Full wwPDB EM Validation Report (i)

Aug 9, 2026 – 03:29 PM JST

PDB ID	:	9V75 / pdb_00009v75
EMDB ID	:	EMD-64810
Title	:	Psl polysaccharide related protein structures
Authors	:	Jiao, L.; Yihua, H.; Jiao, L.
Deposited on	:	2025-05-27
Resolution	:	2.89 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

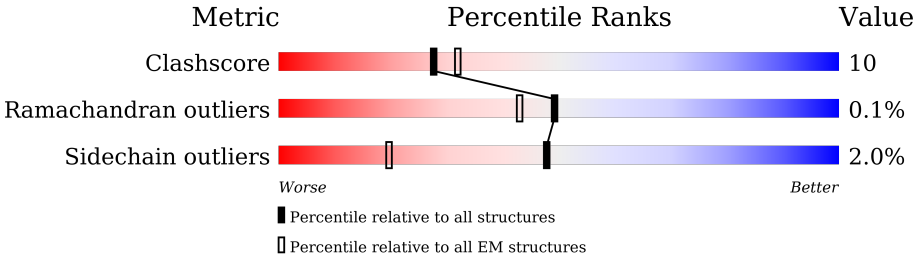
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

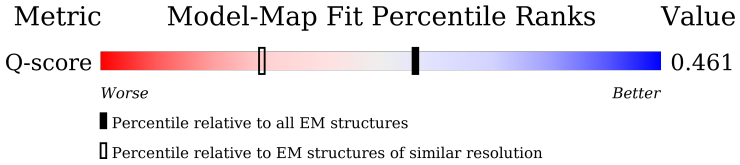
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12148 (2.39 - 3.39)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	662	25% 79% 16%
1	B	662	25% 79% 16%
1	D	662	24% 80% 15%
1	F	662	25% 80% 15%

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Mol	Chain	Length	Quality of chain
1	H	662	24% 79% 14%
1	J	662	25% 82% 14%
1	L	662	24% 80% 15%
1	N	662	25% 80% 15%
2	C	256	80% 11% 9%
2	E	256	82% 9% 9%
2	G	256	82% 9% 9%
2	I	256	82% 9% 9%
2	K	256	82% 9% 9%
2	M	256	82% 10% 9%
2	O	256	81% 11% 9%
2	P	256	82% 10% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 55896 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 Biofilm formation protein PslE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	657	5201	3289	920	983	9	0	0
1	B	657	5201	3289	920	983	9	0	0
1	D	657	5201	3289	920	983	9	0	0
1	F	657	5201	3289	920	983	9	0	0
1	H	657	5201	3289	920	983	9	0	0
1	J	657	5201	3289	920	983	9	0	0
1	L	657	5201	3289	920	983	9	0	0
1	N	657	5201	3289	920	983	9	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	CYS	TYR	conflict	UNP A0A073A0N3
A	595	CYS	ARG	conflict	UNP A0A073A0N3
B	524	CYS	TYR	conflict	UNP A0A073A0N3
B	595	CYS	ARG	conflict	UNP A0A073A0N3
D	524	CYS	TYR	conflict	UNP A0A073A0N3
D	595	CYS	ARG	conflict	UNP A0A073A0N3
F	524	CYS	TYR	conflict	UNP A0A073A0N3
F	595	CYS	ARG	conflict	UNP A0A073A0N3
H	524	CYS	TYR	conflict	UNP A0A073A0N3
H	595	CYS	ARG	conflict	UNP A0A073A0N3
J	524	CYS	TYR	conflict	UNP A0A073A0N3
J	595	CYS	ARG	conflict	UNP A0A073A0N3
L	524	CYS	TYR	conflict	UNP A0A073A0N3
L	595	CYS	ARG	conflict	UNP A0A073A0N3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	524	CYS	TYR	conflict	UNP A0A073A0N3
N	595	CYS	ARG	conflict	UNP A0A073A0N3

- Molecule 2 is a protein called Biofilm formation protein PslD.

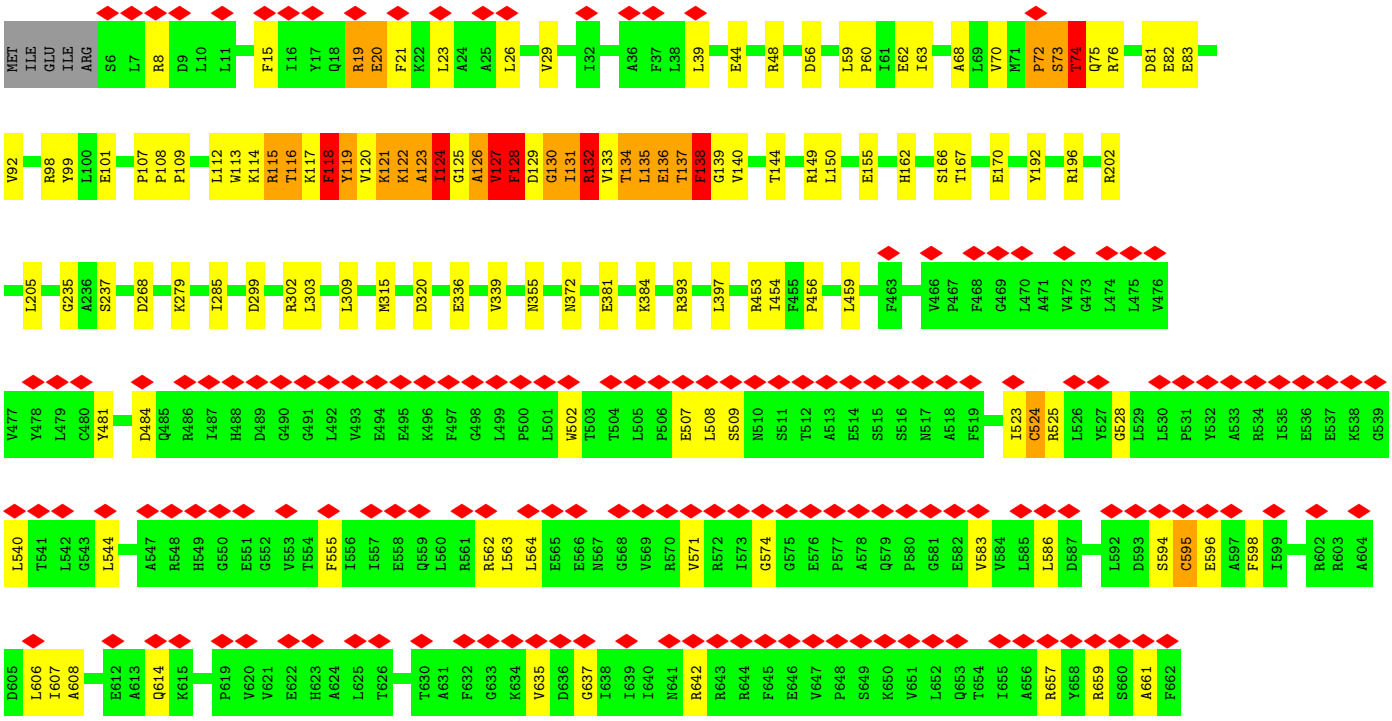
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	234	1786	1125	320	333	8	0	0
2	E	234	1786	1125	320	333	8	0	0
2	G	234	1786	1125	320	333	8	0	0
2	I	234	1786	1125	320	333	8	0	0
2	K	234	1786	1125	320	333	8	0	0
2	M	234	1786	1125	320	333	8	0	0
2	O	234	1786	1125	320	333	8	0	0
2	P	234	1786	1125	320	333	8	0	0

3 Residue-property plots (i)

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.

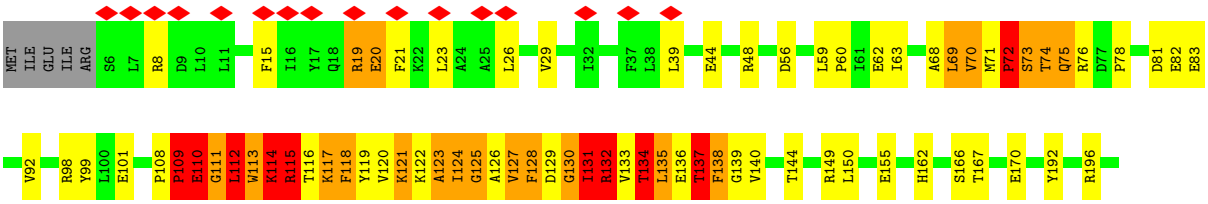
• Molecule 1: Biofilm formation protein PslE

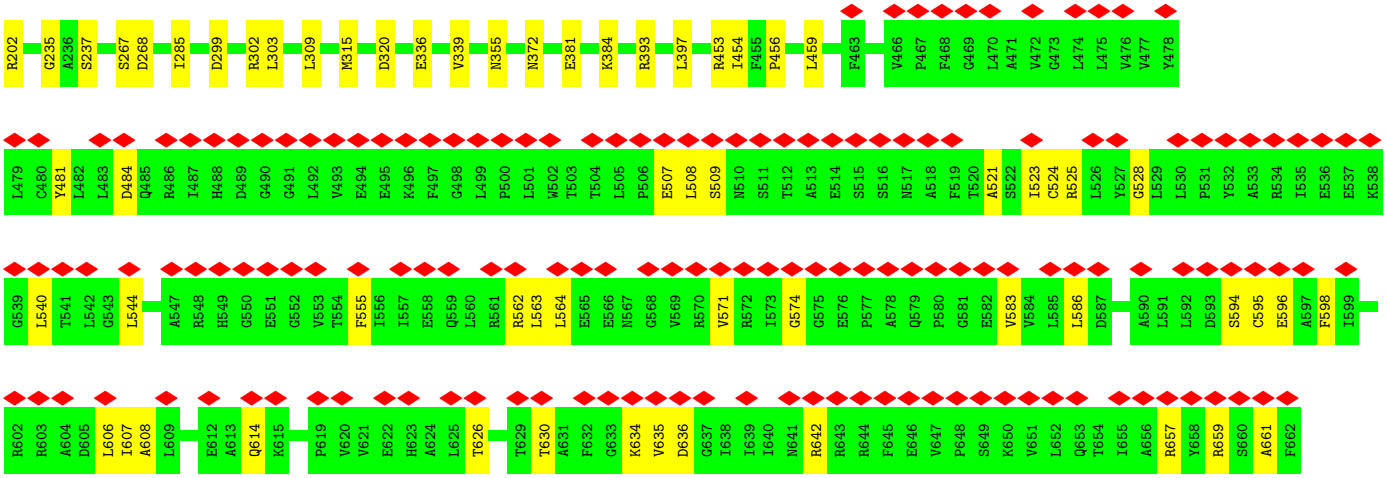
Chain A:



• Molecule 1: Biofilm formation protein PslE

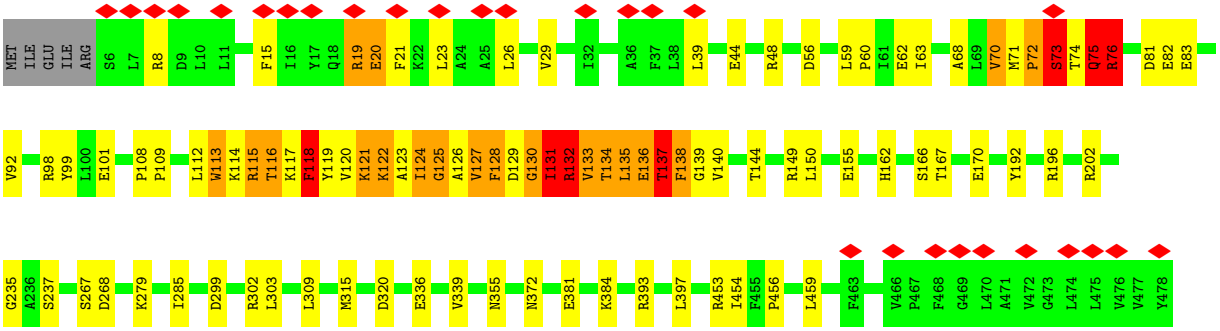
Chain B:

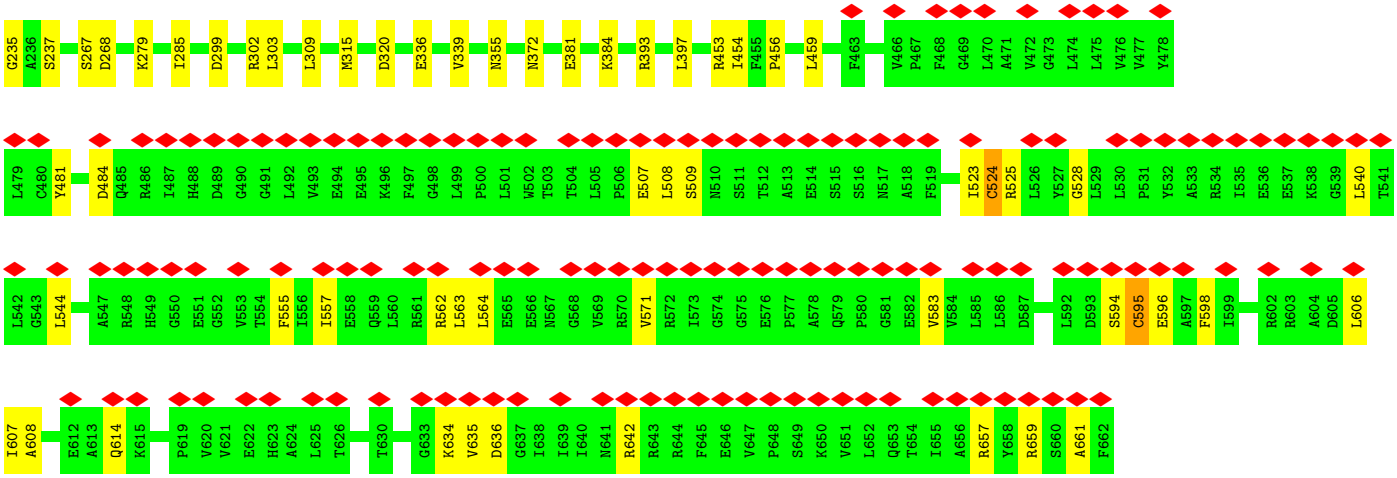




- Molecule 1: Biofilm formation protein PslE

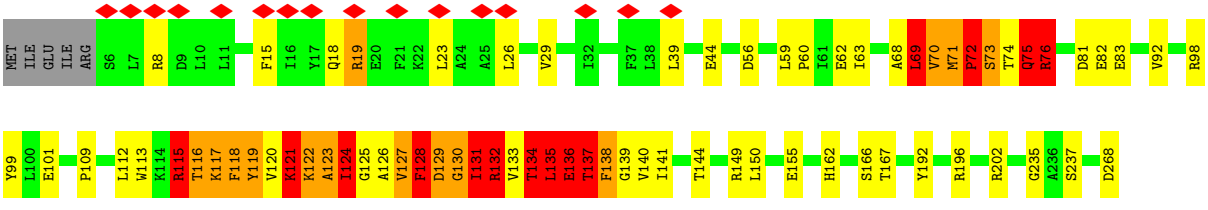
Chain D:

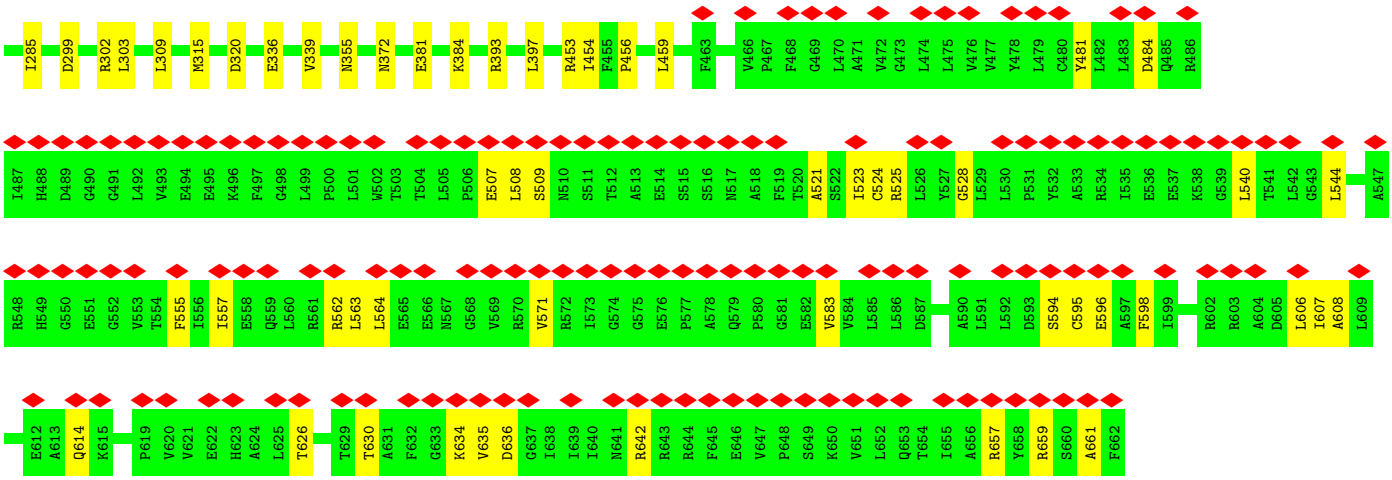




- Molecule 1: Biofilm formation protein PslE

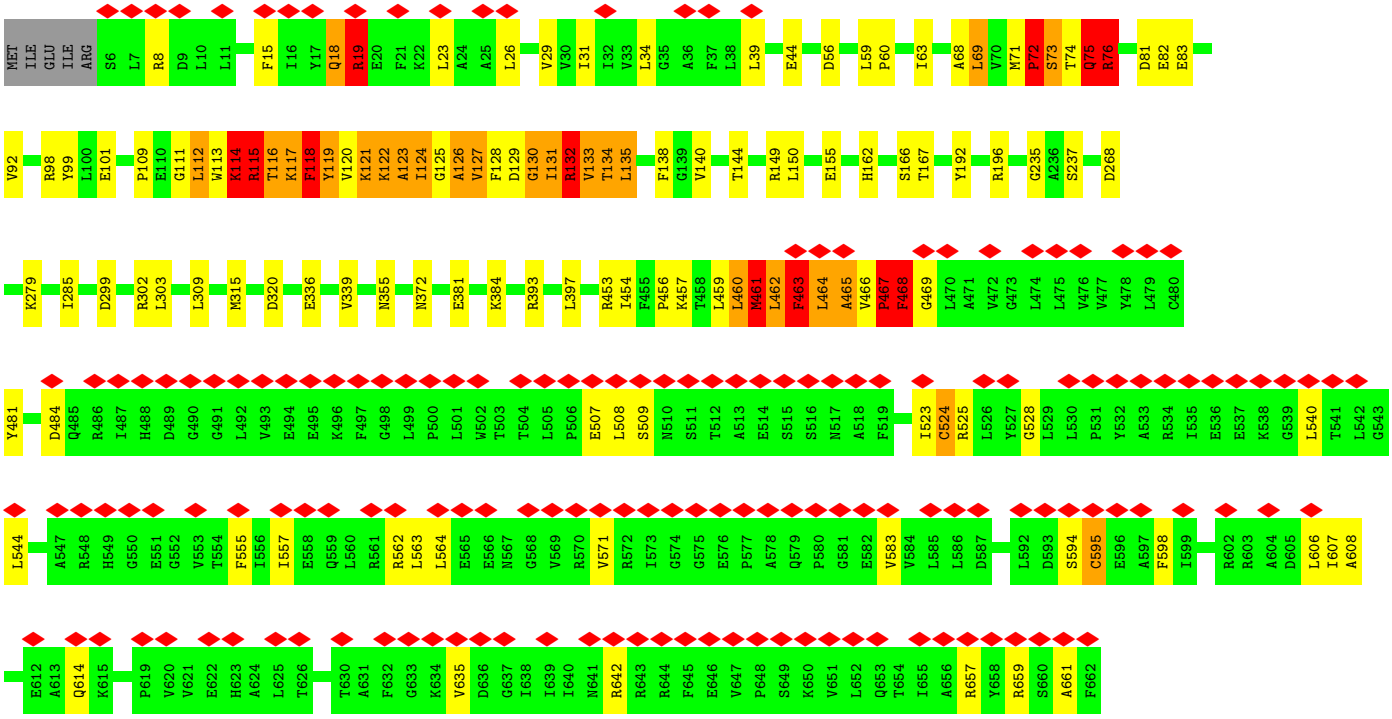
Chain F:





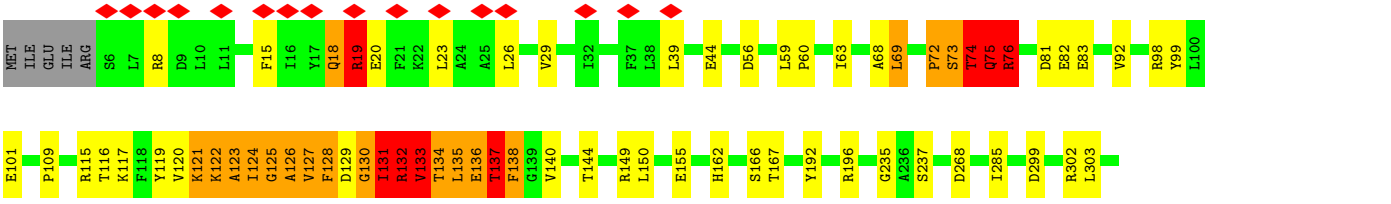
- Molecule 1: Biofilm formation protein PslE

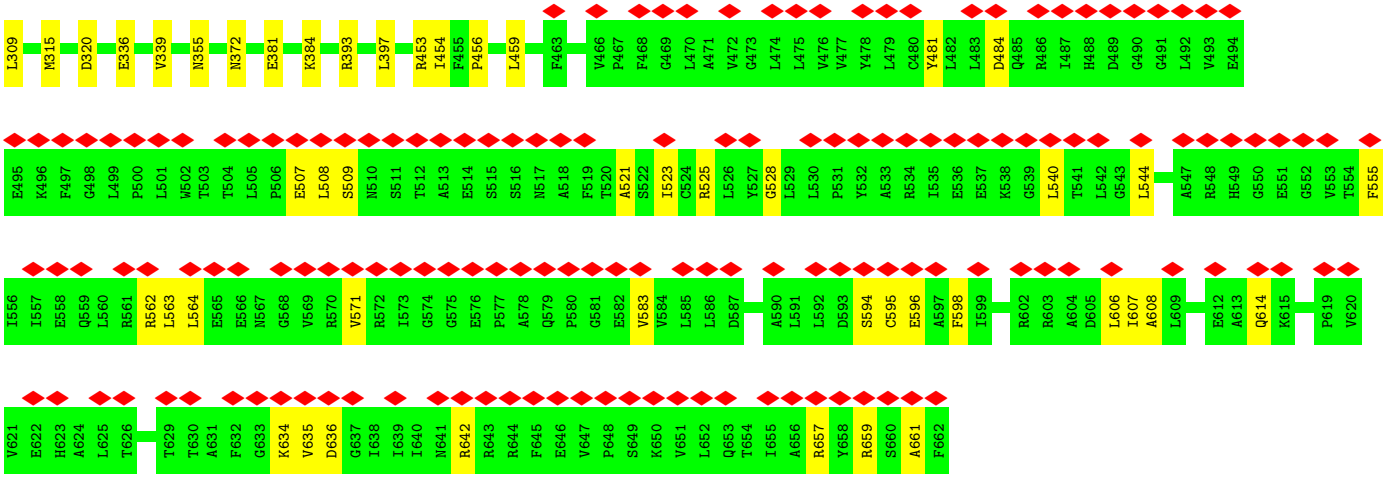
Chain H:



- Molecule 1: Biofilm formation protein PslE

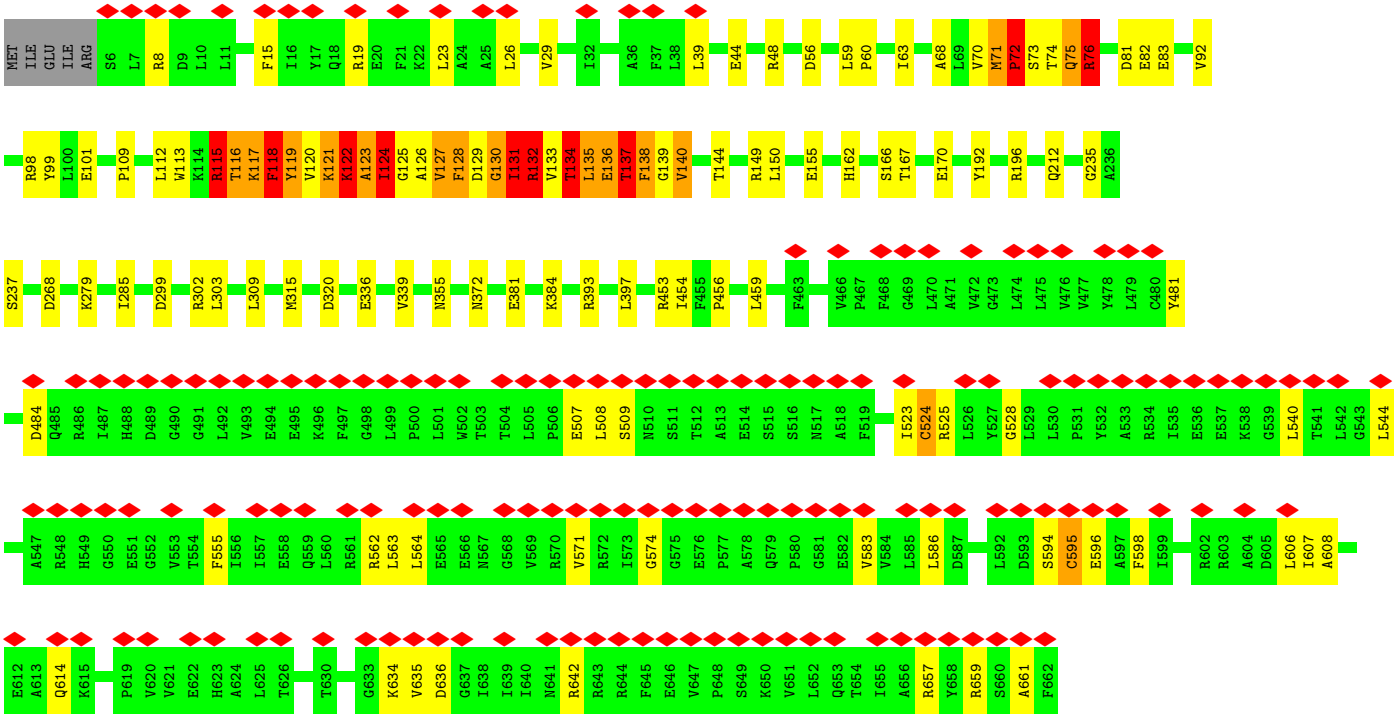
Chain J:





