



Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 06:33 AM EDT

PDB ID : 8FNT
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.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

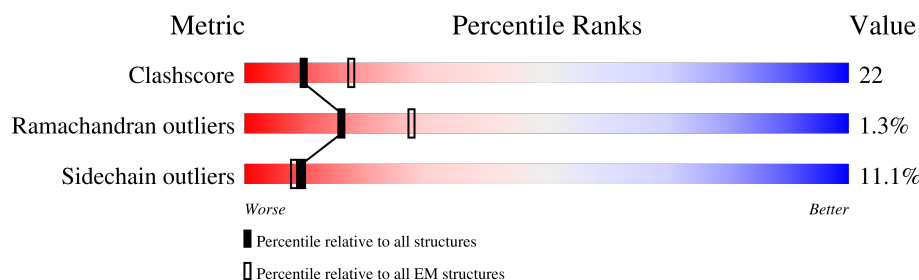
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	<div> <div>13%</div> <div> <div>46%</div> <div>29%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	947	<div> <div>27%</div> <div> <div>46%</div> <div>29%</div> <div>6%</div> <div>17%</div> </div> </div>
1	C	947	<div> <div>22%</div> <div> <div>46%</div> <div>30%</div> <div>6%</div> <div>17%</div> </div> </div>
1	D	947	<div> <div>24%</div> <div> <div>46%</div> <div>29%</div> <div>6%</div> <div>17%</div> </div> </div>
1	E	947	<div> <div>53%</div> <div> <div>45%</div> <div>30%</div> <div>6%</div> <div>18%</div> </div> </div>
1	F	947	<div> <div>25%</div> <div> <div>46%</div> <div>29%</div> <div>5%</div> <div>17%</div> </div> </div>
1	G	947	<div> <div>9%</div> <div> <div>45%</div> <div>31%</div> <div>6%</div> <div>17%</div> </div> </div>

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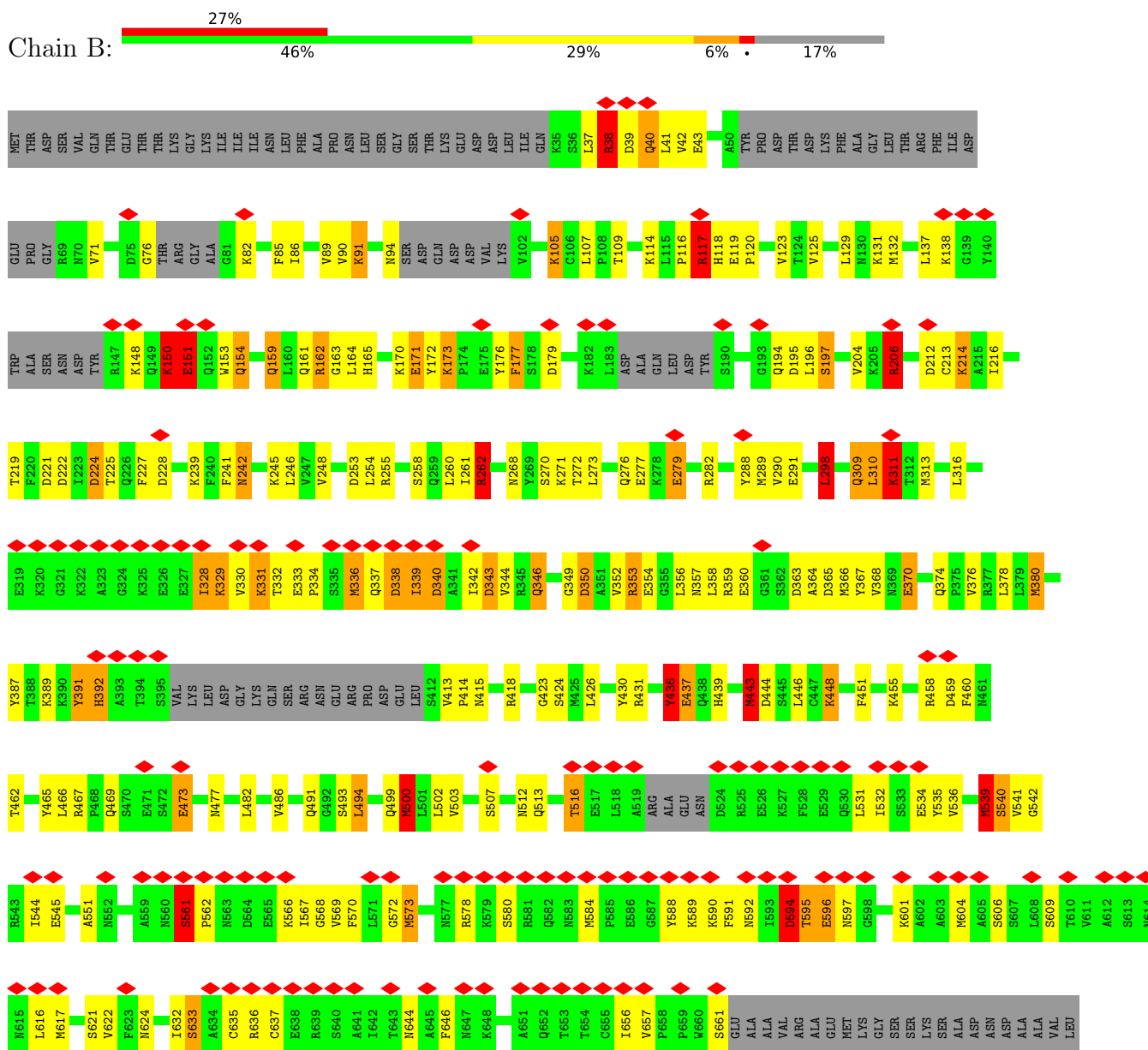
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Chain	Residue	Modelled	Actual	Comment	Reference
E	636	ARG	LEU	conflict	UNP A0A8H9B1T2
E	858	ILE	VAL	conflict	UNP A0A8H9B1T2
A	11	LYS	GLU	conflict	UNP A0A8H9B1T2
A	24	SER	PRO	conflict	UNP A0A8H9B1T2
A	67	PRO	SER	conflict	UNP A0A8H9B1T2
A	335	SER	GLY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

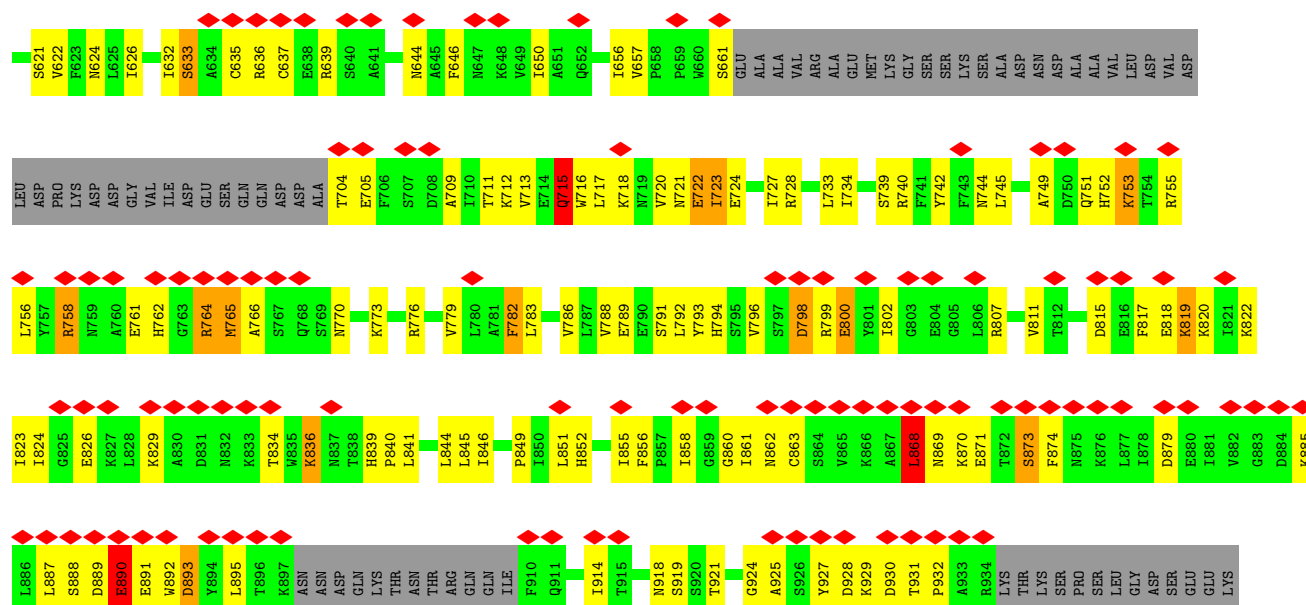
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

