



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:18 AM UTC

PDB ID : 8T8P / pdb_00008t8p
EMDB ID : EMD-41101
Title : 33-mer FliF MS-ring from Salmonella
Authors : Singh, P.K.; Iverson, T.M.
Deposited on : 2023-06-23
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

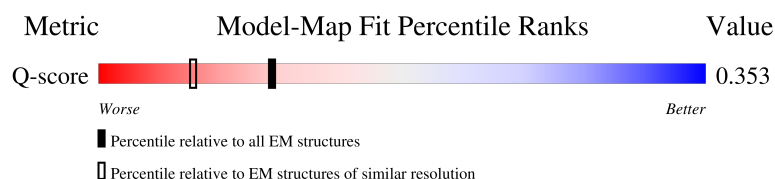
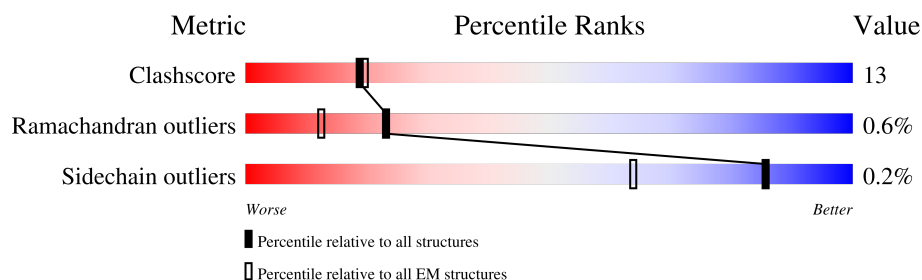
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.



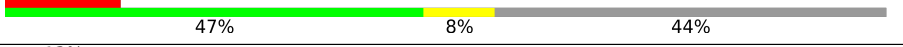
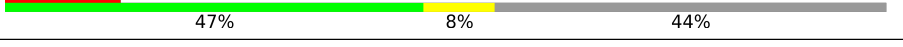
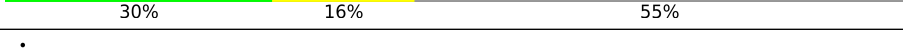
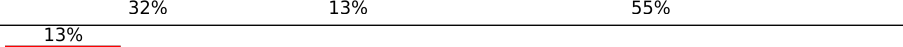
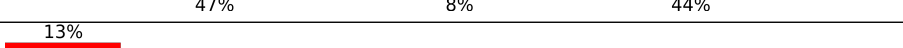
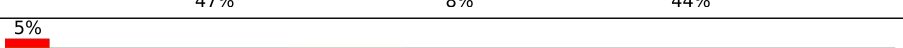
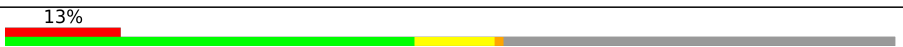
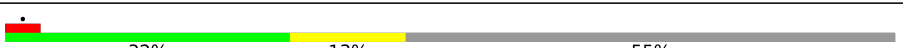
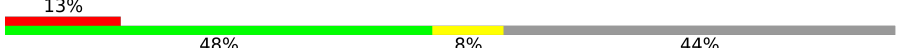
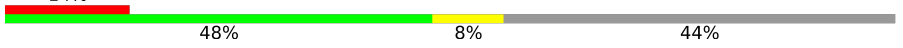
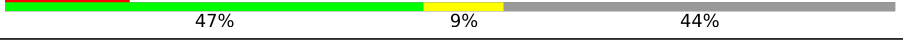
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	560	
1	AA	560	
1	B	560	
1	BA	560	

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Mol	Chain	Length	Quality of chain
1	C	560	
1	CA	560	
1	D	560	
1	DA	560	
1	E	560	
1	EA	560	
1	F	560	
1	FA	560	
1	G	560	
1	GA	560	
1	H	560	
1	HA	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	V	560	

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Mol	Chain	Length	Quality of chain
1	W	560	30%15%55%
1	X	560	14%47%8%44%
1	Y	560	31%14%55%
1	Z	560	30%15%55%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 64845 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	B	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		
1	C	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	D	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	E	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		
1	F	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	G	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	H	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		
1	I	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	J	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	K	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		
1	L	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	M	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	N	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		
1	O	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	P	254	Total	C	N	O	S	0	0
			1945	1190	358	393	4		
1	Q	311	Total	C	N	O	S	0	0
			2005	1209	387	406	3		

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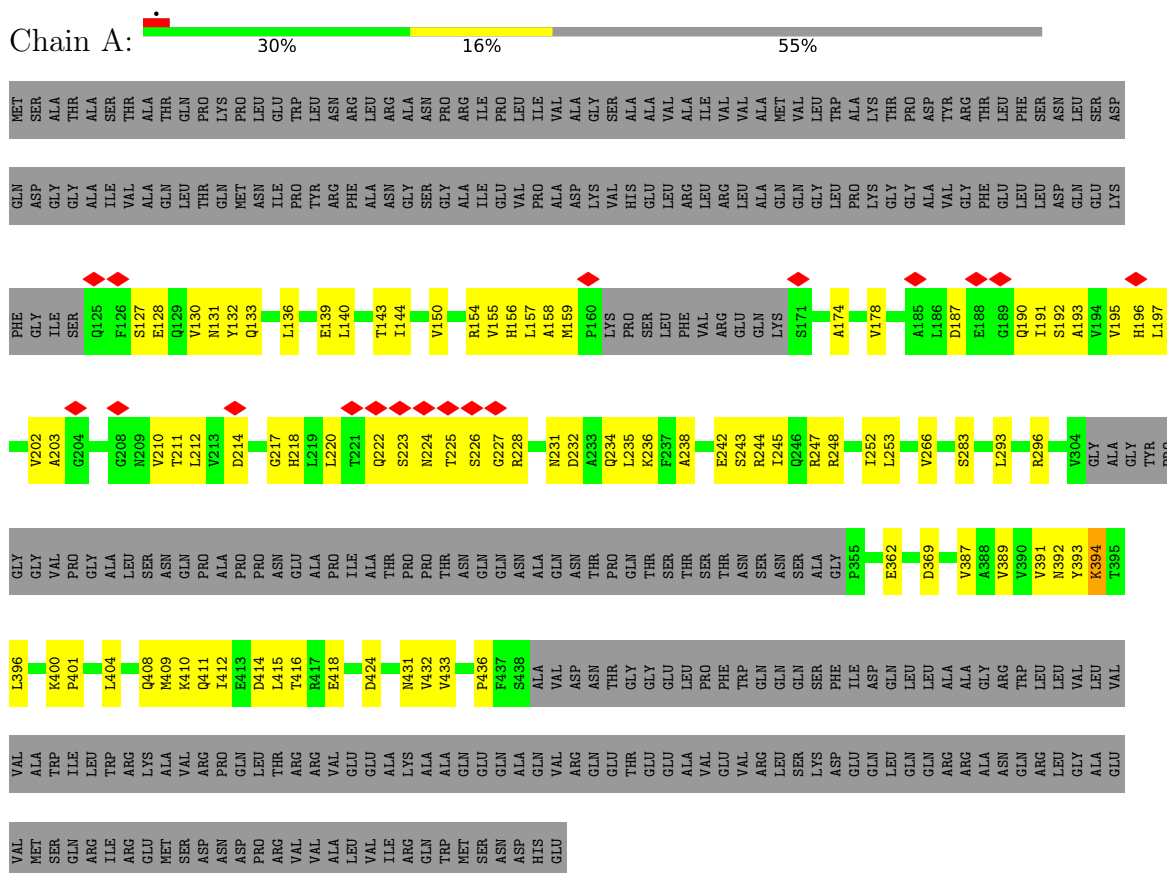
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	S	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	T	311	Total 2005	C 1209	N 387	O 406	S 3	0	0
1	V	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	W	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	X	311	Total 2005	C 1209	N 387	O 406	S 3	0	0
1	Y	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	Z	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	AA	311	Total 2005	C 1209	N 387	O 406	S 3	0	0
1	BA	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	CA	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	DA	311	Total 2005	C 1209	N 387	O 406	S 3	0	0
1	EA	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	FA	254	Total 1945	C 1190	N 358	O 393	S 4	0	0
1	GA	311	Total 2005	C 1209	N 387	O 406	S 3	0	0
1	HA	254	Total 1945	C 1190	N 358	O 393	S 4	0	0

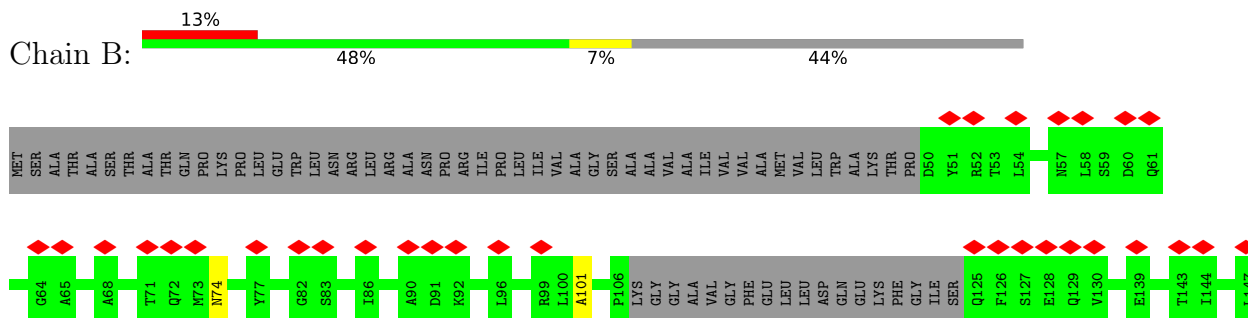
3 Residue-property plots

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

• Molecule 1: Flagellar M-ring protein

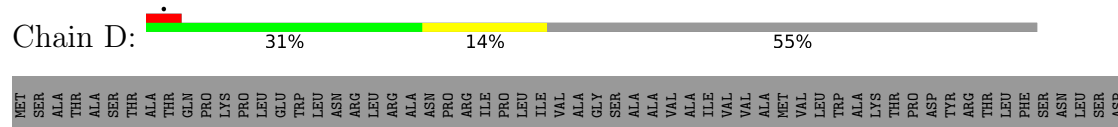


• Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

- Molecule 1: Flagellar M-ring protein



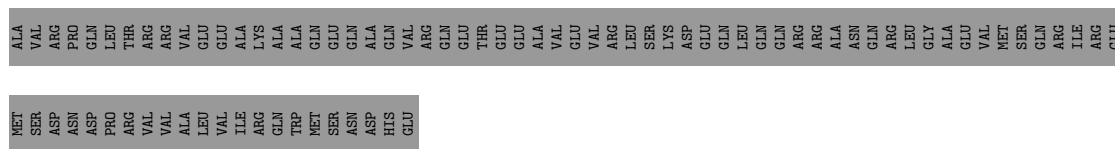


Chain F:

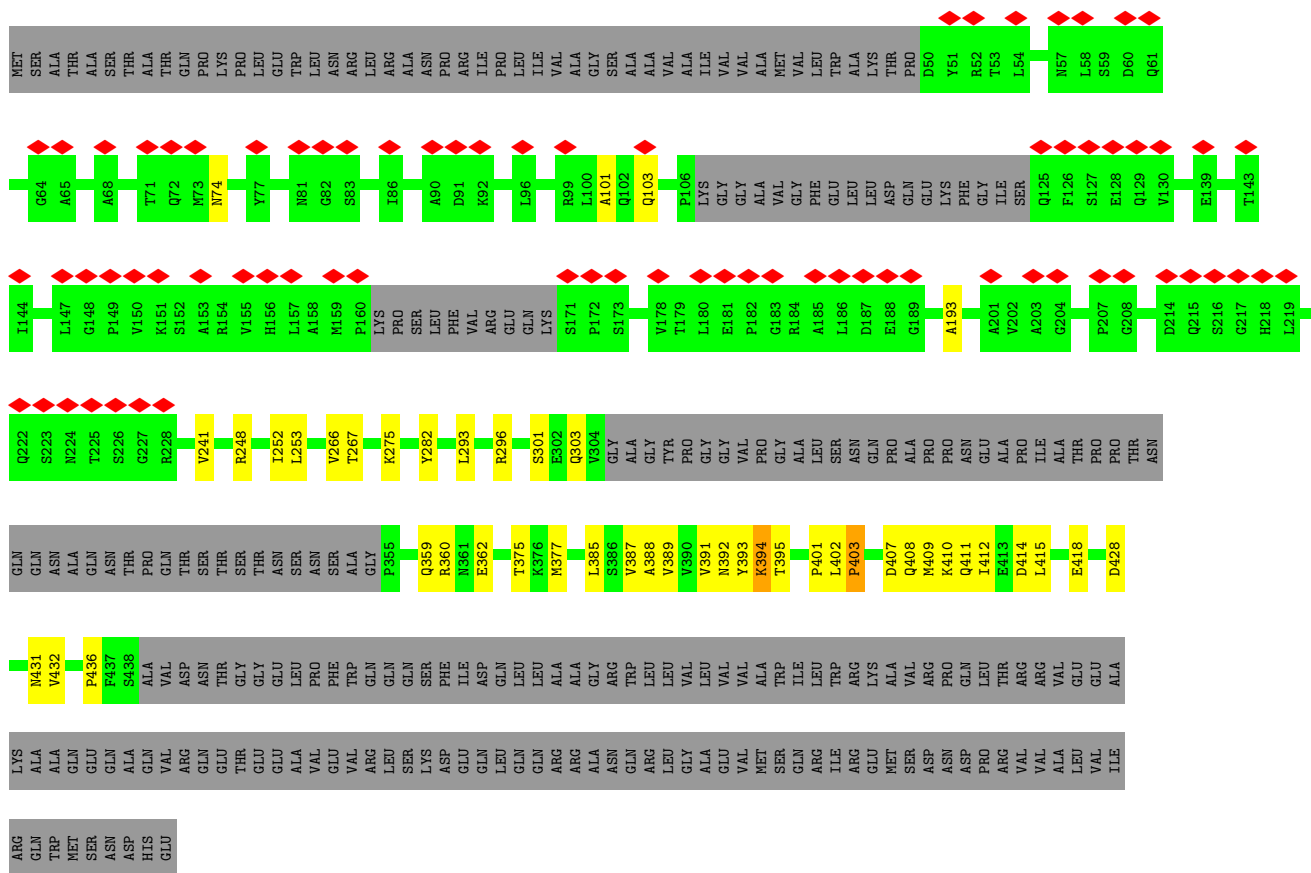


Chain G:

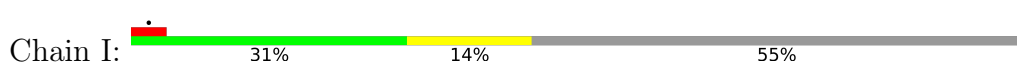


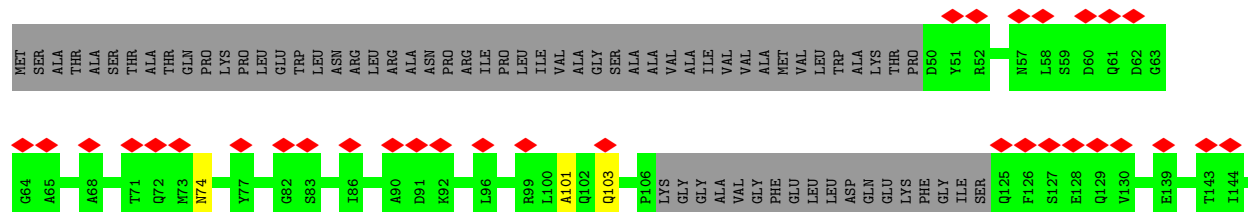


- Molecule 1: Flagellar M-ring protein



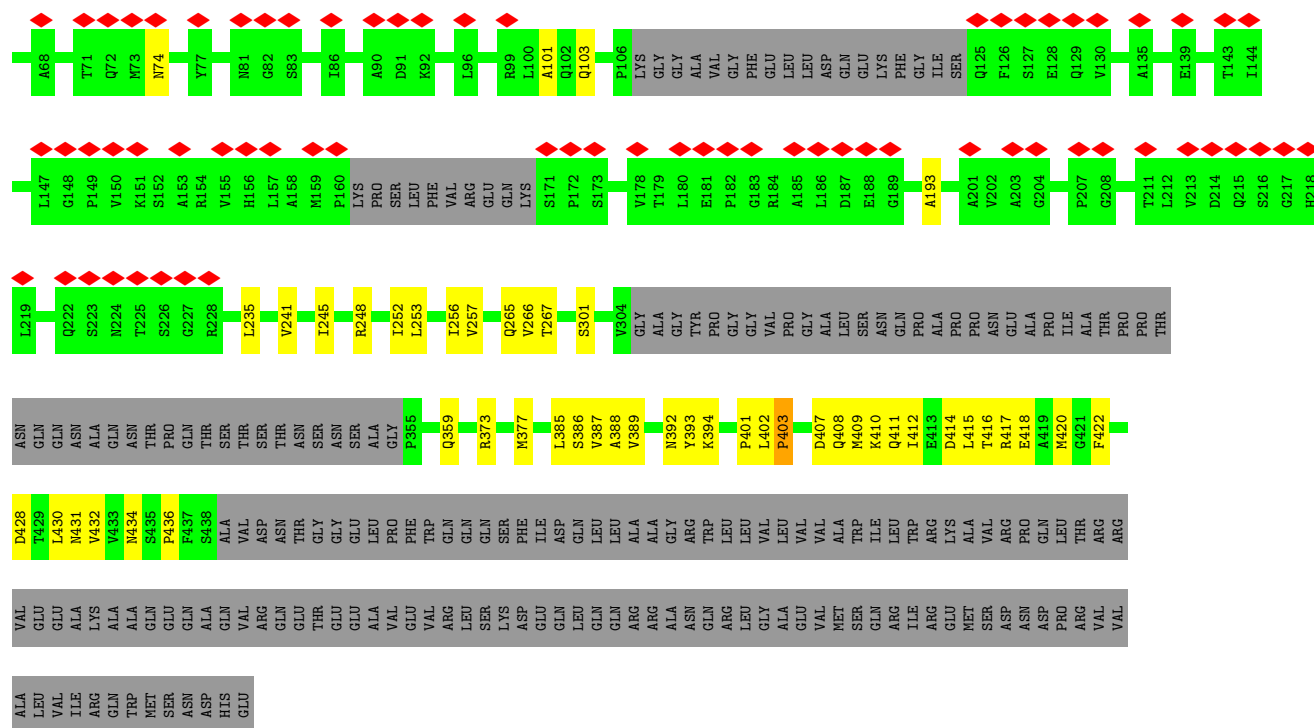
- Molecule 1: Flagellar M-ring protein



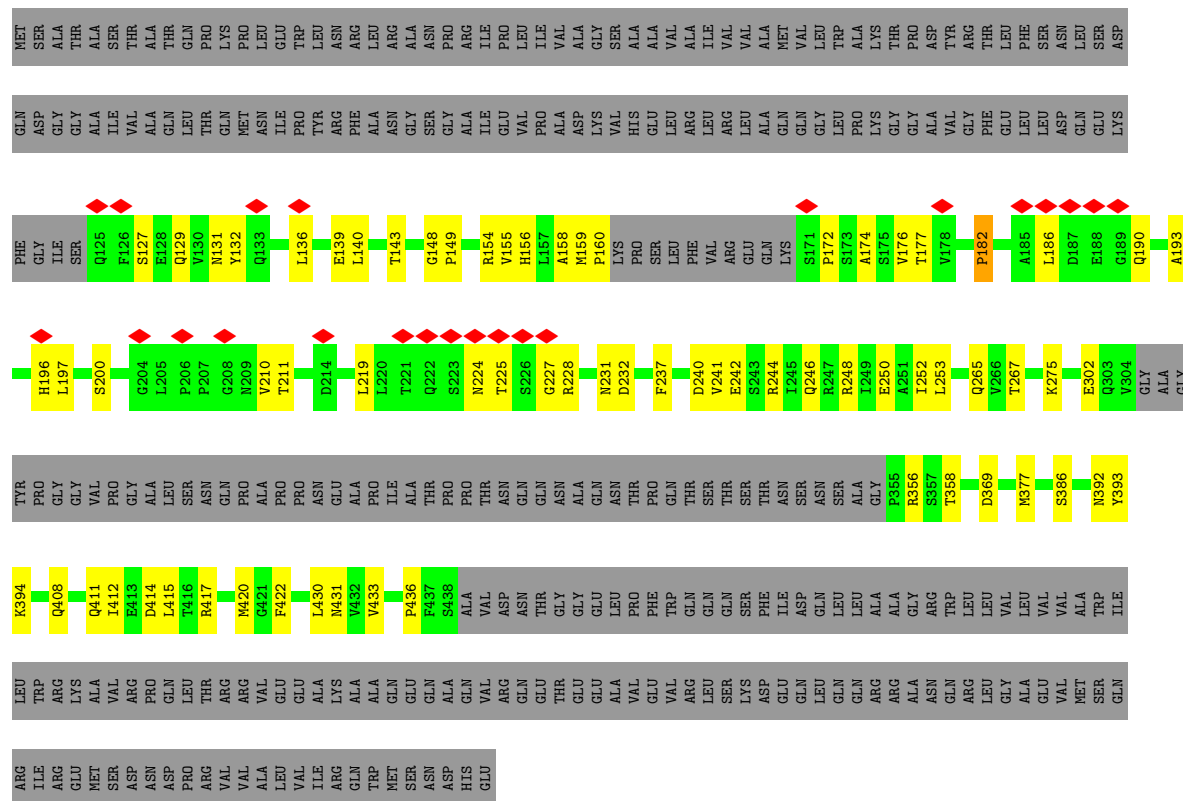
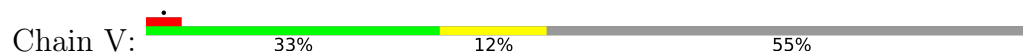




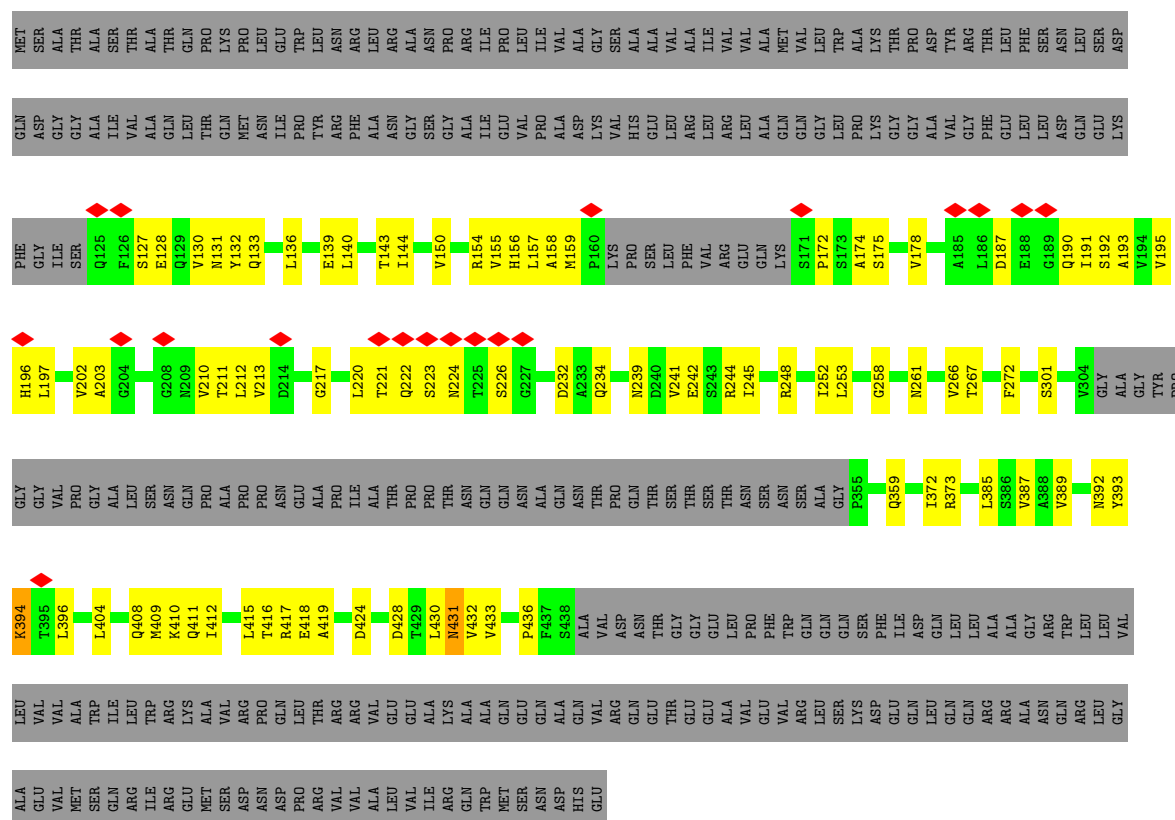
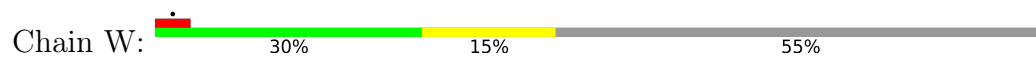




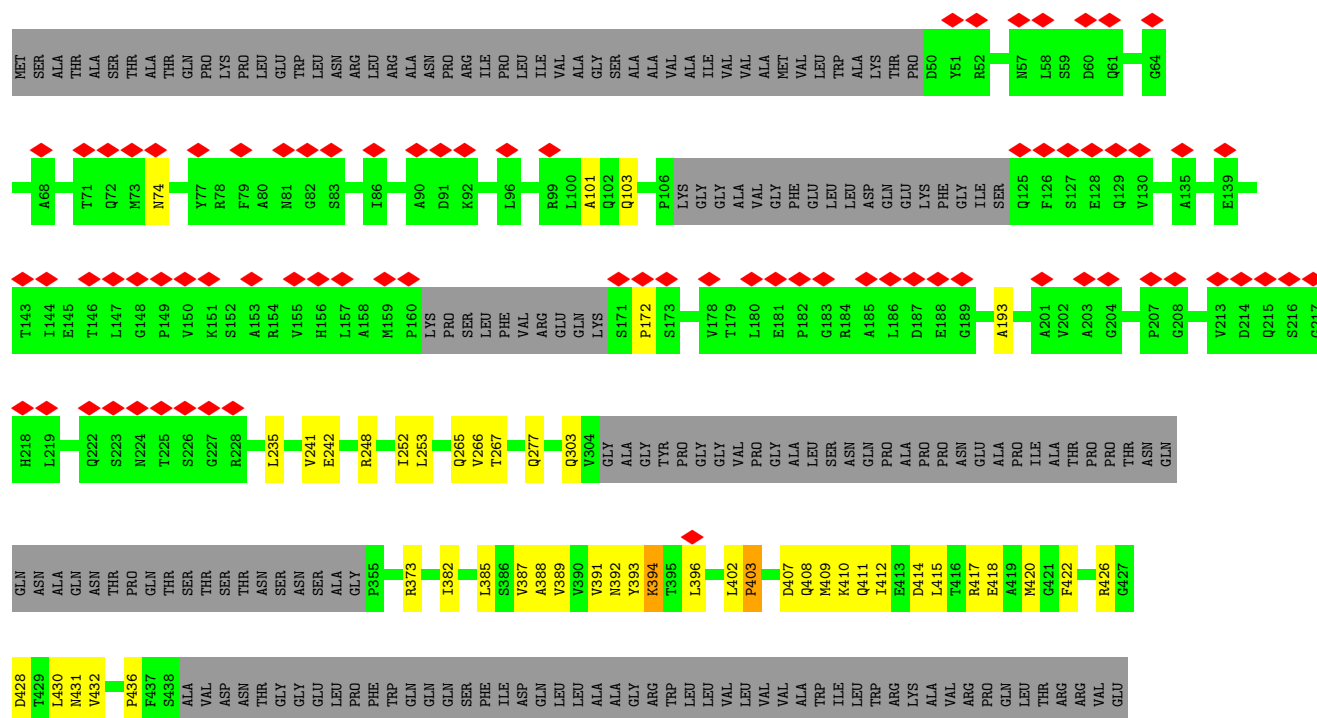
• Molecule 1: Flagellar M-ring protein



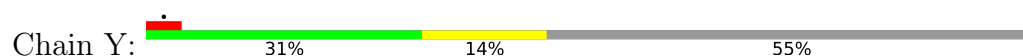
• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein

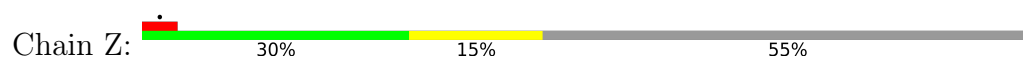
[illegible][illegible][illegible][illegible]