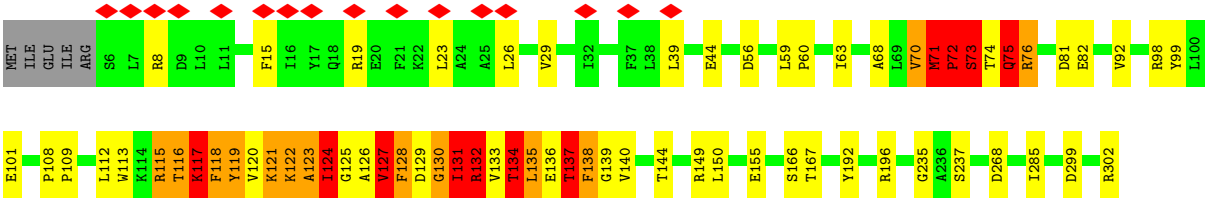
- Molecule 1: Biofilm formation protein PslE

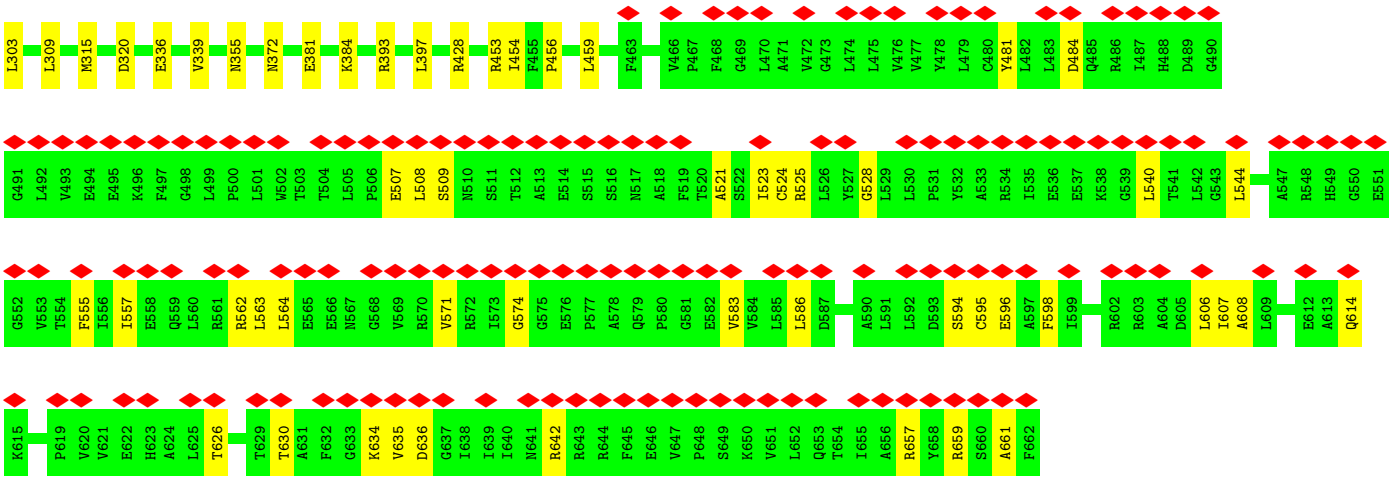
Chain L:



- Molecule 1: Biofilm formation protein PslE

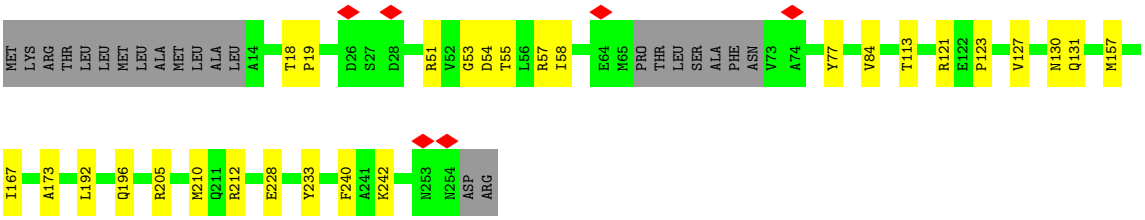
Chain N:





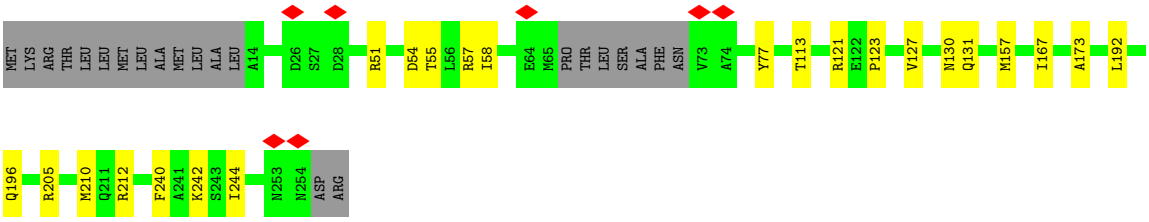
- Molecule 2: Biofilm formation protein PslD

Chain C:



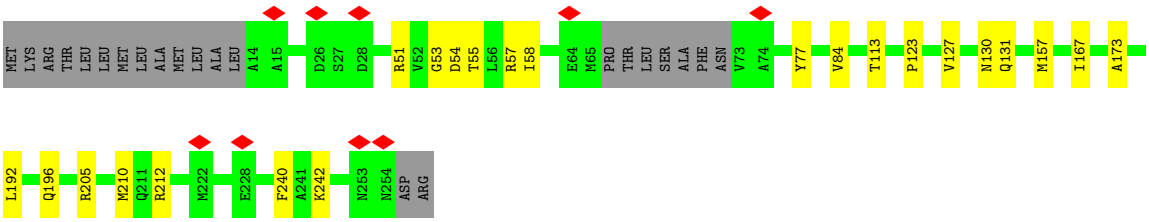
- Molecule 2: Biofilm formation protein PslD

Chain E:



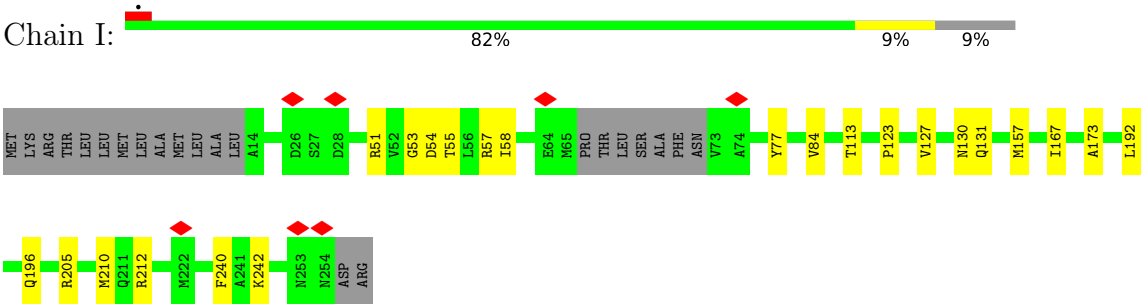
- Molecule 2: Biofilm formation protein PslD

Chain G:



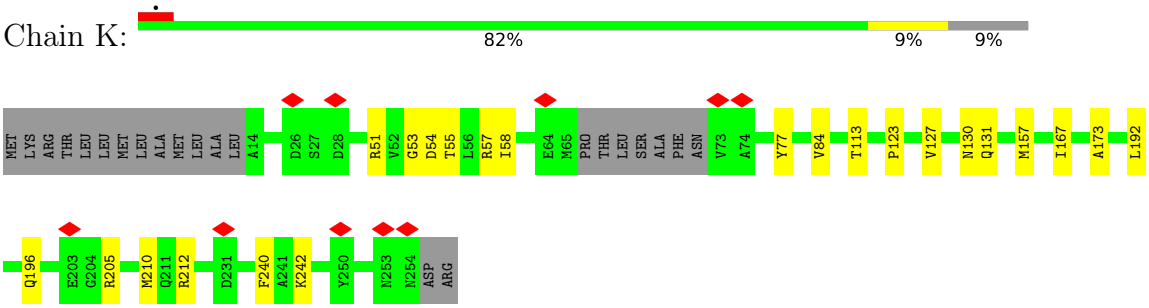
- Molecule 2: Biofilm formation protein PslD

Chain I:



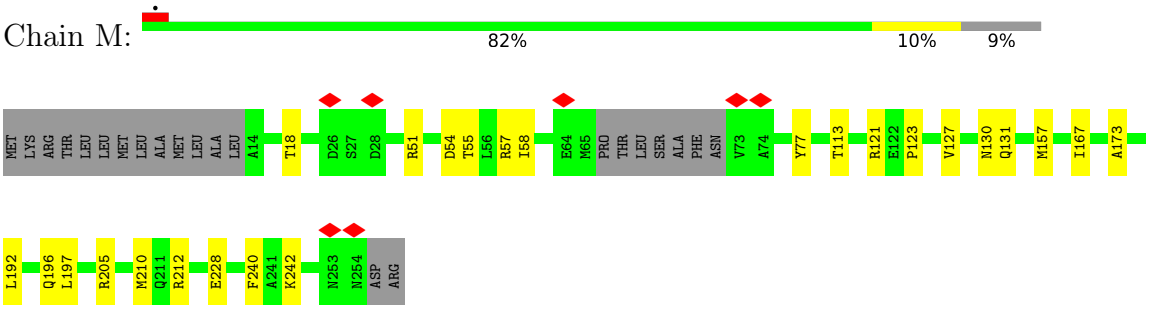
• Molecule 2: Biofilm formation protein PslD

Chain K:



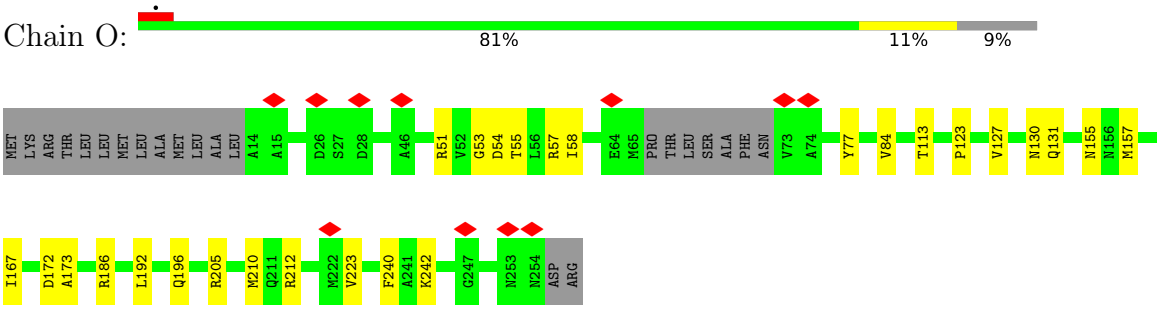
• Molecule 2: Biofilm formation protein PslD

Chain M:



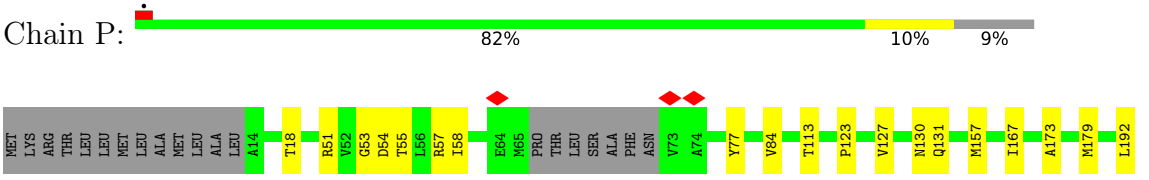
• Molecule 2: Biofilm formation protein PslD

Chain O:



• Molecule 2: Biofilm formation protein PslD

Chain P:



Q196
G204
R205
M210
Q211
R212
E228
Y250
N253
N254
ASP
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116722	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.483	Depositor
Minimum map value	-1.940	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.803	Depositor
Map size (Å)	659.19995, 659.19995, 659.19995	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	3/5278 (0.1%)	1.02	47/7148 (0.7%)
1	B	0.41	4/5278 (0.1%)	1.10	64/7148 (0.9%)
1	D	0.37	1/5278 (0.0%)	0.95	42/7148 (0.6%)
1	F	0.38	3/5278 (0.1%)	0.92	50/7148 (0.7%)
1	H	0.43	4/5278 (0.1%)	1.08	60/7148 (0.8%)
1	J	0.34	1/5278 (0.0%)	0.97	43/7148 (0.6%)
1	L	0.38	4/5278 (0.1%)	0.97	40/7148 (0.6%)
1	N	0.37	2/5278 (0.0%)	0.90	41/7148 (0.6%)
2	C	0.20	0/1819	0.47	0/2473
2	E	0.20	0/1819	0.47	0/2473
2	G	0.20	0/1819	0.47	0/2473
2	I	0.20	0/1819	0.47	0/2473
2	K	0.20	0/1819	0.47	0/2473
2	M	0.20	0/1819	0.47	0/2473
2	O	0.20	0/1819	0.47	0/2473
2	P	0.20	0/1819	0.47	0/2473
All	All	0.35	22/56776 (0.0%)	0.89	387/76968 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
1	D	0	5
1	F	0	6
1	H	0	7
1	J	0	6
1	L	0	6
1	N	0	6
All	All	0	44

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	GLU	C-O	8.30	1.34	1.24
1	H	463	PHE	C-O	8.25	1.30	1.23
1	B	118	PHE	CA-C	-7.11	1.44	1.52
1	A	118	PHE	CA-C	-6.86	1.44	1.52
1	L	118	PHE	CA-C	-6.69	1.44	1.52
1	F	118	PHE	CA-C	-6.52	1.44	1.52
1	L	115	ARG	C-O	6.46	1.32	1.24
1	J	123	ALA	CA-CB	-6.19	1.45	1.53
1	F	115	ARG	C-O	5.95	1.31	1.24
1	H	118	PHE	CA-C	-5.92	1.45	1.52
1	D	116	THR	C-O	-5.77	1.17	1.24
1	H	116	THR	C-O	-5.75	1.17	1.24
1	H	123	ALA	CA-CB	-5.62	1.45	1.53
1	A	107	PRO	CA-C	-5.55	1.48	1.51
1	A	116	THR	C-O	-5.46	1.17	1.24
1	F	116	THR	C-O	-5.39	1.18	1.24
1	L	116	THR	C-O	-5.29	1.18	1.24
1	B	126	ALA	C-O	-5.26	1.17	1.24
1	N	116	THR	C-O	-5.19	1.17	1.24
1	B	123	ALA	CA-CB	-5.11	1.45	1.53
1	N	123	ALA	CA-CB	-5.10	1.45	1.53
1	L	72	PRO	N-CD	5.01	1.54	1.47