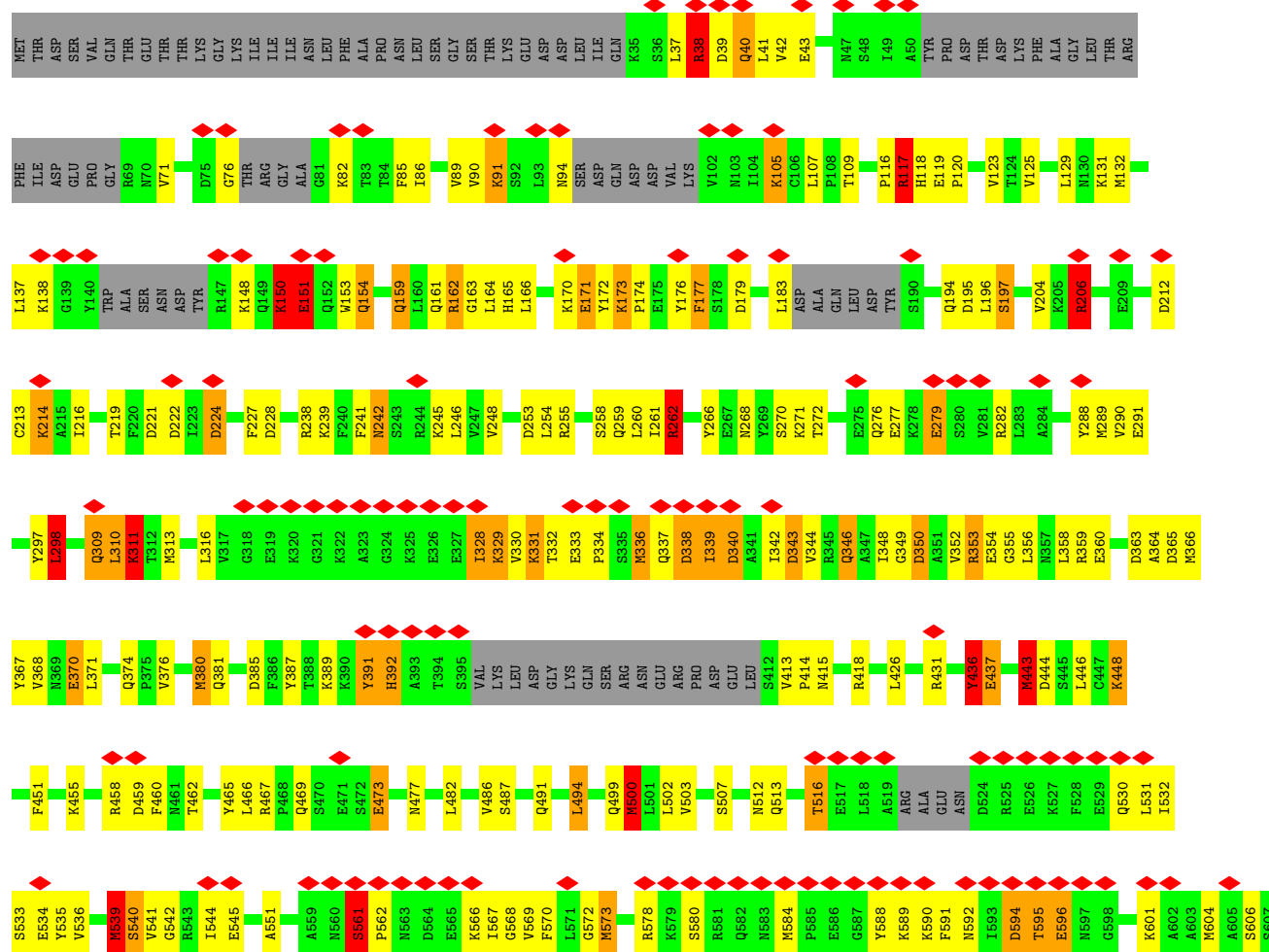
• Molecule 1: Archaeal ATPase



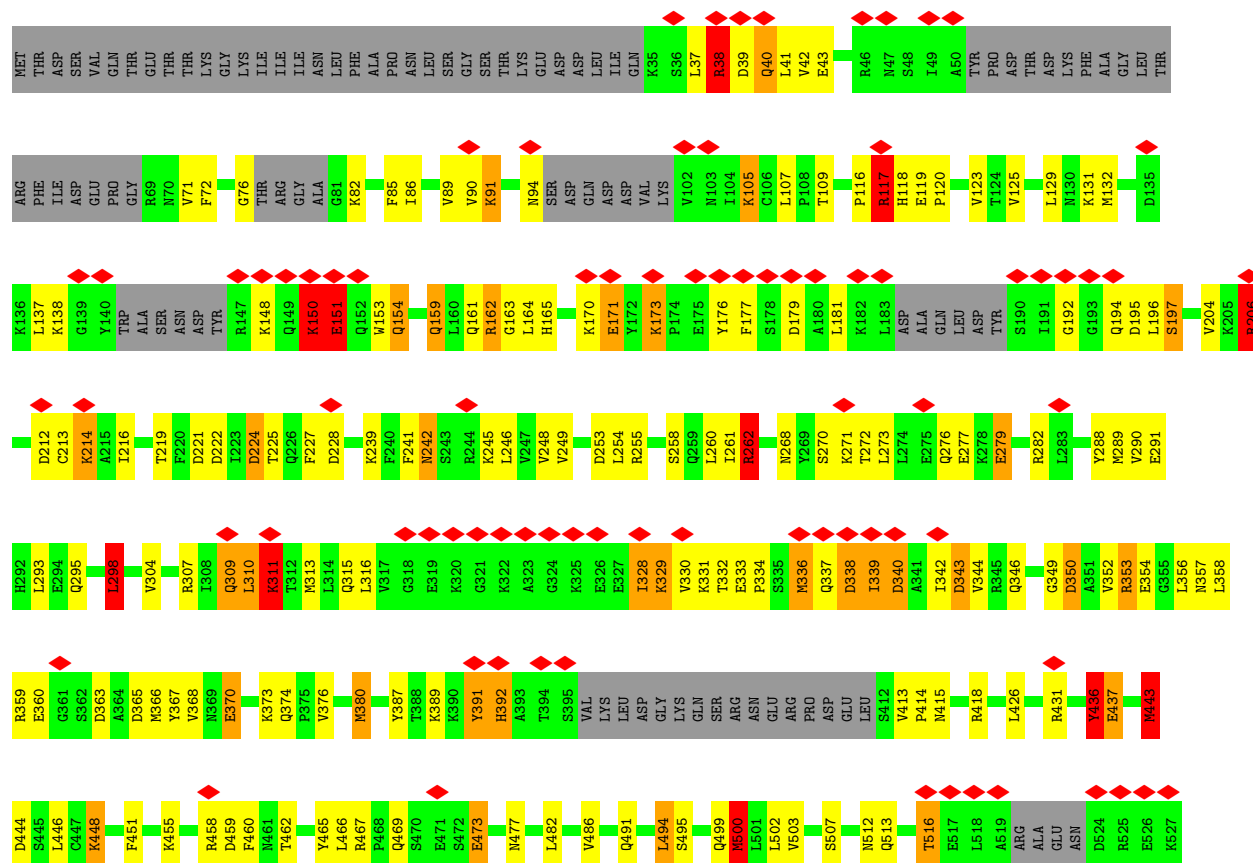


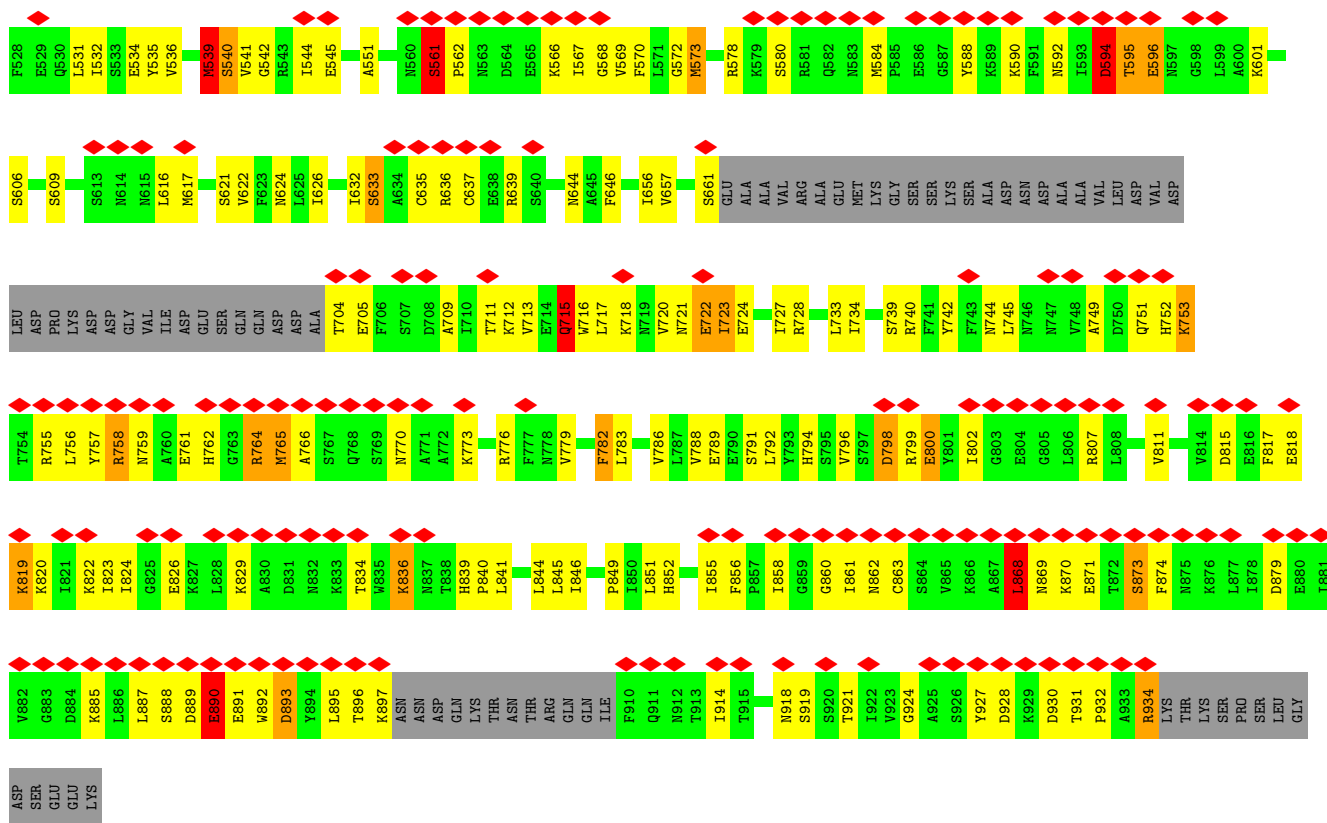


• Molecule 1: Archaeal ATPase

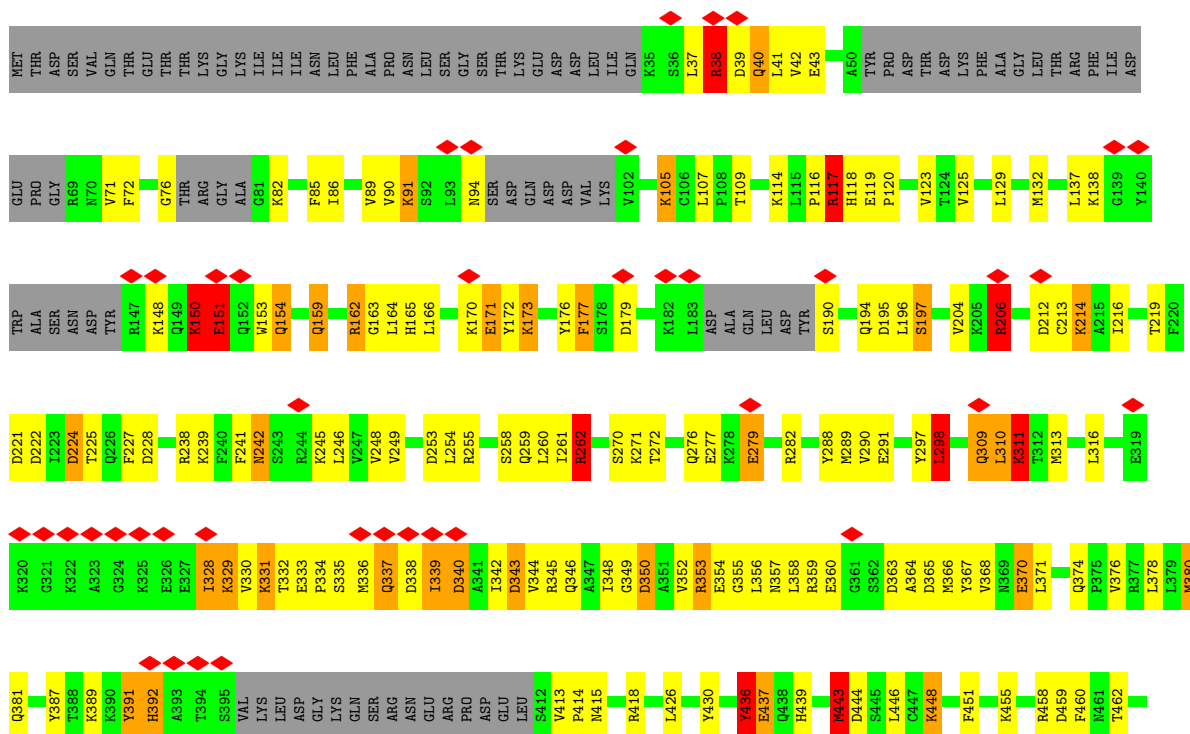
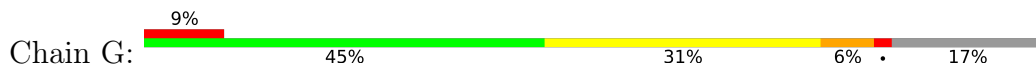