V391	N392	K393	T394	T395	L402	Q408	M409	M410	Q411	D414	L415	E418	A419	M420	R426	Q427	D428	T429	L430	M431	V432	V433	M434	S435	P436	F437	S438	ALA	VAL	ASP	ASN	THR	GLY	GLY	GLU	LEU	PRO	PHE	TRP	THR	GLN	GLN	GLN	SER	PHE	ILE	ASP	CLN	LEU	ALA	ALA	GLY	PRO
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TRP	LEU	LEU	VAL	VAL	TRP	ILE	LEU	TRP	ARG	LYS	ALA	VAL	ARG	PRO	LEU	THR	ARG	VAL	GLU	GLU	ALA	LYS	ALA	GLN	GLU	GLN	ALA	GLN	VAL	ARG	GLN	GLU	THR	GLU	GLU	ALA	VAL	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	GLN	ARG	ARG	ASN
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GLN	ARG	LEU	GLY	ALA	GLU	VAL	MET	SER	GLN	ARG	ILE	ARG	GLU	MET	SER	ASP	ASN	ASP	PRO	ARG	VAL	VAL	ALA	LEU	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU
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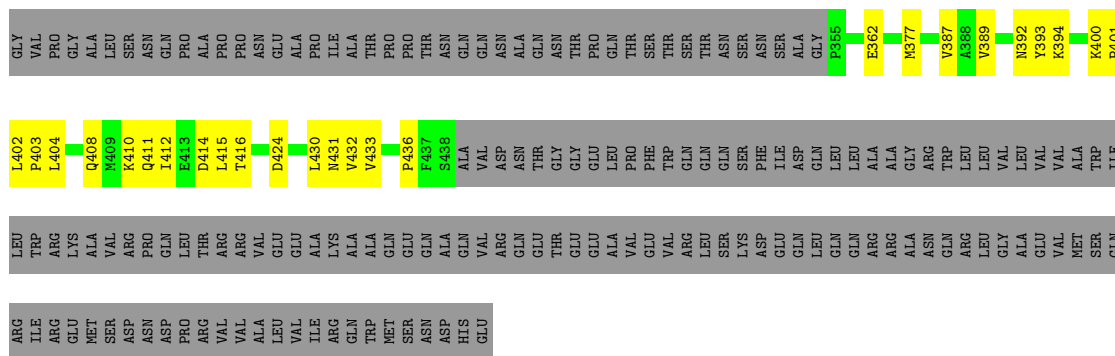
- Molecule 1: Flagellar M-ring protein

[illegible]

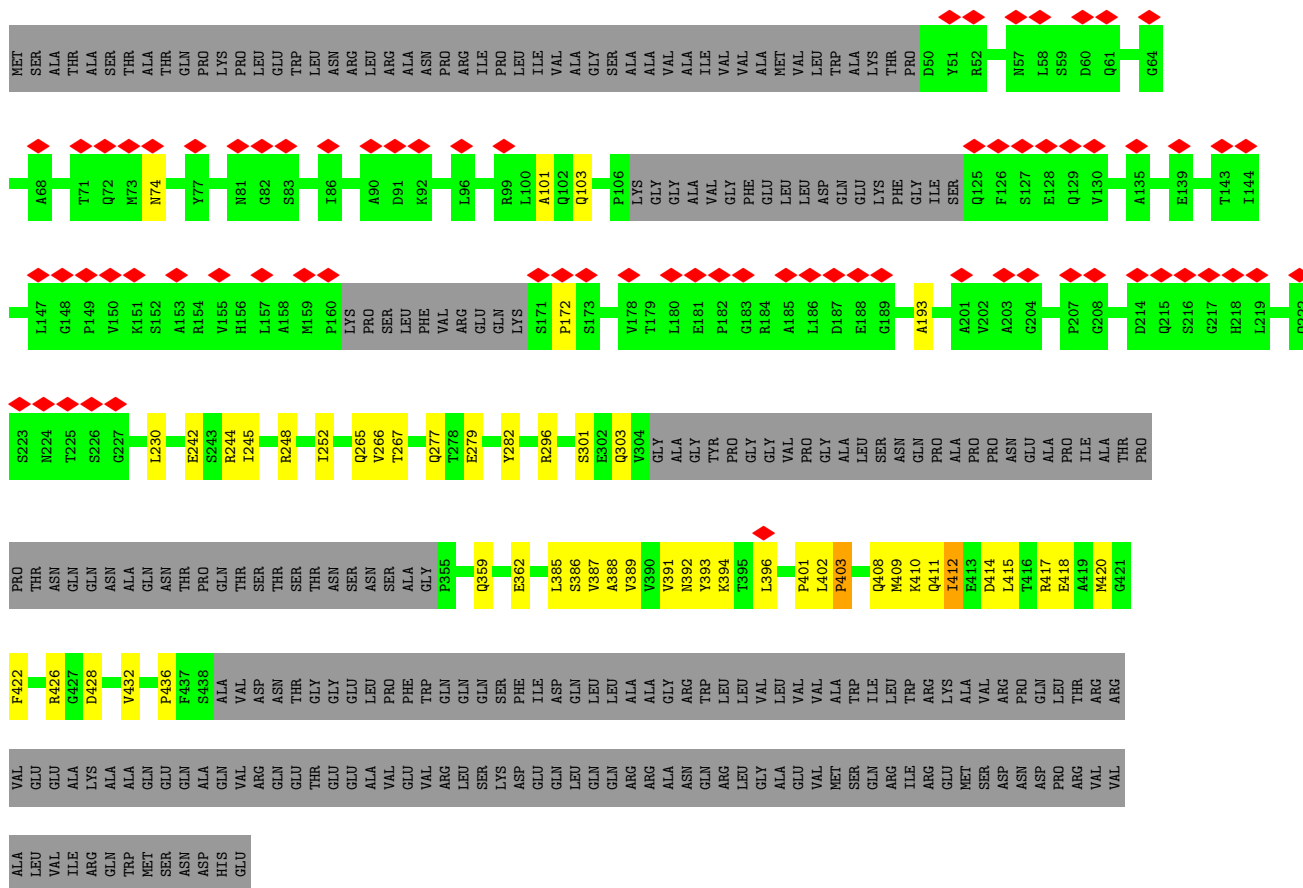
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PHE
 GLY
 ILE
 SER
 Q125
 F126
 E127
 S128
 Q129
 V130
 M131
 Y132
 Q133
 L136
 E139
 L140
 T143
 I144
 F145
 T146
 V150
 R154
 V155
 H156
 L157
 M158
 M159
 F160
 LYS
 PRO
 PRO
 SER
 SER
 LEU
 LEU
 PHE
 PHE
 VAL
 ARG
 GLN
 GLU
 GLN
 LYS
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 V194

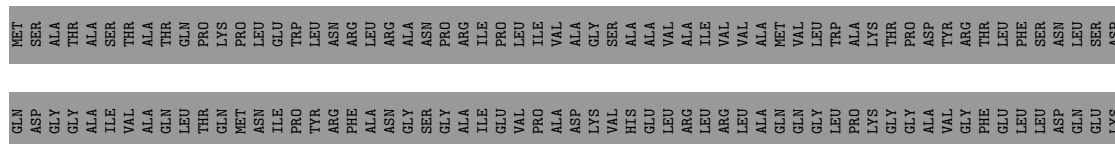
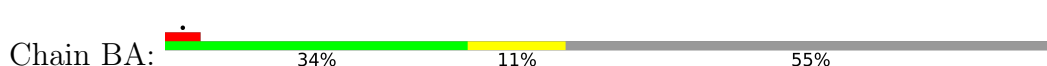
V195	L197	H196	A203	G204	G208	H209	T210	T211	T212	V213	D214	G217	H218	L219	L220	T221	Q222	Q223	N224	T225	S226	G227	L230	N231	D232	L236	V241	E242	S243	R244	T245	R248	L249	L252	V266	T267	K275	T292	R296	V304	GLY	ALA	GLY	TYR	PRO
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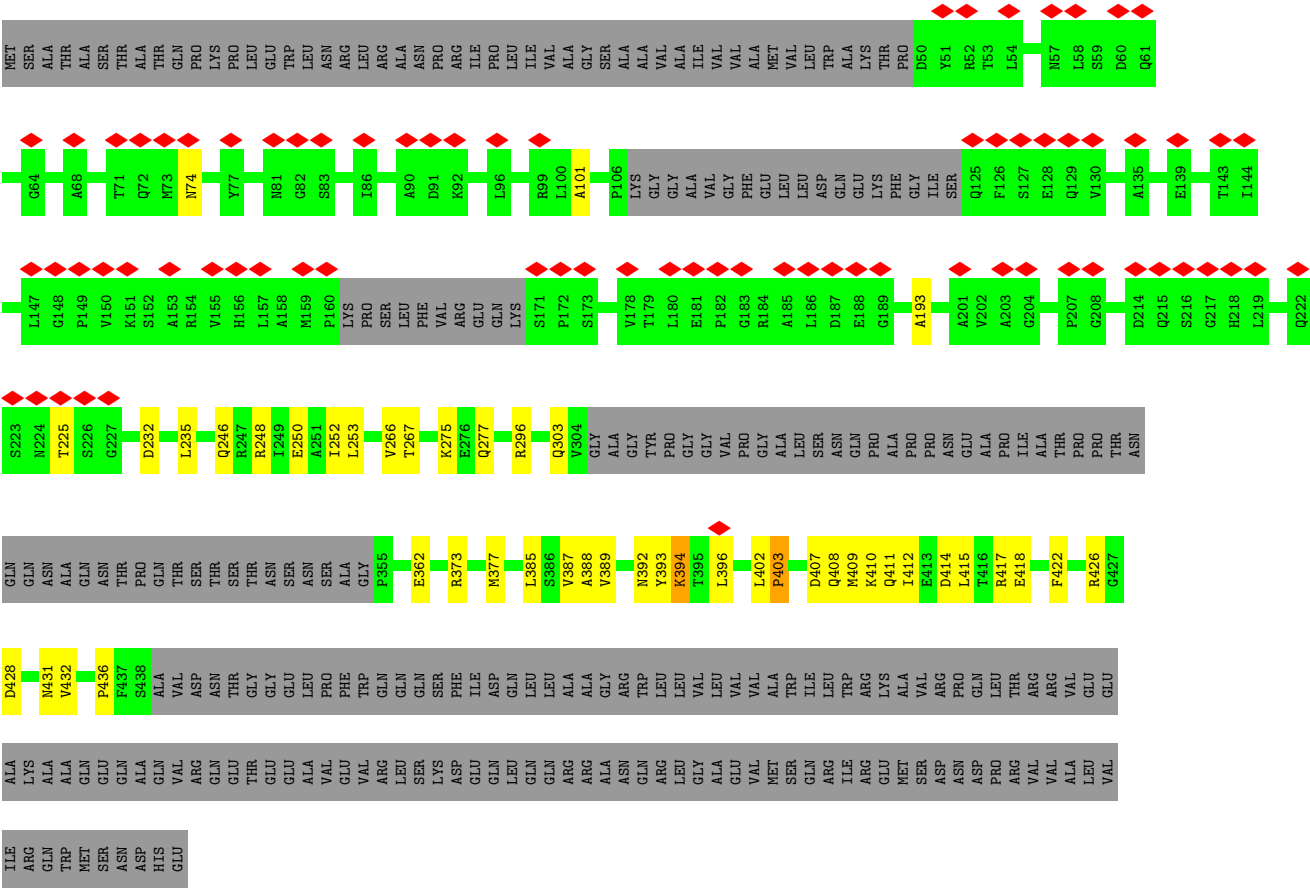
- Molecule 1: Flagellar M-ring protein



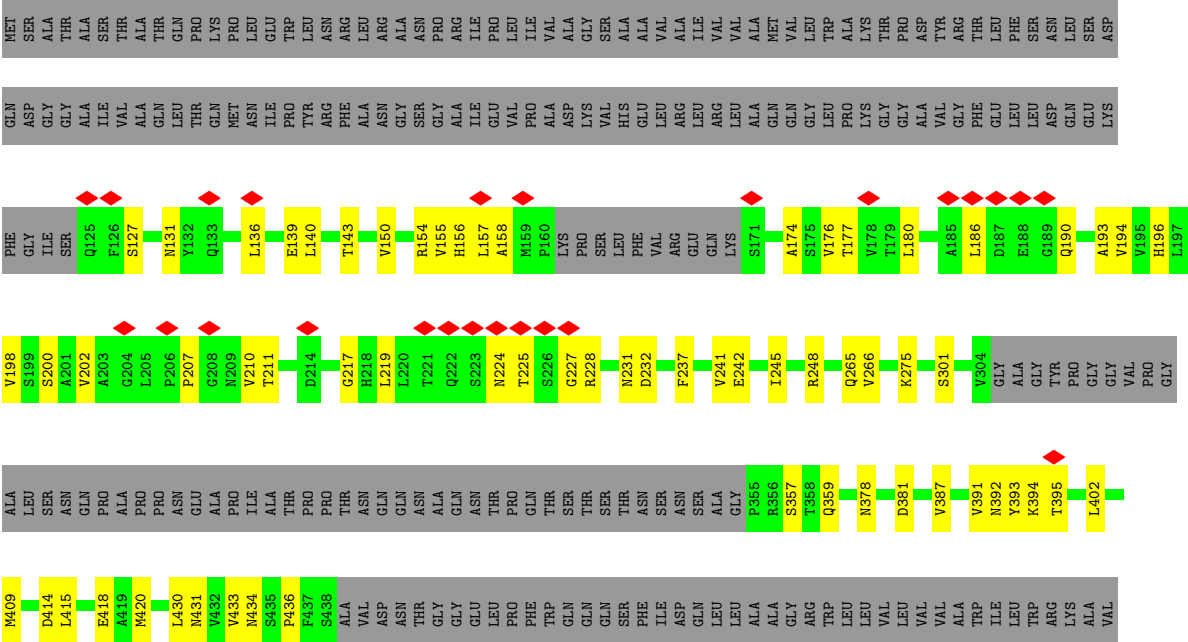
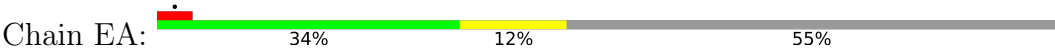
- Molecule 1: Flagellar M-ring protein







• Molecule 1: Flagellar M-ring protein



[illegible]

Chain FA:

[illegible]

H196	H197	A203	A202	G204	G208	N209	T211	D214	G217	L220	T221	Q222	S223	N224	T225	S226	G227	D232	A233	Q234	L235	K236	N239	D240	V241	E242	S243	R244	I245	L248	R249	I252	T256	T257	F272	K275	R296	V304	GLY	ALA	GLY	TYR	PRO	TYR						
PRE	GLY	ILE	SER	Q125	S127	E128	Q129	V130	N131	Y132	L136	E139	L140	T143	I144	E145	T146	V150	R154	V155	H156	L157	A158	M159	P160	LYS	PRO	SER	LEU	PHE	VAL	ARG	GLU	GLN	LYS	S171	A174	S175	V178	A185	L186	D187	E188	G189	Q190	I191	S192	A193	V194	V195

	GLY	VAL	PRO	GLY	ALA	LEU	SER	ASN	GLN	PRO	ALA	ALA	PRO	PRO	ASN	GLY	ALA	ALA	PRO	PRO	THR	THR	ASN	GLN	GLN	ASN	GLN	ALA	ALA	GLN	GLN	THR	THR	THR	SER	SER	ASN	ASN	GLY	P365	E362	M377	L385	V387	A388	V389	V391	N392	V393	T394
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T395	L396	L402	L403	L404	Q408	Q409	Q410	Q411	Q412	E413	D414	D415	T416	T417	E418	A419	Q420	Q421	Q422	Q423	S423	D424	D428	T429	L430	M431	V432	V433	M434	S435	S436	F437	S438	ALA	VAL	ASP	ASN	THR	THR	GLY	GLY	GLY	LEU	PRO	PRO	PHE	TRP	GLN	GLN	GLN	GLN	ASP	LEU	LEU	ALA	ALA
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[illegible]

Chain GA:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C33	Depositor
Number of particles used	16411	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.557	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.981	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	1046.784, 1046.784, 1046.784	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.363, 1.363, 1.363	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/1969	0.42	0/2668
1	AA	0.20	0/2017	0.47	1/2748 (0.0%)
1	B	0.25	1/2017 (0.0%)	0.56	1/2748 (0.0%)
1	BA	0.15	0/1969	0.41	1/2668 (0.0%)
1	C	0.16	0/1969	0.43	2/2668 (0.1%)
1	CA	0.18	0/1969	0.47	0/2668
1	D	0.15	0/1969	0.42	0/2668
1	DA	0.16	0/2017	0.43	0/2748
1	E	0.17	0/2017	0.45	0/2748
1	EA	0.16	0/1969	0.42	1/2668 (0.0%)
1	F	0.16	0/1969	0.42	0/2668
1	FA	0.16	0/1969	0.43	0/2668
1	G	0.16	0/1969	0.42	0/2668
1	GA	0.16	0/2017	0.43	0/2748
1	H	0.16	0/2017	0.45	0/2748
1	HA	0.17	0/1969	0.45	2/2668 (0.1%)
1	I	0.18	0/1969	0.45	4/2668 (0.1%)
1	J	0.17	0/1969	0.44	0/2668
1	K	0.25	1/2017 (0.0%)	0.55	1/2748 (0.0%)
1	L	0.18	0/1969	0.45	2/2668 (0.1%)
1	M	0.17	0/1969	0.46	0/2668
1	N	0.16	0/2017	0.44	0/2748
1	O	0.17	0/1969	0.46	2/2668 (0.1%)
1	P	0.16	0/1969	0.44	0/2668
1	Q	0.16	0/2017	0.43	0/2748
1	R	0.14	0/1969	0.39	0/2668
1	S	0.16	0/1969	0.44	0/2668
1	T	0.17	0/2017	0.45	0/2748
1	V	0.48	2/1969 (0.1%)	0.66	5/2668 (0.2%)
1	W	0.15	0/1969	0.42	0/2668
1	X	0.23	1/2017 (0.0%)	0.53	1/2748 (0.0%)
1	Y	0.15	0/1969	0.39	0/2668
1	Z	0.15	0/1969	0.42	0/2668
All	All	0.19	5/65505 (0.0%)	0.46	23/88924 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	182	PRO	CG-CD	-18.26	0.88	1.50
1	K	172	PRO	CA-CB	-8.08	1.42	1.53
1	B	172	PRO	CA-CB	-8.07	1.42	1.53
1	V	182	PRO	N-CD	7.30	1.57	1.47
1	X	172	PRO	CA-CB	-5.75	1.45	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	182	PRO	N-CD-CG	-19.71	73.63	103.20
1	B	172	PRO	N-CA-CB	-16.49	85.93	103.25
1	K	172	PRO	N-CA-CB	-16.43	85.99	103.25
1	X	172	PRO	N-CA-CB	-15.82	86.64	103.25
1	V	182	PRO	CA-CB-CG	-11.27	83.09	104.50
1	V	182	PRO	CA-N-CD	-9.35	98.90	112.00
1	HA	207	PRO	CA-N-CD	-8.75	99.75	112.00
1	EA	207	PRO	CA-N-CD	-7.99	100.82	112.00
1	O	207	PRO	CA-N-CD	-7.87	100.98	112.00
1	L	207	PRO	CA-N-CD	-7.85	101.01	112.00
1	AA	172	PRO	N-CA-CB	-7.66	93.44	102.86
1	I	172	PRO	CA-N-CD	-6.68	102.64	112.00
1	C	182	PRO	CA-N-CD	-6.48	102.93	112.00
1	I	182	PRO	CA-N-CD	-6.46	102.96	112.00
1	L	182	PRO	CA-N-CD	-6.15	103.39	112.00
1	HA	182	PRO	CA-N-CD	-6.14	103.40	112.00
1	BA	182	PRO	CA-N-CD	-6.09	103.47	112.00
1	V	182	PRO	CB-CG-CD	6.07	125.51	106.10
1	C	182	PRO	N-CD-CG	-5.96	94.26	103.20
1	I	172	PRO	N-CD-CG	-5.74	94.60	103.20
1	I	182	PRO	N-CD-CG	-5.67	94.69	103.20
1	O	182	PRO	CA-N-CD	-5.55	104.22	112.00
1	V	182	PRO	N-CA-CB	-5.25	97.73	103.25

There are no chirality outliers.

There are no planarity outliers.

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	1945	0	1931	79	0
1	AA	2005	0	1599	36	0
1	B	2005	0	1599	36	0
1	BA	1945	0	1931	62	0
1	C	1945	0	1931	61	0
1	CA	1945	0	1931	91	0
1	D	1945	0	1931	77	0
1	DA	2005	0	1599	40	0
1	E	2005	0	1599	37	0
1	EA	1945	0	1931	62	0
1	F	1945	0	1931	75	0
1	FA	1945	0	1931	85	0
1	G	1945	0	1931	75	0
1	GA	2005	0	1599	39	0
1	H	2005	0	1599	37	0
1	HA	1945	0	1931	68	0
1	I	1945	0	1931	71	0
1	J	1945	0	1931	83	0
1	K	2005	0	1599	40	0
1	L	1945	0	1931	65	0
1	M	1945	0	1931	82	0
1	N	2005	0	1599	33	0
1	O	1945	0	1931	62	0
1	P	1945	0	1931	90	0
1	Q	2005	0	1599	39	0
1	R	1945	0	1931	63	0
1	S	1945	0	1931	81	0
1	T	2005	0	1599	38	0
1	V	1945	0	1931	74	0
1	W	1945	0	1931	80	0
1	X	2005	0	1599	39	0
1	Y	1945	0	1931	72	0
1	Z	1945	0	1931	76	0
All	All	64845	0	60071	1608	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 13.

