Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 03:03 PM EDT

PDB ID	:	8FL8 / pdb_00008fl8
EMDB ID	:	EMD-29270
Title	:	Yeast ATP Synthase structure in presence of MgATP
Authors	:	Sharma, S.; Patel, H.; Luo, M.; Mueller, D.M.; Liao, M.
Deposited on	:	2022-12-21
Resolution	:	4.20 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:

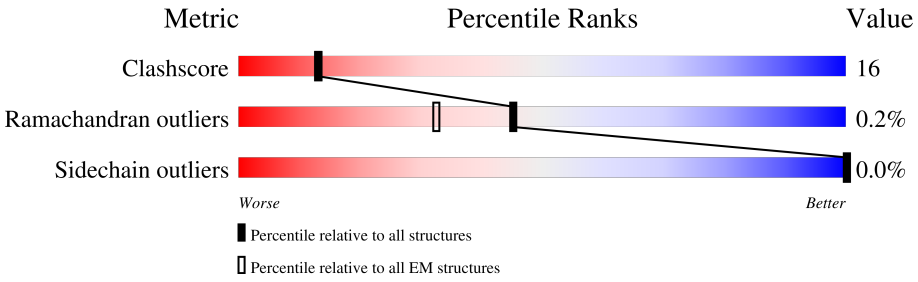
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	8	41	39% 37% 63%
2	J	37	62% 81% 19%
3	Y	166	8% 60% 40%
4	A	507	66% 34%
4	B	507	59% 40%
4	C	507	68% 32%
5	D	473	72% 28%
5	E	473	62% 38%

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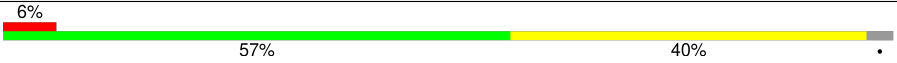
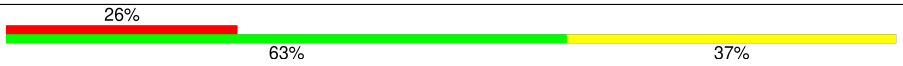
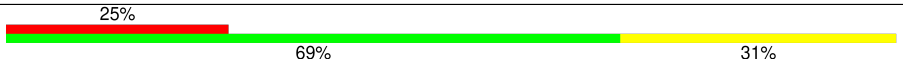
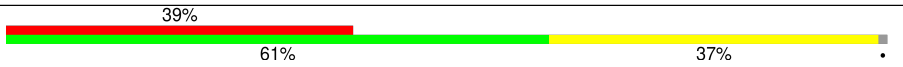
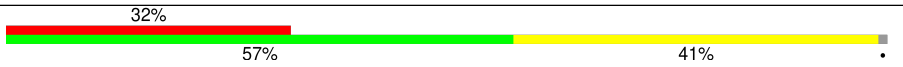
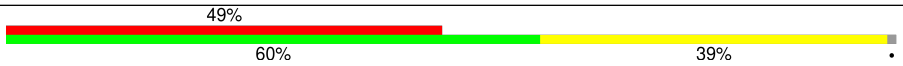
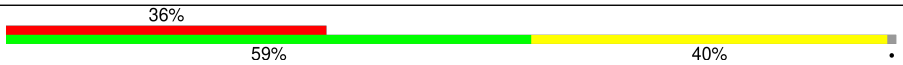
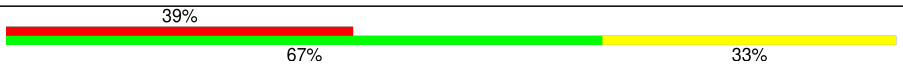
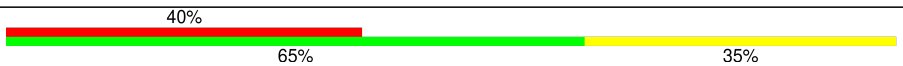
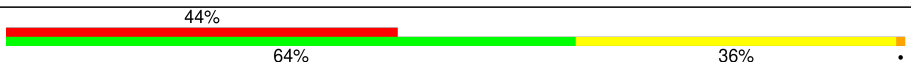
Mol	Chain	Length	Quality of chain
5	F	473	
6	G	270	
7	H	132	
8	I	59	
9	K	75	
9	L	75	
9	M	75	
9	N	75	
9	O	75	
9	P	75	
9	Q	75	
9	R	75	
9	S	75	
9	T	75	
10	X	224	
11	Z	155	
12	7	171	
13	6	89	
14	U	85	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 38784 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 ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	41	356	250	51	52	3	0	0

- Molecule 2 is a protein called ATP18 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	37	292	197	45	48	2	0	0

- Molecule 3 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Y	166	1254	799	217	237	1	0	0

- Molecule 4 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	507	3858	2435	679	741	3	0	0
4	B	506	Total	C	N	O	S	0	0
			3846	2426	678	739	3		
4	C	505	Total	C	N	O	S	0	0
			3844	2426	676	739	3		

- Molecule 5 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	473	3572	2262	608	696	6	0	0
5	E	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

- Molecule 6 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	261	Total	C	N	O	S	0	0
			2032	1276	353	393	10		

- Molecule 7 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	132	Total	C	N	O	S	0	0
			990	624	165	199	2		

- Molecule 8 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	59	Total	C	N	O	0	0
			392	243	71	78		

- Molecule 9 is a protein called ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	T	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	K	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
9	L	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	M	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	N	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	O	74	Total	C	N	O	S	0	0
			533	357	82	90	4		
9	P	75	Total	C	N	O	S	0	0
			537	359	83	91	4		
9	Q	74	Total	C	N	O	S	0	0
			533	357	82	90	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	74	Total	C	N	O	S	0	0
			533	357	82	90	4		

- Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	224	Total	C	N	O	S	0	0
			1772	1210	265	287	10		

- Molecule 11 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	155	Total	C	N	O	S	0	0
			1232	778	211	242	1		

- Molecule 12 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	7	171	Total	C	N	O	S	0	0
			1363	856	236	268	3		

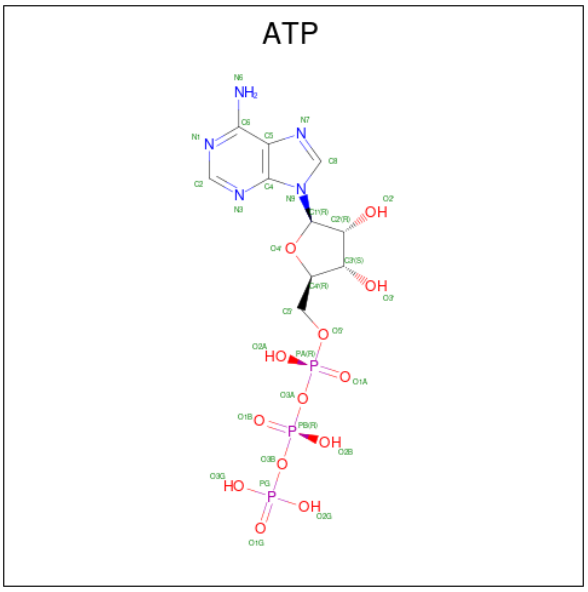
- Molecule 13 is a protein called ATP synthase subunit H, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	6	89	Total	C	N	O	0	0
			710	441	114	155		

- Molecule 14 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	85	Total	C	N	O	S	0	0
			639	420	109	109	1		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

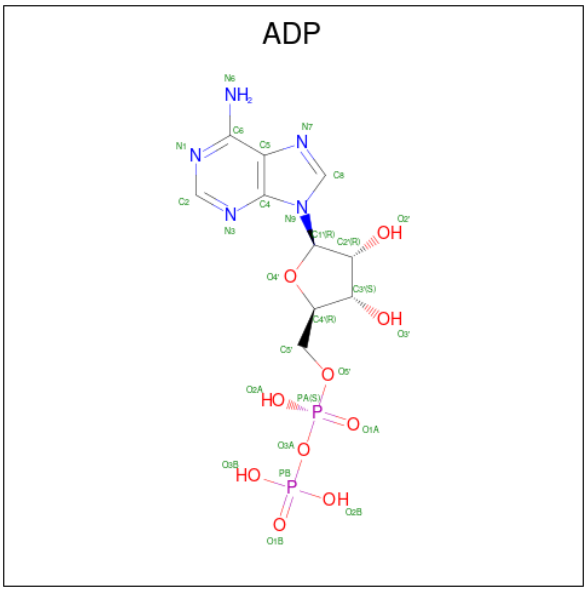


Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	B	1	Total	Mg	0
			1	1	
16	C	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	
16	F	1	Total	Mg	0
			1	1	

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

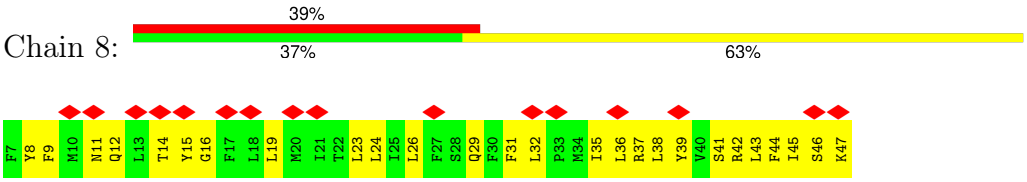


Mol	Chain	Residues	Atoms					AltConf
17	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

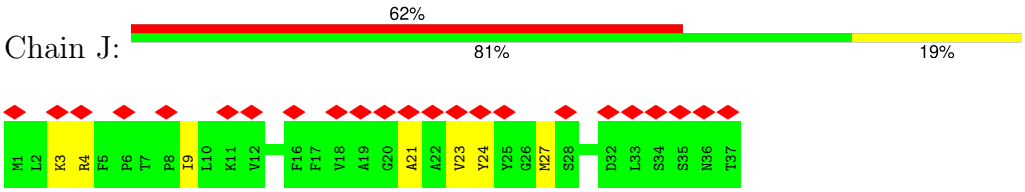
3 Residue-property plots (i)

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

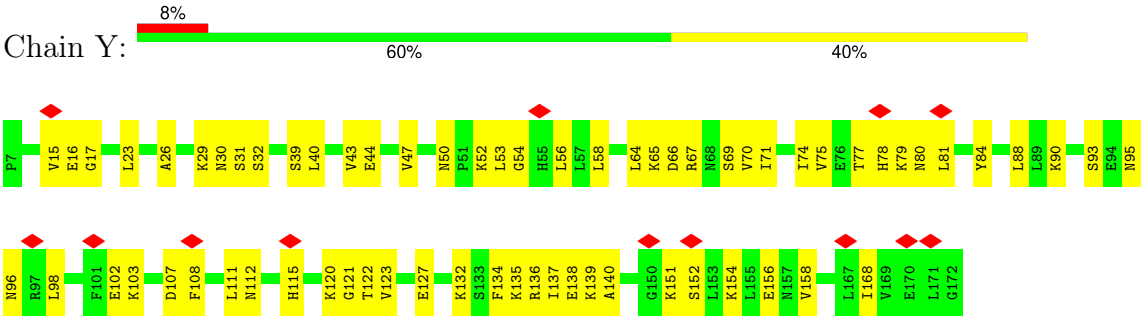
• Molecule 1: ATP synthase protein 8



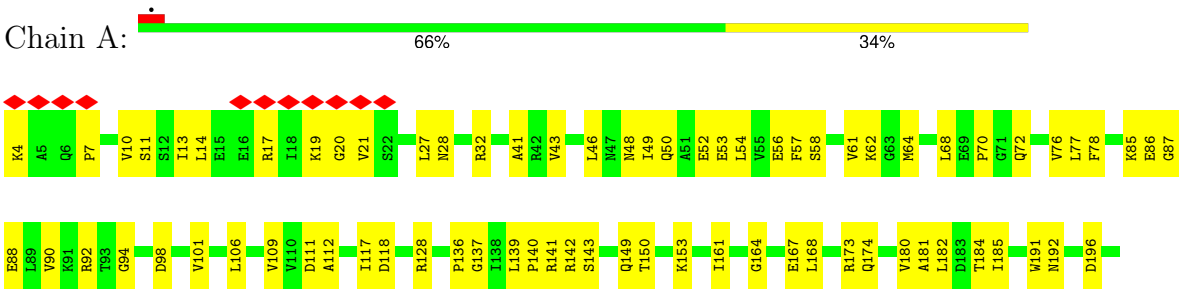
• Molecule 2: ATP18 isoform 1

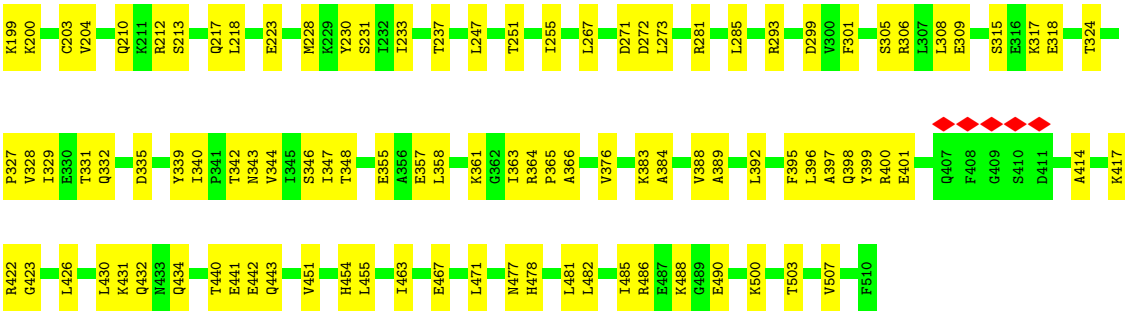


• Molecule 3: ATP synthase subunit 5, mitochondrial



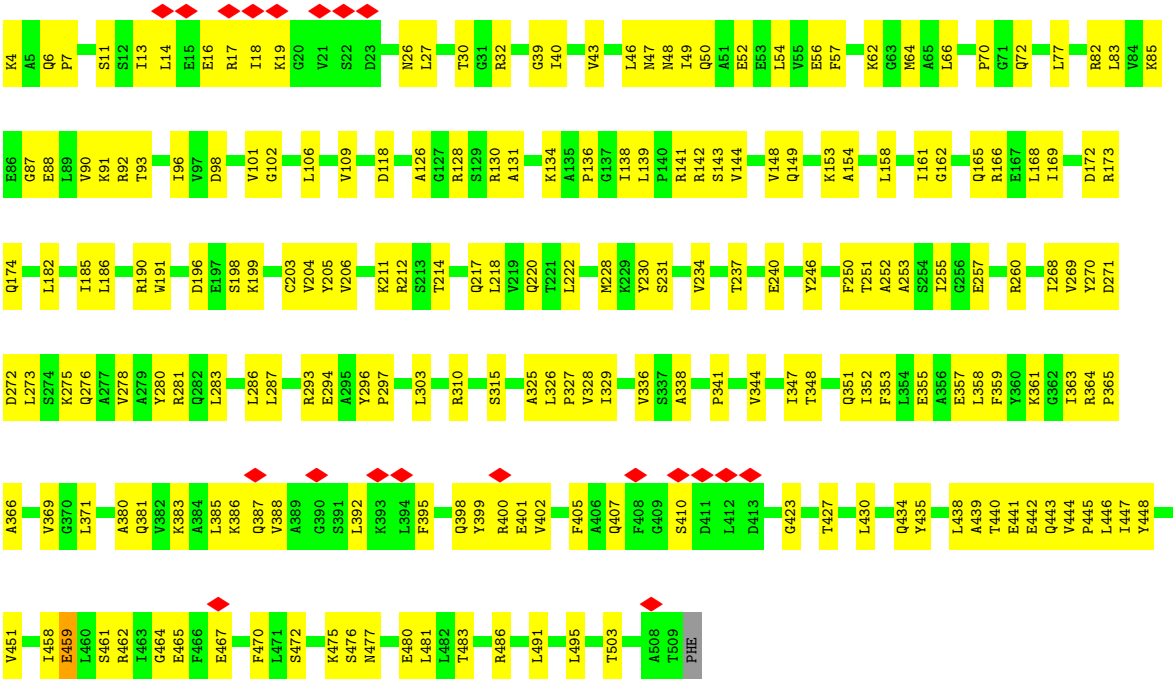
• Molecule 4: ATP synthase subunit alpha





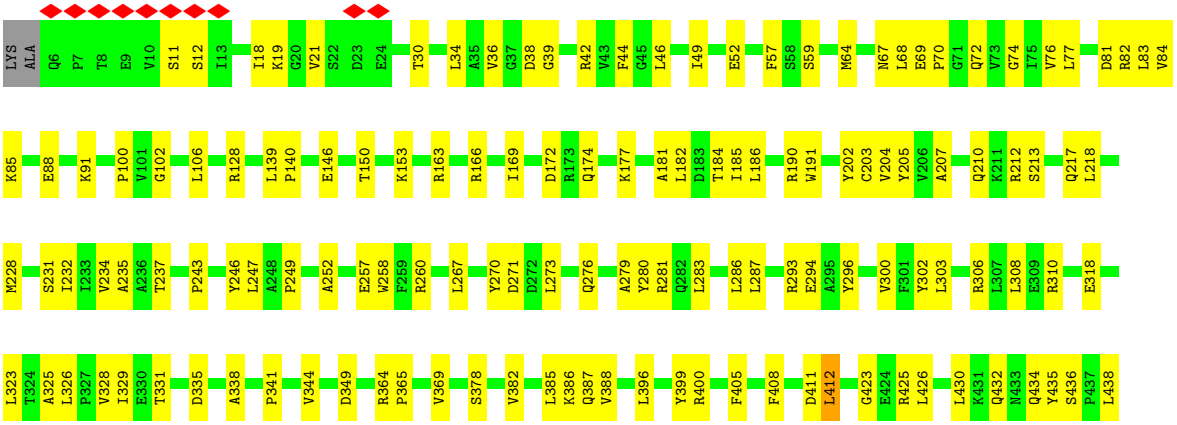
• Molecule 4: ATP synthase subunit alpha

Chain B:



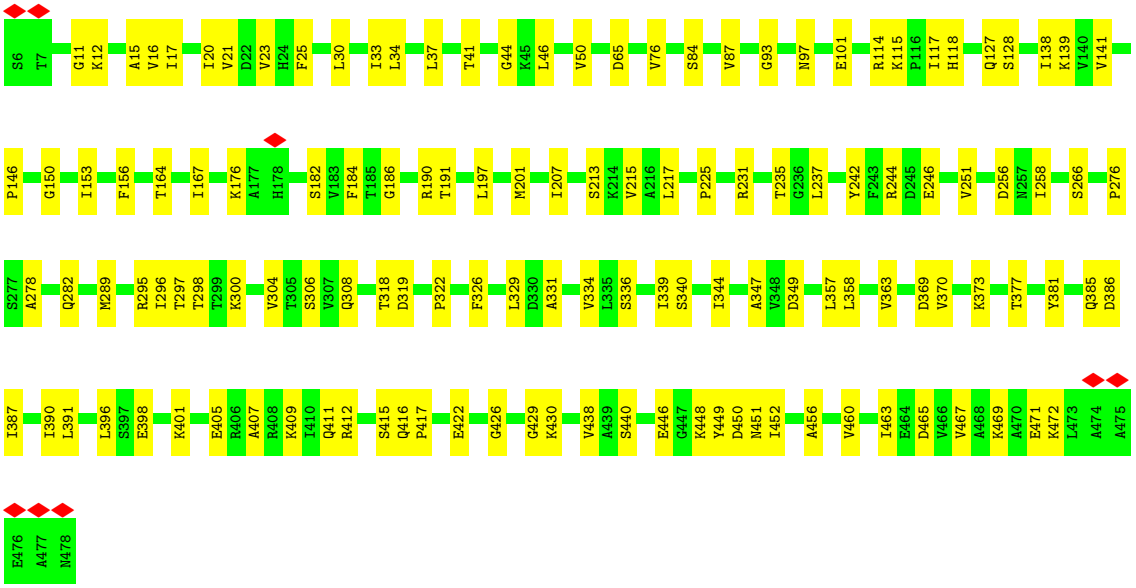
• Molecule 4: ATP synthase subunit alpha

Chain C:



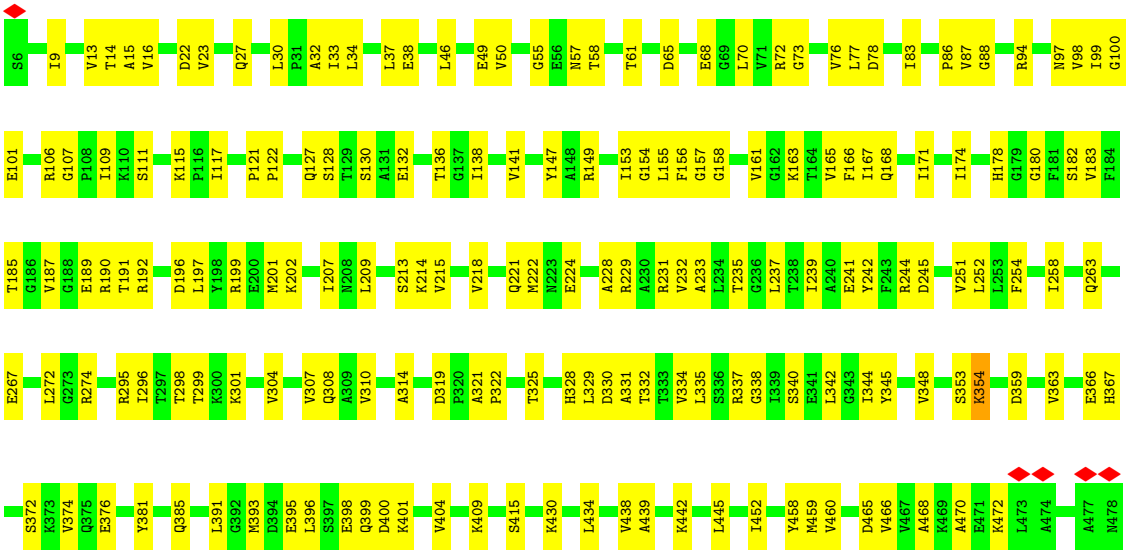
• Molecule 5: ATP synthase subunit beta

Chain D:



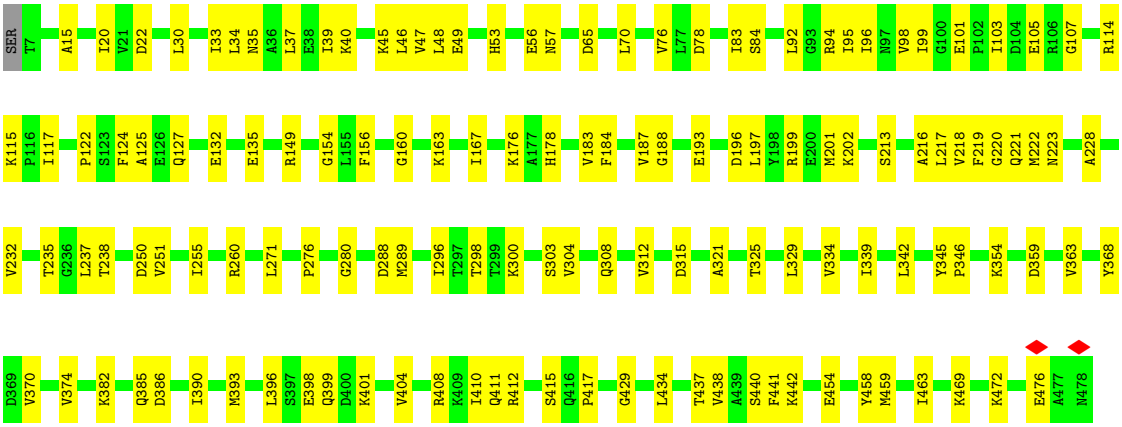
• Molecule 5: ATP synthase subunit beta

Chain E:



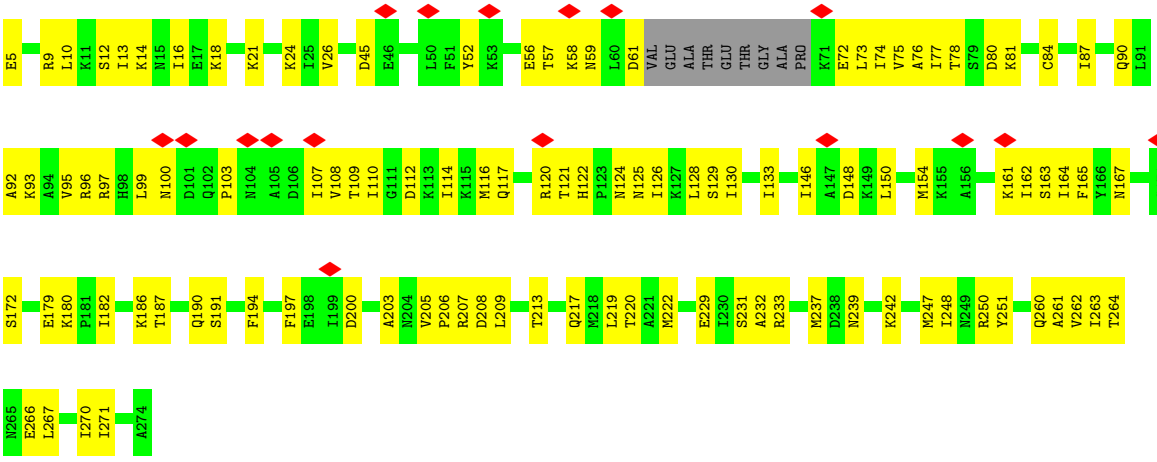
• Molecule 5: ATP synthase subunit beta

Chain F:



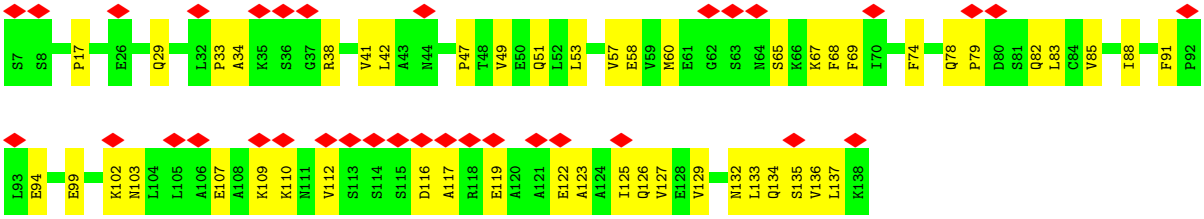
• Molecule 6: ATP synthase subunit gamma, mitochondrial

Chain G:



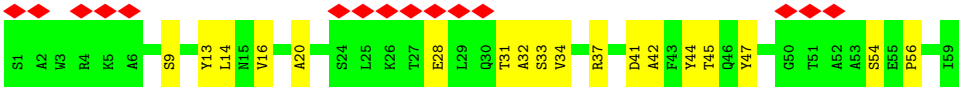
• Molecule 7: ATP synthase subunit delta, mitochondrial

Chain H:



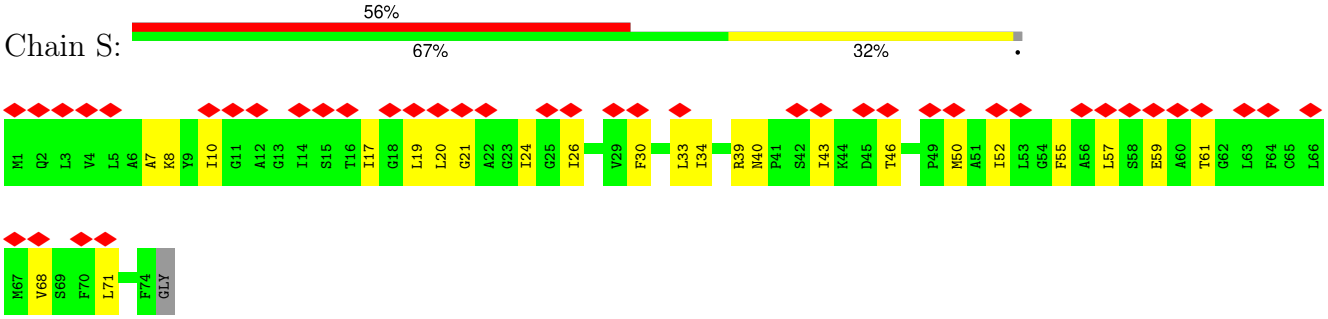
• Molecule 8: ATP synthase subunit epsilon, mitochondrial

Chain I:



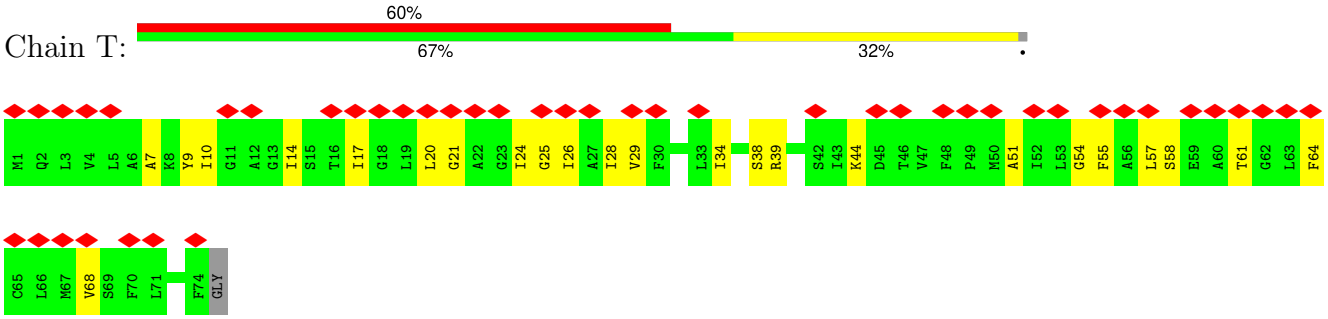
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain S:



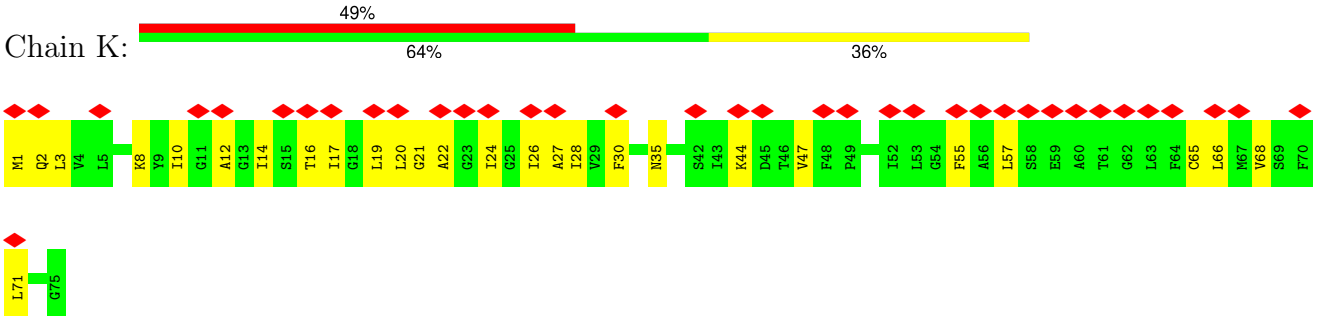
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain T:



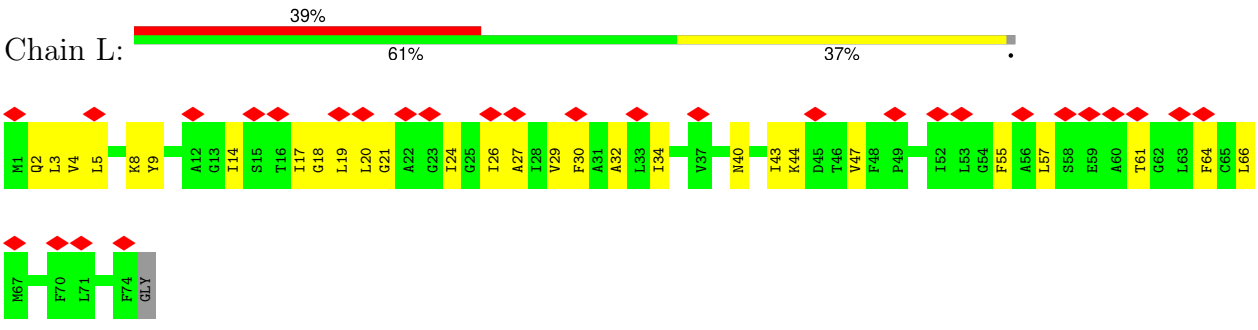
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain K:



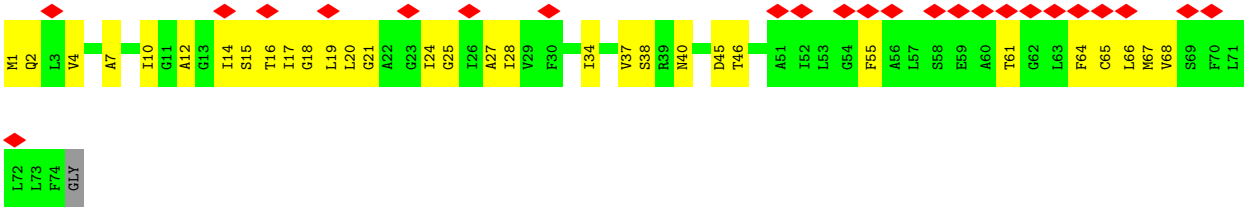
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain L:



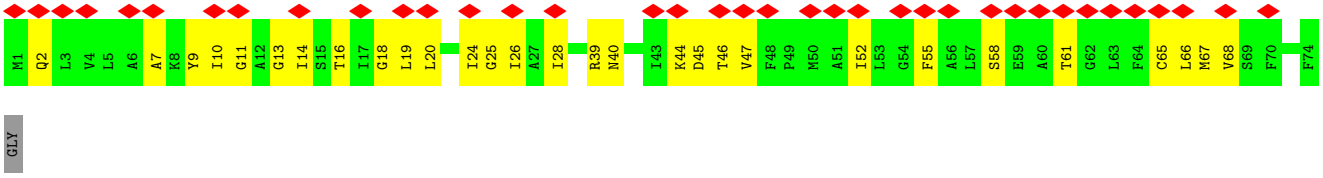
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain M:



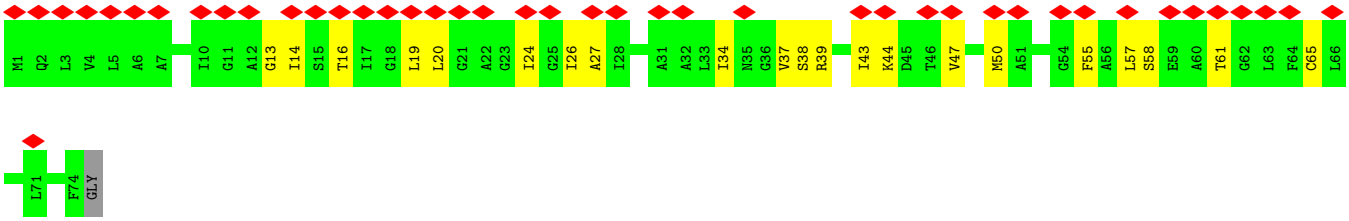
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain N:



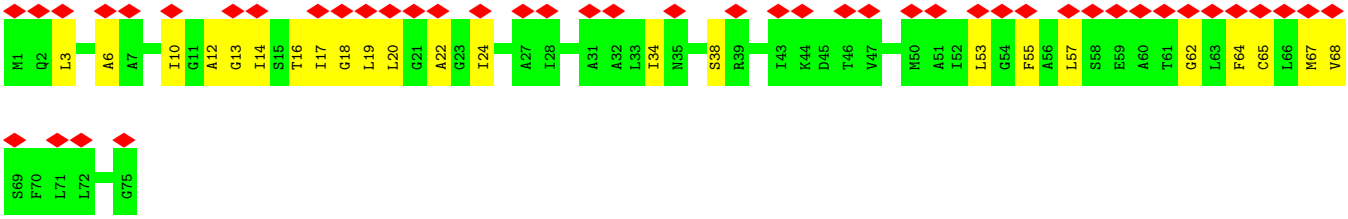
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain O:



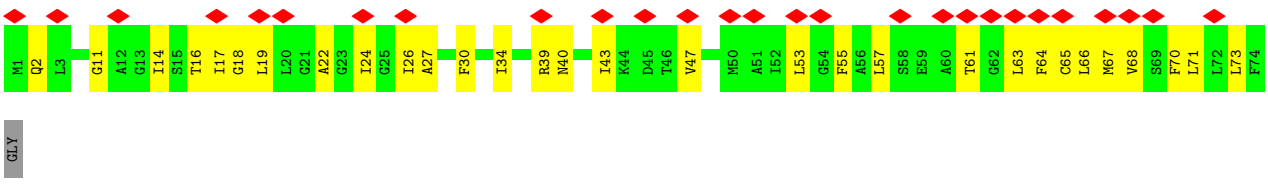
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain P:



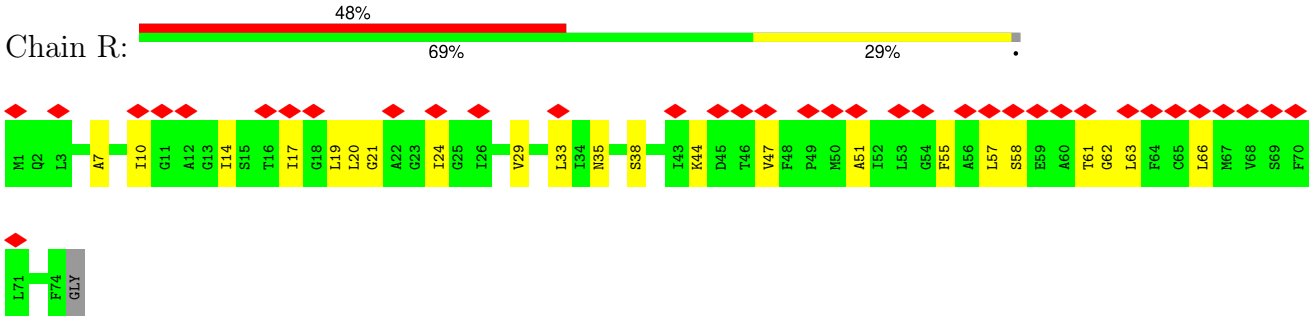
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain Q:



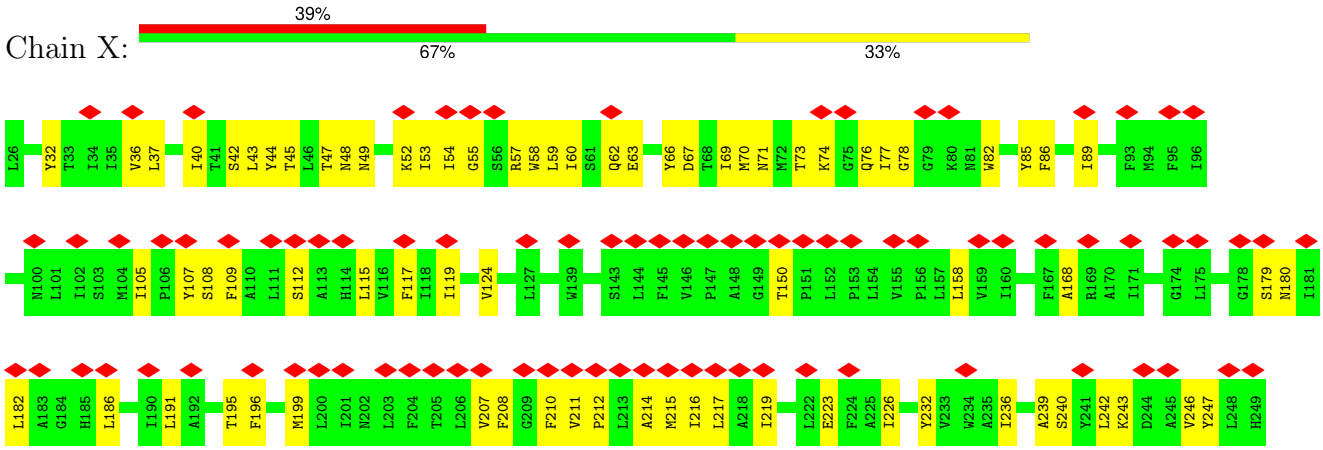
• Molecule 9: ATP synthase subunit 9, mitochondrial

Chain R:



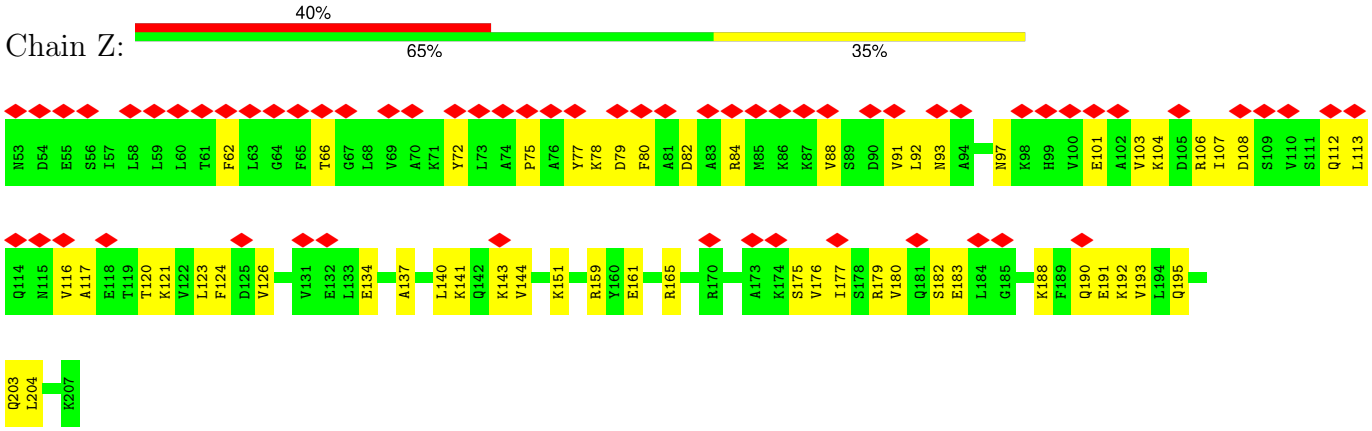
• Molecule 10: ATP synthase subunit a

Chain X:



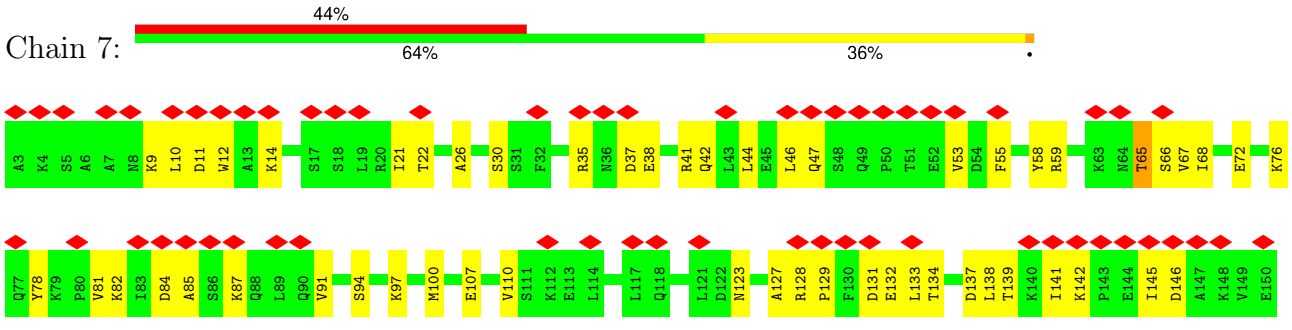
• Molecule 11: ATP synthase subunit 4, mitochondrial

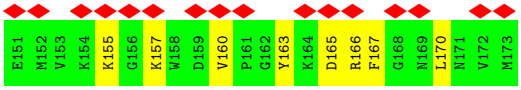
Chain Z:



• Molecule 12: ATP synthase subunit d, mitochondrial

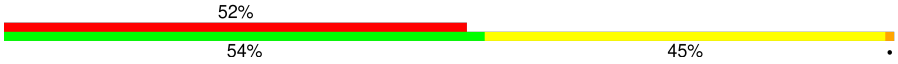
Chain 7:

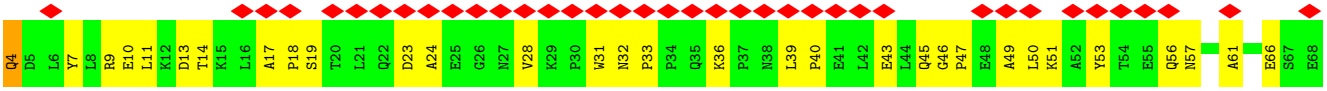


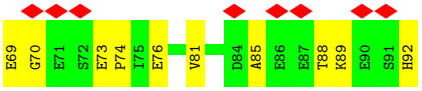


• Molecule 13: ATP synthase subunit H, mitochondrial

Chain 6:

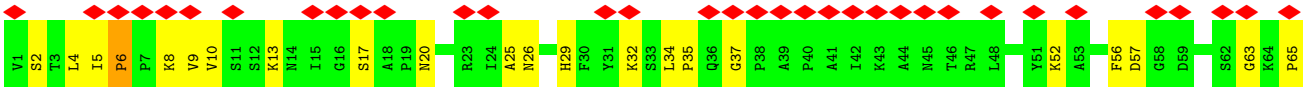






• Molecule 14: ATP synthase subunit f, mitochondrial

Chain U:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65559	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 ($e^-/Å^2$)	51.07	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP

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	8	0.19	0/366	0.38	0/492
2	J	0.18	0/302	0.58	0/410
3	Y	0.15	0/1272	0.41	0/1717
4	A	0.15	0/3916	0.43	0/5298
4	B	0.17	0/3903	0.48	0/5282
4	C	0.16	0/3902	0.42	2/5280 (0.0%)
5	D	0.14	0/3628	0.39	0/4919
5	E	0.15	0/3628	0.42	0/4919
5	F	0.16	0/3622	0.44	0/4911
6	G	0.16	0/2057	0.41	0/2767
7	H	0.12	0/1004	0.31	0/1359
8	I	0.11	0/398	0.29	0/547
9	K	0.17	0/545	0.35	0/737
9	L	0.17	0/541	0.40	0/732
9	M	0.16	0/541	0.32	0/732
9	N	0.17	0/541	0.47	0/732
9	O	0.15	0/541	0.34	0/732
9	P	0.17	0/545	0.38	0/737
9	Q	0.22	0/541	0.41	0/732
9	R	0.17	0/541	0.35	0/732
9	S	0.17	0/541	0.45	0/732
9	T	0.17	0/541	0.33	0/732
10	X	0.13	0/1820	0.36	0/2483
11	Z	0.12	0/1246	0.33	0/1678
12	7	0.11	0/1382	0.35	0/1858
13	6	0.14	0/725	0.41	0/988
14	U	0.14	0/659	0.38	0/895
All	All	0.15	0/39248	0.41	2/53133 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	412	LEU	CA-C-N	5.57	132.17	121.54
4	C	412	LEU	C-N-CA	5.57	132.17	121.54

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	8	356	0	379	26	0
2	J	292	0	298	8	0
3	Y	1254	0	1318	58	0
4	A	3858	0	3941	125	0
4	B	3846	0	3932	159	0
4	C	3844	0	3923	119	0
5	D	3572	0	3638	90	0
5	E	3572	0	3638	131	0
5	F	3566	0	3633	100	0
6	G	2032	0	2093	85	0
7	H	990	0	999	45	0
8	I	392	0	306	17	0
9	K	537	0	582	33	0
9	L	533	0	579	34	0
9	M	533	0	579	35	0
9	N	533	0	579	29	0
9	O	533	0	579	27	0
9	P	537	0	582	22	0
9	Q	533	0	579	33	0
9	R	533	0	579	28	0
9	S	533	0	579	22	0
9	T	533	0	579	26	0
10	X	1772	0	1873	64	0
11	Z	1232	0	1256	59	0
12	7	1363	0	1389	72	0
13	6	710	0	668	40	0
14	U	639	0	615	30	0
15	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	B	31	0	12	0	0
15	C	31	0	12	2	0
15	E	31	0	12	4	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	E	1	0	0	0	0
16	F	1	0	0	0	0
17	F	27	0	12	2	0
All	All	38784	0	39755	1267	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 16.