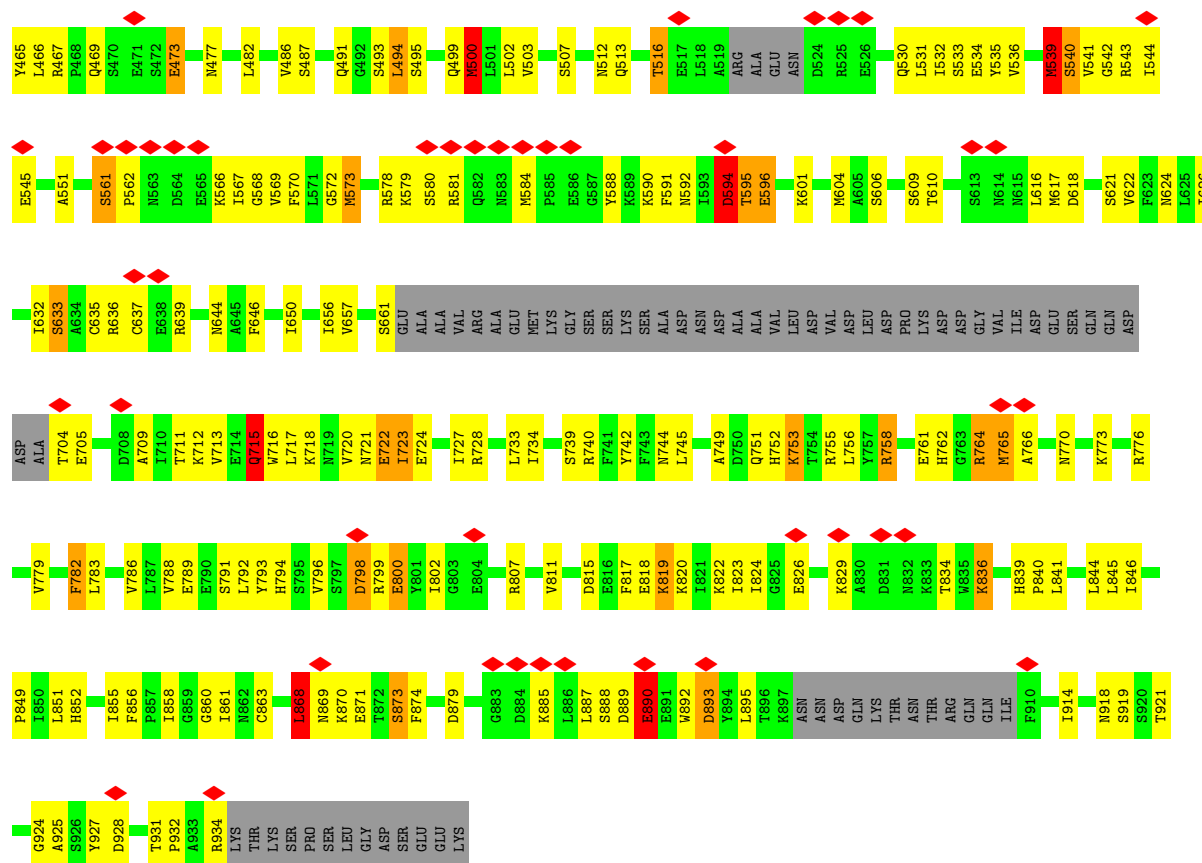
- Molecule 1: Archaeal ATPase



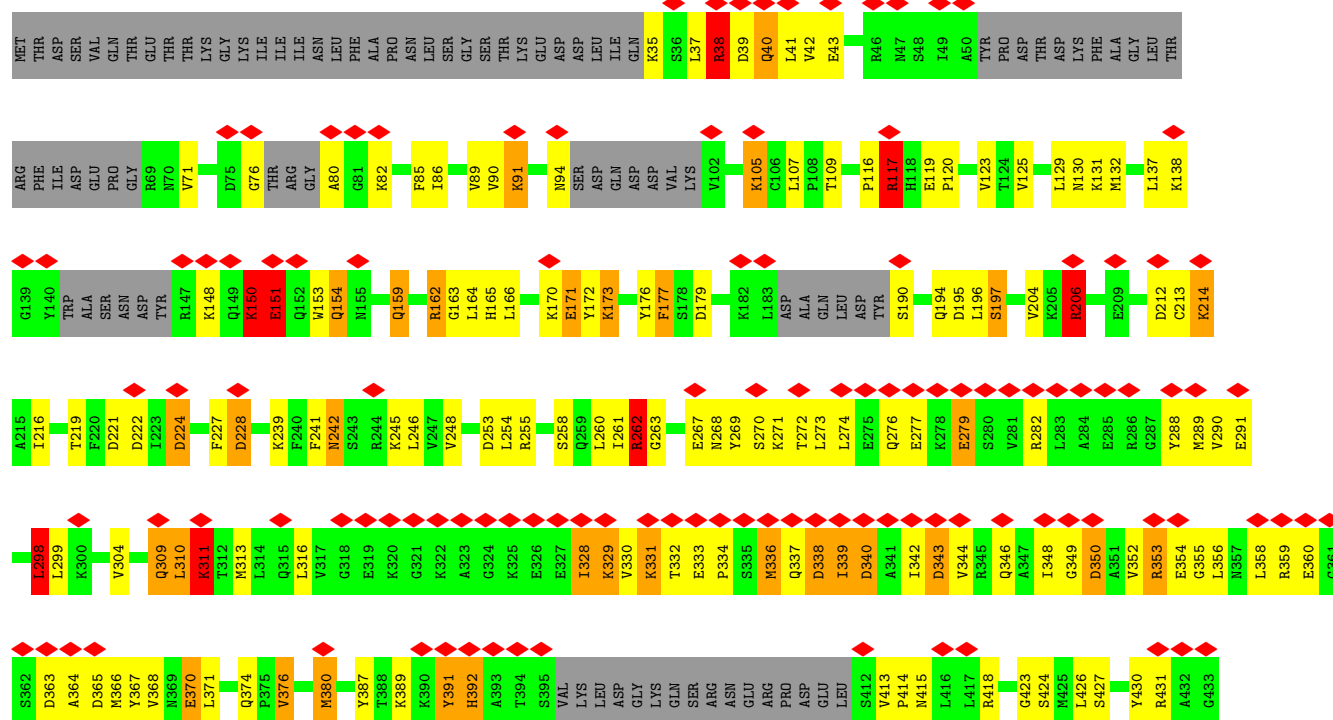


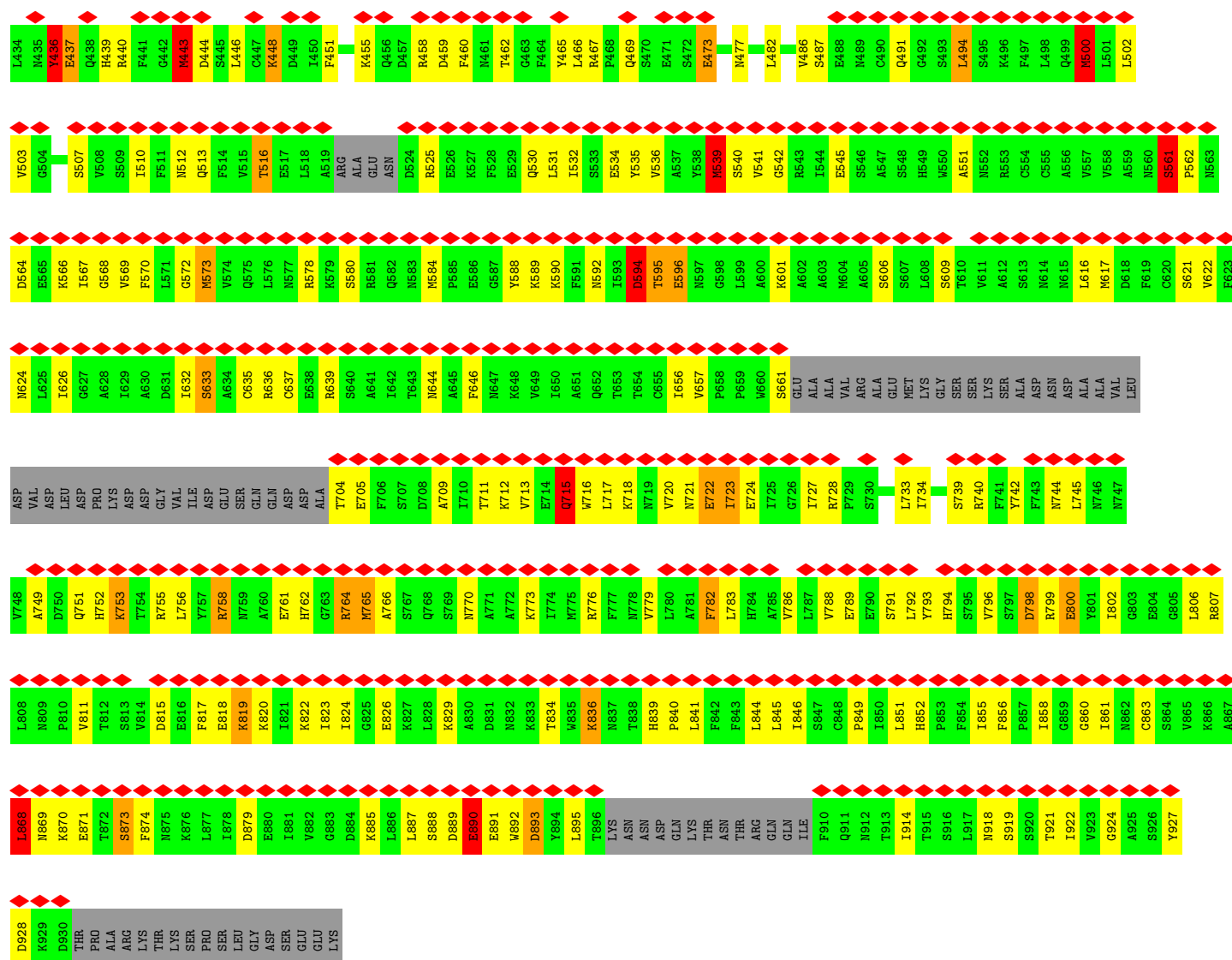
• Molecule 1: Archaeal ATPase



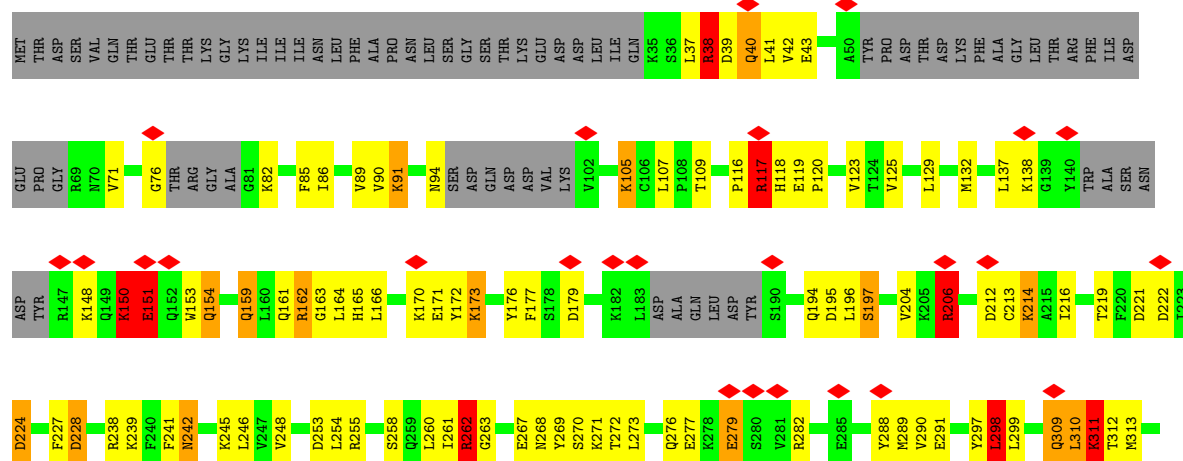


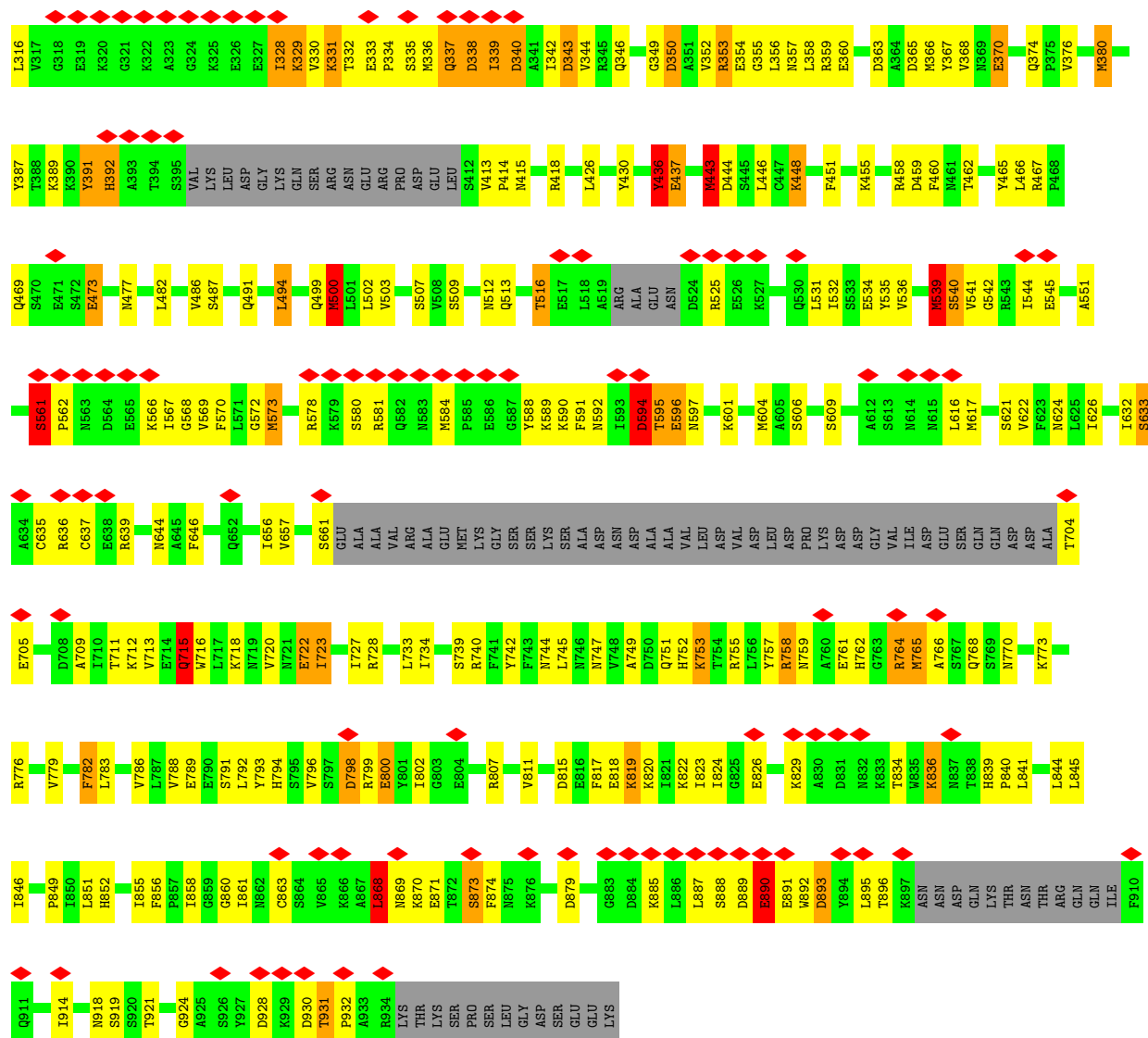
• Molecule 1: Archaeal ATPase





• 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 (\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 (\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	0.47	3/6375 (0.0%)	0.91	49/8586 (0.6%)
1	B	0.47	3/6375 (0.0%)	0.91	49/8586 (0.6%)
1	C	0.47	3/6375 (0.0%)	0.91	49/8586 (0.6%)
1	D	0.47	3/6366 (0.0%)	0.91	48/8575 (0.6%)
1	E	0.47	3/6340 (0.0%)	0.91	49/8539 (0.6%)
1	F	0.48	3/6375 (0.0%)	0.91	47/8586 (0.5%)
1	G	0.47	3/6375 (0.0%)	0.91	49/8586 (0.6%)
All	All	0.47	21/44581 (0.0%)	0.91	340/60044 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	ARG	CG-CD	-5.99	1.36	1.51
1	A	117	ARG	CG-CD	-5.97	1.37	1.51
1	F	117	ARG	CG-CD	-5.97	1.37	1.51
1	E	117	ARG	CG-CD	-5.96	1.37	1.51
1	C	117	ARG	CG-CD	-5.96	1.37	1.51
1	G	117	ARG	CG-CD	-5.96	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	ARG	CG-CD	-5.94	1.37	1.51
1	C	91	LYS	CB-CG	-5.92	1.36	1.52
1	B	91	LYS	CB-CG	-5.92	1.36	1.52
1	E	91	LYS	CB-CG	-5.90	1.36	1.52
1	G	91	LYS	CB-CG	-5.90	1.36	1.52
1	A	91	LYS	CB-CG	-5.90	1.36	1.52
1	F	91	LYS	CB-CG	-5.89	1.36	1.52
1	D	91	LYS	CB-CG	-5.89	1.36	1.52
1	A	310	LEU	C-N	5.19	1.46	1.34
1	F	310	LEU	C-N	5.17	1.46	1.34
1	G	310	LEU	C-N	5.16	1.46	1.34
1	E	310	LEU	C-N	5.16	1.46	1.34
1	D	310	LEU	C-N	5.15	1.45	1.34
1	B	310	LEU	C-N	5.15	1.45	1.34
1	C	310	LEU	C-N	5.14	1.45	1.34