All (1608) 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:FA:191:ILE:HG13	1:FA:220:LEU:HB3	1.57	0.87
1:R:228:ARG:HD3	1:R:231:ASN:HD21	1.38	0.85
1:CA:219:LEU:HD21	1:HA:193:ALA:HA	1.59	0.82
1:CA:191:ILE:HG13	1:CA:220:LEU:HB3	1.65	0.79
1:A:191:ILE:HG13	1:A:220:LEU:HB3	1.66	0.77
1:D:244:ARG:HH12	1:E:235:LEU:HB3	1.50	0.76
1:G:394:LYS:HG2	1:G:395:THR:H	1.50	0.75
1:B:409:MET:HA	1:B:412:ILE:HD12	1.66	0.75
1:A:415:LEU:HD13	1:B:388:ALA:HB1	1.67	0.74
1:P:219:LEU:HD13	1:V:193:ALA:HA	1.69	0.74
1:G:415:LEU:HD13	1:H:388:ALA:HB1	1.70	0.74
1:P:221:THR:O	1:P:224:ASN:ND2	2.20	0.74
1:H:408:GLN:O	1:H:412:ILE:HD12	1.88	0.74
1:S:221:THR:O	1:S:224:ASN:ND2	2.21	0.73
1:CA:415:LEU:HD13	1:DA:388:ALA:HB1	1.71	0.73
1:HA:196:HIS:O	1:HA:196:HIS:ND1	2.22	0.72
1:S:415:LEU:HD13	1:T:388:ALA:HB1	1.72	0.72
1:Z:191:ILE:HG23	1:Z:212:LEU:HD22	1.72	0.72
1:CA:157:LEU:HD21	1:CA:159:MET:HG2	1.71	0.72
1:P:415:LEU:HD13	1:Q:388:ALA:HB1	1.71	0.72
1:Z:191:ILE:HG13	1:Z:220:LEU:HB3	1.70	0.72
1:B:387:VAL:HB	1:B:420:MET:HE2	1.70	0.71
1:M:415:LEU:HD13	1:N:388:ALA:HB1	1.73	0.71
1:AA:248:ARG:NH2	1:BA:242:GLU:OE1	2.23	0.71
1:D:415:LEU:HD13	1:E:388:ALA:HB1	1.71	0.71
1:J:221:THR:OG1	1:J:224:ASN:ND2	2.23	0.71
1:K:248:ARG:NH2	1:L:242:GLU:OE1	2.23	0.71
1:J:221:THR:O	1:J:224:ASN:ND2	2.24	0.71
1:M:191:ILE:HG13	1:M:220:LEU:HB3	1.72	0.71
1:G:221:THR:O	1:G:224:ASN:ND2	2.23	0.70
1:A:217:GLY:HA3	1:F:190:GLN:HG3	1.72	0.70
1:D:221:THR:O	1:D:224:ASN:ND2	2.24	0.70
1:M:191:ILE:HG23	1:M:212:LEU:HD22	1.73	0.70
1:Z:415:LEU:HD13	1:AA:388:ALA:HB1	1.73	0.70
1:B:420:MET:HE1	1:B:430:LEU:HB2	1.73	0.70
1:G:221:THR:OG1	1:G:224:ASN:ND2	2.24	0.70
1:J:408:GLN:O	1:J:412:ILE:HD12	1.92	0.69
1:A:238:ALA:O	1:A:242:GLU:HG3	1.93	0.69
1:O:391:VAL:HG21	1:O:409:MET:HE1	1.74	0.69
1:P:221:THR:OG1	1:P:224:ASN:ND2	2.24	0.69
1:W:157:LEU:HD21	1:W:159:MET:HG2	1.74	0.69
1:W:415:LEU:HD13	1:X:388:ALA:HB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:144:ILE:HD11	1:HA:197:LEU:HD22	1.74	0.69
1:CA:191:ILE:HG23	1:CA:212:LEU:HD22	1.75	0.68
1:A:191:ILE:HG23	1:A:212:LEU:HD22	1.76	0.68
1:V:408:GLN:O	1:V:412:ILE:HD12	1.93	0.68
1:R:225:THR:HG22	1:R:227:GLY:H	1.59	0.68
1:H:248:ARG:NH2	1:I:242:GLU:OE1	2.26	0.68
1:O:408:GLN:O	1:O:412:ILE:HG13	1.93	0.68
1:FA:391:VAL:HG21	1:FA:409:MET:HE1	1.75	0.68
1:S:221:THR:OG1	1:S:224:ASN:ND2	2.26	0.68
1:Q:248:ARG:NH2	1:R:242:GLU:OE1	2.27	0.67
1:M:408:GLN:O	1:M:412:ILE:HD12	1.94	0.67
1:J:415:LEU:HD13	1:K:388:ALA:HB1	1.75	0.67
1:L:144:ILE:HD11	1:L:197:LEU:HD22	1.74	0.67
1:J:191:ILE:HG23	1:J:212:LEU:HD22	1.76	0.67
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	1.77	0.67
1:R:144:ILE:HD11	1:R:197:LEU:HD22	1.74	0.67
1:S:219:LEU:HD13	1:Y:193:ALA:HA	1.76	0.67
1:T:409:MET:HA	1:T:412:ILE:HD12	1.74	0.67
1:Y:225:THR:HG22	1:Y:227:GLY:H	1.59	0.67
1:G:394:LYS:CG	1:G:395:THR:H	2.07	0.67
1:W:221:THR:O	1:W:224:ASN:ND2	2.27	0.67
1:S:191:ILE:HG23	1:S:212:LEU:HD22	1.76	0.67
1:W:175:SER:HB3	1:BA:197:LEU:HD12	1.75	0.67
1:Z:217:GLY:HA3	1:EA:190:GLN:HG3	1.76	0.67
1:T:409:MET:HE1	1:T:434:ASN:HB2	1.76	0.67
1:I:391:VAL:HG21	1:I:409:MET:HE1	1.76	0.67
1:J:175:SER:HB3	1:O:197:LEU:HD12	1.75	0.67
1:CA:408:GLN:O	1:CA:412:ILE:HD12	1.93	0.67
1:GA:248:ARG:NH2	1:HA:242:GLU:OE1	2.27	0.67
1:G:174:ALA:HB3	1:G:210:VAL:HG22	1.77	0.67
1:L:241:VAL:O	1:L:245:ILE:HD12	1.94	0.67
1:Z:221:THR:O	1:Z:224:ASN:ND2	2.28	0.66
1:GA:408:GLN:O	1:GA:412:ILE:HD12	1.94	0.66
1:GA:409:MET:HE1	1:GA:434:ASN:HB2	1.77	0.66
1:M:242:GLU:OE2	1:R:248:ARG:NH2	2.29	0.66
1:P:175:SER:HB3	1:V:197:LEU:HD12	1.77	0.66
1:N:373:ARG:HH21	1:O:275:LYS:HE2	1.59	0.66
1:DA:248:ARG:NH2	1:EA:242:GLU:OE1	2.28	0.66
1:G:244:ARG:HH21	1:G:248:ARG:HH21	1.44	0.66
1:FA:221:THR:OG1	1:FA:224:ASN:ND2	2.25	0.66
1:HA:225:THR:HG22	1:HA:227:GLY:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:296:ARG:NH2	1:K:362:GLU:OE2	2.29	0.65
1:W:221:THR:OG1	1:W:224:ASN:ND2	2.29	0.65
1:N:248:ARG:NH2	1:O:242:GLU:OE1	2.29	0.65
1:FA:244:ARG:HH12	1:GA:235:LEU:HB3	1.61	0.65
1:W:242:GLU:OE2	1:BA:248:ARG:NH2	2.29	0.65
1:E:296:ARG:NH2	1:E:362:GLU:OE2	2.29	0.65
1:J:242:GLU:OE2	1:O:248:ARG:NH2	2.29	0.65
1:W:191:ILE:HG13	1:W:220:LEU:HB3	1.79	0.65
1:B:248:ARG:NH2	1:C:242:GLU:OE1	2.30	0.65
1:T:103:GLN:HA	1:V:182:PRO:HB3	1.79	0.65
1:Y:241:VAL:O	1:Y:245:ILE:HD12	1.97	0.64
1:DA:296:ARG:NH2	1:DA:362:GLU:OE2	2.29	0.64
1:Q:391:VAL:HG21	1:Q:409:MET:HE1	1.78	0.64
1:S:242:GLU:OE1	1:Y:248:ARG:NH2	2.30	0.64
1:Z:408:GLN:O	1:Z:412:ILE:HD12	1.98	0.64
1:B:400:LYS:NZ	1:B:401:PRO:O	2.29	0.64
1:F:391:VAL:O	1:F:434:ASN:ND2	2.31	0.64
1:H:391:VAL:HG21	1:H:409:MET:HE1	1.79	0.64
1:P:191:ILE:HG23	1:P:212:LEU:HD22	1.78	0.64
1:BA:391:VAL:HG21	1:BA:409:MET:HE1	1.77	0.64
1:C:248:ARG:NH2	1:FA:242:GLU:OE1	2.31	0.64
1:D:191:ILE:HG13	1:D:220:LEU:HB3	1.78	0.64
1:P:418:GLU:HG3	1:Q:431:ASN:HB2	1.80	0.64
1:CA:394:LYS:HD3	1:CA:396:LEU:H	1.63	0.64
1:G:223:SER:O	1:G:226:SER:OG	2.16	0.64
1:D:242:GLU:OE1	1:I:248:ARG:NH2	2.31	0.64
1:A:223:SER:O	1:A:226:SER:OG	2.16	0.63
1:I:127:SER:O	1:I:131:ASN:ND2	2.32	0.63
1:FA:223:SER:O	1:FA:226:SER:OG	2.15	0.63
1:C:127:SER:O	1:C:131:ASN:ND2	2.32	0.63
1:G:191:ILE:HG13	1:G:220:LEU:HB3	1.81	0.63
1:BA:225:THR:HG22	1:BA:227:GLY:H	1.63	0.63
1:HA:127:SER:O	1:HA:131:ASN:ND2	2.32	0.63
1:D:221:THR:OG1	1:D:224:ASN:ND2	2.30	0.63
1:Z:248:ARG:NH2	1:AA:242:GLU:OE1	2.31	0.63
1:A:174:ALA:HB3	1:A:210:VAL:HG22	1.81	0.63
1:E:375:THR:HG23	1:F:275:LYS:HG2	1.81	0.63
1:BA:127:SER:O	1:BA:131:ASN:ND2	2.32	0.63
1:GA:266:VAL:HG22	1:GA:387:VAL:HG22	1.80	0.63
1:N:103:GLN:HA	1:O:182:PRO:HB3	1.79	0.63
1:Z:221:THR:OG1	1:Z:224:ASN:ND2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:266:VAL:HG22	1:DA:387:VAL:HG22	1.81	0.63
1:F:127:SER:O	1:F:131:ASN:ND2	2.32	0.62
1:J:223:SER:O	1:J:226:SER:OG	2.17	0.62
1:K:408:GLN:O	1:K:412:ILE:HG12	1.99	0.62
1:X:373:ARG:HH21	1:Y:275:LYS:HE2	1.64	0.62
1:EA:127:SER:O	1:EA:131:ASN:ND2	2.32	0.62
1:F:151:LYS:HZ3	1:F:179:THR:HG22	1.63	0.62
1:T:373:ARG:HH21	1:V:275:LYS:HE2	1.65	0.62
1:B:400:LYS:HD2	1:B:401:PRO:HD2	1.81	0.62
1:L:127:SER:O	1:L:131:ASN:ND2	2.32	0.62
1:Y:127:SER:O	1:Y:131:ASN:ND2	2.32	0.62
1:Q:408:GLN:O	1:Q:412:ILE:HD12	1.99	0.62
1:CA:244:ARG:HH22	1:DA:235:LEU:HB3	1.64	0.62
1:F:151:LYS:NZ	1:F:180:LEU:O	2.32	0.62
1:O:127:SER:O	1:O:131:ASN:ND2	2.32	0.62
1:R:127:SER:O	1:R:131:ASN:ND2	2.32	0.62
1:P:174:ALA:HB3	1:P:210:VAL:HG22	1.81	0.62
1:T:248:ARG:NH2	1:V:242:GLU:OE1	2.31	0.62
1:T:266:VAL:HG22	1:T:387:VAL:HG22	1.81	0.62
1:Y:391:VAL:O	1:Y:434:ASN:ND2	2.32	0.62
1:Y:395:THR:OG1	1:Y:402:LEU:O	2.15	0.62
1:CA:174:ALA:HB3	1:CA:210:VAL:HG22	1.81	0.62
1:V:139:GLU:O	1:V:143:THR:HG23	2.00	0.62
1:Z:223:SER:O	1:Z:226:SER:OG	2.18	0.62
1:AA:266:VAL:HG22	1:AA:387:VAL:HG22	1.81	0.62
1:AA:296:ARG:NH2	1:AA:362:GLU:OE2	2.31	0.62
1:O:174:ALA:HB3	1:O:210:VAL:HG22	1.80	0.62
1:E:244:ARG:NH1	1:F:242:GLU:OE1	2.29	0.62
1:S:409:MET:HA	1:S:412:ILE:HD12	1.79	0.62
1:S:394:LYS:HD3	1:S:396:LEU:H	1.65	0.61
1:V:127:SER:O	1:V:131:ASN:ND2	2.32	0.61
1:W:394:LYS:HD3	1:W:396:LEU:H	1.65	0.61
1:O:266:VAL:HG22	1:O:387:VAL:HG22	1.80	0.61
1:G:400:LYS:NZ	1:G:401:PRO:O	2.34	0.61
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.83	0.61
1:Z:242:GLU:OE1	1:EA:248:ARG:NH2	2.32	0.61
1:M:400:LYS:HD2	1:M:401:PRO:HD2	1.82	0.61
1:O:225:THR:HG22	1:O:227:GLY:H	1.66	0.61
1:FA:408:GLN:O	1:FA:412:ILE:HD12	2.00	0.61
1:E:266:VAL:HG22	1:E:387:VAL:HG22	1.81	0.61
1:X:409:MET:HA	1:X:412:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:400:LYS:HD2	1:G:401:PRO:HD2	1.83	0.61
1:A:242:GLU:OE2	1:F:248:ARG:NH2	2.34	0.61
1:G:242:GLU:OE1	1:L:248:ARG:NH2	2.33	0.61
1:S:133:GLN:HG3	1:S:157:LEU:HD22	1.83	0.61
1:FA:415:LEU:HD13	1:GA:388:ALA:HB1	1.83	0.61
1:O:139:GLU:O	1:O:143:THR:HG23	2.01	0.60
1:P:223:SER:O	1:P:226:SER:OG	2.18	0.60
1:O:301:SER:HB3	1:O:359:GLN:HB2	1.83	0.60
1:P:242:GLU:OE2	1:V:248:ARG:NH2	2.34	0.60
1:HA:186:LEU:HB3	1:HA:190:GLN:HB3	1.84	0.60
1:G:219:LEU:HG	1:L:193:ALA:HA	1.83	0.60
1:I:139:GLU:O	1:I:143:THR:HG23	2.01	0.60
1:A:248:ARG:NH2	1:B:242:GLU:OE2	2.33	0.60
1:B:266:VAL:HG22	1:B:387:VAL:HG22	1.84	0.60
1:D:418:GLU:HG3	1:E:431:ASN:HB2	1.83	0.60
1:BA:139:GLU:O	1:BA:143:THR:HG23	2.02	0.60
1:D:248:ARG:NH2	1:E:242:GLU:OE2	2.34	0.60
1:M:223:SER:O	1:M:226:SER:OG	2.20	0.60
1:P:213:VAL:HG21	1:V:197:LEU:HD22	1.82	0.60
1:D:433:VAL:HG21	1:I:415:LEU:HD11	1.82	0.60
1:K:303:GLN:HG2	1:L:357:SER:HB2	1.84	0.60
1:S:433:VAL:HG21	1:Y:415:LEU:HD11	1.84	0.60
1:CA:242:GLU:OE2	1:HA:248:ARG:NH2	2.34	0.60
1:J:127:SER:O	1:J:131:ASN:ND2	2.35	0.59
1:J:174:ALA:HB3	1:J:210:VAL:HG22	1.83	0.59
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.84	0.59
1:DA:409:MET:HE3	1:DA:409:MET:HA	1.84	0.59
1:EA:139:GLU:O	1:EA:143:THR:HG23	2.01	0.59
1:FA:409:MET:HE3	1:FA:409:MET:HA	1.84	0.59
1:A:400:LYS:HD2	1:A:401:PRO:HD2	1.83	0.59
1:R:139:GLU:O	1:R:143:THR:HG23	2.02	0.59
1:Y:139:GLU:O	1:Y:143:THR:HG23	2.01	0.59
1:A:418:GLU:HG3	1:B:431:ASN:HB2	1.83	0.59
1:F:139:GLU:O	1:F:143:THR:HG23	2.01	0.59
1:I:225:THR:HG22	1:I:227:GLY:H	1.67	0.59
1:K:103:GLN:HA	1:L:182:PRO:HB3	1.84	0.59
1:S:139:GLU:O	1:S:143:THR:HG23	2.01	0.59
1:S:159:MET:HE3	1:S:202:VAL:HG21	1.84	0.59
1:FA:394:LYS:HD3	1:FA:396:LEU:H	1.67	0.59
1:N:266:VAL:HG22	1:N:387:VAL:HG22	1.83	0.59
1:S:127:SER:O	1:S:131:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:193:ALA:HA	1:Y:219:LEU:HD13	1.84	0.59
1:C:139:GLU:O	1:C:143:THR:HG23	2.01	0.59
1:L:225:THR:HG22	1:L:227:GLY:H	1.68	0.59
1:L:395:THR:OG1	1:L:402:LEU:O	2.19	0.59
1:W:409:MET:HA	1:W:412:ILE:HD12	1.85	0.59
1:X:248:ARG:NH2	1:Y:242:GLU:OE2	2.34	0.59
1:R:186:LEU:HD23	1:R:190:GLN:HG2	1.85	0.59
1:W:127:SER:O	1:W:131:ASN:ND2	2.36	0.59
1:C:225:THR:HG22	1:C:227:GLY:H	1.68	0.59
1:L:139:GLU:O	1:L:143:THR:HG23	2.02	0.59
1:S:223:SER:O	1:S:226:SER:OG	2.19	0.59
1:AA:103:GLN:HA	1:BA:182:PRO:HB3	1.84	0.59
1:C:186:LEU:HD23	1:C:190:GLN:HG2	1.84	0.59
1:P:156:HIS:CE1	1:V:143:THR:HG21	2.38	0.59
1:R:186:LEU:HB3	1:R:190:GLN:HB3	1.85	0.59
1:C:186:LEU:HB3	1:C:190:GLN:HB3	1.85	0.59
1:P:140:LEU:O	1:P:144:ILE:HG12	2.03	0.59
1:Z:140:LEU:O	1:Z:144:ILE:HG12	2.03	0.59
1:CA:139:GLU:O	1:CA:143:THR:HG23	2.03	0.59
1:CA:410:LYS:HE2	1:CA:410:LYS:HA	1.84	0.59
1:A:127:SER:O	1:A:131:ASN:ND2	2.36	0.58
1:P:235:LEU:HD21	1:V:241:VAL:HG22	1.85	0.58
1:R:241:VAL:O	1:R:245:ILE:HG13	2.03	0.58
1:CA:127:SER:O	1:CA:131:ASN:ND2	2.36	0.58
1:HA:139:GLU:O	1:HA:143:THR:HG23	2.02	0.58
1:HA:186:LEU:HD23	1:HA:190:GLN:HG2	1.84	0.58
1:A:235:LEU:HD21	1:F:241:VAL:HG22	1.85	0.58
1:D:127:SER:O	1:D:131:ASN:ND2	2.36	0.58
1:M:127:SER:O	1:M:131:ASN:ND2	2.35	0.58
1:Z:174:ALA:HB3	1:Z:210:VAL:HG22	1.84	0.58
1:A:140:LEU:O	1:A:144:ILE:HG12	2.03	0.58
1:C:143:THR:HG21	1:FA:156:HIS:CE1	2.38	0.58
1:G:433:VAL:HG21	1:L:415:LEU:HD11	1.85	0.58
1:O:253:LEU:HD22	1:O:412:ILE:HG23	1.83	0.58
1:P:433:VAL:HG21	1:V:415:LEU:HD11	1.85	0.58
1:W:140:LEU:O	1:W:144:ILE:HG12	2.04	0.58
1:CA:140:LEU:O	1:CA:144:ILE:HG12	2.03	0.58
1:EA:186:LEU:HB3	1:EA:190:GLN:HB3	1.86	0.58
1:A:394:LYS:HD3	1:A:396:LEU:H	1.67	0.58
1:Z:127:SER:O	1:Z:131:ASN:ND2	2.36	0.58
1:M:174:ALA:HB3	1:M:210:VAL:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:174:ALA:HB3	1:Y:210:VAL:HG22	1.84	0.58
1:GA:275:LYS:HB3	1:GA:377:MET:HB2	1.85	0.58
1:G:431:ASN:HB2	1:L:418:GLU:HG3	1.84	0.58
1:R:174:ALA:HB3	1:R:210:VAL:HG22	1.85	0.58
1:S:140:LEU:O	1:S:144:ILE:HG12	2.04	0.58
1:FA:127:SER:O	1:FA:131:ASN:ND2	2.36	0.58
1:FA:418:GLU:HG3	1:GA:431:ASN:HB2	1.86	0.58
1:A:139:GLU:O	1:A:143:THR:HG23	2.04	0.58
1:A:143:THR:HG22	1:C:154:ARG:HG2	1.86	0.58
1:G:140:LEU:O	1:G:144:ILE:HG12	2.03	0.58
1:L:186:LEU:HB3	1:L:190:GLN:HB3	1.86	0.58
1:Z:156:HIS:CE1	1:EA:143:THR:HG21	2.38	0.58
1:EA:391:VAL:O	1:EA:434:ASN:ND2	2.37	0.58
1:J:235:LEU:HD21	1:O:241:VAL:HG22	1.86	0.58
1:W:139:GLU:O	1:W:143:THR:HG23	2.04	0.58
1:W:174:ALA:HB3	1:W:210:VAL:HG22	1.85	0.58
1:Z:139:GLU:O	1:Z:143:THR:HG23	2.03	0.58
1:FA:140:LEU:O	1:FA:144:ILE:HG12	2.04	0.58
1:A:214:ASP:OD2	1:A:218:HIS:ND1	2.32	0.58
1:J:222:GLN:OE1	1:J:222:GLN:N	2.34	0.58
1:M:140:LEU:O	1:M:144:ILE:HG12	2.04	0.58
1:S:157:LEU:HG	1:S:159:MET:HE2	1.85	0.58
1:M:139:GLU:O	1:M:143:THR:HG23	2.04	0.57
1:S:241:VAL:O	1:S:245:ILE:HD12	2.03	0.57
1:FA:248:ARG:NH2	1:GA:242:GLU:OE1	2.37	0.57
1:J:400:LYS:HD2	1:J:401:PRO:HD2	1.85	0.57
1:M:248:ARG:O	1:M:252:ILE:HG22	2.04	0.57
1:Y:409:MET:HA	1:Y:409:MET:HE2	1.86	0.57
1:FA:394:LYS:NZ	1:FA:396:LEU:O	2.27	0.57
1:D:193:ALA:HA	1:F:219:LEU:HD13	1.86	0.57
1:F:159:MET:HE3	1:F:159:MET:HA	1.86	0.57
1:F:420:MET:HE1	1:F:430:LEU:HB2	1.85	0.57
1:G:127:SER:O	1:G:131:ASN:ND2	2.36	0.57
1:P:222:GLN:OE1	1:P:222:GLN:N	2.35	0.57
1:S:156:HIS:CE1	1:Y:143:THR:HG21	2.39	0.57
1:V:174:ALA:HB3	1:V:210:VAL:HG22	1.85	0.57
1:D:156:HIS:CE1	1:I:143:THR:HG21	2.40	0.57
1:I:186:LEU:HD23	1:I:190:GLN:HG2	1.86	0.57
1:P:126:PHE:CZ	1:V:129:GLN:HG2	2.40	0.57
1:X:394:LYS:HD3	1:X:396:LEU:H	1.69	0.57
1:E:409:MET:HE1	1:E:434:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:LEU:O	1:J:144:ILE:HG12	2.04	0.57
1:J:221:THR:HG1	1:J:224:ASN:ND2	2.02	0.57
1:K:275:LYS:HB3	1:K:377:MET:HB2	1.86	0.57
1:A:433:VAL:HG21	1:F:415:LEU:HD11	1.85	0.57
1:E:303:GLN:HG2	1:F:357:SER:HB2	1.86	0.57
1:I:186:LEU:HB3	1:I:190:GLN:HB3	1.87	0.57
1:M:221:THR:OG1	1:M:224:ASN:ND2	2.30	0.57
1:P:394:LYS:HD3	1:P:396:LEU:H	1.69	0.57
1:S:389:VAL:HB	1:S:432:VAL:HG22	1.85	0.57
1:W:301:SER:HB3	1:W:359:GLN:HB3	1.86	0.57
1:CA:193:ALA:HA	1:EA:219:LEU:HD13	1.87	0.57
1:A:394:LYS:NZ	1:A:396:LEU:O	2.26	0.57
1:H:266:VAL:HG22	1:H:387:VAL:HG22	1.84	0.57
1:L:186:LEU:HD23	1:L:190:GLN:HG2	1.87	0.57
1:S:222:GLN:OE1	1:S:222:GLN:N	2.35	0.57
1:W:431:ASN:HB2	1:BA:418:GLU:HG3	1.85	0.57
1:BA:186:LEU:HD23	1:BA:190:GLN:HG2	1.87	0.57
1:CA:433:VAL:HG21	1:HA:415:LEU:HD11	1.85	0.57
1:EA:174:ALA:HB3	1:EA:210:VAL:HG22	1.87	0.57
1:FA:193:ALA:HA	1:HA:219:LEU:HD13	1.87	0.57
1:G:139:GLU:O	1:G:143:THR:HG23	2.04	0.57
1:FA:139:GLU:O	1:FA:143:THR:HG23	2.05	0.57
1:D:222:GLN:OE1	1:D:222:GLN:N	2.35	0.57
1:F:186:LEU:HB3	1:F:190:GLN:HB3	1.87	0.57
1:M:156:HIS:CE1	1:R:143:THR:HG21	2.40	0.57
1:P:139:GLU:O	1:P:143:THR:HG23	2.05	0.57
1:DA:253:LEU:HD22	1:DA:412:ILE:HG23	1.86	0.57
1:G:156:HIS:CE1	1:L:143:THR:HG21	2.40	0.57
1:J:224:ASN:HB3	1:O:196:HIS:CG	2.39	0.57
1:M:217:GLY:HA3	1:R:190:GLN:HG3	1.86	0.57
1:M:433:VAL:HG21	1:R:415:LEU:HD11	1.86	0.57
1:S:143:THR:HG22	1:V:154:ARG:HG2	1.86	0.57
1:S:239:ASN:HB2	1:Y:244:ARG:HH21	1.69	0.57
1:D:248:ARG:O	1:D:252:ILE:HG22	2.05	0.56
1:J:239:ASN:HB2	1:O:244:ARG:HH21	1.70	0.56
1:M:219:LEU:HG	1:R:193:ALA:HA	1.86	0.56
1:W:222:GLN:OE1	1:W:222:GLN:N	2.34	0.56
1:FA:221:THR:O	1:FA:224:ASN:ND2	2.37	0.56
1:GA:303:GLN:HG2	1:HA:357:SER:HB2	1.87	0.56
1:V:408:GLN:O	1:V:411:GLN:HG2	2.05	0.56
1:D:409:MET:HA	1:D:412:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:THR:HG22	1:F:227:GLY:H	1.71	0.56
1:G:224:ASN:HB3	1:L:196:HIS:CG	2.40	0.56
1:J:394:LYS:NZ	1:J:396:LEU:O	2.26	0.56
1:M:221:THR:O	1:M:224:ASN:ND2	2.38	0.56
1:O:186:LEU:HB3	1:O:190:GLN:HB3	1.87	0.56
1:W:223:SER:O	1:W:226:SER:OG	2.21	0.56
1:W:418:GLU:HG3	1:X:431:ASN:HB2	1.88	0.56
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.38	0.56
1:Z:193:ALA:HA	1:BA:219:LEU:HD13	1.87	0.56
1:DA:232:ASP:HA	1:DA:235:LEU:HG	1.86	0.56
1:A:389:VAL:HB	1:A:432:VAL:HG22	1.87	0.56
1:H:296:ARG:NH2	1:H:362:GLU:OE2	2.38	0.56
1:J:156:HIS:CE1	1:O:143:THR:HG21	2.41	0.56
1:J:221:THR:HG1	1:J:224:ASN:HD21	1.54	0.56
1:K:301:SER:HB3	1:K:359:GLN:HB2	1.87	0.56
1:O:241:VAL:O	1:O:245:ILE:HD12	2.05	0.56
1:C:190:GLN:HG3	1:FA:217:GLY:HA3	1.86	0.56
1:D:139:GLU:O	1:D:143:THR:HG23	2.05	0.56
1:D:140:LEU:O	1:D:144:ILE:HG12	2.05	0.56
1:F:192:SER:O	1:F:196:HIS:ND1	2.39	0.56
1:G:143:THR:HG21	1:I:156:HIS:NE2	2.21	0.56
1:H:303:GLN:HG2	1:I:357:SER:HB2	1.88	0.56
1:S:212:LEU:HB3	1:S:220:LEU:HD12	1.86	0.56
1:Y:159:MET:HE1	1:Y:172:PRO:HB3	1.87	0.56
1:CA:143:THR:HG22	1:EA:154:ARG:HG2	1.87	0.56
1:CA:244:ARG:HH22	1:DA:235:LEU:CB	2.18	0.56
1:C:196:HIS:CG	1:FA:224:ASN:HB3	2.39	0.56
1:CA:241:VAL:O	1:CA:245:ILE:HD12	2.06	0.56
1:V:253:LEU:HD22	1:V:412:ILE:HG23	1.87	0.56
1:D:223:SER:O	1:D:226:SER:OG	2.21	0.56
1:DA:418:GLU:HG3	1:EA:431:ASN:HB2	1.87	0.56
1:EA:186:LEU:HD23	1:EA:190:GLN:HG2	1.87	0.56
1:M:224:ASN:HB3	1:R:196:HIS:CG	2.40	0.56
1:CA:222:GLN:OE1	1:CA:222:GLN:N	2.32	0.56
1:F:136:LEU:HD11	1:F:157:LEU:HD22	1.87	0.56
1:J:139:GLU:O	1:J:143:THR:HG23	2.05	0.56
1:P:191:ILE:HG13	1:P:220:LEU:HB3	1.87	0.56
1:S:143:THR:HG21	1:V:156:HIS:NE2	2.21	0.56
1:CA:389:VAL:HB	1:CA:432:VAL:HG22	1.88	0.56
1:CA:296:ARG:NH2	1:CA:362:GLU:OE2	2.40	0.55
1:DA:303:GLN:HG2	1:EA:357:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:196:HIS:O	1:EA:200:SER:OG	2.20	0.55
1:EA:225:THR:HG22	1:EA:227:GLY:H	1.71	0.55
1:EA:420:MET:HE1	1:EA:430:LEU:HB2	1.88	0.55
1:G:410:LYS:HA	1:G:410:LYS:HE2	1.88	0.55
1:N:409:MET:HA	1:N:412:ILE:HD12	1.88	0.55
1:W:156:HIS:CE1	1:BA:143:THR:HG21	2.40	0.55
1:FA:241:VAL:O	1:FA:245:ILE:HG12	2.06	0.55
1:J:418:GLU:HG3	1:K:431:ASN:HB2	1.87	0.55
1:CA:156:HIS:CE1	1:HA:143:THR:HG21	2.41	0.55
1:EA:301:SER:HB3	1:EA:359:GLN:HB2	1.88	0.55
1:I:228:ARG:NH1	1:I:231:ASN:OD1	2.39	0.55
1:J:296:ARG:NH2	1:J:362:GLU:OE2	2.39	0.55
1:L:159:MET:HE1	1:L:172:PRO:HB3	1.88	0.55
1:T:420:MET:HE1	1:T:430:LEU:HB2	1.89	0.55
1:V:186:LEU:HD23	1:V:190:GLN:HG2	1.89	0.55
1:BA:186:LEU:HB3	1:BA:190:GLN:HB3	1.88	0.55
1:A:156:HIS:CE1	1:F:143:THR:HG21	2.42	0.55
1:D:219:LEU:HD21	1:I:193:ALA:HA	1.89	0.55
1:F:186:LEU:HD23	1:F:190:GLN:HG2	1.87	0.55
1:V:225:THR:HG22	1:V:227:GLY:H	1.70	0.55
1:FA:174:ALA:HB3	1:FA:210:VAL:HG22	1.89	0.55
1:G:389:VAL:HB	1:G:432:VAL:HG22	1.88	0.55
1:A:193:ALA:HA	1:C:219:LEU:HD13	1.89	0.55
1:G:193:ALA:HA	1:I:219:LEU:HD13	1.89	0.55
1:I:159:MET:HE3	1:I:159:MET:HA	1.87	0.55
1:P:130:VAL:HG11	1:V:132:TYR:CZ	2.41	0.55
1:P:241:VAL:O	1:P:245:ILE:HG13	2.07	0.55
1:S:193:ALA:HA	1:V:219:LEU:HD13	1.88	0.55
1:Z:433:VAL:HG21	1:EA:415:LEU:HD11	1.89	0.55
1:BA:420:MET:HE1	1:BA:430:LEU:HB2	1.89	0.55
1:EA:392:ASN:OD1	1:EA:393:TYR:N	2.40	0.55
1:A:248:ARG:O	1:A:252:ILE:HG22	2.06	0.55
1:F:174:ALA:HB3	1:F:210:VAL:HG22	1.88	0.55
1:J:433:VAL:HG21	1:O:415:LEU:HD11	1.87	0.55
1:P:127:SER:O	1:P:131:ASN:ND2	2.40	0.55
1:Q:303:GLN:HG2	1:R:357:SER:HB2	1.88	0.55
1:Z:143:THR:HG21	1:BA:156:HIS:NE2	2.22	0.55
1:CA:419:ALA:O	1:DA:267:THR:OG1	2.20	0.55
1:DA:373:ARG:HH21	1:EA:275:LYS:HE2	1.71	0.55
1:DA:392:ASN:OD1	1:DA:393:TYR:N	2.40	0.55
1:EA:241:VAL:O	1:EA:245:ILE:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HG2	1:C:357:SER:HB2	1.89	0.55
1:M:389:VAL:HB	1:M:432:VAL:HG22	1.89	0.55
1:O:186:LEU:HD23	1:O:190:GLN:HG2	1.89	0.55
1:A:266:VAL:HG22	1:A:387:VAL:HG22	1.89	0.54
1:C:241:VAL:O	1:C:245:ILE:HG13	2.07	0.54
1:D:389:VAL:HB	1:D:432:VAL:HG22	1.89	0.54
1:O:275:LYS:HB3	1:O:377:MET:HB2	1.89	0.54
1:CA:414:ASP:O	1:CA:418:GLU:HG2	2.07	0.54
1:C:415:LEU:HD11	1:FA:433:VAL:HG21	1.88	0.54
1:I:174:ALA:HB3	1:I:210:VAL:HG22	1.87	0.54
1:J:394:LYS:HD3	1:J:396:LEU:H	1.72	0.54
1:CA:217:GLY:HA3	1:HA:190:GLN:HG3	1.87	0.54
1:J:244:ARG:HH22	1:K:235:LEU:HA	1.72	0.54
1:N:392:ASN:OD1	1:N:393:TYR:N	2.41	0.54
1:O:228:ARG:NH1	1:O:231:ASN:OD1	2.40	0.54
1:FA:275:LYS:HB3	1:FA:377:MET:HB2	1.88	0.54
1:FA:408:GLN:O	1:FA:411:GLN:HG2	2.07	0.54
1:G:248:ARG:O	1:G:252:ILE:HG22	2.07	0.54
1:M:418:GLU:HG3	1:N:431:ASN:HB2	1.88	0.54
1:A:245:ILE:HG22	1:A:266:VAL:HG21	1.88	0.54
1:L:392:ASN:OD1	1:L:393:TYR:N	2.40	0.54
1:M:266:VAL:HG22	1:M:387:VAL:HG22	1.89	0.54
1:Z:296:ARG:NH2	1:Z:362:GLU:OE2	2.41	0.54
1:D:143:THR:HG21	1:F:156:HIS:NE2	2.22	0.54
1:M:292:THR:HG21	1:N:282:TYR:HB3	1.89	0.54
1:R:395:THR:HB	1:R:402:LEU:HD23	1.88	0.54
1:S:248:ARG:O	1:S:252:ILE:HG22	2.08	0.54
1:W:433:VAL:HG21	1:BA:415:LEU:HD11	1.87	0.54
1:Y:266:VAL:HG22	1:Y:387:VAL:HG22	1.88	0.54
1:FA:402:LEU:HD12	1:FA:403:PRO:HD2	1.90	0.54
1:A:409:MET:HA	1:A:412:ILE:HD12	1.89	0.54
1:F:392:ASN:OD1	1:F:393:TYR:N	2.41	0.54
1:G:253:LEU:HD22	1:G:412:ILE:HG23	1.90	0.54
1:K:392:ASN:OD1	1:K:393:TYR:N	2.41	0.54
1:P:253:LEU:HD22	1:P:412:ILE:HG23	1.89	0.54
1:R:266:VAL:HG22	1:R:387:VAL:HG22	1.89	0.54
1:W:394:LYS:NZ	1:W:396:LEU:O	2.25	0.54
1:AA:420:MET:HE3	1:AA:422:PHE:HB2	1.89	0.54
1:EA:228:ARG:NH1	1:EA:231:ASN:OD1	2.41	0.54
1:A:236:LYS:HZ2	1:B:225:THR:HA	1.72	0.54
1:B:392:ASN:OD1	1:B:393:TYR:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:MET:HA	1:G:412:ILE:HD12	1.89	0.54
1:H:389:VAL:HB	1:H:432:VAL:HG22	1.89	0.54
1:Q:392:ASN:OD1	1:Q:393:TYR:N	2.40	0.54
1:W:232:ASP:OD2	1:W:232:ASP:N	2.35	0.54
1:W:266:VAL:HG22	1:W:387:VAL:HG22	1.89	0.54
1:DA:275:LYS:HB3	1:DA:377:MET:HB2	1.90	0.54
1:HA:392:ASN:OD1	1:HA:393:TYR:N	2.40	0.54
1:M:193:ALA:HA	1:O:219:LEU:HD13	1.90	0.54
1:M:241:VAL:O	1:M:245:ILE:HG12	2.08	0.54
1:N:303:GLN:HG2	1:O:357:SER:HB2	1.90	0.54
1:P:193:ALA:HA	1:R:219:LEU:HD13	1.90	0.54
1:D:253:LEU:HD22	1:D:412:ILE:HG23	1.90	0.54
1:M:408:GLN:O	1:M:411:GLN:HG2	2.08	0.54
1:Y:196:HIS:O	1:Y:200:SER:OG	2.21	0.54
1:CA:143:THR:HG21	1:EA:156:HIS:NE2	2.23	0.54
1:B:252:ILE:HB	1:C:265:GLN:HG3	1.90	0.53
1:I:395:THR:OG1	1:I:402:LEU:O	2.16	0.53
1:W:389:VAL:HB	1:W:432:VAL:HG22	1.91	0.53
1:Z:133:GLN:HG3	1:Z:157:LEU:HD22	1.90	0.53
1:Z:143:THR:HG22	1:BA:154:ARG:HG2	1.88	0.53
1:Z:222:GLN:OE1	1:Z:222:GLN:N	2.34	0.53
1:D:217:GLY:HA3	1:I:190:GLN:HG3	1.90	0.53
1:V:159:MET:HE1	1:V:172:PRO:HB3	1.90	0.53
1:C:174:ALA:HB3	1:C:210:VAL:HG22	1.90	0.53
1:M:143:THR:HG22	1:O:154:ARG:HG2	1.90	0.53
1:Z:408:GLN:O	1:Z:411:GLN:HG2	2.09	0.53
1:CA:408:GLN:O	1:CA:411:GLN:HG2	2.08	0.53
1:F:157:LEU:HD23	1:F:159:MET:SD	2.48	0.53
1:F:196:HIS:O	1:F:200:SER:OG	2.22	0.53
1:J:431:ASN:HB2	1:O:418:GLU:HG3	1.90	0.53
1:L:196:HIS:O	1:L:200:SER:OG	2.23	0.53
1:O:196:HIS:O	1:O:200:SER:OG	2.24	0.53
1:Q:245:ILE:HG22	1:Q:266:VAL:HG21	1.90	0.53
1:S:159:MET:HE1	1:S:205:LEU:HD12	1.89	0.53
1:V:136:LEU:O	1:V:140:LEU:HG	2.08	0.53
1:CA:253:LEU:HD22	1:CA:412:ILE:HG23	1.89	0.53
1:CA:418:GLU:HG3	1:DA:431:ASN:HB2	1.90	0.53
1:A:127:SER:HA	1:A:130:VAL:HG12	1.90	0.53
1:X:253:LEU:HD22	1:X:412:ILE:HG23	1.91	0.53
1:Y:155:VAL:HG13	1:Y:176:VAL:HG22	1.91	0.53
1:AA:414:ASP:HB3	1:BA:431:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:392:ASN:OD1	1:BA:393:TYR:N	2.42	0.53
1:HA:391:VAL:HG21	1:HA:409:MET:HE1	1.90	0.53
1:D:191:ILE:HG23	1:D:212:LEU:HD22	1.90	0.53
1:I:155:VAL:HG13	1:I:176:VAL:HG22	1.90	0.53
1:AA:408:GLN:O	1:AA:412:ILE:HD12	2.09	0.53
1:CA:127:SER:HA	1:CA:130:VAL:HG12	1.91	0.53
1:EA:136:LEU:O	1:EA:140:LEU:HG	2.08	0.53
1:H:393:TYR:HB3	1:H:401:PRO:HB3	1.91	0.53
1:V:186:LEU:HB3	1:V:190:GLN:HB3	1.90	0.53
1:J:389:VAL:HB	1:J:432:VAL:HG22	1.91	0.53
1:W:217:GLY:HA3	1:BA:190:GLN:HG3	1.91	0.53
1:Z:389:VAL:HB	1:Z:432:VAL:HG22	1.91	0.53
1:CA:394:LYS:NZ	1:CA:396:LEU:O	2.29	0.53
1:D:296:ARG:NH2	1:D:362:GLU:OE2	2.42	0.53
1:G:143:THR:HG22	1:I:154:ARG:HG2	1.91	0.53
1:J:253:LEU:HD22	1:J:412:ILE:HG23	1.90	0.53
1:CA:159:MET:HE1	1:CA:172:PRO:HB3	1.90	0.53
1:HA:196:HIS:O	1:HA:200:SER:OG	2.26	0.53
1:A:154:ARG:HG2	1:F:143:THR:HG22	1.91	0.52
1:D:174:ALA:HB3	1:D:210:VAL:HG22	1.91	0.52
1:G:418:GLU:HG3	1:H:431:ASN:HB2	1.91	0.52
1:I:392:ASN:OD1	1:I:393:TYR:N	2.42	0.52
1:O:155:VAL:HG13	1:O:176:VAL:HG22	1.91	0.52
1:W:143:THR:HG21	1:Y:156:HIS:NE2	2.24	0.52
1:X:391:VAL:HG21	1:X:409:MET:HE1	1.90	0.52
1:FA:143:THR:HG22	1:HA:154:ARG:HG2	1.90	0.52
1:GA:392:ASN:OD1	1:GA:393:TYR:N	2.41	0.52
1:A:143:THR:HG21	1:C:156:HIS:NE2	2.24	0.52
1:E:417:ARG:HG3	1:E:422:PHE:HB3	1.90	0.52
1:H:103:GLN:HA	1:I:182:PRO:HB3	1.90	0.52
1:AA:245:ILE:HG22	1:AA:266:VAL:HG21	1.91	0.52
1:I:136:LEU:HD11	1:I:157:LEU:HD22	1.91	0.52
1:P:244:ARG:HH12	1:Q:235:LEU:HB3	1.74	0.52
1:S:431:ASN:HB2	1:Y:418:GLU:HG3	1.90	0.52
1:AA:303:GLN:HG2	1:BA:357:SER:HB2	1.90	0.52
1:A:253:LEU:HD22	1:A:412:ILE:HG23	1.90	0.52
1:J:408:GLN:O	1:J:411:GLN:HG2	2.10	0.52
1:P:133:GLN:HG3	1:P:157:LEU:HD22	1.92	0.52
1:T:414:ASP:HB3	1:V:431:ASN:ND2	2.24	0.52
1:FA:143:THR:HG21	1:HA:156:HIS:NE2	2.24	0.52
1:FA:222:GLN:OE1	1:FA:222:GLN:N	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:389:VAL:HB	1:GA:432:VAL:HG22	1.92	0.52
1:E:389:VAL:HB	1:E:432:VAL:HG22	1.90	0.52
1:F:301:SER:HB3	1:F:359:GLN:HB2	1.90	0.52
1:J:193:ALA:HA	1:L:219:LEU:HD13	1.91	0.52
1:N:246:GLN:O	1:N:250:GLU:HG3	2.09	0.52
1:S:266:VAL:HG22	1:S:387:VAL:HG22	1.91	0.52
1:L:174:ALA:HB3	1:L:210:VAL:HG22	1.90	0.52
1:M:146:THR:HG23	1:M:146:THR:O	2.10	0.52
1:N:418:GLU:HG3	1:O:431:ASN:HB2	1.91	0.52
1:W:143:THR:HG22	1:Y:154:ARG:HG2	1.91	0.52
1:BA:136:LEU:O	1:BA:140:LEU:HG	2.09	0.52
1:HA:395:THR:OG1	1:HA:402:LEU:O	2.20	0.52
1:M:143:THR:HG21	1:O:156:HIS:NE2	2.23	0.52
1:Z:235:LEU:HD21	1:EA:241:VAL:HG22	1.92	0.52
1:B:389:VAL:HB	1:B:432:VAL:HG22	1.92	0.52
1:R:392:ASN:OD1	1:R:393:TYR:N	2.43	0.52
1:S:253:LEU:HD22	1:S:412:ILE:HG23	1.90	0.52
1:W:392:ASN:OD1	1:W:393:TYR:N	2.43	0.52
1:X:417:ARG:HG3	1:X:422:PHE:HB3	1.92	0.52
1:J:143:THR:HG21	1:L:156:HIS:NE2	2.24	0.52
1:P:154:ARG:HG2	1:V:143:THR:HG22	1.92	0.52
1:Z:127:SER:HA	1:Z:130:VAL:HG12	1.92	0.52
1:E:392:ASN:OD1	1:E:393:TYR:N	2.43	0.52
1:H:408:GLN:O	1:H:411:GLN:HG2	2.08	0.52
1:FA:146:THR:HG23	1:FA:146:THR:O	2.10	0.52
1:A:197:LEU:HD11	1:C:177:THR:HG22	1.93	0.51
1:M:133:GLN:HG3	1:M:157:LEU:HD22	1.92	0.51
1:M:296:ARG:NH2	1:M:362:GLU:OE2	2.43	0.51
1:O:392:ASN:OD1	1:O:393:TYR:N	2.43	0.51
1:P:431:ASN:ND2	1:V:414:ASP:HB3	2.25	0.51
1:T:392:ASN:OD1	1:T:393:TYR:N	2.44	0.51
1:GA:414:ASP:HB3	1:HA:431:ASN:ND2	2.25	0.51
1:P:143:THR:HG21	1:R:156:HIS:NE2	2.24	0.51
1:P:267:THR:OG1	1:V:248:ARG:NH1	2.44	0.51
1:S:127:SER:HA	1:S:130:VAL:HG12	1.92	0.51
1:G:217:GLY:HA3	1:L:190:GLN:HG3	1.91	0.51
1:K:252:ILE:HB	1:L:265:GLN:HG3	1.91	0.51
1:Q:418:GLU:HG3	1:R:431:ASN:HB2	1.91	0.51
1:W:127:SER:HA	1:W:130:VAL:HG12	1.93	0.51
1:Z:224:ASN:HB3	1:EA:196:HIS:CG	2.45	0.51
1:BA:174:ALA:HB3	1:BA:210:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:418:GLU:HG3	1:HA:431:ASN:HB2	1.92	0.51
1:A:431:ASN:ND2	1:F:414:ASP:HB3	2.25	0.51
1:E:103:GLN:HA	1:F:182:PRO:HB3	1.93	0.51
1:J:241:VAL:O	1:J:245:ILE:HG12	2.10	0.51
1:W:253:LEU:HD22	1:W:412:ILE:HG23	1.91	0.51
1:DA:389:VAL:HB	1:DA:432:VAL:HG22	1.91	0.51
1:H:248:ARG:NH1	1:I:267:THR:HG22	2.26	0.51
1:DA:246:GLN:O	1:DA:250:GLU:HG3	2.09	0.51
1:FA:127:SER:HA	1:FA:130:VAL:HG12	1.93	0.51
1:FA:266:VAL:HG22	1:FA:387:VAL:HG22	1.92	0.51
1:C:194:VAL:O	1:C:198:VAL:HG22	2.11	0.51
1:D:424:ASP:N	1:D:424:ASP:OD1	2.43	0.51
1:G:267:THR:OG1	1:L:248:ARG:NH1	2.43	0.51
1:I:383:GLU:O	1:I:426:ARG:HB3	2.10	0.51
1:J:127:SER:HA	1:J:130:VAL:HG12	1.92	0.51
1:M:253:LEU:HD22	1:M:412:ILE:HG23	1.92	0.51
1:O:157:LEU:HD23	1:O:159:MET:HE3	1.91	0.51
1:S:244:ARG:HH12	1:T:235:LEU:C	2.17	0.51
1:FA:157:LEU:HD21	1:FA:159:MET:HG2	1.92	0.51
1:HA:241:VAL:O	1:HA:245:ILE:HG12	2.11	0.51
1:C:244:ARG:HH21	1:FA:239:ASN:HB2	1.76	0.51
1:C:248:ARG:NH1	1:FA:267:THR:OG1	2.44	0.51
1:W:157:LEU:HD11	1:W:202:VAL:HG21	1.93	0.51
1:GA:230:LEU:HD11	1:HA:228:ARG:HH21	1.75	0.51
1:B:418:GLU:HG3	1:C:431:ASN:HB2	1.93	0.51
1:F:136:LEU:O	1:F:140:LEU:HG	2.11	0.51
1:J:143:THR:HG22	1:L:154:ARG:HG2	1.93	0.51
1:J:157:LEU:HD21	1:J:159:MET:HG2	1.92	0.51
1:T:418:GLU:HG3	1:V:431:ASN:HB2	1.93	0.51
1:Z:275:LYS:HB3	1:Z:377:MET:HB2	1.93	0.51
1:C:136:LEU:O	1:C:140:LEU:HG	2.10	0.51
1:S:211:THR:HG21	1:Y:197:LEU:HA	1.92	0.51
1:AA:392:ASN:OD1	1:AA:393:TYR:N	2.44	0.51
1:D:143:THR:HG22	1:F:154:ARG:HG2	1.92	0.51
1:D:266:VAL:HG22	1:D:387:VAL:HG22	1.92	0.51
1:M:127:SER:HA	1:M:130:VAL:HG12	1.92	0.51
1:M:235:LEU:HD21	1:R:241:VAL:HG22	1.93	0.51
1:Q:393:TYR:HB3	1:Q:401:PRO:HB3	1.93	0.51
1:V:196:HIS:O	1:V:200:SER:OG	2.23	0.51
1:AA:385:LEU:N	1:AA:428:ASP:OD1	2.34	0.51
1:CA:245:ILE:HD12	1:CA:245:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:SER:HA	1:D:130:VAL:HG12	1.93	0.50
1:G:127:SER:HA	1:G:130:VAL:HG12	1.92	0.50
1:J:408:GLN:HG3	1:J:412:ILE:HD11	1.93	0.50
1:P:392:ASN:OD1	1:P:393:TYR:N	2.44	0.50
1:Q:373:ARG:HH21	1:R:275:LYS:HE2	1.75	0.50
1:R:267:THR:OG1	1:R:386:SER:HB2	2.11	0.50
1:T:415:LEU:HD11	1:V:433:VAL:HG21	1.92	0.50
1:V:356:ARG:HD2	1:V:356:ARG:N	2.26	0.50
1:X:392:ASN:OD1	1:X:393:TYR:N	2.43	0.50
1:A:193:ALA:HB2	1:C:219:LEU:HB2	1.93	0.50
1:H:393:TYR:CE2	1:H:436:PRO:HD3	2.46	0.50
1:J:156:HIS:NE2	1:O:143:THR:HG21	2.27	0.50
1:V:420:MET:HE1	1:V:430:LEU:HB2	1.93	0.50
1:W:248:ARG:NH2	1:X:242:GLU:OE1	2.44	0.50
1:Z:267:THR:OG1	1:EA:248:ARG:NH1	2.45	0.50
1:Z:416:THR:HG23	1:Z:430:LEU:HD21	1.93	0.50
1:H:392:ASN:OD1	1:H:393:TYR:N	2.43	0.50
1:H:415:LEU:HD11	1:I:433:VAL:HG21	1.93	0.50
1:FA:157:LEU:HD11	1:FA:202:VAL:HG21	1.93	0.50
1:FA:389:VAL:HB	1:FA:432:VAL:HG22	1.92	0.50
1:A:392:ASN:OD1	1:A:393:TYR:N	2.44	0.50
1:D:157:LEU:HD11	1:D:202:VAL:HG21	1.94	0.50
1:H:275:LYS:HB3	1:H:377:MET:HB2	1.93	0.50
1:V:155:VAL:HG13	1:V:176:VAL:HG22	1.94	0.50
1:W:193:ALA:HB2	1:Y:219:LEU:HB2	1.92	0.50
1:C:143:THR:HG21	1:FA:156:HIS:NE2	2.26	0.50
1:V:392:ASN:OD1	1:V:393:TYR:N	2.45	0.50
1:X:303:GLN:HG2	1:Y:357:SER:HB2	1.94	0.50
1:CA:392:ASN:OD1	1:CA:393:TYR:N	2.45	0.50
1:B:393:TYR:CE2	1:B:436:PRO:HD3	2.47	0.50
1:G:132:TYR:CZ	1:G:136:LEU:HD11	2.47	0.50
1:J:212:LEU:HB3	1:J:220:LEU:HD12	1.92	0.50
1:J:244:ARG:HH12	1:K:235:LEU:C	2.19	0.50
1:K:418:GLU:HG3	1:L:431:ASN:HB2	1.93	0.50
1:M:414:ASP:O	1:M:418:GLU:HG2	2.12	0.50
1:N:301:SER:HB3	1:N:359:GLN:HB2	1.93	0.50
1:S:392:ASN:OD1	1:S:393:TYR:N	2.44	0.50
1:CA:156:HIS:NE2	1:HA:143:THR:HG21	2.27	0.50
1:CA:193:ALA:HB2	1:EA:219:LEU:HB2	1.93	0.50
1:GA:103:GLN:HA	1:HA:182:PRO:HB3	1.92	0.50
1:E:252:ILE:HB	1:F:265:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:239:ASN:HB2	1:BA:244:ARG:HH21	1.77	0.50
1:X:252:ILE:HB	1:Y:265:GLN:HG3	1.93	0.50
1:CA:197:LEU:HD11	1:EA:177:THR:HG22	1.94	0.50
1:FA:392:ASN:OD1	1:FA:393:TYR:N	2.45	0.50
1:L:356:ARG:HD2	1:L:356:ARG:N	2.27	0.50
1:M:301:SER:HB3	1:M:359:GLN:HB3	1.92	0.50
1:CA:221:THR:O	1:CA:224:ASN:ND2	2.44	0.50
1:B:415:LEU:HD11	1:C:433:VAL:HG21	1.93	0.50
1:D:132:TYR:CZ	1:D:136:LEU:HD11	2.47	0.50
1:D:236:LYS:NZ	1:E:225:THR:HA	2.26	0.50
1:K:415:LEU:HD11	1:L:433:VAL:HG21	1.92	0.50
1:M:394:LYS:HD3	1:M:396:LEU:H	1.77	0.50
1:Y:245:ILE:HD12	1:Y:245:ILE:H	1.77	0.50
1:CA:238:ALA:O	1:CA:242:GLU:HG3	2.12	0.50
1:D:197:LEU:HD11	1:F:177:THR:HG22	1.93	0.49
1:G:193:ALA:HB2	1:I:219:LEU:HB2	1.93	0.49
1:G:197:LEU:HD11	1:I:177:THR:HG22	1.94	0.49
1:G:394:LYS:CG	1:G:395:THR:N	2.75	0.49
1:G:408:GLN:O	1:G:412:ILE:HG13	2.11	0.49
1:R:420:MET:HE1	1:R:430:LEU:HB2	1.93	0.49
1:W:132:TYR:CZ	1:W:136:LEU:HD11	2.47	0.49
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	1.93	0.49
1:Z:392:ASN:OD1	1:Z:393:TYR:N	2.45	0.49
1:H:418:GLU:HG3	1:I:431:ASN:HB2	1.93	0.49
1:K:414:ASP:HB3	1:L:431:ASN:ND2	2.27	0.49
1:M:156:HIS:NE2	1:R:143:THR:HG21	2.27	0.49
1:P:132:TYR:CZ	1:P:136:LEU:HD11	2.47	0.49
1:D:140:LEU:HB3	1:D:155:VAL:HG21	1.94	0.49
1:D:244:ARG:NH1	1:E:235:LEU:HB3	2.24	0.49
1:G:392:ASN:OD1	1:G:393:TYR:N	2.45	0.49
1:J:392:ASN:OD1	1:J:393:TYR:N	2.45	0.49
1:O:385:LEU:N	1:O:428:ASP:OD1	2.38	0.49
1:P:143:THR:HG22	1:R:154:ARG:HG2	1.94	0.49
1:T:389:VAL:HB	1:T:432:VAL:HG22	1.93	0.49
1:W:158:ALA:O	1:W:159:MET:HE2	2.11	0.49
1:X:420:MET:HE1	1:X:430:LEU:HB2	1.93	0.49
1:D:193:ALA:HB2	1:F:219:LEU:HB2	1.95	0.49
1:F:155:VAL:HG13	1:F:176:VAL:HG22	1.94	0.49
1:G:266:VAL:HG22	1:G:387:VAL:HG22	1.94	0.49
1:N:252:ILE:HB	1:O:265:GLN:HG3	1.94	0.49
1:Y:420:MET:HE1	1:Y:430:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:223:SER:O	1:CA:226:SER:OG	2.29	0.49
1:FA:193:ALA:HB2	1:HA:219:LEU:HB2	1.94	0.49
1:D:408:GLN:O	1:D:412:ILE:HG13	2.12	0.49
1:J:154:ARG:HG2	1:O:143:THR:HG22	1.94	0.49
1:M:431:ASN:HB2	1:R:418:GLU:HG3	1.93	0.49
1:P:420:MET:HE3	1:P:422:PHE:HB2	1.93	0.49
1:FA:132:TYR:CZ	1:FA:136:LEU:HD11	2.47	0.49
1:A:391:VAL:HG21	1:A:409:MET:HE1	1.94	0.49
1:E:407:ASP:OD1	1:E:408:GLN:N	2.46	0.49
1:V:275:LYS:HB3	1:V:377:MET:HB2	1.95	0.49
1:CA:245:ILE:O	1:CA:249:ILE:HG13	2.12	0.49
1:D:232:ASP:HA	1:I:237:PHE:HE1	1.77	0.49
1:E:426:ARG:NH2	1:E:428:ASP:OD2	2.43	0.49
1:K:389:VAL:HB	1:K:432:VAL:HG22	1.94	0.49
1:M:132:TYR:CZ	1:M:136:LEU:HD11	2.48	0.49
1:N:414:ASP:HB3	1:O:431:ASN:ND2	2.28	0.49
1:F:395:THR:OG1	1:F:402:LEU:O	2.27	0.49
1:G:292:THR:HG21	1:H:282:TYR:HB3	1.93	0.49
1:J:132:TYR:CZ	1:J:136:LEU:HD11	2.47	0.49
1:L:291:ALA:HB1	1:L:366:TYR:HE1	1.78	0.49
1:M:392:ASN:OD1	1:M:393:TYR:N	2.45	0.49
1:P:156:HIS:NE2	1:V:143:THR:HG21	2.28	0.49
1:Q:103:GLN:HA	1:R:182:PRO:HB3	1.94	0.49
1:W:408:GLN:O	1:W:411:GLN:HG2	2.13	0.49
1:Z:132:TYR:CZ	1:Z:136:LEU:HD11	2.48	0.49
1:CA:132:TYR:CZ	1:CA:136:LEU:HD11	2.48	0.49
1:A:156:HIS:NE2	1:F:143:THR:HG21	2.28	0.49
1:P:244:ARG:NH1	1:Q:235:LEU:HB3	2.27	0.49
1:S:296:ARG:NH2	1:S:362:GLU:OE2	2.46	0.49
1:GA:415:LEU:HD11	1:HA:433:VAL:HG21	1.95	0.49
1:D:187:ASP:OD1	1:D:190:GLN:N	2.44	0.49
1:G:154:ARG:HG2	1:L:143:THR:HG22	1.94	0.49
1:J:140:LEU:HB3	1:J:155:VAL:HG21	1.95	0.49
1:J:416:THR:HG23	1:J:430:LEU:HD21	1.94	0.49
1:N:415:LEU:HD11	1:O:433:VAL:HG21	1.93	0.49
1:X:241:VAL:HG11	1:X:382:ILE:HD11	1.94	0.49
1:DA:252:ILE:HB	1:EA:265:GLN:HG3	1.94	0.49
1:FA:187:ASP:OD1	1:FA:190:GLN:N	2.42	0.49
1:HA:159:MET:HE1	1:HA:172:PRO:HB3	1.94	0.49
1:F:157:LEU:HD21	1:F:202:VAL:HG22	1.95	0.48
1:M:193:ALA:HB2	1:O:219:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:404:LEU:HD23	1:P:408:GLN:HG2	1.94	0.48
1:Z:412:ILE:O	1:Z:416:THR:HG22	2.13	0.48
1:FA:197:LEU:HD11	1:HA:177:THR:HG22	1.95	0.48
1:C:155:VAL:HG13	1:C:176:VAL:HG22	1.95	0.48
1:D:154:ARG:HG2	1:I:143:THR:HG22	1.93	0.48
1:N:389:VAL:HB	1:N:432:VAL:HG22	1.95	0.48
1:P:265:GLN:HG3	1:V:252:ILE:HB	1.95	0.48
1:X:418:GLU:HG3	1:Y:431:ASN:HB2	1.93	0.48
1:Y:225:THR:HG22	1:Y:227:GLY:N	2.28	0.48
1:AA:415:LEU:HD11	1:BA:433:VAL:HG21	1.94	0.48
1:FA:236:LYS:HZ3	1:GA:225:THR:HA	1.77	0.48
1:C:392:ASN:OD1	1:C:393:TYR:N	2.46	0.48
1:D:248:ARG:NH1	1:E:267:THR:OG1	2.46	0.48
1:G:248:ARG:NH1	1:H:267:THR:OG1	2.45	0.48
1:P:244:ARG:HH22	1:Q:235:LEU:HA	1.77	0.48
1:P:391:VAL:HG21	1:P:409:MET:HE1	1.94	0.48
1:S:391:VAL:HG21	1:S:409:MET:HE1	1.95	0.48
1:T:420:MET:HE3	1:T:422:PHE:HB2	1.94	0.48
1:W:408:GLN:O	1:W:412:ILE:HG13	2.13	0.48
1:A:132:TYR:CZ	1:A:136:LEU:HD11	2.47	0.48
1:A:150:VAL:HG13	1:A:178:VAL:HG23	1.95	0.48
1:B:253:LEU:HD22	1:B:412:ILE:HG23	1.95	0.48
1:B:414:ASP:HB3	1:C:431:ASN:ND2	2.28	0.48
1:F:228:ARG:O	1:F:232:ASP:N	2.43	0.48
1:Q:389:VAL:HB	1:Q:432:VAL:HG22	1.95	0.48
1:R:136:LEU:O	1:R:140:LEU:HG	2.13	0.48
1:S:132:TYR:CZ	1:S:136:LEU:HD11	2.48	0.48
1:W:154:ARG:HG2	1:BA:143:THR:HG22	1.95	0.48
1:FA:420:MET:HE3	1:FA:422:PHE:HB2	1.94	0.48
1:C:157:LEU:HD21	1:C:202:VAL:HG22	1.96	0.48
1:P:217:GLY:HA3	1:V:190:GLN:HG3	1.95	0.48
1:T:416:THR:HG23	1:T:430:LEU:HD21	1.95	0.48
1:DA:414:ASP:HB3	1:EA:431:ASN:ND2	2.28	0.48
1:D:392:ASN:OD1	1:D:393:TYR:N	2.46	0.48
1:G:156:HIS:NE2	1:L:143:THR:HG21	2.28	0.48
1:H:252:ILE:HB	1:I:265:GLN:HG3	1.96	0.48
1:I:266:VAL:HG22	1:I:387:VAL:HG22	1.94	0.48
1:O:179:THR:HG23	1:O:215:GLN:HB3	1.96	0.48
1:P:213:VAL:HG11	1:V:197:LEU:HB2	1.96	0.48
1:S:196:HIS:CE1	1:V:224:ASN:HD22	2.32	0.48
1:T:253:LEU:HD22	1:T:412:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:244:ARG:HH12	1:X:235:LEU:HB3	1.78	0.48
1:Z:197:LEU:HD11	1:BA:177:THR:HG22	1.96	0.48
1:BA:271:ASP:O	1:BA:380:GLY:N	2.40	0.48
1:P:400:LYS:HD2	1:P:401:PRO:HD2	1.94	0.48
1:S:408:GLN:O	1:S:412:ILE:HG13	2.12	0.48
1:T:408:GLN:O	1:T:411:GLN:HG2	2.13	0.48
1:X:402:LEU:HA	1:X:403:PRO:HD2	1.60	0.48
1:CA:221:THR:OG1	1:CA:224:ASN:ND2	2.30	0.48
1:DA:393:TYR:CE2	1:DA:436:PRO:HD3	2.49	0.48
1:A:410:LYS:HD2	1:A:410:LYS:O	2.14	0.48
1:E:415:LEU:HD11	1:F:433:VAL:HG21	1.96	0.48
1:F:193:ALA:HA	1:F:196:HIS:CE1	2.49	0.48
1:G:408:GLN:O	1:G:411:GLN:HG2	2.14	0.48
1:J:197:LEU:HD11	1:L:177:THR:HG22	1.96	0.48
1:J:213:VAL:HG21	1:O:197:LEU:HD22	1.95	0.48
1:Q:393:TYR:CE2	1:Q:436:PRO:HD3	2.49	0.48
1:S:175:SER:HA	1:S:211:THR:HG22	1.96	0.48
1:S:408:GLN:O	1:S:411:GLN:HG2	2.13	0.48
1:X:103:GLN:HA	1:Y:182:PRO:HB3	1.95	0.48
1:AA:244:ARG:HH21	1:AA:248:ARG:HH22	1.62	0.48
1:HA:174:ALA:HB3	1:HA:210:VAL:HG22	1.95	0.48
1:D:190:GLN:HG3	1:F:217:GLY:HA3	1.96	0.48
1:I:136:LEU:O	1:I:140:LEU:HG	2.14	0.48
1:J:193:ALA:HB2	1:L:219:LEU:HB2	1.94	0.48
1:M:197:LEU:HD11	1:O:177:THR:HG22	1.95	0.48
1:W:241:VAL:O	1:W:245:ILE:HG12	2.14	0.48
1:C:143:THR:HG22	1:FA:154:ARG:HG2	1.94	0.48
1:D:192:SER:HA	1:D:195:VAL:HG22	1.95	0.48
1:D:402:LEU:HD12	1:D:403:PRO:HD2	1.94	0.48
1:G:221:THR:HG1	1:G:224:ASN:HD21	1.59	0.48
1:G:244:ARG:HH21	1:G:248:ARG:NH2	2.11	0.48
1:I:409:MET:HE2	1:I:409:MET:HA	1.95	0.48
1:P:266:VAL:HG22	1:P:387:VAL:HG22	1.95	0.48
1:R:136:LEU:HD11	1:R:157:LEU:HD22	1.96	0.48
1:DA:385:LEU:N	1:DA:428:ASP:OD1	2.37	0.48
1:A:408:GLN:O	1:A:411:GLN:HG2	2.13	0.47
1:D:128:GLU:HA	1:D:131:ASN:HD21	1.79	0.47
1:D:408:GLN:O	1:D:411:GLN:HG2	2.13	0.47
1:E:393:TYR:HB3	1:E:401:PRO:HB3	1.96	0.47
1:G:222:GLN:OE1	1:G:222:GLN:N	2.39	0.47
1:K:395:THR:OG1	1:K:402:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:239:ASN:HB2	1:R:244:ARG:HH21	1.78	0.47
1:M:408:GLN:HG3	1:M:412:ILE:HD11	1.95	0.47