All (1267) 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)
9:N:25:GLY:HA2	9:O:27:ALA:HB2	1.51	0.92
3:Y:136:ARG:HD3	3:Y:137:ILE:HG23	1.54	0.89
7:H:109:LYS:HZ3	7:H:126:GLN:HB3	1.39	0.87
5:D:456:ALA:HA	5:D:469:LYS:HD2	1.56	0.86
11:Z:123:LEU:HD11	12:7:14:LYS:HB3	1.58	0.85
4:B:82:ARG:NH2	5:E:33:ILE:O	2.09	0.85
9:K:24:ILE:HG23	9:L:24:ILE:HD11	1.59	0.83
9:L:3:LEU:HB3	9:M:2:GLN:HE22	1.42	0.82
13:6:4:GLN:HE21	13:6:4:GLN:N	1.76	0.82
4:A:173:ARG:HG2	4:A:174:GLN:HG2	1.64	0.79
4:B:383:LYS:HZ2	4:B:388:VAL:HG13	1.48	0.78
9:S:26:ILE:HG21	9:S:59:GLU:HG2	1.67	0.77
3:Y:120:LYS:HG3	3:Y:121:GLY:H	1.50	0.76
11:Z:121:LYS:NZ	12:7:100:MET:SD	2.58	0.76
12:7:91:VAL:HG23	13:6:74:PRO:HG3	1.67	0.76
5:D:370:VAL:HG11	5:D:438:VAL:HG23	1.68	0.76
9:Q:39:ARG:NH2	9:R:35:ASN:OD1	2.20	0.75
4:A:305:SER:HB2	5:E:222:MET:HG3	1.68	0.75
5:D:344:ILE:HD12	5:D:415:SER:HB3	1.67	0.75
5:E:196:ASP:OD1	5:E:199:ARG:NH2	2.20	0.75
6:G:76:ALA:HA	6:G:165:PHE:HB2	1.68	0.75
14:U:78:TYR:HA	14:U:82:TYR:HB2	1.68	0.75
10:X:70:MET:SD	10:X:74:LYS:NZ	2.60	0.74
5:E:197:LEU:HD23	5:E:201:MET:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:109:LYS:NZ	7:H:123:ALA:O	2.21	0.74
4:A:389:ALA:HA	4:A:392:LEU:HD13	1.68	0.74
3:Y:67:ARG:NH2	3:Y:95:ASN:O	2.21	0.73
9:S:46:THR:OG1	9:T:44:LYS:NZ	2.21	0.73
4:B:402:VAL:HG21	4:B:423:GLY:HA3	1.69	0.73
4:B:438:LEU:HB3	4:B:443:GLN:HE22	1.52	0.73
4:C:276:GLN:HE22	4:C:303:LEU:HD21	1.52	0.73
5:D:409:LYS:NZ	5:D:452:ILE:O	2.20	0.73
6:G:186:LYS:O	6:G:190:GLN:NE2	2.22	0.73
3:Y:96:ASN:HB3	4:C:11:SER:HB3	1.71	0.72
13:6:39:LEU:HA	13:6:43:GLU:HB3	1.70	0.72
5:E:272:LEU:HD23	5:E:274:ARG:HE	1.54	0.72
4:B:96:ILE:HD13	4:B:130:ARG:HH12	1.52	0.72
4:B:359:PHE:O	4:B:364:ARG:NH2	2.22	0.72
10:X:52:LYS:NZ	12:7:133:LEU:O	2.21	0.72
5:D:296:ILE:HG12	5:D:306:SER:HB2	1.70	0.72
4:A:106:LEU:HD12	4:A:230:TYR:H	1.54	0.72
4:A:363:ILE:HD12	4:A:431:LYS:HG3	1.71	0.71
4:B:13:ILE:HG13	4:B:17:ARG:HH22	1.55	0.71
4:B:329:ILE:HG13	4:B:344:VAL:HG11	1.73	0.71
5:D:251:VAL:HB	5:D:304:VAL:HG12	1.72	0.71
4:A:70:PRO:HD3	5:E:15:ALA:HB2	1.72	0.71
4:C:243:PRO:HG3	4:C:283:LEU:HD11	1.72	0.71
9:K:17:ILE:HD11	9:L:17:ILE:HG12	1.73	0.71
9:N:26:ILE:HG12	9:N:55:PHE:HB2	1.73	0.71
4:B:101:VAL:HG12	4:B:255:ILE:HD13	1.72	0.71
3:Y:140:ALA:HB2	11:Z:204:LEU:HD11	1.73	0.70
4:A:101:VAL:HG12	4:A:255:ILE:HD13	1.73	0.70
4:A:308:LEU:HD11	4:A:327:PRO:HG3	1.72	0.70
5:F:47:VAL:HG21	5:F:99:ILE:HG21	1.73	0.70
6:G:77:ILE:HG21	6:G:222:MET:HA	1.72	0.70
5:E:244:ARG:NH1	5:E:299:THR:HG21	2.06	0.70
9:T:39:ARG:HH22	9:K:35:ASN:HA	1.56	0.70
5:D:97:ASN:HD21	5:D:101:GLU:HB3	1.56	0.70
7:H:109:LYS:NZ	7:H:126:GLN:HB3	2.06	0.70
7:H:99:GLU:HG3	7:H:137:LEU:HD13	1.73	0.70
7:H:126:GLN:HG2	8:I:20:ALA:HB2	1.72	0.70
7:H:134:GLN:HA	7:H:137:LEU:HD12	1.73	0.70
9:O:24:ILE:HG13	9:P:24:ILE:HD11	1.73	0.70
4:C:82:ARG:NH1	5:F:33:ILE:O	2.25	0.70
4:C:364:ARG:NH1	5:F:368:TYR:OH	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:213:THR:O	6:G:217:GLN:NE2	2.24	0.69
12:7:142:LYS:HB2	12:7:145:ILE:HG12	1.74	0.69
6:G:52:TYR:HH	6:G:213:THR:HG1	1.40	0.69
10:X:54:ILE:HG22	10:X:55:GLY:H	1.58	0.69
1:8:29:GLN:HB3	2:J:4:ARG:HG3	1.75	0.69
5:E:153:ILE:HB	5:E:307:VAL:HA	1.73	0.69
5:F:199:ARG:HA	5:F:202:LYS:HG2	1.74	0.69
4:A:212:ARG:HE	4:A:237:THR:HG21	1.58	0.69
3:Y:90:LYS:O	3:Y:93:SER:OG	2.11	0.69
4:A:111:ASP:HB3	4:A:117:ILE:HD11	1.74	0.69
4:B:205:TYR:OH	4:B:271:ASP:OD1	2.09	0.69
6:G:59:ASN:HD21	6:G:187:THR:HB	1.58	0.69
12:7:26:ALA:HB3	14:U:4:LEU:HB2	1.75	0.69
4:B:4:LYS:HZ1	11:Z:165:ARG:HA	1.58	0.68
12:7:65:THR:HG23	12:7:68:ILE:HD12	1.75	0.68
9:P:68:VAL:HG11	9:Q:16:THR:HG21	1.75	0.68
9:N:52:ILE:HA	9:N:55:PHE:CE1	2.29	0.68
1:8:41:SER:O	1:8:45:ILE:HG12	1.94	0.68
11:Z:144:VAL:HG11	12:7:47:GLN:HE22	1.59	0.68
1:8:35:ILE:HD12	10:X:53:ILE:HD11	1.76	0.68
5:D:146:PRO:HB2	5:D:357:LEU:HD11	1.74	0.68
5:E:207:ILE:HD11	5:E:215:VAL:HB	1.76	0.68
5:E:97:ASN:HD21	5:E:101:GLU:HB2	1.58	0.68
6:G:45:ASP:HB2	6:G:220:THR:HG21	1.76	0.68
5:F:382:LYS:HA	5:F:385:GLN:HG2	1.75	0.67
4:C:442:GLU:HB2	4:C:471:LEU:HD11	1.76	0.67
5:F:98:VAL:HG21	5:F:228:ALA:HB1	1.76	0.67
5:D:186:GLY:HA2	5:D:256:ASP:HB2	1.76	0.67
4:C:169:ILE:HD11	4:C:326:LEU:HD12	1.75	0.67
4:A:441:GLU:HB3	4:A:486:ARG:HB3	1.75	0.67
11:Z:191:GLU:OE2	11:Z:195:GLN:NE2	2.27	0.67
5:F:298:THR:HG23	5:F:303:SER:HA	1.76	0.67
4:A:164:GLY:H	4:A:324:THR:HG22	1.59	0.66
4:B:52:GLU:HB2	4:B:64:MET:HE3	1.76	0.66
5:F:30:LEU:HD11	5:F:57:ASN:HA	1.77	0.66
11:Z:72:TYR:HB2	11:Z:75:PRO:HG3	1.77	0.66
3:Y:50:ASN:O	3:Y:54:GLY:N	2.28	0.66
6:G:108:VAL:HG13	6:G:128:LEU:HB3	1.75	0.66
9:R:63:LEU:HD21	10:X:168:ALA:HB1	1.76	0.66
4:C:67:ASN:O	4:C:74:GLY:N	2.28	0.66
4:C:210:GLN:NE2	4:C:271:ASP:OD2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:VAL:HG21	5:E:115:LYS:HG2	1.77	0.66
12:7:87:LYS:HZ1	13:6:69:GLU:H	1.44	0.66
4:A:482:LEU:HA	4:A:485:ILE:HG12	1.78	0.66
5:D:266:SER:HA	5:D:282:GLN:HB3	1.75	0.66
5:E:245:ASP:O	5:E:301:LYS:NZ	2.25	0.66
3:Y:23:LEU:HD12	3:Y:88:LEU:HG	1.78	0.66
4:B:491:LEU:HA	4:B:495:LEU:HD23	1.77	0.66
5:F:412:ARG:HD2	5:F:454:GLU:HB3	1.78	0.65
12:7:132:GLU:HG3	14:U:37:GLY:HA2	1.77	0.65
5:E:94:ARG:NH2	5:E:107:GLY:O	2.27	0.65
12:7:97:LYS:HA	12:7:100:MET:HE2	1.79	0.65
5:F:39:ILE:HD11	5:F:46:LEU:HD23	1.78	0.65
4:A:142:ARG:NH1	4:A:143:SER:OG	2.30	0.65
10:X:49:ASN:ND2	14:U:57:ASP:OD1	2.30	0.65
9:L:18:GLY:HA2	9:M:20:LEU:HB2	1.79	0.65
9:O:20:LEU:HD23	9:P:20:LEU:HD11	1.79	0.65
4:C:174:GLN:O	5:F:354:LYS:NZ	2.29	0.65
9:L:17:ILE:HB	9:M:17:ILE:HD12	1.77	0.65
3:Y:108:PHE:O	3:Y:112:ASN:ND2	2.29	0.65
5:F:96:ILE:HB	5:F:218:VAL:HG12	1.79	0.65
4:A:54:LEU:HD11	4:A:62:LYS:HB3	1.78	0.64
4:C:68:LEU:HD11	5:D:16:VAL:HG22	1.79	0.64
9:N:25:GLY:HA2	9:O:27:ALA:CB	2.25	0.64
3:Y:52:LYS:HG3	3:Y:53:LEU:HD12	1.78	0.64
3:Y:156:GLU:OE1	11:Z:192:LYS:NZ	2.30	0.64
4:B:392:LEU:HD21	4:B:447:ILE:HG21	1.77	0.64
10:X:199:MET:HA	10:X:208:PHE:HE2	1.62	0.64
12:7:138:LEU:HA	12:7:141:ILE:HG22	1.79	0.64
4:B:32:ARG:HG3	4:B:87:GLY:HA2	1.79	0.64
4:B:363:ILE:HG22	4:B:366:ALA:H	1.63	0.64
5:E:132:GLU:HB3	5:E:149:ARG:HD3	1.80	0.64
9:N:68:VAL:HG11	9:O:16:THR:HG21	1.79	0.64
4:B:40:ILE:HG13	4:B:286:LEU:HB3	1.79	0.64
5:D:336:SER:HB2	5:D:339:ILE:HB	1.80	0.64
5:E:55:GLY:O	5:E:58:THR:OG1	2.15	0.64
10:X:57:ARG:HH12	11:Z:78:LYS:HE3	1.63	0.64
5:D:446:GLU:OE1	5:D:448:LYS:NZ	2.26	0.64
3:Y:52:LYS:HA	3:Y:56:LEU:HD13	1.79	0.64
3:Y:53:LEU:HD22	4:A:11:SER:HB3	1.79	0.64
4:A:109:VAL:HG22	4:A:118:ASP:HB3	1.81	0.63
4:C:212:ARG:HG2	4:C:237:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:84:ASP:OD1	12:7:85:ALA:N	2.31	0.63
6:G:103:PRO:O	6:G:125:ASN:ND2	2.30	0.63
3:Y:16:GLU:HG3	4:C:11:SER:HB2	1.80	0.63
5:E:224:GLU:HB3	5:E:228:ALA:HB3	1.79	0.63
11:Z:101:GLU:HG3	11:Z:104:LYS:HD3	1.80	0.63
10:X:47:THR:O	14:U:52:LYS:NZ	2.32	0.63
6:G:186:LYS:HG3	6:G:187:THR:HG23	1.79	0.63
3:Y:58:LEU:HD12	3:Y:98:LEU:HA	1.80	0.63
4:B:220:GLN:OE1	5:E:128:SER:OG	2.16	0.63
6:G:150:LEU:HA	6:G:154:MET:HE2	1.81	0.63
5:D:237:LEU:HD21	5:D:295:ARG:HB2	1.80	0.63
5:F:390:ILE:HG21	6:G:16:ILE:HD11	1.81	0.63
4:B:218:LEU:O	4:B:222:LEU:HD12	1.99	0.63
6:G:130:ILE:HD11	8:I:42:ALA:HB1	1.79	0.63
11:Z:93:ASN:O	12:7:128:ARG:NH2	2.32	0.63
11:Z:143:LYS:HB3	12:7:81:VAL:HG21	1.80	0.63
3:Y:30:ASN:ND2	3:Y:84:TYR:OH	2.31	0.62
5:E:251:VAL:HG23	5:E:304:VAL:HG23	1.80	0.62
4:A:17:ARG:H	4:A:19:LYS:HE3	1.64	0.62
5:D:411:GLN:HE22	5:D:412:ARG:HH21	1.46	0.62
4:C:270:TYR:HB3	4:C:273:LEU:HD21	1.81	0.62
5:D:41:THR:HG21	5:D:46:LEU:HD23	1.81	0.62
9:S:39:ARG:NH2	9:T:38:SER:OG	2.33	0.62
3:Y:70:VAL:HG12	4:A:14:LEU:HD22	1.81	0.62
4:A:56:GLU:HG3	4:A:58:SER:H	1.64	0.62
4:A:136:PRO:O	4:A:141:ARG:NH1	2.32	0.62
9:P:17:ILE:HD11	9:Q:17:ILE:HD12	1.82	0.62
5:E:237:LEU:HD21	5:E:295:ARG:HB2	1.81	0.62
13:6:4:GLN:N	13:6:4:GLN:NE2	2.47	0.62
14:U:52:LYS:HA	14:U:56:PHE:HB2	1.80	0.62
5:D:417:PRO:HB2	5:D:429:GLY:HA2	1.82	0.62
12:7:134:THR:HB	12:7:137:ASP:HB2	1.81	0.62
4:A:315:SER:OG	4:A:318:GLU:OE1	2.16	0.62
5:E:83:ILE:H	5:E:83:ILE:HD12	1.63	0.62
9:K:1:MET:HG2	9:K:2:GLN:HE21	1.65	0.62
5:F:154:GLY:HA3	5:F:329:LEU:HD13	1.82	0.61
4:C:181:ALA:O	4:C:185:ILE:HG12	1.99	0.61
4:C:329:ILE:HG13	4:C:344:VAL:HG11	1.81	0.61
6:G:207:ARG:NH1	6:G:208:ASP:OD1	2.33	0.61
9:L:64:PHE:HZ	9:M:66:LEU:HD13	1.63	0.61
9:P:3:LEU:HD11	9:Q:2:GLN:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:293:ARG:HG2	4:C:294:GLU:OE1	2.00	0.61
4:C:438:LEU:O	4:C:443:GLN:NE2	2.32	0.61
9:K:14:ILE:HD12	9:L:14:ILE:HG13	1.82	0.61
10:X:53:ILE:HG23	10:X:54:ILE:HG12	1.82	0.61
14:U:10:VAL:HA	14:U:13:LYS:HB3	1.83	0.61
4:A:346:SER:O	5:E:190:ARG:NH1	2.34	0.61
5:E:154:GLY:HA2	5:E:329:LEU:HD13	1.81	0.61
4:A:137:GLY:O	4:A:141:ARG:NH1	2.34	0.61
4:C:150:THR:HA	4:C:184:THR:HG23	1.80	0.61
5:F:95:ILE:HG22	5:F:103:ILE:HD12	1.83	0.61
6:G:116:MET:O	6:G:120:ARG:NH2	2.32	0.61
7:H:69:PHE:H	7:H:91:PHE:HB3	1.64	0.61
11:Z:141:LYS:HB2	12:7:44:LEU:HD11	1.83	0.61
11:Z:188:LYS:O	11:Z:192:LYS:N	2.32	0.61
13:6:89:LYS:HD2	14:U:9:VAL:HB	1.81	0.61
5:D:448:LYS:HG3	5:D:449:TYR:CD2	2.35	0.61
10:X:211:VAL:HG12	10:X:215:MET:HE1	1.83	0.61
4:B:381:GLN:HE21	4:B:385:LEU:HB2	1.66	0.60
5:D:244:ARG:NH1	5:D:297:THR:O	2.28	0.60
5:E:396:LEU:O	5:E:401:LYS:NZ	2.34	0.60
9:R:33:LEU:HG	9:R:51:ALA:HB2	1.83	0.60
4:A:329:ILE:HG13	4:A:344:VAL:HG11	1.83	0.60
11:Z:101:GLU:HA	11:Z:104:LYS:HB2	1.81	0.60
4:A:21:VAL:HG12	4:A:32:ARG:HG3	1.83	0.60
4:B:70:PRO:HD3	5:F:15:ALA:HB2	1.83	0.60
5:D:93:GLY:HA2	5:D:207:ILE:HD12	1.82	0.60
5:D:416:GLN:NE2	5:D:430:LYS:O	2.33	0.60
4:B:134:LYS:HZ1	5:F:223:ASN:HD22	1.47	0.60
5:E:191:THR:HG22	5:E:221:GLN:HG3	1.84	0.60
9:L:21:GLY:HA3	9:M:20:LEU:HG	1.82	0.60
14:U:71:LEU:HA	14:U:74:ILE:HD12	1.84	0.60
4:B:438:LEU:HB3	4:B:443:GLN:NE2	2.16	0.60
4:B:483:THR:HA	4:B:486:ARG:HG2	1.84	0.60
5:E:372:SER:O	5:E:376:GLU:HG2	2.02	0.60
4:B:168:LEU:HD11	4:B:329:ILE:HG12	1.84	0.60
4:C:153:LYS:HG3	4:C:430:LEU:HD13	1.82	0.60
4:A:109:VAL:HG12	4:A:233:ILE:HB	1.83	0.60
4:C:85:LYS:HB2	4:C:88:GLU:HG3	1.84	0.60
5:D:17:ILE:HG23	5:D:20:ILE:HB	1.84	0.60
4:A:210:GLN:NE2	4:A:271:ASP:OD2	2.34	0.60
11:Z:137:ALA:HA	11:Z:140:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:348:THR:O	5:E:190:ARG:NH1	2.35	0.59
4:C:260:ARG:HB2	4:C:323:LEU:HG	1.84	0.59
6:G:247:MET:SD	6:G:250:ARG:NH2	2.74	0.59
3:Y:65:LYS:HG3	4:A:17:ARG:NH2	2.17	0.59
4:A:477:ASN:OD1	4:A:478:HIS:N	2.35	0.59
9:S:30:PHE:O	9:S:34:ILE:HG12	2.02	0.59
4:A:11:SER:HA	4:A:14:LEU:HD12	1.84	0.59
4:B:477:ASN:HD22	12:7:12:TRP:NE1	2.00	0.59
5:E:241:GLU:HA	5:E:244:ARG:HG2	1.83	0.59
5:E:396:LEU:HD23	5:E:400:ASP:HB3	1.84	0.59
12:7:163:TYR:CE1	12:7:167:PHE:HB2	2.37	0.59
6:G:163:SER:OG	6:G:179:GLU:OE1	2.19	0.59
4:B:470:PHE:HZ	4:B:503:THR:HG22	1.66	0.59
9:Q:64:PHE:CE2	9:R:19:LEU:HD13	2.38	0.59
5:F:37:LEU:HB2	5:F:48:LEU:HB2	1.85	0.59
6:G:164:ILE:HD11	6:G:180:LYS:HB2	1.83	0.59
4:B:275:LYS:HA	4:B:278:VAL:HG12	1.85	0.59
6:G:172:SER:O	6:G:231:SER:OG	2.20	0.59
9:N:67:MET:HE3	9:N:67:MET:O	2.02	0.59
3:Y:66:ASP:OD1	4:A:17:ARG:NH1	2.35	0.59
4:B:182:LEU:HA	4:B:185:ILE:HD12	1.84	0.59
4:C:85:LYS:NZ	5:F:30:LEU:O	2.35	0.59
4:C:172:ASP:O	4:C:177:LYS:NZ	2.36	0.59
5:F:237:LEU:HD11	5:F:296:ILE:HG12	1.85	0.59
4:B:142:ARG:NH1	4:B:143:SER:OG	2.36	0.59
2:J:23:VAL:O	2:J:27:MET:HB2	2.03	0.59
3:Y:96:ASN:OD1	4:C:12:SER:OG	2.19	0.59
4:B:386:LYS:HG2	4:B:387:GLN:H	1.68	0.59
4:C:18:ILE:HD12	5:F:56:GLU:HG2	1.85	0.59
5:E:46:LEU:HD13	5:E:65:ASP:HB2	1.85	0.58
11:Z:97:ASN:HB2	12:7:128:ARG:HH22	1.68	0.58
4:C:412:LEU:HD21	6:G:26:VAL:HG12	1.85	0.58
9:O:14:ILE:HG12	9:P:14:ILE:HG22	1.86	0.58
4:B:434:GLN:HG3	4:B:435:TYR:HD2	1.68	0.58
5:E:241:GLU:OE1	5:E:295:ARG:NH2	2.36	0.58
5:E:296:ILE:HD11	5:E:304:VAL:HG21	1.85	0.58
5:F:188:GLY:N	5:F:220:GLY:O	2.35	0.58
11:Z:176:VAL:HA	11:Z:179:ARG:HB2	1.84	0.58
6:G:239:ASN:HA	6:G:242:LYS:HZ3	1.69	0.58
4:A:168:LEU:HD11	4:A:344:VAL:HG13	1.86	0.58
4:B:153:LYS:HD2	4:B:430:LEU:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:270:TYR:HE2	4:C:308:LEU:HD23	1.67	0.58
13:6:51:LYS:HD2	13:6:56:GLN:NE2	2.18	0.58
4:C:257:GLU:OE1	4:C:310:ARG:NH2	2.31	0.58
7:H:47:PRO:HB3	7:H:79:PRO:HD3	1.86	0.58
7:H:57:VAL:N	7:H:68:PHE:O	2.35	0.58
4:C:434:GLN:HB2	15:C:601:ATP:N1	2.19	0.58
5:D:207:ILE:HD13	5:D:213:SER:HB3	1.85	0.58
10:X:78:GLY:HA2	10:X:82:TRP:HB3	1.86	0.58
9:O:24:ILE:HG13	9:P:24:ILE:CD1	2.34	0.58
9:O:37:VAL:HG23	9:O:44:LYS:HB2	1.84	0.58
12:7:129:PRO:HB2	12:7:133:LEU:HB2	1.84	0.58
7:H:58:GLU:HA	7:H:67:LYS:HA	1.85	0.58
9:R:7:ALA:HA	9:R:10:ILE:HG12	1.84	0.58
4:A:396:LEU:HB3	4:A:400:ARG:HH12	1.68	0.58
4:B:46:LEU:HB3	4:B:49:ILE:HB	1.86	0.58
6:G:203:ALA:O	7:H:51:GLN:NE2	2.37	0.58
9:N:39:ARG:NH2	9:N:40:ASN:OD1	2.37	0.58
11:Z:117:ALA:HB3	12:7:107:GLU:HG2	1.84	0.58
11:Z:175:SER:C	11:Z:179:ARG:HE	2.12	0.58
3:Y:77:THR:OG1	3:Y:80:ASN:OD1	2.17	0.57
9:S:52:ILE:HA	9:S:55:PHE:CE2	2.39	0.57
9:L:4:VAL:HG13	9:M:2:GLN:HE21	1.69	0.57
4:C:186:LEU:HD11	4:C:435:TYR:HD1	1.68	0.57
5:D:41:THR:HG23	5:D:44:GLY:H	1.69	0.57
5:D:377:THR:HG22	5:D:407:ALA:HB2	1.85	0.57
9:M:18:GLY:HA3	9:M:65:CYS:SG	2.44	0.57
10:X:63:GLU:HA	10:X:66:TYR:HB3	1.85	0.57
4:C:82:ARG:HH12	5:F:35:ASN:CG	2.12	0.57
4:C:439:ALA:N	4:C:442:GLU:OE2	2.35	0.57
5:F:197:LEU:O	5:F:201:MET:HG2	2.04	0.57
4:B:134:LYS:NZ	5:F:223:ASN:HD22	2.01	0.57
9:L:43:ILE:HG13	9:L:47:VAL:HG13	1.85	0.57
9:M:61:THR:HA	9:N:19:LEU:HD12	1.84	0.57
4:B:144:VAL:HG22	4:B:380:ALA:HB2	1.86	0.57
4:B:344:VAL:HA	4:B:347:ILE:HG22	1.86	0.57
7:H:88:ILE:HD13	8:I:14:LEU:HD11	1.86	0.57
9:T:20:LEU:O	9:T:24:ILE:HG12	2.04	0.57
9:L:5:LEU:O	9:L:8:LYS:HG3	2.04	0.57
1:8:46:SER:OG	12:7:166:ARG:NH1	2.37	0.57
5:D:117:ILE:HG21	5:D:235:THR:HG22	1.86	0.57
10:X:69:ILE:HD11	10:X:89:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:137:ASP:O	14:U:32:LYS:NZ	2.38	0.57
4:B:154:ALA:HA	4:B:158:LEU:HD13	1.86	0.57
4:B:399:TYR:HA	4:B:402:VAL:HG12	1.87	0.56
4:C:182:LEU:HD21	4:C:218:LEU:HD11	1.87	0.56
6:G:96:ARG:NH2	6:G:117:GLN:O	2.37	0.56
3:Y:67:ARG:NE	3:Y:93:SER:O	2.38	0.56
4:A:422:ARG:NH2	4:A:451:VAL:O	2.38	0.56
5:F:117:ILE:HG21	5:F:235:THR:HG22	1.87	0.56
6:G:78:THR:HG21	6:G:114:ILE:HB	1.88	0.56
4:A:395:PHE:HD1	4:A:398:GLN:HE22	1.51	0.56
9:S:39:ARG:HH12	9:T:39:ARG:HA	1.70	0.56
9:L:61:THR:HB	9:M:19:LEU:HB3	1.87	0.56
9:P:12:ALA:O	9:P:16:THR:HG23	2.06	0.56
3:Y:132:LYS:HG3	3:Y:134:PHE:H	1.69	0.56
4:C:281:ARG:HD3	4:C:296:TYR:HD1	1.71	0.56
4:C:207:ALA:HB3	4:C:235:ALA:HA	1.87	0.56
5:E:322:PRO:HA	5:E:325:THR:HG22	1.87	0.56
7:H:67:LYS:NZ	7:H:94:GLU:OE2	2.38	0.56
4:A:251:THR:O	4:A:255:ILE:HG12	2.06	0.56
4:A:271:ASP:HA	4:A:328:VAL:HB	1.88	0.56
4:A:376:VAL:HG11	5:E:192:ARG:HD2	1.87	0.56
4:C:69:GLU:OE1	4:C:69:GLU:N	2.38	0.56
5:D:46:LEU:HD13	5:D:65:ASP:HB3	1.87	0.56
5:F:33:ILE:HD12	5:F:34:LEU:HD13	1.87	0.56
9:N:39:ARG:HH22	9:O:38:SER:C	2.14	0.56
11:Z:137:ALA:HB3	12:7:41:ARG:CZ	2.36	0.56
4:B:369:VAL:HG23	4:B:400:ARG:HH22	1.70	0.56
4:C:318:GLU:N	4:C:318:GLU:OE2	2.39	0.56
7:H:38:ARG:NH2	9:M:40:ASN:OD1	2.38	0.56
9:K:12:ALA:O	9:K:16:THR:HG23	2.05	0.56
10:X:150:THR:HG21	10:X:158:LEU:HG	1.88	0.56
9:T:39:ARG:NH2	9:K:35:ASN:OD1	2.39	0.55
10:X:58:TRP:CZ2	14:U:65:PRO:HG2	2.41	0.55
4:A:142:ARG:NH1	4:A:143:SER:O	2.39	0.55
5:D:190:ARG:O	5:D:191:THR:HG22	2.06	0.55
7:H:99:GLU:O	7:H:103:ASN:ND2	2.39	0.55
4:B:43:VAL:HG21	4:B:90:VAL:HG21	1.88	0.55
4:B:72:GLN:OE1	4:B:72:GLN:N	2.36	0.55
4:B:383:LYS:HD2	4:B:386:LYS:HD2	1.88	0.55
9:Q:43:ILE:HD13	9:R:38:SER:HA	1.88	0.55
4:A:28:ASN:ND2	4:A:48:ASN:OD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:183:VAL:HG12	5:F:216:ALA:HB3	1.87	0.55
9:T:26:ILE:HB	9:T:55:PHE:CE1	2.42	0.55
13:6:89:LYS:HA	13:6:92:HIS:HB2	1.89	0.55
4:C:388:VAL:HG12	4:C:447:ILE:HG22	1.87	0.55
5:F:469:LYS:HA	5:F:472:LYS:HG2	1.89	0.55
4:A:331:THR:OG1	4:A:335:ASP:O	2.19	0.55
4:B:402:VAL:HA	4:B:405:PHE:CE2	2.42	0.55
4:C:432:GLN:NE2	4:C:436:SER:O	2.34	0.55
5:E:187:VAL:HG22	5:E:232:VAL:HG13	1.87	0.55
6:G:99:LEU:HD21	6:G:122:HIS:HB3	1.88	0.55
9:M:7:ALA:HA	9:M:10:ILE:HG22	1.88	0.55
13:6:19:SER:O	13:6:24:ALA:N	2.37	0.55
9:K:19:LEU:HD21	9:K:66:LEU:HB2	1.89	0.55
9:Q:30:PHE:CE1	9:Q:34:ILE:HD11	2.42	0.55
10:X:196:PHE:HA	10:X:199:MET:HE2	1.87	0.55
3:Y:168:ILE:HD11	4:B:18:ILE:HD11	1.88	0.54
4:B:293:ARG:HG2	5:F:280:GLY:HA3	1.90	0.54
6:G:209:LEU:HA	7:H:74:PHE:HE2	1.71	0.54
9:L:19:LEU:HD21	9:L:66:LEU:HD21	1.88	0.54
4:C:382:VAL:HB	4:C:385:LEU:HD23	1.89	0.54
5:E:231:ARG:O	5:E:235:THR:HG23	2.08	0.54
9:T:51:ALA:HA	9:K:30:PHE:CZ	2.41	0.54
9:L:64:PHE:CZ	9:M:66:LEU:HD13	2.40	0.54
9:M:64:PHE:HB3	9:N:66:LEU:HD21	1.89	0.54
4:A:355:GLU:HB3	4:A:358:LEU:HB2	1.90	0.54
13:6:36:LYS:O	13:6:40:PRO:HD2	2.07	0.54
1:8:12:GLN:O	1:8:16:GLY:N	2.41	0.54
9:Q:19:LEU:HD12	9:Q:22:ALA:HB3	1.89	0.54
13:6:45:GLN:O	13:6:49:ALA:N	2.41	0.54
3:Y:44:GLU:HA	3:Y:47:VAL:HG12	1.88	0.54
5:F:288:ASP:OD1	5:F:289:MET:N	2.41	0.54
5:D:87:VAL:HG11	5:D:115:LYS:HG2	1.88	0.54
5:E:258:ILE:HG22	5:E:310:VAL:HG22	1.89	0.54
6:G:205:VAL:HG23	6:G:206:PRO:HD3	1.90	0.54
8:I:28:GLU:OE2	8:I:28:GLU:N	2.33	0.54
9:M:34:ILE:HA	9:M:37:VAL:HG12	1.90	0.54
4:A:64:MET:O	4:A:76:VAL:HG12	2.08	0.54
4:B:251:THR:O	4:B:255:ILE:HG12	2.08	0.54
5:E:332:THR:OG1	5:E:353:SER:O	2.26	0.54
5:F:92:LEU:HB3	5:F:213:SER:HB2	1.88	0.54
9:S:52:ILE:HD13	9:S:55:PHE:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:54:GLY:HA2	9:T:57:LEU:HD12	1.90	0.54
9:M:45:ASP:OD1	9:M:46:THR:N	2.41	0.54
4:B:98:ASP:OD2	4:B:128:ARG:NE	2.41	0.54
4:B:106:LEU:HD23	4:B:230:TYR:HA	1.90	0.54
6:G:92:ALA:O	6:G:96:ARG:HD3	2.07	0.54
9:T:29:VAL:HG23	9:K:27:ALA:HB1	1.89	0.54
1:8:44:PHE:HA	1:8:47:LYS:HG2	1.89	0.53
9:K:20:LEU:O	9:K:24:ILE:HG22	2.09	0.53
11:Z:91:VAL:HG21	12:7:167:PHE:HE1	1.72	0.53
4:C:146:GLU:HB2	4:C:163:ARG:HG3	1.90	0.53
5:E:13:VAL:O	5:E:73:GLY:N	2.38	0.53
6:G:90:GLN:O	6:G:93:LYS:HG3	2.07	0.53
13:6:88:THR:O	13:6:92:HIS:N	2.41	0.53
4:A:192:ASN:HA	4:A:200:LYS:HD3	1.91	0.53
4:A:414:ALA:HA	4:A:417:LYS:HB2	1.90	0.53
5:D:37:LEU:HD12	5:D:76:VAL:HG22	1.90	0.53
7:H:33:PRO:HD2	7:H:57:VAL:HG12	1.89	0.53
9:Q:64:PHE:CE1	9:R:66:LEU:HD13	2.43	0.53
9:S:20:LEU:HG	9:R:21:GLY:HA3	1.91	0.53
9:S:33:LEU:HA	9:T:34:ILE:HG21	1.89	0.53
5:E:16:VAL:HG21	5:E:70:LEU:HB3	1.91	0.53
5:E:244:ARG:NH1	5:E:245:ASP:OD1	2.42	0.53
6:G:61:ASP:HB2	6:G:187:THR:HG21	1.91	0.53
4:B:26:ASN:HD22	11:Z:203:GLN:HE21	1.57	0.53
10:X:105:ILE:HG13	10:X:108:SER:HB2	1.90	0.53
6:G:72:GLU:HG2	6:G:161:LYS:HG2	1.91	0.53
4:B:446:LEU:HD22	4:B:467:GLU:HB2	1.89	0.53
6:G:229:GLU:OE2	6:G:233:ARG:NH2	2.42	0.53
9:T:14:ILE:HG21	9:K:14:ILE:HG22	1.89	0.53
10:X:232:TYR:O	10:X:236:ILE:HG12	2.08	0.53
1:8:42:ARG:O	12:7:166:ARG:NH1	2.41	0.53
4:A:182:LEU:HA	4:A:185:ILE:HG22	1.89	0.53
5:D:184:PHE:HB3	5:D:217:LEU:HD13	1.90	0.53
5:D:369:ASP:O	5:D:373:LYS:HG2	2.08	0.53
9:L:44:LYS:HA	9:L:47:VAL:HG22	1.89	0.53
9:N:45:ASP:OD1	9:N:46:THR:N	2.42	0.53
9:P:13:GLY:O	9:P:16:THR:OG1	2.25	0.53
4:A:139:LEU:HG	4:A:140:PRO:HD3	1.89	0.53
5:D:16:VAL:HG12	5:D:21:VAL:HG22	1.91	0.53
5:E:155:LEU:HD11	5:E:166:PHE:CD2	2.44	0.53
9:L:14:ILE:HG21	9:M:14:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:383:LYS:HG3	4:A:490:GLU:HB3	1.91	0.52
4:B:392:LEU:HD23	4:B:395:PHE:CD1	2.43	0.52
6:G:18:LYS:HA	6:G:21:LYS:HZ3	1.74	0.52
5:E:30:LEU:HD21	5:E:57:ASN:HA	1.91	0.52
5:F:458:TYR:CE1	5:F:459:MET:HG2	2.45	0.52
9:O:57:LEU:HD13	9:P:55:PHE:CE1	2.44	0.52
11:Z:134:GLU:O	12:7:41:ARG:NH1	2.41	0.52
5:D:127:GLN:O	5:D:300:LYS:NZ	2.41	0.52
8:I:31:THR:H	8:I:34:VAL:HG22	1.75	0.52
9:K:57:LEU:HD23	9:L:30:PHE:HE2	1.74	0.52
11:Z:137:ALA:H	12:7:41:ARG:NH2	2.07	0.52
11:Z:161:GLU:O	11:Z:165:ARG:HG2	2.10	0.52
4:A:342:THR:HG21	5:E:314:ALA:HA	1.91	0.52
4:B:217:GLN:HE22	5:E:130:SER:HB2	1.75	0.52
5:D:197:LEU:O	5:D:201:MET:HG2	2.08	0.52
6:G:95:VAL:HG23	6:G:165:PHE:HE2	1.74	0.52
9:M:14:ILE:HG21	9:N:14:ILE:HG22	1.92	0.52
10:X:109:PHE:CE2	10:X:112:SER:HA	2.44	0.52
4:A:181:ALA:O	4:A:184:THR:OG1	2.24	0.52
5:D:381:TYR:O	5:D:385:GLN:HG3	2.10	0.52
9:S:52:ILE:HD13	9:S:55:PHE:HE2	1.74	0.52
9:N:39:ARG:NH2	9:O:38:SER:O	2.40	0.52
9:N:47:VAL:HG21	9:O:34:ILE:HG23	1.92	0.52
12:7:22:THR:O	13:6:92:HIS:ND1	2.36	0.52
3:Y:64:LEU:HA	3:Y:67:ARG:HD3	1.90	0.52
9:O:13:GLY:O	9:O:16:THR:OG1	2.27	0.52
4:A:442:GLU:HB2	4:A:471:LEU:HD22	1.92	0.52
4:B:166:ARG:HG2	4:B:325:ALA:HB3	1.92	0.52
4:C:411:ASP:OD1	4:C:412:LEU:N	2.32	0.52
5:D:467:VAL:O	5:D:471:GLU:HG2	2.09	0.52
5:E:87:VAL:HG12	5:E:239:ILE:HD13	1.91	0.52
5:E:244:ARG:HH11	5:E:299:THR:HG21	1.72	0.52
9:Q:26:ILE:HB	9:Q:55:PHE:CD1	2.45	0.52
12:7:139:THR:HG23	12:7:146:ASP:HB2	1.91	0.52
1:8:37:ARG:NH1	12:7:139:THR:OG1	2.43	0.52
4:C:212:ARG:NH1	5:F:122:PRO:O	2.44	0.52
13:6:19:SER:HA	13:6:23:ASP:HB3	1.91	0.52
4:A:70:PRO:HA	5:E:72:ARG:HH12	1.75	0.51
4:B:11:SER:HA	4:B:14:LEU:HD12	1.91	0.51
9:P:6:ALA:O	9:P:10:ILE:HG12	2.09	0.51
9:Q:53:LEU:O	9:Q:57:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:58:TRP:HZ2	14:U:65:PRO:HG2	1.73	0.51
13:6:69:GLU:HG3	13:6:70:GLY:H	1.74	0.51
14:U:25:ALA:O	14:U:29:HIS:ND1	2.43	0.51
5:D:23:VAL:HG11	5:D:76:VAL:HG11	1.92	0.51
3:Y:67:ARG:HA	3:Y:70:VAL:HG22	1.91	0.51
4:C:169:ILE:HB	4:C:328:VAL:HG22	1.91	0.51
5:E:15:ALA:HB3	5:E:22:ASP:HB2	1.90	0.51
6:G:13:ILE:HG22	6:G:248:ILE:HG13	1.92	0.51
2:J:23:VAL:HG21	10:X:124:VAL:HG12	1.92	0.51
4:B:64:MET:HG2	4:B:66:LEU:HD22	1.93	0.51
4:C:281:ARG:HD3	4:C:296:TYR:CD1	2.45	0.51
4:C:434:GLN:HG2	4:C:435:TYR:CD2	2.45	0.51
5:E:430:LYS:NZ	5:E:465:ASP:OD2	2.37	0.51
6:G:87:ILE:HD11	6:G:232:ALA:HB3	1.92	0.51
6:G:110:ILE:HG13	6:G:130:ILE:HG23	1.92	0.51
10:X:212:PRO:HA	10:X:215:MET:HE2	1.92	0.51
5:E:458:TYR:CD1	5:E:459:MET:HG2	2.45	0.51
10:X:76:GLN:NE2	10:X:240:SER:HA	2.25	0.51
12:7:72:GLU:OE2	12:7:76:LYS:NZ	2.34	0.51
5:F:101:GLU:N	5:F:101:GLU:OE1	2.41	0.51
4:B:338:ALA:HB3	4:B:341:PRO:HG2	1.92	0.51
4:C:378:SER:HB2	4:C:386:LYS:HG2	1.93	0.51
4:B:268:ILE:HG23	4:B:325:ALA:HA	1.92	0.51
4:C:506:PHE:O	4:C:510:PHE:N	2.44	0.51
9:S:17:ILE:HG23	9:T:20:LEU:HD11	1.92	0.51
9:L:40:ASN:O	9:L:43:ILE:HG22	2.11	0.51
9:Q:43:ILE:HD12	9:Q:47:VAL:HG11	1.93	0.51
10:X:216:ILE:HA	10:X:219:ILE:HG12	1.92	0.51
13:6:89:LYS:NZ	14:U:9:VAL:H	2.09	0.51
4:A:70:PRO:HG3	5:E:14:THR:HB	1.93	0.51
4:B:26:ASN:ND2	11:Z:203:GLN:HE21	2.08	0.51
6:G:261:ALA:O	6:G:264:THR:OG1	2.27	0.51
11:Z:183:GLU:HA	13:6:9:ARG:HH22	1.76	0.51
4:B:168:LEU:O	4:B:352:ILE:N	2.35	0.50
9:Q:64:PHE:HE1	9:R:66:LEU:HD13	1.76	0.50
3:Y:102:GLU:OE2	3:Y:102:GLU:N	2.40	0.50
5:E:222:MET:HA	5:E:229:ARG:HD3	1.92	0.50
9:S:19:LEU:HD12	9:R:61:THR:HA	1.93	0.50
1:8:38:LEU:HG	10:X:53:ILE:HB	1.93	0.50
4:B:109:VAL:HB	4:B:118:ASP:HB3	1.92	0.50
5:E:9:ILE:HB	5:E:78:ASP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:77:ILE:HA	6:G:110:ILE:HG22	1.92	0.50
9:Q:26:ILE:HB	9:Q:55:PHE:HD1	1.75	0.50
13:6:11:LEU:O	13:6:14:THR:OG1	2.26	0.50
4:C:46:LEU:HB3	4:C:49:ILE:HB	1.94	0.50
5:D:34:LEU:HB3	5:D:118:HIS:CD2	2.46	0.50
5:D:128:SER:HB3	5:D:298:THR:HG23	1.94	0.50
5:E:330:ASP:OD1	5:E:331:ALA:N	2.42	0.50
5:F:15:ALA:HB3	5:F:22:ASP:HB2	1.93	0.50
4:B:13:ILE:HA	4:B:16:GLU:HG2	1.93	0.50
4:C:293:ARG:HA	6:G:267:LEU:HD11	1.94	0.50
5:D:390:ILE:HG22	5:D:391:LEU:HD12	1.93	0.50
5:E:190:ARG:NH2	15:E:501:ATP:O3G	2.40	0.50
5:E:241:GLU:HG2	5:E:244:ARG:HH21	1.77	0.50
5:F:237:LEU:HD11	5:F:296:ILE:CG1	2.42	0.50
9:O:58:SER:O	9:O:61:THR:OG1	2.27	0.50
12:7:127:ALA:HA	14:U:35:PRO:HA	1.92	0.50
4:C:399:TYR:CG	4:C:423:GLY:HA3	2.47	0.50
6:G:9:ARG:NH2	6:G:251:TYR:OH	2.45	0.50
4:B:472:SER:HA	4:B:475:LYS:HG2	1.93	0.50
5:F:34:LEU:HA	5:F:49:GLU:OE2	2.12	0.50
4:A:98:ASP:O	4:A:128:ARG:NH2	2.43	0.50
9:O:44:LYS:HA	9:O:47:VAL:HG12	1.93	0.50
11:Z:134:GLU:OE1	11:Z:134:GLU:N	2.40	0.50
11:Z:137:ALA:H	12:7:41:ARG:HH22	1.60	0.50
11:Z:182:SER:O	13:6:9:ARG:NH2	2.44	0.50
3:Y:107:ASP:O	3:Y:111:LEU:HD23	2.12	0.50
4:A:204:VAL:N	4:A:267:LEU:O	2.45	0.50
4:B:13:ILE:HG13	4:B:17:ARG:NH2	2.23	0.50
4:B:134:LYS:HZ2	5:F:223:ASN:HB2	1.76	0.50
4:B:162:GLY:H	4:B:165:GLN:HG2	1.75	0.50
4:C:166:ARG:HG3	4:C:325:ALA:HB3	1.94	0.50
5:D:422:GLU:OE2	5:D:429:GLY:N	2.28	0.50
9:M:12:ALA:O	9:M:16:THR:HG23	2.11	0.50
12:7:22:THR:C	13:6:92:HIS:HD1	2.20	0.50
4:A:50:GLN:OE1	4:A:92:ARG:NH2	2.44	0.49
4:B:441:GLU:HB3	4:B:486:ARG:HB3	1.93	0.49
5:E:183:VAL:O	5:E:254:PHE:N	2.40	0.49
9:K:21:GLY:H	9:L:20:LEU:HD22	1.77	0.49
12:7:78:TYR:CD2	13:6:61:ALA:HB1	2.46	0.49
12:7:137:ASP:OD1	14:U:32:LYS:NZ	2.26	0.49
13:6:39:LEU:HB3	13:6:40:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:417:PRO:HB2	5:F:429:GLY:HA2	1.94	0.49
6:G:129:SER:OG	8:I:47:TYR:N	2.42	0.49
9:T:7:ALA:HA	9:T:10:ILE:HG22	1.94	0.49
9:N:24:ILE:HB	9:O:24:ILE:HG22	1.93	0.49
4:C:467:GLU:O	4:C:471:LEU:HD23	2.12	0.49
9:R:58:SER:O	9:R:61:THR:OG1	2.30	0.49
10:X:199:MET:HA	10:X:208:PHE:CE2	2.45	0.49
4:B:351:GLN:HE21	4:B:371:LEU:HD23	1.77	0.49
5:D:326:PHE:HD1	5:D:329:LEU:HD11	1.78	0.49
5:E:33:ILE:HD13	5:E:50:VAL:HG12	1.94	0.49
7:H:29:GLN:HE22	7:H:42:LEU:HD22	1.78	0.49
7:H:69:PHE:H	7:H:91:PHE:CB	2.26	0.49
4:A:440:THR:HA	4:A:443:GLN:HB2	1.94	0.49
4:B:13:ILE:O	4:B:16:GLU:HG2	2.13	0.49
4:B:82:ARG:HG3	4:B:83:LEU:HD22	1.94	0.49
4:C:234:VAL:HG21	4:C:252:ALA:HB2	1.94	0.49
7:H:109:LYS:NZ	7:H:127:VAL:HG23	2.28	0.49
7:H:132:ASN:O	7:H:136:VAL:HG23	2.12	0.49
4:B:149:GLN:N	4:B:149:GLN:OE1	2.45	0.49
4:B:270:TYR:HB2	4:B:327:PRO:HA	1.93	0.49
4:B:440:THR:HA	4:B:443:GLN:HG2	1.94	0.49
4:C:478:HIS:HB3	4:C:481:LEU:HD13	1.94	0.49
9:L:4:VAL:HG13	9:M:2:GLN:NE2	2.27	0.49
4:A:463:ILE:O	4:A:467:GLU:HG3	2.12	0.49
5:E:335:LEU:HA	5:E:348:VAL:HA	1.94	0.49
5:F:132:GLU:HB3	5:F:149:ARG:HB3	1.94	0.49
4:A:455:LEU:HD12	4:A:463:ILE:HD12	1.94	0.49
4:B:281:ARG:HA	4:B:297:PRO:HD3	1.94	0.49
5:E:117:ILE:HD12	5:E:235:THR:HA	1.94	0.49
5:E:263:GLN:O	5:E:267:GLU:HG2	2.13	0.49
6:G:112:ASP:HB2	6:G:116:MET:HE1	1.95	0.49
9:K:3:LEU:HD23	9:L:2:GLN:HG2	1.94	0.49
9:K:65:CYS:HB2	9:L:19:LEU:HG	1.94	0.49
9:N:7:ALA:HA	9:N:10:ILE:HG12	1.95	0.49
10:X:59:LEU:HA	10:X:62:GLN:NE2	2.27	0.49
2:J:3:LYS:HZ1	12:7:146:ASP:CG	2.20	0.49
4:C:36:VAL:HG12	5:F:53:HIS:HB2	1.95	0.49
4:C:213:SER:O	4:C:217:GLN:HG2	2.13	0.49
5:E:185:THR:HA	5:E:218:VAL:HB	1.94	0.49
5:F:83:ILE:HD13	5:F:117:ILE:HD11	1.93	0.49
9:O:20:LEU:O	9:O:24:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:127:ALA:O	12:7:129:PRO:HD3	2.12	0.49
4:C:506:PHE:HA	4:C:509:THR:HG22	1.95	0.49
5:D:336:SER:HB3	5:D:349:ASP:HB2	1.94	0.49
9:O:26:ILE:HD12	9:O:55:PHE:CD1	2.47	0.49
5:D:258:ILE:HD11	5:D:289:MET:HE1	1.95	0.48
5:D:469:LYS:O	5:D:472:LYS:HG3	2.13	0.48
5:F:396:LEU:O	5:F:401:LYS:NZ	2.46	0.48
9:Q:57:LEU:HD22	9:R:55:PHE:CZ	2.48	0.48
11:Z:179:ARG:O	11:Z:183:GLU:HG2	2.13	0.48
4:A:68:LEU:HD23	4:A:68:LEU:O	2.13	0.48
4:B:142:ARG:HD3	4:B:143:SER:O	2.13	0.48
5:D:326:PHE:CD1	5:D:329:LEU:HD11	2.48	0.48
9:Q:26:ILE:HD12	9:Q:55:PHE:HE1	1.78	0.48
1:8:36:LEU:HD13	12:7:160:VAL:HG21	1.94	0.48
3:Y:66:ASP:HA	4:A:17:ARG:HH12	1.77	0.48
12:7:37:ASP:OD1	12:7:38:GLU:N	2.45	0.48
4:A:161:ILE:HD13	4:A:167:GLU:HB2	1.95	0.48
4:A:396:LEU:HB3	4:A:400:ARG:NH1	2.29	0.48
4:A:500:LYS:O	4:A:503:THR:OG1	2.25	0.48
6:G:87:ILE:HG23	6:G:167:ASN:ND2	2.29	0.48
9:O:47:VAL:HG21	9:P:34:ILE:HG23	1.95	0.48
3:Y:152:SER:OG	3:Y:154:LYS:NZ	2.47	0.48
4:B:458:ILE:O	4:B:459:GLU:HG3	2.14	0.48
4:B:462:ARG:HB3	4:B:465:GLU:OE2	2.14	0.48
8:I:33:SER:O	8:I:37:ARG:HG3	2.13	0.48
9:R:63:LEU:HA	9:R:66:LEU:HB3	1.94	0.48
3:Y:44:GLU:HG3	3:Y:103:LYS:HG2	1.95	0.48
3:Y:122:THR:OG1	3:Y:123:VAL:N	2.40	0.48
4:A:196:ASP:HB3	4:A:199:LYS:HE3	1.96	0.48
4:B:191:TRP:CD1	4:B:199:LYS:HD3	2.47	0.48
4:C:70:PRO:HD3	5:D:15:ALA:HB2	1.95	0.48
4:C:106:LEU:HD23	4:C:232:ILE:HD11	1.95	0.48
4:C:445:PRO:HB3	4:C:499:LEU:HD11	1.96	0.48
8:I:45:THR:O	8:I:54:SER:N	2.44	0.48
9:Q:14:ILE:HA	9:Q:17:ILE:HG12	1.94	0.48
4:A:223:GLU:HA	4:A:228:MET:HE3	1.95	0.48
4:B:273:LEU:O	4:B:276:GLN:HB3	2.13	0.48
4:C:204:VAL:HG22	4:C:232:ILE:HB	1.95	0.48
9:P:64:PHE:HA	9:P:67:MET:HE2	1.96	0.48
9:Q:40:ASN:HB2	9:Q:43:ILE:HG12	1.94	0.48
10:X:54:ILE:HG13	11:Z:88:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:106:ARG:NH2	14:U:26:ASN:HD21	2.11	0.48
4:B:405:PHE:O	4:B:405:PHE:CD1	2.66	0.48
5:F:187:VAL:HG22	5:F:232:VAL:HG13	1.95	0.48
5:F:440:SER:HB2	5:F:463:ILE:HB	1.96	0.48
6:G:9:ARG:O	6:G:13:ILE:HG12	2.13	0.48
11:Z:177:ILE:HA	11:Z:180:VAL:HG12	1.93	0.48
5:F:345:TYR:HB3	17:F:501:ADP:C6	2.49	0.48
7:H:126:GLN:HA	7:H:129:VAL:HG12	1.95	0.48
9:M:21:GLY:HA2	9:M:24:ILE:HG22	1.96	0.48
11:Z:176:VAL:O	11:Z:180:VAL:N	2.33	0.48
4:B:383:LYS:NZ	4:B:388:VAL:HG13	2.25	0.48
5:D:409:LYS:HE3	5:D:450:ASP:HA	1.96	0.48
5:F:312:VAL:HG23	5:F:315:ASP:HA	1.96	0.48
5:F:346:PRO:HG2	5:F:415:SER:HA	1.95	0.48
9:M:1:MET:HA	9:M:4:VAL:HB	1.96	0.48
9:P:57:LEU:HD13	9:Q:55:PHE:CZ	2.48	0.48
9:P:65:CYS:SG	9:Q:19:LEU:HD23	2.54	0.48
4:A:305:SER:HB2	5:E:222:MET:CG	2.41	0.47
4:A:340:ILE:HA	4:A:343:ASN:HD21	1.79	0.47
4:C:450:GLY:HA2	4:C:455:LEU:HD22	1.96	0.47
5:F:434:LEU:O	5:F:438:VAL:HG23	2.14	0.47
6:G:96:ARG:HE	6:G:121:THR:HG21	1.79	0.47
7:H:102:LYS:HZ1	7:H:133:LEU:HD22	1.79	0.47
7:H:122:GLU:HB3	8:I:16:VAL:HG21	1.95	0.47
9:Q:64:PHE:CZ	9:R:66:LEU:HB2	2.49	0.47
4:A:112:ALA:O	4:A:251:THR:HG21	2.14	0.47
5:E:321:ALA:HB3	5:E:322:PRO:HD3	1.96	0.47
6:G:75:VAL:HB	6:G:164:ILE:HG22	1.96	0.47
14:U:17:SER:OG	14:U:20:ASN:OD1	2.28	0.47
5:E:178:HIS:O	5:E:214:LYS:NZ	2.40	0.47
5:E:337:ARG:O	5:E:340:SER:N	2.47	0.47