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	138	PHE	N-CA-C	-26.12	74.82	110.35
1	B	126	ALA	N-CA-C	-20.31	88.52	113.50
1	L	124	ILE	N-CA-C	-19.43	94.61	111.91
1	H	72	PRO	N-CA-C	19.36	152.35	112.47
1	D	126	ALA	N-CA-C	-18.80	89.28	113.72
1	H	73	SER	N-CA-CB	-18.50	87.96	110.53
1	A	72	PRO	N-CA-C	18.47	150.51	112.47
1	H	72	PRO	N-CA-CB	-18.08	84.26	103.25
1	D	19	ARG	CB-CA-C	-17.74	83.05	110.37
1	H	74	THR	N-CA-C	-17.71	80.56	109.07
1	A	137	THR	N-CA-C	-17.66	94.25	112.97
1	A	74	THR	N-CA-C	-17.64	78.95	108.76
1	B	19	ARG	CB-CA-C	-17.63	83.23	110.37
1	B	72	PRO	N-CA-C	17.59	148.70	112.47
1	D	128	PHE	N-CA-C	-16.75	91.94	113.72
1	L	72	PRO	N-CA-CB	-16.67	85.74	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	138	PHE	N-CA-C	-16.51	89.24	110.53
1	J	128	PHE	N-CA-C	-16.35	92.47	113.72
1	L	139	GLY	N-CA-C	16.33	136.71	115.32
1	A	138	PHE	N-CA-C	-15.78	77.18	110.80
1	B	128	PHE	N-CA-C	-15.72	94.04	113.38
1	N	72	PRO	N-CA-CB	-15.56	86.91	103.25
1	H	76	ARG	N-CA-CB	-15.55	86.91	110.85
1	L	128	PHE	N-CA-C	-15.21	94.67	113.38
1	A	73	SER	N-CA-CB	-14.95	85.20	110.46
1	H	19	ARG	N-CA-CB	-14.76	87.85	111.18
1	B	110	GLU	CB-CA-C	-14.52	85.46	109.27
1	N	138	PHE	N-CA-C	-14.40	90.48	110.35
1	A	19	ARG	CB-CA-C	-14.31	80.39	110.45
1	J	73	SER	N-CA-C	14.16	129.86	112.58
1	N	74	THR	N-CA-C	-13.91	85.85	108.52
1	D	19	ARG	N-CA-C	13.56	134.22	114.16
1	B	19	ARG	N-CA-C	13.55	134.21	114.16
1	A	124	ILE	N-CA-C	-13.51	93.72	112.50
1	J	19	ARG	N-CA-CB	-13.46	87.74	110.49
1	B	112	LEU	N-CA-C	-13.14	96.58	111.82
1	N	128	PHE	N-CA-C	-12.98	95.90	112.90
1	J	126	ALA	N-CA-C	-12.94	97.26	111.36
1	F	124	ILE	N-CA-C	-12.92	96.83	112.98
1	L	124	ILE	CB-CA-C	-12.82	97.45	112.19
1	A	126	ALA	N-CA-C	-12.73	97.77	113.18
1	F	128	PHE	N-CA-C	-12.72	96.04	111.69
1	J	137	THR	N-CA-C	-12.71	96.06	111.69
1	B	111	GLY	N-CA-C	-12.59	83.33	113.18
1	H	126	ALA	N-CA-C	-12.53	97.70	111.36
1	A	19	ARG	N-CA-C	12.45	134.05	113.50
1	F	138	PHE	N-CA-C	-12.34	90.54	109.79
1	B	138	PHE	N-CA-C	-12.29	90.62	109.79
1	L	123	ALA	N-CA-C	12.16	127.21	112.38
1	H	134	THR	N-CA-C	11.98	127.68	113.18
1	D	596	GLU	N-CA-C	-11.87	98.51	113.23
1	D	595	CYS	CB-CA-C	-11.67	92.34	111.13
1	A	73	SER	N-CA-C	11.46	130.20	107.62
1	D	133	VAL	N-CA-C	-11.32	96.27	111.44
1	H	72	PRO	CB-CA-C	-11.31	92.89	111.56
1	B	114	LYS	CB-CA-C	-11.30	93.14	110.88
1	F	135	LEU	N-CA-C	-11.29	97.62	111.40
1	B	114	LYS	N-CA-C	-11.27	99.01	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	524	CYS	CB-CA-C	-11.24	90.36	110.37
1	B	71	MET	N-CA-C	-11.21	93.22	110.14
1	F	118	PHE	N-CA-C	-10.97	99.02	110.97
1	A	75	GLN	N-CA-C	-10.88	91.40	109.46
1	A	73	SER	CB-CA-C	-10.85	92.56	111.22
1	L	595	CYS	CB-CA-C	-10.73	93.75	111.02
1	N	133	VAL	N-CA-C	-10.66	99.38	111.00
1	H	135	LEU	N-CA-C	-10.66	100.41	113.41
1	N	117	LYS	N-CA-C	-10.63	98.62	111.69
1	H	114	LYS	CB-CA-C	-10.60	94.64	110.96
1	D	138	PHE	CB-CA-C	-10.59	92.49	110.81
1	B	110	GLU	CA-C-O	10.53	130.80	118.69
1	N	118	PHE	CB-CA-C	-10.47	93.41	110.79
1	D	139	GLY	N-CA-C	10.35	129.26	115.59
1	B	127	VAL	CB-CA-C	-10.21	95.73	112.26
1	B	110	GLU	CA-C-N	-10.15	101.51	121.41
1	B	110	GLU	C-N-CA	-10.15	101.51	121.41
1	B	73	SER	N-CA-CB	-10.11	91.53	109.93
1	F	19	ARG	N-CA-CB	-10.10	93.43	110.49
1	F	72	PRO	N-CA-CB	-9.91	92.84	103.25
1	B	110	GLU	N-CA-C	9.77	128.56	114.39
1	F	595	CYS	CB-CA-C	-9.69	94.35	110.72
1	J	595	CYS	CB-CA-C	-9.69	94.35	110.72
1	L	596	GLU	N-CA-C	-9.67	100.90	112.89
1	D	132	ARG	N-CA-C	9.62	122.77	111.71
1	F	127	VAL	N-CA-C	9.60	120.44	110.36
1	J	74	THR	N-CA-CB	-9.59	94.15	110.83
1	H	71	MET	CB-CA-C	-9.51	91.43	110.17
1	B	525	ARG	N-CA-C	-9.50	100.05	112.68
1	B	70	VAL	N-CA-C	-9.44	92.16	106.42
1	A	595	CYS	CB-CA-C	-9.29	95.01	110.72
1	F	135	LEU	N-CA-CB	-9.27	96.42	110.13
1	H	73	SER	N-CA-C	-9.24	95.75	109.62
1	B	595	CYS	CB-CA-C	-9.17	95.22	110.72
1	H	468	PHE	CB-CA-C	-9.12	96.45	111.13
1	B	72	PRO	N-CA-CB	-9.11	93.68	103.25
1	B	118	PHE	N-CA-C	-9.11	101.05	110.97
1	N	135	LEU	N-CA-CB	-9.10	96.18	110.28
1	B	118	PHE	CA-CB-CG	9.06	122.86	113.80
1	D	71	MET	N-CA-C	-9.03	89.85	109.81
1	H	465	ALA	CA-C-N	-9.00	113.13	120.33
1	H	465	ALA	C-N-CA	-9.00	113.13	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	LEU	N-CA-CB	-8.98	96.36	110.28
1	B	135	LEU	N-CA-CB	-8.95	96.52	110.30
1	J	127	VAL	N-CA-C	8.94	124.77	111.89
1	F	127	VAL	CB-CA-C	-8.88	100.52	111.88
1	A	118	PHE	CA-CB-CG	8.83	122.63	113.80
1	N	132	ARG	N-CA-C	8.82	120.89	111.28
1	L	133	VAL	N-CA-C	-8.82	101.81	110.72
1	L	135	LEU	N-CA-CB	-8.69	96.92	110.30
1	J	137	THR	CA-C-N	8.67	133.84	120.75
1	J	137	THR	C-N-CA	8.67	133.84	120.75
1	D	132	ARG	CB-CA-C	-8.61	94.71	110.63
1	J	136	GLU	N-CA-C	8.61	122.88	112.38
1	L	118	PHE	CA-CB-CG	8.60	122.40	113.80
1	B	73	SER	N-CA-C	-8.54	101.58	113.20
1	J	74	THR	N-CA-C	-8.54	95.48	109.40
1	J	133	VAL	N-CA-C	-8.53	100.43	111.09
1	A	72	PRO	CB-CA-C	-8.52	97.50	111.56
1	J	72	PRO	N-CA-C	-8.51	94.93	112.47
1	J	596	GLU	N-CA-C	-8.51	102.16	112.54
1	N	132	ARG	CB-CA-C	-8.47	96.72	110.79
1	B	135	LEU	N-CA-C	-8.46	101.57	112.23
1	J	75	GLN	N-CA-C	-8.42	92.09	107.75
1	D	70	VAL	N-CA-C	-8.39	95.00	107.51
1	B	119	TYR	CB-CA-C	8.37	126.12	110.63
1	H	72	PRO	N-CD-CG	-8.36	90.66	103.20
1	L	119	TYR	CB-CA-C	8.34	124.64	110.79
1	N	595	CYS	CB-CA-C	-8.33	96.09	110.17
1	F	596	GLU	N-CA-C	-8.32	102.16	111.82
1	J	132	ARG	N-CA-C	8.32	120.35	111.28
1	A	524	CYS	CB-CA-C	-8.25	94.43	110.11
1	H	76	ARG	N-CA-C	8.20	122.86	110.14
1	B	71	MET	N-CA-CB	8.16	126.00	110.49
1	H	119	TYR	N-CA-CB	-8.08	97.78	110.22
1	A	137	THR	CB-CA-C	-8.06	98.84	111.17
1	A	118	PHE	CB-CA-C	-8.04	98.57	110.96
1	N	139	GLY	N-CA-C	7.98	132.10	113.18
1	H	466	VAL	N-CA-CB	7.96	116.66	110.45
1	D	118	PHE	CA-CB-CG	7.94	121.74	113.80
1	L	132	ARG	N-CA-C	7.94	119.56	111.07
1	N	130	GLY	CA-C-N	-7.82	110.52	120.60
1	N	130	GLY	C-N-CA	-7.82	110.52	120.60
1	F	118	PHE	CA-C-N	-7.82	108.43	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	118	PHE	C-N-CA	-7.82	108.43	120.31
1	H	119	TYR	CB-CA-C	7.76	124.99	110.63
1	J	128	PHE	N-CA-CB	7.74	122.02	110.65
1	H	118	PHE	CA-CB-CG	7.60	121.40	113.80
1	D	128	PHE	N-CA-CB	7.54	121.73	110.65
1	H	73	SER	CB-CA-C	-7.53	100.82	112.12
1	H	134	THR	CB-CA-C	-7.53	94.97	109.95
1	L	135	LEU	N-CA-C	-7.53	102.74	112.23
1	F	71	MET	N-CA-C	-7.53	98.96	110.32
1	B	139	GLY	N-CA-C	7.47	130.88	113.18
1	F	139	GLY	N-CA-C	7.43	130.80	113.18
1	H	130	GLY	CA-C-N	-7.43	110.05	120.53
1	H	130	GLY	C-N-CA	-7.43	110.05	120.53
1	N	118	PHE	CA-CB-CG	7.42	121.22	113.80
1	B	127	VAL	N-CA-C	7.40	120.34	111.09
1	L	118	PHE	CA-C-N	-7.39	110.38	120.28
1	L	118	PHE	C-N-CA	-7.39	110.38	120.28
1	J	130	GLY	CA-C-N	-7.39	110.11	120.53
1	J	130	GLY	C-N-CA	-7.39	110.11	120.53
1	F	130	GLY	CA-C-N	-7.39	110.11	120.53
1	F	130	GLY	C-N-CA	-7.39	110.11	120.53
1	J	125	GLY	N-CA-C	7.38	121.57	112.64
1	F	118	PHE	CA-CB-CG	7.35	121.15	113.80
1	J	119	TYR	N-CA-C	-7.34	104.94	114.04
1	A	596	GLU	N-CA-C	-7.33	103.32	111.82
1	J	132	ARG	CB-CA-C	-7.33	98.63	110.79
1	B	596	GLU	N-CA-C	-7.30	103.36	111.82
1	J	127	VAL	CB-CA-C	-7.28	97.89	111.79
1	B	130	GLY	CA-C-N	-7.27	110.27	120.53
1	B	130	GLY	C-N-CA	-7.27	110.27	120.53
1	L	130	GLY	CA-C-N	-7.22	111.28	120.60
1	L	130	GLY	C-N-CA	-7.22	111.28	120.60
1	F	119	TYR	CB-CA-C	7.20	124.50	110.67
1	D	75	GLN	N-CA-C	7.20	121.32	111.39
1	B	75	GLN	N-CA-C	-7.16	99.71	110.24
1	L	132	ARG	CB-CA-C	-7.14	99.67	110.88
1	N	75	GLN	N-CA-C	-7.13	98.93	110.20
1	J	119	TYR	CB-CA-C	7.10	121.78	109.15
1	L	130	GLY	N-CA-C	-7.08	103.71	112.77
1	A	130	GLY	N-CA-C	-7.08	103.71	112.77
1	A	118	PHE	N-CA-C	-7.07	103.26	110.97
1	L	122	LYS	N-CA-C	-7.07	99.78	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	119	TYR	N-CA-C	-7.04	103.36	112.23
1	N	130	GLY	N-CA-C	-7.00	103.81	112.77
1	B	134	THR	CB-CA-C	-6.99	95.38	109.99
1	H	118	PHE	CB-CA-C	-6.96	100.24	110.96
1	B	119	TYR	N-CA-CB	-6.96	99.50	110.22
1	D	70	VAL	N-CA-CB	-6.95	102.72	111.41
1	H	595	CYS	CB-CA-C	-6.90	98.56	110.09
1	D	130	GLY	N-CA-C	-6.89	103.95	112.77
1	N	73	SER	CB-CA-C	-6.88	101.75	111.80
1	B	128	PHE	N-CA-CB	6.86	120.75	110.53
1	H	462	LEU	N-CA-CB	-6.84	99.25	110.40
1	B	130	GLY	N-CA-C	-6.81	104.24	113.37
1	A	74	THR	N-CA-CB	-6.77	99.09	110.80
1	A	119	TYR	CB-CA-C	6.72	122.11	110.68
1	J	130	GLY	N-CA-C	-6.71	104.18	112.77
1	H	127	VAL	N-CA-C	6.70	117.19	110.23
1	F	130	GLY	N-CA-C	-6.69	104.40	113.37
1	J	19	ARG	N-CA-C	6.65	124.96	110.80
1	D	130	GLY	CA-C-N	-6.62	111.20	120.53
1	D	130	GLY	C-N-CA	-6.62	111.20	120.53
1	L	134	THR	CB-CA-C	-6.61	96.19	109.99
1	A	525	ARG	N-CA-C	-6.60	103.35	111.40
1	H	524	CYS	CB-CA-C	-6.58	96.86	109.95
1	F	75	GLN	CA-C-N	-6.58	111.44	122.29
1	F	75	GLN	C-N-CA	-6.58	111.44	122.29
1	J	135	LEU	N-CA-CB	-6.57	98.55	109.72
1	N	524	CYS	CB-CA-C	-6.57	96.88	109.95
1	A	128	PHE	N-CA-C	-6.57	104.16	111.71
1	F	76	ARG	N-CA-CB	-6.56	99.33	111.53
1	H	461	MET	CB-CA-C	-6.52	98.30	109.65
1	F	524	CYS	CB-CA-C	-6.52	96.97	109.95
1	L	128	PHE	N-CA-CB	6.49	120.21	110.53
1	F	123	ALA	N-CA-C	6.49	119.67	111.69
1	N	137	THR	CA-CB-OG1	-6.45	99.92	109.60
1	A	137	THR	CA-CB-OG1	-6.45	99.92	109.60
1	B	137	THR	CA-CB-OG1	-6.45	99.93	109.60
1	N	116	THR	CB-CA-C	-6.44	98.31	110.67
1	D	135	LEU	N-CA-CB	-6.42	99.31	109.78
1	F	137	THR	CA-CB-OG1	-6.42	99.97	109.60
1	D	119	TYR	CB-CA-C	6.37	122.42	110.63
1	F	74	THR	N-CA-C	-6.36	97.25	110.80
1	F	134	THR	CB-CA-C	-6.34	96.73	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	112	LEU	N-CA-CB	6.33	121.20	110.49
1	N	596	GLU	N-CA-C	-6.32	104.49	111.82
1	L	131	ILE	N-CA-C	-6.30	103.74	110.36
1	B	72	PRO	CB-CA-C	-6.22	101.30	111.56
1	D	75	GLN	CB-CA-C	-6.21	103.07	111.89
1	H	466	VAL	N-CA-C	-6.21	104.90	112.35
1	H	462	LEU	N-CA-C	-6.20	105.20	112.89
1	D	118	PHE	CB-CA-C	-6.20	98.09	110.42
1	L	118	PHE	N-CA-C	-6.20	104.22	110.97
1	A	70	VAL	N-CA-C	-6.19	106.40	111.91
1	H	118	PHE	N-CA-C	-6.19	104.22	110.97
1	L	122	LYS	CB-CA-C	6.19	121.11	110.84
1	B	525	ARG	CA-CB-CG	6.14	126.39	114.10
1	J	525	ARG	CA-CB-CG	6.14	126.39	114.10
1	A	525	ARG	CA-CB-CG	6.13	126.37	114.10
1	D	525	ARG	CA-CB-CG	6.13	126.37	114.10
1	H	525	ARG	CA-CB-CG	6.13	126.37	114.10
1	L	525	ARG	CA-CB-CG	6.13	126.37	114.10
1	H	74	THR	CB-CA-C	6.13	120.33	109.72
1	A	130	GLY	CA-C-N	-6.12	111.50	121.54
1	A	130	GLY	C-N-CA	-6.12	111.50	121.54
1	L	137	THR	CA-CB-OG1	-6.12	100.42	109.60
1	N	525	ARG	CA-CB-CG	6.12	126.34	114.10
1	F	525	ARG	CA-CB-CG	6.12	126.33	114.10
1	H	463	PHE	CB-CA-C	6.08	122.88	112.00
1	B	110	GLU	N-CA-CB	6.07	118.99	110.98
1	L	123	ALA	CB-CA-C	-6.07	97.52	110.32
1	L	117	LYS	CB-CA-C	6.02	120.78	110.79
1	B	125	GLY	N-CA-C	6.01	122.11	114.66
1	D	71	MET	N-CA-CB	6.01	121.06	110.37
1	F	123	ALA	N-CA-CB	-6.00	101.26	110.20
1	B	524	CYS	N-CA-C	-5.97	105.86	113.02
1	L	524	CYS	CB-CA-C	-5.96	98.08	109.95
1	N	131	ILE	N-CA-C	-5.95	104.11	110.36
1	D	73	SER	N-CA-C	-5.93	103.74	111.74
1	B	131	ILE	N-CA-C	-5.91	103.88	110.62
1	B	112	LEU	CB-CA-C	5.87	121.94	110.67
1	A	127	VAL	N-CA-CB	5.87	117.28	110.65
1	D	594	SER	CA-C-N	-5.84	113.92	122.86
1	D	594	SER	C-N-CA	-5.84	113.92	122.86
1	D	119	TYR	N-CA-CB	-5.84	101.22	110.22
1	J	123	ALA	N-CA-CB	-5.84	101.81	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	69	LEU	CA-C-N	-5.82	117.43	122.96
1	B	69	LEU	C-N-CA	-5.82	117.43	122.96
1	F	70	VAL	N-CA-C	-5.78	97.32	109.34
1	N	525	ARG	N-CA-C	-5.78	104.35	111.40
1	F	128	PHE	CB-CA-C	5.77	121.26	110.70
1	N	72	PRO	N-CD-CG	-5.76	94.55	103.20
1	D	136	GLU	N-CA-CB	5.76	118.34	109.98
1	F	123	ALA	CB-CA-C	-5.76	100.16	110.70
1	H	525	ARG	N-CA-C	-5.76	104.92	111.14
1	F	131	ILE	N-CA-C	-5.76	104.06	110.62
1	F	136	GLU	N-CA-C	5.76	117.24	110.97
1	F	525	ARG	N-CA-C	-5.75	104.93	111.14
1	D	131	ILE	N-CA-C	-5.74	104.08	110.62
1	F	127	VAL	N-CA-CB	5.74	116.88	110.51
1	N	71	MET	N-CA-C	5.72	118.18	110.29
1	L	140	VAL	N-CA-C	5.72	120.04	112.04
1	A	119	TYR	N-CA-CB	-5.71	101.49	110.06
1	A	115	ARG	N-CA-CB	-5.70	101.45	110.22
1	N	135	LEU	N-CA-C	-5.70	105.21	111.82
1	N	124	ILE	N-CA-C	-5.68	103.34	111.17
1	A	118	PHE	CA-C-N	-5.67	112.61	120.38
1	A	118	PHE	C-N-CA	-5.67	112.61	120.38
1	F	71	MET	N-CA-CB	5.66	122.16	110.45
1	D	73	SER	CB-CA-C	-5.65	103.71	111.73
1	H	75	GLN	CB-CA-C	-5.65	103.22	112.03
1	J	137	THR	CA-CB-OG1	-5.64	101.14	109.60
1	D	138	PHE	N-CA-C	5.64	119.24	112.93
1	F	19	ARG	CA-CB-CG	5.63	125.37	114.10
1	H	18	GLN	CA-C-N	-5.63	110.89	121.63
1	H	18	GLN	C-N-CA	-5.63	110.89	121.63
1	H	465	ALA	N-CA-C	5.62	117.09	110.97
1	H	133	VAL	CB-CA-C	5.60	120.22	112.05
1	J	136	GLU	CB-CA-C	-5.58	98.55	110.32
1	B	525	ARG	CB-CG-CD	5.56	124.08	111.30
1	J	525	ARG	CB-CG-CD	5.56	124.08	111.30
1	A	594	SER	CA-C-N	-5.55	113.94	122.60
1	A	594	SER	C-N-CA	-5.55	113.94	122.60
1	N	525	ARG	CB-CG-CD	5.55	124.07	111.30
1	F	525	ARG	CB-CG-CD	5.54	124.05	111.30
1	A	525	ARG	CB-CG-CD	5.54	124.05	111.30
1	D	525	ARG	CB-CG-CD	5.54	124.05	111.30
1	H	525	ARG	CB-CG-CD	5.54	124.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	525	ARG	CB-CG-CD	5.54	124.05	111.30
1	H	69	LEU	O-C-N	-5.54	114.94	122.36
1	A	128	PHE	CB-CA-C	5.54	120.87	110.63
1	B	123	ALA	N-CA-CB	-5.53	101.94	110.07
1	F	69	LEU	O-C-N	-5.53	114.95	122.36
1	N	127	VAL	CB-CA-C	-5.52	103.16	112.16
1	B	594	SER	CA-C-N	-5.52	113.99	122.60
1	B	594	SER	C-N-CA	-5.52	113.99	122.60
1	F	594	SER	CA-C-N	-5.51	114.00	122.60
1	F	594	SER	C-N-CA	-5.51	114.00	122.60
1	J	131	ILE	N-CA-C	-5.51	104.34	110.62
1	H	135	LEU	CB-CA-C	5.50	118.86	109.24
1	D	137	THR	CA-CB-OG1	-5.49	101.36	109.60
1	J	18	GLN	CA-C-N	-5.49	111.06	121.54
1	J	18	GLN	C-N-CA	-5.49	111.06	121.54
1	J	594	SER	CA-C-N	-5.49	114.04	122.60
1	J	594	SER	C-N-CA	-5.49	114.04	122.60
1	L	594	SER	CA-C-N	-5.48	113.96	122.67
1	L	594	SER	C-N-CA	-5.48	113.96	122.67
1	N	594	SER	CA-C-N	-5.47	114.01	122.49
1	N	594	SER	C-N-CA	-5.47	114.01	122.49
1	D	70	VAL	CB-CA-C	5.46	118.95	111.31
1	H	468	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	123	ALA	CB-CA-C	-5.44	98.51	109.55
1	H	469	GLY	CA-C-N	5.44	133.84	122.58
1	H	469	GLY	C-N-CA	5.44	133.84	122.58
1	B	70	VAL	N-CA-CB	-5.41	107.24	112.65
1	B	113	TRP	CA-C-N	-5.40	113.42	120.44
1	B	113	TRP	C-N-CA	-5.40	113.42	120.44
1	F	129	ASP	N-CA-C	5.40	117.59	111.11
1	B	74	THR	N-CA-C	-5.38	97.87	107.98
1	J	69	LEU	O-C-N	-5.35	116.12	122.65
1	A	116	THR	N-CA-C	-5.33	105.16	110.97
1	B	109	PRO	CA-C-N	-5.33	113.82	121.98
1	B	109	PRO	C-N-CA	-5.33	113.82	121.98
1	A	125	GLY	N-CA-C	5.32	119.58	112.77
1	L	118	PHE	CB-CA-C	-5.31	102.78	110.96
1	D	125	GLY	N-CA-C	5.31	122.27	115.32
1	F	121	LYS	N-CA-C	-5.30	105.42	111.14
1	B	69	LEU	O-C-N	-5.29	115.27	122.36
1	N	74	THR	CB-CA-C	5.28	118.84	110.19
1	N	75	GLN	CA-C-N	-5.27	111.94	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	75	GLN	C-N-CA	-5.27	111.94	121.69
1	D	76	ARG	N-CA-C	5.27	117.33	108.96
1	H	465	ALA	N-CA-CB	-5.26	102.22	109.91
1	A	134	THR	CB-CA-C	-5.24	101.12	110.70
1	H	468	PHE	CA-C-O	-5.24	114.22	120.55
1	J	136	GLU	N-CA-CB	5.24	119.22	110.32
1	F	115	ARG	N-CA-C	-5.23	106.40	112.89
1	N	128	PHE	N-CA-CB	5.21	118.14	110.33
1	H	594	SER	CA-C-N	-5.21	113.95	122.54
1	H	594	SER	C-N-CA	-5.21	113.95	122.54
1	H	75	GLN	CA-C-N	-5.21	113.76	122.92
1	H	75	GLN	C-N-CA	-5.21	113.76	122.92
1	N	70	VAL	CB-CA-C	5.20	119.81	111.29
1	F	18	GLN	CA-C-N	-5.17	111.66	121.54
1	F	18	GLN	C-N-CA	-5.17	111.66	121.54
1	B	20	GLU	CB-CA-C	-5.15	100.17	110.42
1	D	524	CYS	CB-CA-C	-5.12	99.28	109.99
1	A	20	GLU	CB-CA-C	-5.12	100.24	110.42
1	D	20	GLU	CB-CA-C	-5.11	100.25	110.42
1	A	139	GLY	N-CA-C	5.09	125.25	113.18
1	N	134	THR	CB-CA-C	-5.08	100.02	110.38
1	L	117	LYS	N-CA-CB	-5.07	102.67	110.12
1	H	114	LYS	N-CA-C	-5.07	105.45	110.97
1	J	20	GLU	N-CA-C	-5.03	104.79	112.04
1	B	114	LYS	O-C-N	5.03	127.25	122.07
1	L	525	ARG	N-CA-C	-5.03	105.71	111.14
1	H	467	PRO	N-CA-CB	-5.03	97.97	103.25
1	N	166	SER	CA-CB-OG	5.02	121.14	111.10
1	F	166	SER	CA-CB-OG	5.02	121.13	111.10
1	A	166	SER	CA-CB-OG	5.02	121.13	111.10
1	D	166	SER	CA-CB-OG	5.02	121.13	111.10
1	H	166	SER	CA-CB-OG	5.02	121.13	111.10
1	L	166	SER	CA-CB-OG	5.02	121.13	111.10
1	B	166	SER	CA-CB-OG	5.01	121.12	111.10
1	J	166	SER	CA-CB-OG	5.01	121.12	111.10

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	132	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	15	PHE	Sidechain
1	B	109	PRO	Mainchain
1	B	115	ARG	Sidechain
1	B	132	ARG	Sidechain
1	B	15	PHE	Sidechain
1	B	69	LEU	Mainchain
1	D	113	TRP	Mainchain
1	D	115	ARG	Sidechain
1	D	132	ARG	Sidechain
1	D	15	PHE	Sidechain
1	D	76	ARG	Sidechain
1	F	115	ARG	Sidechain
1	F	132	ARG	Sidechain
1	F	15	PHE	Sidechain
1	F	19	ARG	Sidechain
1	F	69	LEU	Mainchain
1	F	76	ARG	Sidechain
1	H	111	GLY	Mainchain
1	H	115	ARG	Sidechain
1	H	132	ARG	Sidechain
1	H	15	PHE	Sidechain
1	H	18	GLN	Mainchain
1	H	19	ARG	Sidechain
1	H	69	LEU	Mainchain
1	J	132	ARG	Sidechain
1	J	15	PHE	Sidechain
1	J	18	GLN	Mainchain
1	J	19	ARG	Sidechain
1	J	69	LEU	Mainchain
1	J	76	ARG	Sidechain
1	L	115	ARG	Sidechain
1	L	132	ARG	Sidechain
1	L	15	PHE	Sidechain
1	L	19	ARG	Peptide
1	L	70	VAL	Mainchain
1	L	76	ARG	Sidechain
1	N	115	ARG	Sidechain
1	N	132	ARG	Sidechain
1	N	15	PHE	Sidechain
1	N	19	ARG	Peptide
1	N	70	VAL	Mainchain
1	N	76	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5201	0	5349	135	0
1	B	5201	0	5347	157	0
1	D	5201	0	5346	123	0
1	F	5201	0	5346	120	0
1	H	5201	0	5349	141	0
1	J	5201	0	5349	137	0
1	L	5201	0	5346	128	0
1	N	5201	0	5349	140	0
2	C	1786	0	1806	18	0
2	E	1786	0	1806	14	0
2	G	1786	0	1806	14	0
2	I	1786	0	1806	13	0
2	K	1786	0	1806	13	0
2	M	1786	0	1806	15	0
2	O	1786	0	1806	17	0
2	P	1786	0	1806	15	0
All	All	55896	0	57229	1100	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 10.