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	LEU	CB-CG-CD1	13.19	133.42	111.00
1	E	502	LEU	CB-CG-CD1	13.18	133.41	111.00
1	B	502	LEU	CB-CG-CD1	13.18	133.41	111.00
1	D	502	LEU	CB-CG-CD1	13.18	133.41	111.00
1	F	502	LEU	CB-CG-CD1	13.18	133.41	111.00
1	G	502	LEU	CB-CG-CD1	13.18	133.41	111.00
1	C	502	LEU	CB-CG-CD1	13.16	133.38	111.00
1	E	822	LYS	CD-CE-NZ	11.27	137.62	111.70
1	B	822	LYS	CD-CE-NZ	11.26	137.60	111.70
1	A	822	LYS	CD-CE-NZ	11.26	137.60	111.70
1	C	822	LYS	CD-CE-NZ	11.26	137.59	111.70
1	F	822	LYS	CD-CE-NZ	11.26	137.59	111.70
1	G	822	LYS	CD-CE-NZ	11.26	137.59	111.70
1	D	822	LYS	CD-CE-NZ	11.25	137.57	111.70
1	B	443	MET	CB-CG-SD	10.73	144.60	112.40
1	F	443	MET	CB-CG-SD	10.73	144.61	112.40
1	C	443	MET	CB-CG-SD	10.73	144.60	112.40
1	E	443	MET	CB-CG-SD	10.73	144.59	112.40
1	A	443	MET	CB-CG-SD	10.73	144.58	112.40
1	G	443	MET	CB-CG-SD	10.72	144.56	112.40
1	D	443	MET	CB-CG-SD	10.72	144.56	112.40
1	B	298	LEU	CB-CG-CD1	10.63	129.07	111.00
1	C	298	LEU	CB-CG-CD1	10.62	129.06	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	298	LEU	CB-CG-CD1	10.62	129.05	111.00
1	A	298	LEU	CB-CG-CD1	10.61	129.04	111.00
1	D	298	LEU	CB-CG-CD1	10.60	129.03	111.00
1	E	298	LEU	CB-CG-CD1	10.60	129.02	111.00
1	F	298	LEU	CB-CG-CD1	10.60	129.01	111.00
1	D	868	LEU	CB-CG-CD2	10.36	128.61	111.00
1	F	868	LEU	CB-CG-CD2	10.35	128.59	111.00
1	B	868	LEU	CB-CG-CD2	10.34	128.58	111.00
1	A	868	LEU	CB-CG-CD2	10.34	128.58	111.00
1	C	868	LEU	CB-CG-CD2	10.33	128.56	111.00
1	G	868	LEU	CB-CG-CD2	10.33	128.56	111.00
1	E	868	LEU	CB-CG-CD2	10.33	128.55	111.00
1	G	311	LYS	CB-CG-CD	9.87	137.27	111.60
1	F	311	LYS	CB-CG-CD	9.86	137.24	111.60
1	C	311	LYS	CB-CG-CD	9.85	137.22	111.60
1	A	311	LYS	CB-CG-CD	9.85	137.22	111.60
1	E	311	LYS	CB-CG-CD	9.85	137.20	111.60
1	B	311	LYS	CB-CG-CD	9.84	137.19	111.60
1	D	311	LYS	CB-CG-CD	9.84	137.18	111.60
1	B	879	ASP	CB-CG-OD2	8.98	126.38	118.30
1	F	879	ASP	CB-CG-OD2	8.97	126.38	118.30
1	C	879	ASP	CB-CG-OD2	8.96	126.37	118.30
1	A	879	ASP	CB-CG-OD2	8.96	126.36	118.30
1	G	879	ASP	CB-CG-OD2	8.96	126.36	118.30
1	D	879	ASP	CB-CG-OD2	8.95	126.36	118.30
1	E	879	ASP	CB-CG-OD2	8.93	126.34	118.30
1	B	584	MET	CA-CB-CG	-8.92	98.14	113.30
1	A	584	MET	CA-CB-CG	-8.92	98.14	113.30
1	E	584	MET	CA-CB-CG	-8.91	98.14	113.30
1	D	584	MET	CA-CB-CG	-8.91	98.15	113.30
1	F	584	MET	CA-CB-CG	-8.91	98.16	113.30
1	G	584	MET	CA-CB-CG	-8.90	98.16	113.30
1	C	584	MET	CA-CB-CG	-8.90	98.17	113.30
1	C	455	LYS	CD-CE-NZ	8.54	131.33	111.70
1	E	455	LYS	CD-CE-NZ	8.54	131.33	111.70
1	A	455	LYS	CD-CE-NZ	8.53	131.32	111.70
1	D	455	LYS	CD-CE-NZ	8.53	131.31	111.70
1	F	455	LYS	CD-CE-NZ	8.53	131.31	111.70
1	B	455	LYS	CD-CE-NZ	8.52	131.31	111.70
1	G	455	LYS	CD-CE-NZ	8.52	131.29	111.70
1	F	890	GLU	CA-CB-CG	8.14	131.31	113.40
1	C	890	GLU	CA-CB-CG	8.14	131.31	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	GLU	CA-CB-CG	8.14	131.30	113.40
1	A	890	GLU	CA-CB-CG	8.13	131.29	113.40
1	D	890	GLU	CA-CB-CG	8.13	131.28	113.40
1	E	890	GLU	CA-CB-CG	8.12	131.27	113.40
1	G	890	GLU	CA-CB-CG	8.12	131.26	113.40
1	G	298	LEU	CB-CG-CD2	-8.04	97.34	111.00
1	C	298	LEU	CB-CG-CD2	-8.03	97.35	111.00
1	D	298	LEU	CB-CG-CD2	-8.02	97.36	111.00
1	B	298	LEU	CB-CG-CD2	-8.02	97.36	111.00
1	E	298	LEU	CB-CG-CD2	-8.02	97.37	111.00
1	A	298	LEU	CB-CG-CD2	-8.01	97.39	111.00
1	F	298	LEU	CB-CG-CD2	-8.00	97.39	111.00
1	A	740	ARG	CG-CD-NE	7.83	128.24	111.80
1	G	740	ARG	CG-CD-NE	7.83	128.24	111.80
1	F	43	GLU	CA-CB-CG	7.83	130.62	113.40
1	C	740	ARG	CG-CD-NE	7.82	128.23	111.80
1	B	43	GLU	CA-CB-CG	7.82	130.60	113.40
1	G	43	GLU	CA-CB-CG	7.82	130.61	113.40
1	F	740	ARG	CG-CD-NE	7.82	128.22	111.80
1	A	43	GLU	CA-CB-CG	7.81	130.58	113.40
1	D	740	ARG	CG-CD-NE	7.81	128.20	111.80
1	D	43	GLU	CA-CB-CG	7.80	130.57	113.40
1	E	43	GLU	CA-CB-CG	7.80	130.57	113.40
1	E	740	ARG	CG-CD-NE	7.80	128.19	111.80
1	C	43	GLU	CA-CB-CG	7.80	130.57	113.40
1	B	740	ARG	CG-CD-NE	7.79	128.15	111.80
1	B	722	GLU	CA-CB-CG	7.62	130.16	113.40
1	D	722	GLU	CA-CB-CG	7.62	130.16	113.40
1	C	722	GLU	CA-CB-CG	7.61	130.14	113.40
1	F	722	GLU	CA-CB-CG	7.60	130.12	113.40
1	A	722	GLU	CA-CB-CG	7.60	130.12	113.40
1	G	722	GLU	CA-CB-CG	7.59	130.11	113.40
1	B	566	LYS	CD-CE-NZ	7.59	129.16	111.70
1	C	566	LYS	CD-CE-NZ	7.59	129.16	111.70
1	E	722	GLU	CA-CB-CG	7.59	130.10	113.40
1	D	566	LYS	CD-CE-NZ	7.58	129.13	111.70
1	A	566	LYS	CD-CE-NZ	7.58	129.12	111.70
1	E	566	LYS	CD-CE-NZ	7.57	129.10	111.70
1	G	566	LYS	CD-CE-NZ	7.56	129.09	111.70
1	F	566	LYS	CD-CE-NZ	7.56	129.09	111.70
1	D	868	LEU	CB-CG-CD1	-7.54	98.18	111.00
1	F	868	LEU	CB-CG-CD1	-7.53	98.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	868	LEU	CB-CG-CD1	-7.53	98.20	111.00
1	A	868	LEU	CB-CG-CD1	-7.53	98.20	111.00
1	E	868	LEU	CB-CG-CD1	-7.53	98.21	111.00
1	C	868	LEU	CB-CG-CD1	-7.52	98.22	111.00
1	B	868	LEU	CB-CG-CD1	-7.51	98.23	111.00
1	F	117	ARG	CA-CB-CG	-7.46	97.00	113.40
1	G	117	ARG	CA-CB-CG	-7.44	97.03	113.40
1	E	117	ARG	CA-CB-CG	-7.44	97.04	113.40
1	A	117	ARG	CA-CB-CG	-7.43	97.05	113.40
1	B	117	ARG	CA-CB-CG	-7.42	97.06	113.40
1	C	117	ARG	CA-CB-CG	-7.42	97.09	113.40
1	D	117	ARG	CA-CB-CG	-7.41	97.10	113.40
1	E	91	LYS	CD-CE-NZ	7.40	128.73	111.70
1	D	91	LYS	CD-CE-NZ	7.39	128.70	111.70
1	B	91	LYS	CD-CE-NZ	7.38	128.68	111.70
1	G	91	LYS	CD-CE-NZ	7.38	128.67	111.70
1	A	91	LYS	CD-CE-NZ	7.38	128.67	111.70
1	C	91	LYS	CD-CE-NZ	7.38	128.66	111.70
1	F	91	LYS	CD-CE-NZ	7.37	128.64	111.70
1	B	601	LYS	CD-CE-NZ	7.16	128.18	111.70
1	E	601	LYS	CD-CE-NZ	7.16	128.18	111.70
1	D	601	LYS	CD-CE-NZ	7.16	128.17	111.70
1	A	601	LYS	CD-CE-NZ	7.16	128.16	111.70
1	C	601	LYS	CD-CE-NZ	7.15	128.16	111.70
1	G	601	LYS	CD-CE-NZ	7.15	128.15	111.70
1	F	601	LYS	CD-CE-NZ	7.15	128.14	111.70
1	G	117	ARG	CG-CD-NE	6.98	126.45	111.80
1	E	117	ARG	CG-CD-NE	6.97	126.43	111.80
1	A	117	ARG	CG-CD-NE	6.96	126.42	111.80
1	F	117	ARG	CG-CD-NE	6.96	126.42	111.80
1	C	117	ARG	CG-CD-NE	6.96	126.41	111.80
1	B	117	ARG	CG-CD-NE	6.95	126.39	111.80
1	G	289	MET	CB-CG-SD	-6.95	91.55	112.40
1	F	289	MET	CB-CG-SD	-6.94	91.58	112.40
1	C	289	MET	CB-CG-SD	-6.94	91.58	112.40
1	D	117	ARG	CG-CD-NE	6.93	126.36	111.80
1	A	289	MET	CB-CG-SD	-6.93	91.60	112.40
1	B	289	MET	CB-CG-SD	-6.93	91.61	112.40
1	E	289	MET	CB-CG-SD	-6.93	91.61	112.40
1	D	289	MET	CB-CG-SD	-6.92	91.63	112.40
1	E	494	LEU	CB-CG-CD1	6.80	122.57	111.00
1	D	494	LEU	CB-CG-CD1	6.79	122.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	GLN	CB-CG-CD	6.79	129.25	111.60
1	A	494	LEU	CB-CG-CD1	6.79	122.54	111.00
1	B	40	GLN	CB-CG-CD	6.78	129.23	111.60
1	B	494	LEU	CB-CG-CD1	6.78	122.53	111.00
1	G	494	LEU	CB-CG-CD1	6.77	122.51	111.00
1	C	494	LEU	CB-CG-CD1	6.77	122.51	111.00
1	F	40	GLN	CB-CG-CD	6.77	129.20	111.60
1	F	494	LEU	CB-CG-CD1	6.77	122.51	111.00
1	A	40	GLN	CB-CG-CD	6.77	129.20	111.60
1	D	40	GLN	CB-CG-CD	6.76	129.19	111.60
1	G	40	GLN	CB-CG-CD	6.76	129.19	111.60
1	C	40	GLN	CB-CG-CD	6.76	129.16	111.60
1	D	819	LYS	CD-CE-NZ	-6.70	96.30	111.70
1	C	819	LYS	CD-CE-NZ	-6.70	96.30	111.70
1	A	819	LYS	CD-CE-NZ	-6.70	96.30	111.70
1	G	819	LYS	CD-CE-NZ	-6.69	96.31	111.70
1	E	819	LYS	CD-CE-NZ	-6.69	96.31	111.70
1	F	819	LYS	CD-CE-NZ	-6.68	96.33	111.70
1	B	819	LYS	CD-CE-NZ	-6.68	96.33	111.70
1	F	617	MET	CB-CG-SD	-6.67	92.40	112.40
1	D	617	MET	CB-CG-SD	-6.66	92.43	112.40
1	G	617	MET	CB-CG-SD	-6.66	92.43	112.40
1	C	617	MET	CB-CG-SD	-6.65	92.44	112.40
1	A	617	MET	CB-CG-SD	-6.65	92.44	112.40
1	B	617	MET	CB-CG-SD	-6.64	92.47	112.40
1	E	617	MET	CB-CG-SD	-6.64	92.47	112.40
1	C	105	LYS	CB-CG-CD	6.62	128.81	111.60
1	B	105	LYS	CB-CG-CD	6.62	128.81	111.60
1	D	105	LYS	CB-CG-CD	6.62	128.80	111.60
1	A	105	LYS	CB-CG-CD	6.61	128.78	111.60
1	E	105	LYS	CB-CG-CD	6.61	128.78	111.60
1	F	105	LYS	CB-CG-CD	6.61	128.78	111.60
1	G	105	LYS	CB-CG-CD	6.60	128.76	111.60
1	B	836	LYS	CD-CE-NZ	-6.55	96.64	111.70
1	E	836	LYS	CD-CE-NZ	-6.55	96.64	111.70
1	F	836	LYS	CD-CE-NZ	-6.55	96.64	111.70
1	A	836	LYS	CD-CE-NZ	-6.55	96.64	111.70
1	G	836	LYS	CD-CE-NZ	-6.54	96.65	111.70
1	C	836	LYS	CD-CE-NZ	-6.54	96.66	111.70
1	D	836	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	B	879	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	D	214	LYS	CD-CE-NZ	6.38	126.38	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	214	LYS	CD-CE-NZ	6.38	126.37	111.70
1	G	214	LYS	CD-CE-NZ	6.38	126.37	111.70
1	E	214	LYS	CD-CE-NZ	6.38	126.37	111.70
1	B	214	LYS	CD-CE-NZ	6.37	126.35	111.70
1	D	879	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	214	LYS	CD-CE-NZ	6.37	126.34	111.70
1	C	214	LYS	CD-CE-NZ	6.36	126.33	111.70
1	A	879	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	C	879	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	E	879	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	G	879	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	D	138	LYS	CG-CD-CE	6.31	130.84	111.90
1	F	879	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	B	138	LYS	CG-CD-CE	6.31	130.83	111.90
1	G	138	LYS	CG-CD-CE	6.31	130.82	111.90
1	A	138	LYS	CG-CD-CE	6.30	130.81	111.90
1	E	138	LYS	CG-CD-CE	6.30	130.81	111.90
1	C	138	LYS	CG-CD-CE	6.30	130.79	111.90
1	F	138	LYS	CG-CD-CE	6.30	130.79	111.90
1	A	753	LYS	CD-CE-NZ	6.29	126.17	111.70
1	C	753	LYS	CD-CE-NZ	6.28	126.15	111.70
1	D	753	LYS	CD-CE-NZ	6.27	126.12	111.70
1	E	753	LYS	CD-CE-NZ	6.27	126.12	111.70
1	F	753	LYS	CD-CE-NZ	6.27	126.11	111.70
1	G	753	LYS	CD-CE-NZ	6.27	126.12	111.70
1	B	753	LYS	CD-CE-NZ	6.26	126.10	111.70
1	B	329	LYS	CD-CE-NZ	6.16	125.88	111.70
1	C	329	LYS	CD-CE-NZ	6.16	125.87	111.70
1	E	329	LYS	CD-CE-NZ	6.16	125.86	111.70
1	A	329	LYS	CD-CE-NZ	6.15	125.85	111.70
1	D	329	LYS	CD-CE-NZ	6.15	125.85	111.70
1	G	329	LYS	CD-CE-NZ	6.15	125.84	111.70
1	F	329	LYS	CD-CE-NZ	6.15	125.84	111.70
1	F	494	LEU	CA-CB-CG	5.97	129.03	115.30
1	E	494	LEU	CA-CB-CG	5.96	129.02	115.30
1	D	494	LEU	CA-CB-CG	5.96	129.01	115.30
1	G	494	LEU	CA-CB-CG	5.96	129.00	115.30
1	C	494	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	494	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	494	LEU	CA-CB-CG	5.94	128.96	115.30
1	E	500	MET	CB-CG-SD	5.88	130.03	112.40
1	A	500	MET	CB-CG-SD	5.87	130.02	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	MET	CB-CG-SD	5.87	130.02	112.40
1	F	500	MET	CB-CG-SD	5.86	129.99	112.40
1	D	500	MET	CB-CG-SD	5.86	129.97	112.40
1	C	500	MET	CB-CG-SD	5.86	129.97	112.40
1	G	500	MET	CB-CG-SD	5.85	129.95	112.40
1	B	151	GLU	CA-CB-CG	5.75	126.05	113.40
1	F	151	GLU	CA-CB-CG	5.75	126.05	113.40
1	E	151	GLU	CA-CB-CG	5.74	126.03	113.40
1	A	151	GLU	CA-CB-CG	5.74	126.02	113.40
1	G	151	GLU	CA-CB-CG	5.73	126.01	113.40
1	C	151	GLU	CA-CB-CG	5.72	125.99	113.40
1	D	151	GLU	CA-CB-CG	5.71	125.97	113.40
1	F	221	ASP	CB-CG-OD2	5.44	123.20	118.30
1	G	298	LEU	CA-CB-CG	-5.44	102.78	115.30
1	A	221	ASP	CB-CG-OD2	5.44	123.19	118.30
1	B	298	LEU	CA-CB-CG	-5.43	102.81	115.30
1	F	298	LEU	CA-CB-CG	-5.43	102.81	115.30
1	D	298	LEU	CA-CB-CG	-5.43	102.82	115.30
1	C	298	LEU	CA-CB-CG	-5.42	102.83	115.30
1	G	221	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	117	ARG	CB-CG-CD	5.42	125.69	111.60
1	E	117	ARG	CB-CG-CD	5.42	125.68	111.60
1	E	298	LEU	CA-CB-CG	-5.42	102.84	115.30
1	B	117	ARG	CB-CG-CD	5.41	125.67	111.60
1	D	221	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	117	ARG	CB-CG-CD	5.41	125.66	111.60
1	D	117	ARG	CB-CG-CD	5.41	125.66	111.60
1	G	117	ARG	CB-CG-CD	5.41	125.65	111.60
1	A	298	LEU	CA-CB-CG	-5.40	102.88	115.30
1	A	117	ARG	CB-CG-CD	5.38	125.60	111.60
1	B	221	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	221	ASP	CB-CG-OD2	5.37	123.14	118.30
1	E	221	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	715	GLN	CA-CB-CG	5.35	125.16	113.40
1	G	138	LYS	CB-CG-CD	5.34	125.48	111.60
1	C	138	LYS	CB-CG-CD	5.33	125.47	111.60
1	E	138	LYS	CB-CG-CD	5.33	125.46	111.60
1	D	138	LYS	CB-CG-CD	5.33	125.45	111.60
1	D	715	GLN	CA-CB-CG	5.33	125.12	113.40
1	F	138	LYS	CB-CG-CD	5.33	125.45	111.60
1	B	138	LYS	CB-CG-CD	5.33	125.45	111.60
1	E	715	GLN	CA-CB-CG	5.33	125.11	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	715	GLN	CA-CB-CG	5.33	125.11	113.40
1	F	715	GLN	CA-CB-CG	5.32	125.11	113.40
1	A	138	LYS	CB-CG-CD	5.32	125.44	111.60
1	G	715	GLN	CA-CB-CG	5.32	125.11	113.40
1	B	715	GLN	CA-CB-CG	5.31	125.07	113.40
1	G	40	GLN	CA-CB-CG	5.29	125.04	113.40
1	A	40	GLN	CA-CB-CG	5.29	125.04	113.40
1	C	40	GLN	CA-CB-CG	5.29	125.03	113.40
1	F	40	GLN	CA-CB-CG	5.29	125.03	113.40
1	D	40	GLN	CA-CB-CG	5.27	125.00	113.40
1	E	40	GLN	CA-CB-CG	5.27	124.99	113.40
1	B	40	GLN	CA-CB-CG	5.26	124.98	113.40
1	B	350	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	350	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	350	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	350	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	350	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	350	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	350	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	380	MET	CB-CG-SD	5.17	127.90	112.40
1	C	380	MET	CB-CG-SD	5.17	127.90	112.40
1	D	380	MET	CB-CG-SD	5.17	127.89	112.40
1	G	380	MET	CB-CG-SD	5.16	127.88	112.40
1	E	380	MET	CB-CG-SD	5.16	127.88	112.40
1	A	380	MET	CB-CG-SD	5.16	127.87	112.40
1	F	380	MET	CB-CG-SD	5.15	127.85	112.40
1	F	594	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	594	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	539	MET	CA-CB-CG	5.06	121.90	113.30
1	E	594	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	594	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	539	MET	CA-CB-CG	5.06	121.89	113.30
1	D	436	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	436	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	594	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	539	MET	CA-CB-CG	5.05	121.89	113.30
1	G	539	MET	CA-CB-CG	5.05	121.88	113.30
1	D	150	LYS	CB-CG-CD	5.04	124.71	111.60
1	B	309	GLN	CA-CB-CG	5.04	124.48	113.40
1	E	539	MET	CA-CB-CG	5.04	121.87	113.30
1	A	309	GLN	CA-CB-CG	5.04	124.48	113.40
1	F	150	LYS	CB-CG-CD	5.04	124.69	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	539	MET	CA-CB-CG	5.03	121.86	113.30
1	G	150	LYS	CB-CG-CD	5.03	124.69	111.60
1	G	436	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	D	309	GLN	CA-CB-CG	5.03	124.47	113.40
1	F	539	MET	CA-CB-CG	5.03	121.85	113.30
1	E	436	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	331	LYS	CD-CE-NZ	-5.03	100.13	111.70
1	C	150	LYS	CB-CG-CD	5.03	124.67	111.60
1	B	436	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	C	309	GLN	CA-CB-CG	5.03	124.46	113.40
1	A	150	LYS	CB-CG-CD	5.03	124.67	111.60
1	F	309	GLN	CA-CB-CG	5.03	124.45	113.40
1	E	309	GLN	CA-CB-CG	5.02	124.45	113.40
1	G	309	GLN	CA-CB-CG	5.02	124.45	113.40
1	E	150	LYS	CB-CG-CD	5.02	124.66	111.60
1	B	150	LYS	CB-CG-CD	5.02	124.65	111.60
1	D	331	LYS	CD-CE-NZ	-5.02	100.16	111.70
1	C	436	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	B	331	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	E	331	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	G	331	LYS	CD-CE-NZ	-5.01	100.18	111.70
1	C	331	LYS	CD-CE-NZ	-5.01	100.19	111.70

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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 ⓘ

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	282	0
1	B	6273	0	6322	289	0
1	C	6273	0	6322	295	0
1	D	6264	0	6309	301	0
1	E	6239	0	6282	323	0
1	F	6273	0	6321	308	0
1	G	6273	0	6322	285	0
All	All	43868	0	44200	1934	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 22.

