:G:493:SER:H	1:G:727:ILE:HD11	1.84	0.42
1:E:888:SER:O	1:E:891:GLU:N	2.51	0.42
1:A:332:THR:HB	1:A:336:MET:HE3	2.00	0.42
1:A:358:LEU:O	1:A:359:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CD1	1:B:260:LEU:HD13	2.54	0.42
1:B:358:LEU:O	1:B:359:ARG:HB2	2.19	0.42
1:B:491:GLN:CD	1:B:728:ARG:HG2	2.45	0.42
1:B:717:LEU:C	1:B:721:ASN:HD22	2.21	0.42
1:C:38:ARG:HE	1:C:38:ARG:HB3	1.54	0.42
1:C:354:GLU:OE1	1:C:413:VAL:HG11	2.20	0.42
1:C:391:TYR:CD1	1:C:391:TYR:C	2.98	0.42
1:C:834:THR:OG1	1:C:836:LYS:HB2	2.20	0.42
1:F:328:ILE:O	1:F:329:LYS:HB2	2.20	0.42
1:F:342:ILE:HD13	1:F:346:GLN:OE1	2.19	0.42
1:F:444:ASP:O	1:F:542:GLY:HA2	2.19	0.42
1:A:227:PHE:CD1	1:A:260:LEU:HD13	2.54	0.42
1:A:779:VAL:HG13	1:A:851:LEU:HD22	2.02	0.42
1:B:162:ARG:O	1:B:165:HIS:CD2	2.73	0.42
1:B:925:ALA:HB3	1:B:927:TYR:CE2	2.54	0.42
1:C:794:HIS:ND1	1:C:796:VAL:HG22	2.35	0.42
1:C:869:ASN:O	1:C:873:SER:HB3	2.20	0.42
1:D:82:LYS:HE3	1:D:222:ASP:HB2	2.02	0.42
1:D:116:PRO:HD2	1:D:119:GLU:OE2	2.20	0.42
1:D:330:VAL:HG22	1:D:331:LYS:N	2.35	0.42
1:D:338:ASP:C	1:D:339:ILE:CG1	2.93	0.42
1:D:717:LEU:C	1:D:721:ASN:HD22	2.21	0.42
1:F:592:ASN:HB3	1:F:595:THR:HG23	2.02	0.42
1:F:849:PRO:HA	1:F:852:HIS:ND1	2.35	0.42
1:G:204:VAL:HG12	1:G:245:LYS:HB3	2.02	0.42
1:G:204:VAL:HG21	1:G:246:LEU:HD11	2.00	0.42
1:G:342:ILE:HD13	1:G:346:GLN:OE1	2.19	0.42
1:G:354:GLU:OE1	1:G:413:VAL:HG11	2.20	0.42
1:E:116:PRO:HD2	1:E:119:GLU:OE2	2.20	0.42
1:E:391:TYR:C	1:E:391:TYR:CD1	2.98	0.42
1:E:761:GLU:O	1:E:762:HIS:HB2	2.20	0.42
1:E:834:THR:OG1	1:E:836:LYS:HB2	2.20	0.42
1:E:849:PRO:HA	1:E:852:HIS:ND1	2.35	0.42
1:A:82:LYS:O	1:A:86:ILE:HG12	2.20	0.42
1:A:204:VAL:HG12	1:A:245:LYS:HB3	2.02	0.42
1:A:357:ASN:ND2	1:A:728:ARG:HB3	2.33	0.42
1:B:82:LYS:O	1:B:86:ILE:HG12	2.20	0.41
1:B:338:ASP:C	1:B:339:ILE:CG1	2.93	0.41
1:B:834:THR:OG1	1:B:836:LYS:HB2	2.20	0.41
1:B:893:ASP:O	1:B:897:LYS:HG2	2.20	0.41
1:C:162:ARG:O	1:C:165:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:VAL:HG22	1:C:331:LYS:N	2.35	0.41
1:C:482:LEU:O	1:C:486:VAL:HG23	2.19	0.41
1:C:596:GLU:C	1:C:597:ASN:OD1	2.62	0.41
1:D:436:TYR:CD2	1:E:255:ARG:NE	2.88	0.41
1:D:500:MET:HG3	1:D:734:ILE:HD13	2.01	0.41
1:F:120:PRO:HG2	1:F:123:VAL:HG23	2.01	0.41
1:G:543:ARG:NH2	1:A:459:ASP:CG	2.78	0.41
1:G:592:ASN:HB3	1:G:595:THR:HG23	2.02	0.41
1:G:849:PRO:HA	1:G:852:HIS:ND1	2.35	0.41
1:E:204:VAL:HG12	1:E:245:LYS:HB3	2.02	0.41
1:E:330:VAL:HG22	1:E:331:LYS:N	2.35	0.41
1:A:162:ARG:O	1:A:165:HIS:CD2	2.73	0.41
1:A:656:ILE:HG22	1:A:657:VAL:O	2.19	0.41
1:B:330:VAL:HG22	1:B:331:LYS:N	2.35	0.41
1:B:768:GLN:HG3	1:B:931:THR:HG21	2.01	0.41
1:C:279:GLU:H	1:C:279:GLU:CD	2.25	0.41
1:D:262:ARG:HH11	1:E:277:GLU:CD	2.27	0.41
1:D:639:ARG:HH21	1:D:711:THR:HG23	1.85	0.41
1:D:892:TRP:CE3	1:D:895:LEU:HD12	2.56	0.41
1:F:540:SER:HB3	1:F:544:ILE:HG22	2.03	0.41
1:E:82:LYS:HE3	1:E:222:ASP:HB2	2.02	0.41
1:A:592:ASN:HB3	1:A:595:THR:HG23	2.02	0.41
1:A:758:ARG:HD3	1:A:928:ASP:C	2.45	0.41
1:A:849:PRO:HA	1:A:852:HIS:ND1	2.35	0.41
1:B:849:PRO:HA	1:B:852:HIS:ND1	2.35	0.41
1:C:493:SER:H	1:C:727:ILE:HD11	1.85	0.41
1:C:892:TRP:CE3	1:C:895:LEU:HD12	2.56	0.41
1:D:342:ILE:HD13	1:D:346:GLN:OE1	2.19	0.41
1:F:391:TYR:CD1	1:F:391:TYR:C	2.98	0.41
1:F:551:ALA:HB1	1:F:624:ASN:OD1	2.20	0.41
1:F:626:ILE:HG12	1:F:782:PHE:CE2	2.56	0.41
1:F:711:THR:O	1:F:715:GLN:N	2.42	0.41
1:G:162:ARG:O	1:G:165:HIS:CD2	2.73	0.41
1:G:567:ILE:HA	1:G:924:GLY:HA3	2.02	0.41
1:G:728:ARG:HG3	1:G:728:ARG:HH11	1.84	0.41
1:E:82:LYS:O	1:E:86:ILE:HG12	2.20	0.41
1:E:328:ILE:O	1:E:329:LYS:HB2	2.20	0.41
1:A:116:PRO:HD2	1:A:119:GLU:OE2	2.20	0.41
1:A:330:VAL:HG22	1:A:331:LYS:N	2.35	0.41
1:C:540:SER:HB3	1:C:544:ILE:HG22	2.03	0.41
1:C:639:ARG:HH21	1:C:711:THR:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:PHE:CD1	1:C:782:PHE:C	2.99	0.41
1:C:792:LEU:CD2	1:C:800:GLU:OE1	2.69	0.41
1:C:849:PRO:HA	1:C:852:HIS:ND1	2.35	0.41
1:D:348:ILE:HG23	1:D:371:LEU:HD23	2.03	0.41
1:D:441:PHE:O	1:D:442:GLY:C	2.64	0.41
1:D:568:GLY:HA2	1:D:570:PHE:HE1	1.85	0.41
1:D:761:GLU:O	1:D:762:HIS:HB2	2.20	0.41
1:G:430:TYR:CE1	1:A:255:ARG:HG2	2.55	0.41
1:G:540:SER:HB3	1:G:544:ILE:HG22	2.03	0.41
1:G:568:GLY:HA2	1:G:570:PHE:HE1	1.85	0.41
1:E:338:ASP:C	1:E:339:ILE:CG1	2.93	0.41
1:E:756:LEU:CA	1:E:927:TYR:HE1	2.30	0.41
1:A:568:GLY:HA2	1:A:570:PHE:HE1	1.85	0.41
1:B:139:GLY:O	1:B:140:TYR:C	2.63	0.41
1:B:391:TYR:C	1:B:391:TYR:CD1	2.98	0.41
1:B:568:GLY:HA2	1:B:570:PHE:HE1	1.85	0.41
1:B:592:ASN:HB3	1:B:595:THR:HG23	2.03	0.41
1:B:779:VAL:HG13	1:B:851:LEU:HD22	2.02	0.41
1:B:892:TRP:CE3	1:B:895:LEU:HD12	2.56	0.41
1:C:204:VAL:HG12	1:C:245:LYS:CB	2.51	0.41
1:C:591:PHE:CZ	1:C:604:MET:HE2	2.56	0.41
1:D:374:GLN:NE2	1:D:477:ASN:OD1	2.44	0.41
1:D:626:ILE:HG12	1:D:782:PHE:CE2	2.56	0.41
1:D:779:VAL:HG13	1:D:851:LEU:HD22	2.02	0.41
1:D:794:HIS:ND1	1:D:796:VAL:HG22	2.35	0.41
1:F:91:LYS:C	1:F:93:LEU:N	2.78	0.41
1:F:591:PHE:CZ	1:F:604:MET:HE2	2.56	0.41
1:G:591:PHE:CZ	1:G:604:MET:HE2	2.56	0.41
1:E:568:GLY:HA2	1:E:570:PHE:HE1	1.85	0.41
1:E:594:ASP:OD1	1:E:594:ASP:N	2.50	0.41
1:E:782:PHE:CD1	1:E:782:PHE:C	2.99	0.41
1:A:191:ILE:HG22	1:A:198:GLU:CD	2.46	0.41
1:A:892:TRP:CE3	1:A:895:LEU:HD12	2.56	0.41
1:B:540:SER:HB3	1:B:544:ILE:HG22	2.03	0.41
1:C:191:ILE:HG22	1:C:198:GLU:CD	2.46	0.41
1:C:364:ALA:O	1:C:368:VAL:HG23	2.21	0.41
1:D:364:ALA:O	1:D:368:VAL:HG23	2.21	0.41
1:D:540:SER:HB3	1:D:544:ILE:HG22	2.03	0.41
1:D:782:PHE:C	1:D:782:PHE:CD1	2.99	0.41
1:F:330:VAL:HG22	1:F:331:LYS:N	2.35	0.41
1:F:568:GLY:HA2	1:F:570:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:VAL:HG22	1:G:331:LYS:N	2.36	0.41
1:G:551:ALA:HB1	1:G:624:ASN:OD1	2.20	0.41
1:G:892:TRP:CE3	1:G:895:LEU:HD12	2.56	0.41
1:E:165:HIS:CE1	1:E:176:TYR:HD2	2.39	0.41
1:E:348:ILE:HG23	1:E:371:LEU:HD23	2.03	0.41
1:E:500:MET:HG3	1:E:734:ILE:HD13	2.01	0.41
1:A:82:LYS:HE3	1:A:222:ASP:HB2	2.02	0.41
1:A:482:LEU:O	1:A:486:VAL:HG23	2.20	0.41
1:A:591:PHE:CZ	1:A:604:MET:HE2	2.56	0.41
1:A:861:ILE:HD12	1:A:895:LEU:HD22	2.03	0.41
1:B:191:ILE:HG22	1:B:198:GLU:CD	2.46	0.41
1:B:493:SER:H	1:B:727:ILE:HD11	1.85	0.41
1:B:561:SER:H	1:B:562:PRO:HD2	1.86	0.41
1:B:567:ILE:HA	1:B:924:GLY:HA3	2.02	0.41
1:B:861:ILE:HD12	1:B:895:LEU:HD22	2.03	0.41
1:C:431:ARG:NH1	1:E:277:GLU:OE2	2.53	0.41
1:C:441:PHE:O	1:C:442:GLY:C	2.64	0.41
1:C:567:ILE:HA	1:C:924:GLY:HA3	2.02	0.41
1:D:861:ILE:HD12	1:D:895:LEU:HD22	2.03	0.41
1:F:116:PRO:HD2	1:F:119:GLU:OE2	2.20	0.41
1:G:91:LYS:C	1:G:93:LEU:N	2.78	0.41
1:G:116:PRO:HD2	1:G:119:GLU:OE2	2.20	0.41
1:G:191:ILE:HG22	1:G:198:GLU:CD	2.46	0.41
1:G:391:TYR:C	1:G:391:TYR:CD1	2.98	0.41
1:G:626:ILE:HG12	1:G:782:PHE:CE2	2.56	0.41
1:G:639:ARG:HH21	1:G:711:THR:HG23	1.85	0.41
1:E:171:GLU:N	1:E:171:GLU:OE2	2.54	0.41
1:A:244:ARG:C	1:A:246:LEU:H	2.29	0.41
1:A:626:ILE:HG12	1:A:782:PHE:CE2	2.56	0.41
1:A:639:ARG:HH21	1:A:711:THR:HG23	1.85	0.41
1:A:782:PHE:C	1:A:782:PHE:CD1	2.99	0.41
1:A:834:THR:OG1	1:A:836:LYS:HB2	2.20	0.41
1:B:589:LYS:O	1:B:921:THR:HG23	2.21	0.41
1:B:792:LEU:CD2	1:B:800:GLU:OE1	2.69	0.41
1:C:171:GLU:OE2	1:C:171:GLU:N	2.54	0.41
1:C:568:GLY:HA2	1:C:570:PHE:HE1	1.85	0.41
1:C:592:ASN:HB3	1:C:595:THR:HG23	2.02	0.41