9:Q:18:GLY:HA2	9:R:20:LEU:HD11	1.96	0.47
11:Z:108:ASP:O	11:Z:112:GLN:HG2	2.14	0.47
3:Y:26:ALA:O	3:Y:29:LYS:HG2	2.14	0.47
4:A:118:ASP:OD1	4:A:118:ASP:N	2.46	0.47
4:B:136:PRO:O	4:B:141:ARG:NH2	2.42	0.47
4:B:353:PHE:HD2	4:B:371:LEU:HD22	1.79	0.47
5:D:139:LYS:NZ	5:D:460:VAL:O	2.46	0.47
5:E:458:TYR:CE1	5:E:459:MET:HG2	2.50	0.47
7:H:133:LEU:O	7:H:137:LEU:N	2.47	0.47
9:K:8:LYS:HG3	9:L:9:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:24:ILE:HB	9:R:24:ILE:HD11	1.97	0.47
10:X:85:TYR:HD2	10:X:242:LEU:HD21	1.80	0.47
10:X:242:LEU:O	10:X:246:VAL:HG22	2.15	0.47
11:Z:151:LYS:O	12:7:58:TYR:OH	2.33	0.47
4:B:272:ASP:H	4:B:328:VAL:HB	1.79	0.47
4:C:42:ARG:HB3	4:C:72:GLN:HG3	1.95	0.47
4:C:68:LEU:HD12	4:C:68:LEU:O	2.14	0.47
5:E:23:VAL:HG11	5:E:76:VAL:HG11	1.95	0.47
5:E:158:GLY:O	5:E:163:LYS:NZ	2.38	0.47
5:E:182:SER:HB3	5:E:252:LEU:HB2	1.97	0.47
5:E:393:MET:HA	5:E:396:LEU:HD13	1.96	0.47
9:R:14:ILE:O	9:R:17:ILE:HG12	2.13	0.47
10:X:67:ASP:O	10:X:71:ASN:ND2	2.47	0.47
4:A:182:LEU:HD11	4:A:218:LEU:HD11	1.96	0.47
4:C:270:TYR:CE2	4:C:308:LEU:HD23	2.49	0.47
5:D:386:ASP:O	5:D:390:ILE:HG13	2.14	0.47
5:E:127:GLN:OE1	5:E:298:THR:HG23	2.15	0.47
5:F:37:LEU:HD13	5:F:78:ASP:HA	1.96	0.47
9:L:26:ILE:HG12	9:L:55:PHE:CD1	2.49	0.47
3:Y:31:SER:OG	3:Y:32:SER:N	2.48	0.47
3:Y:127:GLU:OE1	3:Y:152:SER:OG	2.29	0.47
4:B:139:LEU:O	4:B:141:ARG:N	2.45	0.47
4:B:203:CYS:O	4:B:231:SER:HA	2.14	0.47
4:C:249:PRO:HG2	4:C:276:GLN:HG3	1.96	0.47
4:C:280:TYR:HD2	4:C:300:VAL:HG12	1.80	0.47
7:H:109:LYS:HZ2	7:H:127:VAL:HG23	1.80	0.47
7:H:125:ILE:HG21	8:I:13:TYR:HD1	1.80	0.47
4:A:57:PHE:HD1	4:A:61:VAL:HG23	1.79	0.47
4:C:369:VAL:HG13	4:C:400:ARG:NH1	2.30	0.47
5:E:97:ASN:OD1	5:E:100:GLY:N	2.41	0.47
3:Y:40:LEU:HG	3:Y:103:LYS:HD3	1.96	0.47
4:B:85:LYS:HE2	5:E:32:ALA:HA	1.95	0.47
4:C:190:ARG:HB2	4:C:191:TRP:CE3	2.50	0.47
4:C:425:ARG:NH1	4:C:460:LEU:HB3	2.30	0.47
5:E:147:TYR:CD1	5:E:153:ILE:HD12	2.50	0.47
5:F:196:ASP:O	5:F:199:ARG:HD3	2.15	0.47
6:G:148:ASP:OD1	8:I:9:SER:OG	2.30	0.47
9:T:21:GLY:N	9:K:20:LEU:HG	2.30	0.47
11:Z:113:LEU:HD11	14:U:10:VAL:HG21	1.97	0.47
3:Y:111:LEU:O	3:Y:115:HIS:N	2.34	0.47
4:A:293:ARG:HD3	4:A:339:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:54:LEU:HD11	4:B:62:LYS:HB3	1.97	0.47
4:B:56:GLU:O	4:B:91:LYS:N	2.47	0.47
4:B:212:ARG:HG3	4:B:237:THR:HG21	1.96	0.47
5:D:84:SER:HB2	5:D:114:ARG:HG3	1.97	0.47
6:G:80:ASP:OD2	6:G:133:ILE:N	2.48	0.47
9:K:57:LEU:HD21	9:L:55:PHE:CZ	2.50	0.47
9:M:14:ILE:O	9:M:17:ILE:HG12	2.15	0.47
9:O:39:ARG:NH1	9:O:39:ARG:HB3	2.30	0.47
14:U:9:VAL:HG12	14:U:9:VAL:O	2.14	0.47
4:A:398:GLN:HA	4:A:401:GLU:CD	2.40	0.46
4:B:46:LEU:HD11	4:B:92:ARG:HB2	1.97	0.46
9:Q:67:MET:HG3	10:X:179:SER:HB2	1.98	0.46
3:Y:132:LYS:HD2	3:Y:134:PHE:HD1	1.80	0.46
4:A:7:PRO:HA	4:A:10:VAL:HG12	1.95	0.46
4:A:434:GLN:HB2	15:A:601:ATP:C6	2.49	0.46
4:C:39:GLY:N	4:C:81:ASP:OD2	2.36	0.46
5:D:276:PRO:HD2	6:G:271:ILE:HD11	1.98	0.46
5:E:98:VAL:HG21	5:E:228:ALA:HA	1.97	0.46
5:F:321:ALA:O	5:F:325:THR:HG23	2.14	0.46
11:Z:116:VAL:O	11:Z:120:THR:HG23	2.15	0.46
12:7:30:SER:OG	14:U:2:SER:O	2.33	0.46
3:Y:65:LYS:HG3	4:A:17:ARG:HH22	1.79	0.46
3:Y:138:GLU:OE1	3:Y:138:GLU:N	2.44	0.46
4:A:399:TYR:CG	4:A:423:GLY:HA3	2.50	0.46
4:C:19:LYS:HG3	4:C:21:VAL:HG23	1.96	0.46
4:C:52:GLU:HB2	4:C:64:MET:HE2	1.97	0.46
4:C:364:ARG:HB3	4:C:365:PRO:HD3	1.97	0.46
4:B:30:THR:HG23	4:B:90:VAL:O	2.15	0.46
5:E:187:VAL:HG21	5:E:233:ALA:HB2	1.96	0.46
9:L:32:ALA:HB3	9:M:34:ILE:HD11	1.96	0.46
3:Y:44:GLU:HG3	3:Y:103:LYS:HE3	1.98	0.46
3:Y:120:LYS:HE2	4:B:27:LEU:O	2.16	0.46
4:B:148:VAL:HB	4:B:161:ILE:HG13	1.95	0.46
4:B:211:LYS:HG3	4:B:214:THR:HG23	1.96	0.46
4:B:439:ALA:O	4:B:443:GLN:HG2	2.16	0.46
4:C:34:LEU:HD11	4:C:44:PHE:HB2	1.98	0.46
4:C:349:ASP:OD1	5:D:190:ARG:HD3	2.15	0.46
12:7:35:ARG:NH2	12:7:38:GLU:OE1	2.41	0.46
3:Y:98:LEU:HG	4:C:11:SER:OG	2.15	0.46
4:A:20:GLY:C	4:A:27:LEU:HD21	2.41	0.46
4:C:77:LEU:HD12	4:C:81:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:HIS:CD2	5:E:252:LEU:HD11	2.50	0.46
5:E:241:GLU:HG2	5:E:244:ARG:HE	1.81	0.46
6:G:146:ILE:O	6:G:150:LEU:HD23	2.15	0.46
7:H:132:ASN:O	7:H:135:SER:OG	2.23	0.46
9:K:26:ILE:HG23	9:K:55:PHE:HD1	1.80	0.46
4:C:202:TYR:O	4:C:267:LEU:N	2.36	0.46
4:C:279:ALA:O	4:C:283:LEU:HD23	2.16	0.46
10:X:73:THR:HG22	10:X:82:TRP:HB2	1.97	0.46
1:8:23:LEU:HA	1:8:26:LEU:HG	1.98	0.46
4:A:57:PHE:HA	4:A:90:VAL:HG12	1.97	0.46
4:A:86:GLU:HB3	5:D:30:LEU:HD11	1.98	0.46
4:C:64:MET:O	4:C:76:VAL:HG22	2.15	0.46
5:E:37:LEU:HD13	5:E:78:ASP:HA	1.97	0.46
5:F:250:ASP:OD1	5:F:250:ASP:N	2.48	0.46
5:F:458:TYR:O	5:F:469:LYS:NZ	2.49	0.46
9:R:19:LEU:HD12	9:R:62:GLY:CA	2.46	0.46
11:Z:179:ARG:HG3	13:6:13:ASP:CG	2.41	0.46
4:A:281:ARG:O	4:A:285:LEU:HG	2.14	0.46
6:G:263:ILE:O	6:G:267:LEU:HD23	2.16	0.46
7:H:126:GLN:HE21	8:I:20:ALA:HA	1.81	0.46
5:D:451:ASN:OD1	5:D:452:ILE:HD12	2.15	0.46
5:F:40:LYS:HD3	5:F:45:LYS:NZ	2.31	0.46
7:H:107:GLU:HA	7:H:110:LYS:NZ	2.31	0.46
13:6:28:VAL:HG11	13:6:31:TRP:CE3	2.51	0.46
13:6:47:PRO:O	13:6:51:LYS:HG2	2.15	0.46
14:U:80:MET:HE2	14:U:80:MET:HA	1.97	0.46
4:C:57:PHE:CE2	4:C:77:LEU:HD22	2.51	0.45
9:S:24:ILE:HD11	9:R:24:ILE:HB	1.97	0.45
9:K:44:LYS:HA	9:K:47:VAL:HG22	1.97	0.45
9:R:19:LEU:HD12	9:R:62:GLY:HA3	1.98	0.45
13:6:17:ALA:HB3	13:6:18:PRO:HD3	1.98	0.45
4:B:56:GLU:OE2	4:B:93:THR:HG22	2.16	0.45
4:B:57:PHE:CD1	4:B:90:VAL:HG12	2.51	0.45
4:B:253:ALA:HB2	4:B:270:TYR:OH	2.17	0.45
4:B:336:VAL:HG11	4:B:353:PHE:HE2	1.81	0.45
4:C:30:THR:HG22	4:C:91:LYS:HG3	1.98	0.45
5:D:231:ARG:O	5:D:235:THR:HG23	2.16	0.45
5:E:468:ALA:HB1	5:E:472:LYS:NZ	2.31	0.45
5:F:84:SER:O	5:F:114:ARG:NH2	2.48	0.45
5:F:410:ILE:HG23	5:F:441:PHE:HE2	1.81	0.45
9:T:21:GLY:CA	9:K:20:LEU:HG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:62:PHE:O	11:Z:66:THR:N	2.32	0.45
4:A:305:SER:HA	4:A:347:ILE:HG12	1.98	0.45
5:E:168:GLN:O	5:E:171:ILE:HG22	2.16	0.45
5:E:468:ALA:HB1	5:E:472:LYS:HZ3	1.81	0.45
3:Y:151:LYS:HG2	3:Y:154:LYS:HG3	1.98	0.45
4:B:169:ILE:HD11	4:B:326:LEU:HG	1.98	0.45
4:B:280:TYR:CD2	4:B:303:LEU:HD22	2.51	0.45
4:B:448:TYR:O	4:B:451:VAL:HG12	2.15	0.45
5:E:132:GLU:N	5:E:132:GLU:OE1	2.50	0.45
5:E:157:GLY:HA3	5:E:161:VAL:HG21	1.98	0.45
5:E:189:GLU:C	5:E:222:MET:HE1	2.41	0.45
9:Q:63:LEU:HD13	9:Q:66:LEU:HD23	1.99	0.45
11:Z:190:GLN:O	11:Z:193:VAL:HG12	2.17	0.45
4:C:57:PHE:HE2	4:C:77:LEU:HD22	1.80	0.45
5:D:289:MET:HA	5:D:289:MET:HE2	1.98	0.45
9:N:61:THR:HB	9:O:19:LEU:HD21	1.99	0.45
13:6:7:TYR:O	13:6:10:GLU:HG3	2.16	0.45
4:C:76:VAL:HG11	4:C:283:LEU:HD12	1.99	0.45
5:D:65:ASP:C	5:D:225:PRO:HG2	2.40	0.45
5:E:38:GLU:HB3	5:E:77:LEU:HB3	1.98	0.45
9:K:21:GLY:HA3	9:L:20:LEU:HA	1.97	0.45
9:M:4:VAL:HG23	9:N:2:GLN:OE1	2.16	0.45
9:R:44:LYS:HA	9:R:47:VAL:HG12	1.98	0.45
9:R:57:LEU:O	9:R:61:THR:HG23	2.16	0.45
12:7:165:ASP:N	12:7:165:ASP:OD1	2.49	0.45
4:B:448:TYR:HD2	4:B:503:THR:HG21	1.81	0.45
5:D:278:ALA:O	6:G:264:THR:HG22	2.16	0.45
5:F:37:LEU:HD12	5:F:76:VAL:HG12	1.99	0.45
6:G:122:HIS:CE1	6:G:124:ASN:HD21	2.35	0.45
9:K:28:ILE:HG22	9:L:27:ALA:HB1	1.98	0.45
9:M:15:SER:HB3	9:N:13:GLY:HA2	1.99	0.45
12:7:37:ASP:O	12:7:41:ARG:HG2	2.16	0.45
1:8:37:ARG:NH2	12:7:146:ASP:HA	2.32	0.45
4:B:142:ARG:HB2	4:B:315:SER:HA	1.99	0.45
4:C:405:PHE:HD1	4:C:408:PHE:HZ	1.64	0.45
5:E:38:GLU:N	5:E:77:LEU:O	2.50	0.45
10:X:207:VAL:O	10:X:207:VAL:HG13	2.17	0.45
1:8:35:ILE:HG13	1:8:39:TYR:CZ	2.52	0.45
3:Y:65:LYS:NZ	3:Y:69:SER:HB3	2.32	0.45
4:B:441:GLU:HG2	4:B:442:GLU:OE1	2.17	0.45
5:E:345:TYR:HD1	15:E:501:ATP:C4	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:366:GLU:HG2	5:E:367:HIS:N	2.32	0.45
5:F:98:VAL:HG22	5:F:232:VAL:HB	1.99	0.45
5:F:472:LYS:O	5:F:476:GLU:OE1	2.34	0.45
6:G:107:ILE:HG22	6:G:107:ILE:O	2.17	0.45
6:G:130:ILE:HD12	8:I:44:TYR:CE1	2.52	0.45
7:H:116:ASP:O	7:H:119:GLU:N	2.49	0.45
11:Z:77:TYR:HA	11:Z:80:PHE:HB3	1.99	0.45
12:7:65:THR:O	12:7:67:VAL:N	2.50	0.45
13:6:32:ASN:HB2	13:6:33:PRO:HD3	1.99	0.45
14:U:5:ILE:HD11	14:U:8:LYS:HD2	1.98	0.45
1:8:19:LEU:HD13	10:X:37:LEU:HD21	1.98	0.45
1:8:43:LEU:HD12	12:7:166:ARG:NH2	2.32	0.45
4:B:353:PHE:CD2	4:B:371:LEU:HD22	2.52	0.45
4:C:100:PRO:HD3	4:C:128:ARG:CZ	2.47	0.45
5:D:150:GLY:HA2	5:D:304:VAL:O	2.17	0.45
7:H:60:MET:HG3	7:H:65:SER:HB3	1.99	0.45
9:P:22:ALA:HB2	9:P:62:GLY:HA3	1.98	0.45
4:A:272:ASP:H	4:A:328:VAL:HB	1.83	0.44
5:E:153:ILE:O	5:E:308:GLN:HB2	2.16	0.44
9:N:19:LEU:HD21	9:N:66:LEU:HG	1.99	0.44
9:Q:26:ILE:HG13	9:Q:27:ALA:N	2.32	0.44
3:Y:70:VAL:O	3:Y:74:ILE:HG13	2.17	0.44
4:A:426:LEU:O	4:A:430:LEU:HD23	2.17	0.44
4:B:459:GLU:OE2	4:B:461:SER:OG	2.31	0.44
5:E:106:ARG:NH2	5:E:209:LEU:O	2.51	0.44
5:E:374:VAL:HG23	5:E:445:LEU:HD11	1.99	0.44
5:F:255:ILE:O	5:F:308:GLN:HA	2.17	0.44
6:G:191:SER:HB2	6:G:194:PHE:HB2	1.97	0.44
6:G:239:ASN:HA	6:G:242:LYS:NZ	2.30	0.44
6:G:262:VAL:O	6:G:266:GLU:OE1	2.35	0.44
9:M:18:GLY:HA2	9:N:20:LEU:HD22	2.00	0.44
4:A:43:VAL:O	4:A:72:GLN:HB2	2.17	0.44
4:C:462:ARG:NH2	4:C:465:GLU:OE1	2.49	0.44
5:D:340:SER:HB2	5:D:347:ALA:HA	1.99	0.44
5:E:83:ILE:O	5:E:117:ILE:HG12	2.17	0.44
5:E:452:ILE:HG23	5:E:470:ALA:HB2	1.99	0.44
5:F:94:ARG:NH2	5:F:107:GLY:O	2.45	0.44
6:G:76:ALA:O	6:G:110:ILE:HG22	2.18	0.44
7:H:17:PRO:HD2	7:H:88:ILE:O	2.17	0.44
1:8:8:TYR:OH	1:8:11:ASN:ND2	2.51	0.44
1:8:15:TYR:O	1:8:19:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:71:ILE:HA	3:Y:74:ILE:HD12	2.00	0.44
3:Y:75:VAL:HA	3:Y:81:LEU:HD23	2.00	0.44
4:A:180:VAL:O	4:A:184:THR:HG23	2.17	0.44
4:B:131:ALA:O	4:B:250:PHE:HB3	2.18	0.44
5:D:138:ILE:HB	5:D:141:VAL:HB	1.99	0.44
5:E:121:PRO:HA	5:E:122:PRO:HD3	1.85	0.44
5:E:156:PHE:HB2	5:E:334:VAL:HA	1.99	0.44
6:G:12:SER:O	6:G:16:ILE:HG12	2.18	0.44
9:S:17:ILE:HG21	9:T:17:ILE:HG12	1.98	0.44
9:L:21:GLY:CA	9:M:20:LEU:HG	2.48	0.44
5:E:344:ILE:HG23	5:E:415:SER:HB3	1.99	0.44
6:G:213:THR:HG23	6:G:217:GLN:NE2	2.33	0.44
9:S:7:ALA:HA	9:S:10:ILE:HD12	2.00	0.44
4:A:306:ARG:HA	4:A:309:GLU:OE2	2.18	0.44
4:C:67:ASN:ND2	4:C:287:LEU:HB3	2.32	0.44
5:D:296:ILE:HG23	5:D:296:ILE:O	2.18	0.44
5:F:472:LYS:HE2	5:F:472:LYS:HB2	1.85	0.44
4:A:481:LEU:O	4:A:485:ILE:HG23	2.17	0.44
4:C:102:GLY:HA2	4:C:258:TRP:CE2	2.53	0.44
5:D:182:SER:O	5:D:215:VAL:HA	2.18	0.44
5:F:196:ASP:HA	5:F:199:ARG:CD	2.48	0.44
5:F:386:ASP:O	5:F:390:ILE:HG22	2.18	0.44
9:M:68:VAL:HG11	9:N:16:THR:OG1	2.18	0.44
9:Q:11:GLY:HA2	9:Q:14:ILE:HG12	1.99	0.44
11:Z:75:PRO:HB2	11:Z:78:LYS:HD3	1.99	0.44
4:C:396:LEU:O	4:C:400:ARG:NE	2.43	0.44
5:E:319:ASP:HB3	5:E:322:PRO:HD2	2.00	0.44
6:G:56:GLU:O	6:G:58:LYS:N	2.51	0.44
12:7:55:PHE:HB2	12:7:59:ARG:HE	1.83	0.44
4:B:206:VAL:HG22	4:B:269:VAL:O	2.18	0.44
4:C:293:ARG:HE	6:G:263:ILE:HD11	1.82	0.44
5:D:12:LYS:HA	5:D:12:LYS:HD3	1.71	0.44
5:D:319:ASP:HB3	5:D:322:PRO:HD2	2.00	0.44
5:F:95:ILE:HB	5:F:103:ILE:HB	2.00	0.44
5:F:156:PHE:HB2	5:F:334:VAL:HA	1.99	0.44
6:G:97:ARG:HA	6:G:100:ASN:ND2	2.33	0.44
9:S:68:VAL:O	9:S:71:LEU:HG	2.17	0.44
10:X:105:ILE:HD12	10:X:107:TYR:CZ	2.53	0.44
12:7:53:VAL:HG13	12:7:58:TYR:CD2	2.53	0.44
4:B:102:GLY:HA3	4:B:126:ALA:H	1.83	0.43
4:B:398:GLN:O	4:B:401:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:46:LEU:HD13	5:F:65:ASP:HB3	2.00	0.43
5:F:217:LEU:HD12	5:F:219:PHE:CZ	2.53	0.43
5:F:255:ILE:HB	5:F:308:GLN:HB3	2.00	0.43
6:G:73:LEU:HD21	6:G:150:LEU:HD12	2.00	0.43
9:O:24:ILE:O	9:O:27:ALA:HB3	2.18	0.43
11:Z:79:ASP:HA	11:Z:82:ASP:HB2	1.99	0.43
4:B:182:LEU:O	4:B:186:LEU:HG	2.18	0.43
5:F:125:ALA:O	5:F:300:LYS:NZ	2.41	0.43
6:G:219:LEU:O	6:G:222:MET:HG3	2.17	0.43
9:S:21:GLY:HA2	9:T:24:ILE:HD11	1.99	0.43
9:S:46:THR:O	9:S:50:MET:HE1	2.18	0.43
2:J:21:ALA:HA	2:J:24:TYR:CD2	2.53	0.43
4:A:149:GLN:HB2	4:A:191:TRP:CH2	2.53	0.43
4:C:38:ASP:O	4:C:286:LEU:HD13	2.18	0.43
5:D:396:LEU:O	5:D:401:LYS:NZ	2.49	0.43
5:F:20:ILE:HG13	5:F:271:LEU:HB3	1.99	0.43
5:F:458:TYR:CD1	5:F:459:MET:HG2	2.53	0.43
7:H:109:LYS:HD3	7:H:123:ALA:HB1	2.00	0.43
9:N:18:GLY:HA3	9:N:65:CYS:SG	2.58	0.43
9:R:63:LEU:CD2	10:X:168:ALA:HB1	2.47	0.43
4:A:182:LEU:HD21	4:A:218:LEU:HD11	2.00	0.43
4:B:6:GLN:HB2	4:B:7:PRO:HD3	2.00	0.43
4:B:260:ARG:NH1	4:B:310:ARG:O	2.52	0.43
4:B:400:ARG:HA	4:B:400:ARG:NE	2.33	0.43
4:B:440:THR:O	4:B:444:VAL:HG23	2.18	0.43
5:E:138:ILE:HB	5:E:141:VAL:HG12	2.00	0.43
5:F:105:GLU:O	5:F:105:GLU:HG2	2.19	0.43
11:Z:126:VAL:HG11	12:7:10:LEU:HD21	1.99	0.43
3:Y:71:ILE:HD13	3:Y:93:SER:HB3	2.00	0.43
4:A:46:LEU:HB3	4:A:49:ILE:HB	2.00	0.43
4:B:470:PHE:CZ	4:B:503:THR:HG22	2.51	0.43
5:D:153:ILE:HD12	5:D:331:ALA:HB3	2.00	0.43
5:E:163:LYS:NZ	15:E:501:ATP:O1B	2.42	0.43
6:G:107:ILE:O	6:G:109:THR:HG23	2.18	0.43
6:G:260:GLN:O	6:G:264:THR:HG23	2.18	0.43
12:7:21:ILE:HG23	12:7:21:ILE:O	2.19	0.43
12:7:53:VAL:HG13	12:7:58:TYR:HD2	1.84	0.43
4:A:41:ALA:HB2	4:A:77:LEU:HD21	2.01	0.43
4:A:153:LYS:HG3	4:A:432:GLN:HE21	1.82	0.43
5:E:199:ARG:HA	5:E:202:LYS:HE2	2.00	0.43
5:E:439:ALA:O	5:E:442:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:160:GLY:HA2	17:F:501:ADP:H5'1	1.99	0.43
5:F:339:ILE:HA	5:F:342:LEU:HB2	2.00	0.43
5:F:434:LEU:O	5:F:437:THR:OG1	2.36	0.43
6:G:107:ILE:HB	6:G:126:ILE:HA	2.00	0.43
7:H:83:LEU:HG	7:H:85:VAL:HG23	2.01	0.43
9:S:57:LEU:O	9:S:61:THR:HG23	2.19	0.43
9:O:65:CYS:SG	9:P:19:LEU:HB2	2.59	0.43
11:Z:140:LEU:HD12	11:Z:143:LYS:HD2	2.00	0.43
12:7:42:GLN:O	12:7:46:LEU:HD23	2.18	0.43
4:A:357:GLU:OE1	4:A:361:LYS:NZ	2.51	0.43
4:B:257:GLU:OE1	4:B:310:ARG:NH2	2.44	0.43
5:D:244:ARG:NH1	5:D:304:VAL:HG22	2.34	0.43
5:F:393:MET:SD	5:F:393:MET:N	2.79	0.43
9:S:34:ILE:HD12	9:R:47:VAL:HG22	2.01	0.43
9:T:25:GLY:O	9:T:28:ILE:HG22	2.18	0.43
9:T:51:ALA:HA	9:K:30:PHE:CE2	2.54	0.43
9:R:29:VAL:O	9:R:33:LEU:HD23	2.19	0.43
10:X:52:LYS:HE2	12:7:131:ASP:C	2.44	0.43
10:X:57:ARG:HA	10:X:60:ILE:HD12	2.01	0.43
10:X:58:TRP:CZ3	14:U:56:PHE:HA	2.53	0.43
11:Z:88:VAL:O	11:Z:92:LEU:HD23	2.18	0.43
3:Y:16:GLU:HB2	4:C:12:SER:HB2	2.00	0.43
5:D:242:TYR:CE1	5:D:246:GLU:HG3	2.53	0.43
5:D:440:SER:HB3	5:D:463:ILE:HB	2.01	0.43
5:E:86:PRO:HB3	5:E:111:SER:HB3	2.00	0.43
5:F:251:VAL:HG22	5:F:304:VAL:HG12	2.00	0.43
11:Z:91:VAL:HG21	12:7:167:PHE:CE1	2.51	0.43
12:7:141:ILE:HB	14:U:32:LYS:NZ	2.34	0.43
1:8:14:THR:HG22	2:J:24:TYR:CE2	2.53	0.43
1:8:24:LEU:HG	2:J:9:ILE:HD12	2.01	0.43
4:B:294:GLU:HG2	4:B:296:TYR:HD2	1.83	0.43
4:B:476:SER:O	4:B:477:ASN:OD1	2.36	0.43
5:F:163:LYS:O	5:F:167:ILE:HG12	2.18	0.43
7:H:78:GLN:HG2	7:H:79:PRO:HD2	2.00	0.43
9:P:24:ILE:HA	9:P:24:ILE:HD13	1.78	0.43
9:P:53:LEU:O	9:P:57:LEU:HG	2.18	0.43
9:Q:68:VAL:O	9:Q:71:LEU:HG	2.19	0.43
10:X:243:LYS:HG3	10:X:247:TYR:HD2	1.83	0.43
13:6:89:LYS:HE3	14:U:6:PRO:O	2.19	0.43
4:A:32:ARG:NH1	4:A:87:GLY:O	2.52	0.43
4:A:153:LYS:HZ1	4:A:432:GLN:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:358:LEU:O	4:A:363:ILE:HG22	2.18	0.43
5:D:386:ASP:OD1	5:D:387:ILE:N	2.50	0.43
5:F:193:GLU:HA	5:F:196:ASP:OD2	2.18	0.43
5:F:221:GLN:HB2	5:F:223:ASN:OD1	2.19	0.43
4:B:50:GLN:HG3	4:B:92:ARG:HH21	1.83	0.42
4:B:190:ARG:NH1	4:B:439:ALA:HB2	2.34	0.42
4:B:196:ASP:OD1	4:B:198:SER:OG	2.37	0.42
4:C:36:VAL:HG21	4:C:84:VAL:HG21	2.01	0.42
4:C:411:ASP:CG	4:C:412:LEU:H	2.25	0.42
5:D:164:THR:O	5:D:167:ILE:N	2.51	0.42
9:T:57:LEU:HD13	9:K:55:PHE:CE1	2.53	0.42
9:T:58:SER:O	9:T:61:THR:OG1	2.30	0.42
9:K:68:VAL:O	9:K:71:LEU:HG	2.19	0.42
10:X:69:ILE:HG23	10:X:86:PHE:HE1	1.84	0.42
12:7:123:ASN:C	12:7:123:ASN:HD22	2.27	0.42
3:Y:39:SER:O	3:Y:43:VAL:HG23	2.19	0.42
4:B:228:MET:HA	4:B:231:SER:OG	2.19	0.42
5:E:359:ASP:O	5:E:363:VAL:HG12	2.19	0.42
5:F:124:PHE:HA	5:F:127:GLN:HG2	2.01	0.42
7:H:88:ILE:HD11	8:I:14:LEU:HD21	2.00	0.42
10:X:42:SER:O	10:X:43:LEU:HD22	2.19	0.42
11:Z:84:ARG:CZ	12:7:170:LEU:HD12	2.50	0.42
12:7:87:LYS:NZ	13:6:69:GLU:H	2.14	0.42
3:Y:75:VAL:HG13	3:Y:75:VAL:O	2.19	0.42
4:C:139:LEU:N	4:C:140:PRO:HD2	2.34	0.42
4:C:260:ARG:NH1	4:C:310:ARG:O	2.52	0.42
5:E:165:VAL:HG23	15:E:501:ATP:O2A	2.19	0.42
5:E:189:GLU:N	5:E:189:GLU:OE1	2.51	0.42
8:I:41:ASP:N	8:I:41:ASP:OD1	2.52	0.42
9:K:47:VAL:HB	9:L:34:ILE:HD11	2.01	0.42
4:A:273:LEU:HD12	4:A:327:PRO:HB3	2.01	0.42
4:A:454:HIS:HB3	4:A:507:VAL:HG21	2.01	0.42
6:G:84:CYS:SG	6:G:237:MET:HE3	2.59	0.42
9:K:22:ALA:O	9:K:26:ILE:HG13	2.19	0.42
11:Z:103:VAL:O	11:Z:107:ILE:HG12	2.19	0.42
1:8:14:THR:HG22	2:J:24:TYR:CZ	2.54	0.42
4:A:397:ALA:O	4:A:401:GLU:OE1	2.38	0.42
4:B:273:LEU:HD12	4:B:276:GLN:HB3	2.02	0.42
4:B:283:LEU:O	4:B:287:LEU:HG	2.19	0.42
5:E:381:TYR:O	5:E:385:GLN:HG2	2.20	0.42
5:F:115:LYS:HA	5:F:115:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:5:GLU:N	6:G:5:GLU:OE1	2.53	0.42
7:H:41:VAL:HG11	7:H:83:LEU:HD13	2.02	0.42
9:L:43:ILE:HG12	9:M:38:SER:HA	2.02	0.42
10:X:210:PHE:O	10:X:214:ALA:N	2.51	0.42
1:8:9:PHE:HD1	10:X:117:PHE:CZ	2.38	0.42
4:A:10:VAL:HA	4:A:13:ILE:HG12	2.00	0.42
4:A:78:PHE:CZ	4:A:247:LEU:HD22	2.54	0.42
4:A:150:THR:HB	4:A:184:THR:HG22	2.01	0.42
4:B:19:LYS:HD3	13:6:7:TYR:HB2	2.01	0.42
5:F:359:ASP:O	5:F:363:VAL:HG22	2.20	0.42
9:P:18:GLY:HA3	9:P:65:CYS:SG	2.60	0.42
11:Z:84:ARG:NE	12:7:170:LEU:HD12	2.35	0.42
1:8:37:ARG:O	1:8:41:SER:HB3	2.19	0.42
3:Y:16:GLU:HB2	4:C:12:SER:H	1.85	0.42
4:A:85:LYS:HB3	4:A:88:GLU:HG3	2.02	0.42
4:A:185:ILE:HG13	4:A:203:CYS:SG	2.60	0.42
4:C:153:LYS:NZ	4:C:432:GLN:HB2	2.35	0.42
5:D:358:LEU:HD12	5:D:363:VAL:HG21	2.01	0.42
5:F:222:MET:HE3	5:F:222:MET:HB2	1.91	0.42
8:I:31:THR:OG1	8:I:32:ALA:N	2.51	0.42
9:S:40:ASN:O	9:S:43:ILE:HG22	2.20	0.42
12:7:9:LYS:HA	12:7:12:TRP:CD1	2.55	0.42
4:A:203:CYS:O	4:A:231:SER:HA	2.19	0.42
5:D:405:GLU:OE1	5:D:409:LYS:HE2	2.19	0.42
5:E:86:PRO:HG2	5:E:109:ILE:HG21	2.02	0.42
5:F:117:ILE:HA	5:F:238:THR:OG1	2.20	0.42
7:H:51:GLN:HA	7:H:74:PHE:CD1	2.54	0.42
9:N:52:ILE:HD13	9:N:55:PHE:CZ	2.55	0.42
9:Q:65:CYS:SG	9:R:19:LEU:HD22	2.60	0.42
4:A:299:ASP:OD1	4:A:299:ASP:N	2.44	0.42
4:A:363:ILE:HG23	4:A:366:ALA:HA	2.01	0.42
4:B:355:GLU:OE2	4:B:358:LEU:HD13	2.20	0.42
4:B:357:GLU:O	4:B:361:LYS:HG2	2.19	0.42
4:B:369:VAL:HG23	4:B:400:ARG:HH12	1.84	0.42
4:C:228:MET:HE2	4:C:228:MET:HA	2.01	0.42
5:E:391:LEU:HD23	5:E:395:GLU:HG2	2.02	0.42
5:F:176:LYS:O	5:F:178:HIS:N	2.50	0.42
5:F:184:PHE:HB3	5:F:217:LEU:HD13	2.02	0.42
5:F:398:GLU:HG2	5:F:399:GLN:N	2.35	0.42
6:G:162:ILE:HB	6:G:182:ILE:HB	2.02	0.42
9:K:10:ILE:O	9:K:14:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:37:LEU:HD22	10:X:40:ILE:HD12	2.02	0.42
12:7:41:ARG:HA	12:7:41:ARG:HD2	1.86	0.42
12:7:155:LYS:HE2	12:7:157:LYS:HB2	2.01	0.42
13:6:73:GLU:OE1	13:6:76:GLU:HB2	2.19	0.42
13:6:81:VAL:O	13:6:85:ALA:N	2.44	0.42
4:A:52:GLU:OE2	5:E:68:GLU:HG3	2.19	0.42
4:B:217:GLN:CD	5:E:128:SER:HB2	2.45	0.42
5:D:156:PHE:HB2	5:D:334:VAL:HG22	2.02	0.42
6:G:10:LEU:O	6:G:14:LYS:HG2	2.20	0.42
6:G:21:LYS:O	6:G:24:LYS:HG2	2.20	0.42
6:G:77:ILE:N	6:G:165:PHE:O	2.47	0.42
10:X:180:ASN:HD22	10:X:180:ASN:C	2.25	0.42
12:7:107:GLU:HA	12:7:110:VAL:HG22	2.02	0.42
12:7:129:PRO:HG3	14:U:34:LEU:O	2.20	0.42
13:6:43:GLU:C	13:6:46:GLY:H	2.27	0.42
4:B:47:ASN:OD1	4:B:48:ASN:N	2.53	0.41
4:B:464:GLY:O	4:B:467:GLU:HG2	2.20	0.41
4:C:302:TYR:CZ	4:C:306:ARG:HD3	2.55	0.41
4:C:331:THR:OG1	4:C:335:ASP:O	2.36	0.41
4:C:387:GLN:HE22	4:C:491:LEU:H	1.66	0.41
5:E:163:LYS:O	5:E:167:ILE:HG12	2.20	0.41
9:T:51:ALA:HA	9:K:30:PHE:HZ	1.85	0.41
9:N:44:LYS:HA	9:N:47:VAL:HG12	2.01	0.41
4:A:332:GLN:NE2	5:D:318:THR:HA	2.35	0.41
4:B:211:LYS:O	4:B:214:THR:OG1	2.29	0.41
4:C:426:LEU:O	4:C:430:LEU:HD23	2.21	0.41
4:C:442:GLU:HB2	4:C:471:LEU:CD1	2.46	0.41
5:E:338:GLY:O	5:E:342:LEU:HD23	2.20	0.41
9:M:25:GLY:HA2	9:M:28:ILE:HG12	2.01	0.41
9:O:26:ILE:HD12	9:O:55:PHE:CE1	2.55	0.41
14:U:52:LYS:HA	14:U:52:LYS:HD2	1.87	0.41
1:8:31:PHE:CE2	10:X:44:TYR:HD2	2.37	0.41
4:A:191:TRP:HD1	4:A:199:LYS:HD2	1.85	0.41
5:D:460:VAL:HG13	5:D:465:ASP:HB3	2.02	0.41
9:O:43:ILE:HG12	9:P:38:SER:HA	2.02	0.41
9:Q:70:PHE:HA	9:Q:73:LEU:HD12	2.02	0.41
9:R:20:LEU:H	9:R:20:LEU:HD12	1.85	0.41
10:X:32:TYR:O	10:X:36:VAL:HG23	2.20	0.41
10:X:77:ILE:HD11	10:X:239:ALA:HB1	2.03	0.41
13:6:46:GLY:N	13:6:47:PRO:HD2	2.35	0.41
3:Y:135:LYS:NZ	3:Y:139:LYS:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:4:LYS:C	4:A:7:PRO:HD2	2.44	0.41
4:A:53:GLU:OE1	4:A:94:GLY:N	2.53	0.41
4:A:301:PHE:HD1	4:A:343:ASN:HB2	1.85	0.41
4:A:488:LYS:HG2	4:A:490:GLU:OE1	2.20	0.41
4:B:85:LYS:H	4:B:88:GLU:CD	2.28	0.41
4:B:240:GLU:OE1	4:B:240:GLU:N	2.53	0.41
5:F:187:VAL:HG12	5:F:260:ARG:HB2	2.01	0.41
5:F:374:VAL:HG23	5:F:410:ILE:HG21	2.03	0.41
7:H:60:MET:HA	7:H:65:SER:HA	2.02	0.41
7:H:78:GLN:HB3	7:H:82:GLN:HB3	2.01	0.41
9:T:64:PHE:O	9:T:68:VAL:HG23	2.20	0.41
9:M:64:PHE:HA	9:M:67:MET:HG3	2.02	0.41
10:X:57:ARG:HH21	11:Z:77:TYR:HD2	1.68	0.41
10:X:115:LEU:HD23	10:X:182:LEU:HD21	2.01	0.41
10:X:191:LEU:O	10:X:195:THR:HG23	2.21	0.41
14:U:63:GLY:O	14:U:66:LEU:HG	2.21	0.41
1:8:37:ARG:HH22	12:7:146:ASP:HA	1.86	0.41
4:A:49:ILE:HD11	4:A:53:GLU:HB3	2.03	0.41
4:A:140:PRO:HA	4:A:317:LYS:HZ1	1.85	0.41
4:B:6:GLN:H	4:B:6:GLN:CD	2.28	0.41
4:B:161:ILE:HB	4:B:165:GLN:NE2	2.35	0.41
4:B:174:GLN:HG3	5:E:354:LYS:HE3	2.01	0.41
4:B:423:GLY:O	4:B:427:THR:HG23	2.20	0.41
4:C:364:ARG:HD2	15:C:601:ATP:C2	2.55	0.41
4:C:470:PHE:O	4:C:474:LEU:HD23	2.20	0.41
5:D:318:THR:C	6:G:260:GLN:HE22	2.28	0.41
5:E:27:GLN:O	5:E:27:GLN:HG2	2.20	0.41
5:E:460:VAL:HG21	5:E:466:VAL:HG22	2.03	0.41
5:F:408:ARG:HA	5:F:411:GLN:HG2	2.02	0.41
6:G:200:ASP:OD1	6:G:200:ASP:N	2.51	0.41
9:Q:61:THR:CG2	9:R:19:LEU:HD21	2.50	0.41
12:7:11:ASP:O	12:7:14:LYS:HG2	2.20	0.41
4:A:340:ILE:HA	4:A:343:ASN:ND2	2.36	0.41
4:A:384:ALA:O	4:A:388:VAL:HG22	2.20	0.41
4:B:357:GLU:OE1	4:B:358:LEU:HD12	2.20	0.41
4:B:364:ARG:HB2	4:B:365:PRO:HD3	2.01	0.41
5:D:33:ILE:HG22	5:D:50:VAL:HG12	2.01	0.41
5:D:344:ILE:HD11	5:D:412:ARG:HA	2.01	0.41
9:M:64:PHE:O	9:M:67:MET:HG3	2.20	0.41
10:X:53:ILE:HA	10:X:53:ILE:HD12	1.80	0.41
11:Z:124:PHE:CE1	14:U:5:ILE:HB	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:156:GLU:O	3:Y:158:VAL:N	2.54	0.41
4:B:407:GLN:O	4:B:410:SER:OG	2.30	0.41
4:C:446:LEU:HD13	4:C:446:LEU:HA	1.96	0.41
9:S:8:LYS:HG3	9:T:9:TYR:CD2	2.56	0.41
12:7:94:SER:O	12:7:97:LYS:HG2	2.21	0.41
4:B:168:LEU:HB2	4:B:348:THR:HG21	2.02	0.41
4:B:172:ASP:CG	4:B:173:ARG:H	2.29	0.41
4:B:234:VAL:HG21	4:B:252:ALA:HB2	2.03	0.41
4:B:246:TYR:HA	4:B:276:GLN:OE1	2.21	0.41
4:B:483:THR:O	4:B:486:ARG:HG2	2.21	0.41
5:D:398:GLU:HA	5:D:401:LYS:HE2	2.03	0.41
5:F:276:PRO:O	6:G:270:ILE:HD11	2.21	0.41
10:X:45:THR:O	10:X:48:ASN:ND2	2.53	0.41
13:6:53:TYR:HA	13:6:57:ASN:ND2	2.36	0.41
3:Y:15:VAL:C	3:Y:17:GLY:H	2.29	0.41
4:B:39:GLY:HA2	4:B:77:LEU:HD12	2.02	0.41
4:B:272:ASP:OD2	4:B:275:LYS:HE2	2.21	0.41
4:B:355:GLU:OE1	4:B:355:GLU:N	2.54	0.41
4:B:480:GLU:HG2	4:B:481:LEU:N	2.35	0.41
4:C:59:SER:OG	4:C:83:LEU:HB3	2.21	0.41
4:C:205:TYR:OH	4:C:271:ASP:OD2	2.25	0.41
5:D:11:GLY:HA3	5:D:25:PHE:CD1	2.56	0.41
5:E:99:ILE:HB	5:E:101:GLU:OE1	2.21	0.41
5:E:398:GLU:HG2	5:E:399:GLN:N	2.35	0.41
5:E:409:LYS:NZ	5:E:452:ILE:O	2.30	0.41
6:G:233:ARG:O	6:G:237:MET:HG2	2.21	0.41
9:N:28:ILE:CG1	9:O:27:ALA:HB1	2.50	0.41
9:N:58:SER:O	9:N:61:THR:OG1	2.37	0.41
10:X:217:LEU:HD12	10:X:217:LEU:HA	1.91	0.41
11:Z:179:ARG:NH1	13:6:14:THR:HG22	2.35	0.41
4:B:434:GLN:HG3	4:B:435:TYR:CD2	2.52	0.41
4:C:465:GLU:O	4:C:469:SER:OG	2.35	0.41
5:E:434:LEU:O	5:E:438:VAL:HG12	2.21	0.41
5:F:386:ASP:OD1	5:F:386:ASP:N	2.54	0.41
9:O:47:VAL:HG23	9:O:50:MET:HE2	2.03	0.41
10:X:119:ILE:H	10:X:119:ILE:HD12	1.86	0.41
3:Y:78:HIS:C	3:Y:79:LYS:HG3	2.46	0.40
4:B:341:PRO:HA	4:B:344:VAL:HG12	2.02	0.40
5:D:11:GLY:HA3	5:D:25:PHE:HD1	1.86	0.40
5:E:50:VAL:HG22	5:E:61:THR:HG22	2.02	0.40
5:E:180:GLY:O	5:E:214:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:296:ILE:HG23	5:E:296:ILE:O	2.21	0.40
6:G:74:ILE:HG21	6:G:165:PHE:CZ	2.56	0.40
6:G:81:LYS:HB3	6:G:233:ARG:HH22	1.86	0.40
12:7:82:LYS:NZ	13:6:66:GLU:OE1	2.42	0.40
4:A:213:SER:O	4:A:217:GLN:HG2	2.21	0.40
4:B:444:VAL:HB	4:B:445:PRO:HD3	2.02	0.40
4:C:246:TYR:HD2	4:C:247:LEU:HD22	1.85	0.40
5:D:176:LYS:HA	5:D:176:LYS:HD3	1.82	0.40
5:D:308:GLN:N	5:D:308:GLN:OE1	2.53	0.40
5:F:39:ILE:HD12	5:F:70:LEU:HD11	2.03	0.40
6:G:197:PHE:HB3	7:H:49:VAL:HG22	2.03	0.40
9:N:11:GLY:HA2	9:N:14:ILE:HG12	2.02	0.40
10:X:195:THR:HG22	10:X:212:PRO:HB2	2.02	0.40
4:B:204:VAL:HG13	4:B:268:ILE:HD13	2.04	0.40
4:B:388:VAL:HB	4:B:491:LEU:HB2	2.03	0.40
4:C:203:CYS:O	4:C:231:SER:HA	2.22	0.40
4:C:302:TYR:OH	5:D:225:PRO:HG3	2.21	0.40
5:D:156:PHE:HZ	5:D:326:PHE:HE1	1.68	0.40
5:D:164:THR:HA	5:D:167:ILE:HD12	2.03	0.40
5:F:135:GLU:OE1	5:F:434:LEU:HB2	2.22	0.40
6:G:74:ILE:HG23	6:G:163:SER:HB3	2.04	0.40
7:H:109:LYS:HG2	7:H:112:VAL:CG2	2.51	0.40
7:H:123:ALA:O	7:H:127:VAL:HG23	2.21	0.40
9:K:57:LEU:HD23	9:L:30:PHE:CE2	2.54	0.40
9:L:57:LEU:HD13	9:M:55:PHE:CE1	2.56	0.40
9:Q:70:PHE:CE2	10:X:186:LEU:HD11	2.56	0.40
10:X:223:GLU:HA	10:X:226:ILE:HG12	2.02	0.40
1:8:32:LEU:HA	1:8:35:ILE:HG22	2.03	0.40
4:A:364:ARG:HB3	4:A:365:PRO:HD3	2.03	0.40
4:A:364:ARG:HD2	15:A:601:ATP:C5	2.56	0.40
4:B:138:ILE:HD12	4:B:138:ILE:HA	1.98	0.40
4:C:338:ALA:HB3	4:C:341:PRO:HG2	2.03	0.40
4:C:479:ASN:O	4:C:483:THR:HG23	2.21	0.40
5:E:34:LEU:HD23	5:E:49:GLU:OE2	2.21	0.40
5:E:37:LEU:HD12	5:E:76:VAL:HG22	2.03	0.40
5:E:154:GLY:HA3	5:E:332:THR:HA	2.03	0.40
5:F:370:VAL:HG22	5:F:442:LYS:HD3	2.02	0.40
5:F:404:VAL:O	5:F:408:ARG:HG3	2.22	0.40
6:G:129:SER:O	8:I:45:THR:OG1	2.27	0.40
7:H:34:ALA:HA	7:H:53:LEU:H	1.86	0.40
9:T:21:GLY:HA3	9:K:20:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:57:LEU:HD13	9:Q:55:PHE:CE1	2.57	0.40
10:X:62:GLN:HG2	10:X:63:GLU:N	2.36	0.40
10:X:215:MET:O	10:X:219:ILE:HG23	2.21	0.40
11:Z:159:ARG:NH2	13:6:50:LEU:HD22	2.37	0.40
11:Z:179:ARG:NH1	13:6:18:PRO:HG3	2.36	0.40
1:8:12:GLN:HB3	10:X:117:PHE:CZ	2.56	0.40
5:E:88:GLY:HA2	5:E:242:TYR:CE1	2.57	0.40
5:E:136:THR:HA	5:E:174:ILE:HD11	2.04	0.40
5:E:241:GLU:HA	5:E:244:ARG:NE	2.36	0.40
5:E:401:LYS:HA	5:E:404:VAL:HG12	2.04	0.40
9:L:29:VAL:HG13	9:M:27:ALA:HB1	2.03	0.40
9:M:4:VAL:HG13	9:N:9:TYR:HE2	1.87	0.40
11:Z:113:LEU:H	11:Z:113:LEU:HD23	1.87	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	8	39/41 (95%)	34 (87%)	5 (13%)	0	100	100
2	J	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
3	Y	164/166 (99%)	141 (86%)	23 (14%)	0	100	100
4	A	505/507 (100%)	483 (96%)	22 (4%)	0	100	100
4	B	504/507 (99%)	474 (94%)	29 (6%)	1 (0%)	44	77
4	C	503/507 (99%)	477 (95%)	26 (5%)	0	100	100
5	D	471/473 (100%)	442 (94%)	28 (6%)	1 (0%)	44	77
5	E	471/473 (100%)	444 (94%)	25 (5%)	2 (0%)	30	67
5	F	470/473 (99%)	453 (96%)	17 (4%)	0	100	100
6	G	257/270 (95%)	239 (93%)	17 (7%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	H	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	16 54
8	I	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	7 36
9	K	73/75 (97%)	71 (97%)	2 (3%)	0	100 100
9	L	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
9	M	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
9	N	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
9	O	72/75 (96%)	70 (97%)	2 (3%)	0	100 100
9	P	73/75 (97%)	72 (99%)	1 (1%)	0	100 100
9	Q	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
9	R	72/75 (96%)	70 (97%)	2 (3%)	0	100 100
9	S	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
9	T	72/75 (96%)	71 (99%)	1 (1%)	0	100 100
10	X	222/224 (99%)	202 (91%)	20 (9%)	0	100 100
11	Z	153/155 (99%)	144 (94%)	9 (6%)	0	100 100
12	7	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	11 44
13	6	87/89 (98%)	72 (83%)	15 (17%)	0	100 100
14	U	83/85 (98%)	75 (90%)	7 (8%)	1 (1%)	11 44
All	All	5042/5119 (98%)	4747 (94%)	285 (6%)	10 (0%)	45 77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	459	GLU
7	H	117	ALA
8	I	56	PRO
5	E	354	LYS
6	G	57	THR
5	E	213	SER
12	7	66	SER
14	U	6	PRO
12	7	65	THR
5	D	426	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	8	40/40 (100%)	40 (100%)	0	100 100
2	J	30/30 (100%)	30 (100%)	0	100 100
3	Y	139/139 (100%)	139 (100%)	0	100 100
4	A	410/410 (100%)	410 (100%)	0	100 100
4	B	409/410 (100%)	409 (100%)	0	100 100
4	C	409/410 (100%)	409 (100%)	0	100 100
5	D	382/382 (100%)	382 (100%)	0	100 100
5	E	382/382 (100%)	381 (100%)	1 (0%)	91 92
5	F	381/382 (100%)	381 (100%)	0	100 100
6	G	224/230 (97%)	224 (100%)	0	100 100
7	H	111/111 (100%)	111 (100%)	0	100 100
8	I	25/46 (54%)	25 (100%)	0	100 100
9	K	55/55 (100%)	55 (100%)	0	100 100
9	L	55/55 (100%)	55 (100%)	0	100 100
9	M	55/55 (100%)	55 (100%)	0	100 100
9	N	55/55 (100%)	55 (100%)	0	100 100
9	O	55/55 (100%)	55 (100%)	0	100 100
9	P	55/55 (100%)	55 (100%)	0	100 100
9	Q	55/55 (100%)	55 (100%)	0	100 100
9	R	55/55 (100%)	55 (100%)	0	100 100
9	S	55/55 (100%)	55 (100%)	0	100 100
9	T	55/55 (100%)	55 (100%)	0	100 100
10	X	193/193 (100%)	193 (100%)	0	100 100
11	Z	137/138 (99%)	137 (100%)	0	100 100
12	7	154/156 (99%)	154 (100%)	0	100 100
13	6	79/79 (100%)	78 (99%)	1 (1%)	65 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	U	60/68 (88%)	60 (100%)	0	100	100
All	All	4115/4156 (99%)	4113 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	328	HIS
13	6	4	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	Y	112	ASN
4	A	210	GLN
4	A	418	GLN
4	A	432	GLN
4	A	443	GLN
4	A	452	ASN
4	A	478	HIS
4	B	50	GLN
4	B	217	GLN
4	B	332	GLN
4	B	343	ASN
4	C	132	GLN
4	C	245	GLN
4	C	262	ASN
4	C	276	GLN
4	C	381	GLN
4	C	387	GLN
4	C	418	GLN
4	C	479	ASN
5	D	35	ASN
5	D	221	GLN
5	D	365	GLN
5	D	455	HIS
5	E	35	ASN
5	E	399	GLN
5	F	53	HIS
5	F	173	ASN
5	F	208	ASN
5	F	223	ASN