All (1100) 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:N:124:ILE:CG1	1:N:128:PHE:CZ	1.83	1.57
1:A:121:LYS:NZ	1:A:124:ILE:CD1	1.73	1.50
1:A:121:LYS:NZ	1:A:124:ILE:CG1	1.75	1.48
1:B:121:LYS:CA	1:B:124:ILE:HD11	1.44	1.45
1:H:121:LYS:CA	1:H:124:ILE:HD11	1.44	1.45
1:N:124:ILE:HG13	1:N:128:PHE:CZ	1.50	1.37
1:B:108:PRO:HA	1:B:118:PHE:CE2	1.58	1.37
1:B:121:LYS:HA	1:B:124:ILE:CD1	1.58	1.31
1:N:39:LEU:CD1	1:N:124:ILE:HD12	1.61	1.30
1:F:121:LYS:HA	1:F:124:ILE:CD1	1.61	1.28
1:A:121:LYS:HA	1:A:124:ILE:CD1	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:LYS:HA	1:H:124:ILE:CD1	1.61	1.28
1:A:121:LYS:HZ1	1:A:124:ILE:CG1	1.35	1.27
1:H:121:LYS:O	1:H:124:ILE:CD1	1.84	1.26
1:D:121:LYS:HA	1:D:124:ILE:CD1	1.65	1.25
1:L:121:LYS:HA	1:L:124:ILE:CD1	1.66	1.25
1:B:121:LYS:O	1:B:124:ILE:HD12	1.08	1.25
1:A:131:ILE:O	1:A:135:LEU:HD12	1.33	1.24
1:J:121:LYS:HA	1:J:124:ILE:CD1	1.68	1.24
1:A:121:LYS:NZ	1:A:124:ILE:HD11	1.30	1.23
1:B:121:LYS:O	1:B:124:ILE:CD1	1.88	1.22
1:N:124:ILE:HG12	1:N:128:PHE:CE2	1.75	1.22
1:B:108:PRO:CA	1:B:118:PHE:HE2	1.50	1.21
1:B:109:PRO:HG2	1:B:114:LYS:CB	1.68	1.21
1:H:468:PHE:CG	1:H:468:PHE:O	1.90	1.21
1:H:121:LYS:O	1:H:124:ILE:HD12	1.04	1.20
1:B:109:PRO:CG	1:B:114:LYS:HB3	1.74	1.16
1:L:121:LYS:HA	1:L:124:ILE:HD11	1.21	1.16
1:N:124:ILE:CG1	1:N:128:PHE:HZ	1.39	1.12
1:H:468:PHE:O	1:H:468:PHE:CD1	2.02	1.12
1:N:121:LYS:NZ	1:N:124:ILE:CG2	2.13	1.11
1:A:121:LYS:HA	1:A:124:ILE:HD11	1.25	1.11
1:A:121:LYS:HZ3	1:A:124:ILE:CD1	1.44	1.11
1:A:121:LYS:O	1:A:124:ILE:HD13	1.48	1.11
1:A:19:ARG:O	1:A:23:LEU:HD12	1.50	1.11
1:H:121:LYS:NZ	1:H:124:ILE:HD13	1.65	1.10
1:N:39:LEU:HD12	1:N:124:ILE:HD12	1.15	1.10
1:D:121:LYS:O	1:D:124:ILE:HD13	1.51	1.10
1:J:121:LYS:CA	1:J:124:ILE:HD11	1.82	1.10
1:N:121:LYS:HZ3	1:N:124:ILE:HG21	1.13	1.09
1:N:121:LYS:NZ	1:N:124:ILE:HG21	1.67	1.09
1:B:19:ARG:O	1:B:23:LEU:HD12	1.52	1.09
1:N:39:LEU:CD1	1:N:124:ILE:CD1	2.29	1.09
1:D:19:ARG:O	1:D:23:LEU:HD12	1.52	1.09
1:L:121:LYS:O	1:L:124:ILE:HD13	1.52	1.09
1:H:31:ILE:HG13	1:H:465:ALA:HB1	1.17	1.08
1:H:75:GLN:CG	1:H:75:GLN:O	2.00	1.08
1:D:121:LYS:HA	1:D:124:ILE:HD11	1.27	1.08
1:N:116:THR:O	1:N:120:VAL:HG13	1.52	1.08
1:N:124:ILE:HG12	1:N:128:PHE:CZ	1.64	1.07
1:A:121:LYS:O	1:A:124:ILE:CD1	2.02	1.07
1:A:121:LYS:HZ2	1:A:124:ILE:CD1	1.50	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:121:LYS:O	1:L:124:ILE:CD1	2.04	1.05
1:A:121:LYS:CA	1:A:124:ILE:CD1	2.34	1.04
1:J:121:LYS:HA	1:J:124:ILE:HD11	1.09	1.04
1:F:121:LYS:HA	1:F:124:ILE:HD11	1.05	1.04
1:A:121:LYS:HZ1	1:A:124:ILE:HG13	0.89	1.03
1:J:121:LYS:HD2	1:J:124:ILE:HD11	1.38	1.03
1:N:39:LEU:HD12	1:N:124:ILE:CD1	1.86	1.03
1:D:121:LYS:CA	1:D:124:ILE:CD1	2.37	1.02
1:L:121:LYS:CA	1:L:124:ILE:CD1	2.36	1.02
1:L:121:LYS:CA	1:L:124:ILE:HD11	1.89	1.02
1:A:121:LYS:CA	1:A:124:ILE:HD11	1.90	1.02
1:D:121:LYS:O	1:D:124:ILE:CD1	2.08	1.01
1:J:121:LYS:CD	1:J:124:ILE:HD11	1.90	1.01
1:J:39:LEU:HD11	1:J:124:ILE:HG21	1.42	1.01
1:A:121:LYS:NZ	1:A:124:ILE:HG13	1.50	1.00
1:H:121:LYS:CA	1:H:124:ILE:CD1	2.27	1.00
1:N:124:ILE:CD1	1:N:128:PHE:CZ	2.44	0.99
1:F:121:LYS:CA	1:F:124:ILE:HD11	1.93	0.99
1:J:121:LYS:CA	1:J:124:ILE:CD1	2.41	0.98
1:B:70:VAL:O	1:B:70:VAL:HG13	1.63	0.97
1:H:121:LYS:C	1:H:124:ILE:CD1	2.35	0.97
1:N:124:ILE:CD1	1:N:128:PHE:HZ	1.78	0.97
1:B:19:ARG:O	1:B:23:LEU:CD1	2.12	0.96
1:H:75:GLN:O	1:H:75:GLN:OE1	1.82	0.96
1:H:75:GLN:O	1:H:75:GLN:HG3	1.62	0.96
1:J:121:LYS:O	1:J:124:ILE:CD1	2.13	0.96
1:B:121:LYS:C	1:B:124:ILE:CD1	2.39	0.95
1:D:19:ARG:O	1:D:23:LEU:CD1	2.12	0.95
1:B:121:LYS:CA	1:B:124:ILE:CD1	2.27	0.95
1:N:124:ILE:CG1	1:N:128:PHE:CE2	2.40	0.95
1:A:19:ARG:O	1:A:23:LEU:CD1	2.15	0.94
1:H:121:LYS:C	1:H:124:ILE:HD12	1.89	0.94
1:B:121:LYS:C	1:B:124:ILE:HD12	1.93	0.94
1:H:75:GLN:O	1:H:75:GLN:CD	2.09	0.94
1:D:127:VAL:O	1:D:127:VAL:CG1	2.13	0.94
1:B:109:PRO:HB2	1:B:114:LYS:CG	1.97	0.94
1:F:121:LYS:CA	1:F:124:ILE:CD1	2.45	0.93
1:D:121:LYS:CA	1:D:124:ILE:HD11	1.94	0.92
1:B:109:PRO:HG2	1:B:114:LYS:HB3	0.93	0.91
1:F:70:VAL:HG13	1:F:70:VAL:O	1.69	0.91
1:J:127:VAL:CG1	1:J:127:VAL:O	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:LYS:O	1:J:124:ILE:HD13	1.72	0.89
1:A:131:ILE:O	1:A:135:LEU:CD1	2.21	0.89
1:F:127:VAL:O	1:F:131:ILE:HG23	1.71	0.89
1:H:121:LYS:HZ2	1:H:124:ILE:HD13	1.34	0.89
1:N:121:LYS:NZ	1:N:124:ILE:HG23	1.86	0.89
1:B:108:PRO:HA	1:B:118:PHE:HE2	0.73	0.89
1:F:135:LEU:O	1:F:138:PHE:HB2	1.73	0.88
1:B:127:VAL:O	1:B:131:ILE:HG23	1.74	0.88
1:L:124:ILE:HD13	1:L:124:ILE:H	1.38	0.87
1:H:39:LEU:HD11	1:H:124:ILE:HG12	1.57	0.86
1:A:124:ILE:HD13	1:A:124:ILE:H	1.38	0.86
1:J:136:GLU:C	1:J:138:PHE:O	2.18	0.86
1:F:75:GLN:O	1:F:75:GLN:HG3	1.72	0.86
1:B:115:ARG:HH11	1:B:115:ARG:CG	1.89	0.85
1:J:117:LYS:NZ	1:J:120:VAL:HG21	1.90	0.85
1:F:120:VAL:O	1:F:123:ALA:HB3	1.74	0.85
1:A:121:LYS:C	1:A:124:ILE:HD13	2.02	0.84
1:H:460:LEU:HD12	1:H:460:LEU:O	1.76	0.84
1:N:127:VAL:O	1:N:131:ILE:HG23	1.77	0.84
1:F:39:LEU:HD11	1:F:124:ILE:HG21	1.59	0.84
1:J:120:VAL:O	1:J:124:ILE:HD13	1.77	0.84
1:A:121:LYS:HA	1:A:124:ILE:HD12	1.59	0.83
1:A:121:LYS:HZ2	1:A:124:ILE:HD11	0.87	0.83
1:A:39:LEU:HD11	1:A:124:ILE:HG21	1.60	0.83
1:B:127:VAL:O	1:B:127:VAL:HG12	1.78	0.83
1:F:123:ALA:O	1:F:127:VAL:HG23	1.79	0.83
1:B:39:LEU:HD11	1:B:124:ILE:HG12	1.60	0.83
1:N:121:LYS:HZ1	1:N:124:ILE:HD13	1.43	0.82
1:A:121:LYS:C	1:A:124:ILE:CD1	2.50	0.82
1:B:70:VAL:O	1:B:70:VAL:CG1	2.27	0.82
1:B:109:PRO:CB	1:B:114:LYS:HG3	2.09	0.82
1:B:109:PRO:HB2	1:B:114:LYS:HG2	1.61	0.82
1:D:39:LEU:HD11	1:D:124:ILE:HG21	1.62	0.82
1:L:71:MET:HG3	1:L:72:PRO:N	1.95	0.82
1:L:121:LYS:C	1:L:124:ILE:HD13	2.05	0.81
1:D:121:LYS:C	1:D:124:ILE:HD13	2.06	0.81
1:F:124:ILE:HD13	1:F:124:ILE:H	1.45	0.81
1:F:124:ILE:HB	1:F:128:PHE:CZ	2.15	0.81
1:H:120:VAL:O	1:H:124:ILE:HG13	1.81	0.81
1:B:109:PRO:HB2	1:B:114:LYS:HG3	1.61	0.81
1:D:121:LYS:HA	1:D:124:ILE:HD12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:468:PHE:CD1	1:H:468:PHE:C	2.59	0.80
1:L:39:LEU:HD11	1:L:124:ILE:HG21	1.63	0.80
1:L:121:LYS:C	1:L:124:ILE:CD1	2.53	0.80
1:H:463:PHE:O	1:H:467:PRO:HD2	1.82	0.80
1:J:19:ARG:O	1:J:23:LEU:HG	1.82	0.80
1:N:124:ILE:HD11	1:N:128:PHE:CZ	2.15	0.80
1:F:120:VAL:O	1:F:124:ILE:HD13	1.82	0.80
1:J:117:LYS:HA	1:J:120:VAL:HG22	1.63	0.80
1:H:130:GLY:HA2	1:H:133:VAL:HG12	1.65	0.79
1:J:123:ALA:O	1:J:124:ILE:C	2.24	0.79
1:J:76:ARG:NH2	1:L:167:THR:CG2	2.46	0.79
1:D:121:LYS:C	1:D:124:ILE:CD1	2.56	0.78
1:B:127:VAL:O	1:B:127:VAL:CG1	2.33	0.77
1:J:117:LYS:CE	1:J:120:VAL:HG21	2.14	0.77
1:N:116:THR:O	1:N:120:VAL:CG1	2.31	0.77
1:D:127:VAL:O	1:D:127:VAL:HG12	1.84	0.77
1:L:127:VAL:CG1	1:L:127:VAL:O	2.31	0.76
1:B:109:PRO:CB	1:B:114:LYS:CG	2.63	0.76
1:A:109:PRO:HB2	1:A:114:LYS:HG2	1.67	0.76
1:H:461:MET:O	1:H:465:ALA:HB2	1.85	0.76
1:N:124:ILE:HG13	1:N:128:PHE:HZ	0.99	0.76
1:B:120:VAL:O	1:B:124:ILE:HG13	1.84	0.75
1:J:127:VAL:O	1:J:127:VAL:HG13	1.84	0.75
1:B:112:LEU:O	1:B:115:ARG:HB2	1.86	0.75
1:B:109:PRO:CG	1:B:114:LYS:CG	2.64	0.74
1:J:121:LYS:C	1:J:124:ILE:CD1	2.61	0.74
1:N:124:ILE:HG13	1:N:128:PHE:CE1	2.19	0.74
1:N:121:LYS:O	1:N:124:ILE:HG23	1.88	0.74
1:L:127:VAL:O	1:L:131:ILE:HG23	1.87	0.74
1:D:127:VAL:O	1:D:127:VAL:HG13	1.86	0.73
1:J:127:VAL:O	1:J:131:ILE:HG23	1.87	0.73
1:H:121:LYS:C	1:H:124:ILE:HD11	2.06	0.73
1:B:109:PRO:CG	1:B:114:LYS:HG3	2.18	0.73
1:A:121:LYS:HZ1	1:A:124:ILE:HG12	1.47	0.73
1:J:135:LEU:O	1:J:138:PHE:O	2.07	0.73
1:D:117:LYS:HA	1:D:120:VAL:HG22	1.69	0.72
1:H:130:GLY:O	1:H:131:ILE:C	2.30	0.72
1:L:130:GLY:O	1:L:131:ILE:C	2.30	0.72
1:D:19:ARG:O	1:D:23:LEU:CG	2.37	0.72
1:J:120:VAL:O	1:J:124:ILE:CD1	2.36	0.72
1:J:137:THR:C	1:J:138:PHE:O	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TRP:HA	1:B:116:THR:HG23	1.72	0.72
1:N:128:PHE:O	1:N:131:ILE:HG12	1.90	0.72
1:B:19:ARG:O	1:B:23:LEU:CG	2.37	0.72
1:B:109:PRO:CG	1:B:114:LYS:CB	2.49	0.72
1:A:112:LEU:O	1:A:116:THR:HG23	1.90	0.71
1:A:121:LYS:NZ	1:A:124:ILE:HG12	1.98	0.71
1:N:124:ILE:CD1	1:N:128:PHE:CE2	2.70	0.71
1:B:74:THR:HG22	1:D:76:ARG:O	1.91	0.71
1:J:73:SER:HB3	1:L:75:GLN:HA	1.72	0.71
1:H:121:LYS:HA	1:H:124:ILE:HD11	0.73	0.70
1:L:124:ILE:HB	1:L:128:PHE:CZ	2.27	0.70
1:B:115:ARG:HH11	1:B:115:ARG:HG2	1.56	0.70
1:D:130:GLY:O	1:D:131:ILE:C	2.30	0.70
1:N:39:LEU:HD13	1:N:124:ILE:HD13	1.74	0.70
1:A:121:LYS:HZ3	1:A:124:ILE:HD12	1.53	0.69
1:F:125:GLY:O	1:F:126:ALA:C	2.33	0.69
1:D:112:LEU:O	1:D:116:THR:HG23	1.92	0.69
1:N:39:LEU:HD13	1:N:124:ILE:CD1	2.21	0.69
1:F:70:VAL:O	1:F:70:VAL:CG1	2.41	0.69
1:H:117:LYS:HA	1:H:120:VAL:HG22	1.74	0.69
1:N:39:LEU:CD1	1:N:124:ILE:HD13	2.23	0.69
1:B:39:LEU:CD1	1:B:124:ILE:HG12	2.21	0.69
1:J:121:LYS:HD2	1:J:124:ILE:CD1	2.18	0.69
1:N:39:LEU:HD11	1:N:124:ILE:HD12	1.68	0.69
1:L:121:LYS:HA	1:L:124:ILE:HD12	1.67	0.69
1:H:31:ILE:CG1	1:H:465:ALA:HB1	2.09	0.69
1:H:121:LYS:NZ	1:H:124:ILE:CD1	2.51	0.68
1:N:124:ILE:HD11	1:N:128:PHE:CE2	2.28	0.68
1:H:73:SER:CB	1:J:74:THR:O	2.41	0.68
1:J:130:GLY:O	1:J:131:ILE:C	2.34	0.68
1:H:31:ILE:HG13	1:H:465:ALA:CB	2.10	0.68
1:H:121:LYS:HZ3	1:H:124:ILE:HD13	1.56	0.68
1:A:128:PHE:HA	1:A:131:ILE:HG23	1.75	0.68
1:J:124:ILE:HB	1:J:128:PHE:CZ	2.29	0.68
1:L:124:ILE:O	1:L:128:PHE:CE2	2.47	0.68
1:L:121:LYS:O	1:L:124:ILE:HD11	1.91	0.68
1:D:123:ALA:C	1:D:125:GLY:N	2.50	0.68
1:H:116:THR:O	1:H:120:VAL:HG13	1.94	0.68
1:J:135:LEU:O	1:J:138:PHE:HB2	1.94	0.68
1:A:121:LYS:O	1:A:124:ILE:HD11	1.90	0.68
1:N:121:LYS:NZ	1:N:124:ILE:HD13	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:CG	1:B:115:ARG:NH1	2.55	0.67
1:H:128:PHE:HA	1:H:131:ILE:HG23	1.76	0.67
1:L:112:LEU:O	1:L:116:THR:HG23	1.94	0.67
1:N:123:ALA:O	1:N:124:ILE:C	2.38	0.67
1:N:121:LYS:HZ1	1:N:124:ILE:CG2	2.05	0.67
1:A:136:GLU:C	1:A:138:PHE:H	2.00	0.67
1:B:123:ALA:C	1:B:125:GLY:N	2.48	0.67
1:H:39:LEU:CD1	1:H:124:ILE:HG12	2.24	0.67
1:N:121:LYS:HZ2	1:N:124:ILE:HG23	1.60	0.67
1:B:127:VAL:O	1:B:131:ILE:CG2	2.43	0.67
1:H:131:ILE:O	1:H:134:THR:OG1	2.13	0.67
1:N:121:LYS:O	1:N:124:ILE:CG2	2.42	0.67
1:B:130:GLY:O	1:B:131:ILE:C	2.35	0.66
1:N:130:GLY:O	1:N:131:ILE:C	2.36	0.66
1:F:121:LYS:O	1:F:124:ILE:HD13	1.95	0.66
1:A:108:PRO:HA	1:A:118:PHE:CE2	2.31	0.66
1:B:109:PRO:HD2	1:B:118:PHE:CD2	2.31	0.66
1:N:112:LEU:O	1:N:116:THR:HG23	1.96	0.66
1:D:127:VAL:O	1:D:131:ILE:HG23	1.96	0.66
1:J:120:VAL:O	1:J:123:ALA:HB3	1.96	0.66
1:B:128:PHE:O	1:B:131:ILE:HG12	1.96	0.65
1:J:121:LYS:C	1:J:124:ILE:HD13	2.19	0.65
1:A:116:THR:O	1:A:120:VAL:HG13	1.96	0.65
1:F:120:VAL:O	1:F:124:ILE:CD1	2.43	0.65
1:D:121:LYS:O	1:D:124:ILE:HD11	1.97	0.65
1:N:121:LYS:HZ3	1:N:124:ILE:CG2	1.89	0.65
1:A:117:LYS:HA	1:A:120:VAL:HG22	1.78	0.65
1:J:121:LYS:C	1:J:124:ILE:HD11	2.20	0.65
1:J:128:PHE:O	1:J:131:ILE:HG12	1.97	0.64
1:A:76:ARG:NH1	1:B:78:PRO:HD2	2.12	0.64
1:F:113:TRP:HA	1:F:116:THR:HG23	1.79	0.64
1:D:73:SER:HB3	1:F:75:GLN:HA	1.79	0.64
1:D:116:THR:O	1:D:120:VAL:HG13	1.97	0.64
1:J:19:ARG:O	1:J:23:LEU:CG	2.45	0.64
1:H:127:VAL:O	1:H:131:ILE:HG23	1.98	0.64
1:B:121:LYS:HA	1:B:124:ILE:HD11	0.67	0.64
1:L:123:ALA:C	1:L:125:GLY:H	2.06	0.64
1:J:121:LYS:CD	1:J:124:ILE:CD1	2.73	0.64
1:L:122:LYS:O	1:L:125:GLY:N	2.31	0.63
1:L:122:LYS:O	1:L:125:GLY:CA	2.47	0.63
1:F:72:PRO:HG2	1:H:72:PRO:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:PHE:HA	1:L:131:ILE:HG23	1.79	0.63
1:H:463:PHE:O	1:H:464:LEU:C	2.38	0.63
1:B:123:ALA:O	1:B:124:ILE:C	2.41	0.63
1:J:123:ALA:C	1:J:125:GLY:N	2.54	0.63
1:F:113:TRP:O	1:F:116:THR:OG1	2.17	0.62
2:G:157:MET:HA	2:G:210:MET:HE2	1.81	0.62
1:J:39:LEU:CD1	1:J:124:ILE:HG21	2.24	0.62
1:N:117:LYS:HA	1:N:120:VAL:HG22	1.82	0.62
1:B:108:PRO:CA	1:B:118:PHE:CE2	2.42	0.62
1:H:131:ILE:HG13	1:H:132:ARG:N	2.14	0.62
2:I:157:MET:HA	2:I:210:MET:HE2	1.81	0.62
1:L:128:PHE:O	1:L:131:ILE:HG12	2.00	0.62
1:F:130:GLY:O	1:F:131:ILE:C	2.36	0.62
1:H:123:ALA:C	1:H:125:GLY:N	2.50	0.62
1:J:121:LYS:HD3	1:J:124:ILE:HD11	1.76	0.62
1:L:122:LYS:O	1:L:125:GLY:HA3	2.00	0.62
2:E:157:MET:HA	2:E:210:MET:HE2	1.81	0.62
2:C:157:MET:HA	2:C:210:MET:HE2	1.81	0.62
1:L:121:LYS:C	1:L:124:ILE:HD11	2.21	0.61
1:H:657:ARG:O	1:H:661:ALA:HB3	2.01	0.61
1:J:657:ARG:O	1:J:661:ALA:HB3	2.00	0.61
1:F:128:PHE:O	1:F:131:ILE:HG12	1.99	0.61
1:L:657:ARG:O	1:L:661:ALA:HB3	2.01	0.61
1:B:657:ARG:O	1:B:661:ALA:HB3	2.01	0.61
1:J:121:LYS:O	1:J:124:ILE:HD11	1.95	0.61
2:K:157:MET:HA	2:K:210:MET:HE2	1.81	0.61
1:A:124:ILE:HB	1:A:128:PHE:CZ	2.36	0.61
1:A:127:VAL:O	1:A:131:ILE:HG23	1.99	0.61
2:P:157:MET:HA	2:P:210:MET:HE2	1.81	0.61
1:D:124:ILE:HB	1:D:128:PHE:CZ	2.35	0.61
1:L:127:VAL:O	1:L:127:VAL:HG13	2.00	0.61
1:A:121:LYS:C	1:A:124:ILE:HD11	2.21	0.61
1:A:657:ARG:O	1:A:661:ALA:HB3	2.01	0.61
1:D:123:ALA:O	1:D:124:ILE:C	2.42	0.61
1:D:109:PRO:O	1:D:115:ARG:NE	2.34	0.60
1:F:657:ARG:O	1:F:661:ALA:HB3	2.01	0.60
1:H:123:ALA:O	1:H:124:ILE:C	2.44	0.60
2:O:157:MET:HA	2:O:210:MET:HE2	1.81	0.60
1:B:109:PRO:HD2	1:B:118:PHE:HD2	1.66	0.60
1:F:75:GLN:O	1:F:75:GLN:CG	2.43	0.60
1:L:120:VAL:O	1:L:124:ILE:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:MET:HA	2:M:210:MET:HE2	1.81	0.60
1:N:657:ARG:O	1:N:661:ALA:HB3	2.01	0.60
1:D:657:ARG:O	1:D:661:ALA:HB3	2.01	0.60
1:L:120:VAL:O	1:L:123:ALA:HB3	2.01	0.60
1:N:123:ALA:C	1:N:125:GLY:N	2.50	0.60
1:B:115:ARG:HH11	1:B:115:ARG:HG3	1.63	0.60
1:D:128:PHE:HA	1:D:131:ILE:HG23	1.84	0.60
1:B:123:ALA:C	1:B:125:GLY:H	2.10	0.60
1:B:120:VAL:O	1:B:123:ALA:HB3	2.01	0.60
1:L:121:LYS:O	1:L:122:LYS:C	2.43	0.60
1:N:39:LEU:HD13	1:N:121:LYS:HZ3	1.66	0.60
1:N:71:MET:HG3	1:N:72:PRO:N	2.16	0.60
1:B:131:ILE:O	1:B:134:THR:OG1	2.20	0.59
1:D:135:LEU:O	1:D:138:PHE:HB2	2.02	0.59
1:A:128:PHE:O	1:A:131:ILE:HG12	2.01	0.59
1:F:131:ILE:O	1:F:134:THR:OG1	2.21	0.59
1:L:109:PRO:O	1:L:115:ARG:NE	2.35	0.59
1:F:116:THR:O	1:F:120:VAL:HG13	2.02	0.59
1:L:117:LYS:HA	1:L:120:VAL:HG22	1.84	0.59
1:F:121:LYS:O	1:F:124:ILE:CD1	2.50	0.59
1:H:19:ARG:HG3	1:H:23:LEU:HD11	1.83	0.59
1:J:131:ILE:O	1:J:134:THR:OG1	2.21	0.59
1:B:39:LEU:HD13	1:B:121:LYS:NZ	2.18	0.59
1:D:131:ILE:O	1:D:134:THR:OG1	2.21	0.59
1:H:113:TRP:HA	1:H:116:THR:CG2	2.32	0.59
1:B:137:THR:C	1:B:138:PHE:O	2.40	0.59
1:F:141:ILE:HD11	1:H:459:LEU:HD21	1.85	0.59
1:J:117:LYS:HZ2	1:J:120:VAL:HG21	1.65	0.59
1:A:113:TRP:O	1:A:116:THR:OG1	2.20	0.59
1:H:113:TRP:HA	1:H:116:THR:HG23	1.85	0.59
1:B:109:PRO:HG2	1:B:114:LYS:CG	2.27	0.59
1:F:109:PRO:O	1:F:115:ARG:NE	2.35	0.59
1:D:128:PHE:O	1:D:131:ILE:HG12	2.03	0.58
1:F:112:LEU:O	1:F:116:THR:HG23	2.02	0.58
1:N:39:LEU:HD13	1:N:121:LYS:NZ	2.18	0.58
1:H:120:VAL:O	1:H:124:ILE:CG1	2.51	0.58
1:A:562:ARG:HH21	1:A:563:LEU:HD23	1.69	0.58
1:L:562:ARG:HH21	1:L:563:LEU:HD23	1.69	0.58
1:D:113:TRP:O	1:D:116:THR:OG1	2.20	0.58
1:N:562:ARG:HH21	1:N:563:LEU:HD23	1.69	0.58
1:B:19:ARG:O	1:B:23:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ARG:HH21	1:B:563:LEU:HD23	1.69	0.58
1:F:132:ARG:O	1:F:133:VAL:C	2.46	0.58
1:H:39:LEU:HD13	1:H:121:LYS:NZ	2.17	0.58
1:B:73:SER:HB2	1:D:75:GLN:HA	1.86	0.58
1:D:562:ARG:HH21	1:D:563:LEU:HD23	1.69	0.58
1:J:19:ARG:HG3	1:J:23:LEU:HD11	1.86	0.58
1:H:121:LYS:HZ3	1:H:124:ILE:CD1	2.14	0.57
1:A:453:ARG:HD2	1:A:456:PRO:HG2	1.86	0.57
1:D:136:GLU:O	1:D:137:THR:C	2.46	0.57
1:H:562:ARG:HH21	1:H:563:LEU:HD23	1.69	0.57
1:J:453:ARG:HD2	1:J:456:PRO:HG2	1.86	0.57
1:N:131:ILE:O	1:N:134:THR:OG1	2.22	0.57
1:B:453:ARG:HD2	1:B:456:PRO:HG2	1.86	0.57
1:J:562:ARG:HH21	1:J:563:LEU:HD23	1.69	0.57
1:L:120:VAL:O	1:L:124:ILE:CD1	2.52	0.57
1:L:131:ILE:O	1:L:134:THR:OG1	2.22	0.57
1:A:39:LEU:HD13	1:A:121:LYS:NZ	2.20	0.57
1:D:19:ARG:O	1:D:23:LEU:HG	2.04	0.57
1:H:109:PRO:O	1:H:115:ARG:NE	2.38	0.57
1:F:562:ARG:HH21	1:F:563:LEU:HD23	1.69	0.57
1:N:137:THR:C	1:N:138:PHE:O	2.43	0.57
1:N:453:ARG:HD2	1:N:456:PRO:HG2	1.86	0.57
1:B:116:THR:O	1:B:120:VAL:HG13	2.04	0.57
1:D:453:ARG:HD2	1:D:456:PRO:HG2	1.86	0.57
1:H:453:ARG:HD2	1:H:456:PRO:HG2	1.86	0.57
1:B:92:VAL:HG11	1:B:155:GLU:HG3	1.87	0.56
1:D:92:VAL:HG11	1:D:155:GLU:HG3	1.87	0.56
1:F:128:PHE:O	1:F:131:ILE:N	2.38	0.56
1:H:75:GLN:OE1	1:H:75:GLN:C	2.48	0.56
1:J:75:GLN:HG3	1:J:75:GLN:O	2.05	0.56
1:J:120:VAL:HG23	1:J:121:LYS:N	2.20	0.56
1:L:76:ARG:NH2	1:N:167:THR:CG2	2.68	0.56
1:L:92:VAL:HG11	1:L:155:GLU:HG3	1.87	0.56
1:F:453:ARG:HD2	1:F:456:PRO:HG2	1.86	0.56
1:L:127:VAL:O	1:L:127:VAL:HG12	2.04	0.56
1:D:121:LYS:C	1:D:124:ILE:HD11	2.28	0.56
2:E:157:MET:HG2	2:E:192:LEU:HD22	1.88	0.56
1:F:92:VAL:HG11	1:F:155:GLU:HG3	1.87	0.56
1:F:127:VAL:O	1:F:131:ILE:CG2	2.49	0.56
1:J:92:VAL:HG11	1:J:155:GLU:HG3	1.87	0.56
1:H:44:GLU:HB2	1:H:454:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:LEU:O	1:H:116:THR:HG23	2.06	0.56
2:K:157:MET:HG2	2:K:192:LEU:HD22	1.88	0.56
1:L:44:GLU:HB2	1:L:454:ILE:HD11	1.88	0.56
1:A:19:ARG:O	1:A:23:LEU:CG	2.54	0.56
1:A:507:GLU:HG3	1:A:509:SER:H	1.71	0.56
1:B:132:ARG:O	1:B:133:VAL:C	2.45	0.56
1:F:121:LYS:CA	1:F:124:ILE:HD13	2.32	0.56
2:G:157:MET:HG2	2:G:192:LEU:HD22	1.88	0.56
2:I:157:MET:HG2	2:I:192:LEU:HD22	1.88	0.56
2:C:157:MET:HG2	2:C:192:LEU:HD22	1.88	0.56
1:F:137:THR:C	1:F:138:PHE:O	2.40	0.56
1:J:117:LYS:HA	1:J:120:VAL:CG2	2.34	0.56
1:L:75:GLN:O	1:L:75:GLN:HG3	2.05	0.56
2:M:157:MET:HG2	2:M:192:LEU:HD22	1.88	0.56
1:A:136:GLU:C	1:A:138:PHE:N	2.63	0.55
1:B:123:ALA:O	1:B:125:GLY:N	2.39	0.55
1:F:135:LEU:O	1:F:138:PHE:CB	2.51	0.55
1:L:453:ARG:HD2	1:L:456:PRO:HG2	1.86	0.55
1:N:92:VAL:HG11	1:N:155:GLU:HG3	1.87	0.55
1:N:507:GLU:HG3	1:N:509:SER:H	1.71	0.55
2:P:157:MET:HG2	2:P:192:LEU:HD22	1.88	0.55
2:K:57:ARG:HB2	2:K:130:ASN:HB2	1.89	0.55
1:A:92:VAL:HG11	1:A:155:GLU:HG3	1.87	0.55
1:H:564:LEU:HD21	1:H:583:VAL:HB	1.88	0.55
2:O:157:MET:HG2	2:O:192:LEU:HD22	1.88	0.55
1:H:92:VAL:HG11	1:H:155:GLU:HG3	1.87	0.55
1:J:127:VAL:O	1:J:131:ILE:CG2	2.54	0.55
2:O:57:ARG:HB2	2:O:130:ASN:HB2	1.89	0.55
1:A:132:ARG:O	1:A:133:VAL:C	2.46	0.55
1:B:507:GLU:HG3	1:B:509:SER:H	1.71	0.55
1:F:44:GLU:HB2	1:F:454:ILE:HD11	1.88	0.55
2:P:57:ARG:HB2	2:P:130:ASN:HB2	1.89	0.55
1:A:564:LEU:HD21	1:A:583:VAL:HB	1.88	0.55
1:L:614:GLN:NE2	1:L:642:ARG:O	2.39	0.55
1:N:44:GLU:HB2	1:N:454:ILE:HD11	1.88	0.55
1:N:109:PRO:O	1:N:115:ARG:NE	2.39	0.55
2:E:51:ARG:HD3	2:E:212:ARG:HD2	1.89	0.55
1:A:74:THR:O	1:N:73:SER:CB	2.55	0.55
1:B:44:GLU:HB2	1:B:454:ILE:HD11	1.88	0.55
1:F:507:GLU:HG3	1:F:509:SER:H	1.71	0.55
1:F:564:LEU:HD21	1:F:583:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:507:GLU:HG3	1:H:509:SER:H	1.71	0.55
1:J:564:LEU:HD21	1:J:583:VAL:HB	1.88	0.55
1:L:126:ALA:HA	1:L:129:ASP:HB3	1.88	0.55
2:O:51:ARG:HD3	2:O:212:ARG:HD2	1.89	0.55
1:B:564:LEU:HD21	1:B:583:VAL:HB	1.88	0.55
1:D:123:ALA:C	1:D:125:GLY:H	2.13	0.55
1:H:123:ALA:C	1:H:125:GLY:H	2.13	0.55
2:I:51:ARG:HD3	2:I:212:ARG:HD2	1.89	0.55
1:L:507:GLU:HG3	1:L:509:SER:H	1.71	0.55
1:N:564:LEU:HD21	1:N:583:VAL:HB	1.88	0.55
2:G:57:ARG:HB2	2:G:130:ASN:HB2	1.89	0.54
1:H:109:PRO:HG2	1:H:114:LYS:HB3	1.89	0.54
1:J:44:GLU:HB2	1:J:454:ILE:HD11	1.88	0.54
1:L:39:LEU:HD13	1:L:121:LYS:NZ	2.22	0.54
1:L:116:THR:O	1:L:120:VAL:HG13	2.07	0.54
2:K:51:ARG:HD3	2:K:212:ARG:HD2	1.89	0.54
1:A:39:LEU:HD13	1:A:121:LYS:HZ3	1.72	0.54
2:C:57:ARG:HB2	2:C:130:ASN:HB2	1.89	0.54
1:D:136:GLU:C	1:D:138:PHE:N	2.65	0.54
1:D:507:GLU:HG3	1:D:509:SER:H	1.71	0.54
2:M:51:ARG:HD3	2:M:212:ARG:HD2	1.89	0.54
1:N:75:GLN:O	1:N:75:GLN:HG3	2.05	0.54
1:A:44:GLU:HB2	1:A:454:ILE:HD11	1.88	0.54
1:D:44:GLU:HB2	1:D:454:ILE:HD11	1.88	0.54
2:G:51:ARG:HD3	2:G:212:ARG:HD2	1.89	0.54
1:J:507:GLU:HG3	1:J:509:SER:H	1.71	0.54
2:M:57:ARG:HB2	2:M:130:ASN:HB2	1.89	0.54
2:E:57:ARG:HB2	2:E:130:ASN:HB2	1.89	0.54
1:L:285:ILE:HG12	1:L:355:ASN:HB3	1.90	0.54
1:F:285:ILE:HG12	1:F:355:ASN:HB3	1.90	0.54
2:I:57:ARG:HB2	2:I:130:ASN:HB2	1.89	0.54
1:N:121:LYS:HZ2	1:N:124:ILE:CG2	2.12	0.54
1:J:285:ILE:HG12	1:J:355:ASN:HB3	1.90	0.54
1:L:564:LEU:HD21	1:L:583:VAL:HB	1.88	0.54
1:A:128:PHE:HA	1:A:131:ILE:CG2	2.38	0.54
2:C:51:ARG:HD3	2:C:212:ARG:HD2	1.89	0.54
1:D:564:LEU:HD21	1:D:583:VAL:HB	1.88	0.54
2:P:51:ARG:HD3	2:P:212:ARG:HD2	1.89	0.54
1:J:614:GLN:NE2	1:J:642:ARG:O	2.39	0.53
1:F:39:LEU:HD13	1:F:121:LYS:NZ	2.23	0.53
1:N:127:VAL:O	1:N:131:ILE:CG2	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:523:ILE:HG13	1:N:563:LEU:HD11	1.91	0.53
1:A:121:LYS:HZ3	1:A:124:ILE:CG1	1.82	0.53
1:A:523:ILE:HG13	1:A:563:LEU:HD11	1.91	0.53
1:J:523:ILE:HG13	1:J:563:LEU:HD11	1.91	0.53
1:H:285:ILE:HG12	1:H:355:ASN:HB3	1.90	0.53
1:L:523:ILE:HG13	1:L:563:LEU:HD11	1.91	0.53
1:B:111:GLY:H	1:B:114:LYS:HG2	1.73	0.53
1:A:285:ILE:HG12	1:A:355:ASN:HB3	1.90	0.53
1:B:115:ARG:HD3	1:B:115:ARG:N	2.22	0.53
1:F:523:ILE:HG13	1:F:563:LEU:HD11	1.91	0.53
1:N:108:PRO:HA	1:N:118:PHE:CE2	2.43	0.53
1:D:523:ILE:HG13	1:D:563:LEU:HD11	1.91	0.53
1:B:285:ILE:HG12	1:B:355:ASN:HB3	1.90	0.53
1:D:39:LEU:HD13	1:D:121:LYS:NZ	2.22	0.53
1:N:285:ILE:HG12	1:N:355:ASN:HB3	1.90	0.53
1:B:120:VAL:O	1:B:124:ILE:CG1	2.56	0.53
1:D:120:VAL:O	1:D:124:ILE:HD13	2.09	0.53
1:F:136:GLU:C	1:F:138:PHE:N	2.65	0.53
1:N:125:GLY:O	1:N:126:ALA:C	2.52	0.52
1:B:115:ARG:NH1	1:B:115:ARG:HG3	2.22	0.52
1:J:127:VAL:O	1:J:127:VAL:HG12	1.96	0.52
1:B:614:GLN:NE2	1:B:642:ARG:O	2.39	0.52
1:J:122:LYS:NZ	1:J:122:LYS:HB3	2.25	0.52
1:B:128:PHE:HA	1:B:131:ILE:HG23	1.92	0.52
1:F:128:PHE:HA	1:F:131:ILE:HG23	1.91	0.52
1:J:76:ARG:NH2	1:L:167:THR:HG23	2.23	0.52
1:D:285:ILE:HG12	1:D:355:ASN:HB3	1.90	0.52
1:D:614:GLN:NE2	1:D:642:ARG:O	2.39	0.52
1:J:120:VAL:CG2	1:J:121:LYS:N	2.72	0.52
1:B:26:LEU:HA	1:B:29:VAL:HG12	1.92	0.52
1:N:26:LEU:HA	1:N:29:VAL:HG12	1.92	0.52
1:B:109:PRO:CD	1:B:118:PHE:CD2	2.92	0.52
1:D:121:LYS:CA	1:D:124:ILE:HD13	2.33	0.52
1:J:76:ARG:HH11	1:J:76:ARG:HB2	1.75	0.52
1:L:26:LEU:HA	1:L:29:VAL:HG12	1.92	0.52
1:N:136:GLU:C	1:N:138:PHE:N	2.66	0.52
1:A:130:GLY:C	1:A:132:ARG:N	2.67	0.52
1:B:523:ILE:HG13	1:B:563:LEU:HD11	1.91	0.52
1:D:315:MET:O	2:E:121:ARG:NH1	2.41	0.52
1:H:126:ALA:O	1:H:129:ASP:HB3	2.10	0.52
1:B:315:MET:O	2:C:121:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:LEU:HA	1:H:29:VAL:HG12	1.92	0.52
1:H:128:PHE:HA	1:H:131:ILE:CG2	2.40	0.52
1:H:523:ILE:HG13	1:H:563:LEU:HD11	1.91	0.52
1:A:120:VAL:O	1:A:124:ILE:HD13	2.09	0.51
1:J:134:THR:O	1:J:135:LEU:C	2.53	0.51
1:J:26:LEU:HA	1:J:29:VAL:HG12	1.92	0.51
1:F:26:LEU:HA	1:F:29:VAL:HG12	1.92	0.51
1:H:463:PHE:C	1:H:465:ALA:N	2.68	0.51
1:D:607:ILE:HD11	1:D:635:VAL:HA	1.93	0.51
1:F:607:ILE:HD11	1:F:635:VAL:HA	1.93	0.51
1:H:135:LEU:HA	1:H:138:PHE:HB2	1.91	0.51
2:K:113:THR:OG1	2:K:123:PRO:O	2.29	0.51
1:N:122:LYS:HZ3	1:N:123:ALA:N	2.09	0.51
2:O:113:THR:OG1	2:O:123:PRO:O	2.29	0.51
1:A:614:GLN:NE2	1:A:642:ARG:O	2.39	0.51
1:H:607:ILE:HD11	1:H:635:VAL:HA	1.93	0.51
1:H:614:GLN:NE2	1:H:642:ARG:O	2.39	0.51
2:I:113:THR:OG1	2:I:123:PRO:O	2.29	0.51
1:J:121:LYS:HD3	1:J:124:ILE:CD1	2.40	0.51
2:K:54:ASP:OD2	2:K:212:ARG:NH1	2.44	0.51
1:L:8:ARG:HH12	1:L:659:ARG:HH22	1.59	0.51
1:N:123:ALA:C	1:N:125:GLY:H	2.18	0.51
2:G:54:ASP:OD2	2:G:212:ARG:NH1	2.44	0.51
1:N:8:ARG:HH12	1:N:659:ARG:HH22	1.59	0.51
1:B:99:TYR:HB3	1:B:150:LEU:HD21	1.93	0.51
1:D:99:TYR:HB3	1:D:150:LEU:HD21	1.93	0.51
1:J:8:ARG:HH12	1:J:659:ARG:HH22	1.59	0.51
2:M:54:ASP:OD2	2:M:212:ARG:NH1	2.44	0.51
1:N:99:TYR:HB3	1:N:150:LEU:HD21	1.93	0.51
2:P:54:ASP:OD2	2:P:212:ARG:NH1	2.44	0.51
2:P:113:THR:OG1	2:P:123:PRO:O	2.29	0.51
1:B:607:ILE:HD11	1:B:635:VAL:HA	1.93	0.51
1:F:8:ARG:HH12	1:F:659:ARG:HH22	1.59	0.51
1:F:614:GLN:NE2	1:F:642:ARG:O	2.39	0.51
1:H:8:ARG:HH12	1:H:659:ARG:HH22	1.59	0.51
2:M:113:THR:OG1	2:M:123:PRO:O	2.29	0.51
1:A:8:ARG:HH12	1:A:659:ARG:HH22	1.59	0.51
1:D:8:ARG:HH12	1:D:659:ARG:HH22	1.59	0.51
1:B:8:ARG:HH12	1:B:659:ARG:HH22	1.59	0.50
1:N:119:TYR:O	1:N:122:LYS:NZ	2.44	0.50
2:O:54:ASP:OD2	2:O:212:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HA	1:A:29:VAL:HG12	1.92	0.50
1:D:120:VAL:O	1:D:124:ILE:CD1	2.60	0.50
2:E:54:ASP:OD2	2:E:212:ARG:NH1	2.44	0.50
1:F:81:ASP:OD2	1:H:167:THR:OG1	2.30	0.50
1:F:113:TRP:HA	1:F:116:THR:CG2	2.41	0.50
1:H:125:GLY:O	1:H:129:ASP:HB2	2.11	0.50
1:J:607:ILE:HD11	1:J:635:VAL:HA	1.93	0.50
1:A:120:VAL:O	1:A:124:ILE:CD1	2.59	0.50
1:A:607:ILE:HD11	1:A:635:VAL:HA	1.93	0.50
1:B:113:TRP:HA	1:B:116:THR:CG2	2.42	0.50
2:C:54:ASP:OD2	2:C:212:ARG:NH1	2.44	0.50
1:H:117:LYS:HD2	1:H:120:VAL:HG21	1.93	0.50
1:L:607:ILE:HD11	1:L:635:VAL:HA	1.93	0.50
1:D:26:LEU:HA	1:D:29:VAL:HG12	1.92	0.50
1:D:116:THR:OG1	1:D:117:LYS:N	2.43	0.50
1:F:117:LYS:HA	1:F:120:VAL:HG22	1.94	0.50
1:F:121:LYS:C	1:F:124:ILE:HD13	2.36	0.50
1:H:116:THR:HG1	1:H:117:LYS:H	1.59	0.50
1:J:544:LEU:HG	1:J:608:ALA:HB3	1.94	0.50
1:N:607:ILE:HD11	1:N:635:VAL:HA	1.93	0.50
1:N:39:LEU:HD13	1:N:124:ILE:HG21	1.93	0.50
1:H:23:LEU:HD23	1:H:26:LEU:HD21	1.93	0.50
1:J:130:GLY:HA2	1:J:133:VAL:CG1	2.41	0.50
1:L:99:TYR:HB3	1:L:150:LEU:HD21	1.93	0.50
1:A:99:TYR:HB3	1:A:150:LEU:HD21	1.93	0.50
1:B:544:LEU:HG	1:B:608:ALA:HB3	1.94	0.50
2:I:54:ASP:OD2	2:I:212:ARG:NH1	2.44	0.50