1:D:204:VAL:HG12	1:D:245:LYS:HB3	2.02	0.41
1:D:204:VAL:HG12	1:D:245:LYS:CB	2.51	0.41
1:D:354:GLU:OE1	1:D:413:VAL:HG11	2.20	0.41
1:D:467:ARG:HB2	1:D:469:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:789:GLU:O	1:D:793:TYR:N	2.46	0.41
1:D:792:LEU:CD2	1:D:800:GLU:OE1	2.69	0.41
1:D:799:ARG:NE	1:D:800:GLU:O	2.48	0.41
1:F:834:THR:OG1	1:F:836:LYS:HB2	2.20	0.41
1:F:892:TRP:CE3	1:F:895:LEU:HD12	2.56	0.41
1:G:467:ARG:HB2	1:G:469:GLN:OE1	2.21	0.41
1:G:782:PHE:C	1:G:782:PHE:CD1	2.99	0.41
1:G:834:THR:OG1	1:G:836:LYS:HB2	2.20	0.41
1:G:861:ILE:HD12	1:G:895:LEU:HD22	2.03	0.41
1:E:426:LEU:CD1	1:E:436:TYR:HE1	2.27	0.41
1:E:441:PHE:O	1:E:442:GLY:C	2.64	0.41
1:E:591:PHE:CZ	1:E:604:MET:HE2	2.56	0.41
1:E:711:THR:O	1:E:715:GLN:N	2.42	0.41
1:A:467:ARG:HB2	1:A:469:GLN:OE1	2.21	0.41
1:A:792:LEU:CD2	1:A:800:GLU:OE1	2.69	0.41
1:B:195:ASP:OD1	1:B:197:SER:N	2.54	0.41
1:B:204:VAL:HG12	1:B:245:LYS:CB	2.51	0.41
1:B:244:ARG:C	1:B:246:LEU:H	2.29	0.41
1:B:364:ALA:O	1:B:368:VAL:HG23	2.21	0.41
1:B:591:PHE:CZ	1:B:604:MET:HE2	2.56	0.41
1:B:782:PHE:C	1:B:782:PHE:CD1	2.99	0.41
1:C:328:ILE:O	1:C:329:LYS:HB2	2.20	0.41
1:C:467:ARG:HB2	1:C:469:GLN:OE1	2.21	0.41
1:C:626:ILE:HG12	1:C:782:PHE:CE2	2.56	0.41
1:C:761:GLU:O	1:C:762:HIS:HB2	2.20	0.41
1:D:328:ILE:O	1:D:329:LYS:HB2	2.20	0.41
1:D:589:LYS:O	1:D:921:THR:HG23	2.21	0.41
1:D:591:PHE:CZ	1:D:604:MET:HE2	2.56	0.41
1:F:162:ARG:O	1:F:165:HIS:CD2	2.73	0.41
1:F:173:LYS:HD2	1:F:176:TYR:HE1	1.85	0.41
1:F:173:LYS:CD	1:F:176:TYR:CE1	3.04	0.41
1:F:191:ILE:HG22	1:F:198:GLU:CD	2.46	0.41
1:F:293:LEU:HD22	1:E:224:ASP:O	2.20	0.41
1:F:338:ASP:C	1:F:339:ILE:CG1	2.93	0.41
1:F:354:GLU:OE1	1:F:413:VAL:HG11	2.20	0.41
1:F:561:SER:H	1:F:562:PRO:HD2	1.86	0.41
1:F:757:TYR:CE1	1:F:932:PRO:HD2	2.55	0.41
1:F:782:PHE:C	1:F:782:PHE:CD1	2.99	0.41
1:G:204:VAL:HG12	1:G:245:LYS:CB	2.51	0.41
1:G:244:ARG:C	1:G:246:LEU:H	2.29	0.41
1:G:758:ARG:HD3	1:G:928:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:792:LEU:CD2	1:G:800:GLU:OE1	2.69	0.41
1:E:204:VAL:HG12	1:E:245:LYS:CB	2.51	0.41
1:E:561:SER:H	1:E:562:PRO:HD2	1.86	0.41
1:E:794:HIS:ND1	1:E:796:VAL:HG22	2.35	0.41
1:E:861:ILE:HD12	1:E:895:LEU:HD22	2.03	0.41
1:A:204:VAL:HG12	1:A:245:LYS:CB	2.51	0.41
1:A:540:SER:HB3	1:A:544:ILE:HG22	2.03	0.41
1:A:561:SER:H	1:A:562:PRO:HD2	1.86	0.41
1:A:567:ILE:HA	1:A:924:GLY:HA3	2.02	0.41
1:A:589:LYS:O	1:A:921:THR:HG23	2.21	0.41
1:C:195:ASP:OD1	1:C:197:SER:N	2.54	0.41
1:C:330:VAL:HG22	1:C:331:LYS:H	1.86	0.41
1:C:779:VAL:HG13	1:C:851:LEU:HD22	2.02	0.41
1:D:790:GLU:CD	1:D:839:HIS:HA	2.46	0.41
1:F:171:GLU:OE2	1:F:171:GLU:N	2.54	0.41
1:F:204:VAL:HG12	1:F:245:LYS:HB3	2.02	0.41
1:F:261:ILE:CD1	1:F:298:LEU:CD1	2.96	0.41
1:F:315:GLN:NE2	1:E:439:HIS:CB	2.84	0.41
1:G:38:ARG:HG2	1:G:89:VAL:HG22	2.02	0.41
1:E:195:ASP:OD1	1:E:197:SER:N	2.54	0.41
1:E:364:ALA:O	1:E:368:VAL:HG23	2.21	0.41
1:E:510:ILE:HD13	1:E:510:ILE:HA	1.90	0.41
1:E:589:LYS:O	1:E:921:THR:HG23	2.21	0.41
1:E:639:ARG:HH21	1:E:711:THR:HG23	1.85	0.41
1:E:790:GLU:CD	1:E:839:HIS:HA	2.46	0.41
1:A:888:SER:O	1:A:891:GLU:N	2.51	0.41
1:B:91:LYS:C	1:B:93:LEU:N	2.78	0.40
1:B:116:PRO:HD2	1:B:119:GLU:OE2	2.20	0.40
1:C:153:TRP:CE3	1:C:206:ARG:HB3	2.56	0.40
1:D:171:GLU:N	1:D:171:GLU:OE2	2.54	0.40
1:D:244:ARG:C	1:D:246:LEU:H	2.29	0.40
1:D:330:VAL:HG22	1:D:331:LYS:H	1.86	0.40
1:F:38:ARG:HG2	1:F:89:VAL:HG22	2.03	0.40
1:F:139:GLY:O	1:F:140:TYR:C	2.63	0.40
1:F:495:SER:HB2	1:F:633:SER:HB3	2.04	0.40
1:F:792:LEU:CD2	1:F:800:GLU:OE1	2.69	0.40
1:G:495:SER:HB2	1:G:633:SER:HB3	2.03	0.40
1:E:162:ARG:O	1:E:165:HIS:CD2	2.73	0.40
1:A:91:LYS:C	1:A:93:LEU:N	2.78	0.40
1:B:171:GLU:OE2	1:B:171:GLU:N	2.54	0.40
1:B:330:VAL:HG22	1:B:331:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:THR:HB	1:B:336:MET:CE	2.52	0.40
1:B:462:THR:HG22	1:B:465:TYR:HE1	1.86	0.40
1:B:773:LYS:NZ	1:B:862:ASN:OD1	2.34	0.40
1:C:589:LYS:O	1:C:921:THR:HG23	2.21	0.40
1:C:889:ASP:O	1:C:893:ASP:N	2.41	0.40
1:D:165:HIS:CE1	1:D:176:TYR:HD2	2.39	0.40
1:D:758:ARG:HD3	1:D:928:ASP:C	2.46	0.40
1:D:834:THR:OG1	1:D:836:LYS:HB2	2.20	0.40
1:F:761:GLU:O	1:F:762:HIS:HB2	2.20	0.40
1:F:861:ILE:HD12	1:F:895:LEU:HD22	2.03	0.40
1:E:792:LEU:CD2	1:E:800:GLU:OE1	2.69	0.40
1:A:38:ARG:HG2	1:A:89:VAL:HG22	2.02	0.40
1:A:462:THR:HG22	1:A:465:TYR:HE1	1.86	0.40
1:C:165:HIS:CE1	1:C:176:TYR:HD2	2.39	0.40
1:C:495:SER:HB2	1:C:633:SER:HB3	2.03	0.40
1:C:790:GLU:CD	1:C:839:HIS:HA	2.46	0.40
1:C:861:ILE:HD12	1:C:895:LEU:HD22	2.03	0.40
1:D:162:ARG:O	1:D:165:HIS:CD2	2.73	0.40
1:D:191:ILE:HG22	1:D:198:GLU:CD	2.46	0.40
1:F:139:GLY:C	1:F:140:TYR:CD1	3.00	0.40
1:F:181:LEU:HD22	1:E:130:ASN:ND2	2.36	0.40
1:F:639:ARG:HH21	1:F:711:THR:HG23	1.85	0.40
1:G:139:GLY:O	1:G:140:TYR:C	2.63	0.40
1:G:330:VAL:HG22	1:G:331:LYS:H	1.87	0.40
1:G:364:ALA:O	1:G:368:VAL:HG23	2.21	0.40
1:E:38:ARG:HG2	1:E:89:VAL:HG22	2.02	0.40
1:E:330:VAL:HG22	1:E:331:LYS:H	1.86	0.40
1:E:592:ASN:HB3	1:E:595:THR:HG23	2.03	0.40
1:E:626:ILE:HG12	1:E:782:PHE:CE2	2.56	0.40
1:B:38:ARG:HG2	1:B:89:VAL:HG22	2.02	0.40
1:B:272:THR:HG21	1:A:267:GLU:HA	2.02	0.40
1:B:439:HIS:HB3	1:C:312:THR:CG2	2.51	0.40
1:B:441:PHE:O	1:B:442:GLY:C	2.63	0.40
1:C:499:GLN:O	1:C:500:MET:C	2.65	0.40
1:C:595:THR:O	1:C:597:ASN:OD1	2.40	0.40
1:C:646:PHE:O	1:C:650:ILE:HG12	2.22	0.40
1:C:773:LYS:NZ	1:C:862:ASN:OD1	2.34	0.40
1:D:195:ASP:OD1	1:D:197:SER:N	2.54	0.40
1:D:462:THR:HG22	1:D:465:TYR:HE1	1.86	0.40
1:D:592:ASN:HB3	1:D:595:THR:HG23	2.02	0.40
1:D:646:PHE:O	1:D:650:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:PHE:HB2	1:F:249:VAL:HG22	2.04	0.40
1:F:330:VAL:HG22	1:F:331:LYS:H	1.86	0.40
1:G:72:PHE:HB2	1:G:249:VAL:HG22	2.04	0.40
1:G:139:GLY:C	1:G:140:TYR:CD1	3.00	0.40
1:G:171:GLU:OE2	1:G:171:GLU:N	2.54	0.40
1:G:462:THR:HG22	1:G:465:TYR:HE1	1.86	0.40
1:G:646:PHE:O	1:G:650:ILE:HG12	2.22	0.40
1:G:761:GLU:O	1:G:762:HIS:HB2	2.20	0.40
1:G:790:GLU:CD	1:G:839:HIS:HA	2.47	0.40
1:E:789:GLU:O	1:E:793:TYR:N	2.46	0.40
1:A:330:VAL:HG22	1:A:331:LYS:H	1.87	0.40
1:A:761:GLU:O	1:A:762:HIS:HB2	2.20	0.40
1:B:467:ARG:HB2	1:B:469:GLN:OE1	2.21	0.40
1:B:595:THR:O	1:B:597:ASN:OD1	2.40	0.40
1:B:761:GLU:O	1:B:762:HIS:HB2	2.20	0.40
1:B:790:GLU:CD	1:B:839:HIS:HA	2.46	0.40
1:C:38:ARG:HG2	1:C:89:VAL:HG22	2.02	0.40
1:C:159:GLN:HA	1:C:162:ARG:NE	2.37	0.40
1:D:153:TRP:CE3	1:D:206:ARG:HB3	2.56	0.40
1:D:561:SER:H	1:D:562:PRO:HD2	1.86	0.40
1:D:752:HIS:NE2	1:D:811:VAL:O	2.37	0.40
1:F:467:ARG:HB2	1:F:469:GLN:OE1	2.21	0.40
1:G:344:VAL:CG1	1:G:345:ARG:N	2.85	0.40
1:G:348:ILE:HG23	1:G:371:LEU:HD23	2.03	0.40
1:E:261:ILE:CD1	1:E:298:LEU:CD1	2.96	0.40
1:A:139:GLY:O	1:A:140:TYR:C	2.63	0.40
1:A:139:GLY:C	1:A:140:TYR:CD1	3.00	0.40
1:A:595:THR:O	1:A:597:ASN:OD1	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	765/947 (81%)	687 (90%)	69 (9%)	9 (1%)	10	19
1	B	765/947 (81%)	685 (90%)	70 (9%)	10 (1%)	9	17
1	C	765/947 (81%)	688 (90%)	68 (9%)	9 (1%)	10	19
1	D	764/947 (81%)	686 (90%)	68 (9%)	10 (1%)	9	17
1	E	761/947 (80%)	684 (90%)	67 (9%)	10 (1%)	9	17
1	F	765/947 (81%)	687 (90%)	68 (9%)	10 (1%)	9	17
1	G	765/947 (81%)	687 (90%)	69 (9%)	9 (1%)	10	19
All	All	5350/6629 (81%)	4804 (90%)	479 (9%)	67 (1%)	12	17