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Mol	Chain	Res	Type
5	F	365	GLN
5	F	367	HIS
6	G	49	GLN
6	G	59	ASN
6	G	141	GLN
6	G	190	GLN
6	G	217	GLN
6	G	260	GLN
7	H	111	ASN
9	S	2	GLN
9	T	35	ASN
9	L	35	ASN
9	M	2	GLN
10	X	114	HIS
11	Z	203	GLN
12	7	47	GLN
12	7	88	GLN
13	6	56	GLN
13	6	57	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	ATP	E	501	16	28,33,33	0.63	0	34,52,52	0.62	1 (2%)
15	ATP	B	601	16	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
17	ADP	F	501	16	24,29,29	0.90	0	29,45,45	1.16	2 (6%)
15	ATP	A	601	16	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
15	ATP	C	601	16	28,33,33	0.63	0	34,52,52	0.60	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ATP	E	501	16	-	5/18/38/38	0/3/3/3
15	ATP	B	601	16	-	4/18/38/38	0/3/3/3
17	ADP	F	501	16	-	0/12/32/32	0/3/3/3
15	ATP	A	601	16	-	4/18/38/38	0/3/3/3
15	ATP	C	601	16	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	501	ADP	N3-C2-N1	-3.60	123.79	128.67
17	F	501	ADP	C4-C5-N7	-2.52	106.67	109.34
15	C	601	ATP	C5-C6-N6	2.35	123.89	120.31
15	B	601	ATP	C5-C6-N6	2.34	123.87	120.31
15	A	601	ATP	C5-C6-N6	2.31	123.83	120.31
15	E	501	ATP	C5-C6-N6	2.30	123.82	120.31