1:S:172:PRO:O	1:S:209:ASN:ND2	2.30	0.47
1:S:197:LEU:HD11	1:V:177:THR:HG22	1.96	0.47
1:HA:196:HIS:HA	1:HA:199:SER:OG	2.15	0.47
1:E:414:ASP:HB3	1:F:431:ASN:ND2	2.29	0.47
1:G:387:VAL:HG21	1:G:420:MET:HG3	1.95	0.47
1:M:412:ILE:HD12	1:M:412:ILE:H	1.79	0.47
1:S:187:ASP:OD1	1:S:190:GLN:N	2.46	0.47
1:Y:136:LEU:O	1:Y:140:LEU:HG	2.14	0.47
1:Z:140:LEU:HB3	1:Z:155:VAL:HG21	1.95	0.47
1:AA:393:TYR:CE2	1:AA:436:PRO:HD3	2.49	0.47
1:CA:244:ARG:NH2	1:DA:235:LEU:HB3	2.28	0.47
1:FA:192:SER:HA	1:FA:195:VAL:HG22	1.96	0.47
1:HA:293:LEU:HD21	1:HA:296:ARG:HH11	1.80	0.47
1:A:197:LEU:HA	1:C:211:THR:HG21	1.95	0.47
1:E:418:GLU:HG3	1:F:431:ASN:HB2	1.97	0.47
1:N:409:MET:HE1	1:N:434:ASN:HB2	1.95	0.47
1:V:225:THR:HG22	1:V:227:GLY:N	2.29	0.47
1:BA:409:MET:HE2	1:BA:409:MET:HA	1.96	0.47
1:HA:157:LEU:HD21	1:HA:202:VAL:HG22	1.96	0.47
1:F:376:LYS:HB2	1:F:376:LYS:NZ	2.29	0.47
1:P:193:ALA:HB2	1:R:219:LEU:HB2	1.94	0.47
1:S:128:GLU:HA	1:S:131:ASN:HD21	1.79	0.47
1:W:213:VAL:HG21	1:BA:197:LEU:HD22	1.97	0.47
1:Z:193:ALA:HB2	1:BA:219:LEU:HB2	1.96	0.47
1:BA:385:LEU:N	1:BA:428:ASP:OD1	2.37	0.47
1:A:244:ARG:HD2	1:A:244:ARG:HA	1.71	0.47
1:B:101:ALA:HB1	1:B:193:ALA:HA	1.96	0.47
1:B:393:TYR:CE2	1:B:403:PRO:HD3	2.49	0.47
1:C:418:GLU:HG3	1:FA:431:ASN:HB2	1.97	0.47
1:D:431:ASN:ND2	1:I:414:ASP:HB3	2.29	0.47
1:G:424:ASP:N	1:G:424:ASP:OD1	2.48	0.47
1:H:395:THR:OG1	1:H:402:LEU:HG	2.14	0.47
1:J:196:HIS:CE1	1:L:224:ASN:HD22	2.33	0.47
1:L:408:GLN:O	1:L:411:GLN:HG2	2.15	0.47
1:S:150:VAL:HG13	1:S:178:VAL:HG23	1.97	0.47
1:W:404:LEU:HD23	1:W:408:GLN:HG2	1.96	0.47
1:Z:128:GLU:HA	1:Z:131:ASN:HD21	1.79	0.47
1:Z:232:ASP:C	1:Z:232:ASP:OD1	2.58	0.47
1:AA:418:GLU:HG3	1:BA:431:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HA	1:FA:211:THR:HG21	1.96	0.47
1:D:157:LEU:HD21	1:D:159:MET:HG2	1.96	0.47
1:K:402:LEU:HA	1:K:403:PRO:HD2	1.63	0.47
1:L:302:GLU:HG3	1:L:358:THR:HG22	1.96	0.47
1:M:232:ASP:OD2	1:M:232:ASP:C	2.58	0.47
1:O:136:LEU:O	1:O:140:LEU:HG	2.15	0.47
1:O:408:GLN:O	1:O:411:GLN:HG2	2.13	0.47
1:P:146:THR:HG23	1:P:146:THR:O	2.15	0.47
1:S:154:ARG:HG2	1:Y:143:THR:HG22	1.96	0.47
1:T:241:VAL:O	1:T:245:ILE:HG12	2.14	0.47
1:CA:140:LEU:HB3	1:CA:155:VAL:HG21	1.97	0.47
1:FA:128:GLU:HA	1:FA:131:ASN:HD21	1.80	0.47
1:E:405:THR:HG23	1:E:408:GLN:HB2	1.96	0.47
1:G:128:GLU:HA	1:G:131:ASN:HD21	1.80	0.47
1:G:232:ASP:OD1	1:G:232:ASP:C	2.58	0.47
1:P:232:ASP:HA	1:V:237:PHE:HE1	1.79	0.47
1:Q:415:LEU:HD11	1:R:433:VAL:HG21	1.95	0.47
1:T:385:LEU:N	1:T:428:ASP:OD1	2.41	0.47
1:V:246:GLN:O	1:V:250:GLU:HG3	2.14	0.47
1:X:101:ALA:HB1	1:X:193:ALA:HA	1.96	0.47
1:Y:186:LEU:HB3	1:Y:190:GLN:HB3	1.96	0.47
1:Y:373:ARG:NH1	1:Y:373:ARG:HB3	2.30	0.47
1:CA:128:GLU:HA	1:CA:131:ASN:HD21	1.79	0.47
1:CA:232:ASP:OD2	1:CA:232:ASP:C	2.58	0.47
1:CA:248:ARG:O	1:CA:252:ILE:HG22	2.15	0.47
1:FA:412:ILE:O	1:FA:416:THR:HG22	2.15	0.47
1:B:407:ASP:OD1	1:B:408:GLN:N	2.48	0.47
1:C:370:ARG:HD2	1:C:372:ILE:HD11	1.96	0.47
1:D:156:HIS:NE2	1:I:143:THR:HG21	2.30	0.47
1:F:144:ILE:HD11	1:F:194:VAL:HG23	1.96	0.47
1:F:293:LEU:HD21	1:F:296:ARG:HH11	1.80	0.47
1:J:266:VAL:HG22	1:J:387:VAL:HG22	1.95	0.47
1:P:393:TYR:CE2	1:P:436:PRO:HD3	2.49	0.47
1:T:267:THR:OG1	1:T:386:SER:HB2	2.14	0.47
1:W:156:HIS:NE2	1:BA:143:THR:HG21	2.30	0.47
1:X:407:ASP:OD1	1:X:408:GLN:N	2.48	0.47
1:CA:236:LYS:NZ	1:DA:225:THR:HA	2.30	0.47
1:CA:412:ILE:HD12	1:CA:412:ILE:H	1.79	0.47
1:H:414:ASP:HB3	1:I:431:ASN:ND2	2.29	0.47
1:N:408:GLN:O	1:N:411:GLN:HG2	2.14	0.47
1:GA:393:TYR:CE2	1:GA:436:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:HA	1:F:237:PHE:HE1	1.80	0.47
1:B:245:ILE:HG22	1:B:266:VAL:HG21	1.96	0.47
1:J:192:SER:HA	1:J:195:VAL:HG22	1.97	0.47
1:M:373:ARG:NH1	1:N:277:GLN:OE1	2.48	0.47
1:P:373:ARG:NH1	1:Q:277:GLN:OE1	2.48	0.47
1:Z:424:ASP:N	1:Z:424:ASP:OD1	2.47	0.47
1:EA:266:VAL:HG22	1:EA:387:VAL:HG22	1.96	0.47
1:A:211:THR:OG1	1:A:224:ASN:OD1	2.17	0.46
1:B:402:LEU:HA	1:B:403:PRO:HD2	1.58	0.46
1:J:376:LYS:HB2	1:J:376:LYS:NZ	2.31	0.46
1:J:424:ASP:OD1	1:J:424:ASP:N	2.47	0.46
1:O:136:LEU:HD11	1:O:157:LEU:HD22	1.96	0.46
1:P:408:GLN:O	1:P:412:ILE:HG13	2.15	0.46
1:S:158:ALA:O	1:S:172:PRO:HA	2.15	0.46
1:S:193:ALA:HB2	1:V:219:LEU:HB2	1.96	0.46
1:W:140:LEU:HB3	1:W:155:VAL:HG21	1.96	0.46
1:Z:225:THR:O	1:Z:225:THR:OG1	2.31	0.46
1:EA:150:VAL:HA	1:EA:180:LEU:HA	1.97	0.46
1:FA:414:ASP:O	1:FA:418:GLU:HG2	2.15	0.46
1:GA:407:ASP:OD1	1:GA:408:GLN:N	2.48	0.46
1:M:154:ARG:HG2	1:R:143:THR:HG22	1.96	0.46
1:P:197:LEU:HA	1:R:211:THR:HG21	1.98	0.46
1:P:232:ASP:OD2	1:P:232:ASP:C	2.58	0.46
1:S:192:SER:HA	1:S:195:VAL:HG22	1.96	0.46
1:W:128:GLU:HA	1:W:131:ASN:HD21	1.80	0.46
1:W:424:ASP:OD1	1:W:424:ASP:N	2.47	0.46
1:G:275:LYS:HB3	1:G:377:MET:HB2	1.97	0.46
1:H:360:ARG:NH1	1:H:362:GLU:OE1	2.45	0.46
1:T:393:TYR:CE2	1:T:436:PRO:HD3	2.50	0.46
1:AA:426:ARG:NH2	1:AA:428:ASP:OD2	2.44	0.46
1:GA:402:LEU:HD12	1:GA:402:LEU:O	2.16	0.46
1:HA:420:MET:HE1	1:HA:430:LEU:HB2	1.97	0.46
1:A:408:GLN:O	1:A:412:ILE:HG13	2.14	0.46
1:C:420:MET:HE3	1:C:422:PHE:HB2	1.97	0.46
1:M:412:ILE:O	1:M:416:THR:HG22	2.15	0.46
1:S:416:THR:HG23	1:S:430:LEU:HD21	1.98	0.46
1:X:393:TYR:CE2	1:X:436:PRO:HD3	2.49	0.46
1:Y:158:ALA:O	1:Y:159:MET:HE2	2.16	0.46
1:Z:196:HIS:CE1	1:BA:224:ASN:HD22	2.33	0.46
1:CA:394:LYS:HA	1:CA:394:LYS:HE2	1.98	0.46
1:CA:408:GLN:HG3	1:CA:412:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:140:LEU:HB3	1:FA:155:VAL:HG21	1.98	0.46
1:FA:232:ASP:OD1	1:FA:232:ASP:N	2.46	0.46
1:FA:248:ARG:NH1	1:GA:267:THR:HG23	2.31	0.46
1:E:393:TYR:CE2	1:E:436:PRO:HD3	2.51	0.46
1:M:187:ASP:OD1	1:M:190:GLN:N	2.47	0.46
1:S:245:ILE:O	1:S:249:ILE:HG13	2.16	0.46
1:T:101:ALA:HB1	1:T:193:ALA:HA	1.96	0.46
1:CA:266:VAL:HG22	1:CA:387:VAL:HG22	1.96	0.46
1:A:128:GLU:HA	1:A:131:ASN:HD21	1.81	0.46
1:D:150:VAL:HG13	1:D:178:VAL:HG23	1.98	0.46
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.79	0.46
1:J:245:ILE:O	1:J:249:ILE:HG13	2.16	0.46
1:M:128:GLU:HA	1:M:131:ASN:HD21	1.80	0.46
1:N:393:TYR:CE2	1:N:436:PRO:HD3	2.50	0.46
1:P:127:SER:HA	1:P:130:VAL:HG12	1.98	0.46
1:R:424:ASP:N	1:R:424:ASP:OD2	2.48	0.46
1:W:197:LEU:HD11	1:Y:177:THR:HG22	1.97	0.46
1:Z:431:ASN:HB2	1:EA:418:GLU:HG3	1.96	0.46
1:BA:150:VAL:HA	1:BA:180:LEU:HA	1.98	0.46
1:DA:426:ARG:NH2	1:DA:428:ASP:OD2	2.39	0.46
1:G:404:LEU:HD23	1:G:408:GLN:HG2	1.98	0.46
1:K:101:ALA:HB1	1:K:193:ALA:HA	1.98	0.46
1:K:409:MET:SD	1:K:412:ILE:HD11	2.56	0.46
1:S:156:HIS:NE2	1:Y:143:THR:HG21	2.31	0.46
1:V:302:GLU:HG3	1:V:358:THR:HG22	1.96	0.46
1:Y:383:GLU:O	1:Y:426:ARG:HB3	2.16	0.46
1:CA:133:GLN:HG3	1:CA:157:LEU:HD22	1.97	0.46
1:CA:197:LEU:HA	1:EA:211:THR:HG21	1.98	0.46
1:CA:431:ASN:ND2	1:HA:414:ASP:HB3	2.31	0.46
1:HA:136:LEU:O	1:HA:140:LEU:HG	2.15	0.46
1:HA:225:THR:HG22	1:HA:227:GLY:N	2.29	0.46
1:P:203:ALA:N	1:R:158:ALA:HB1	2.30	0.46
1:P:424:ASP:N	1:P:424:ASP:OD1	2.49	0.46
1:CA:154:ARG:HG2	1:HA:143:THR:HG22	1.97	0.46
1:DA:417:ARG:HG3	1:DA:422:PHE:HB3	1.98	0.46
1:FA:424:ASP:N	1:FA:424:ASP:OD1	2.49	0.46
1:B:408:GLN:O	1:B:411:GLN:HG2	2.16	0.46
1:H:301:SER:HB3	1:H:359:GLN:HB2	1.97	0.46
1:K:385:LEU:N	1:K:428:ASP:OD1	2.37	0.46
1:K:407:ASP:OD1	1:K:408:GLN:N	2.49	0.46
1:L:136:LEU:O	1:L:140:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:424:ASP:OD1	1:M:424:ASP:N	2.49	0.46
1:P:140:LEU:HB3	1:P:155:VAL:HG21	1.97	0.46
1:S:385:LEU:N	1:S:428:ASP:OD1	2.35	0.46
1:Z:410:LYS:HZ1	1:Z:414:ASP:CG	2.18	0.46
1:F:177:THR:O	1:F:177:THR:OG1	2.32	0.46
1:S:140:LEU:HB3	1:S:155:VAL:HG21	1.97	0.46
1:Z:244:ARG:HH21	1:Z:248:ARG:HH21	1.63	0.46
1:AA:389:VAL:HB	1:AA:432:VAL:HG22	1.98	0.46
1:BA:196:HIS:O	1:BA:200:SER:OG	2.34	0.46
1:CA:393:TYR:CE2	1:CA:436:PRO:HD3	2.51	0.46
1:A:393:TYR:CE2	1:A:436:PRO:HD3	2.51	0.45
1:D:146:THR:HG23	1:D:146:THR:O	2.16	0.45
1:J:412:ILE:O	1:J:416:THR:HG22	2.15	0.45
1:L:157:LEU:HD21	1:L:202:VAL:HG22	1.98	0.45
1:T:417:ARG:HG3	1:T:422:PHE:HB3	1.98	0.45
1:W:187:ASP:OD1	1:W:190:GLN:N	2.43	0.45
1:W:195:VAL:HG12	1:W:212:LEU:HD13	1.98	0.45
1:W:393:TYR:CE2	1:W:436:PRO:HD3	2.51	0.45
1:AA:417:ARG:HG3	1:AA:422:PHE:HB3	1.99	0.45
1:F:196:HIS:HA	1:F:199:SER:OG	2.16	0.45
1:G:150:VAL:HG13	1:G:178:VAL:HG23	1.98	0.45
1:I:196:HIS:O	1:I:200:SER:OG	2.24	0.45
1:J:203:ALA:N	1:L:158:ALA:HB1	2.31	0.45
1:K:241:VAL:O	1:K:245:ILE:HG12	2.16	0.45
1:K:393:TYR:CE2	1:K:436:PRO:HD3	2.50	0.45
1:P:127:SER:HA	1:V:132:TYR:OH	2.15	0.45
1:R:245:ILE:HD12	1:R:266:VAL:HG11	1.98	0.45
1:S:377:MET:HE3	1:S:377:MET:HB3	1.82	0.45
1:CA:187:ASP:OD1	1:CA:190:GLN:N	2.46	0.45
1:EA:391:VAL:HG23	1:EA:434:ASN:ND2	2.31	0.45
1:A:140:LEU:HB3	1:A:155:VAL:HG21	1.99	0.45
1:E:408:GLN:O	1:E:411:GLN:HG2	2.17	0.45
1:G:192:SER:HA	1:G:195:VAL:HG22	1.96	0.45
1:J:128:GLU:HA	1:J:131:ASN:HD21	1.80	0.45
1:J:265:GLN:HG3	1:O:252:ILE:HB	1.99	0.45
1:M:385:LEU:N	1:M:428:ASP:OD1	2.36	0.45
1:Q:301:SER:HB3	1:Q:359:GLN:HB3	1.98	0.45
1:Y:177:THR:O	1:Y:177:THR:OG1	2.33	0.45
1:E:409:MET:HA	1:E:412:ILE:HD12	1.98	0.45
1:P:192:SER:HA	1:P:195:VAL:HG22	1.98	0.45
1:Q:252:ILE:HB	1:R:265:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:409:MET:HE2	1:Q:409:MET:HA	1.99	0.45
1:S:143:THR:CG2	1:V:154:ARG:HG2	2.47	0.45
1:S:146:THR:O	1:S:146:THR:OG1	2.34	0.45
1:S:393:TYR:CE2	1:S:436:PRO:HD3	2.51	0.45
1:Z:192:SER:HA	1:Z:195:VAL:HG22	1.98	0.45
1:Z:225:THR:O	1:Z:227:GLY:N	2.48	0.45
1:Z:241:VAL:O	1:Z:245:ILE:HG12	2.17	0.45
1:P:150:VAL:HG13	1:P:178:VAL:HG23	1.99	0.45
1:S:424:ASP:N	1:S:424:ASP:OD1	2.49	0.45
1:T:402:LEU:HA	1:T:403:PRO:HD2	1.61	0.45
1:AA:244:ARG:NH2	1:AA:248:ARG:HH22	2.13	0.45
1:C:225:THR:HG22	1:C:227:GLY:N	2.31	0.45
1:D:232:ASP:OD2	1:D:232:ASP:C	2.60	0.45
1:F:225:THR:HG22	1:F:227:GLY:N	2.32	0.45
1:G:143:THR:HG21	1:I:156:HIS:CE1	2.52	0.45
1:I:196:HIS:HD2	1:I:207:PRO:HG3	1.82	0.45
1:J:157:LEU:HD11	1:J:202:VAL:HG21	1.99	0.45
1:J:252:ILE:HB	1:K:265:GLN:HG3	1.99	0.45
1:L:376:LYS:HE3	1:L:376:LYS:HB2	1.66	0.45
1:Q:414:ASP:HB3	1:R:431:ASN:ND2	2.30	0.45
1:X:414:ASP:HB3	1:Y:431:ASN:ND2	2.32	0.45
1:Z:393:TYR:CE2	1:Z:436:PRO:HD3	2.51	0.45
1:AA:101:ALA:HB1	1:AA:193:ALA:HA	1.99	0.45
1:GA:101:ALA:HB1	1:GA:193:ALA:HA	1.98	0.45
1:HA:245:ILE:O	1:HA:249:ILE:HG13	2.17	0.45
1:M:140:LEU:HB3	1:M:155:VAL:HG21	1.98	0.45
1:N:101:ALA:HB1	1:N:193:ALA:HA	1.98	0.45
1:S:197:LEU:HA	1:V:211:THR:HG21	1.99	0.45
1:X:408:GLN:O	1:X:411:GLN:HG2	2.16	0.45
1:AA:417:ARG:HG3	1:AA:422:PHE:CB	2.46	0.45
1:DA:409:MET:HA	1:DA:412:ILE:HD12	1.99	0.45
1:A:203:ALA:N	1:C:158:ALA:HB1	2.32	0.45
1:D:143:THR:HG21	1:F:156:HIS:CE1	2.51	0.45
1:D:410:LYS:O	1:D:410:LYS:HD3	2.17	0.45
1:L:393:TYR:CE2	1:L:436:PRO:HD3	2.52	0.45
1:P:197:LEU:HD11	1:R:177:THR:HG22	1.98	0.45
1:P:408:GLN:O	1:P:411:GLN:HG2	2.17	0.45
1:P:416:THR:HG23	1:P:430:LEU:HD21	1.99	0.45
1:W:258:GLY:HA3	1:W:261:ASN:HD22	1.81	0.45
1:Y:196:HIS:CD2	1:Y:207:PRO:HG3	2.52	0.45
1:Y:356:ARG:HD2	1:Y:356:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:159:MET:HE2	1:BA:159:MET:HA	1.99	0.45
1:CA:150:VAL:HG13	1:CA:178:VAL:HG23	1.99	0.45
1:E:417:ARG:HG3	1:E:422:PHE:CB	2.47	0.45
1:G:296:ARG:NH2	1:G:362:GLU:OE2	2.50	0.45
1:P:187:ASP:OD1	1:P:190:GLN:N	2.48	0.45
1:P:196:HIS:CE1	1:R:224:ASN:HD22	2.35	0.45
1:P:248:ARG:O	1:P:252:ILE:HG22	2.17	0.45
1:Y:408:GLN:O	1:Y:411:GLN:HG2	2.16	0.45
1:Z:154:ARG:HG2	1:EA:143:THR:HG22	1.98	0.45
1:CA:424:ASP:OD1	1:CA:424:ASP:N	2.50	0.45
1:EA:225:THR:HG22	1:EA:227:GLY:N	2.32	0.45
1:FA:244:ARG:NH1	1:GA:235:LEU:HB3	2.29	0.45
1:GA:407:ASP:O	1:GA:411:GLN:HG3	2.17	0.45
1:GA:410:LYS:HD2	1:GA:410:LYS:O	2.16	0.45
1:HA:301:SER:HB3	1:HA:359:GLN:HB2	1.98	0.45
1:D:196:HIS:CE1	1:F:224:ASN:HD22	2.35	0.45
1:I:271:ASP:O	1:I:380:GLY:N	2.50	0.45
1:J:146:THR:O	1:J:146:THR:HG23	2.17	0.45
1:P:409:MET:HA	1:P:412:ILE:HD12	1.98	0.45
1:Q:377:MET:HE3	1:Q:377:MET:HB3	1.91	0.45
1:S:244:ARG:NH1	1:T:235:LEU:O	2.31	0.45
1:S:394:LYS:HE2	1:S:394:LYS:HA	1.98	0.45
1:S:414:ASP:HB3	1:T:431:ASN:ND2	2.32	0.45
1:V:196:HIS:O	1:V:196:HIS:ND1	2.50	0.45
1:Y:145:GLU:HG2	1:Y:152:SER:HA	1.99	0.45
1:Y:186:LEU:HD23	1:Y:190:GLN:HG2	1.98	0.45
1:BA:225:THR:HG22	1:BA:227:GLY:N	2.30	0.45
1:BA:408:GLN:O	1:BA:411:GLN:HG2	2.16	0.45
1:HA:404:LEU:H	1:HA:434:ASN:ND2	2.15	0.45
1:H:101:ALA:HB1	1:H:193:ALA:HA	1.99	0.44
1:H:394:LYS:H	1:H:395:THR:HG23	1.82	0.44
1:I:373:ARG:HB3	1:I:373:ARG:NH1	2.31	0.44
1:L:155:VAL:HG13	1:L:176:VAL:HG22	1.98	0.44
1:L:355:PRO:N	1:L:356:ARG:HH11	2.15	0.44
1:P:248:ARG:NH2	1:Q:242:GLU:OE1	2.50	0.44
1:T:256:ILE:HG23	1:T:257:VAL:HG13	1.98	0.44
1:W:159:MET:HE1	1:W:172:PRO:HB3	1.99	0.44
1:W:192:SER:HA	1:W:195:VAL:HG22	1.98	0.44
1:W:417:ARG:HH21	1:W:430:LEU:HD23	1.82	0.44
1:Y:136:LEU:HD11	1:Y:157:LEU:HD22	1.98	0.44
1:Z:211:THR:OG1	1:Z:224:ASN:OD1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:393:TYR:CE2	1:FA:436:PRO:HD3	2.52	0.44
1:B:241:VAL:HG22	1:C:235:LEU:HD21	1.99	0.44
1:E:385:LEU:N	1:E:428:ASP:OD1	2.38	0.44
1:J:400:LYS:HD2	1:J:401:PRO:CD	2.48	0.44
1:J:412:ILE:HD12	1:J:412:ILE:H	1.82	0.44
1:M:190:GLN:HG3	1:O:217:GLY:HA3	1.99	0.44
1:M:377:MET:HE3	1:M:377:MET:HB3	1.90	0.44
1:AA:230:LEU:HD11	1:BA:228:ARG:HH21	1.81	0.44
1:DA:393:TYR:CE2	1:DA:403:PRO:HD3	2.52	0.44
1:EA:194:VAL:O	1:EA:198:VAL:HG22	2.17	0.44
1:F:385:LEU:N	1:F:428:ASP:OD1	2.40	0.44
1:G:235:LEU:HD21	1:L:241:VAL:HG22	1.99	0.44
1:M:159:MET:HE1	1:M:172:PRO:HB3	1.98	0.44
1:M:225:THR:HG22	1:R:196:HIS:NE2	2.32	0.44
1:Q:417:ARG:HG3	1:Q:422:PHE:HB3	1.99	0.44
1:W:143:THR:CG2	1:Y:154:ARG:HG2	2.48	0.44
1:W:196:HIS:CE1	1:Y:224:ASN:HD22	2.35	0.44
1:Z:252:ILE:HB	1:AA:265:GLN:HG3	1.99	0.44
1:AA:393:TYR:HB3	1:AA:401:PRO:HB3	1.99	0.44
1:BA:136:LEU:HD11	1:BA:157:LEU:HD22	1.98	0.44
1:CA:225:THR:O	1:CA:225:THR:OG1	2.33	0.44
1:CA:416:THR:HG23	1:CA:430:LEU:HD21	1.99	0.44
1:GA:252:ILE:HB	1:HA:265:GLN:HG3	1.99	0.44
1:D:211:THR:HG21	1:I:197:LEU:HA	1.98	0.44
1:E:275:LYS:HB3	1:E:377:MET:HB2	1.99	0.44
1:G:239:ASN:HB2	1:L:244:ARG:HH21	1.82	0.44
1:J:232:ASP:HA	1:O:237:PHE:HE1	1.83	0.44
1:S:143:THR:HG21	1:V:156:HIS:CE1	2.53	0.44
1:T:407:ASP:OD1	1:T:408:GLN:N	2.50	0.44
1:AA:252:ILE:HB	1:BA:265:GLN:HG3	2.00	0.44
1:CA:186:LEU:HB2	1:CA:191:ILE:HD11	1.99	0.44
1:CA:258:GLY:HA3	1:CA:261:ASN:HD22	1.83	0.44
1:CA:412:ILE:O	1:CA:416:THR:HG22	2.18	0.44
1:A:400:LYS:HD2	1:A:401:PRO:CD	2.48	0.44
1:D:175:SER:HA	1:D:211:THR:HG22	1.99	0.44
1:E:402:LEU:HA	1:E:403:PRO:HD2	1.71	0.44
1:I:225:THR:HG22	1:I:227:GLY:N	2.32	0.44
1:J:410:LYS:O	1:J:410:LYS:HD3	2.18	0.44
1:K:360:ARG:NH1	1:K:362:GLU:OE1	2.51	0.44
1:P:275:LYS:HB3	1:P:377:MET:HB2	1.98	0.44
1:Y:385:LEU:N	1:Y:428:ASP:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:187:ASP:OD1	1:Z:190:GLN:N	2.47	0.44
1:CA:196:HIS:CE1	1:EA:224:ASN:HD22	2.35	0.44
1:FA:408:GLN:HG3	1:FA:412:ILE:HD11	1.99	0.44
1:A:143:THR:CG2	1:C:154:ARG:HG2	2.48	0.44
1:A:236:LYS:NZ	1:B:225:THR:HA	2.32	0.44
1:K:408:GLN:O	1:K:411:GLN:HG2	2.18	0.44
1:W:234:GLN:HB3	1:W:272:PHE:CZ	2.53	0.44
1:W:373:ARG:NH1	1:X:277:GLN:OE1	2.51	0.44
1:Z:150:VAL:HG13	1:Z:178:VAL:HG23	1.99	0.44
1:Z:292:THR:HG21	1:AA:282:TYR:HB3	1.98	0.44
1:DA:402:LEU:HA	1:DA:403:PRO:HD2	1.61	0.44
1:HA:159:MET:HE2	1:HA:159:MET:HA	1.99	0.44
1:A:424:ASP:OD1	1:A:424:ASP:N	2.50	0.44
1:K:409:MET:CE	1:K:434:ASN:HB2	2.46	0.44
1:W:244:ARG:HH22	1:X:235:LEU:HA	1.82	0.44
1:CA:267:THR:OG1	1:HA:248:ARG:NH1	2.51	0.44
1:FA:150:VAL:HG13	1:FA:178:VAL:HG23	2.00	0.44
1:FA:175:SER:HA	1:FA:211:THR:HG22	2.00	0.44
1:C:150:VAL:HA	1:C:180:LEU:HA	2.00	0.44
1:E:101:ALA:HB1	1:E:193:ALA:HA	2.00	0.44
1:G:140:LEU:HB3	1:G:155:VAL:HG21	2.00	0.44
1:G:196:HIS:CE1	1:I:224:ASN:HD22	2.35	0.44
1:G:393:TYR:CE2	1:G:436:PRO:HD3	2.53	0.44
1:J:187:ASP:OD1	1:J:190:GLN:N	2.49	0.44
1:M:232:ASP:HA	1:R:237:PHE:HE1	1.83	0.44
1:N:407:ASP:OD1	1:N:408:GLN:N	2.51	0.44
1:S:267:THR:OG1	1:Y:248:ARG:NH1	2.51	0.44
1:CA:143:THR:HG21	1:EA:156:HIS:CE1	2.52	0.44
1:CA:190:GLN:HG3	1:EA:217:GLY:HA3	2.00	0.44
1:CA:203:ALA:N	1:EA:158:ALA:HB1	2.33	0.44
1:CA:417:ARG:HE	1:CA:417:ARG:HB2	1.71	0.44
1:A:196:HIS:CE1	1:C:224:ASN:HD22	2.35	0.44
1:B:417:ARG:HG3	1:B:422:PHE:HB3	2.00	0.44
1:D:412:ILE:O	1:D:416:THR:HG22	2.18	0.44
1:L:417:ARG:HG3	1:L:422:PHE:HB3	2.00	0.44
1:P:157:LEU:HD21	1:P:159:MET:HG2	2.00	0.44
1:V:228:ARG:O	1:V:232:ASP:N	2.51	0.44
1:Z:154:ARG:HG2	1:EA:143:THR:CG2	2.48	0.44
1:CA:221:THR:HG1	1:CA:224:ASN:HD21	1.56	0.44
1:DA:407:ASP:OD1	1:DA:408:GLN:N	2.50	0.44
1:EA:186:LEU:HD12	1:EA:186:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:HE1	1:D:172:PRO:HB3	2.00	0.43
1:P:130:VAL:HB	1:V:132:TYR:CE1	2.53	0.43
1:P:143:THR:HG21	1:R:156:HIS:CE1	2.53	0.43
1:P:154:ARG:HG2	1:V:143:THR:CG2	2.48	0.43
1:R:391:VAL:HG21	1:R:409:MET:HE1	1.99	0.43
1:X:385:LEU:N	1:X:428:ASP:OD1	2.39	0.43
1:Z:146:THR:HG23	1:Z:146:THR:O	2.16	0.43
1:D:275:LYS:HG3	1:I:375:THR:HG23	2.00	0.43
1:Z:400:LYS:HD2	1:Z:401:PRO:HD2	1.98	0.43
1:CA:245:ILE:HG22	1:CA:249:ILE:HD11	2.00	0.43
1:FA:190:GLN:HG3	1:HA:217:GLY:HA3	2.00	0.43
1:HA:393:TYR:CE2	1:HA:436:PRO:HD3	2.54	0.43
1:A:157:LEU:HD11	1:A:202:VAL:HG21	2.00	0.43
1:A:187:ASP:OD1	1:A:190:GLN:N	2.48	0.43
1:A:228:ARG:HB3	1:A:231:ASN:OD1	2.18	0.43
1:K:417:ARG:HG3	1:K:422:PHE:HB3	2.00	0.43
1:L:150:VAL:HA	1:L:180:LEU:HA	2.00	0.43
1:M:234:GLN:HB3	1:M:272:PHE:CE2	2.54	0.43
1:M:244:ARG:HH12	1:N:235:LEU:HB3	1.83	0.43
1:W:385:LEU:N	1:W:428:ASP:OD1	2.35	0.43
1:AA:277:GLN:HG2	1:AA:279:GLU:OE2	2.18	0.43
1:AA:391:VAL:HG21	1:AA:409:MET:HE1	2.00	0.43
1:AA:408:GLN:O	1:AA:411:GLN:HG2	2.19	0.43
1:CA:400:LYS:HD3	1:CA:400:LYS:C	2.44	0.43
1:FA:203:ALA:N	1:HA:158:ALA:HB1	2.34	0.43
1:A:192:SER:HA	1:A:195:VAL:HG22	2.00	0.43
1:C:186:LEU:HD12	1:C:186:LEU:H	1.84	0.43
1:C:291:ALA:HB1	1:C:366:TYR:HE1	1.84	0.43
1:J:217:GLY:HA3	1:O:190:GLN:HG3	1.99	0.43
1:O:157:LEU:HD21	1:O:202:VAL:HG22	2.01	0.43
1:O:225:THR:HG22	1:O:227:GLY:N	2.33	0.43
1:S:235:LEU:HD21	1:Y:241:VAL:HG22	2.01	0.43
1:CA:143:THR:CG2	1:EA:154:ARG:HG2	2.49	0.43
1:FA:416:THR:HG23	1:FA:430:LEU:HD21	2.00	0.43
1:GA:402:LEU:HA	1:GA:403:PRO:HD2	1.67	0.43
1:HA:267:THR:OG1	1:HA:386:SER:HB2	2.18	0.43
1:J:393:TYR:CE2	1:J:436:PRO:HD3	2.54	0.43
1:L:290:LYS:HB2	1:L:290:LYS:HE3	1.75	0.43
1:M:244:ARG:NH1	1:N:235:LEU:HB3	2.33	0.43
1:W:412:ILE:O	1:W:416:THR:HG22	2.18	0.43
1:X:408:GLN:O	1:X:412:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:426:ARG:NH2	1:X:428:ASP:OD2	2.42	0.43
1:Z:194:VAL:HG21	1:Z:212:LEU:HD21	2.01	0.43
1:BA:394:LYS:HE2	1:BA:396:LEU:O	2.19	0.43
1:BA:396:LEU:HD23	1:BA:396:LEU:HA	1.93	0.43
1:CA:219:LEU:CD2	1:HA:193:ALA:HA	2.40	0.43
1:CA:275:LYS:HB3	1:CA:377:MET:HB2	2.01	0.43
1:DA:101:ALA:HB1	1:DA:193:ALA:HA	1.99	0.43
1:EA:157:LEU:HD21	1:EA:202:VAL:HG22	2.00	0.43
1:GA:238:ALA:O	1:GA:242:GLU:HG2	2.19	0.43
1:HA:199:SER:OG	1:HA:207:PRO:HD3	2.18	0.43
1:A:394:LYS:HA	1:A:394:LYS:HE2	2.00	0.43
1:B:253:LEU:HD23	1:B:253:LEU:HA	1.86	0.43
1:D:219:LEU:CD2	1:I:193:ALA:HA	2.49	0.43
1:G:377:MET:HE3	1:G:377:MET:HB3	1.82	0.43
1:I:196:HIS:CD2	1:I:207:PRO:HG3	2.54	0.43
1:N:253:LEU:HD22	1:N:412:ILE:HG23	1.99	0.43
1:S:199:SER:HA	1:S:205:LEU:HD22	2.00	0.43
1:Z:232:ASP:HA	1:EA:237:PHE:HE1	1.84	0.43
1:BA:186:LEU:H	1:BA:186:LEU:HD12	1.84	0.43
1:CA:192:SER:HA	1:CA:195:VAL:HG22	2.01	0.43
1:CA:194:VAL:HG21	1:CA:212:LEU:HD21	2.01	0.43
1:DA:408:GLN:O	1:DA:411:GLN:HG2	2.18	0.43
1:DA:409:MET:HE3	1:DA:412:ILE:HD12	2.01	0.43
1:GA:244:ARG:NH2	1:GA:248:ARG:HH22	2.16	0.43
1:K:244:ARG:NH2	1:K:248:ARG:HH22	2.17	0.43
1:R:186:LEU:HD12	1:R:186:LEU:H	1.83	0.43
1:S:191:ILE:HG13	1:S:220:LEU:HB3	2.00	0.43
1:Z:143:THR:HG21	1:BA:156:HIS:CE1	2.54	0.43
1:CA:253:LEU:CD2	1:CA:412:ILE:HG23	2.48	0.43
1:EA:391:VAL:HG21	1:EA:409:MET:HE1	2.00	0.43
1:FA:197:LEU:HD12	1:HA:175:SER:HB2	2.00	0.43
1:A:154:ARG:HG2	1:F:143:THR:CG2	2.49	0.43
1:A:296:ARG:NH2	1:A:362:GLU:OE2	2.51	0.43
1:B:393:TYR:HB3	1:B:401:PRO:HB2	2.01	0.43
1:G:187:ASP:OD1	1:G:190:GLN:N	2.44	0.43
1:I:393:TYR:CE2	1:I:436:PRO:HD3	2.54	0.43
1:M:143:THR:HG21	1:O:156:HIS:CE1	2.53	0.43
1:M:244:ARG:HH22	1:N:235:LEU:HA	1.83	0.43
1:M:253:LEU:CD2	1:M:412:ILE:HG23	2.48	0.43
1:S:217:GLY:HA3	1:Y:190:GLN:HG3	1.99	0.43
1:HA:186:LEU:HD12	1:HA:186:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:O	1:A:418:GLU:HG2	2.19	0.43
1:J:234:GLN:HB3	1:J:272:PHE:CE2	2.54	0.43
1:M:402:LEU:HD12	1:M:403:PRO:HD2	1.99	0.43
1:Q:417:ARG:HG3	1:Q:422:PHE:CB	2.49	0.43
1:S:293:LEU:HD13	1:S:296:ARG:HD2	2.01	0.43
1:T:377:MET:HE3	1:T:377:MET:HB3	1.91	0.43
1:Z:244:ARG:HD2	1:Z:244:ARG:HA	1.78	0.43
1:AA:402:LEU:HA	1:AA:403:PRO:HD2	1.67	0.43
1:BA:194:VAL:O	1:BA:198:VAL:HG22	2.19	0.43
1:CA:385:LEU:N	1:CA:428:ASP:OD1	2.34	0.43
1:A:222:GLN:OE1	1:A:222:GLN:N	2.40	0.43
1:C:136:LEU:HD11	1:C:157:LEU:HD22	2.01	0.43
1:H:402:LEU:HD12	1:H:402:LEU:O	2.19	0.43
1:L:158:ALA:C	1:L:159:MET:HE2	2.44	0.43
1:N:414:ASP:O	1:N:418:GLU:HG2	2.19	0.43
1:O:186:LEU:HD12	1:O:186:LEU:H	1.84	0.43
1:O:394:LYS:HE2	1:O:396:LEU:O	2.19	0.43
1:Q:407:ASP:OD1	1:Q:408:GLN:N	2.52	0.43
1:R:420:MET:HE3	1:R:422:PHE:HB2	2.01	0.43
1:X:396:LEU:HD23	1:X:396:LEU:HA	1.91	0.43
1:Z:173:SER:HB2	1:EA:200:SER:O	2.19	0.43
1:BA:196:HIS:HA	1:BA:199:SER:OG	2.19	0.43
1:FA:404:LEU:H	1:FA:434:ASN:ND2	2.17	0.43
1:GA:409:MET:HB2	1:GA:409:MET:HE2	1.74	0.43
1:D:154:ARG:HG2	1:I:143:THR:CG2	2.49	0.42
1:F:393:TYR:CE2	1:F:436:PRO:HD3	2.54	0.42
1:F:402:LEU:HA	1:F:403:PRO:HD2	1.91	0.42
1:G:385:LEU:HD23	1:G:385:LEU:HA	1.91	0.42
1:I:291:ALA:HB1	1:I:366:TYR:HE1	1.84	0.42
1:J:143:THR:HG21	1:L:156:HIS:CE1	2.53	0.42
1:L:385:LEU:N	1:L:428:ASP:OD1	2.43	0.42
1:P:417:ARG:HE	1:P:417:ARG:HB2	1.74	0.42
1:S:232:ASP:OD2	1:S:232:ASP:C	2.62	0.42
1:T:410:LYS:HD2	1:T:410:LYS:O	2.19	0.42
1:Y:414:ASP:O	1:Y:418:GLU:HG2	2.18	0.42
1:Z:143:THR:CG2	1:BA:154:ARG:HG2	2.49	0.42
1:CA:244:ARG:HH22	1:DA:235:LEU:CA	2.32	0.42
1:A:190:GLN:HG3	1:C:217:GLY:HA3	2.01	0.42
1:M:197:LEU:HA	1:O:211:THR:HG21	2.01	0.42
1:M:252:ILE:HB	1:N:265:GLN:HG3	2.01	0.42
1:P:126:PHE:CE2	1:V:129:GLN:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:271:ASP:O	1:Y:380:GLY:N	2.47	0.42
1:EA:155:VAL:HG13	1:EA:176:VAL:HG22	2.01	0.42
1:F:267:THR:OG1	1:F:386:SER:HB2	2.19	0.42
1:G:391:VAL:HG21	1:G:409:MET:HE1	2.01	0.42
1:J:197:LEU:HA	1:L:211:THR:HG21	2.01	0.42
1:J:275:LYS:HB3	1:J:377:MET:HB2	2.01	0.42
1:L:378:ASN:HB3	1:L:381:ASP:OD1	2.19	0.42
1:M:360:ARG:N	1:R:300:ILE:O	2.50	0.42
1:P:404:LEU:H	1:P:434:ASN:ND2	2.17	0.42
1:Q:402:LEU:HD12	1:Q:402:LEU:O	2.18	0.42
1:R:155:VAL:HG13	1:R:176:VAL:HG22	2.00	0.42
1:R:179:THR:HG23	1:R:215:GLN:HB3	2.02	0.42
1:T:301:SER:HB3	1:T:359:GLN:HB2	2.00	0.42
1:V:228:ARG:HA	1:V:231:ASN:OD1	2.18	0.42
1:W:203:ALA:N	1:Y:158:ALA:HB1	2.34	0.42
1:Y:291:ALA:HB1	1:Y:366:TYR:HE1	1.84	0.42
1:Y:393:TYR:CE2	1:Y:436:PRO:HD3	2.53	0.42
1:FA:196:HIS:CE1	1:HA:224:ASN:HD22	2.37	0.42
1:HA:194:VAL:O	1:HA:198:VAL:HG22	2.19	0.42
1:HA:228:ARG:HA	1:HA:231:ASN:OD1	2.20	0.42
1:A:143:THR:HG21	1:C:156:HIS:CE1	2.55	0.42
1:I:378:ASN:HB3	1:I:381:ASP:OD2	2.20	0.42
1:J:244:ARG:NH1	1:K:235:LEU:O	2.48	0.42
1:M:143:THR:CG2	1:O:154:ARG:HG2	2.49	0.42
1:N:290:LYS:HB2	1:N:290:LYS:HE2	1.85	0.42
1:P:175:SER:HA	1:P:211:THR:HG22	2.00	0.42
1:Q:412:ILE:HD12	1:Q:412:ILE:H	1.85	0.42
1:T:252:ILE:HB	1:V:265:GLN:HG3	2.02	0.42
1:W:191:ILE:HD13	1:W:191:ILE:HA	1.84	0.42
1:Y:240:ASP:O	1:Y:244:ARG:HG3	2.19	0.42
1:Z:156:HIS:NE2	1:EA:143:THR:HG21	2.33	0.42
1:Z:190:GLN:HG3	1:BA:217:GLY:HA3	2.01	0.42
1:CA:219:LEU:HA	1:CA:219:LEU:HD22	1.83	0.42
1:FA:394:LYS:HE2	1:FA:394:LYS:HA	2.00	0.42
1:HA:150:VAL:HA	1:HA:180:LEU:HA	2.02	0.42
1:C:196:HIS:O	1:C:200:SER:OG	2.27	0.42
1:C:414:ASP:HB3	1:FA:431:ASN:ND2	2.34	0.42
1:D:234:GLN:HB3	1:D:272:PHE:CE2	2.55	0.42
1:F:383:GLU:O	1:F:426:ARG:HB3	2.19	0.42
1:H:407:ASP:OD1	1:H:408:GLN:N	2.52	0.42
1:I:408:GLN:O	1:I:411:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:253:LEU:CD2	1:J:412:ILE:HG23	2.48	0.42
1:M:192:SER:HA	1:M:195:VAL:HG22	2.00	0.42
1:M:196:HIS:CE1	1:O:224:ASN:HD22	2.37	0.42
1:N:417:ARG:HG3	1:N:422:PHE:HB3	2.01	0.42
1:P:211:THR:HG21	1:V:197:LEU:HA	2.01	0.42
1:Q:101:ALA:HB1	1:Q:193:ALA:HA	1.99	0.42
1:T:373:ARG:NH2	1:V:275:LYS:HE2	2.33	0.42
1:W:234:GLN:HB3	1:W:272:PHE:CE2	2.55	0.42
1:W:394:LYS:HA	1:W:394:LYS:HE2	2.00	0.42
1:X:415:LEU:HD11	1:Y:433:VAL:HG21	1.99	0.42
1:Z:159:MET:SD	1:Z:159:MET:N	2.93	0.42
1:BA:393:TYR:CE2	1:BA:436:PRO:HD3	2.55	0.42
1:D:420:MET:HE2	1:D:420:MET:HB3	1.92	0.42
1:F:266:VAL:HG22	1:F:387:VAL:HG22	2.02	0.42
1:L:186:LEU:HD12	1:L:186:LEU:H	1.84	0.42
1:M:133:GLN:NE2	1:M:157:LEU:O	2.52	0.42
1:M:393:TYR:CE2	1:M:436:PRO:HD3	2.55	0.42
1:W:252:ILE:HB	1:X:265:GLN:HG3	2.01	0.42
1:Y:144:ILE:HG22	1:Y:153:ALA:HB2	2.01	0.42
1:CA:157:LEU:HD11	1:CA:202:VAL:HG21	2.01	0.42
1:FA:252:ILE:HB	1:GA:265:GLN:HG3	2.00	0.42
1:FA:296:ARG:NH2	1:FA:362:GLU:OE2	2.52	0.42
1:HA:196:HIS:HA	1:HA:199:SER:HG	1.84	0.42
1:A:133:GLN:HG3	1:A:157:LEU:HD22	2.02	0.42
1:A:234:GLN:H	1:A:234:GLN:HG3	1.65	0.42
1:A:293:LEU:HD13	1:A:296:ARG:HD2	2.02	0.42
1:I:194:VAL:O	1:I:198:VAL:HG22	2.20	0.42
1:P:402:LEU:HD12	1:P:403:PRO:HD2	2.00	0.42
1:Q:426:ARG:NH2	1:Q:428:ASP:OD2	2.44	0.42
1:S:194:VAL:HG21	1:S:212:LEU:HD21	2.01	0.42
1:V:186:LEU:H	1:V:186:LEU:HD12	1.83	0.42
1:FA:404:LEU:HD23	1:FA:408:GLN:HG2	2.02	0.42
1:FA:411:GLN:O	1:FA:415:LEU:HD23	2.20	0.42
1:HA:192:SER:HA	1:HA:195:VAL:HB	2.02	0.42
1:C:158:ALA:O	1:C:159:MET:HE2	2.19	0.42
1:I:186:LEU:HD12	1:I:186:LEU:H	1.83	0.42
1:I:402:LEU:HA	1:I:403:PRO:HD2	1.92	0.42
1:J:377:MET:HE3	1:J:377:MET:HB3	1.82	0.42
1:R:225:THR:HG22	1:R:227:GLY:N	2.30	0.42
1:S:191:ILE:O	1:S:195:VAL:HG13	2.20	0.42
1:Z:159:MET:HE1	1:Z:172:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:267:THR:OG1	1:BA:386:SER:HB2	2.20	0.42
1:FA:245:ILE:O	1:FA:249:ILE:HG13	2.19	0.42
1:D:203:ALA:N	1:F:158:ALA:HB1	2.34	0.42
1:F:151:LYS:NZ	1:F:179:THR:HG22	2.34	0.42
1:F:245:ILE:HG22	1:F:266:VAL:HG21	2.01	0.42
1:J:150:VAL:HG13	1:J:178:VAL:HG23	2.02	0.42
1:N:275:LYS:HB3	1:N:377:MET:HB2	2.01	0.42
1:P:425:LYS:HB3	1:P:425:LYS:HE3	1.84	0.42
1:R:396:LEU:HD23	1:R:396:LEU:HA	1.95	0.42
1:S:252:ILE:HB	1:T:265:GLN:HG3	2.02	0.42
1:A:227:GLY:HA3	1:F:230:LEU:HD13	2.02	0.42
1:B:393:TYR:CZ	1:B:403:PRO:HD3	2.54	0.42
1:G:197:LEU:HA	1:I:211:THR:HG21	2.01	0.42
1:G:225:THR:HG22	1:L:196:HIS:NE2	2.35	0.42
1:I:404:LEU:H	1:I:434:ASN:ND2	2.17	0.42
1:K:291:ALA:HB1	1:K:366:TYR:HE1	1.85	0.42
1:P:234:GLN:HB3	1:P:272:PHE:CE2	2.55	0.42
1:P:412:ILE:O	1:P:416:THR:HG22	2.19	0.42
1:W:211:THR:OG1	1:W:224:ASN:OD1	2.24	0.42
1:Z:402:LEU:HD12	1:Z:403:PRO:HD2	2.02	0.42
1:CA:411:GLN:O	1:CA:415:LEU:HD23	2.20	0.42
1:A:130:VAL:HG11	1:F:132:TYR:CZ	2.55	0.41
1:D:292:THR:HG21	1:E:282:TYR:HB3	2.01	0.41
1:I:420:MET:HE1	1:I:430:LEU:HB2	2.01	0.41
1:M:410:LYS:O	1:M:410:LYS:HD3	2.20	0.41
1:P:394:LYS:HE2	1:P:394:LYS:HA	2.00	0.41
1:R:408:GLN:O	1:R:411:GLN:HG2	2.20	0.41
1:S:203:ALA:N	1:V:158:ALA:HB1	2.34	0.41
1:FA:248:ARG:O	1:FA:252:ILE:HG22	2.20	0.41
1:C:266:VAL:HG22	1:C:387:VAL:HG22	2.01	0.41
1:I:414:ASP:O	1:I:418:GLU:HG2	2.20	0.41
1:K:230:LEU:HD12	1:K:230:LEU:O	2.20	0.41
1:M:157:LEU:HD21	1:M:159:MET:HG2	2.01	0.41
1:O:290:LYS:HE3	1:O:290:LYS:HB2	1.76	0.41
1:P:389:VAL:HB	1:P:432:VAL:HG22	2.02	0.41
1:R:194:VAL:O	1:R:198:VAL:HG22	2.19	0.41
1:AA:396:LEU:HD23	1:AA:396:LEU:HA	1.94	0.41
1:BA:158:ALA:O	1:BA:159:MET:HE2	2.21	0.41
1:CA:234:GLN:HB3	1:CA:272:PHE:CE2	2.56	0.41
1:CA:244:ARG:HH12	1:DA:235:LEU:HB3	1.86	0.41
1:DA:410:LYS:HD2	1:DA:410:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:415:LEU:HD11	1:EA:433:VAL:HG21	2.00	0.41
1:DA:417:ARG:HG3	1:DA:422:PHE:CB	2.49	0.41
1:GA:259:ASN:OD1	1:GA:259:ASN:C	2.63	0.41
1:C:159:MET:HE2	1:C:159:MET:HA	2.02	0.41
1:C:252:ILE:HD12	1:C:252:ILE:HA	1.94	0.41
1:G:143:THR:CG2	1:I:154:ARG:HG2	2.49	0.41
1:I:228:ARG:O	1:I:232:ASP:N	2.51	0.41
1:I:271:ASP:OD2	1:I:383:GLU:HG3	2.20	0.41
1:L:417:ARG:HG3	1:L:422:PHE:CB	2.50	0.41
1:M:222:GLN:OE1	1:M:222:GLN:N	2.38	0.41
1:V:253:LEU:HD23	1:V:253:LEU:HA	1.88	0.41
1:V:253:LEU:CD2	1:V:412:ILE:HG23	2.48	0.41
1:W:372:ILE:O	1:X:277:GLN:HA	2.20	0.41
1:AA:410:LYS:HD2	1:AA:410:LYS:C	2.45	0.41
1:EA:393:TYR:CE2	1:EA:436:PRO:HD3	2.55	0.41
1:FA:191:ILE:HD13	1:FA:191:ILE:HA	1.83	0.41
1:A:158:ALA:O	1:A:159:MET:HE2	2.21	0.41
1:H:253:LEU:HD22	1:H:412:ILE:HG23	2.02	0.41
1:J:186:LEU:HB3	1:J:190:GLN:HB3	2.03	0.41
1:J:232:ASP:OD2	1:J:232:ASP:C	2.62	0.41
1:L:228:ARG:O	1:L:232:ASP:N	2.49	0.41
1:M:150:VAL:HG13	1:M:178:VAL:HG23	2.02	0.41
1:M:420:MET:HE3	1:M:420:MET:HB3	1.84	0.41
1:P:186:LEU:HB3	1:P:190:GLN:HB3	2.02	0.41
1:Q:253:LEU:HD23	1:Q:253:LEU:HA	1.90	0.41
1:Q:362:GLU:OE2	1:Q:364:SER:OG	2.27	0.41
1:V:132:TYR:N	1:V:132:TYR:CD2	2.86	0.41
1:X:410:LYS:HD2	1:X:410:LYS:O	2.20	0.41
1:BA:383:GLU:O	1:BA:426:ARG:HB3	2.20	0.41
1:EA:136:LEU:HD11	1:EA:157:LEU:HD22	2.02	0.41
1:FA:143:THR:HG21	1:HA:156:HIS:CE1	2.55	0.41
1:B:248:ARG:NH1	1:C:267:THR:HG22	2.34	0.41
1:E:253:LEU:HD23	1:E:253:LEU:HA	1.90	0.41
1:F:195:VAL:HA	1:F:210:VAL:HG11	2.03	0.41
1:G:203:ALA:N	1:I:158:ALA:HB1	2.36	0.41
1:G:227:GLY:HA3	1:L:230:LEU:HD13	2.02	0.41
1:L:225:THR:HG22	1:L:227:GLY:N	2.32	0.41
1:M:194:VAL:HG21	1:M:212:LEU:HD21	2.03	0.41
1:P:128:GLU:HA	1:P:131:ASN:HD21	1.85	0.41
1:P:244:ARG:HH22	1:Q:235:LEU:CA	2.33	0.41
1:T:393:TYR:CZ	1:T:403:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:150:VAL:HG13	1:W:178:VAL:HG23	2.02	0.41
1:X:389:VAL:HB	1:X:432:VAL:HG22	2.02	0.41
1:Z:411:GLN:O	1:Z:415:LEU:HD23	2.20	0.41
1:BA:228:ARG:HA	1:BA:231:ASN:OD1	2.21	0.41
1:GA:248:ARG:NH1	1:HA:267:THR:HG22	2.36	0.41
1:D:143:THR:CG2	1:F:154:ARG:HG2	2.50	0.41
1:D:197:LEU:HA	1:F:211:THR:HG21	2.01	0.41
1:D:234:GLN:H	1:D:234:GLN:HG3	1.63	0.41
1:F:140:LEU:HB2	1:F:155:VAL:HG21	2.03	0.41
1:H:293:LEU:HD13	1:H:296:ARG:HD2	2.03	0.41
1:T:393:TYR:CE2	1:T:403:PRO:HD3	2.55	0.41
1:W:143:THR:HG21	1:Y:156:HIS:CE1	2.56	0.41
1:Y:228:ARG:HA	1:Y:231:ASN:OD1	2.20	0.41
1:EA:140:LEU:HB2	1:EA:155:VAL:HG21	2.02	0.41
1:C:143:THR:CG2	1:FA:154:ARG:HG2	2.51	0.41
1:P:410:LYS:O	1:P:410:LYS:HD3	2.20	0.41
1:S:186:LEU:HB3	1:S:190:GLN:HB3	2.02	0.41
1:W:154:ARG:HG2	1:BA:143:THR:CG2	2.50	0.41
1:W:190:GLN:HG3	1:Y:217:GLY:HA3	2.02	0.41
1:HA:252:ILE:HD12	1:HA:252:ILE:HA	1.94	0.41
1:K:393:TYR:O	1:K:394:LYS:HB2	2.21	0.41
1:L:402:LEU:HA	1:L:403:PRO:HD2	1.93	0.41
1:O:393:TYR:CE2	1:O:436:PRO:HD3	2.56	0.41
1:R:394:LYS:HE2	1:R:396:LEU:O	2.20	0.41
1:W:267:THR:OG1	1:BA:248:ARG:NH1	2.54	0.41
1:Z:245:ILE:O	1:Z:249:ILE:HG13	2.21	0.41
1:CA:157:LEU:CD2	1:CA:159:MET:HG2	2.45	0.41
1:FA:412:ILE:HD12	1:FA:412:ILE:H	1.85	0.41
1:FA:417:ARG:HE	1:FA:417:ARG:HB2	1.58	0.41
1:GA:385:LEU:N	1:GA:428:ASP:OD1	2.47	0.41
1:A:412:ILE:O	1:A:416:THR:HG22	2.21	0.41
1:B:377:MET:HE3	1:B:377:MET:HB3	1.91	0.41
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.96	0.41
1:C:267:THR:OG1	1:C:386:SER:HB2	2.20	0.41
1:D:241:VAL:O	1:D:245:ILE:HG12	2.21	0.41
1:D:431:ASN:HB2	1:I:418:GLU:HG3	2.03	0.41
1:G:402:LEU:HD12	1:G:403:PRO:HD2	2.03	0.41
1:J:191:ILE:HG13	1:J:220:LEU:HB3	2.03	0.41
1:J:385:LEU:HD23	1:J:385:LEU:HA	1.91	0.41
1:K:248:ARG:NH1	1:L:267:THR:HG22	2.36	0.41
1:K:271:ASP:OD1	1:K:383:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:245:ILE:HG22	1:S:249:ILE:HD11	2.02	0.41
1:S:414:ASP:O	1:S:418:GLU:HG2	2.21	0.41
1:S:425:LYS:HD3	1:S:425:LYS:N	2.36	0.41
1:X:394:LYS:HE2	1:X:394:LYS:HA	2.03	0.41
1:Y:148:GLY:HA3	1:Y:149:PRO:HD3	1.83	0.41
1:Y:194:VAL:O	1:Y:198:VAL:HG22	2.21	0.41
1:Z:410:LYS:HZ2	1:Z:410:LYS:HG3	1.68	0.41
1:AA:301:SER:HB3	1:AA:359:GLN:HB3	2.01	0.41
1:BA:155:VAL:HG13	1:BA:176:VAL:HG22	2.03	0.41
1:EA:395:THR:HB	1:EA:402:LEU:HG	2.03	0.41
1:FA:385:LEU:N	1:FA:428:ASP:OD1	2.33	0.41
1:HA:195:VAL:HA	1:HA:210:VAL:HG11	2.03	0.41
1:HA:408:GLN:O	1:HA:411:GLN:HG2	2.21	0.41
1:A:225:THR:O	1:A:227:GLY:N	2.51	0.41
1:A:243:SER:OG	1:A:247:ARG:NH1	2.54	0.41
1:C:420:MET:HE1	1:C:430:LEU:HB2	2.03	0.41
1:E:418:GLU:HB2	1:F:388:ALA:HB2	2.02	0.41
1:F:186:LEU:H	1:F:186:LEU:HD12	1.86	0.41
1:G:411:GLN:O	1:G:415:LEU:HD23	2.21	0.41
1:H:375:THR:HG23	1:I:275:LYS:HG2	2.03	0.41
1:J:213:VAL:HG11	1:O:197:LEU:HB2	2.03	0.41
1:M:211:THR:HG21	1:R:197:LEU:HA	2.03	0.41
1:P:190:GLN:HG3	1:R:217:GLY:HA3	2.03	0.41
1:R:148:GLY:HA3	1:R:149:PRO:HD3	1.87	0.41
1:W:133:GLN:HG3	1:W:157:LEU:HD22	2.03	0.41
1:W:410:LYS:O	1:W:410:LYS:HD3	2.21	0.41
1:W:419:ALA:O	1:X:267:THR:OG1	2.28	0.41
1:Z:219:LEU:HD21	1:EA:193:ALA:N	2.36	0.41
1:AA:267:THR:HB	1:AA:386:SER:OG	2.21	0.41
1:EA:378:ASN:HB3	1:EA:381:ASP:OD1	2.20	0.41
1:FA:402:LEU:HD12	1:FA:403:PRO:CD	2.51	0.41
1:FA:419:ALA:O	1:GA:267:THR:OG1	2.38	0.41
1:HA:290:LYS:HB2	1:HA:290:LYS:HE2	1.76	0.41
1:A:404:LEU:HD23	1:A:408:GLN:HG2	2.04	0.40
1:C:228:ARG:O	1:C:232:ASP:N	2.53	0.40
1:H:241:VAL:HG22	1:I:235:LEU:HD21	2.03	0.40
1:H:410:LYS:HE3	1:H:410:LYS:HB3	1.92	0.40
1:K:410:LYS:HD2	1:K:410:LYS:O	2.21	0.40
1:N:228:ARG:NH2	1:N:230:LEU:HD13	2.37	0.40
1:P:373:ARG:NH2	1:Q:275:LYS:HE2	2.34	0.40
1:V:148:GLY:HA3	1:V:149:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:356:ARG:HD2	1:BA:356:ARG:N	2.35	0.40
1:GA:393:TYR:HB3	1:GA:401:PRO:HB3	2.03	0.40
1:B:405:THR:HG23	1:B:408:GLN:HB2	2.03	0.40
1:C:393:TYR:CE2	1:C:436:PRO:HD3	2.56	0.40
1:H:253:LEU:CD2	1:H:412:ILE:HG23	2.51	0.40
1:H:385:LEU:N	1:H:428:ASP:OD1	2.48	0.40
1:H:402:LEU:O	1:H:403:PRO:O	2.40	0.40
1:I:150:VAL:HA	1:I:180:LEU:HA	2.02	0.40
1:J:234:GLN:H	1:J:234:GLN:HG3	1.65	0.40
1:V:159:MET:HA	1:V:160:PRO:HD3	1.94	0.40
1:V:267:THR:OG1	1:V:386:SER:HB2	2.21	0.40
1:V:417:ARG:HG3	1:V:422:PHE:HB3	2.04	0.40
1:Y:186:LEU:H	1:Y:186:LEU:HD12	1.87	0.40
1:Z:203:ALA:N	1:BA:158:ALA:HB1	2.36	0.40
1:DA:394:LYS:HD3	1:DA:396:LEU:H	1.85	0.40
1:GA:420:MET:HE3	1:GA:422:PHE:HB2	2.04	0.40
1:D:393:TYR:CE2	1:D:436:PRO:HD3	2.57	0.40
1:F:389:VAL:O	1:F:432:VAL:HA	2.21	0.40
1:G:190:GLN:HG3	1:I:217:GLY:HA3	2.03	0.40
1:Q:248:ARG:NH1	1:R:267:THR:HG22	2.36	0.40
1:V:240:ASP:O	1:V:244:ARG:HG3	2.22	0.40
1:W:197:LEU:HA	1:Y:211:THR:HG21	2.04	0.40
1:Y:196:HIS:HA	1:Y:199:SER:OG	2.20	0.40
1:EA:228:ARG:O	1:EA:232:ASP:N	2.52	0.40
1:D:394:LYS:HD3	1:D:396:LEU:H	1.86	0.40
1:D:416:THR:HG23	1:D:430:LEU:HD21	2.02	0.40
1:E:417:ARG:HH21	1:E:430:LEU:HD23	1.86	0.40
1:G:154:ARG:HG2	1:L:143:THR:CG2	2.51	0.40
1:Q:402:LEU:O	1:Q:403:PRO:O	2.40	0.40
1:S:389:VAL:HG12	1:S:432:VAL:HG13	2.03	0.40
1:V:248:ARG:O	1:V:252:ILE:HG22	2.22	0.40
1:V:393:TYR:CE2	1:V:436:PRO:HD3	2.56	0.40
1:W:234:GLN:H	1:W:234:GLN:HG3	1.67	0.40
1:X:253:LEU:HD23	1:X:253:LEU:HA	1.86	0.40
1:Y:391:VAL:HG23	1:Y:434:ASN:ND2	2.36	0.40
1:Z:404:LEU:HD23	1:Z:408:GLN:HG2	2.04	0.40
1:Z:431:ASN:ND2	1:EA:414:ASP:HB3	2.36	0.40
1:BA:140:LEU:HB2	1:BA:155:VAL:HG21	2.03	0.40
1:HA:266:VAL:HG22	1:HA:387:VAL:HG22	2.04	0.40
1:A:227:GLY:CA	1:F:230:LEU:HD13	2.52	0.40
1:A:283:SER:HB2	1:A:369:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:GLU:O	1:C:426:ARG:HB3	2.22	0.40
1:F:391:VAL:HG23	1:F:434:ASN:ND2	2.37	0.40
1:J:373:ARG:NH1	1:K:277:GLN:OE1	2.54	0.40
1:T:393:TYR:HB3	1:T:401:PRO:HB3	2.03	0.40
1:CA:372:ILE:O	1:DA:277:GLN:HA	2.22	0.40
1:FA:234:GLN:HB3	1:FA:272:PHE:CE2	2.56	0.40
1:GA:395:THR:OG1	1:GA:402:LEU:HG	2.21	0.40
1:HA:396:LEU:HD23	1:HA:396:LEU:HA	1.95	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	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	30	59
1	AA	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	12	40
1	B	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	12	40
1	BA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	C	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	CA	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	30	59
1	D	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	30	59
1	DA	303/560 (54%)	292 (96%)	8 (3%)	3 (1%)	12	40
1	E	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	12	40
1	EA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	F	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	FA	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	30	59
1	G	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GA	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	12	40
1	H	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	12	40
1	HA	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	I	248/560 (44%)	240 (97%)	7 (3%)	1 (0%)	30	59
1	J	248/560 (44%)	239 (96%)	8 (3%)	1 (0%)	30	59
1	K	303/560 (54%)	292 (96%)	8 (3%)	3 (1%)	12	40
1	L	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	M	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	30	59
1	N	303/560 (54%)	293 (97%)	8 (3%)	2 (1%)	18	47
1	O	248/560 (44%)	243 (98%)	4 (2%)	1 (0%)	30	59
1	P	248/560 (44%)	238 (96%)	9 (4%)	1 (0%)	30	59
1	Q	303/560 (54%)	290 (96%)	10 (3%)	3 (1%)	12	40
1	R	248/560 (44%)	243 (98%)	4 (2%)	1 (0%)	30	59
1	S	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	30	59
1	T	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	12	40
1	V	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	W	248/560 (44%)	240 (97%)	7 (3%)	1 (0%)	30	59
1	X	303/560 (54%)	291 (96%)	9 (3%)	3 (1%)	12	40
1	Y	248/560 (44%)	242 (98%)	5 (2%)	1 (0%)	30	59
1	Z	248/560 (44%)	237 (96%)	10 (4%)	1 (0%)	30	59
All	All	8789/18480 (48%)	8483 (96%)	252 (3%)	54 (1%)	23	50