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	LYS
1	C	311	LYS
1	D	311	LYS
1	F	311	LYS
1	G	311	LYS
1	E	311	LYS
1	A	311	LYS
1	B	337	GLN
1	B	339	ILE
1	B	459	ASP
1	B	561	SER
1	C	339	ILE
1	C	459	ASP
1	C	561	SER
1	D	337	GLN
1	D	339	ILE
1	D	459	ASP
1	D	561	SER
1	F	337	GLN
1	F	339	ILE
1	F	459	ASP
1	F	561	SER
1	G	339	ILE
1	G	459	ASP
1	G	561	SER
1	E	337	GLN
1	E	339	ILE
1	E	459	ASP
1	E	561	SER

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Mol	Chain	Res	Type
1	A	339	ILE
1	A	459	ASP
1	A	561	SER
1	B	151	GLU
1	B	336	MET
1	C	151	GLU
1	C	337	GLN
1	D	151	GLU
1	D	336	MET
1	F	151	GLU
1	F	336	MET
1	G	151	GLU
1	G	337	GLN
1	E	151	GLU
1	E	336	MET
1	A	151	GLU
1	A	337	GLN
1	B	343	ASP
1	C	343	ASP
1	D	343	ASP
1	F	343	ASP
1	G	343	ASP
1	E	117	ARG
1	E	343	ASP
1	A	343	ASP
1	B	117	ARG
1	B	309	GLN
1	C	117	ARG
1	C	309	GLN
1	D	117	ARG
1	D	309	GLN
1	F	117	ARG
1	F	309	GLN
1	G	117	ARG
1	G	309	GLN
1	E	309	GLN
1	A	117	ARG
1	A	309	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	697/837 (83%)	621 (89%)	76 (11%)	6	12
1	B	697/837 (83%)	624 (90%)	73 (10%)	6	13
1	C	697/837 (83%)	623 (89%)	74 (11%)	6	12
1	D	696/837 (83%)	625 (90%)	71 (10%)	7	14
1	E	693/837 (83%)	623 (90%)	70 (10%)	7	14
1	F	697/837 (83%)	624 (90%)	73 (10%)	6	13
1	G	697/837 (83%)	626 (90%)	71 (10%)	7	14
All	All	4874/5859 (83%)	4366 (90%)	508 (10%)	9	13

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ARG
1	B	39	ASP
1	B	40	GLN
1	B	105	LYS
1	B	150	LYS
1	B	151	GLU
1	B	154	GLN
1	B	170	LYS
1	B	171	GLU
1	B	173	LYS
1	B	197	SER
1	B	206	ARG
1	B	212	ASP
1	B	224	ASP
1	B	228	ASP
1	B	242	ASN
1	B	258	SER
1	B	262	ARG
1	B	270	SER
1	B	271	LYS

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Mol	Chain	Res	Type
1	B	278	LYS
1	B	279	GLU
1	B	298	LEU
1	B	311	LYS
1	B	313	MET
1	B	328	ILE
1	B	338	ASP
1	B	340	ASP
1	B	360	GLU
1	B	370	GLU
1	B	376	VAL
1	B	380	MET
1	B	392	HIS
1	B	436	TYR
1	B	437	GLU
1	B	443	MET
1	B	473	GLU
1	B	516	THR
1	B	526	GLU
1	B	531	LEU
1	B	539	MET
1	B	540	SER
1	B	545	GLU
1	B	561	SER
1	B	573	MET
1	B	584	MET
1	B	595	THR
1	B	596	GLU
1	B	606	SER
1	B	617	MET
1	B	621	SER
1	B	632	ILE
1	B	633	SER
1	B	636	ARG
1	B	661	SER
1	B	715	GLN
1	B	723	ILE
1	B	725	ILE
1	B	728	ARG
1	B	739	SER
1	B	765	MET
1	B	798	ASP