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	601	ATP	C5'-O5'-PA-O1A
15	B	601	ATP	C5'-O5'-PA-O3A
15	C	601	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
15	C	601	ATP	C5'-O5'-PA-O3A
15	E	501	ATP	C5'-O5'-PA-O1A
15	E	501	ATP	C5'-O5'-PA-O3A
15	B	601	ATP	PB-O3A-PA-O1A
15	A	601	ATP	C5'-O5'-PA-O1A
15	C	601	ATP	C5'-O5'-PA-O2A
15	E	501	ATP	C5'-O5'-PA-O2A
15	B	601	ATP	PB-O3A-PA-O2A
15	E	501	ATP	PA-O3A-PB-O2B
15	A	601	ATP	PG-O3B-PB-O3A
15	E	501	ATP	PA-O3A-PB-O1B
15	A	601	ATP	PG-O3B-PB-O1B
15	A	601	ATP	PG-O3B-PB-O2B

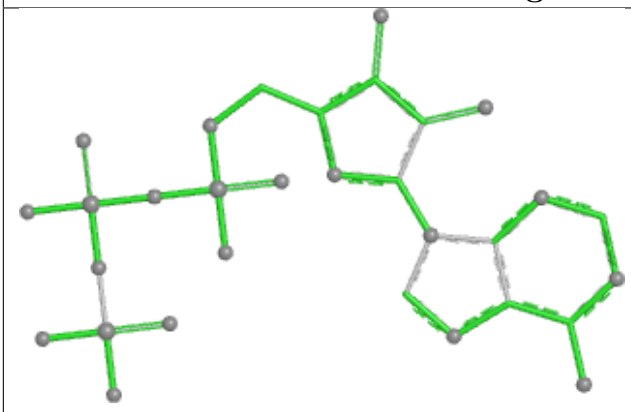
There are no ring outliers.