All (1934) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:338:ASP:O	1:G:339:ILE:HD13	1.77	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:D:646:PHE:HZ	1:D:713:VAL:HG21	1.42	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: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: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:C:751:GLN:CD	1:C:811:VAL:HG11	2.02	0.80
1:A:751:GLN:CD	1:A:811:VAL:HG11	2.02	0.80
1:E:414:PRO:HG2	1:E:491:GLN:OE1	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:751:GLN:CD	1:D:811:VAL:HG11	2.03	0.79
1:G:340:ASP:OD1	1:G:340:ASP:N	2.13	0.79
1:B:751:GLN:CD	1:B:811:VAL:HG11	2.02	0.79
1:F:340:ASP:OD1	1:F:340:ASP:N	2.14	0.79
1:F:758:ARG:HD3	1:F:928:ASP:C	2.02	0.79
1:F:295:GLN:HE21	1:E:427:SER:HB2	1.47	0.79
1:G:751:GLN:CD	1:G:811:VAL:HG11	2.02	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:E:751:GLN:CD	1:E:811:VAL:HG11	2.02	0.79
1:A:578:ARG:O	1:A:590:LYS:NZ	2.14	0.78
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:751:GLN:CD	1:F:811:VAL:HG11	2.02	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:D:340:ASP:N	1:D:340:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:41:LEU:HD23	1:G:89:VAL:HG21	1.70	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:F:578:ARG:O	1:F:590:LYS:NZ	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:764:ARG:CZ	1:F:897:LYS:C	2.61	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:N	1:A:798:ASP:OD2	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:B:197:SER:OG	1:B:239:LYS:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:443:MET:HG3	1:E:446:LEU:HD23	1.75	0.67
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: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: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: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:F:291:GLU:OE1	1:E:431:ARG:CG	2.43	0.66
1:B:798:ASP:OD2	1:B:798:ASP:N	2.28	0.66
1:B:885:LYS:HZ2	1:B:888:SER:HA	1.60	0.66
1:F:722:GLU:HB2	1:F:723:ILE:CG2	2.25	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: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: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:798:ASP:OD2	1:D:798:ASP:N	2.28	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:N	1:D:336:MET:HE3	2.13	0.64
1:D:436:TYR:HB3	1:D:437:GLU:OE1	1.97	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:A:357:ASN:CG	1:A:728:ARG:HB3	2.18	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: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:535:TYR:O	1:E:539:MET:HB2	1.98	0.63
1:D:333:GLU:H	1:D: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:885:LYS:HZ2	1:A:888:SER:HA	1.62	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:357:ASN:CG	1:G:728:ARG:HB3	2.20	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
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:C:357:ASN:CG	1:C:728:ARG:HB3	2.20	0.62
1:D:137:LEU:HD13	1:D:150:LYS:HG3	1.82	0.62
1:F:333:GLU:N	1:F:336:MET:HE3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:333:GLU:N	1:E:336:MET:HE3	2.14	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:F:333:GLU:H	1:F:336:MET:HE3	1.66	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:333:GLU:N	1:B:336:MET:HE3	2.15	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:C:431:ARG:HH12	1:E:277:GLU:CD	2.04	0.61
1:C:704:THR:OG1	1:C:705:GLU:N	2.33	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
1:E:333:GLU:H	1:E:336:MET:HE3	1.64	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:333:GLU:H	1:B:336:MET:HE3	1.65	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:E:885:LYS:HZ2	1:E:888:SER:HA	1.66	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:F:704:THR:OG1	1:F:705:GLU:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:CG	1:B:728:ARG:HB3	2.22	0.59
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
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:D:367:TYR:OH	1:D:466:LEU:O	2.15	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:F:758:ARG:CD	1:F:928:ASP:C	2.70	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:C:885:LYS:HZ2	1:C:888:SER:HA	1.68	0.59
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: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:G:885:LYS:HZ2	1:G:888:SER:HA	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:885:LYS:HZ2	1:D:888:SER:HA	1.68	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:333:GLU:H	1:C:336:MET:HE3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:333:GLU:H	1:A:336:MET:HE3	1.70	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: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:G:503:VAL:O	1:G:507:SER:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:HG3	1:A:290:VAL:CG1	2.36	0.56
1:D:354:GLU:HB3	1:D:413:VAL:HG11	1.87	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:G:443:MET:HE3	1:G:499:GLN:HB3	1.89	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: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: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:F:764:ARG:NH1	1:F:897:LYS:C	2.62	0.54
1:E:262:ARG:HG3	1:E:290:VAL:HG11	1.90	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
1:C:370:GLU:O	1:C:370:GLU:OE2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:333:GLU:H	1:G:336:MET:HE3	1.74	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:885:LYS:NZ	1:B:888:SER:HA	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:443:MET:HE3	1:C:499:GLN:HB3	1.91	0.52
1:C:709:ALA:O	1:C:713:VAL:HG23	2.10	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: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:E:885:LYS:NZ	1:E:888:SER:HA	2.24	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:462:THR:HG22	1:C:465:TYR:CE1	2.45	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
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:A:443:MET:HE3	1:A:499:GLN:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:431:ARG:HH12	1:A:277:GLU:CD	2.13	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: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
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:F:357:ASN:CG	1:F:728:ARG:HB3	2.30	0.51
1:G:206:ARG:HA	1:G:206:ARG:NE	2.24	0.51
1:B:443:MET:HE3	1:B:499:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:885:LYS:NZ	1:A:888:SER:HA	2.24	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:C:885:LYS:NZ	1:C:888:SER:HA	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:131:LYS:HE2	1:E:190:SER:C	2.32	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:ASN:OD1	1:D:242:ASN:C	2.51	0.49
1:D:567:ILE:HG22	1:D:569:VAL:HG23	1.94	0.49
1:F:242:ASN:OD1	1:F:242:ASN:C	2.51	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:A:242:ASN:OD1	1:A:242:ASN:C	2.51	0.49
1:B:242:ASN:OD1	1:B:242:ASN:C	2.51	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
1:D:86:ILE:O	1:D:90:VAL:HG23	2.13	0.49
1:D:443:MET:HE3	1:D:499:GLN:HB3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:443:MET:HE3	1:E:500:MET:H	1.78	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:242:ASN:OD1	1:C:242:ASN:C	2.51	0.48
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: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:G:242:ASN:OD1	1:G:242:ASN:C	2.51	0.48
1:G:338:ASP:C	1:G:339:ILE:HG12	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:770:ASN:OD1	1:D:770:ASN:N	2.46	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:35:LYS:HZ1	1:E:80:ALA:N	2.11	0.48
1:E:343:ASP:HB3	1:E:346:GLN:HB2	1.95	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:TRP:HD1	1:E:154:GLN:OE1	1.96	0.48
1:E:242:ASN:OD1	1:E:242:ASN:C	2.51	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:338:ASP:C	1:B:339:ILE:HG12	2.35	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
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: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:C:338:ASP:C	1:C:339:ILE:HG12	2.35	0.47
1:C:431:ARG:CB	1:D:291:GLU:OE1	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:567:ILE:HG22	1:F:569:VAL:N	2.30	0.47
1:F:724:GLU:O	1:F:727:ILE:CG1	2.52	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:338:ASP:C	1:D:339:ILE:HG12	2.35	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: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:A:752:HIS:NE2	1:A:811:VAL:O	2.37	0.47
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:E:338:ASP:C	1:E:339:ILE:HG12	2.35	0.46
1:E:349:GLY:HA2	1:E:368:VAL:CG2	2.45	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:D:355:GLY:O	1:D:487:SER:OG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:38:ARG:HB2	1:A:85:PHE:CE1	2.50	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:338:ASP:C	1:F:339:ILE:HG12	2.35	0.46
1:F:562:PRO:HG2	1:F:570:PHE:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LYS:HE2	1:G:190:SER:C	2.37	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: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: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: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:E:758:ARG:HD3	1:E:928:ASP:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:443:MET:HE3	1:F:500:MET:H	1.82	0.45
1:E:465:TYR:HB3	1:E:467:ARG:HG3	1.99	0.45
1:E:594:ASP:N	1:E:594:ASP:OD1	2.50	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
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: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:E:443:MET:HE3	1:E:500:MET:N	2.32	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:E:328:ILE:HG13	1:E:329:LYS:N	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:591:PHE:CE1	1:G:604:MET:HE2	2.54	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: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:D:591:PHE:CE1	1:D:604:MET:HE2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:A:591:PHE:CE1	1:A:604:MET:HE2	2.54	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:195:ASP:OD1	1:E:195:ASP:C	2.58	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:G:195:ASP:OD1	1:G:195:ASP:C	2.58	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:C:195:ASP:OD1	1:C:195:ASP:C	2.58	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: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
1:E:788:VAL:O	1:E:791:SER:OG	2.24	0.42
1:B:195:ASP:OD1	1:B:195:ASP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:195:ASP:OD1	1:F:195:ASP:C	2.58	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:591:PHE:CE1	1:C:604:MET:HE2	2.54	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: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:195:ASP:OD1	1:D:195:ASP:C	2.58	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:443:MET:HE3	1:F:499:GLN:HB3	2.00	0.42
1:F:443:MET:HE3	1:F:500:MET:N	2.35	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
1:G:227:PHE:CD1	1:G:260:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:ILE:O	1:G:329:LYS:HB2	2.20	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: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: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: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: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: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: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:358:LEU:O	1:A:359:ARG:HB2	2.19	0.42
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:C:330:VAL:HG22	1:C:331:LYS:N	2.35	0.41
1:C:333:GLU:N	1:C:336:MET:HE3	2.33	0.41
1:C:482:LEU:O	1:C:486:VAL:HG23	2.19	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: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:E:355:GLY:O	1:E:487:SER:OG	2.24	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:335:SER:O	1:C:336:MET:C	2.58	0.41
1:D:639:ARG:HH21	1:D:711:THR:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:758:ARG:HD3	1:G:928:ASP:C	2.40	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:849:PRO:HA	1:A:852:HIS:ND1	2.35	0.41
1:B:591:PHE:CE1	1:B:604:MET:HE2	2.55	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: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:195:ASP:OD1	1:A:195:ASP:C	2.58	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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:610:THR:OG1	1:G:618:ASP:OD2	2.28	0.41
1:E:568:GLY:HA2	1:E:570:PHE:HE1	1.85	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: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: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
1:G:330:VAL:HG22	1:G:331:LYS:N	2.36	0.41
1:G:335:SER:O	1:G:336:MET:C	2.59	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:861:ILE:HD12	1:A:895:LEU:HD22	2.03	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: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:116:PRO:HD2	1:G:119:GLU:OE2	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:364:ALA:O	1:B:368:VAL:HG23	2.21	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: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:293:LEU:HD22	1:E:224:ASP:O	2.20	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:G:204:VAL:HG12	1:G:245:LYS:CB	2.51	0.41
1:G:758:ARG:HD3	1:G:928:ASP:HA	2.03	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:888:SER:O	1:A:891:GLU:N	2.51	0.41
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: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: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:333:GLU:N	1:A:336:MET:HE3	2.34	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
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: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:335:SER:O	1:A:336:MET:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:355:GLY:O	1:G:487:SER:OG	2.24	0.40
1:E:261:ILE:CD1	1:E:298:LEU:CD1	2.96	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%)	13	22
1	B	765/947 (81%)	685 (90%)	70 (9%)	10 (1%)	12	20
1	C	765/947 (81%)	688 (90%)	68 (9%)	9 (1%)	13	22
1	D	764/947 (81%)	686 (90%)	68 (9%)	10 (1%)	12	20
1	E	761/947 (80%)	684 (90%)	67 (9%)	10 (1%)	12	20
1	F	765/947 (81%)	687 (90%)	68 (9%)	10 (1%)	12	20
1	G	765/947 (81%)	687 (90%)	69 (9%)	9 (1%)	13	22
All	All	5350/6629 (81%)	4804 (90%)	479 (9%)	67 (1%)	16	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	616 (88%)	81 (12%)	5	9
1	B	697/837 (83%)	619 (89%)	78 (11%)	6	10
1	C	697/837 (83%)	619 (89%)	78 (11%)	6	10
1	D	696/837 (83%)	619 (89%)	77 (11%)	6	10
1	E	693/837 (83%)	618 (89%)	75 (11%)	6	11
1	F	697/837 (83%)	620 (89%)	77 (11%)	6	11
1	G	697/837 (83%)	621 (89%)	76 (11%)	6	11
All	All	4874/5859 (83%)	4332 (89%)	542 (11%)	9	10

All (542) 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	117	ARG
1	B	148	LYS
1	B	150	LYS
1	B	151	GLU
1	B	154	GLN
1	B	159	GLN
1	B	162	ARG
1	B	170	LYS
1	B	171	GLU
1	B	173	LYS
1	B	177	PHE
1	B	179	ASP
1	B	197	SER
1	B	206	ARG
1	B	212	ASP
1	B	213	CYS
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
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	346	GLN
1	B	360	GLU
1	B	365	ASP
1	B	370	GLU
1	B	376	VAL
1	B	380	MET
1	B	391	TYR
1	B	392	HIS

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Mol	Chain	Res	Type
1	B	436	TYR
1	B	437	GLU
1	B	443	MET
1	B	448	LYS
1	B	473	GLU
1	B	500	MET
1	B	516	THR
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	594	ASP
1	B	595	THR
1	B	606	SER
1	B	621	SER
1	B	632	ILE
1	B	633	SER
1	B	661	SER
1	B	715	GLN
1	B	723	ILE
1	B	739	SER
1	B	744	ASN
1	B	765	MET
1	B	782	PHE
1	B	798	ASP
1	B	800	GLU
1	B	817	PHE
1	B	818	GLU
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	117	ARG
1	C	148	LYS

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Mol	Chain	Res	Type
1	C	150	LYS
1	C	151	GLU
1	C	154	GLN
1	C	159	GLN
1	C	162	ARG
1	C	170	LYS
1	C	171	GLU
1	C	173	LYS
1	C	177	PHE
1	C	179	ASP
1	C	197	SER
1	C	206	ARG
1	C	212	ASP
1	C	213	CYS
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	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	365	ASP
1	C	370	GLU
1	C	376	VAL
1	C	380	MET
1	C	391	TYR
1	C	392	HIS
1	C	436	TYR
1	C	437	GLU
1	C	443	MET
1	C	448	LYS
1	C	473	GLU
1	C	500	MET

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Mol	Chain	Res	Type
1	C	516	THR
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	594	ASP
1	C	595	THR
1	C	606	SER
1	C	621	SER
1	C	632	ILE
1	C	633	SER
1	C	661	SER
1	C	715	GLN
1	C	723	ILE
1	C	739	SER
1	C	744	ASN
1	C	765	MET
1	C	782	PHE
1	C	798	ASP
1	C	800	GLU
1	C	817	PHE
1	C	818	GLU
1	C	868	LEU
1	C	873	SER
1	C	890	GLU
1	C	893	ASP
1	C	929	LYS
1	C	930	ASP
1	D	38	ARG
1	D	39	ASP
1	D	40	GLN
1	D	105	LYS
1	D	117	ARG
1	D	148	LYS
1	D	150	LYS
1	D	151	GLU
1	D	154	GLN
1	D	159	GLN
1	D	162	ARG
1	D	170	LYS

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Mol	Chain	Res	Type
1	D	171	GLU
1	D	173	LYS
1	D	177	PHE
1	D	179	ASP
1	D	197	SER
1	D	206	ARG
1	D	212	ASP
1	D	213	CYS
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	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	346	GLN
1	D	360	GLU
1	D	365	ASP
1	D	370	GLU
1	D	376	VAL
1	D	380	MET
1	D	391	TYR
1	D	392	HIS
1	D	436	TYR
1	D	437	GLU
1	D	443	MET
1	D	448	LYS
1	D	473	GLU
1	D	500	MET
1	D	516	THR
1	D	531	LEU
1	D	539	MET
1	D	540	SER
1	D	545	GLU
1	D	561	SER