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Mol	Chain	Res	Type
1	B	800	GLU
1	B	818	GLU
1	B	834	THR
1	B	836	LYS
1	B	855	ILE
1	B	868	LEU
1	B	873	SER
1	B	890	GLU
1	B	893	ASP
1	B	930	ASP
1	B	931	THR
1	C	38	ARG
1	C	39	ASP
1	C	40	GLN
1	C	105	LYS
1	C	150	LYS
1	C	151	GLU
1	C	154	GLN
1	C	170	LYS
1	C	171	GLU
1	C	173	LYS
1	C	197	SER
1	C	206	ARG
1	C	212	ASP
1	C	224	ASP
1	C	228	ASP
1	C	242	ASN
1	C	258	SER
1	C	262	ARG
1	C	270	SER
1	C	271	LYS
1	C	278	LYS
1	C	279	GLU
1	C	298	LEU
1	C	311	LYS
1	C	313	MET
1	C	328	ILE
1	C	337	GLN
1	C	338	ASP
1	C	340	ASP
1	C	360	GLU
1	C	370	GLU

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Mol	Chain	Res	Type
1	C	376	VAL
1	C	380	MET
1	C	392	HIS
1	C	436	TYR
1	C	437	GLU
1	C	443	MET
1	C	473	GLU
1	C	516	THR
1	C	526	GLU
1	C	531	LEU
1	C	539	MET
1	C	540	SER
1	C	545	GLU
1	C	561	SER
1	C	573	MET
1	C	584	MET
1	C	595	THR
1	C	596	GLU
1	C	606	SER
1	C	617	MET
1	C	621	SER
1	C	632	ILE
1	C	633	SER
1	C	636	ARG
1	C	661	SER
1	C	715	GLN
1	C	723	ILE
1	C	725	ILE
1	C	739	SER
1	C	765	MET
1	C	798	ASP
1	C	800	GLU
1	C	818	GLU
1	C	834	THR
1	C	836	LYS
1	C	855	ILE
1	C	868	LEU
1	C	873	SER
1	C	890	GLU
1	C	893	ASP
1	C	929	LYS
1	C	930	ASP

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Mol	Chain	Res	Type
1	C	931	THR
1	D	38	ARG
1	D	39	ASP
1	D	40	GLN
1	D	105	LYS
1	D	150	LYS
1	D	151	GLU
1	D	154	GLN
1	D	170	LYS
1	D	171	GLU
1	D	173	LYS
1	D	197	SER
1	D	206	ARG
1	D	212	ASP
1	D	224	ASP
1	D	228	ASP
1	D	242	ASN
1	D	258	SER
1	D	262	ARG
1	D	270	SER
1	D	271	LYS
1	D	278	LYS
1	D	279	GLU
1	D	298	LEU
1	D	311	LYS
1	D	313	MET
1	D	328	ILE
1	D	338	ASP
1	D	340	ASP
1	D	360	GLU
1	D	370	GLU
1	D	376	VAL
1	D	380	MET
1	D	392	HIS
1	D	436	TYR
1	D	437	GLU
1	D	443	MET
1	D	473	GLU
1	D	516	THR
1	D	526	GLU
1	D	531	LEU
1	D	539	MET

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Mol	Chain	Res	Type
1	D	540	SER
1	D	545	GLU
1	D	561	SER
1	D	573	MET
1	D	584	MET
1	D	595	THR
1	D	596	GLU
1	D	606	SER
1	D	617	MET
1	D	621	SER
1	D	632	ILE
1	D	633	SER
1	D	636	ARG
1	D	661	SER
1	D	715	GLN
1	D	723	ILE
1	D	725	ILE
1	D	739	SER
1	D	765	MET
1	D	798	ASP
1	D	800	GLU
1	D	818	GLU
1	D	834	THR
1	D	836	LYS
1	D	855	ILE
1	D	868	LEU
1	D	873	SER
1	D	890	GLU
1	D	893	ASP
1	D	930	ASP
1	F	38	ARG
1	F	39	ASP
1	F	40	GLN
1	F	105	LYS
1	F	150	LYS
1	F	151	GLU
1	F	154	GLN
1	F	170	LYS
1	F	171	GLU
1	F	173	LYS
1	F	197	SER
1	F	206	ARG

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Mol	Chain	Res	Type
1	F	212	ASP
1	F	224	ASP
1	F	228	ASP
1	F	242	ASN
1	F	258	SER
1	F	262	ARG
1	F	270	SER
1	F	271	LYS
1	F	278	LYS
1	F	279	GLU
1	F	298	LEU
1	F	311	LYS
1	F	313	MET
1	F	328	ILE
1	F	338	ASP
1	F	340	ASP
1	F	360	GLU
1	F	370	GLU
1	F	376	VAL
1	F	380	MET
1	F	392	HIS
1	F	436	TYR
1	F	437	GLU
1	F	443	MET
1	F	473	GLU
1	F	516	THR
1	F	526	GLU
1	F	531	LEU
1	F	539	MET
1	F	540	SER
1	F	545	GLU
1	F	561	SER
1	F	573	MET
1	F	584	MET
1	F	595	THR
1	F	596	GLU
1	F	606	SER
1	F	617	MET
1	F	621	SER
1	F	632	ILE
1	F	633	SER
1	F	636	ARG

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Mol	Chain	Res	Type
1	F	661	SER
1	F	715	GLN
1	F	723	ILE
1	F	725	ILE
1	F	739	SER
1	F	765	MET
1	F	798	ASP
1	F	800	GLU
1	F	818	GLU
1	F	834	THR
1	F	836	LYS
1	F	855	ILE
1	F	868	LEU
1	F	873	SER
1	F	890	GLU
1	F	893	ASP
1	F	926	SER
1	F	931	THR
1	F	934	ARG
1	G	38	ARG
1	G	39	ASP
1	G	40	GLN
1	G	105	LYS
1	G	150	LYS
1	G	151	GLU
1	G	154	GLN
1	G	170	LYS
1	G	171	GLU
1	G	173	LYS
1	G	197	SER
1	G	206	ARG
1	G	212	ASP
1	G	224	ASP
1	G	228	ASP
1	G	242	ASN
1	G	258	SER
1	G	262	ARG
1	G	270	SER
1	G	271	LYS
1	G	278	LYS
1	G	279	GLU
1	G	298	LEU

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Mol	Chain	Res	Type
1	G	311	LYS
1	G	313	MET
1	G	328	ILE
1	G	337	GLN
1	G	338	ASP
1	G	340	ASP
1	G	360	GLU
1	G	370	GLU
1	G	376	VAL
1	G	380	MET
1	G	392	HIS
1	G	436	TYR
1	G	437	GLU
1	G	443	MET
1	G	473	GLU
1	G	516	THR
1	G	526	GLU
1	G	531	LEU
1	G	539	MET
1	G	540	SER
1	G	545	GLU
1	G	561	SER
1	G	573	MET
1	G	584	MET
1	G	595	THR
1	G	596	GLU
1	G	606	SER
1	G	617	MET
1	G	621	SER
1	G	632	ILE
1	G	633	SER
1	G	636	ARG
1	G	661	SER
1	G	715	GLN
1	G	723	ILE
1	G	725	ILE
1	G	739	SER
1	G	765	MET
1	G	798	ASP
1	G	800	GLU
1	G	818	GLU
1	G	834	THR

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Mol	Chain	Res	Type
1	G	836	LYS
1	G	855	ILE
1	G	868	LEU
1	G	873	SER
1	G	890	GLU
1	G	893	ASP
1	E	38	ARG
1	E	39	ASP
1	E	40	GLN
1	E	105	LYS
1	E	150	LYS
1	E	151	GLU
1	E	154	GLN
1	E	170	LYS
1	E	171	GLU
1	E	173	LYS
1	E	197	SER
1	E	206	ARG
1	E	212	ASP
1	E	224	ASP
1	E	228	ASP
1	E	242	ASN
1	E	258	SER
1	E	262	ARG
1	E	270	SER
1	E	271	LYS
1	E	278	LYS
1	E	279	GLU
1	E	298	LEU
1	E	311	LYS
1	E	313	MET
1	E	328	ILE
1	E	338	ASP
1	E	340	ASP
1	E	360	GLU
1	E	370	GLU
1	E	376	VAL
1	E	380	MET
1	E	392	HIS
1	E	436	TYR
1	E	437	GLU
1	E	443	MET

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Mol	Chain	Res	Type
1	E	473	GLU
1	E	516	THR
1	E	526	GLU
1	E	531	LEU
1	E	539	MET
1	E	540	SER
1	E	545	GLU
1	E	561	SER
1	E	573	MET
1	E	584	MET
1	E	595	THR
1	E	596	GLU
1	E	606	SER
1	E	617	MET
1	E	621	SER
1	E	632	ILE
1	E	633	SER
1	E	636	ARG
1	E	661	SER
1	E	715	GLN
1	E	723	ILE
1	E	725	ILE
1	E	739	SER
1	E	765	MET
1	E	798	ASP
1	E	800	GLU
1	E	818	GLU
1	E	834	THR
1	E	836	LYS
1	E	855	ILE
1	E	868	LEU
1	E	873	SER
1	E	890	GLU
1	E	893	ASP
1	A	38	ARG
1	A	39	ASP
1	A	40	GLN
1	A	105	LYS
1	A	150	LYS
1	A	151	GLU
1	A	154	GLN
1	A	170	LYS

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Mol	Chain	Res	Type
1	A	171	GLU
1	A	173	LYS
1	A	197	SER
1	A	206	ARG
1	A	212	ASP
1	A	224	ASP
1	A	228	ASP
1	A	242	ASN
1	A	258	SER
1	A	262	ARG
1	A	270	SER
1	A	271	LYS
1	A	278	LYS
1	A	279	GLU
1	A	298	LEU
1	A	311	LYS
1	A	313	MET
1	A	328	ILE
1	A	337	GLN
1	A	338	ASP
1	A	339	ILE
1	A	340	ASP
1	A	360	GLU
1	A	370	GLU
1	A	376	VAL
1	A	380	MET
1	A	392	HIS
1	A	436	TYR
1	A	437	GLU
1	A	443	MET
1	A	473	GLU
1	A	509	SER
1	A	516	THR
1	A	526	GLU
1	A	531	LEU
1	A	539	MET
1	A	540	SER
1	A	545	GLU
1	A	561	SER
1	A	573	MET
1	A	584	MET
1	A	595	THR

Continued on next page...