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	ASN
1	B	394	LYS
1	B	403	PRO
1	C	394	LYS
1	E	394	LYS
1	E	403	PRO
1	F	394	LYS
1	H	394	LYS
1	H	403	PRO
1	I	394	LYS

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Mol	Chain	Res	Type
1	K	394	LYS
1	K	403	PRO
1	N	74	ASN
1	N	394	LYS
1	O	394	LYS
1	Q	74	ASN
1	Q	394	LYS
1	Q	403	PRO
1	R	394	LYS
1	T	74	ASN
1	T	394	LYS
1	T	403	PRO
1	V	394	LYS
1	X	394	LYS
1	X	403	PRO
1	Z	394	LYS
1	AA	394	LYS
1	AA	403	PRO
1	BA	394	LYS
1	DA	74	ASN
1	DA	394	LYS
1	DA	403	PRO
1	EA	394	LYS
1	GA	394	LYS
1	GA	403	PRO
1	HA	394	LYS
1	A	394	LYS
1	D	394	LYS
1	E	74	ASN
1	G	394	LYS
1	H	74	ASN
1	J	394	LYS
1	K	74	ASN
1	L	394	LYS
1	M	394	LYS
1	P	394	LYS
1	S	394	LYS
1	W	394	LYS
1	X	74	ASN
1	Y	394	LYS
1	AA	74	ASN
1	CA	394	LYS