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Mol	Chain	Res	Type
1	D	573	MET
1	D	594	ASP
1	D	595	THR
1	D	606	SER
1	D	621	SER
1	D	632	ILE
1	D	633	SER
1	D	661	SER
1	D	715	GLN
1	D	723	ILE
1	D	739	SER
1	D	744	ASN
1	D	765	MET
1	D	782	PHE
1	D	798	ASP
1	D	800	GLU
1	D	817	PHE
1	D	818	GLU
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	117	ARG
1	F	148	LYS
1	F	150	LYS
1	F	151	GLU
1	F	154	GLN
1	F	159	GLN
1	F	162	ARG
1	F	170	LYS
1	F	171	GLU
1	F	173	LYS
1	F	177	PHE
1	F	179	ASP
1	F	197	SER
1	F	206	ARG
1	F	212	ASP

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Mol	Chain	Res	Type
1	F	213	CYS
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	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	365	ASP
1	F	370	GLU
1	F	376	VAL
1	F	380	MET
1	F	391	TYR
1	F	392	HIS
1	F	436	TYR
1	F	437	GLU
1	F	443	MET
1	F	448	LYS
1	F	473	GLU
1	F	500	MET
1	F	516	THR
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	594	ASP
1	F	595	THR
1	F	606	SER
1	F	621	SER
1	F	632	ILE
1	F	633	SER
1	F	661	SER

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Mol	Chain	Res	Type
1	F	715	GLN
1	F	723	ILE
1	F	739	SER
1	F	744	ASN
1	F	765	MET
1	F	782	PHE
1	F	798	ASP
1	F	800	GLU
1	F	817	PHE
1	F	818	GLU
1	F	868	LEU
1	F	873	SER
1	F	890	GLU
1	F	893	ASP
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	117	ARG
1	G	148	LYS
1	G	150	LYS
1	G	151	GLU
1	G	154	GLN
1	G	159	GLN
1	G	162	ARG
1	G	170	LYS
1	G	171	GLU
1	G	173	LYS
1	G	177	PHE
1	G	179	ASP
1	G	197	SER
1	G	206	ARG
1	G	212	ASP
1	G	213	CYS
1	G	224	ASP
1	G	228	ASP
1	G	242	ASN
1	G	258	SER
1	G	262	ARG
1	G	270	SER

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Mol	Chain	Res	Type
1	G	271	LYS
1	G	279	GLU
1	G	298	LEU
1	G	311	LYS
1	G	313	MET
1	G	328	ILE
1	G	337	GLN
1	G	340	ASP
1	G	360	GLU
1	G	365	ASP
1	G	370	GLU
1	G	376	VAL
1	G	380	MET
1	G	391	TYR
1	G	392	HIS
1	G	436	TYR
1	G	437	GLU
1	G	443	MET
1	G	448	LYS
1	G	473	GLU
1	G	500	MET
1	G	516	THR
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	594	ASP
1	G	595	THR
1	G	606	SER
1	G	621	SER
1	G	632	ILE
1	G	633	SER
1	G	661	SER
1	G	715	GLN
1	G	723	ILE
1	G	739	SER
1	G	744	ASN
1	G	765	MET
1	G	782	PHE
1	G	798	ASP

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Mol	Chain	Res	Type
1	G	800	GLU
1	G	817	PHE
1	G	818	GLU
1	G	868	LEU
1	G	873	SER
1	G	890	GLU
1	G	893	ASP
1	G	934	ARG
1	E	38	ARG
1	E	39	ASP
1	E	40	GLN
1	E	105	LYS
1	E	117	ARG
1	E	148	LYS
1	E	150	LYS
1	E	151	GLU
1	E	154	GLN
1	E	159	GLN
1	E	162	ARG
1	E	170	LYS
1	E	171	GLU
1	E	173	LYS
1	E	177	PHE
1	E	179	ASP
1	E	197	SER
1	E	206	ARG
1	E	212	ASP
1	E	213	CYS
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	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

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Mol	Chain	Res	Type
1	E	360	GLU
1	E	365	ASP
1	E	370	GLU
1	E	376	VAL
1	E	380	MET
1	E	391	TYR
1	E	392	HIS
1	E	436	TYR
1	E	437	GLU
1	E	443	MET
1	E	448	LYS
1	E	473	GLU
1	E	500	MET
1	E	516	THR
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	594	ASP
1	E	595	THR
1	E	606	SER
1	E	621	SER
1	E	632	ILE
1	E	633	SER
1	E	661	SER
1	E	715	GLN
1	E	723	ILE
1	E	739	SER
1	E	744	ASN
1	E	765	MET
1	E	782	PHE
1	E	798	ASP
1	E	800	GLU
1	E	817	PHE
1	E	818	GLU
1	E	868	LEU
1	E	873	SER
1	E	890	GLU
1	E	893	ASP
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	39	ASP
1	A	40	GLN
1	A	105	LYS
1	A	117	ARG
1	A	148	LYS
1	A	150	LYS
1	A	151	GLU
1	A	154	GLN
1	A	159	GLN
1	A	162	ARG
1	A	170	LYS
1	A	171	GLU
1	A	173	LYS
1	A	177	PHE
1	A	179	ASP
1	A	197	SER
1	A	206	ARG
1	A	212	ASP
1	A	213	CYS
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	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	365	ASP
1	A	370	GLU
1	A	376	VAL
1	A	380	MET
1	A	391	TYR
1	A	392	HIS

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Mol	Chain	Res	Type
1	A	436	TYR
1	A	437	GLU
1	A	443	MET
1	A	448	LYS
1	A	473	GLU
1	A	500	MET
1	A	509	SER
1	A	516	THR
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	594	ASP
1	A	595	THR
1	A	606	SER
1	A	621	SER
1	A	632	ILE
1	A	633	SER
1	A	661	SER
1	A	715	GLN
1	A	723	ILE
1	A	739	SER
1	A	744	ASN
1	A	747	ASN
1	A	765	MET
1	A	782	PHE
1	A	798	ASP
1	A	800	GLU
1	A	817	PHE
1	A	818	GLU
1	A	868	LEU
1	A	873	SER
1	A	890	GLU
1	A	893	ASP
1	A	930	ASP
1	A	931	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	GLN
1	C	194	GLN
1	D	194	GLN
1	D	530	GLN
1	F	194	GLN
1	F	276	GLN
1	F	295	GLN
1	F	759	ASN
1	G	194	GLN
1	E	194	GLN
1	A	194	GLN
1	A	768	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

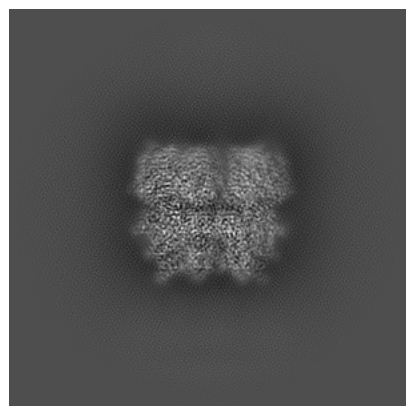
6 Map visualisation [i](#)

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.

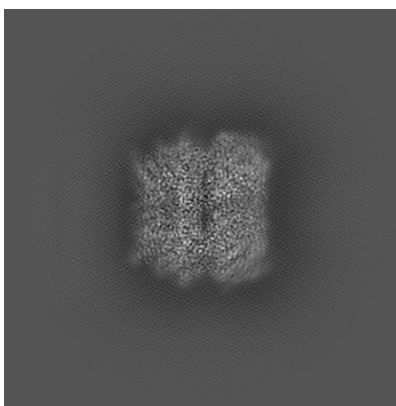
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

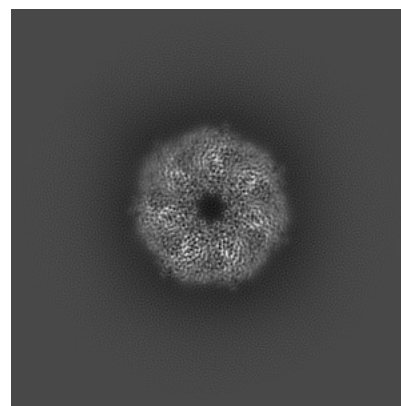
6.1.1 Primary map



X

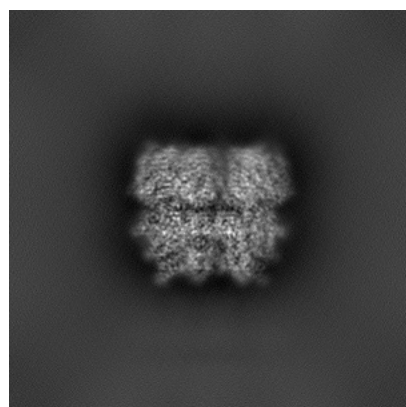


Y

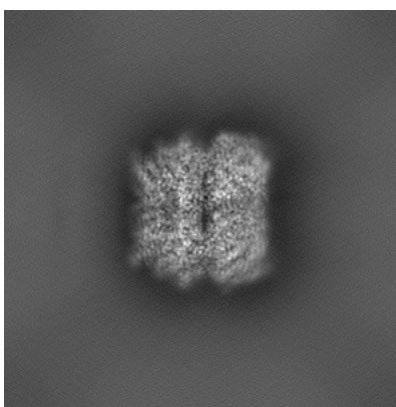


Z

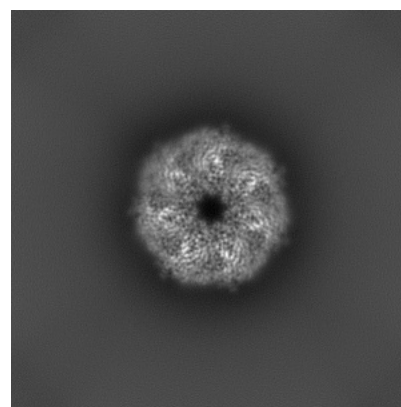
6.1.2 Raw map



X



Y

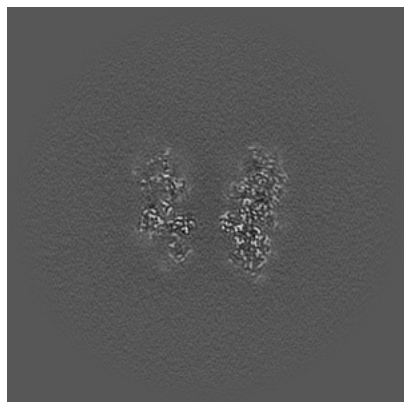


Z

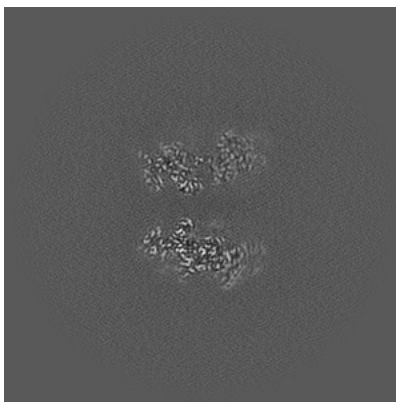
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

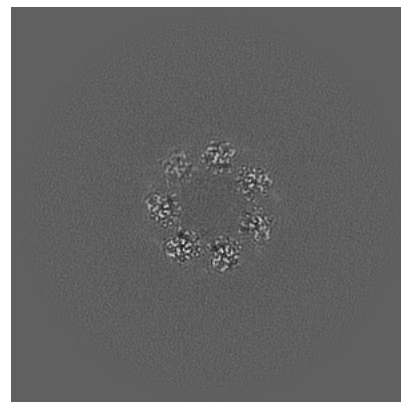
6.2.1 Primary map



X Index: 208

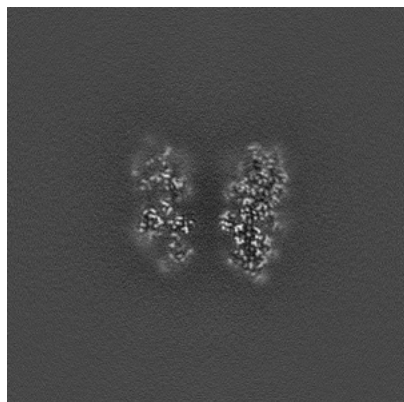


Y Index: 208

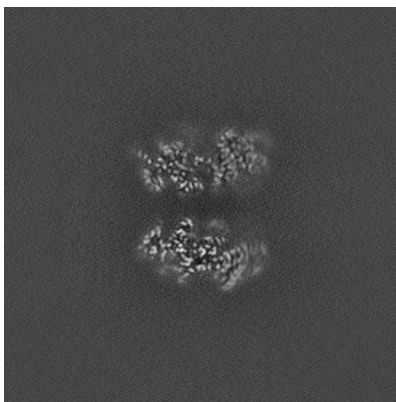


Z Index: 208

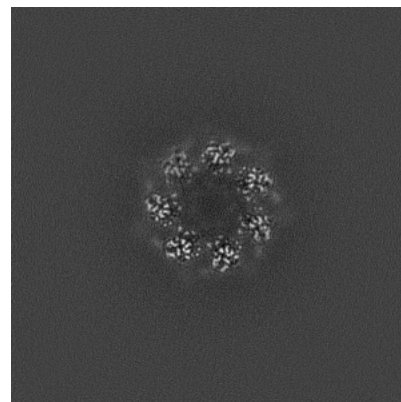
6.2.2 Raw map



X Index: 208



Y Index: 208

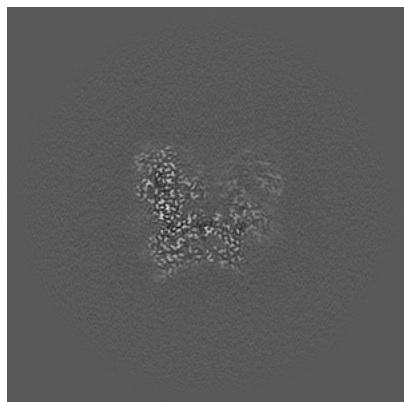


Z Index: 208

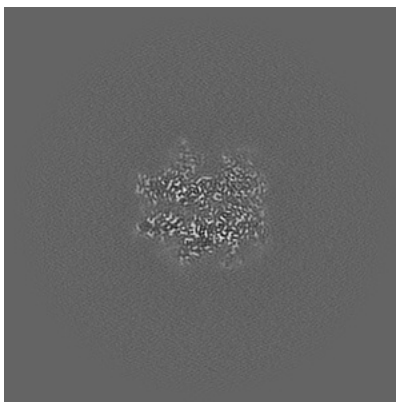
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

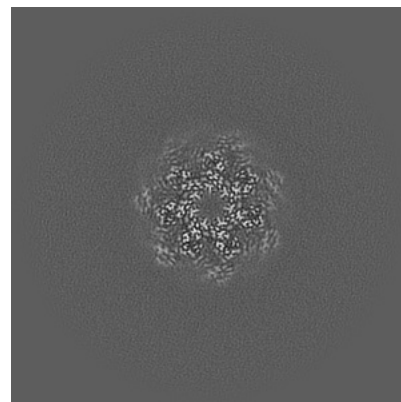
6.3.1 Primary map



X Index: 182

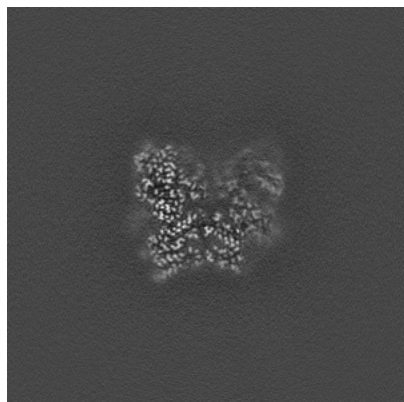


Y Index: 165

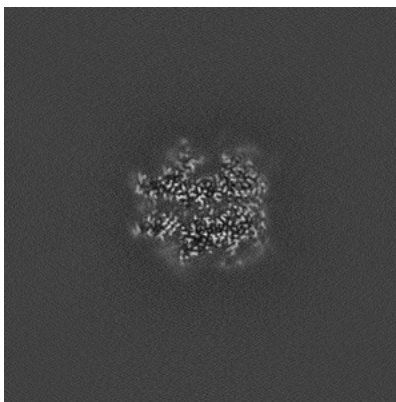


Z Index: 184

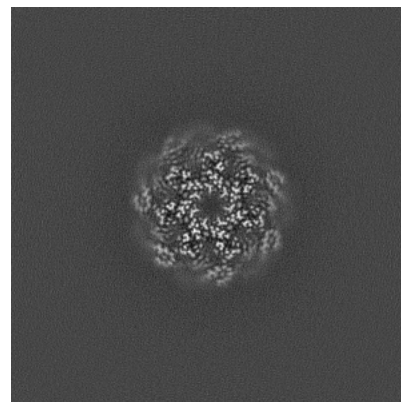
6.3.2 Raw map



X Index: 182



Y Index: 164

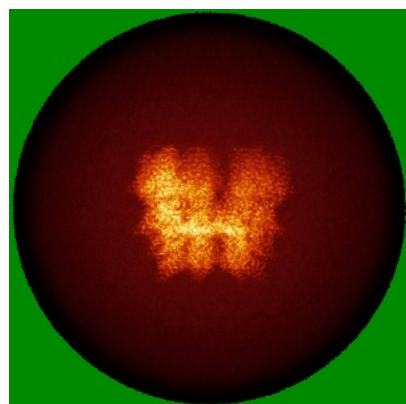


Z Index: 184

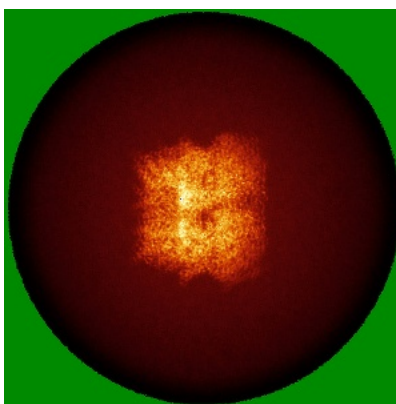
The images above show the largest variance slices of the map in three orthogonal directions.