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Mol	Chain	Res	Type
1	A	596	GLU
1	A	606	SER
1	A	617	MET
1	A	621	SER
1	A	632	ILE
1	A	633	SER
1	A	636	ARG
1	A	661	SER
1	A	715	GLN
1	A	723	ILE
1	A	725	ILE
1	A	739	SER
1	A	765	MET
1	A	798	ASP
1	A	800	GLU
1	A	818	GLU
1	A	834	THR
1	A	836	LYS
1	A	855	ILE
1	A	868	LEU
1	A	873	SER
1	A	890	GLU
1	A	893	ASP
1	A	929	LYS
1	A	930	ASP
1	A	931	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	156	HIS
1	B	159	GLN
1	B	194	GLN
1	B	276	GLN
1	B	309	GLN
1	C	118	HIS
1	C	156	HIS
1	C	159	GLN
1	C	194	GLN
1	C	276	GLN
1	C	309	GLN
1	D	156	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	159	GLN
1	D	194	GLN
1	D	276	GLN
1	D	295	GLN
1	D	309	GLN
1	D	530	GLN
1	F	194	GLN
1	F	276	GLN
1	F	295	GLN
1	F	461	ASN
1	F	759	ASN
1	G	156	HIS
1	G	159	GLN
1	G	194	GLN
1	G	276	GLN
1	G	309	GLN
1	E	194	GLN
1	E	276	GLN
1	E	295	GLN
1	E	309	GLN
1	E	461	ASN
1	E	530	GLN
1	A	94	ASN
1	A	156	HIS
1	A	159	GLN
1	A	194	GLN
1	A	276	GLN
1	A	309	GLN
1	A	768	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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](#)

There are no chain breaks in this entry.

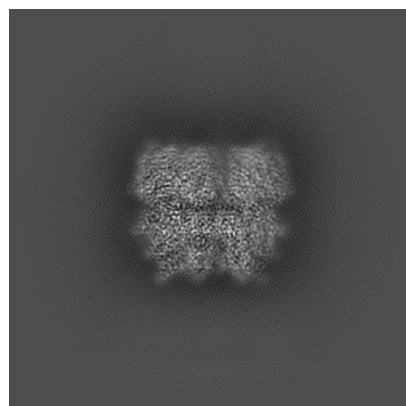
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29323. These allow visual inspection of the internal detail of the map and identification of artifacts.

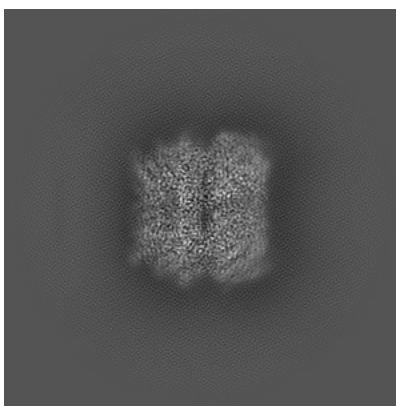
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

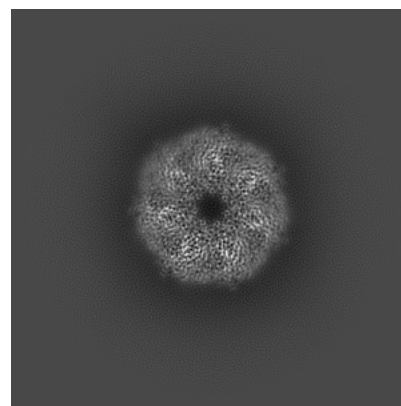
6.1.1 Primary map



X

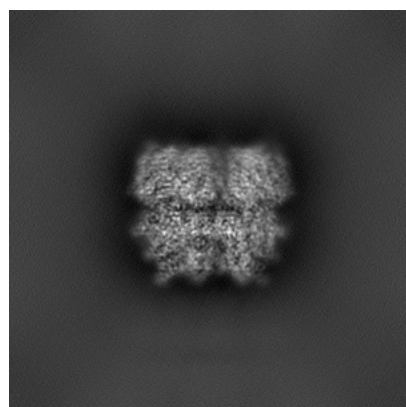


Y

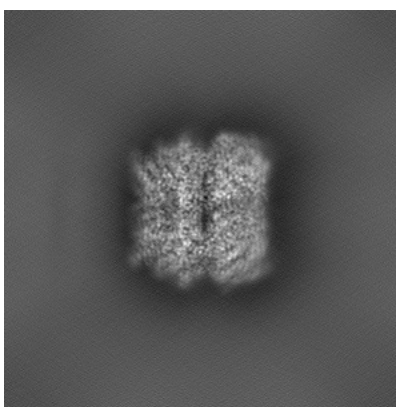


Z

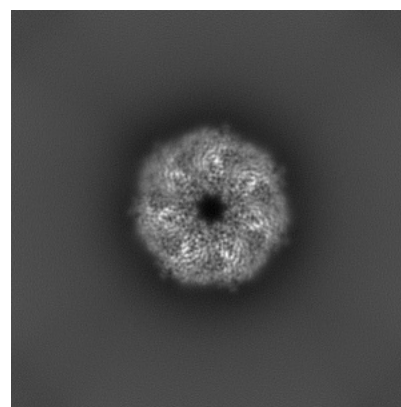
6.1.2 Raw map



X



Y

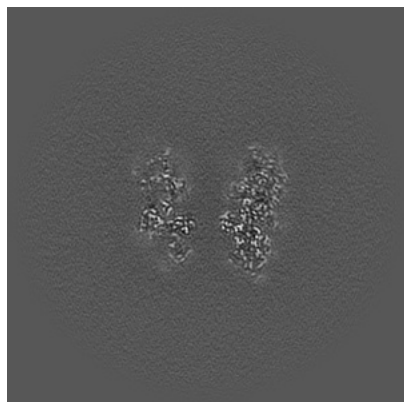


Z

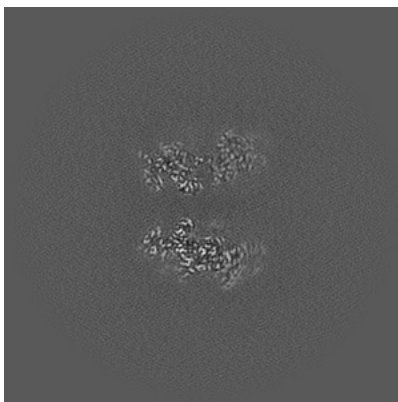
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

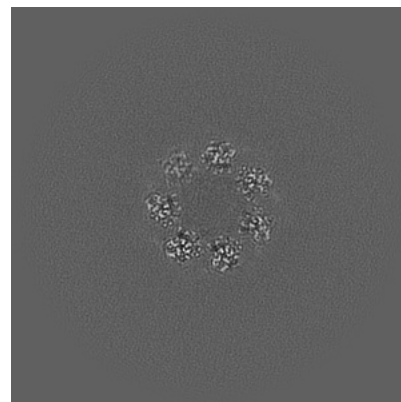
6.2.1 Primary map



X Index: 208

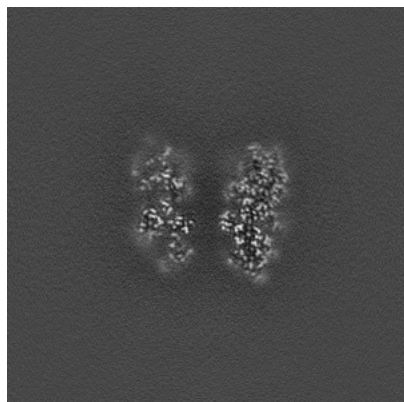


Y Index: 208

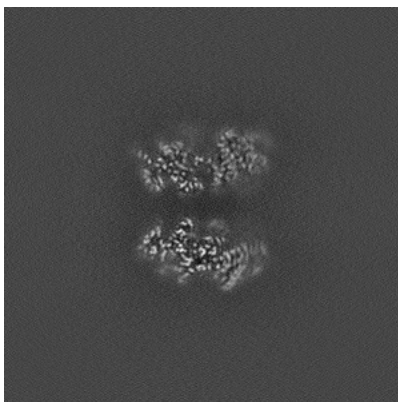


Z Index: 208

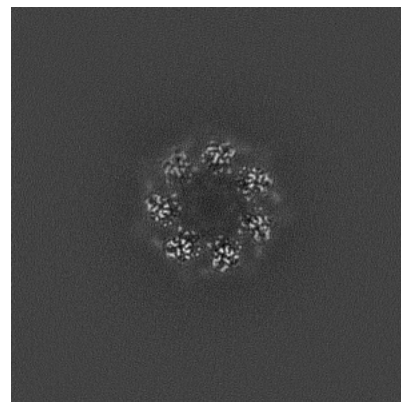
6.2.2 Raw map



X Index: 208



Y Index: 208

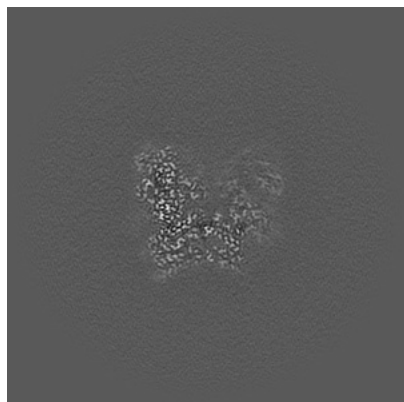


Z Index: 208

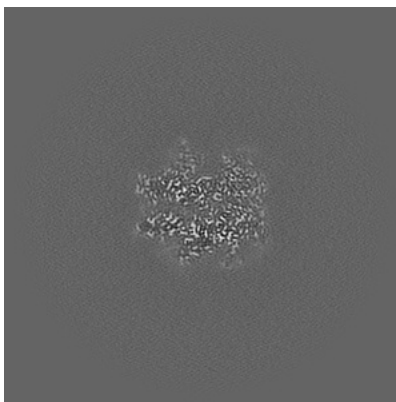
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