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Mol	Chain	Res	Type
1	FA	394	LYS
1	GA	74	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/467 (47%)	218 (100%)	0	100	100
1	AA	142/467 (30%)	141 (99%)	1 (1%)	76	78
1	B	142/467 (30%)	142 (100%)	0	100	100
1	BA	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	C	218/467 (47%)	218 (100%)	0	100	100
1	CA	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	D	218/467 (47%)	218 (100%)	0	100	100
1	DA	142/467 (30%)	142 (100%)	0	100	100
1	E	142/467 (30%)	142 (100%)	0	100	100
1	EA	218/467 (47%)	218 (100%)	0	100	100
1	F	218/467 (47%)	216 (99%)	2 (1%)	70	76
1	FA	218/467 (47%)	218 (100%)	0	100	100
1	G	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	GA	142/467 (30%)	142 (100%)	0	100	100
1	H	142/467 (30%)	142 (100%)	0	100	100
1	HA	218/467 (47%)	218 (100%)	0	100	100
1	I	218/467 (47%)	218 (100%)	0	100	100
1	J	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	K	142/467 (30%)	141 (99%)	1 (1%)	76	78
1	L	218/467 (47%)	218 (100%)	0	100	100
1	M	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	N	142/467 (30%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	218/467 (47%)	218 (100%)	0	100	100
1	P	218/467 (47%)	218 (100%)	0	100	100
1	Q	142/467 (30%)	142 (100%)	0	100	100
1	R	218/467 (47%)	218 (100%)	0	100	100
1	S	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	T	142/467 (30%)	142 (100%)	0	100	100
1	V	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	W	218/467 (47%)	217 (100%)	1 (0%)	81	81
1	X	142/467 (30%)	142 (100%)	0	100	100
1	Y	218/467 (47%)	218 (100%)	0	100	100
1	Z	218/467 (47%)	217 (100%)	1 (0%)	81	81
All	All	6358/15411 (41%)	6345 (100%)	13 (0%)	85	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	231	ASN
1	F	402	LEU
1	G	431	ASN
1	J	431	ASN
1	K	409	MET
1	M	431	ASN
1	S	415	LEU
1	V	369	ASP
1	W	431	ASN
1	Z	230	LEU
1	AA	412	ILE
1	BA	369	ASP
1	CA	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	A	299	ASN
1	A	434	ASN
1	B	361	ASN