4 monomers are involved in 10 short contacts:

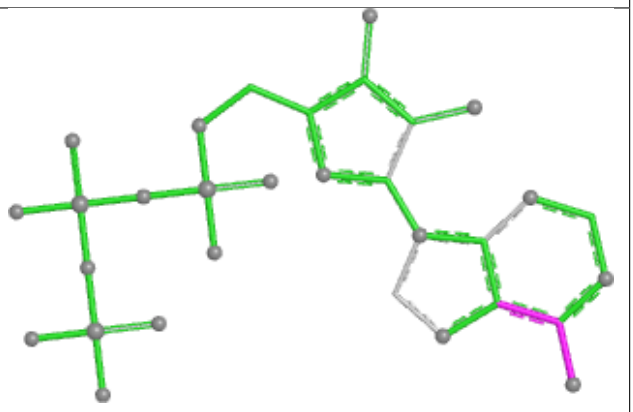
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	501	ATP	4	0
17	F	501	ADP	2	0
15	A	601	ATP	2	0
15	C	601	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

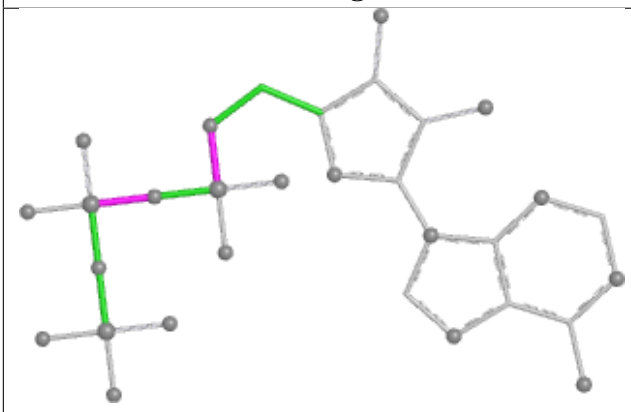
Ligand ATP E 501



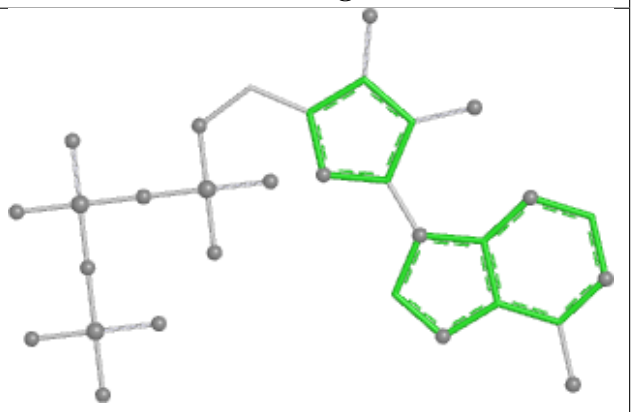
Bond lengths



Bond angles

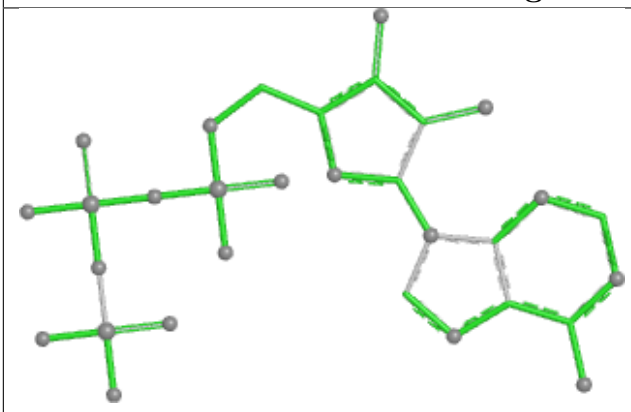


Torsions

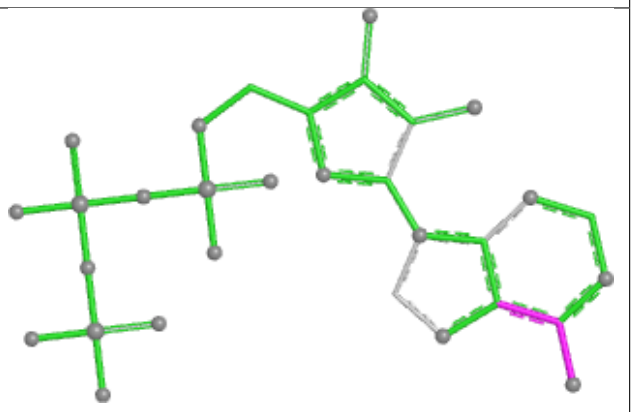


Rings

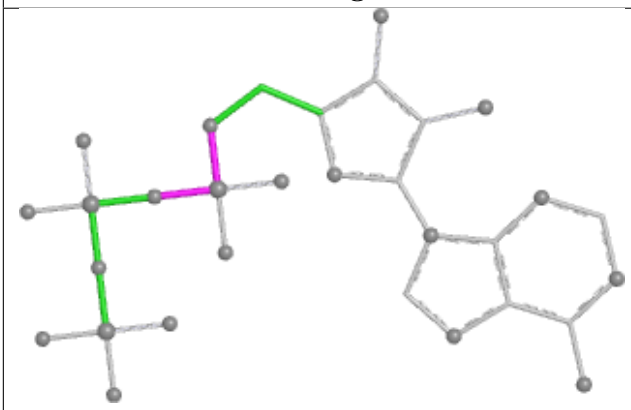
Ligand ATP B 601



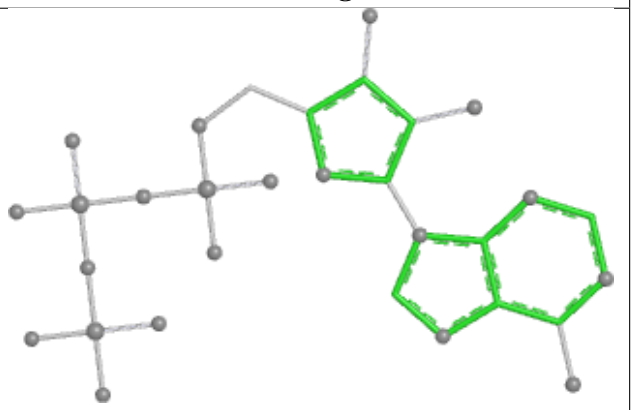
Bond lengths



Bond angles

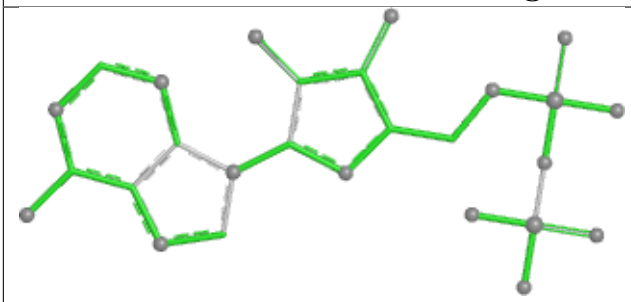


Torsions

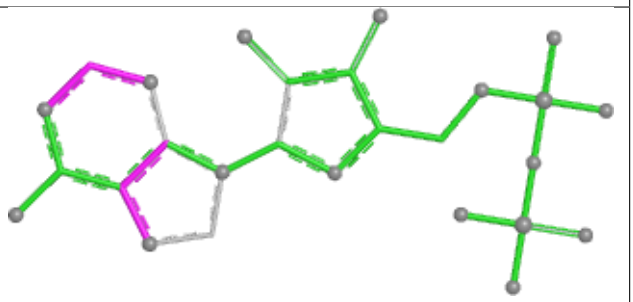


Rings

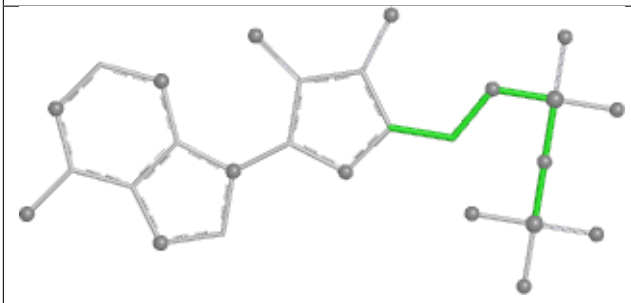
Ligand ADP F 501



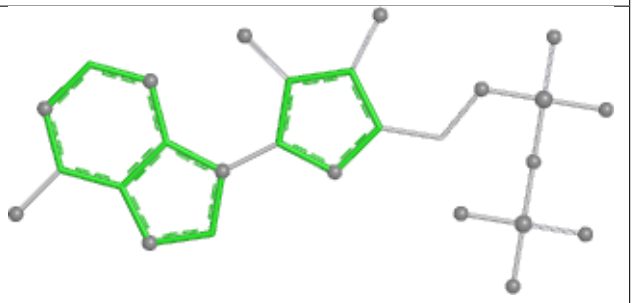
Bond lengths



Bond angles

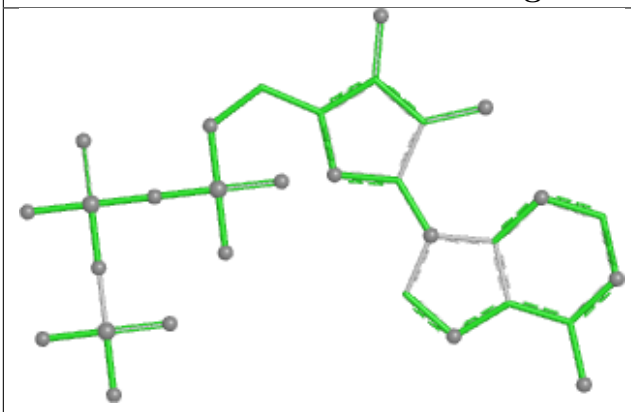


Torsions

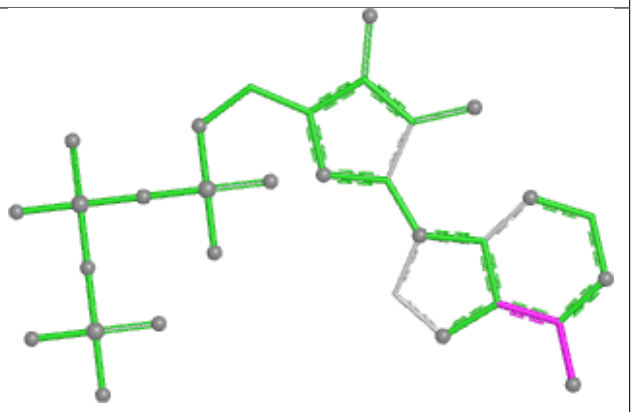


Rings

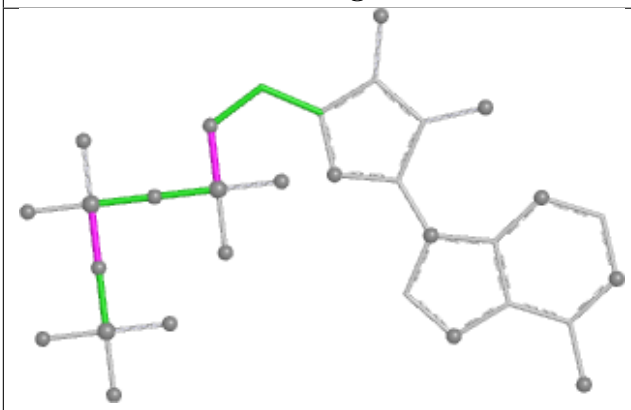
Ligand ATP A 601



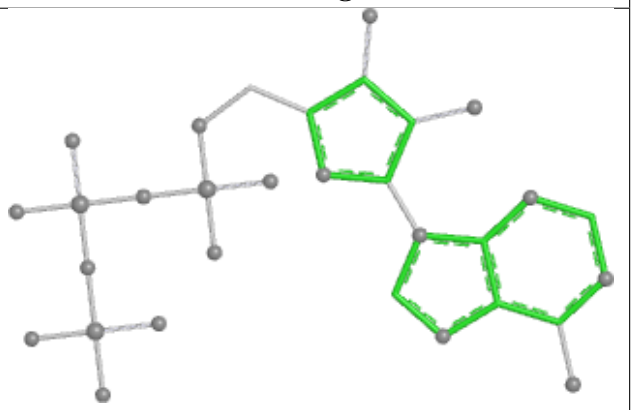
Bond lengths



Bond angles

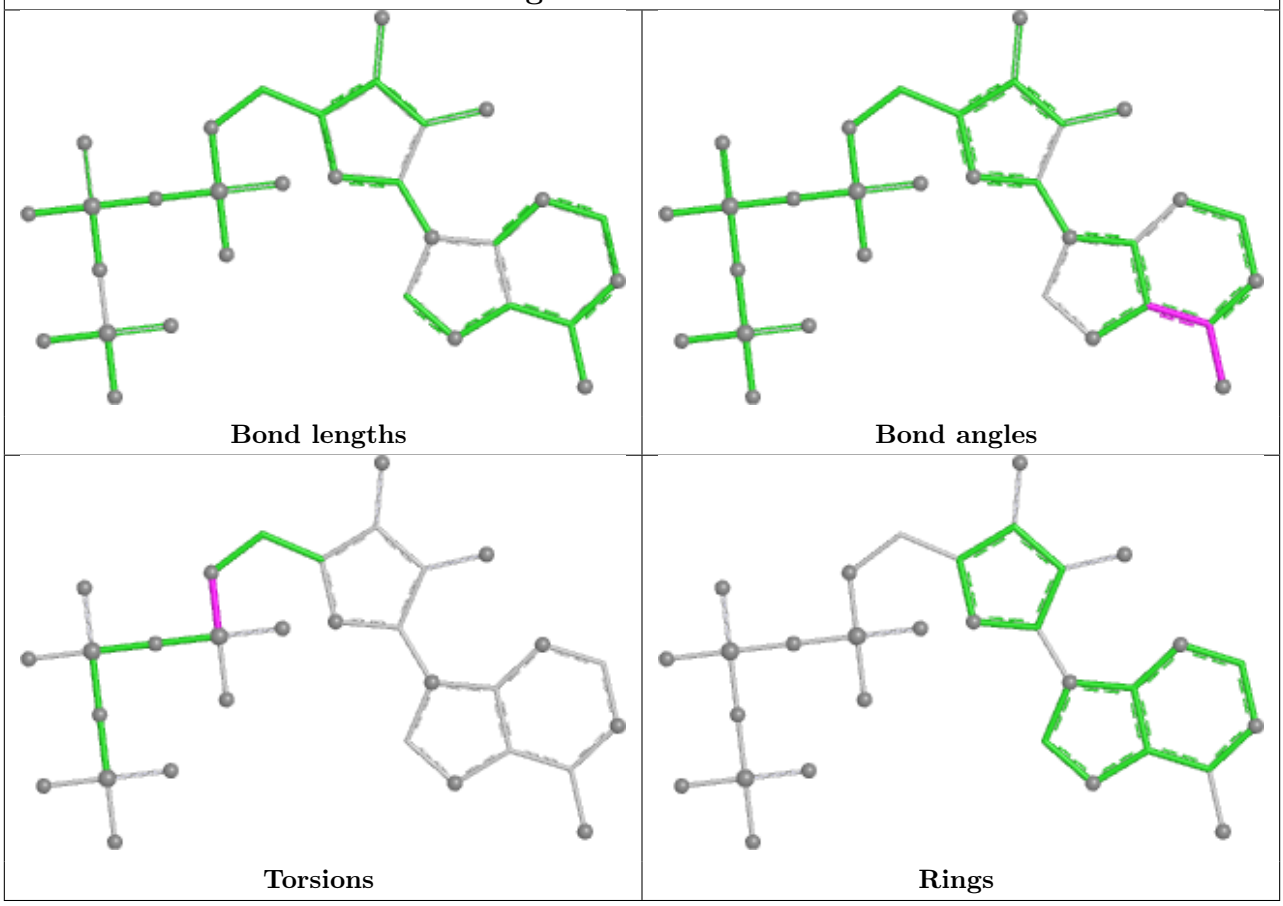


Torsions



Rings

Ligand ATP C 601



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.

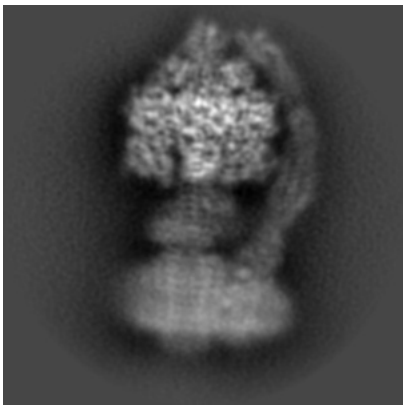
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29270. These allow visual inspection of the internal detail of the map and identification of artifacts.