1:N:121:LYS:HA	1:N:124:ILE:CG2	2.41	0.50
1:N:544:LEU:HG	1:N:608:ALA:HB3	1.94	0.50
1:N:614:GLN:NE2	1:N:642:ARG:O	2.39	0.50
1:F:123:ALA:C	1:F:125:GLY:N	2.68	0.50
1:F:544:LEU:HG	1:F:608:ALA:HB3	1.94	0.50
1:B:23:LEU:HD23	1:B:26:LEU:HD21	1.93	0.50
1:B:135:LEU:O	1:B:138:PHE:HB2	2.12	0.50
1:H:39:LEU:HD13	1:H:121:LYS:HZ1	1.77	0.50
1:A:23:LEU:HD23	1:A:26:LEU:HD21	1.93	0.49
1:A:81:ASP:OD2	1:B:167:THR:OG1	2.30	0.49
1:B:110:GLU:OE1	1:B:112:LEU:CA	2.60	0.49
1:D:544:LEU:HG	1:D:608:ALA:HB3	1.94	0.49
1:F:23:LEU:HD23	1:F:26:LEU:HD21	1.93	0.49
1:F:99:TYR:HB3	1:F:150:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:LEU:O	1:N:138:PHE:HB2	2.12	0.49
1:B:116:THR:OG1	1:B:117:LYS:N	2.45	0.49
1:D:540:LEU:HD11	1:D:606:LEU:HG	1.94	0.49
1:J:130:GLY:HA2	1:J:133:VAL:HG13	1.92	0.49
1:L:81:ASP:OD2	1:N:167:THR:OG1	2.30	0.49
1:L:315:MET:O	2:M:121:ARG:NH1	2.41	0.49
1:A:544:LEU:HG	1:A:608:ALA:HB3	1.94	0.49
1:D:123:ALA:O	1:D:125:GLY:N	2.45	0.49
1:F:626:THR:O	1:F:630:THR:OG1	2.29	0.49
1:H:81:ASP:OD2	1:J:167:THR:OG1	2.30	0.49
1:B:72:PRO:C	1:B:74:THR:H	2.19	0.49
1:B:540:LEU:HD11	1:B:606:LEU:HG	1.94	0.49
1:A:124:ILE:CD1	1:A:124:ILE:H	2.15	0.49
1:A:167:THR:OG1	1:N:81:ASP:OD2	2.31	0.49
1:D:81:ASP:OD2	1:F:167:THR:OG1	2.30	0.49
1:J:23:LEU:HD23	1:J:26:LEU:HD21	1.93	0.49
1:L:136:GLU:C	1:L:138:PHE:N	2.68	0.49
1:D:23:LEU:HD23	1:D:26:LEU:HD21	1.93	0.49
1:H:120:VAL:O	1:H:124:ILE:CD1	2.60	0.49
1:H:544:LEU:HG	1:H:608:ALA:HB3	1.94	0.49
1:L:23:LEU:HD23	1:L:26:LEU:HD21	1.93	0.49
1:L:128:PHE:HA	1:L:131:ILE:CG2	2.42	0.49
1:L:544:LEU:HG	1:L:608:ALA:HB3	1.94	0.49
1:N:128:PHE:HA	1:N:131:ILE:HG23	1.94	0.49
1:A:118:PHE:O	1:A:119:TYR:C	2.53	0.49
1:J:99:TYR:HB3	1:J:150:LEU:HD21	1.93	0.49
1:L:125:GLY:C	1:L:127:VAL:N	2.68	0.49
2:O:240:PHE:O	2:O:242:LYS:NZ	2.37	0.49
2:C:233:TYR:CD1	2:O:223:VAL:HG21	2.48	0.49
1:J:81:ASP:OD2	1:L:167:THR:OG1	2.30	0.49
1:N:23:LEU:HD23	1:N:26:LEU:HD21	1.93	0.49
1:N:125:GLY:C	1:N:127:VAL:N	2.69	0.49
1:A:540:LEU:HD11	1:A:606:LEU:HG	1.94	0.49
1:B:112:LEU:O	1:B:115:ARG:N	2.46	0.49
1:B:136:GLU:C	1:B:138:PHE:N	2.65	0.49
1:H:464:LEU:O	1:H:467:PRO:HB2	2.13	0.49
1:J:121:LYS:CA	1:J:124:ILE:HD13	2.39	0.49
1:L:540:LEU:HD11	1:L:606:LEU:HG	1.94	0.49
1:F:136:GLU:O	1:F:137:THR:C	2.56	0.49
1:H:99:TYR:HB3	1:H:150:LEU:HD21	1.93	0.49
1:J:540:LEU:HD11	1:J:606:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:598:PHE:HZ	1:H:528:GLY:HA3	1.78	0.48
1:H:463:PHE:O	1:H:467:PRO:CD	2.57	0.48
1:N:39:LEU:CD1	1:N:124:ILE:HG21	2.43	0.48
1:N:136:GLU:O	1:N:137:THR:C	2.56	0.48
2:C:58:ILE:HG12	2:C:127:VAL:HG22	1.95	0.48
1:F:299:ASP:OD1	1:F:302:ARG:NH2	2.47	0.48
1:L:118:PHE:O	1:L:119:TYR:C	2.53	0.48
1:F:540:LEU:HD11	1:F:606:LEU:HG	1.94	0.48
1:J:126:ALA:O	1:J:129:ASP:HB3	2.13	0.48
1:A:598:PHE:HZ	1:B:528:GLY:HA3	1.79	0.48
1:B:81:ASP:OD2	1:D:167:THR:OG1	2.30	0.48
1:B:136:GLU:O	1:B:137:THR:C	2.55	0.48
2:E:58:ILE:HG12	2:E:127:VAL:HG22	1.95	0.48
1:J:128:PHE:HA	1:J:131:ILE:HG23	1.94	0.48
2:O:58:ILE:HG12	2:O:127:VAL:HG22	1.95	0.48
1:D:299:ASP:OD1	1:D:302:ARG:NH2	2.47	0.48
1:L:135:LEU:CD2	1:N:459:LEU:HD21	2.44	0.48
1:L:393:ARG:NH2	1:N:235:GLY:O	2.47	0.48
1:H:299:ASP:OD1	1:H:302:ARG:NH2	2.47	0.48
1:J:135:LEU:HD22	1:L:459:LEU:HD21	1.96	0.48
1:N:540:LEU:HD11	1:N:606:LEU:HG	1.94	0.48
2:O:186:ARG:HB3	2:P:204:GLY:HA3	1.95	0.48
1:H:76:ARG:NH2	1:J:167:THR:CG2	2.77	0.48
1:J:299:ASP:OD1	1:J:302:ARG:NH2	2.47	0.48
1:B:393:ARG:NH2	1:D:235:GLY:O	2.47	0.48
2:E:55:THR:HB	2:E:131:GLN:HB2	1.96	0.48
1:F:82:GLU:OE1	1:F:192:TYR:OH	2.30	0.48
1:L:76:ARG:HB2	1:L:76:ARG:HH11	1.77	0.48
2:C:57:ARG:HD2	2:C:77:TYR:HE1	1.79	0.48
2:E:57:ARG:HD2	2:E:77:TYR:HE1	1.79	0.48
1:H:118:PHE:HD2	1:H:119:TYR:CE1	2.32	0.48
1:J:136:GLU:C	1:J:136:GLU:CD	2.82	0.48
2:K:240:PHE:O	2:K:242:LYS:NZ	2.37	0.48
2:P:58:ILE:HG12	2:P:127:VAL:HG22	1.95	0.48
1:A:299:ASP:OD1	1:A:302:ARG:NH2	2.47	0.47
1:F:393:ARG:NH2	1:H:235:GLY:O	2.47	0.47
1:H:540:LEU:HD11	1:H:606:LEU:HG	1.94	0.47
1:L:598:PHE:HZ	1:N:528:GLY:HA3	1.79	0.47
2:M:240:PHE:O	2:M:242:LYS:NZ	2.37	0.47
1:D:74:THR:HA	1:F:76:ARG:O	2.14	0.47
1:F:121:LYS:C	1:F:123:ALA:N	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:ILE:HG12	2:G:127:VAL:HG22	1.95	0.47
1:H:598:PHE:HZ	1:J:528:GLY:HA3	1.79	0.47
1:L:71:MET:O	1:L:72:PRO:HB3	2.10	0.47
1:L:113:TRP:O	1:L:116:THR:OG1	2.26	0.47
1:D:131:ILE:HG13	1:D:132:ARG:N	2.28	0.47
1:F:39:LEU:HD13	1:F:121:LYS:CE	2.45	0.47
2:G:55:THR:HB	2:G:131:GLN:HB2	1.96	0.47
1:H:73:SER:HB2	1:J:74:THR:O	2.13	0.47
1:N:123:ALA:O	1:N:125:GLY:N	2.47	0.47
2:O:57:ARG:HD2	2:O:77:TYR:HE1	1.79	0.47
1:A:116:THR:OG1	1:A:117:LYS:N	2.47	0.47
1:B:60:PRO:HD2	1:B:63:ILE:HD11	1.97	0.47
1:F:121:LYS:C	1:F:124:ILE:CD1	2.88	0.47
1:H:123:ALA:O	1:H:125:GLY:N	2.47	0.47
2:K:58:ILE:HG12	2:K:127:VAL:HG22	1.95	0.47
1:L:299:ASP:OD1	1:L:302:ARG:NH2	2.47	0.47
1:A:140:VAL:O	1:B:453:ARG:NH2	2.48	0.47
1:B:598:PHE:HZ	1:D:528:GLY:HA3	1.79	0.47
2:C:55:THR:HB	2:C:131:GLN:HB2	1.96	0.47
1:D:60:PRO:HD2	1:D:63:ILE:HD11	1.97	0.47
1:D:598:PHE:HZ	1:F:528:GLY:HA3	1.79	0.47
1:H:117:LYS:HD2	1:H:120:VAL:CG2	2.44	0.47
1:J:109:PRO:O	1:J:115:ARG:NE	2.44	0.47
1:N:60:PRO:HD2	1:N:63:ILE:HD11	1.97	0.47
1:N:299:ASP:OD1	1:N:302:ARG:NH2	2.46	0.47
1:A:60:PRO:HD2	1:A:63:ILE:HD11	1.97	0.47
1:B:111:GLY:O	1:B:114:LYS:HB2	2.15	0.47
1:F:72:PRO:CG	1:H:72:PRO:O	2.62	0.47
1:F:124:ILE:CD1	1:F:124:ILE:H	2.21	0.47
1:H:60:PRO:HD2	1:H:63:ILE:HD11	1.97	0.47
1:H:393:ARG:NH2	1:J:235:GLY:O	2.47	0.47
1:J:60:PRO:HD2	1:J:63:ILE:HD11	1.97	0.47
1:A:39:LEU:HD13	1:A:124:ILE:HG13	1.95	0.47
1:A:235:GLY:O	1:N:393:ARG:NH2	2.48	0.47
1:B:108:PRO:CB	1:B:118:PHE:CE2	2.97	0.47
1:B:140:VAL:O	1:D:453:ARG:NH2	2.48	0.47
1:B:144:THR:O	1:B:149:ARG:NH1	2.48	0.47
1:B:299:ASP:OD1	1:B:302:ARG:NH2	2.47	0.47
2:E:240:PHE:O	2:E:242:LYS:NZ	2.37	0.47
1:F:60:PRO:HD2	1:F:63:ILE:HD11	1.97	0.47
1:F:144:THR:O	1:F:149:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ARG:HD2	2:G:77:TYR:HE1	1.79	0.47
2:G:113:THR:OG1	2:G:123:PRO:O	2.29	0.47
2:I:58:ILE:HG12	2:I:127:VAL:HG22	1.95	0.47
1:J:76:ARG:NH2	1:L:167:THR:HG22	2.29	0.47
1:J:598:PHE:HZ	1:L:528:GLY:HA3	1.79	0.47
1:L:60:PRO:HD2	1:L:63:ILE:HD11	1.97	0.47
1:L:117:LYS:O	1:L:120:VAL:HG22	2.14	0.47
1:L:124:ILE:CD1	1:L:124:ILE:H	2.14	0.47
1:L:127:VAL:O	1:L:131:ILE:CG2	2.59	0.47
2:M:58:ILE:HG12	2:M:127:VAL:HG22	1.95	0.47
1:N:564:LEU:HD23	1:N:571:VAL:HG22	1.97	0.47
1:A:144:THR:O	1:A:149:ARG:NH1	2.48	0.47
1:A:528:GLY:HA3	1:N:598:PHE:HZ	1.79	0.47
1:D:393:ARG:NH2	1:F:235:GLY:O	2.48	0.47
1:F:73:SER:HB2	1:H:75:GLN:HA	1.96	0.47
1:H:122:LYS:HE2	1:H:122:LYS:HB2	1.77	0.47
1:D:144:THR:O	1:D:149:ARG:NH1	2.48	0.47
1:H:457:LYS:HB2	1:H:460:LEU:HD23	1.97	0.47
1:J:393:ARG:NH2	1:L:235:GLY:O	2.48	0.47
1:L:137:THR:C	1:L:138:PHE:O	2.53	0.47
1:L:564:LEU:HD23	1:L:571:VAL:HG22	1.97	0.47
1:N:144:THR:O	1:N:149:ARG:NH1	2.48	0.47
1:N:626:THR:O	1:N:630:THR:OG1	2.29	0.47
1:A:393:ARG:NH2	1:B:235:GLY:O	2.47	0.47
1:B:82:GLU:OE1	1:B:192:TYR:OH	2.30	0.47
2:E:113:THR:OG1	2:E:123:PRO:O	2.29	0.47
1:F:268:ASP:OD1	1:F:372:ASN:ND2	2.47	0.47
1:H:268:ASP:OD1	1:H:372:ASN:ND2	2.47	0.47
2:I:55:THR:HB	2:I:131:GLN:HB2	1.96	0.47
1:J:144:THR:O	1:J:149:ARG:NH1	2.48	0.47
1:A:76:ARG:HH12	1:B:78:PRO:HD2	1.76	0.46
1:A:453:ARG:NH2	1:N:140:VAL:O	2.49	0.46
1:A:564:LEU:HD23	1:A:571:VAL:HG22	1.97	0.46
1:B:70:VAL:HG11	1:D:70:VAL:HG23	1.97	0.46
1:D:83:GLU:OE2	1:D:162:HIS:ND1	2.43	0.46
1:J:136:GLU:O	1:J:138:PHE:O	2.34	0.46
1:B:124:ILE:HG22	1:B:128:PHE:CZ	2.51	0.46
1:B:564:LEU:HD23	1:B:571:VAL:HG22	1.97	0.46
1:D:20:GLU:HB3	1:D:21:PHE:H	1.52	0.46
1:F:141:ILE:HD11	1:H:459:LEU:CD2	2.46	0.46
1:L:140:VAL:O	1:N:453:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:121:LYS:HA	1:N:124:ILE:HG22	1.97	0.46
1:D:134:THR:O	1:D:135:LEU:C	2.57	0.46
1:D:136:GLU:O	1:D:138:PHE:N	2.48	0.46
1:J:116:THR:O	1:J:120:VAL:HG13	2.15	0.46
1:J:268:ASP:OD1	1:J:372:ASN:ND2	2.47	0.46
1:J:564:LEU:HD23	1:J:571:VAL:HG22	1.97	0.46
2:P:57:ARG:HD2	2:P:77:TYR:HE1	1.79	0.46
1:D:140:VAL:O	1:F:453:ARG:NH2	2.48	0.46
1:D:268:ASP:OD1	1:D:372:ASN:ND2	2.47	0.46
1:J:140:VAL:O	1:L:453:ARG:NH2	2.48	0.46
1:L:144:THR:O	1:L:149:ARG:NH1	2.48	0.46
1:N:82:GLU:OE1	1:N:192:TYR:OH	2.30	0.46
1:H:564:LEU:HD23	1:H:571:VAL:HG22	1.97	0.46
1:L:128:PHE:CA	1:L:131:ILE:HG23	2.46	0.46
1:L:136:GLU:O	1:L:137:THR:C	2.57	0.46
2:M:55:THR:HB	2:M:131:GLN:HB2	1.96	0.46
1:N:120:VAL:O	1:N:124:ILE:HG22	2.15	0.46
1:F:69:LEU:HD13	1:F:71:MET:HE3	1.98	0.46
1:J:123:ALA:O	1:J:125:GLY:N	2.47	0.46
1:L:136:GLU:HG3	1:L:137:THR:N	2.30	0.46
1:L:268:ASP:OD1	1:L:372:ASN:ND2	2.47	0.46
1:A:135:LEU:CD2	1:B:459:LEU:HD21	2.45	0.46
1:D:564:LEU:HD23	1:D:571:VAL:HG22	1.97	0.46
1:H:82:GLU:OE1	1:H:192:TYR:OH	2.30	0.46
2:I:57:ARG:HD2	2:I:77:TYR:HE1	1.79	0.46
1:L:39:LEU:HD13	1:L:124:ILE:HG13	1.97	0.46
1:F:140:VAL:O	1:H:453:ARG:NH2	2.48	0.46
1:H:34:LEU:HD22	1:H:461:MET:HB3	1.97	0.46
1:H:140:VAL:O	1:J:453:ARG:NH2	2.48	0.46
1:H:144:THR:O	1:H:149:ARG:NH1	2.48	0.46
1:J:124:ILE:HD13	1:J:124:ILE:H	1.80	0.46
2:P:55:THR:HB	2:P:131:GLN:HB2	1.96	0.46
1:A:59:LEU:HD11	1:A:68:ALA:HB2	1.98	0.46
1:J:121:LYS:HA	1:J:121:LYS:HD3	1.75	0.46
2:M:57:ARG:HD2	2:M:77:TYR:HE1	1.79	0.46
1:N:98:ARG:HA	1:N:101:GLU:HG2	1.98	0.46
1:N:113:TRP:O	1:N:116:THR:OG1	2.20	0.46
1:N:268:ASP:OD1	1:N:372:ASN:ND2	2.47	0.46
1:A:98:ARG:HA	1:A:101:GLU:HG2	1.98	0.46
1:D:128:PHE:HA	1:D:131:ILE:CG2	2.46	0.46
1:F:564:LEU:HD23	1:F:571:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:55:THR:HB	2:K:131:GLN:HB2	1.97	0.46
1:L:98:ARG:HA	1:L:101:GLU:HG2	1.98	0.46
1:N:59:LEU:HD11	1:N:68:ALA:HB2	1.98	0.46
2:C:113:THR:OG1	2:C:123:PRO:O	2.29	0.45
1:F:121:LYS:O	1:F:122:LYS:C	2.56	0.45
1:H:126:ALA:HA	1:H:129:ASP:HB3	1.98	0.45
2:K:57:ARG:HD2	2:K:77:TYR:HE1	1.79	0.45
1:L:71:MET:HB2	1:L:71:MET:HE2	1.49	0.45
1:B:121:LYS:C	1:B:123:ALA:N	2.72	0.45
1:H:116:THR:OG1	1:H:117:LYS:N	2.50	0.45
1:N:481:TYR:HA	1:N:484:ASP:HB2	1.99	0.45
1:B:59:LEU:HD11	1:B:68:ALA:HB2	1.98	0.45
1:B:121:LYS:HA	1:B:121:LYS:NZ	2.24	0.45
1:B:268:ASP:OD1	1:B:372:ASN:ND2	2.47	0.45
2:O:55:THR:HB	2:O:131:GLN:HB2	1.96	0.45
2:C:19:PRO:HB2	2:O:172:ASP:HB3	1.98	0.45
1:J:98:ARG:HA	1:J:101:GLU:HG2	1.98	0.45
1:L:59:LEU:HD11	1:L:68:ALA:HB2	1.98	0.45
1:L:481:TYR:HA	1:L:484:ASP:HB2	1.99	0.45
1:N:127:VAL:O	1:N:127:VAL:HG13	2.15	0.45
1:A:130:GLY:O	1:A:131:ILE:C	2.58	0.45
1:D:122:LYS:HE2	1:D:122:LYS:HB2	1.84	0.45
1:F:59:LEU:HD11	1:F:68:ALA:HB2	1.98	0.45
1:H:98:ARG:HA	1:H:101:GLU:HG2	1.98	0.45
1:J:117:LYS:CA	1:J:120:VAL:HG22	2.39	0.45
1:A:268:ASP:OD1	1:A:372:ASN:ND2	2.47	0.45
1:B:98:ARG:HA	1:B:101:GLU:HG2	1.99	0.45
1:B:125:GLY:O	1:B:129:ASP:HB2	2.16	0.45
1:J:121:LYS:C	1:J:123:ALA:N	2.73	0.45
1:A:83:GLU:OE2	1:A:162:HIS:ND1	2.43	0.45
1:A:336:GLU:HA	1:A:339:VAL:HG12	1.99	0.45
1:D:39:LEU:HD13	1:D:124:ILE:HG13	1.97	0.45
1:F:83:GLU:OE2	1:F:162:HIS:ND1	2.43	0.45
1:D:481:TYR:HA	1:D:484:ASP:HB2	1.99	0.45
1:F:336:GLU:HA	1:F:339:VAL:HG12	1.99	0.45
1:F:481:TYR:HA	1:F:484:ASP:HB2	1.99	0.45
1:J:121:LYS:HA	1:J:124:ILE:HD12	1.84	0.45
1:L:125:GLY:O	1:L:126:ALA:C	2.57	0.45
1:L:135:LEU:HD22	1:N:459:LEU:HD21	1.99	0.45
1:A:126:ALA:HA	1:A:129:ASP:HB3	1.98	0.45
1:A:481:TYR:HA	1:A:484:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HA	1:B:120:VAL:HG22	1.98	0.45
1:D:98:ARG:HA	1:D:101:GLU:HG2	1.98	0.45
1:D:336:GLU:HA	1:D:339:VAL:HG12	1.99	0.45
1:J:481:TYR:HA	1:J:484:ASP:HB2	1.99	0.45
1:B:117:LYS:HD2	1:B:120:VAL:HG21	1.99	0.44
1:F:98:ARG:HA	1:F:101:GLU:HG2	1.99	0.44
1:H:59:LEU:HD11	1:H:68:ALA:HB2	1.98	0.44
1:N:336:GLU:HA	1:N:339:VAL:HG12	1.99	0.44
2:C:240:PHE:O	2:C:242:LYS:NZ	2.37	0.44
1:D:59:LEU:HD11	1:D:68:ALA:HB2	1.98	0.44
1:D:121:LYS:C	1:D:123:ALA:N	2.74	0.44
1:J:135:LEU:O	1:J:138:PHE:C	2.60	0.44
1:L:23:LEU:HA	1:L:26:LEU:HG	1.99	0.44
1:A:192:TYR:CZ	1:A:196:ARG:HD2	2.53	0.44
2:C:196:GLN:O	2:C:205:ARG:NH1	2.51	0.44
1:D:23:LEU:HA	1:D:26:LEU:HG	1.99	0.44
1:A:82:GLU:OE1	1:A:192:TYR:OH	2.30	0.44
2:G:240:PHE:O	2:G:242:LYS:NZ	2.37	0.44
1:J:23:LEU:HA	1:J:26:LEU:HG	1.99	0.44
1:L:124:ILE:O	1:L:128:PHE:CZ	2.70	0.44
1:N:23:LEU:HA	1:N:26:LEU:HG	1.99	0.44
1:N:192:TYR:CZ	1:N:196:ARG:HD2	2.53	0.44
1:B:117:LYS:HA	1:B:117:LYS:HD2	1.87	0.44
1:D:108:PRO:HA	1:D:118:PHE:CE2	2.52	0.44
1:D:127:VAL:O	1:D:131:ILE:CG2	2.65	0.44
1:F:123:ALA:C	1:F:125:GLY:H	2.18	0.44
1:L:135:LEU:O	1:L:138:PHE:HB2	2.18	0.44
2:O:196:GLN:O	2:O:205:ARG:NH1	2.51	0.44
1:A:128:PHE:CA	1:A:131:ILE:HG23	2.46	0.44
1:B:192:TYR:CZ	1:B:196:ARG:HD2	2.53	0.44
1:F:118:PHE:O	1:F:119:TYR:C	2.57	0.44
1:F:128:PHE:HA	1:F:131:ILE:CG2	2.48	0.44
1:N:56:ASP:N	1:N:56:ASP:OD1	2.51	0.44
1:A:459:LEU:HD21	1:N:135:LEU:CD2	2.48	0.44
1:B:135:LEU:CD2	1:D:459:LEU:HD21	2.47	0.44
1:F:192:TYR:CZ	1:F:196:ARG:HD2	2.53	0.44
1:H:73:SER:OG	1:J:74:THR:O	2.34	0.44
1:H:127:VAL:C	1:H:129:ASP:N	2.75	0.44
1:J:657:ARG:O	1:J:661:ALA:CB	2.66	0.44
1:L:657:ARG:O	1:L:661:ALA:CB	2.66	0.44
1:N:113:TRP:HA	1:N:116:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:196:GLN:O	2:P:205:ARG:NH1	2.51	0.44
1:B:111:GLY:H	1:B:114:LYS:CG	2.30	0.44
1:D:39:LEU:HD13	1:D:121:LYS:CE	2.48	0.44
2:I:196:GLN:O	2:I:205:ARG:NH1	2.51	0.44
1:J:59:LEU:HD11	1:J:68:ALA:HB2	1.98	0.44
1:J:192:TYR:CZ	1:J:196:ARG:HD2	2.53	0.44
1:D:135:LEU:HD22	1:F:459:LEU:HD21	1.99	0.44
1:H:336:GLU:HA	1:H:339:VAL:HG12	1.99	0.44
1:H:481:TYR:HA	1:H:484:ASP:HB2	1.99	0.44
1:L:192:TYR:CZ	1:L:196:ARG:HD2	2.53	0.44
1:L:279:LYS:HB2	1:L:279:LYS:HE3	1.83	0.44
1:B:20:GLU:HB3	1:B:21:PHE:H	1.51	0.43
1:B:336:GLU:HA	1:B:339:VAL:HG12	1.99	0.43
1:A:315:MET:HE1	1:A:320:ASP:HA	2.00	0.43
2:E:196:GLN:O	2:E:205:ARG:NH1	2.51	0.43
1:F:136:GLU:HG3	1:F:137:THR:N	2.34	0.43
1:H:23:LEU:HA	1:H:26:LEU:HG	1.99	0.43
1:L:315:MET:HE1	1:L:320:ASP:HA	2.00	0.43
1:L:336:GLU:HA	1:L:339:VAL:HG12	1.99	0.43
1:A:135:LEU:O	1:A:138:PHE:HB2	2.18	0.43
1:B:56:ASP:N	1:B:56:ASP:OD1	2.51	0.43
1:B:481:TYR:HA	1:B:484:ASP:HB2	1.99	0.43
1:D:56:ASP:N	1:D:56:ASP:OD1	2.51	0.43
1:D:192:TYR:CZ	1:D:196:ARG:HD2	2.53	0.43
1:F:56:ASP:OD1	1:F:56:ASP:N	2.51	0.43
1:F:126:ALA:HA	1:F:129:ASP:HB3	2.00	0.43
1:J:82:GLU:OE1	1:J:192:TYR:OH	2.30	0.43
1:J:124:ILE:HG12	1:J:125:GLY:N	2.32	0.43
2:K:196:GLN:O	2:K:205:ARG:NH1	2.51	0.43
1:A:23:LEU:HA	1:A:26:LEU:HG	1.99	0.43
1:A:56:ASP:OD1	1:A:56:ASP:N	2.51	0.43
1:H:83:GLU:OE2	1:H:162:HIS:ND1	2.43	0.43
1:H:192:TYR:CZ	1:H:196:ARG:HD2	2.53	0.43
1:H:508:LEU:HD12	1:H:555:PHE:HZ	1.84	0.43
1:D:128:PHE:CA	1:D:131:ILE:HG23	2.48	0.43
1:H:315:MET:HE1	1:H:320:ASP:HA	2.00	0.43
1:H:397:LEU:HD21	1:J:237:SER:HA	2.01	0.43
2:M:196:GLN:O	2:M:205:ARG:NH1	2.51	0.43
1:B:23:LEU:HA	1:B:26:LEU:HG	1.99	0.43
1:B:124:ILE:HG13	1:B:124:ILE:H	1.49	0.43
1:H:56:ASP:OD1	1:H:56:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:508:LEU:HD12	1:L:555:PHE:HZ	1.84	0.43
2:G:196:GLN:O	2:G:205:ARG:NH1	2.51	0.43
1:H:463:PHE:O	1:H:465:ALA:N	2.52	0.43
1:H:135:LEU:HB3	1:H:140:VAL:HG23	2.01	0.43
1:J:39:LEU:HD13	1:J:124:ILE:HG13	2.01	0.43
1:J:56:ASP:OD1	1:J:56:ASP:N	2.51	0.43
1:J:124:ILE:HD13	1:J:124:ILE:N	2.34	0.43
1:J:315:MET:HE1	1:J:320:ASP:HA	2.00	0.43
1:A:397:LEU:HD21	1:B:237:SER:HA	2.01	0.43
1:D:315:MET:HE1	1:D:320:ASP:HA	2.00	0.43
1:F:128:PHE:CA	1:F:131:ILE:HG23	2.47	0.43
1:H:381:GLU:HG3	1:H:384:LYS:HE3	2.01	0.43
1:L:397:LEU:HD21	1:N:237:SER:HA	2.01	0.43
1:N:126:ALA:HA	1:N:129:ASP:HB3	2.01	0.43
2:P:18:THR:OG1	2:P:228:GLU:OE1	2.32	0.43
1:A:130:GLY:C	1:A:132:ARG:H	2.26	0.43
1:D:279:LYS:HE3	1:D:279:LYS:HB2	1.83	0.43
1:F:540:LEU:HB3	1:F:583:VAL:HG13	2.01	0.43
1:B:120:VAL:CG2	1:B:121:LYS:N	2.82	0.42
1:B:121:LYS:C	1:B:123:ALA:H	2.27	0.42
1:F:23:LEU:HA	1:F:26:LEU:HG	1.99	0.42
1:J:336:GLU:HA	1:J:339:VAL:HG12	1.99	0.42
1:L:56:ASP:OD1	1:L:56:ASP:N	2.51	0.42
1:A:279:LYS:HE3	1:A:279:LYS:HB2	1.83	0.42
1:A:595:CYS:SG	1:B:521:ALA:HA	2.59	0.42
1:B:136:GLU:HG3	1:B:137:THR:N	2.34	0.42
1:B:657:ARG:O	1:B:661:ALA:CB	2.66	0.42
1:D:109:PRO:HB2	1:D:114:LYS:HE3	2.01	0.42
1:D:309:LEU:HD22	1:F:303:LEU:HD22	2.01	0.42
1:H:135:LEU:HD13	1:J:459:LEU:HD21	1.99	0.42
1:J:381:GLU:HG3	1:J:384:LYS:HE3	2.01	0.42
1:L:212:GLN:OE1	1:N:428:ARG:NH2	2.46	0.42
1:N:136:GLU:HG3	1:N:137:THR:N	2.34	0.42
1:A:20:GLU:HB3	1:A:21:PHE:H	1.52	0.42
1:B:397:LEU:HD21	1:D:237:SER:HA	2.01	0.42
1:D:397:LEU:HD21	1:F:237:SER:HA	2.01	0.42
1:J:117:LYS:HE3	1:J:120:VAL:HG21	1.98	0.42
1:J:540:LEU:HB3	1:J:583:VAL:HG13	2.01	0.42
1:N:315:MET:HE1	1:N:320:ASP:HA	2.01	0.42
1:B:120:VAL:O	1:B:124:ILE:CD1	2.67	0.42
1:B:508:LEU:HD12	1:B:555:PHE:HZ	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:LEU:HB3	1:B:583:VAL:HG13	2.01	0.42
1:L:82:GLU:OE1	1:L:192:TYR:OH	2.30	0.42
1:A:303:LEU:HD22	1:N:309:LEU:HD22	2.02	0.42
1:A:309:LEU:HD22	1:B:303:LEU:HD22	2.01	0.42
1:D:508:LEU:HD12	1:D:555:PHE:HZ	1.84	0.42
1:D:657:ARG:O	1:D:661:ALA:CB	2.66	0.42
2:E:167:ILE:HG13	2:E:173:ALA:HB2	2.02	0.42
1:H:109:PRO:O	1:H:115:ARG:NH2	2.52	0.42
1:H:540:LEU:HB3	1:H:583:VAL:HG13	2.01	0.42
1:N:131:ILE:HG13	1:N:135:LEU:HD12	2.02	0.42
2:C:167:ILE:HG13	2:C:173:ALA:HB2	2.02	0.42
1:D:82:GLU:OE1	1:D:192:TYR:OH	2.30	0.42
1:F:309:LEU:HD22	1:H:303:LEU:HD22	2.02	0.42
1:F:397:LEU:HD21	1:H:237:SER:HA	2.01	0.42
2:I:240:PHE:O	2:I:242:LYS:NZ	2.37	0.42
1:L:381:GLU:HG3	1:L:384:LYS:HE3	2.01	0.42
1:A:121:LYS:HZ3	1:A:124:ILE:HG13	1.56	0.42
1:A:657:ARG:O	1:A:661:ALA:CB	2.66	0.42
1:B:315:MET:HE1	1:B:320:ASP:HA	2.00	0.42
1:D:381:GLU:HG3	1:D:384:LYS:HE3	2.01	0.42
1:F:315:MET:HE1	1:F:320:ASP:HA	2.01	0.42
1:F:381:GLU:HG3	1:F:384:LYS:HE3	2.02	0.42
2:G:167:ILE:HG13	2:G:173:ALA:HB2	2.02	0.42
1:J:508:LEU:HD12	1:J:555:PHE:HZ	1.84	0.42
1:L:122:LYS:HE2	1:L:122:LYS:HB2	1.85	0.42
2:O:167:ILE:HG13	2:O:173:ALA:HB2	2.02	0.42
1:A:459:LEU:HD21	1:N:135:LEU:HD22	2.01	0.42
1:H:117:LYS:HA	1:H:117:LYS:HD2	1.62	0.42
1:J:76:ARG:HH21	1:L:167:THR:CG2	2.25	0.42
1:D:135:LEU:CD2	1:F:459:LEU:HD21	2.49	0.42
1:H:34:LEU:HD22	1:H:461:MET:CB	2.49	0.42
1:H:595:CYS:SG	1:J:521:ALA:HA	2.60	0.42
1:J:309:LEU:HD22	1:L:303:LEU:HD22	2.01	0.42
1:L:74:THR:HG22	1:N:76:ARG:O	2.20	0.42
1:B:128:PHE:HA	1:B:131:ILE:CG2	2.50	0.42
1:B:626:THR:O	1:B:630:THR:OG1	2.29	0.42
1:D:120:VAL:O	1:D:123:ALA:HB3	2.20	0.42
1:D:540:LEU:HB3	1:D:583:VAL:HG13	2.01	0.42
1:H:116:THR:HG1	1:H:117:LYS:N	2.18	0.42
1:A:508:LEU:HD12	1:A:555:PHE:HZ	1.84	0.41
1:B:135:LEU:HD22	1:D:459:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:133:VAL:O	1:J:136:GLU:HG3	2.20	0.41
1:J:135:LEU:CD2	1:L:459:LEU:HD21	2.49	0.41
1:J:397:LEU:HD21	1:L:237:SER:HA	2.02	0.41
1:N:71:MET:HA	1:N:72:PRO:HD3	1.84	0.41
1:N:113:TRP:HA	1:N:116:THR:CG2	2.50	0.41
1:N:657:ARG:O	1:N:661:ALA:CB	2.66	0.41
1:A:109:PRO:CB	1:A:114:LYS:HG2	2.44	0.41
1:D:595:CYS:SG	1:F:521:ALA:HA	2.59	0.41
1:F:508:LEU:HD12	1:F:555:PHE:HZ	1.84	0.41
1:J:130:GLY:O	1:J:134:THR:OG1	2.33	0.41
1:L:540:LEU:HB3	1:L:583:VAL:HG13	2.01	0.41
2:M:18:THR:OG1	2:M:228:GLU:OE1	2.32	0.41
1:N:540:LEU:HB3	1:N:583:VAL:HG13	2.01	0.41
2:P:167:ILE:HG13	2:P:173:ALA:HB2	2.02	0.41
1:A:117:LYS:HA	1:A:117:LYS:HD2	1.83	0.41
1:A:120:VAL:CG2	1:A:121:LYS:N	2.84	0.41
1:A:237:SER:HA	1:N:397:LEU:HD21	2.01	0.41
1:B:112:LEU:O	1:B:115:ARG:CB	2.64	0.41
1:D:117:LYS:HA	1:D:120:VAL:CG2	2.47	0.41
1:L:309:LEU:HD22	1:N:303:LEU:HD22	2.02	0.41
1:N:508:LEU:HD12	1:N:555:PHE:HZ	1.84	0.41
1:H:279:LYS:HE3	1:H:279:LYS:HB2	1.83	0.41
1:J:83:GLU:OE2	1:J:162:HIS:ND1	2.43	0.41
1:L:131:ILE:HG13	1:L:132:ARG:N	2.35	0.41
1:A:62:GLU:OE2	1:A:202:ARG:NH1	2.50	0.41
1:A:381:GLU:HG3	1:A:384:LYS:HE3	2.01	0.41
2:C:53:GLY:H	2:C:84:VAL:HG23	1.86	0.41
1:F:657:ARG:O	1:F:661:ALA:CB	2.66	0.41
2:M:167:ILE:HG13	2:M:173:ALA:HB2	2.02	0.41
1:N:381:GLU:HG3	1:N:384:LYS:HE3	2.01	0.41
1:B:381:GLU:HG3	1:B:384:LYS:HE3	2.01	0.41
1:H:460:LEU:HD12	1:H:460:LEU:C	2.42	0.41
1:J:75:GLN:O	1:J:75:GLN:CG	2.67	0.41
1:N:121:LYS:HZ1	1:N:124:ILE:HG23	1.71	0.41
2:P:53:GLY:H	2:P:84:VAL:HG23	1.86	0.41
1:B:62:GLU:OE2	1:B:202:ARG:NH1	2.50	0.41
1:F:39:LEU:HD13	1:F:124:ILE:HG13	2.03	0.41
2:G:53:GLY:H	2:G:84:VAL:HG23	1.86	0.41
1:L:595:CYS:SG	1:N:521:ALA:HA	2.61	0.41
1:N:71:MET:HG3	1:N:72:PRO:CD	2.51	0.41
1:N:109:PRO:O	1:N:115:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.96	0.41
1:A:135:LEU:HD22	1:B:459:LEU:HD21	2.01	0.41
1:A:540:LEU:HB3	1:A:583:VAL:HG13	2.01	0.41
1:B:110:GLU:OE1	1:B:112:LEU:N	2.51	0.41
1:B:117:LYS:HA	1:B:120:VAL:HG13	2.03	0.41
1:F:124:ILE:HB	1:F:128:PHE:HZ	1.77	0.41
2:I:167:ILE:HG13	2:I:173:ALA:HB2	2.02	0.41
1:J:121:LYS:C	1:J:123:ALA:H	2.28	0.41
2:K:53:GLY:H	2:K:84:VAL:HG23	1.86	0.41
1:A:121:LYS:C	1:A:123:ALA:N	2.74	0.41
1:A:136:GLU:C	1:A:136:GLU:CD	2.89	0.41
1:B:83:GLU:OE2	1:B:162:HIS:ND1	2.43	0.41
1:B:309:LEU:HD22	1:D:303:LEU:HD22	2.02	0.41
2:C:18:THR:OG1	2:C:228:GLU:OE1	2.32	0.41
1:D:634:LYS:NZ	1:D:636:ASP:OD2	2.54	0.41
1:F:508:LEU:HD23	1:F:508:LEU:HA	1.95	0.41
1:H:117:LYS:O	1:H:118:PHE:C	2.61	0.41
1:H:120:VAL:CG2	1:H:121:LYS:N	2.83	0.41
1:J:634:LYS:NZ	1:J:636:ASP:OD2	2.54	0.41
1:L:39:LEU:HD13	1:L:121:LYS:CE	2.51	0.41
1:L:71:MET:HA	1:L:72:PRO:HD3	1.84	0.41
2:M:197:LEU:HG	2:P:179:MET:HE3	2.03	0.41
1:N:574:GLY:HA2	1:N:586:LEU:HG	2.03	0.41
1:A:39:LEU:CD1	1:A:124:ILE:HG13	2.51	0.41
1:A:74:THR:O	1:N:73:SER:OG	2.39	0.41
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.91	0.41
1:B:117:LYS:HD2	1:B:120:VAL:CG2	2.51	0.41
1:B:574:GLY:HA2	1:B:586:LEU:HG	2.03	0.41
1:B:634:LYS:NZ	1:B:636:ASP:OD2	2.54	0.41
1:D:62:GLU:OE2	1:D:202:ARG:NH1	2.50	0.41
1:F:634:LYS:NZ	1:F:636:ASP:OD2	2.54	0.41
1:H:544:LEU:HB2	1:H:557:ILE:HD11	2.03	0.41
1:L:48:ARG:HG2	1:L:170:GLU:HG2	2.03	0.41
1:H:309:LEU:HD22	1:J:303:LEU:HD22	2.02	0.40
2:K:167:ILE:HG13	2:K:173:ALA:HB2	2.02	0.40
1:N:127:VAL:O	1:N:127:VAL:CG1	2.59	0.40
1:N:634:LYS:NZ	1:N:636:ASP:OD2	2.54	0.40
1:A:48:ARG:HG2	1:A:170:GLU:HG2	2.03	0.40
2:C:51:ARG:HE	2:O:155:ASN:HD22	1.68	0.40
1:J:131:ILE:HG13	1:J:135:LEU:HD12	2.02	0.40
2:O:53:GLY:H	2:O:84:VAL:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:CA	1:A:118:PHE:CE2	3.02	0.40
1:A:574:GLY:HA2	1:A:586:LEU:HG	2.03	0.40
1:B:48:ARG:HG2	1:B:170:GLU:HG2	2.03	0.40
1:D:544:LEU:HB2	1:D:557:ILE:HD11	2.03	0.40
2:E:244:ILE:HD11	2:G:240:PHE:HD2	1.86	0.40
2:I:53:GLY:H	2:I:84:VAL:HG23	1.86	0.40
1:L:83:GLU:OE2	1:L:162:HIS:ND1	2.43	0.40
1:D:48:ARG:HG2	1:D:170:GLU:HG2	2.03	0.40
1:D:120:VAL:CG2	1:D:121:LYS:N	2.85	0.40
1:F:122:LYS:HB3	1:F:122:LYS:HE3	1.72	0.40
1:F:544:LEU:HB2	1:F:557:ILE:HD11	2.03	0.40
1:L:574:GLY:HA2	1:L:586:LEU:HG	2.03	0.40
1:L:634:LYS:NZ	1:L:636:ASP:OD2	2.54	0.40
1:A:117:LYS:O	1:A:118:PHE:C	2.63	0.40
1:A:120:VAL:O	1:A:123:ALA:HB3	2.20	0.40
1:A:122:LYS:HE2	1:A:122:LYS:HB2	1.86	0.40
1:A:502:TRP:CD2	1:A:637:GLY:HA3	2.57	0.40
1:B:267:SER:OG	1:B:372:ASN:OD1	2.40	0.40
1:D:267:SER:OG	1:D:372:ASN:OD1	2.40	0.40
1:F:62:GLU:OE2	1:F:202:ARG:NH1	2.50	0.40
1:H:508:LEU:HD23	1:H:508:LEU:HA	1.95	0.40
1:N:117:LYS:CA	1:N:120:VAL:HG22	2.50	0.40
1:N:544:LEU:HB2	1:N:557:ILE:HD11	2.03	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	655/662 (99%)	613 (94%)	41 (6%)	1 (0%)	43 72
1	B	655/662 (99%)	613 (94%)	40 (6%)	2 (0%)	36 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	655/662 (99%)	613 (94%)	41 (6%)	1 (0%)	43	72
1	F	655/662 (99%)	616 (94%)	38 (6%)	1 (0%)	43	72
1	H	655/662 (99%)	611 (93%)	43 (7%)	1 (0%)	43	72
1	J	655/662 (99%)	616 (94%)	38 (6%)	1 (0%)	43	72
1	L	655/662 (99%)	616 (94%)	38 (6%)	1 (0%)	43	72
1	N	655/662 (99%)	618 (94%)	36 (6%)	1 (0%)	43	72
2	C	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	E	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	G	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	I	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	K	230/256 (90%)	217 (94%)	13 (6%)	0	100	100
2	M	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	O	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
2	P	230/256 (90%)	216 (94%)	14 (6%)	0	100	100
All	All	7080/7344 (96%)	6645 (94%)	426 (6%)	9 (0%)	49	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	PRO
1	D	72	PRO
1	F	72	PRO
1	L	72	PRO
1	N	72	PRO
1	H	72	PRO
1	J	72	PRO
1	A	72	PRO
1	B	109	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	562/567 (99%)	547 (97%)	15 (3%)	39	73
1	B	562/567 (99%)	547 (97%)	15 (3%)	39	73
1	D	562/567 (99%)	546 (97%)	16 (3%)	38	72
1	F	562/567 (99%)	548 (98%)	14 (2%)	42	74
1	H	562/567 (99%)	541 (96%)	21 (4%)	30	64
1	J	562/567 (99%)	550 (98%)	12 (2%)	47	77
1	L	562/567 (99%)	546 (97%)	16 (3%)	38	72
1	N	562/567 (99%)	549 (98%)	13 (2%)	44	76
2	C	189/208 (91%)	189 (100%)	0	100	100
2	E	189/208 (91%)	189 (100%)	0	100	100
2	G	189/208 (91%)	189 (100%)	0	100	100
2	I	189/208 (91%)	189 (100%)	0	100	100
2	K	189/208 (91%)	189 (100%)	0	100	100
2	M	189/208 (91%)	189 (100%)	0	100	100
2	O	189/208 (91%)	189 (100%)	0	100	100
2	P	189/208 (91%)	189 (100%)	0	100	100
All	All	6008/6200 (97%)	5886 (98%)	122 (2%)	48	78