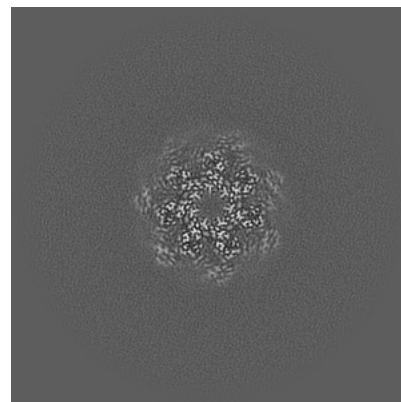
6.3.1 Primary map



X Index: 182

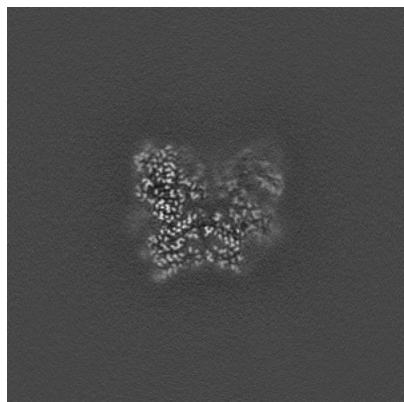


Y Index: 165

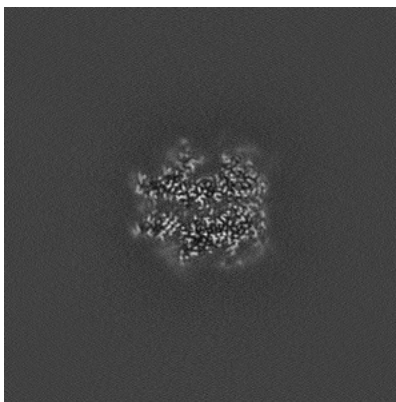


Z Index: 184

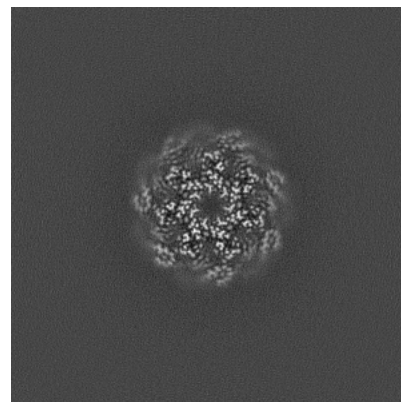
6.3.2 Raw map



X Index: 182



Y Index: 164

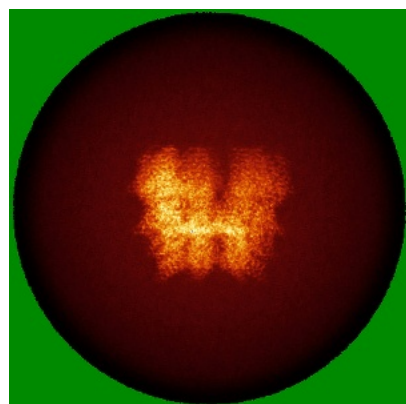


Z Index: 184

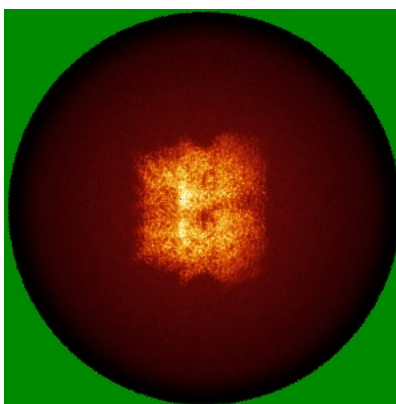
The images above show the largest variance slices of the map in three orthogonal directions.

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

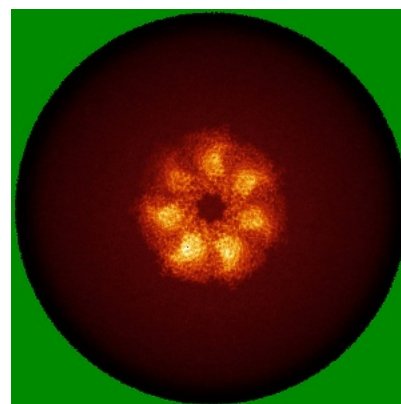
6.4.1 Primary map



X

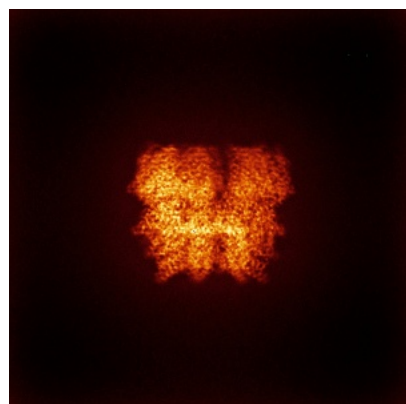


Y

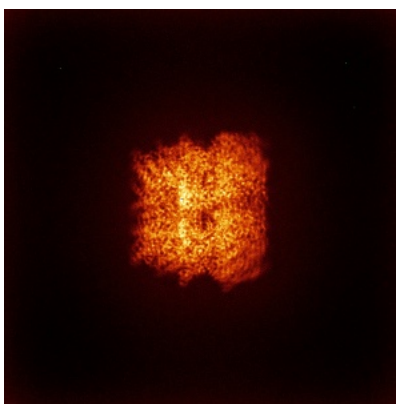


Z

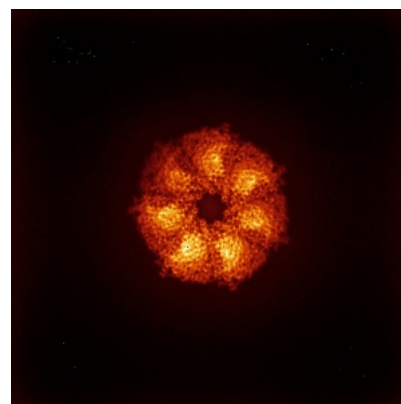
6.4.2 Raw map



X



Y

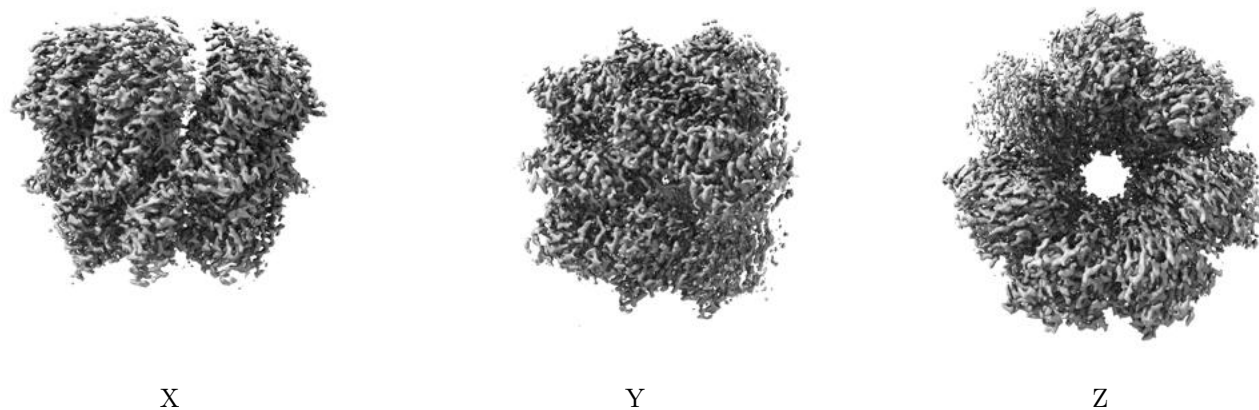


Z

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.

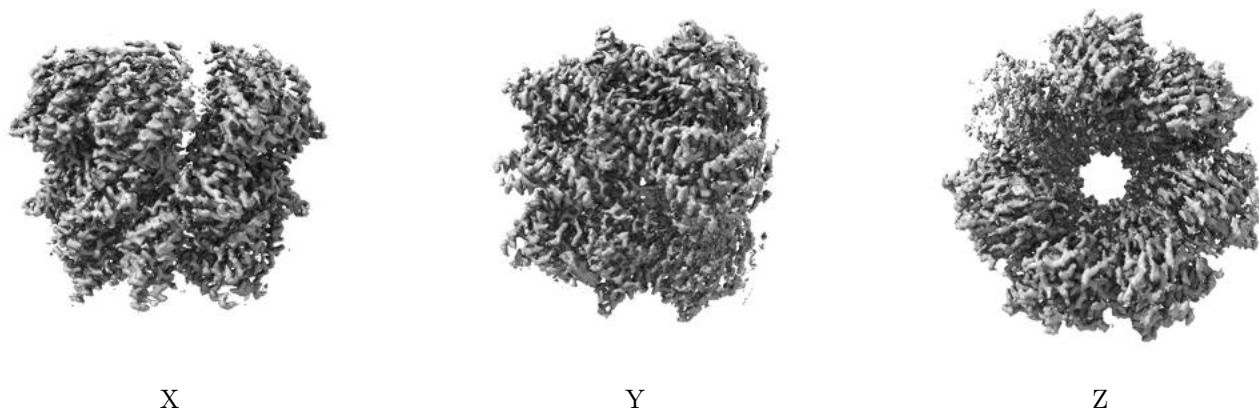
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

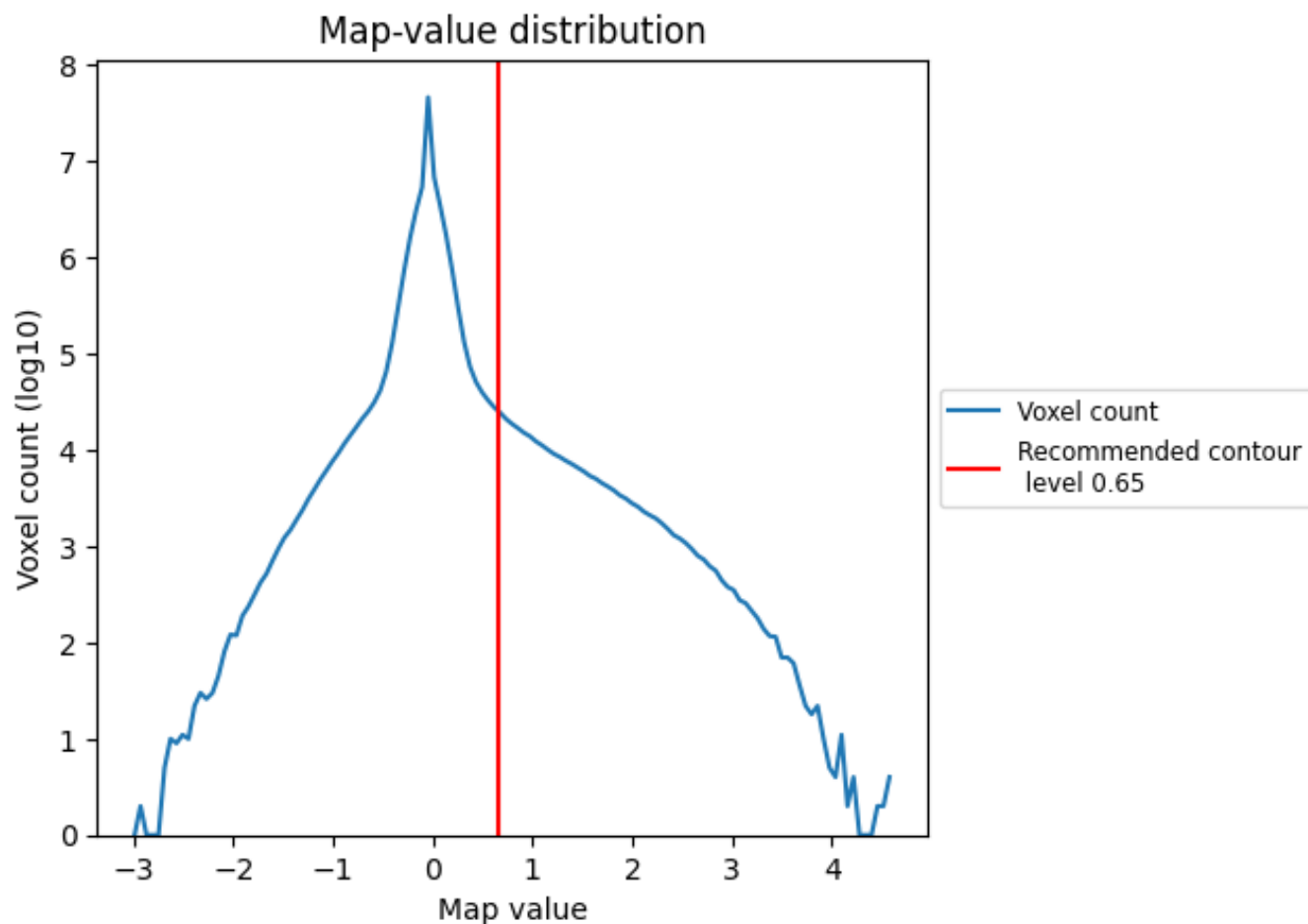
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