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

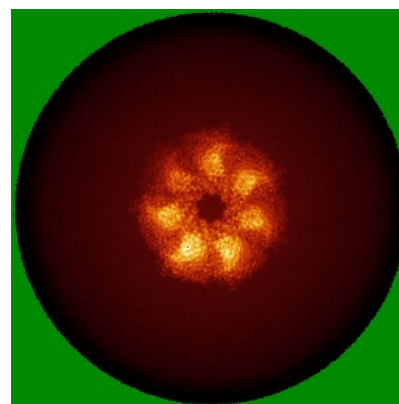
6.4.1 Primary map



X

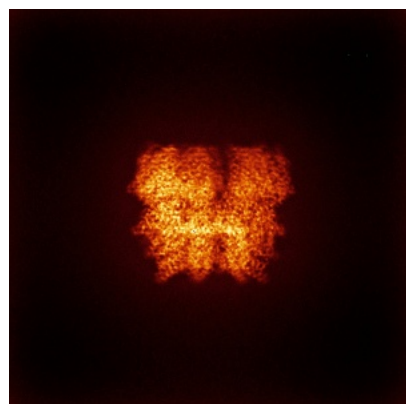


Y

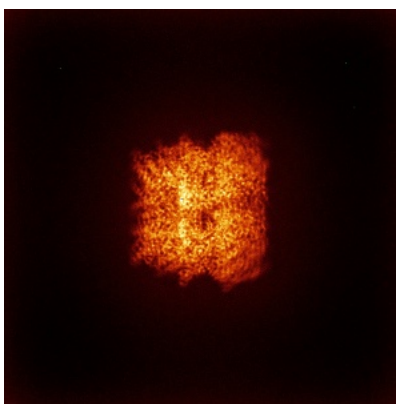


Z

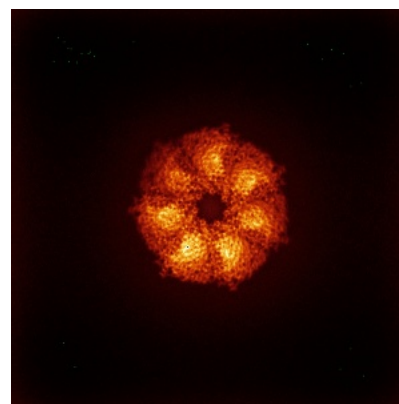
6.4.2 Raw map



X



Y

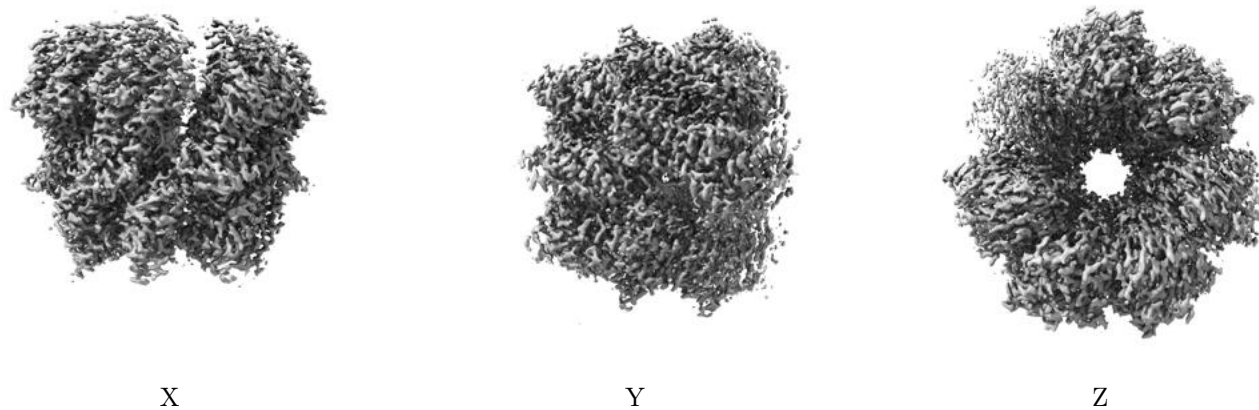


Z

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.

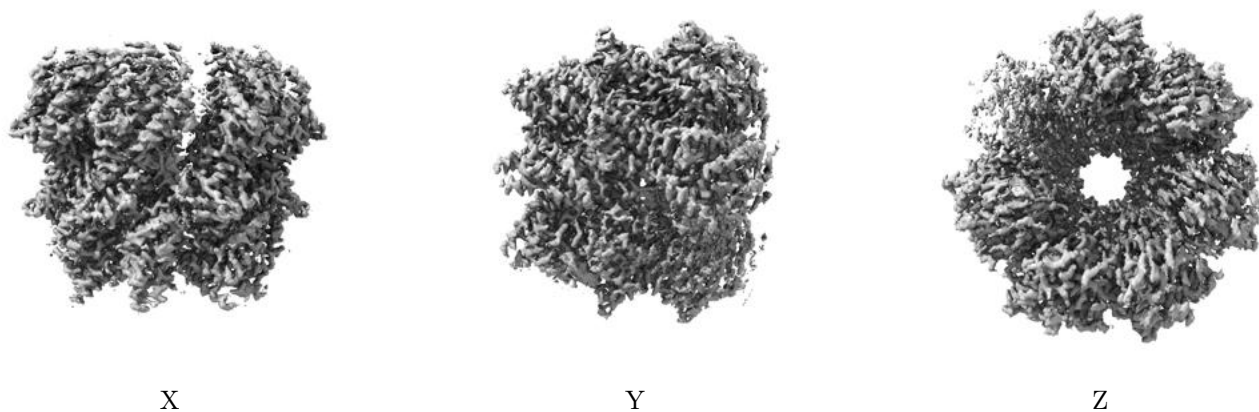
6.5 Orthogonal surface views [i](#)

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.

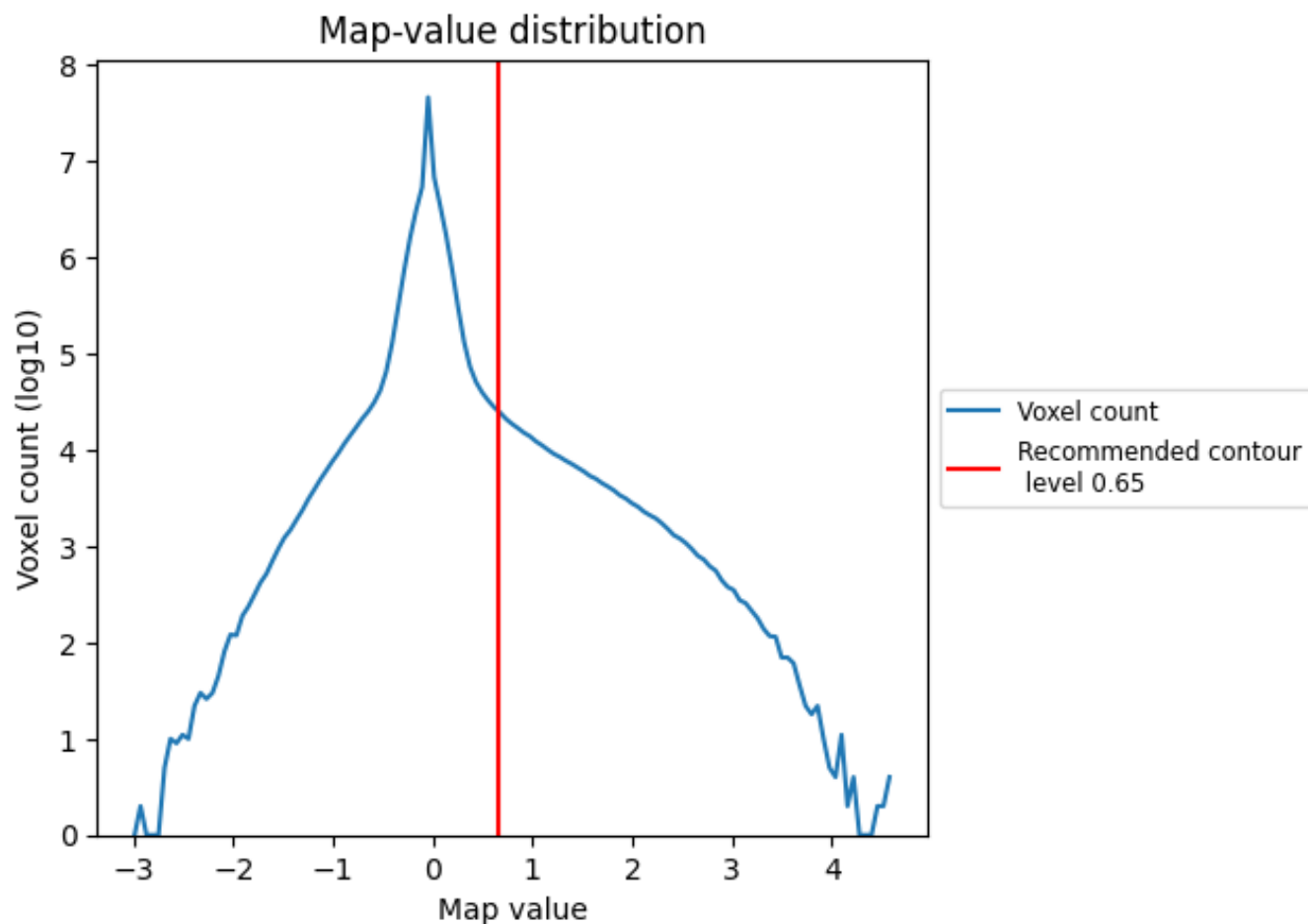
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

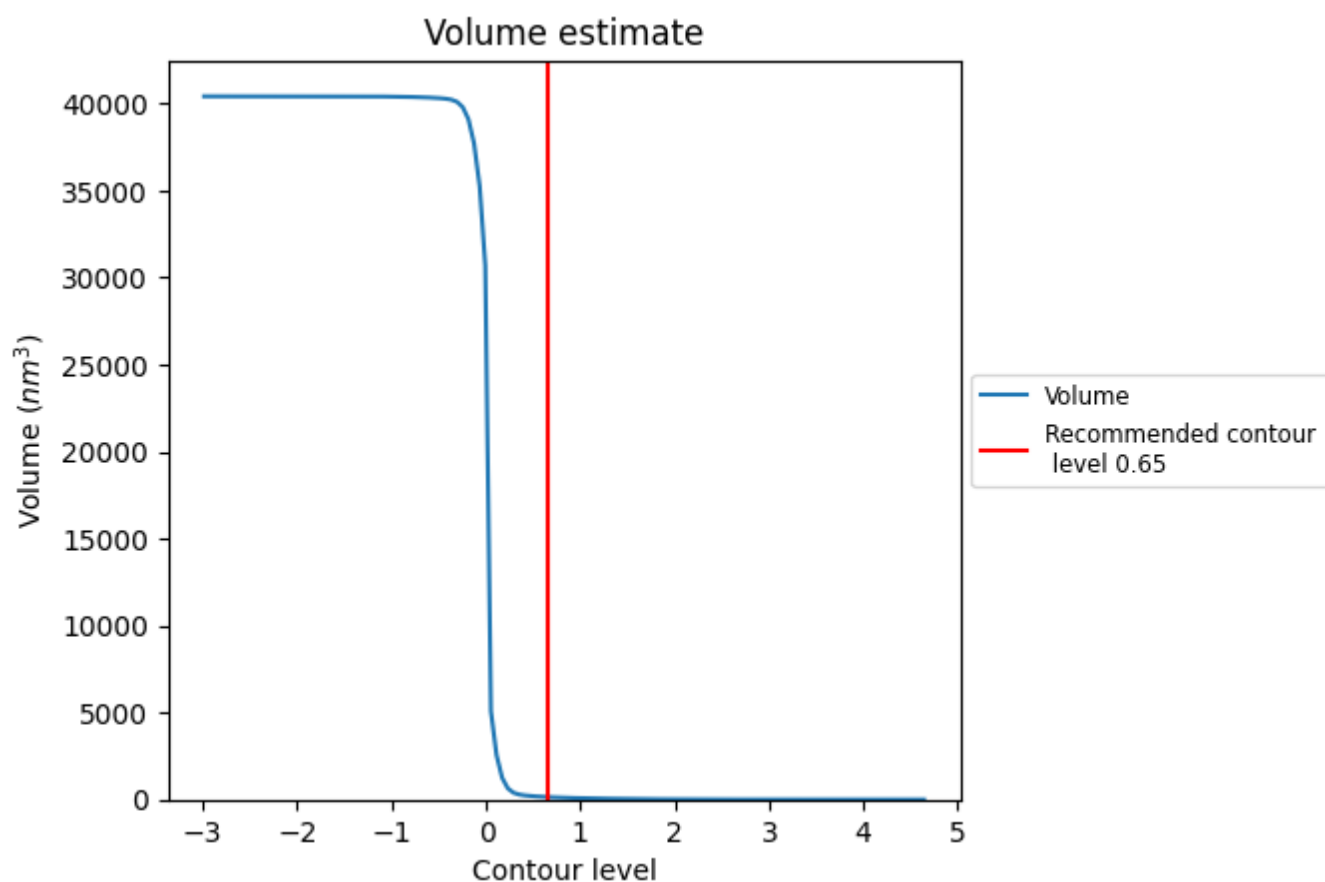
This section contains the results of statistical analysis of the map.

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.