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	74	THR
1	A	118	PHE
1	A	121	LYS
1	A	122	LYS
1	A	124	ILE
1	A	127	VAL
1	A	128	PHE
1	A	131	ILE
1	A	132	ARG
1	A	134	THR
1	A	136	GLU
1	A	137	THR
1	A	138	PHE
1	A	524	CYS
1	B	72	PRO

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	76	ARG
1	B	110	GLU
1	B	112	LEU
1	B	114	LYS
1	B	115	ARG
1	B	117	LYS
1	B	121	LYS
1	B	122	LYS
1	B	124	ILE
1	B	131	ILE
1	B	132	ARG
1	B	134	THR
1	B	137	THR
1	D	72	PRO
1	D	73	SER
1	D	75	GLN
1	D	76	ARG
1	D	118	PHE
1	D	121	LYS
1	D	122	LYS
1	D	124	ILE
1	D	127	VAL
1	D	129	ASP
1	D	131	ILE
1	D	132	ARG
1	D	133	VAL
1	D	134	THR
1	D	137	THR
1	D	524	CYS
1	F	72	PRO
1	F	73	SER
1	F	75	GLN
1	F	117	LYS
1	F	121	LYS
1	F	122	LYS
1	F	124	ILE
1	F	128	PHE
1	F	131	ILE
1	F	132	ARG
1	F	134	THR
1	F	135	LEU