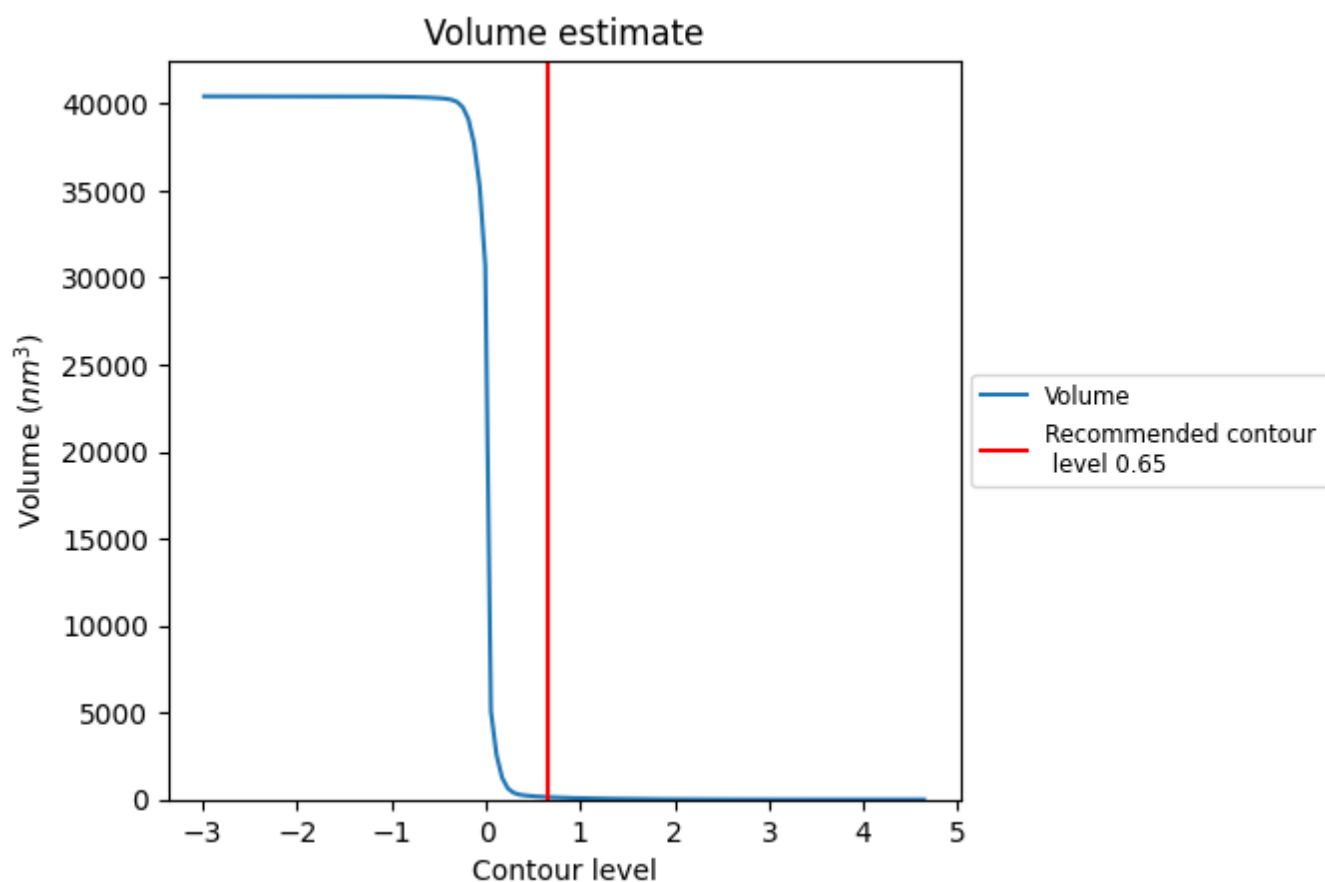
This section contains the results of statistical analysis of the map.

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.

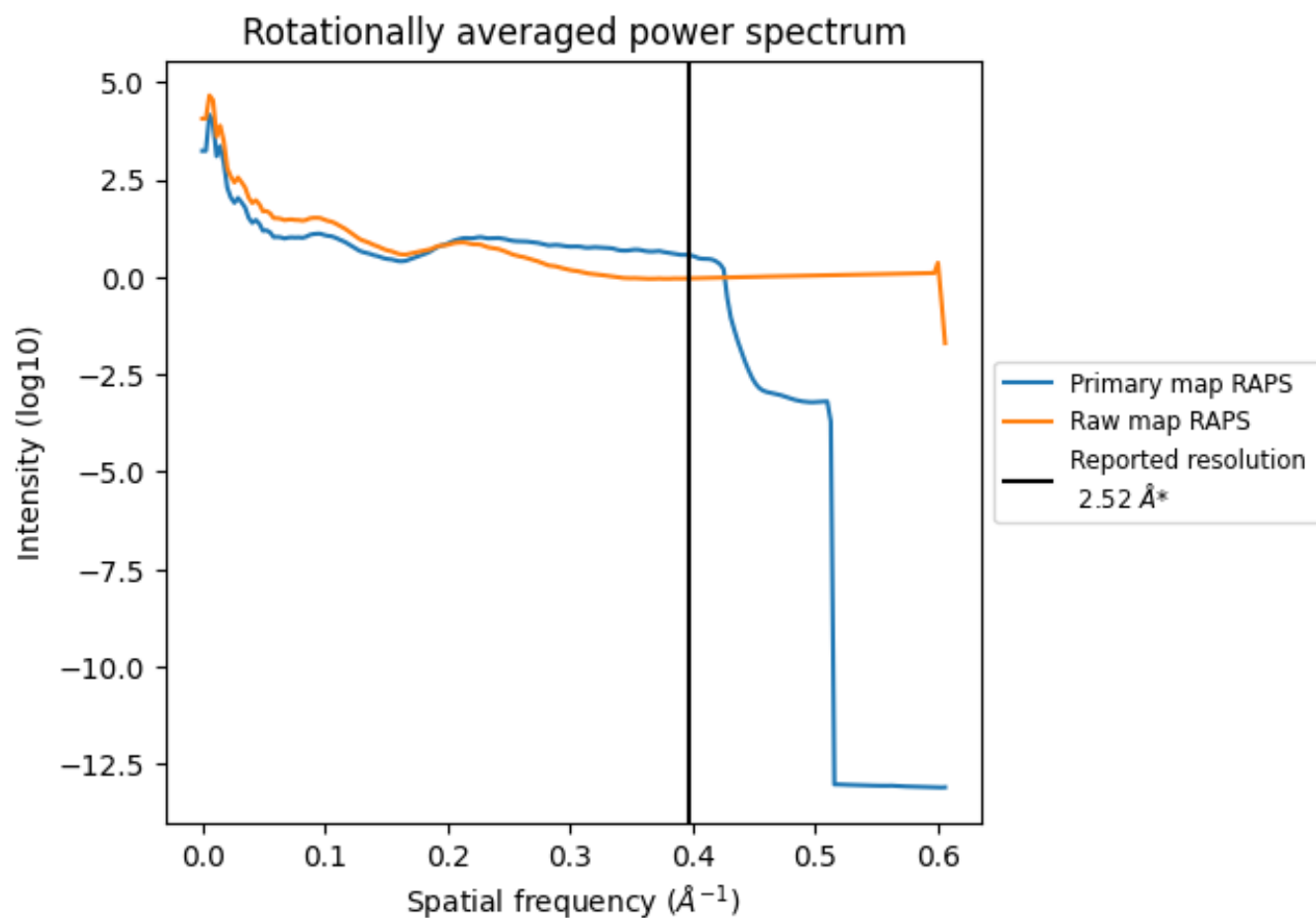
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