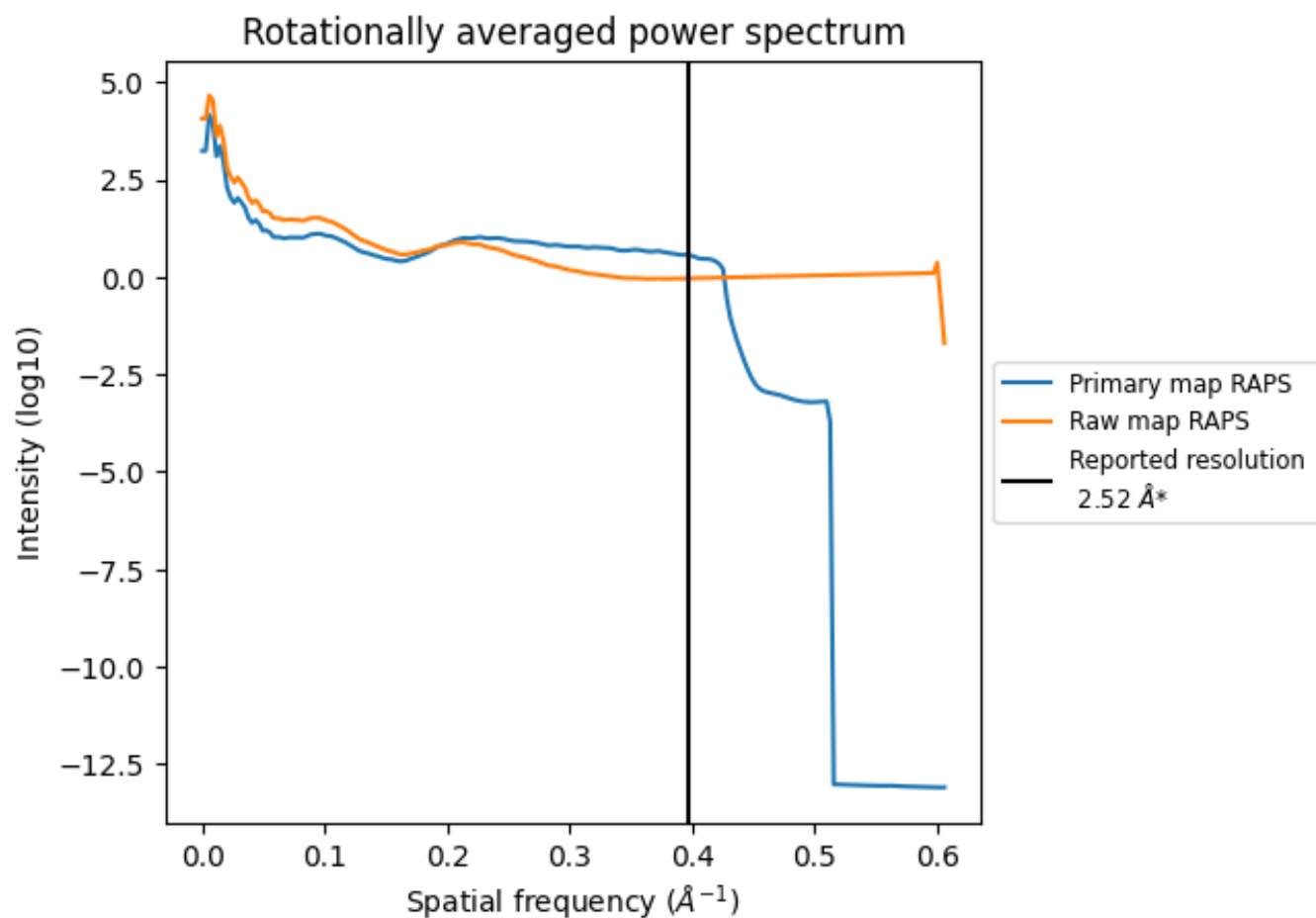
7.2 Volume estimate [i](#)



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 ⓘ

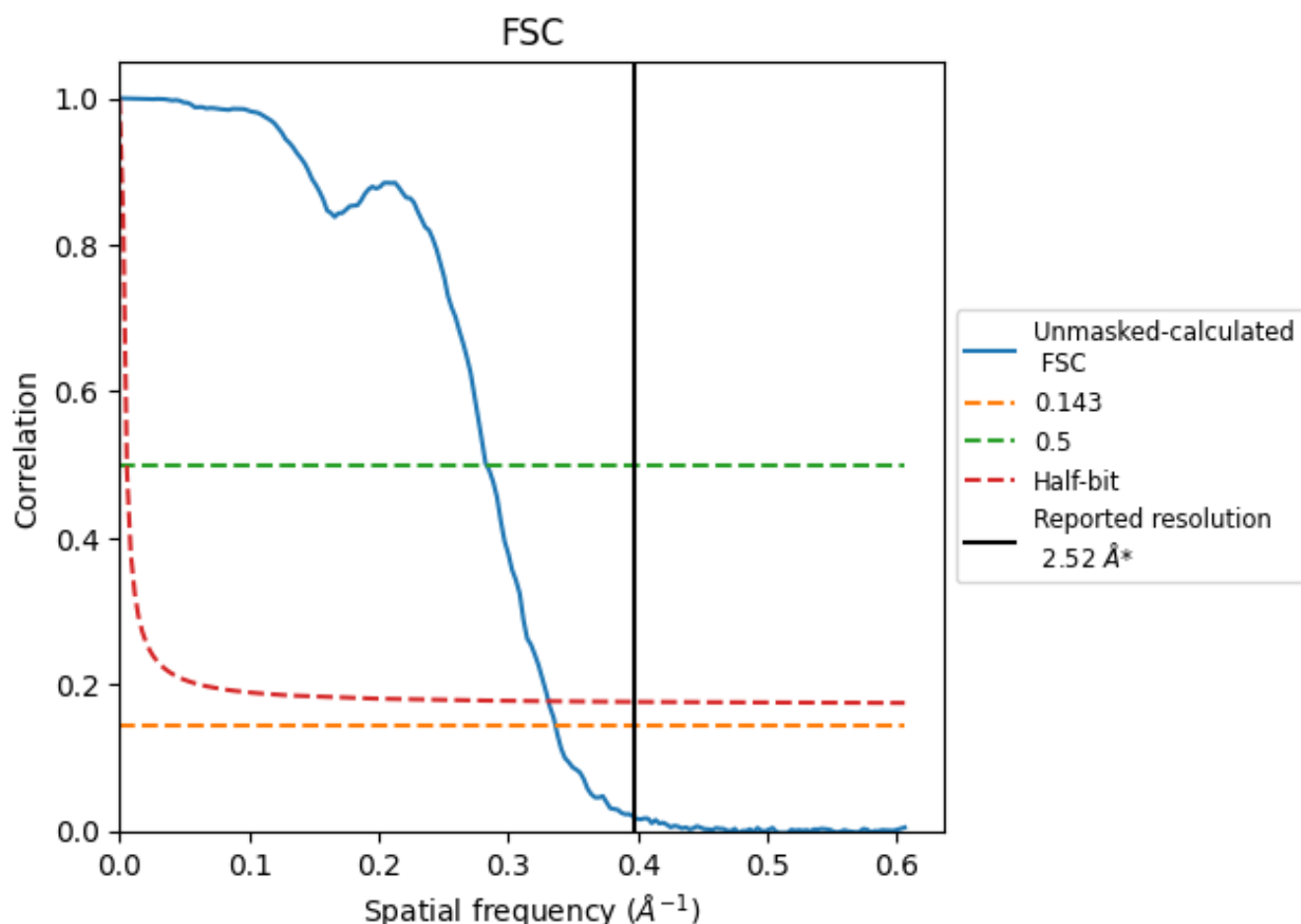


*Reported resolution corresponds to spatial frequency of 0.397 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

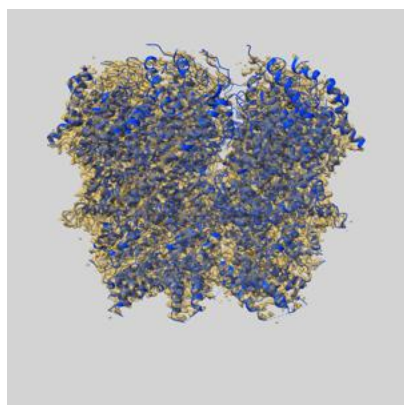
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.53	3.02

*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 %

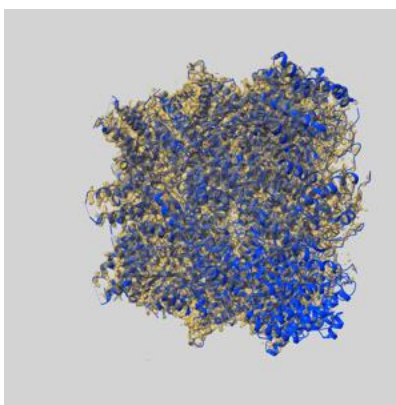
9 Map-model fit [i](#)

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 [6](#).

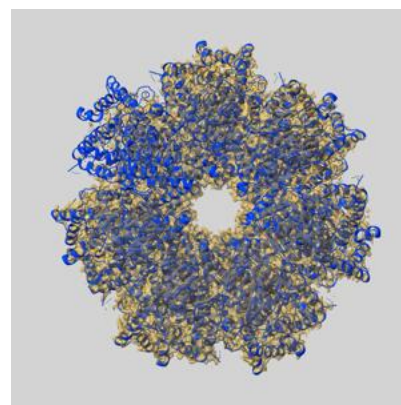
9.1 Map-model overlay [i](#)



X



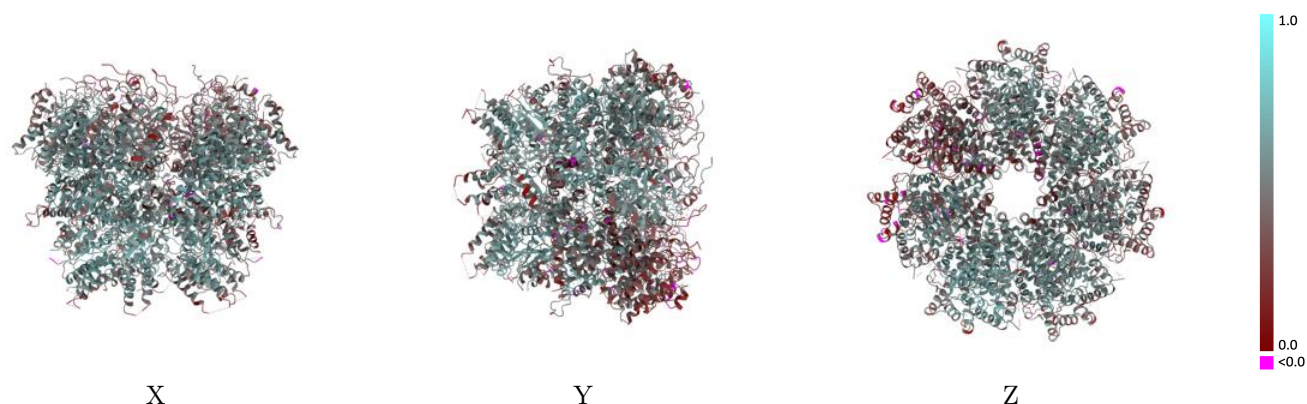
Y



Z

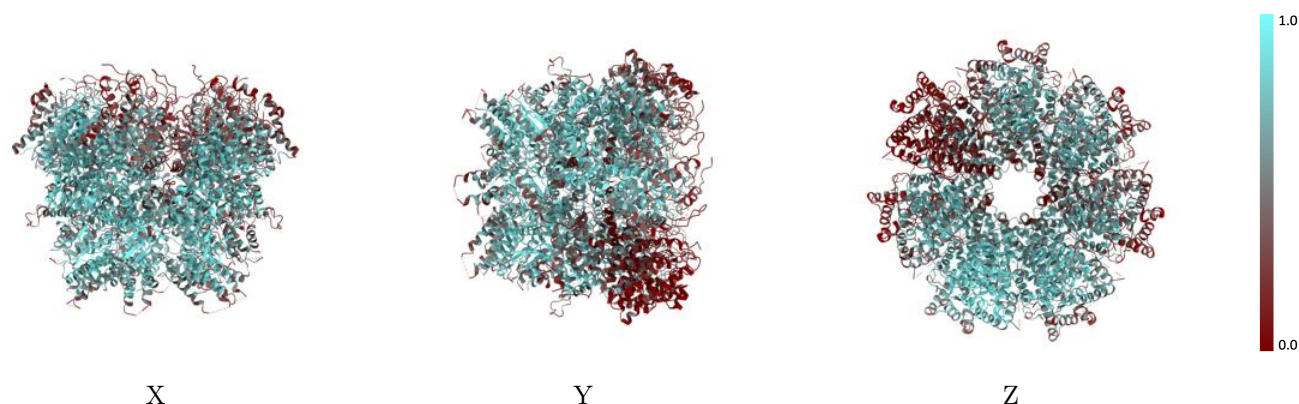
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



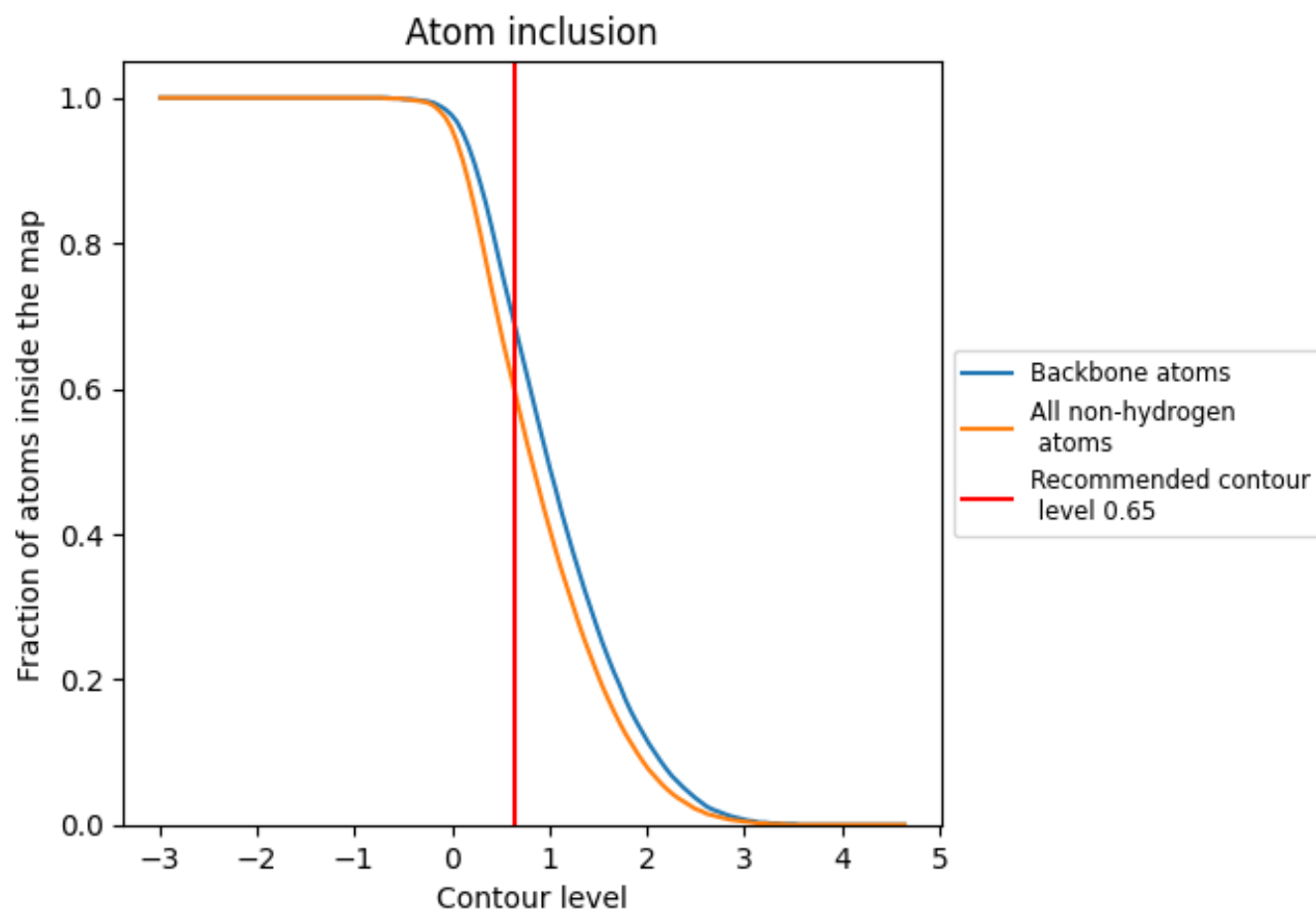
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.5930	<div></div> 0.4860
A	<div></div> 0.6990	<div></div> 0.5250
B	<div></div> 0.5660	<div></div> 0.4910
C	<div></div> 0.6200	<div></div> 0.5090
D	<div></div> 0.5980	<div></div> 0.5040
E	<div></div> 0.3140	<div></div> 0.3470
F	<div></div> 0.5930	<div></div> 0.4640
G	<div></div> 0.7570	<div></div> 0.5590

1.0

0.0

<0.0