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Mol	Chain	Res	Type
1	F	136	GLU
1	F	137	THR
1	H	19	ARG
1	H	72	PRO
1	H	75	GLN
1	H	76	ARG
1	H	114	LYS
1	H	115	ARG
1	H	117	LYS
1	H	118	PHE
1	H	121	LYS
1	H	122	LYS
1	H	124	ILE
1	H	131	ILE
1	H	132	ARG
1	H	460	LEU
1	H	461	MET
1	H	462	LEU
1	H	463	PHE
1	H	464	LEU
1	H	467	PRO
1	H	468	PHE
1	H	524	CYS
1	J	19	ARG
1	J	74	THR
1	J	75	GLN
1	J	76	ARG
1	J	121	LYS
1	J	122	LYS
1	J	124	ILE
1	J	131	ILE
1	J	132	ARG
1	J	133	VAL
1	J	134	THR
1	J	137	THR
1	L	71	MET
1	L	72	PRO
1	L	73	SER
1	L	75	GLN
1	L	76	ARG
1	L	118	PHE
1	L	121	LYS

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Mol	Chain	Res	Type
1	L	122	LYS
1	L	124	ILE
1	L	127	VAL
1	L	131	ILE
1	L	132	ARG
1	L	134	THR
1	L	136	GLU
1	L	137	THR
1	L	524	CYS
1	N	71	MET
1	N	72	PRO
1	N	73	SER
1	N	75	GLN
1	N	117	LYS
1	N	121	LYS
1	N	122	LYS
1	N	124	ILE
1	N	127	VAL
1	N	131	ILE
1	N	132	ARG
1	N	134	THR
1	N	137	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	65	ASN
1	A	230	HIS
1	A	251	ASN
1	A	382	GLN
1	A	567	ASN
1	B	46	ASN
1	B	65	ASN
1	B	230	HIS
1	B	251	ASN
1	B	382	GLN
1	B	567	ASN
1	B	623	HIS
2	C	155	ASN
2	C	188	HIS
1	D	46	ASN

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Mol	Chain	Res	Type
1	D	65	ASN
1	D	230	HIS
1	D	251	ASN
1	D	382	GLN
1	D	567	ASN
2	E	86	ASN
2	E	159	GLN
2	E	188	HIS
1	F	46	ASN
1	F	65	ASN
1	F	230	HIS
1	F	251	ASN
1	F	382	GLN
1	F	567	ASN
1	F	623	HIS
2	G	159	GLN
2	G	188	HIS
2	G	235	ASN
1	H	46	ASN
1	H	65	ASN
1	H	230	HIS
1	H	251	ASN
1	H	382	GLN
1	H	567	ASN
1	H	623	HIS
2	I	159	GLN
2	I	188	HIS
2	I	235	ASN
1	J	46	ASN
1	J	65	ASN
1	J	230	HIS
1	J	251	ASN
1	J	382	GLN
1	J	567	ASN
1	J	623	HIS
2	K	131	GLN
2	K	159	GLN
2	K	188	HIS
1	L	46	ASN
1	L	65	ASN
1	L	230	HIS
1	L	251	ASN

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Mol	Chain	Res	Type
1	L	382	GLN
1	L	567	ASN
1	L	623	HIS
2	M	131	GLN
2	M	155	ASN
2	M	188	HIS
2	M	235	ASN
1	N	46	ASN
1	N	65	ASN
1	N	230	HIS
1	N	251	ASN
1	N	382	GLN
1	N	488	HIS
1	N	567	ASN
2	O	131	GLN
2	O	155	ASN
2	O	159	GLN
2	O	188	HIS
2	O	235	ASN
2	P	86	ASN
2	P	106	GLN
2	P	159	GLN
2	P	188	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

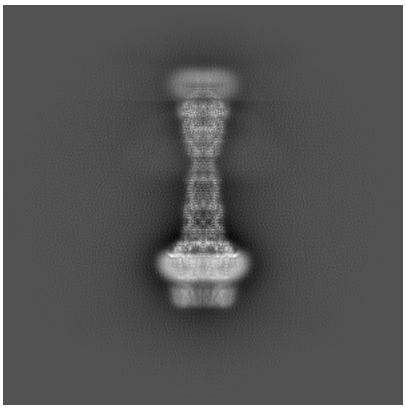
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-64810. These allow visual inspection of the internal detail of the map and identification of artifacts.

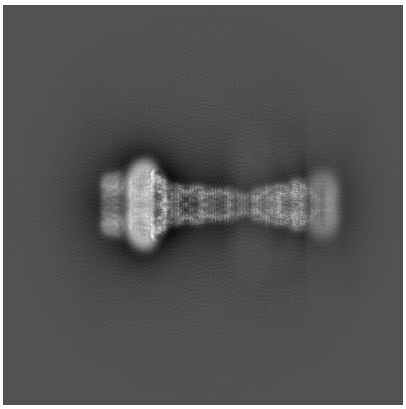
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

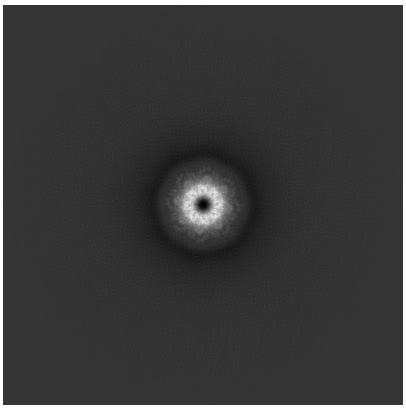
6.1.1 Primary map



X

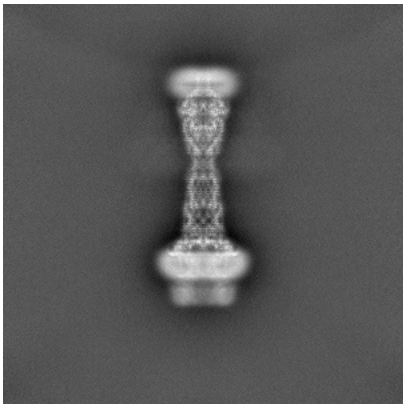


Y

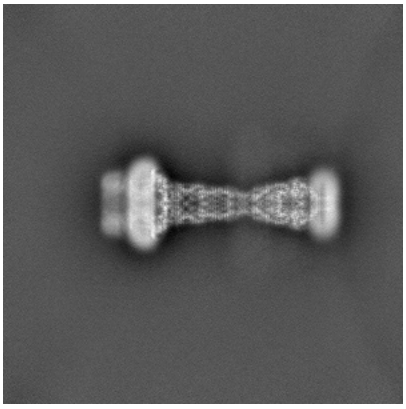


Z

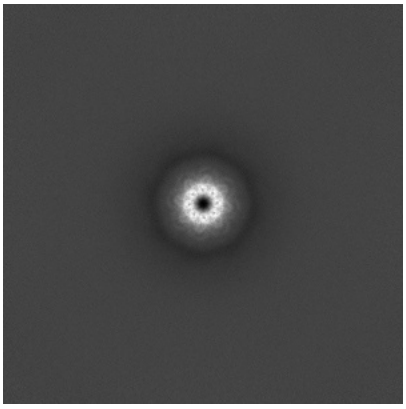
6.1.2 Raw map



X



Y

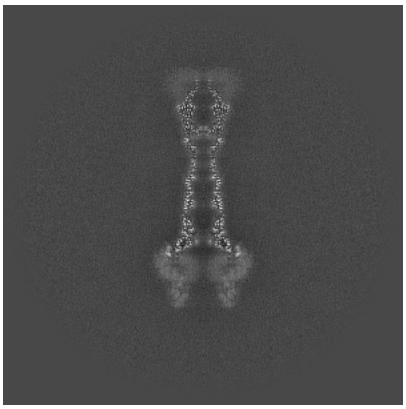


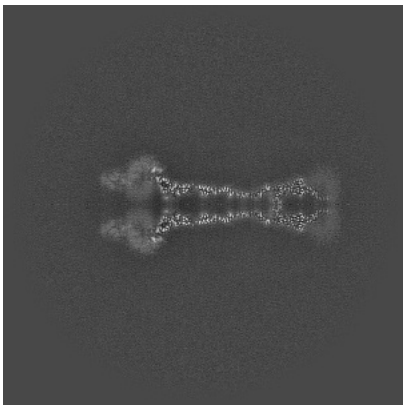
Z

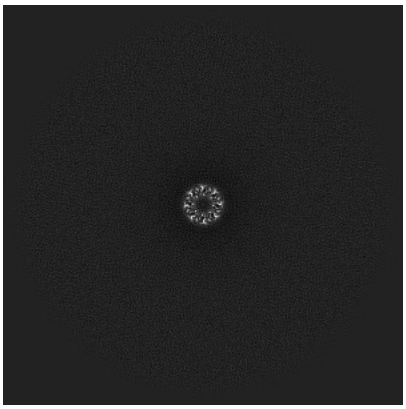
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

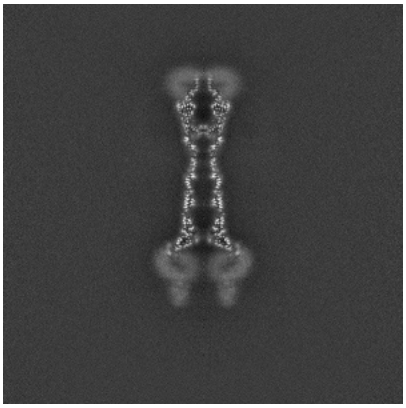
6.2.1 Primary map

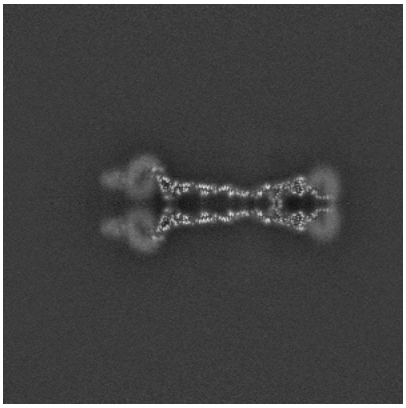

X Index: 320

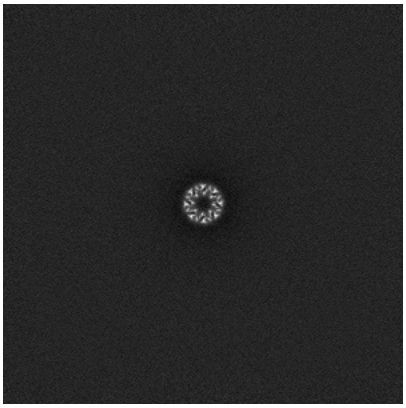

Y Index: 320


Z Index: 320

6.2.2 Raw map


X Index: 320

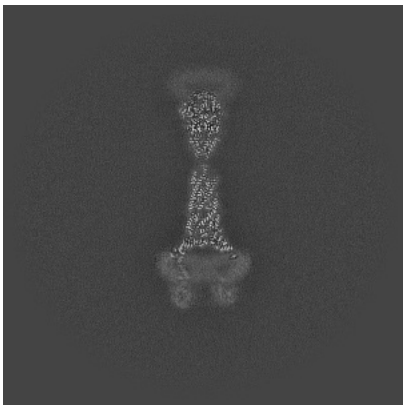

Y Index: 320

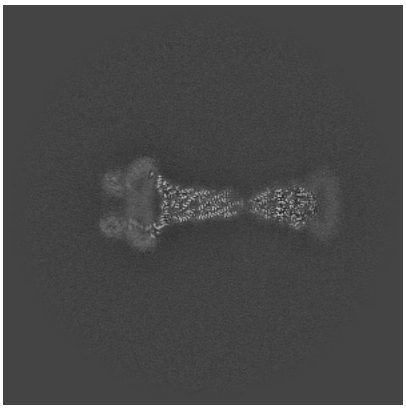

Z Index: 320

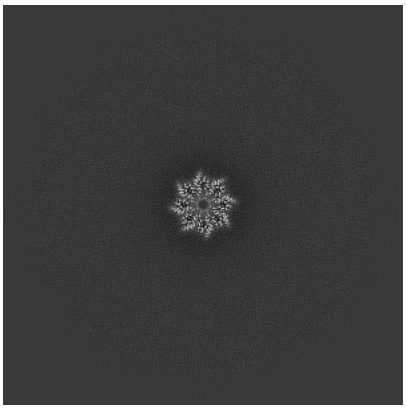
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

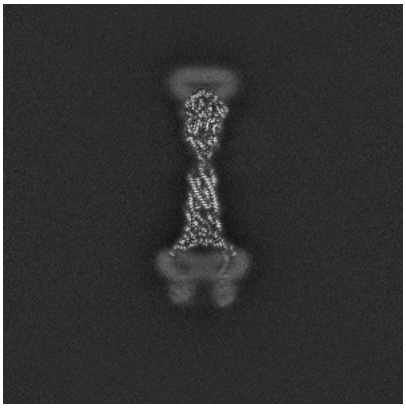
6.3.1 Primary map

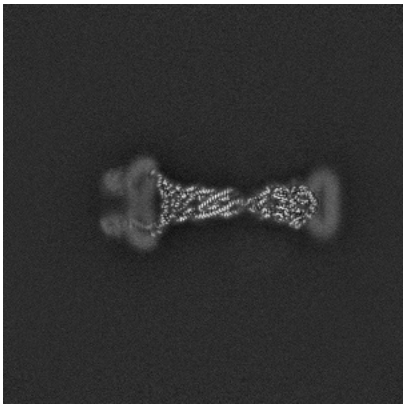

X Index: 340

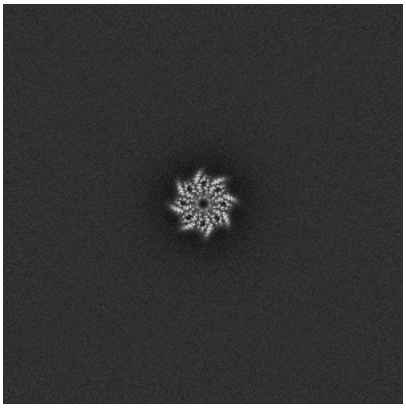

Y Index: 300


Z Index: 258

6.3.2 Raw map


X Index: 301

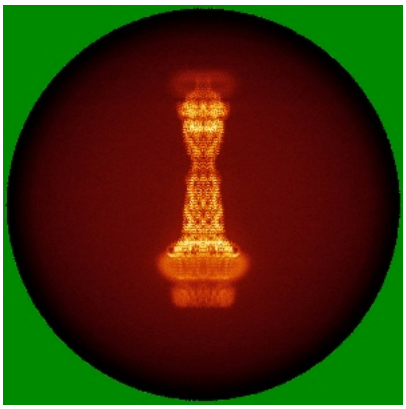

Y Index: 301

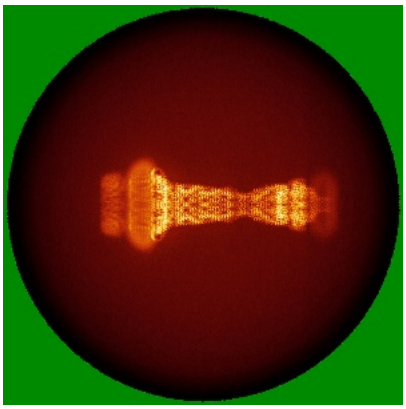

Z Index: 259

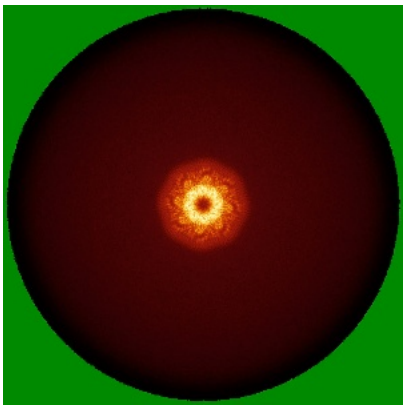
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

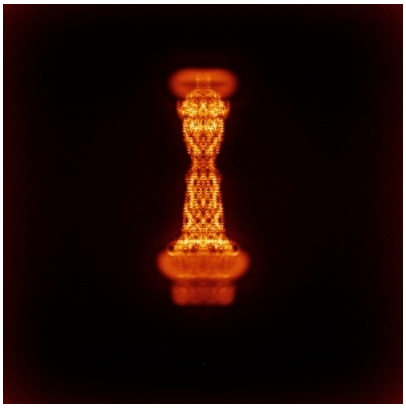
6.4.1 Primary map

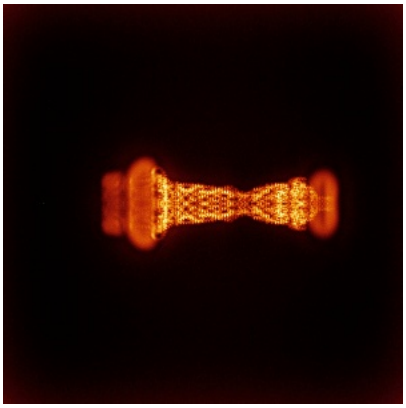

X

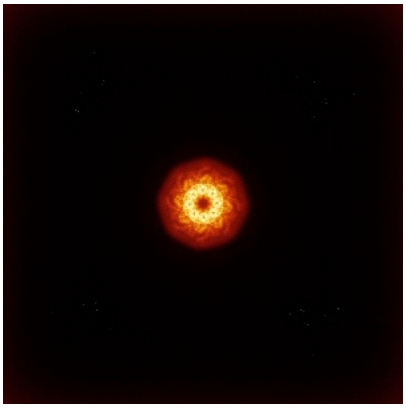

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.803. 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

X Y Z

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.