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Mol	Chain	Res	Type
1	B	434	ASN
1	C	239	ASN
1	C	411	GLN
1	D	133	GLN
1	D	411	GLN
1	D	434	ASN
1	E	361	ASN
1	F	131	ASN
1	F	196	HIS
1	F	218	HIS
1	F	365	ASN
1	G	133	GLN
1	G	365	ASN
1	G	434	ASN
1	H	434	ASN
1	I	131	ASN
1	I	434	ASN
1	J	131	ASN
1	J	133	GLN
1	J	261	ASN
1	J	434	ASN
1	K	299	ASN
1	K	361	ASN
1	L	131	ASN
1	L	218	HIS
1	M	274	ASN
1	M	299	ASN
1	M	411	GLN
1	M	434	ASN
1	N	431	ASN
1	O	218	HIS
1	O	299	ASN
1	P	131	ASN
1	P	434	ASN
1	Q	361	ASN
1	Q	434	ASN
1	R	299	ASN
1	S	133	GLN
1	S	261	ASN
1	S	299	ASN
1	S	431	ASN
1	S	434	ASN

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Mol	Chain	Res	Type
1	T	361	ASN
1	V	359	GLN
1	W	434	ASN
1	X	431	ASN
1	X	434	ASN
1	Y	365	ASN
1	Y	411	GLN
1	Z	133	GLN
1	Z	239	ASN
1	Z	299	ASN
1	Z	365	ASN
1	Z	431	ASN
1	AA	361	ASN
1	BA	299	ASN
1	BA	365	ASN
1	CA	133	GLN
1	CA	261	ASN
1	CA	411	GLN
1	CA	434	ASN
1	DA	365	ASN
1	DA	431	ASN
1	DA	434	ASN
1	EA	131	ASN
1	EA	218	HIS
1	FA	131	ASN
1	FA	133	GLN
1	FA	261	ASN
1	FA	411	GLN
1	FA	431	ASN
1	FA	434	ASN
1	GA	361	ASN
1	GA	434	ASN
1	HA	299	ASN
1	HA	359	GLN
1	HA	365	ASN
1	HA	434	ASN

5.3.3 RNA ⓘ

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.

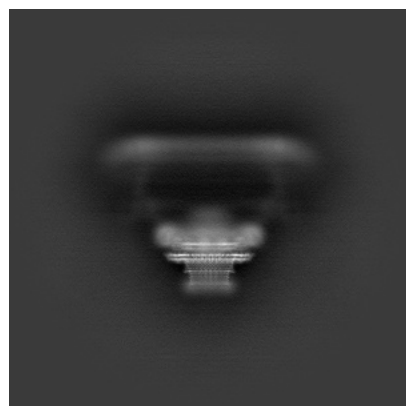
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41101. These allow visual inspection of the internal detail of the map and identification of artifacts.

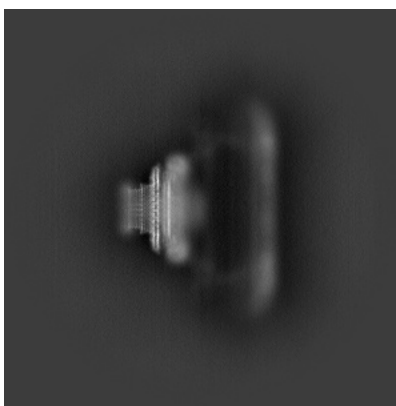
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

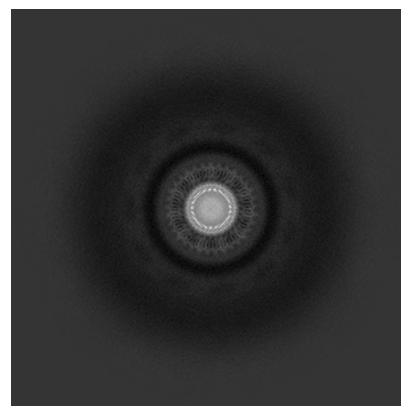
6.1.1 Primary map



X

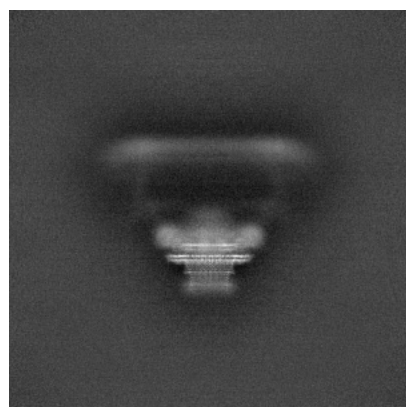


Y

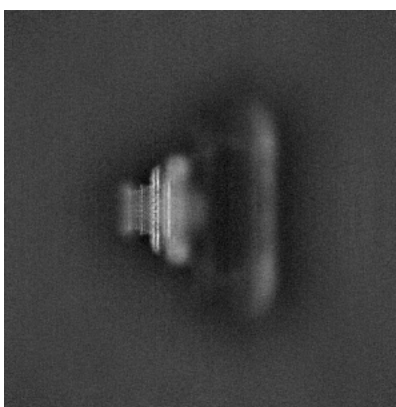


Z

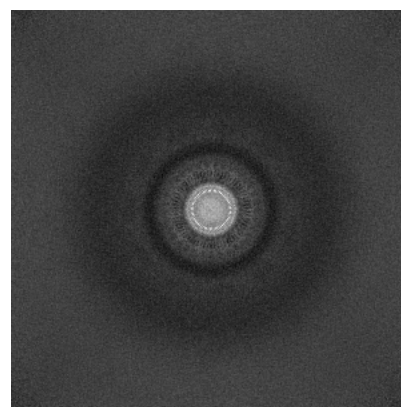
6.1.2 Raw map



X



Y

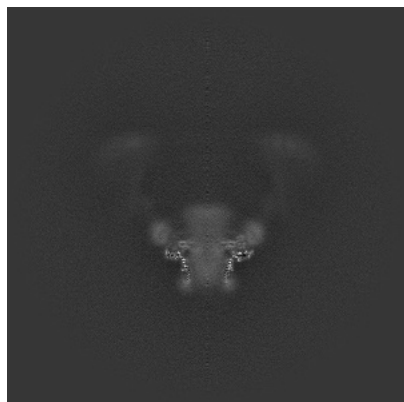


Z

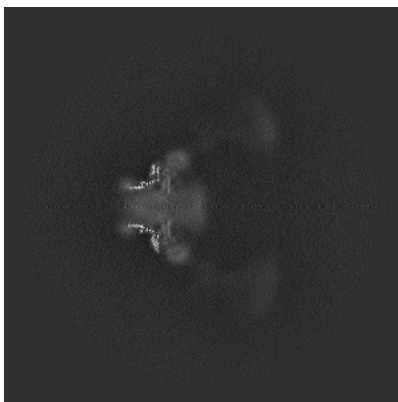
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

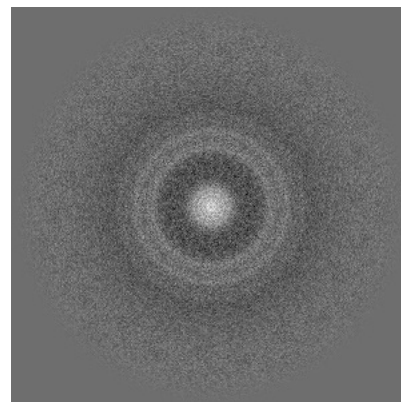
6.2.1 Primary map



X Index: 384



Y Index: 384



Z Index: 384

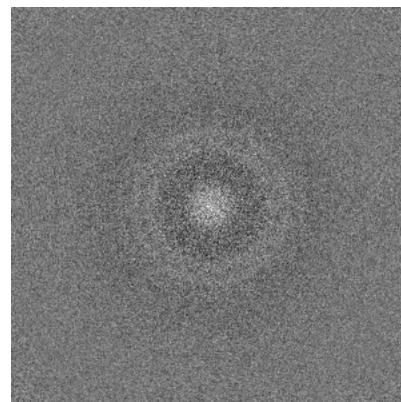
6.2.2 Raw map



X Index: 384



Y Index: 384

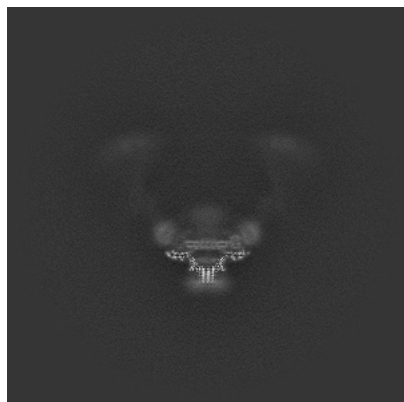


Z Index: 384

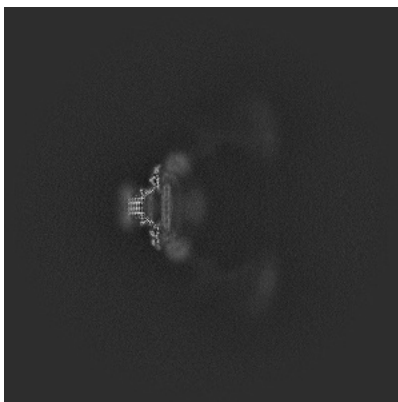
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

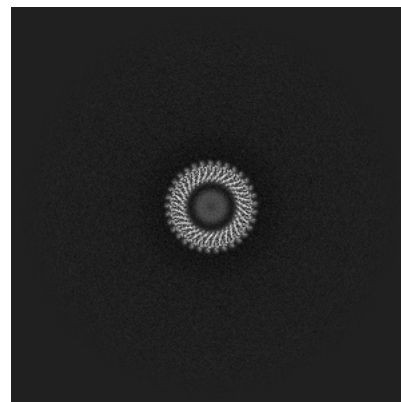
6.3.1 Primary map



X Index: 348



Y Index: 419



Z Index: 295

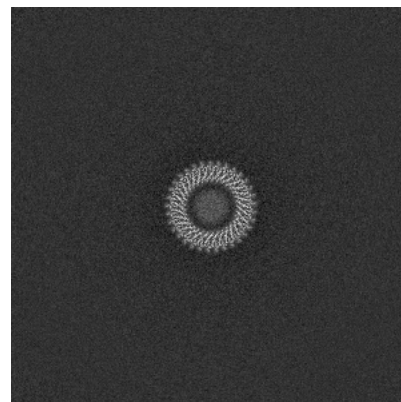
6.3.2 Raw map



X Index: 348



Y Index: 384

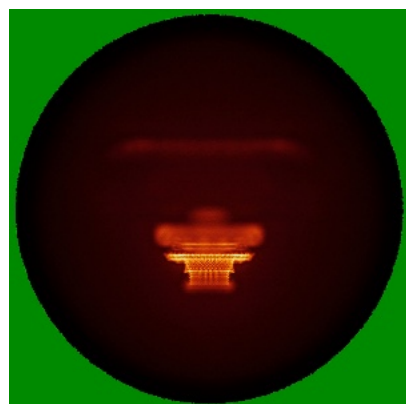


Z Index: 295

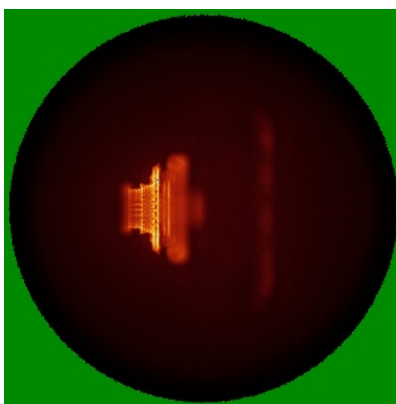
The images above show the largest variance slices of the map in three orthogonal directions.