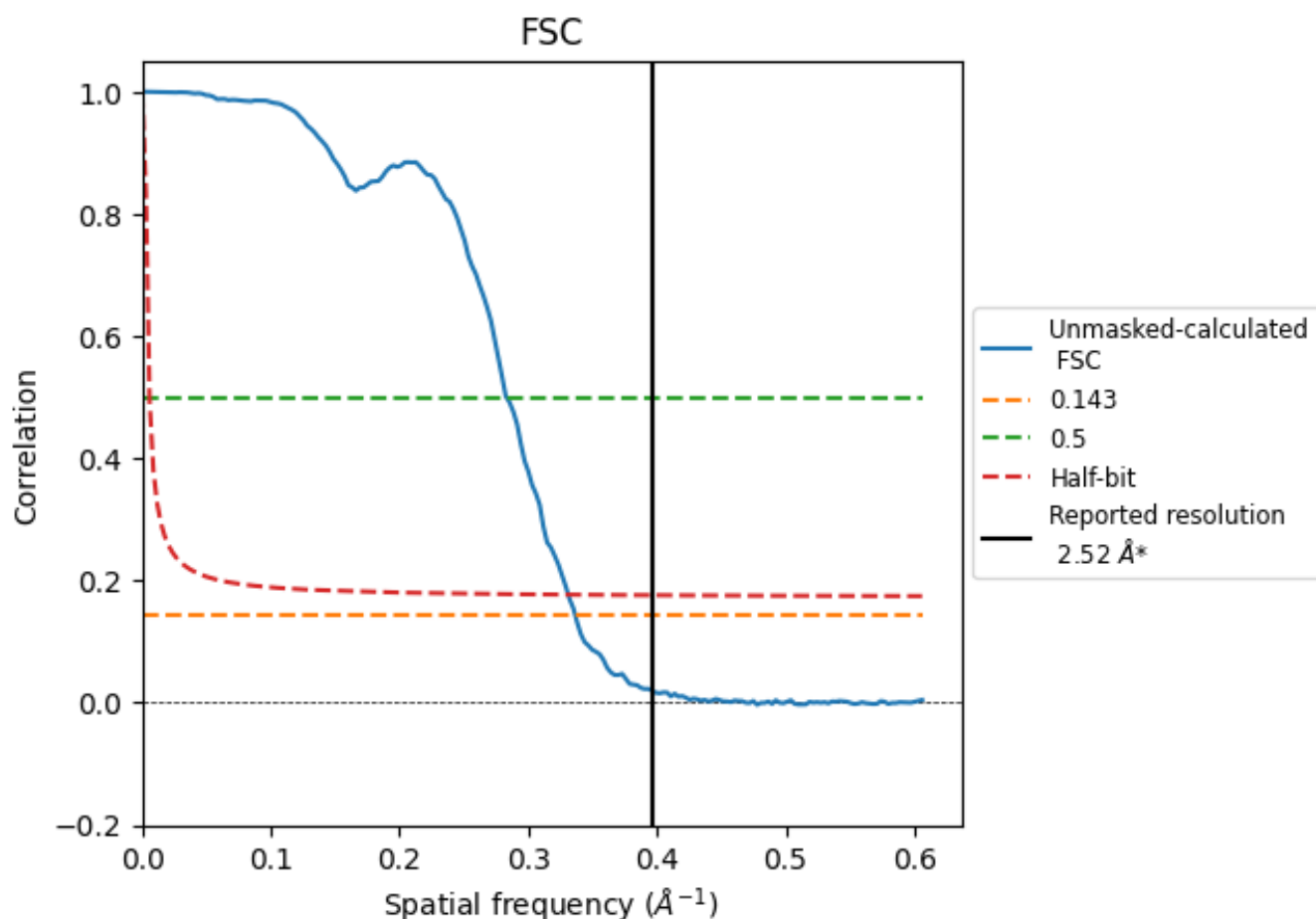


*Reported resolution corresponds to spatial frequency of 0.397 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.397 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.53	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.52 by more than 10 %

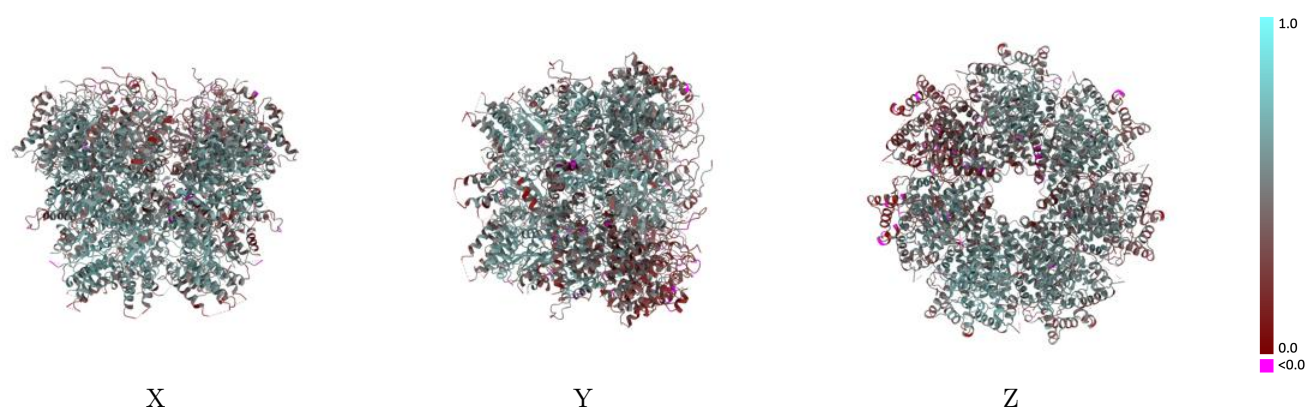
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29323 and PDB model 8FNT. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

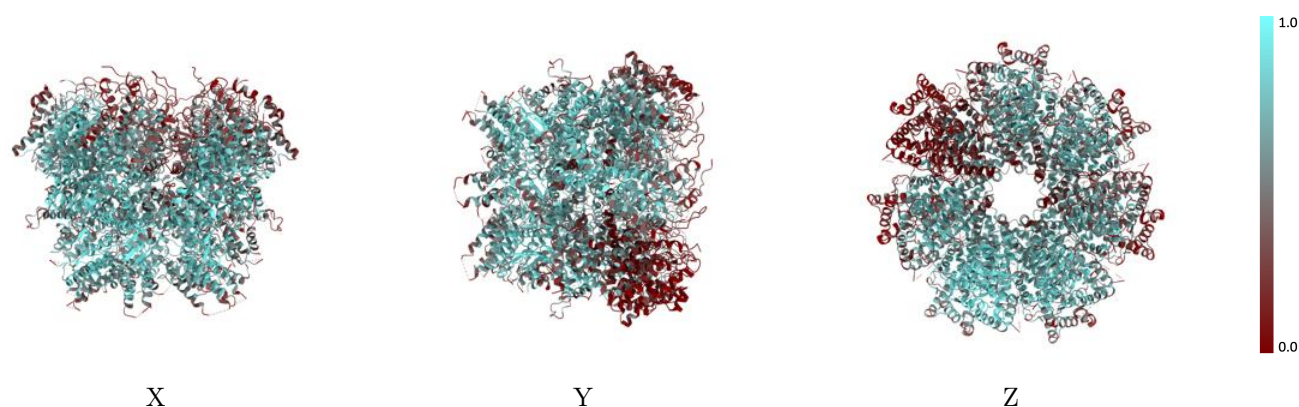
This section was not generated.

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



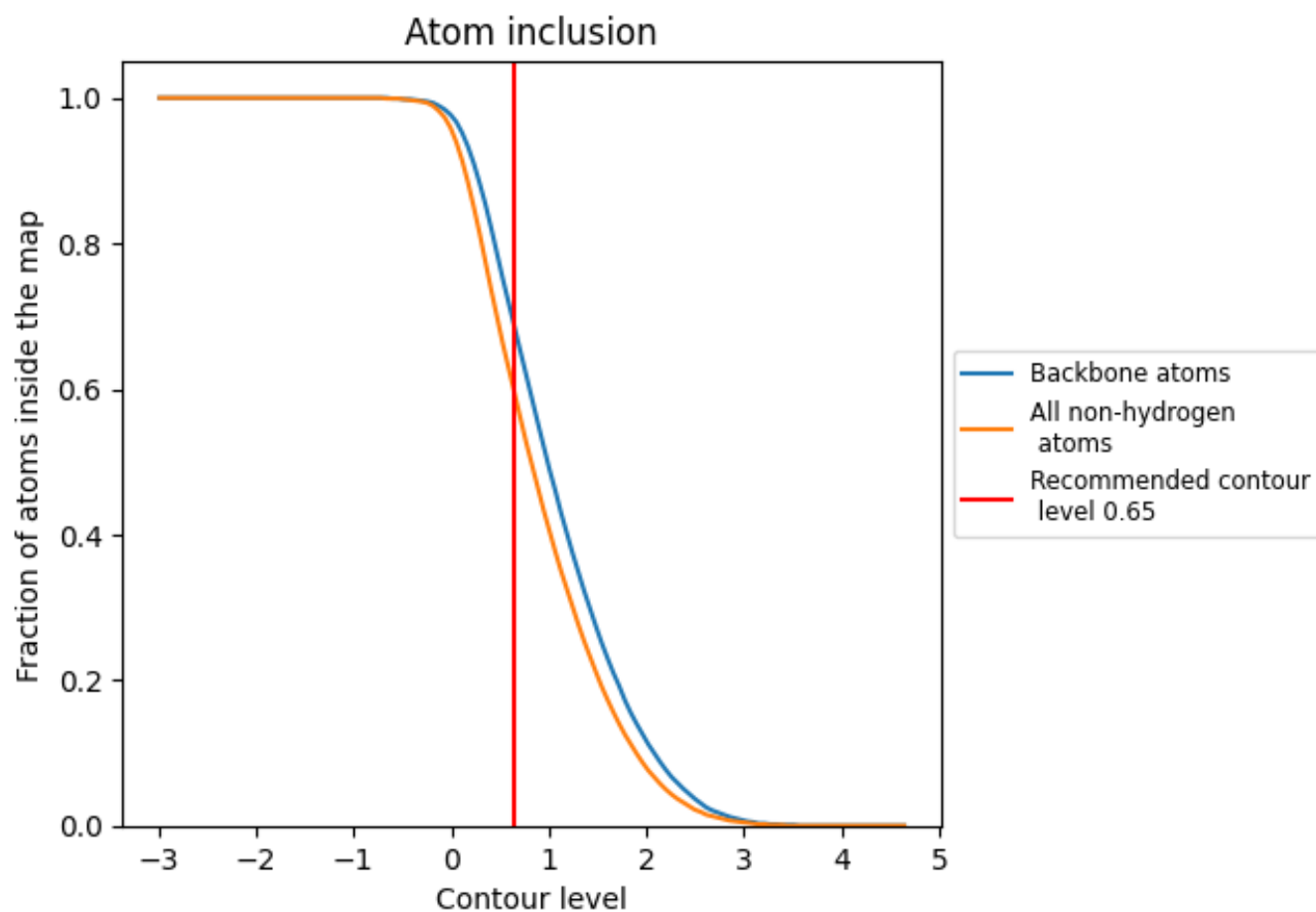
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5930	0.4860
A	0.6990	0.5250
B	0.5660	0.4910
C	0.6200	0.5090
D	0.5980	0.5040
E	0.3140	0.3470
F	0.5930	0.4640
G	0.7570	0.5590

1.0

0.0

<0.0