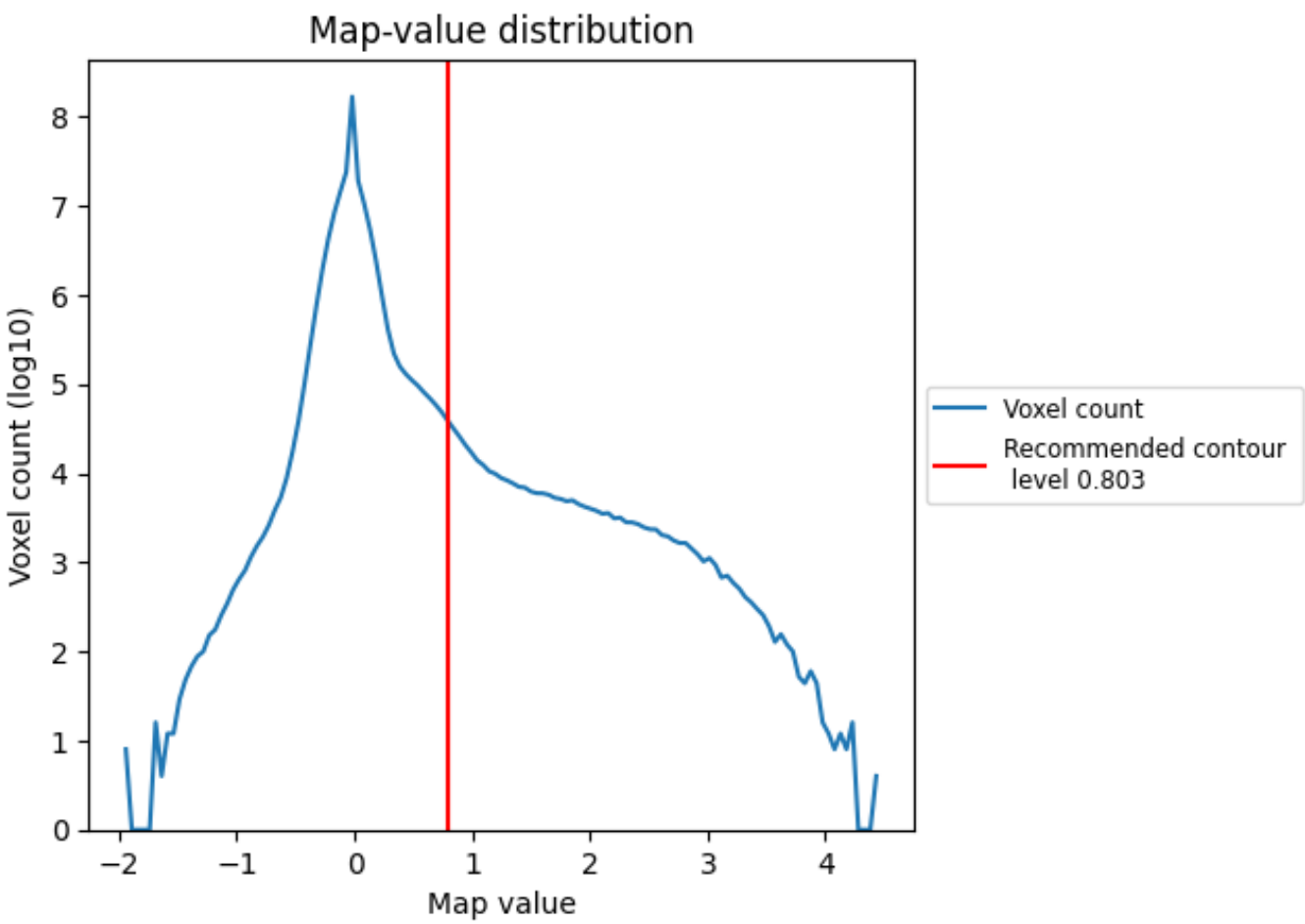
6.6 Mask visualisation (i)

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

7 Map analysis (i)

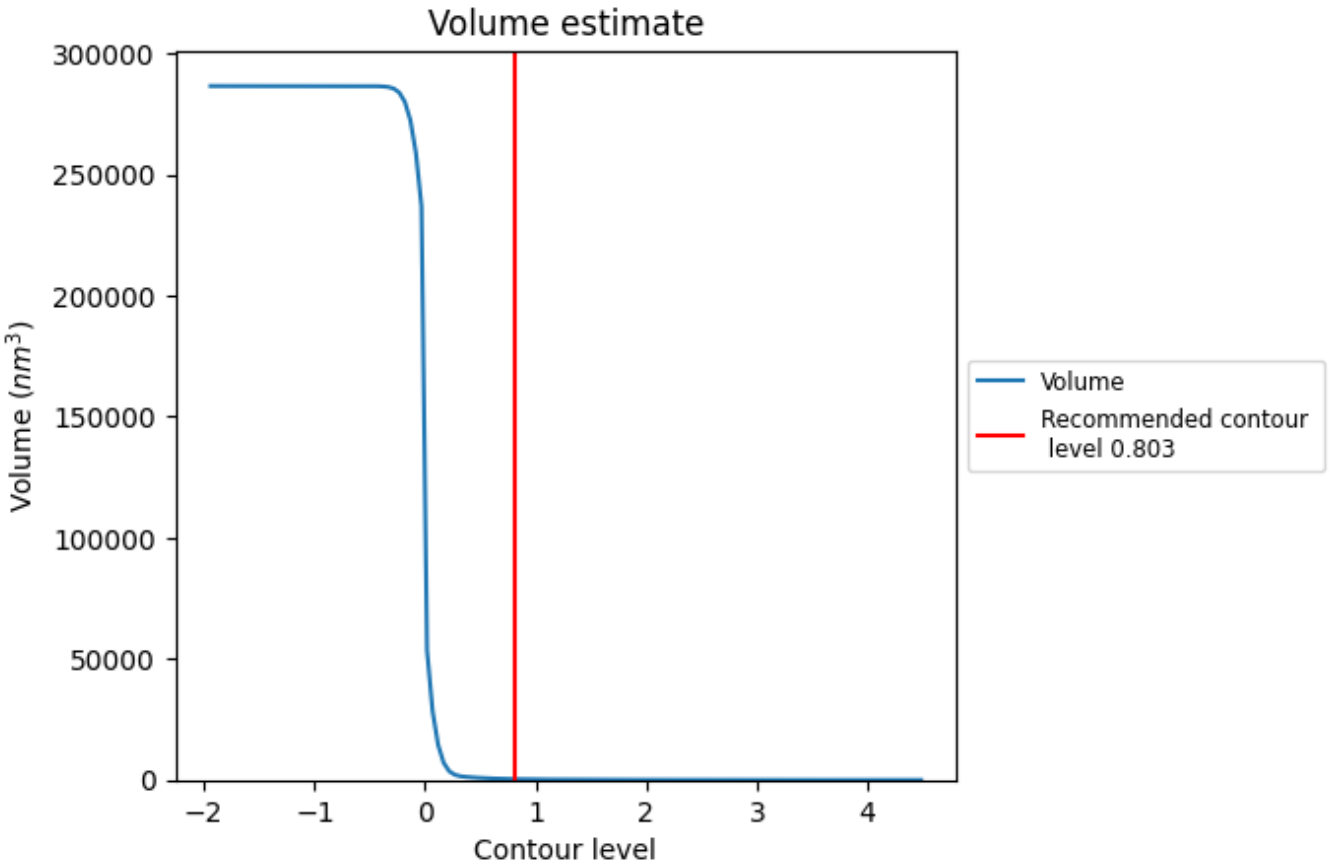
This section contains the results of statistical analysis of the map.

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.

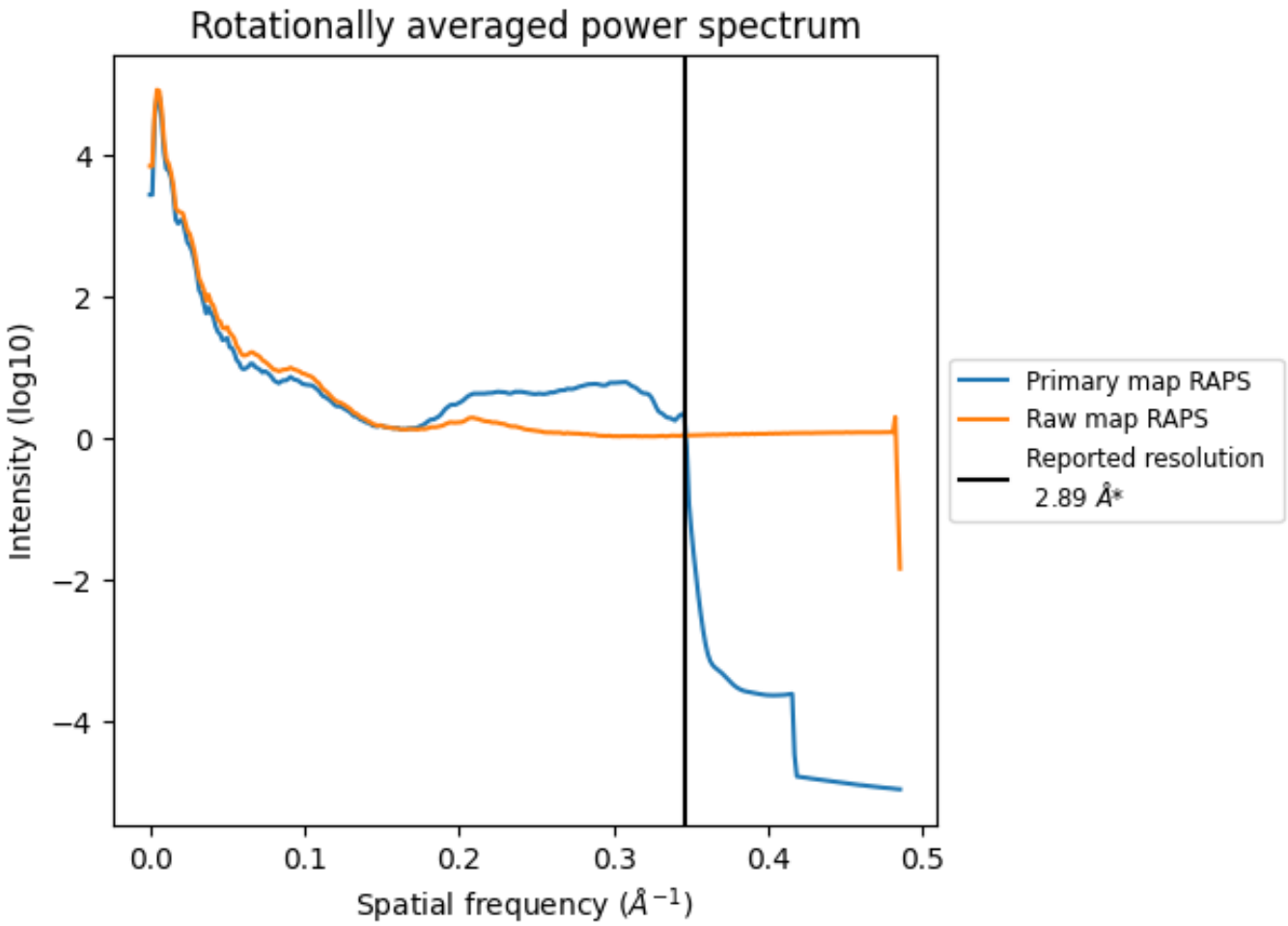
7.2 Volume estimate (i)



The volume at the recommended contour level is 350 nm^3; this corresponds to an approximate mass of 316 kDa.

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

7.3 Rotationally averaged power spectrum (i)

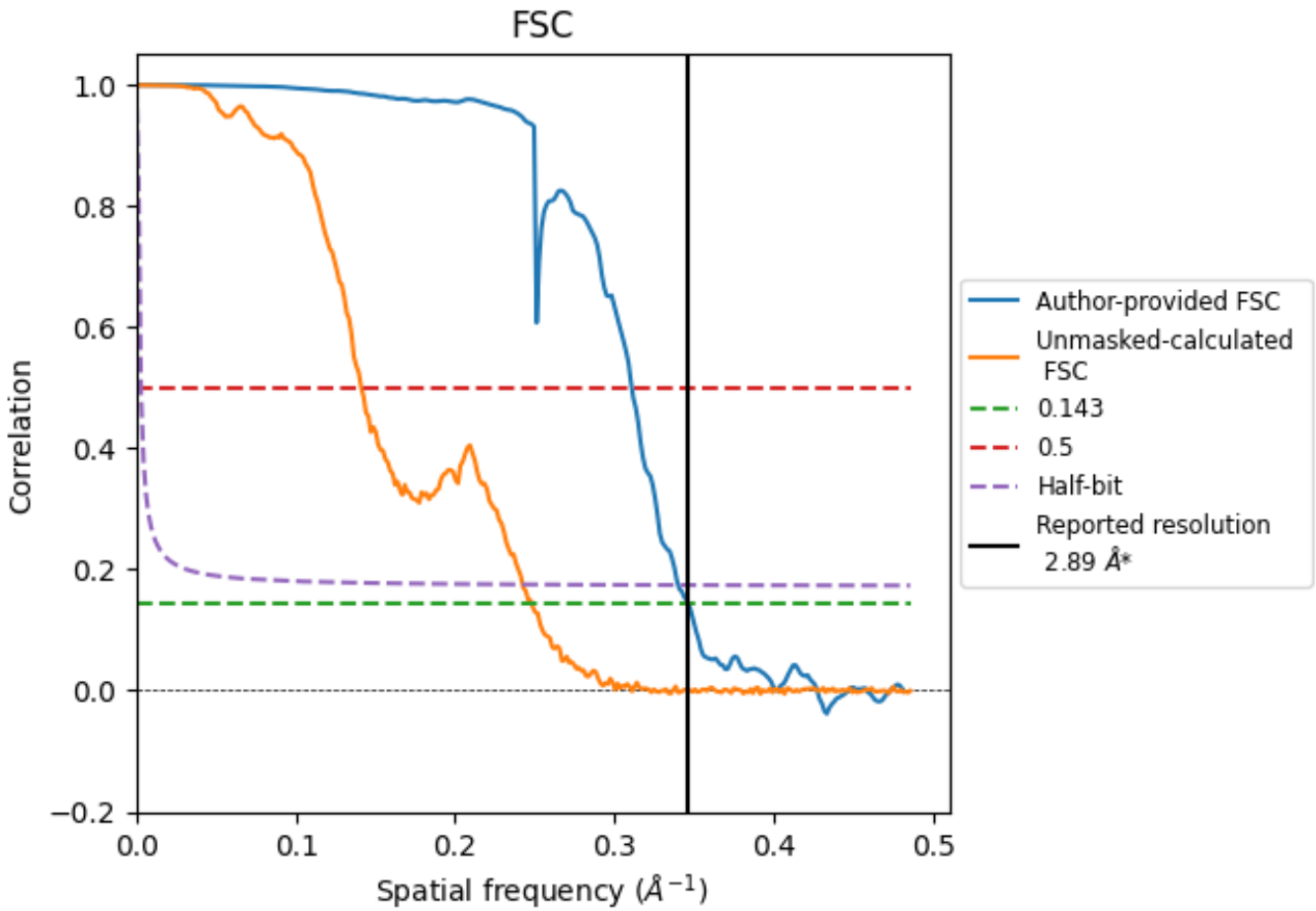


*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

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 0.346 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.22	2.94
Unmasked-calculated*	4.03	7.09	4.13

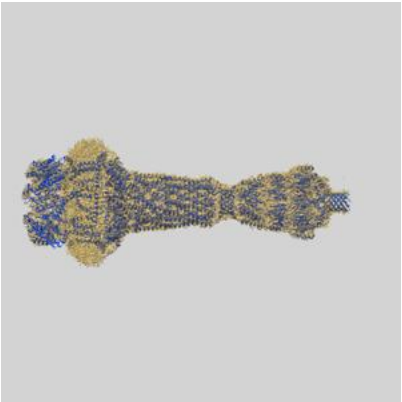
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.89 by more than 10 %

9 Map-model fit (i)

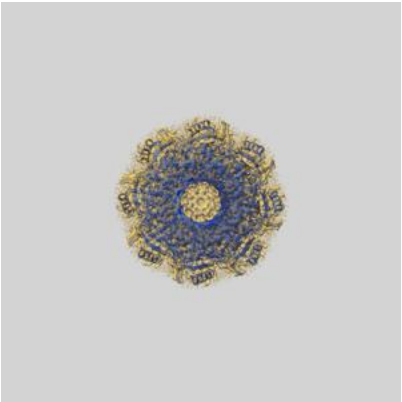
This section contains information regarding the fit between EMDB map EMD-64810 and PDB model 9V75. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

X



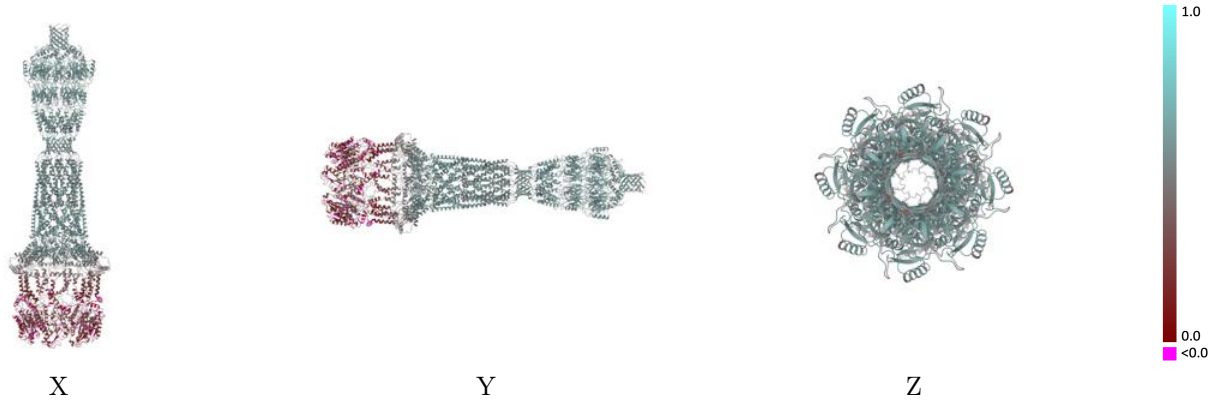
Y



Z

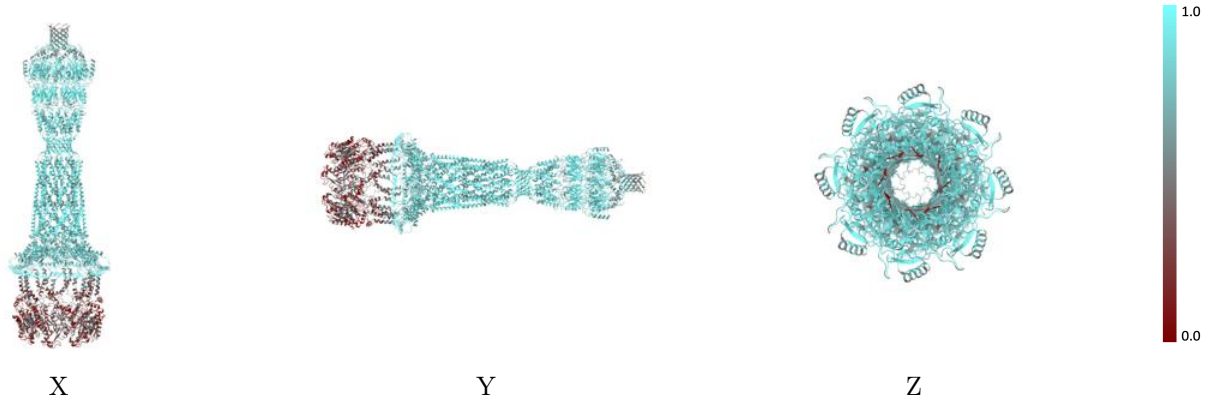
The images above show the 3D surface view of the map at the recommended contour level 0.803 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



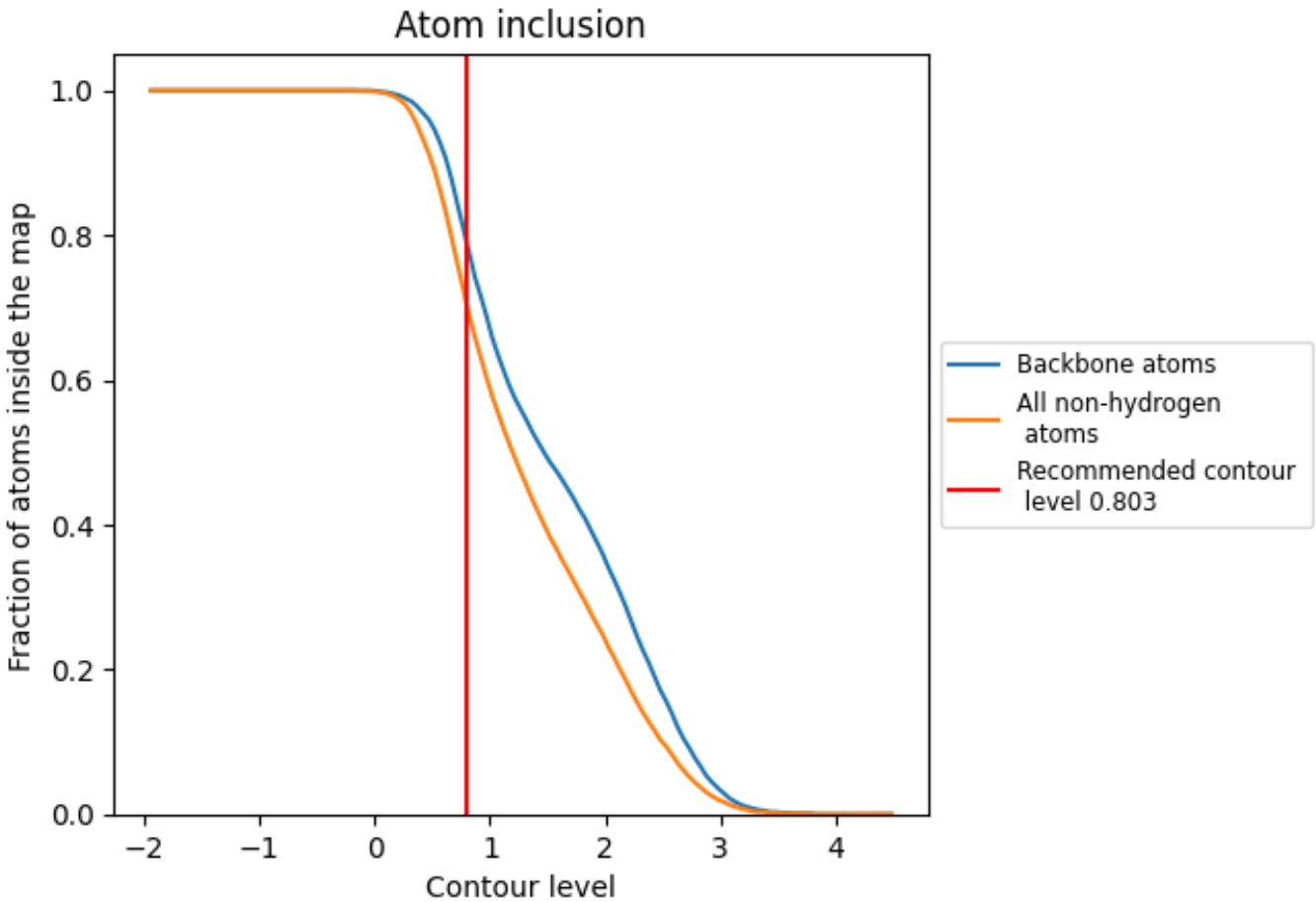
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.803).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.803) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.4610
A	0.6550	0.4220
B	0.6530	0.4240
C	0.8380	0.5720
D	0.6560	0.4240
E	0.8430	0.5730
F	0.6540	0.4230
G	0.8250	0.5650
H	0.6570	0.4260
I	0.8330	0.5690
J	0.6520	0.4230
K	0.8330	0.5650
L	0.6580	0.4230
M	0.8420	0.5740
N	0.6540	0.4230
O	0.8280	0.5590
P	0.8390	0.5710