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

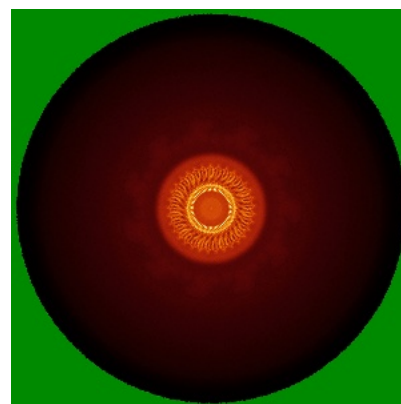
6.4.1 Primary map



X

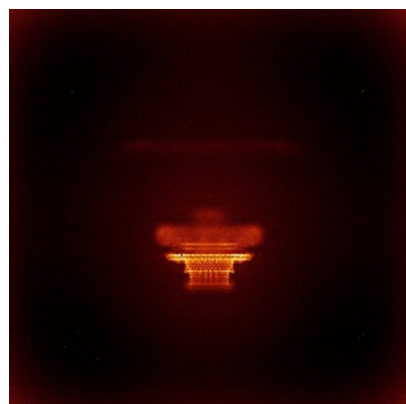


Y

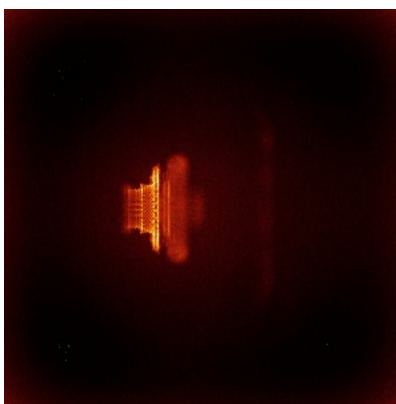


Z

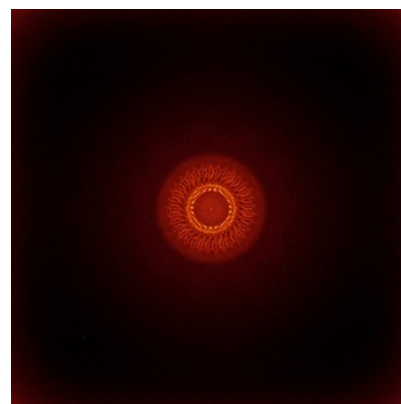
6.4.2 Raw map



X



Y

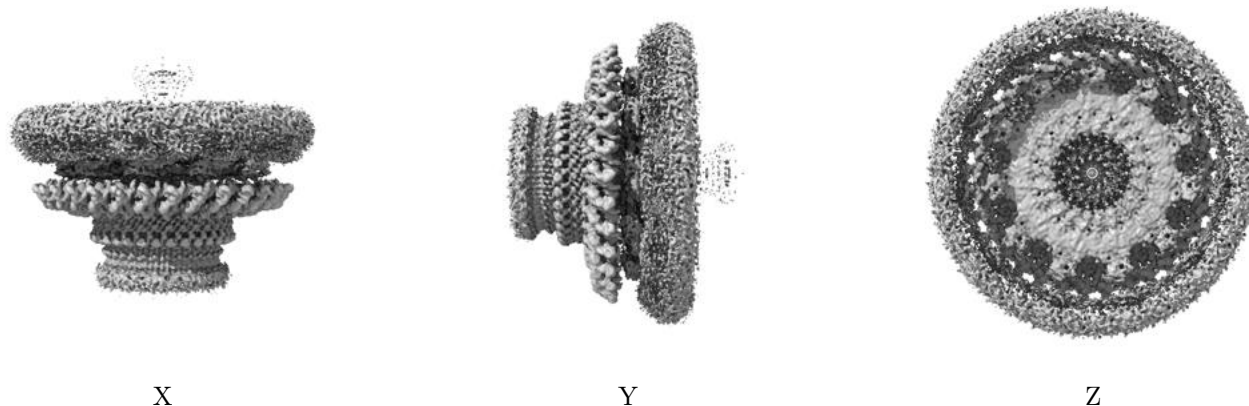


Z

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

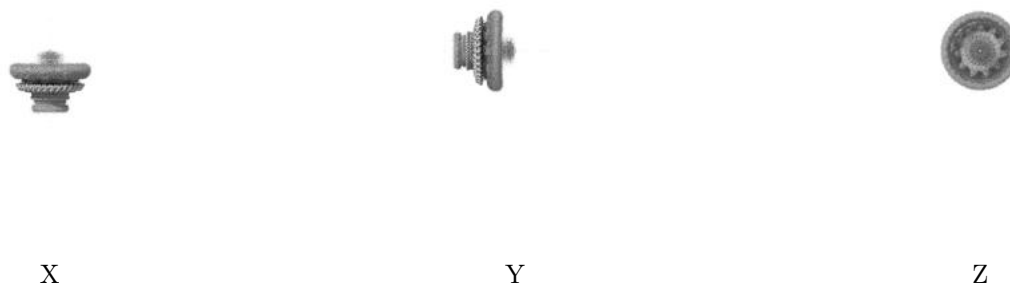
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

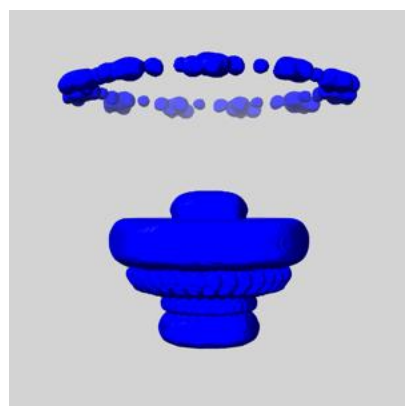
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

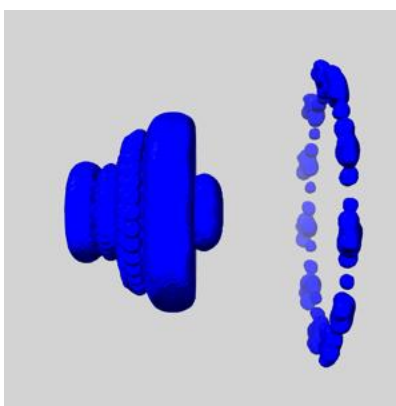
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

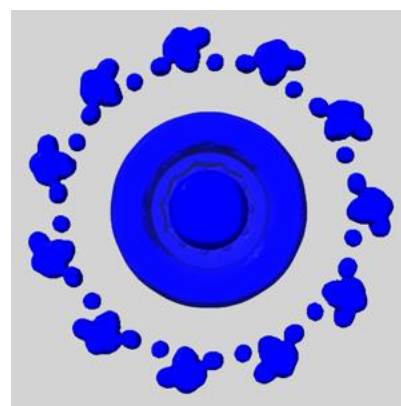
6.6.1 emd_41101_msk_1.map [i](#)



X



Y

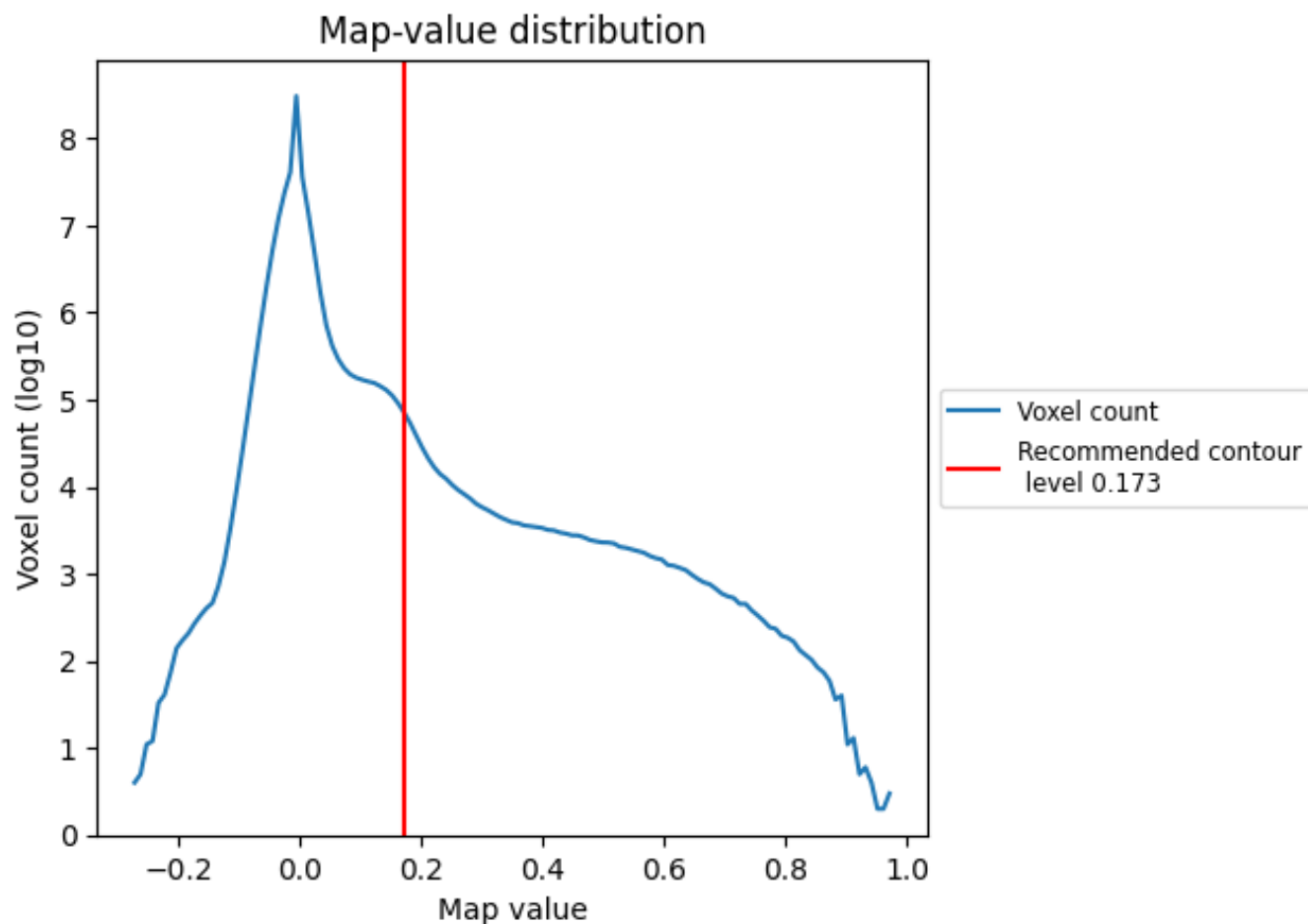


Z

7 Map analysis [i](#)

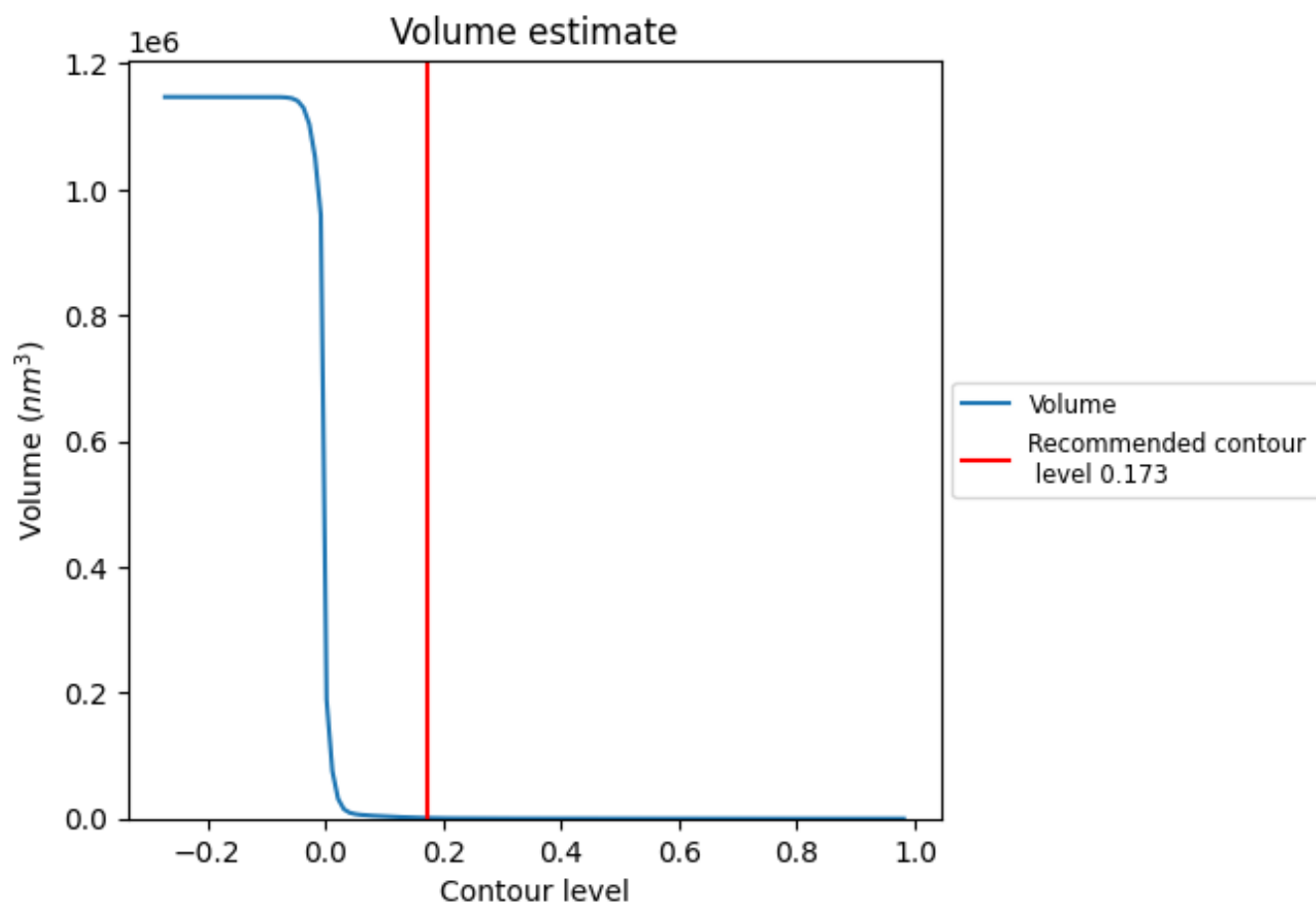
This section contains the results of statistical analysis of the map.

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.

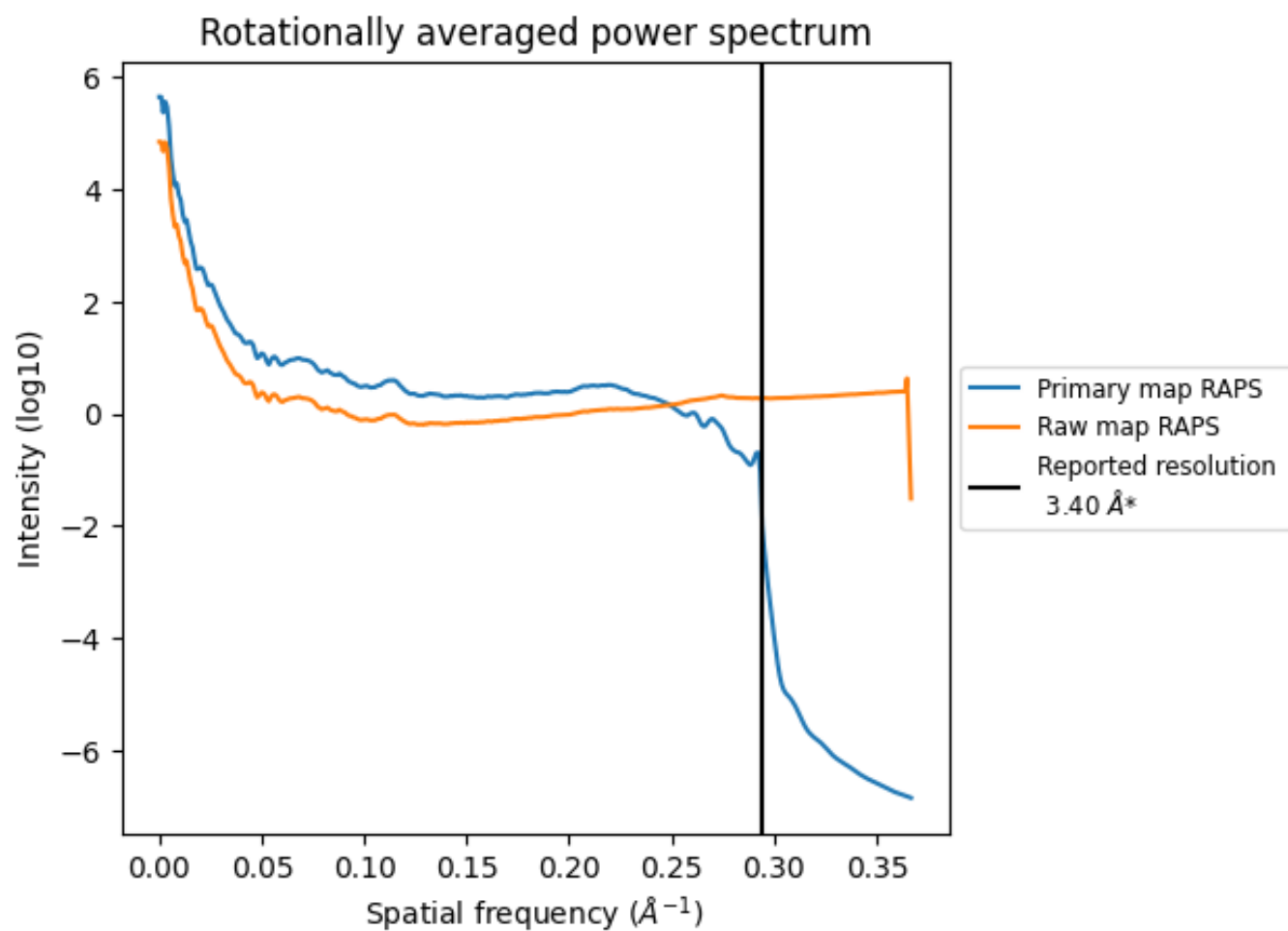
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1012 nm^3 ; this corresponds to an approximate mass of 914 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

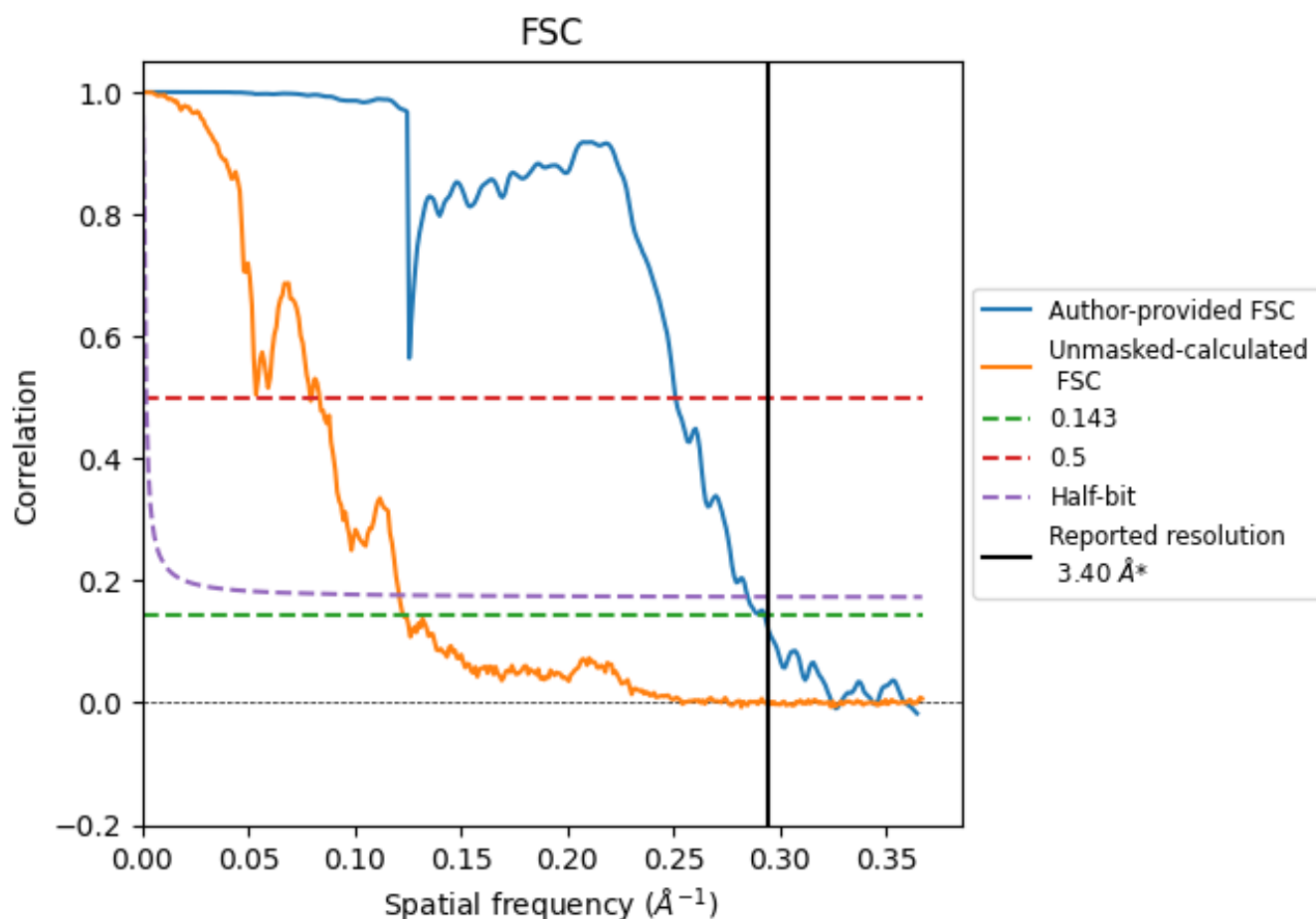


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

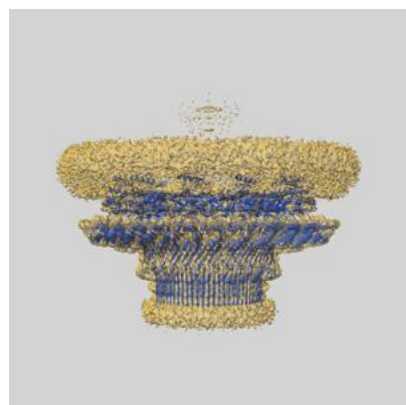
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.99	3.51
Unmasked-calculated*	8.14	12.64	8.28

*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 8.14 differs from the reported value 3.4 by more than 10 %

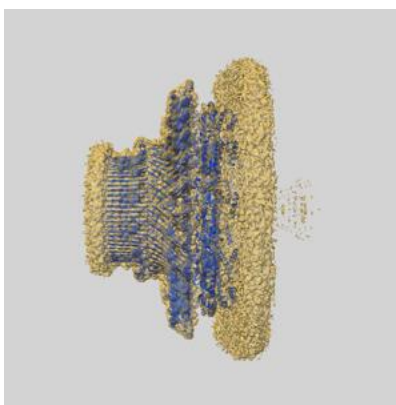
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41101 and PDB model 8T8P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

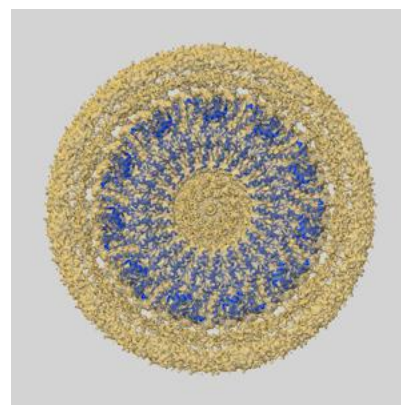
9.1 Map-model overlay [i](#)



X



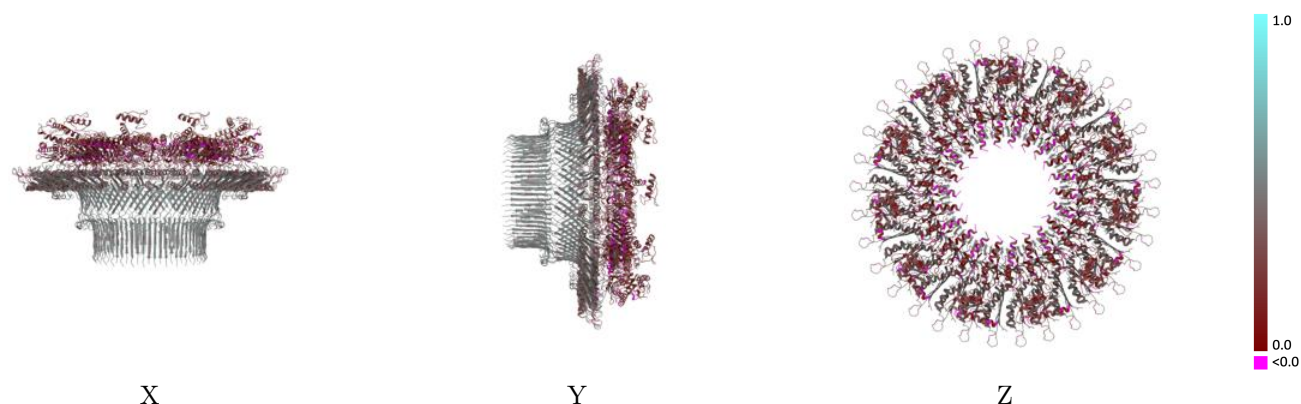
Y



Z

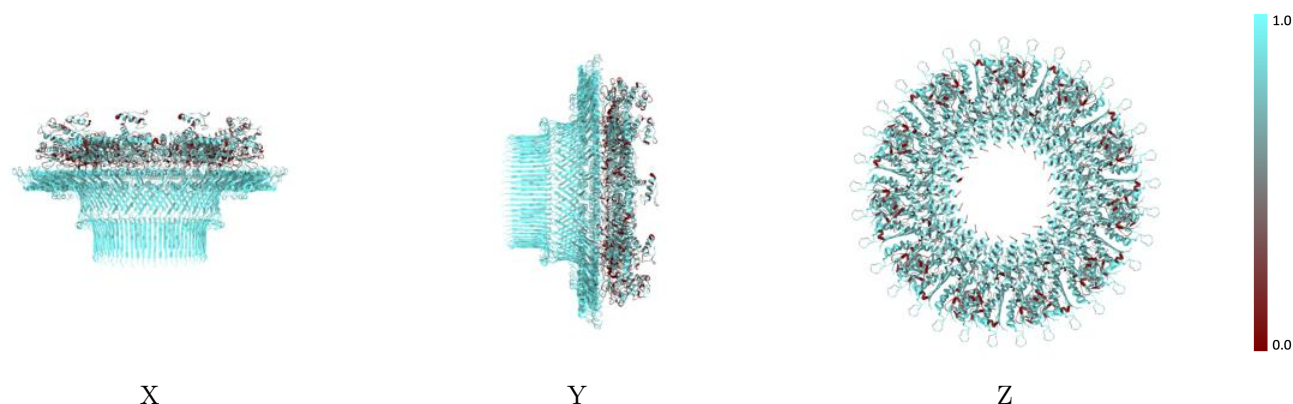
The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



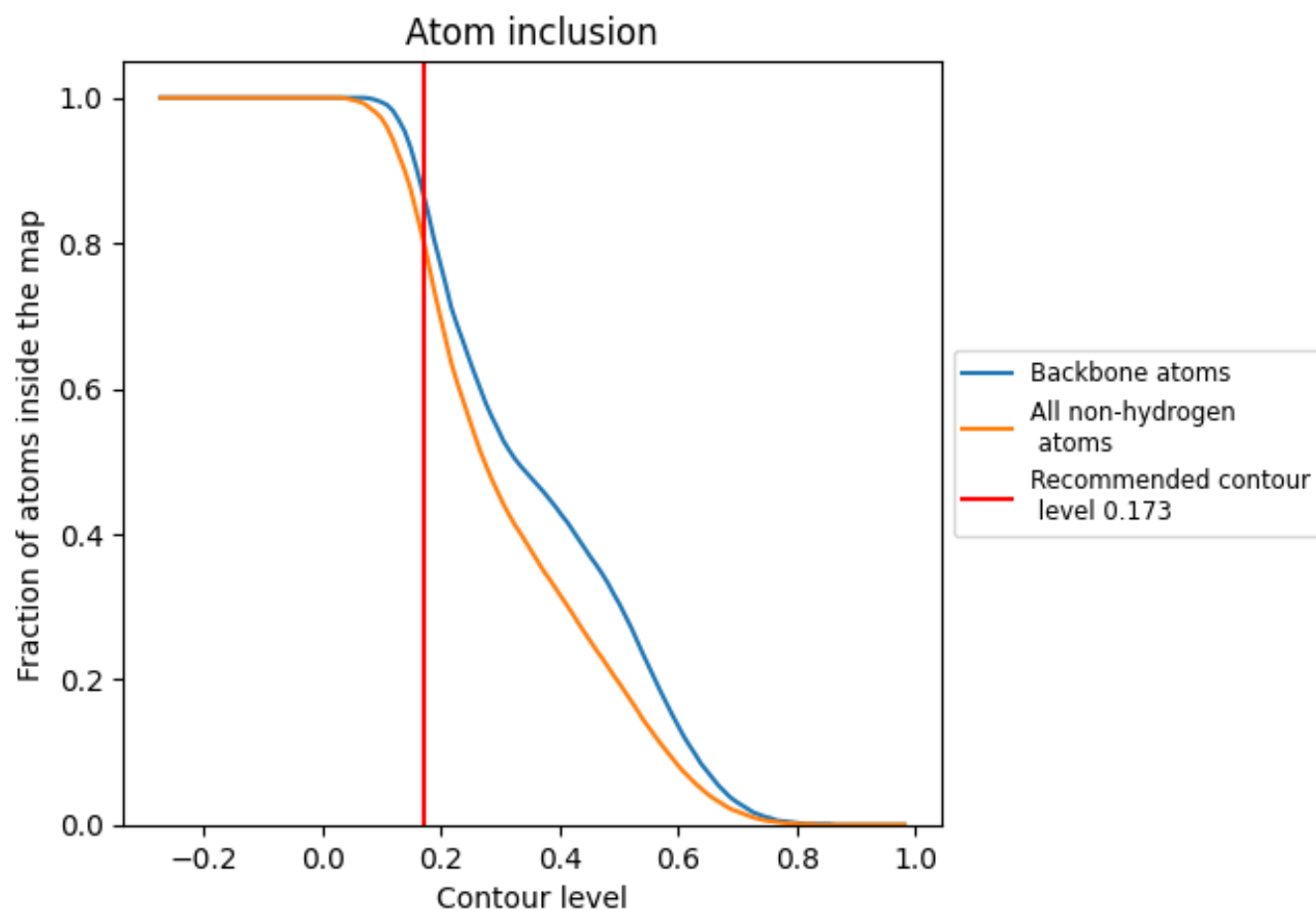
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.173).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.3530
A	 0.8170	 0.3420
AA	 0.7580	 0.3710
B	 0.7590	 0.3650
BA	 0.8150	 0.3460
C	 0.8150	 0.3470
CA	 0.8160	 0.3400
D	 0.8210	 0.3430
DA	 0.7590	 0.3660
E	 0.7550	 0.3680
EA	 0.8100	 0.3460
F	 0.8170	 0.3470
FA	 0.8210	 0.3420
G	 0.8130	 0.3430
GA	 0.7550	 0.3670
H	 0.7540	 0.3700
HA	 0.8110	 0.3440
I	 0.8170	 0.3470
J	 0.8180	 0.3430
K	 0.7590	 0.3700
L	 0.8170	 0.3480
M	 0.8180	 0.3410
N	 0.7590	 0.3690
O	 0.8130	 0.3480
P	 0.8170	 0.3420
Q	 0.7580	 0.3680
R	 0.8100	 0.3460
S	 0.8210	 0.3420
T	 0.7520	 0.3700
V	 0.8130	 0.3490
W	 0.8230	 0.3430
X	 0.7500	 0.3680
Y	 0.8120	 0.3460
Z	 0.8240	 0.3450