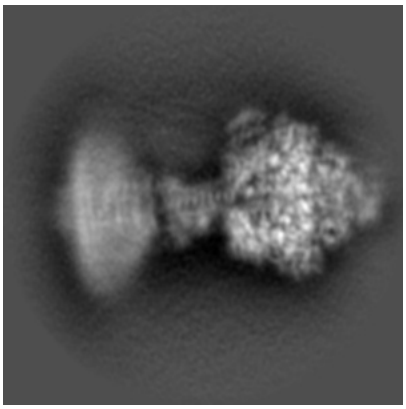
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

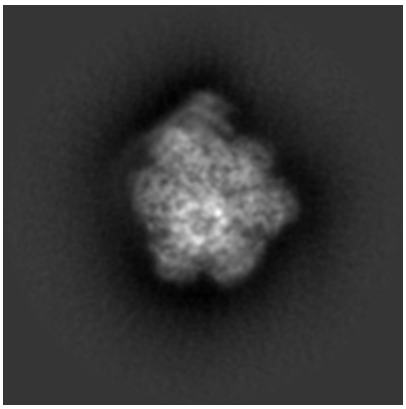
6.1.1 Primary map



X

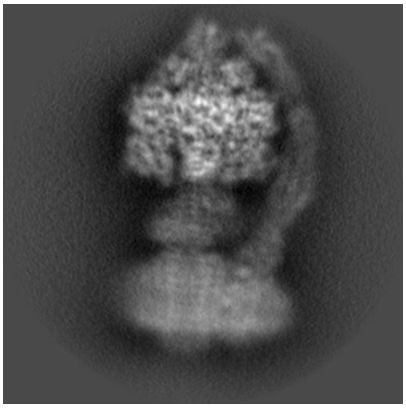


Y

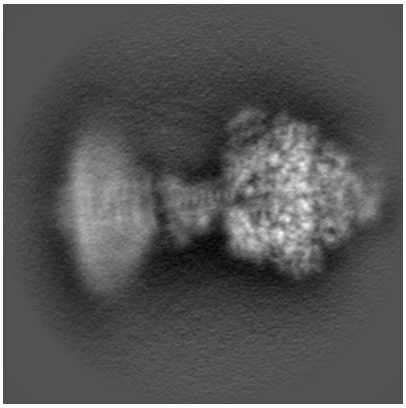


Z

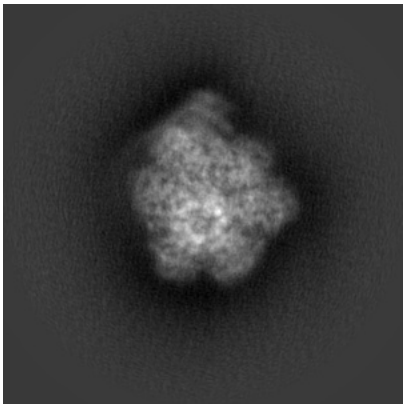
6.1.2 Raw map



X



Y

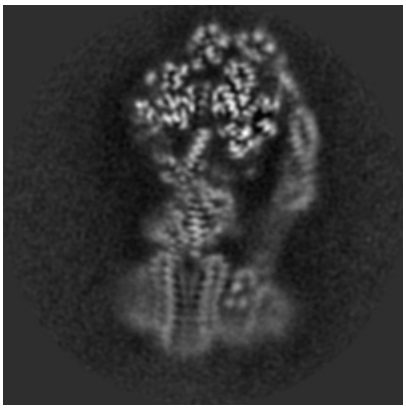


Z

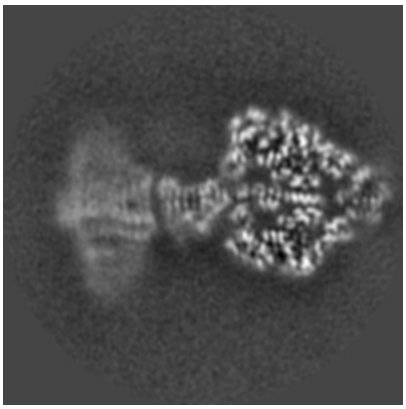
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

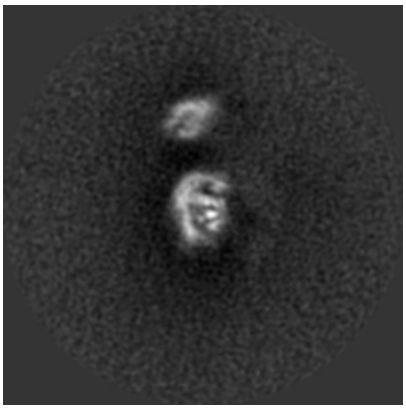
6.2.1 Primary map



X Index: 128

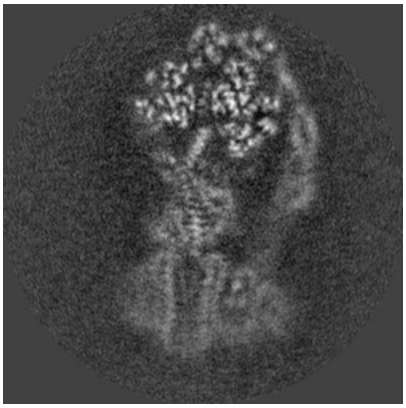


Y Index: 128

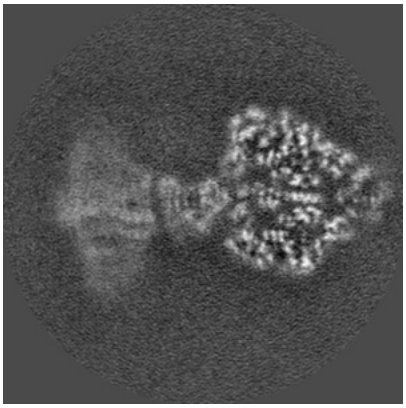


Z Index: 128

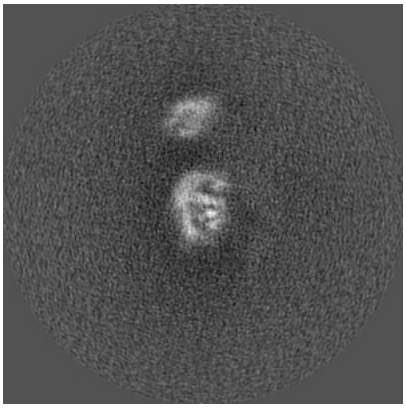
6.2.2 Raw map



X Index: 128



Y Index: 128

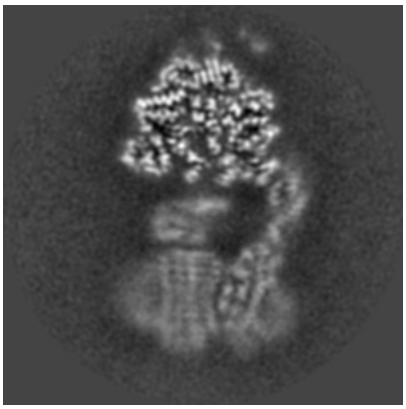


Z Index: 128

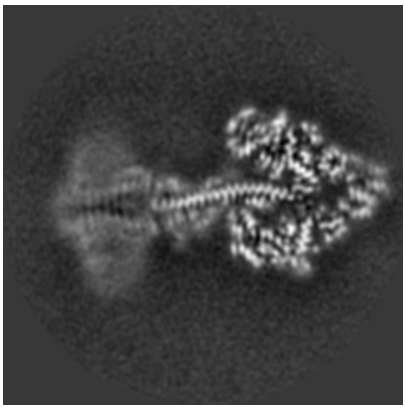
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

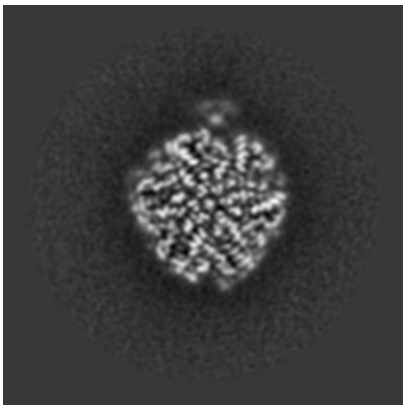
6.3.1 Primary map



X Index: 114

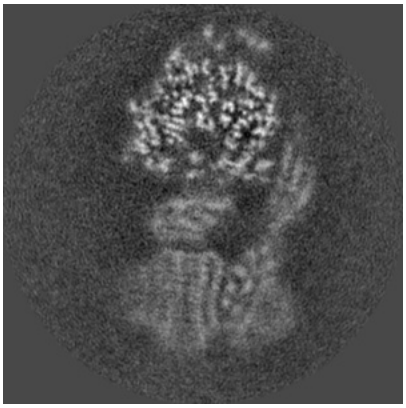


Y Index: 123

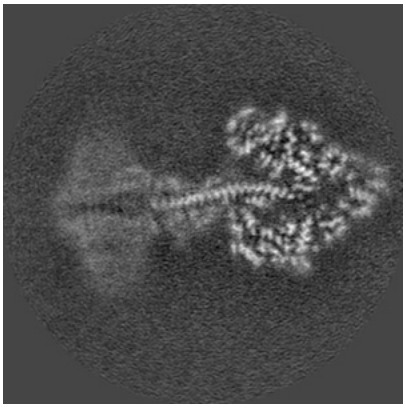


Z Index: 191

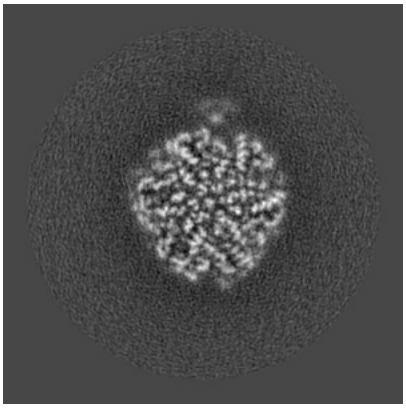
6.3.2 Raw map



X Index: 118



Y Index: 123

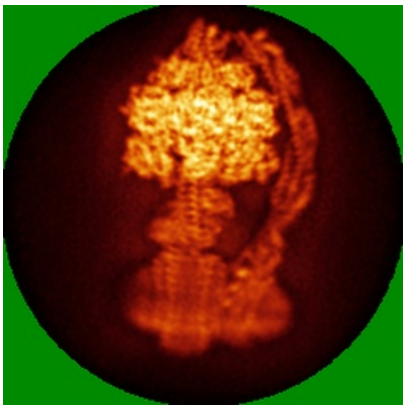


Z Index: 191

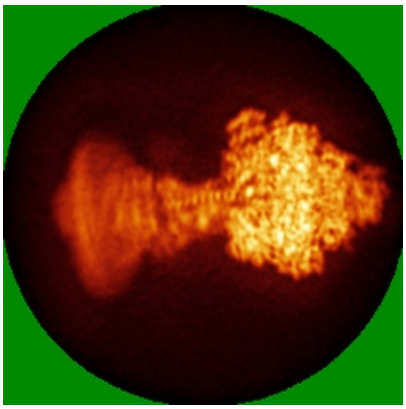
The images above show the largest variance slices of the map in three orthogonal directions.

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

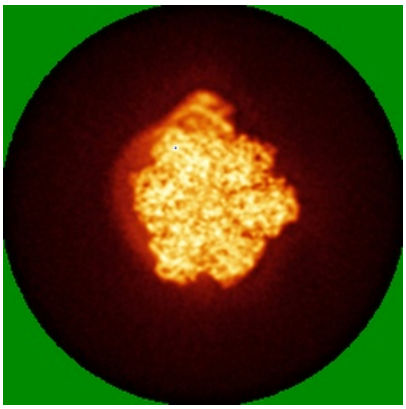
6.4.1 Primary map



X

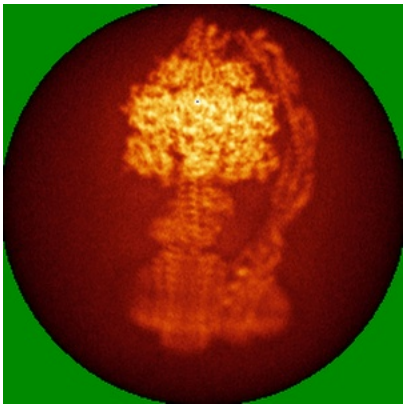


Y

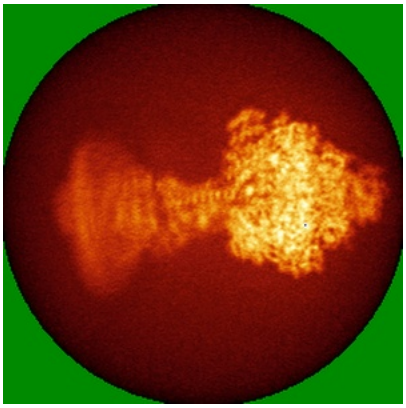


Z

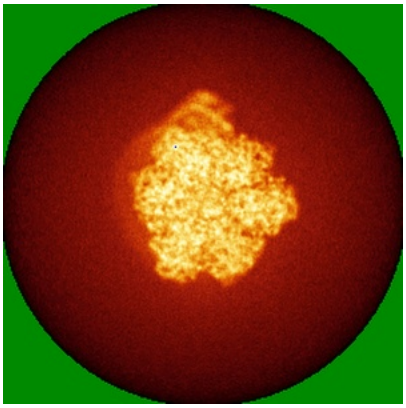
6.4.2 Raw map



X



Y

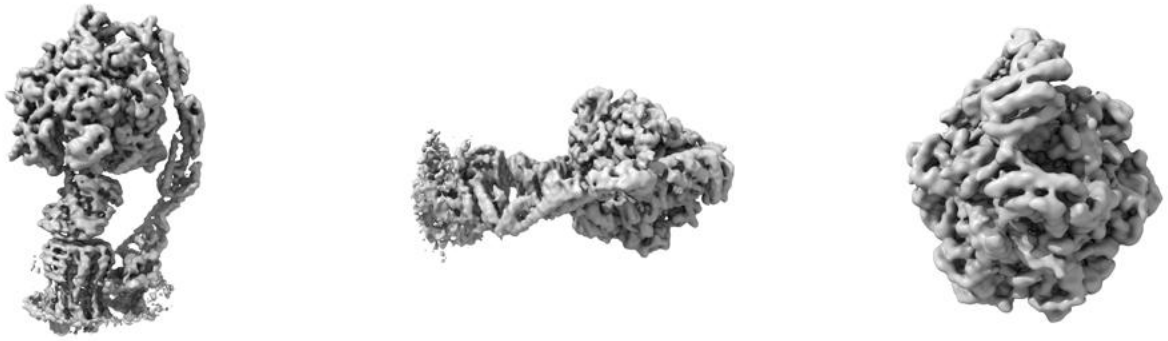


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

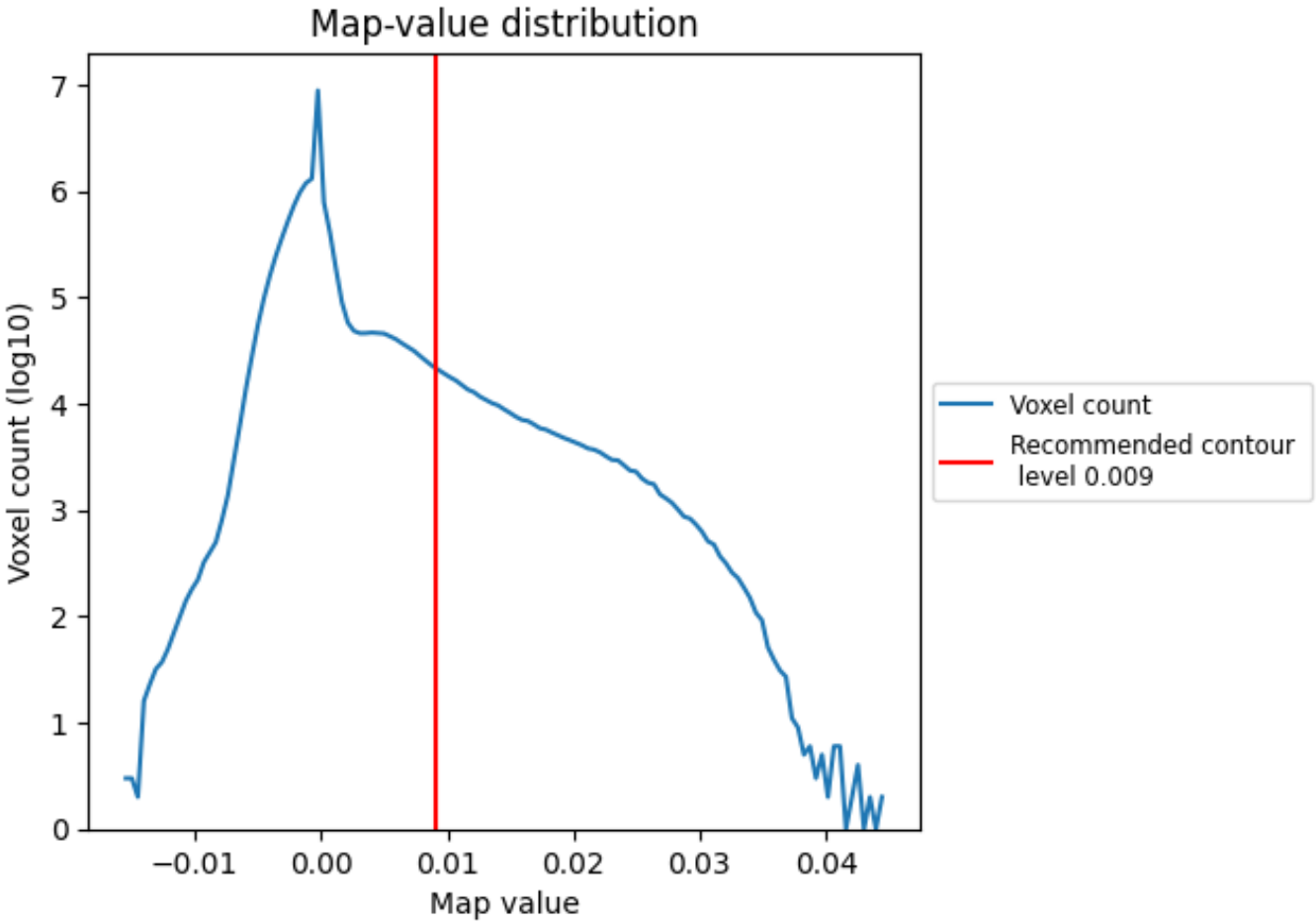
6.6 Mask visualisation (i)

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

7 Map analysis

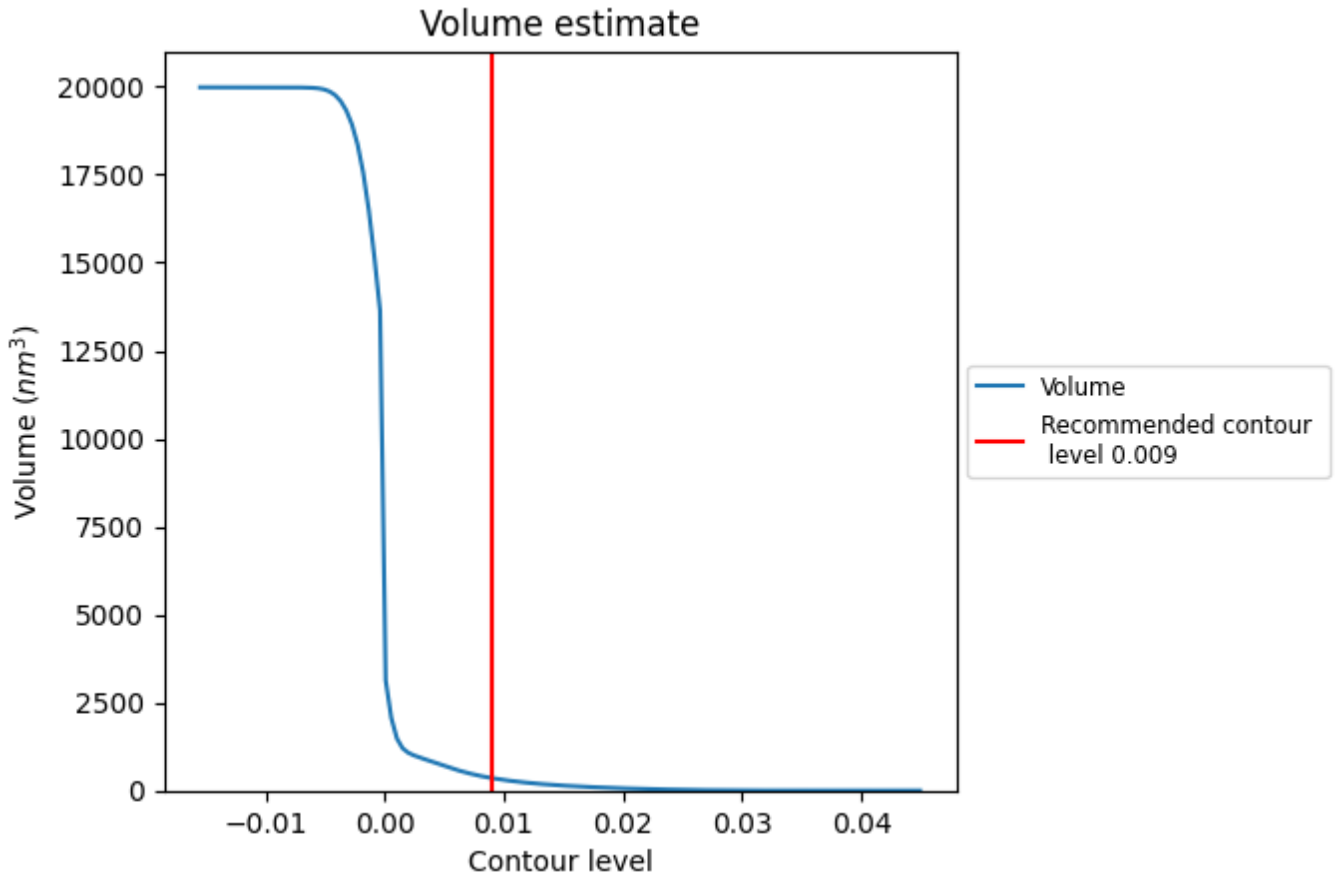
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

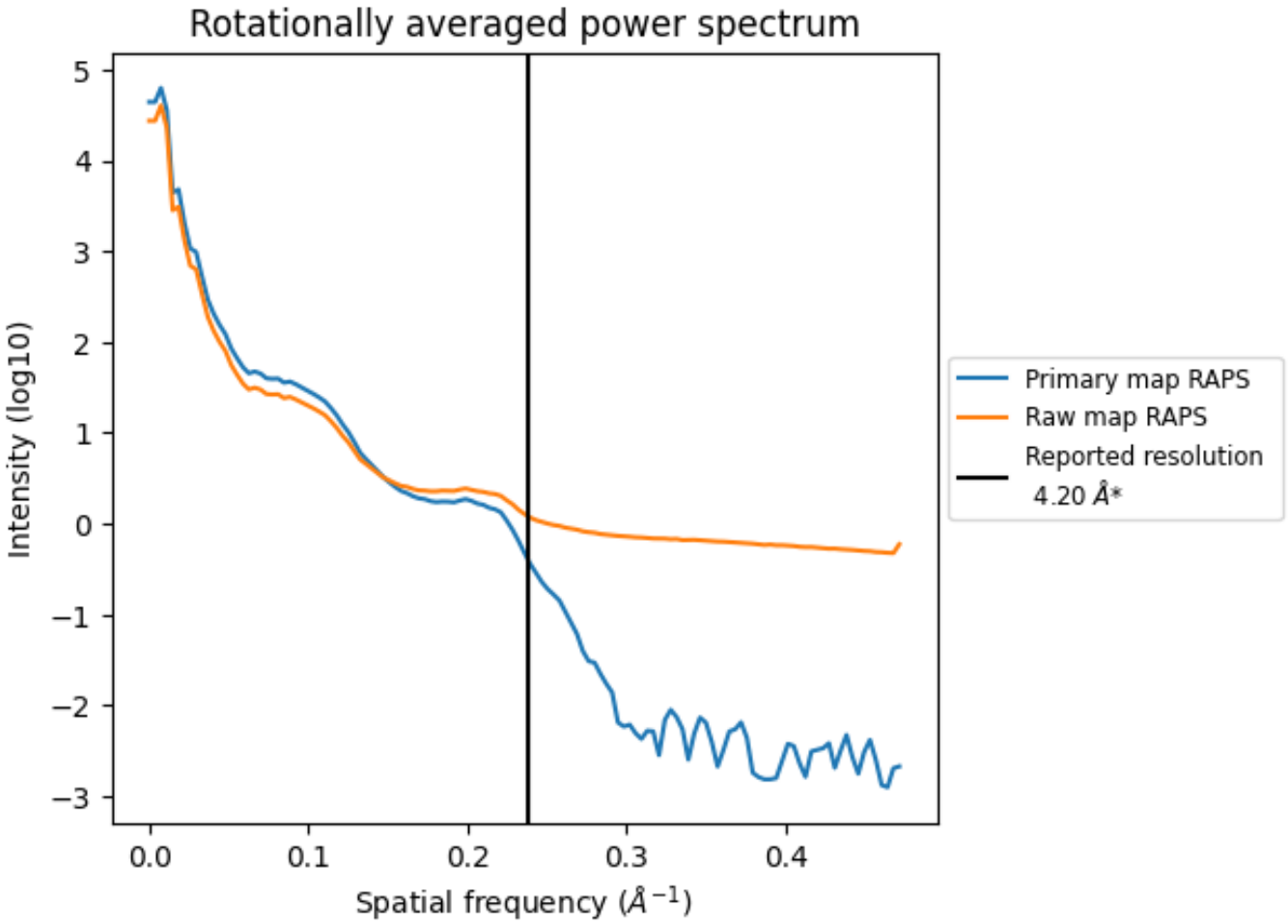
7.2 Volume estimate



The volume at the recommended contour level is 354 nm^3; this corresponds to an approximate mass of 320 kDa.

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

7.3 Rotationally averaged power spectrum (i)

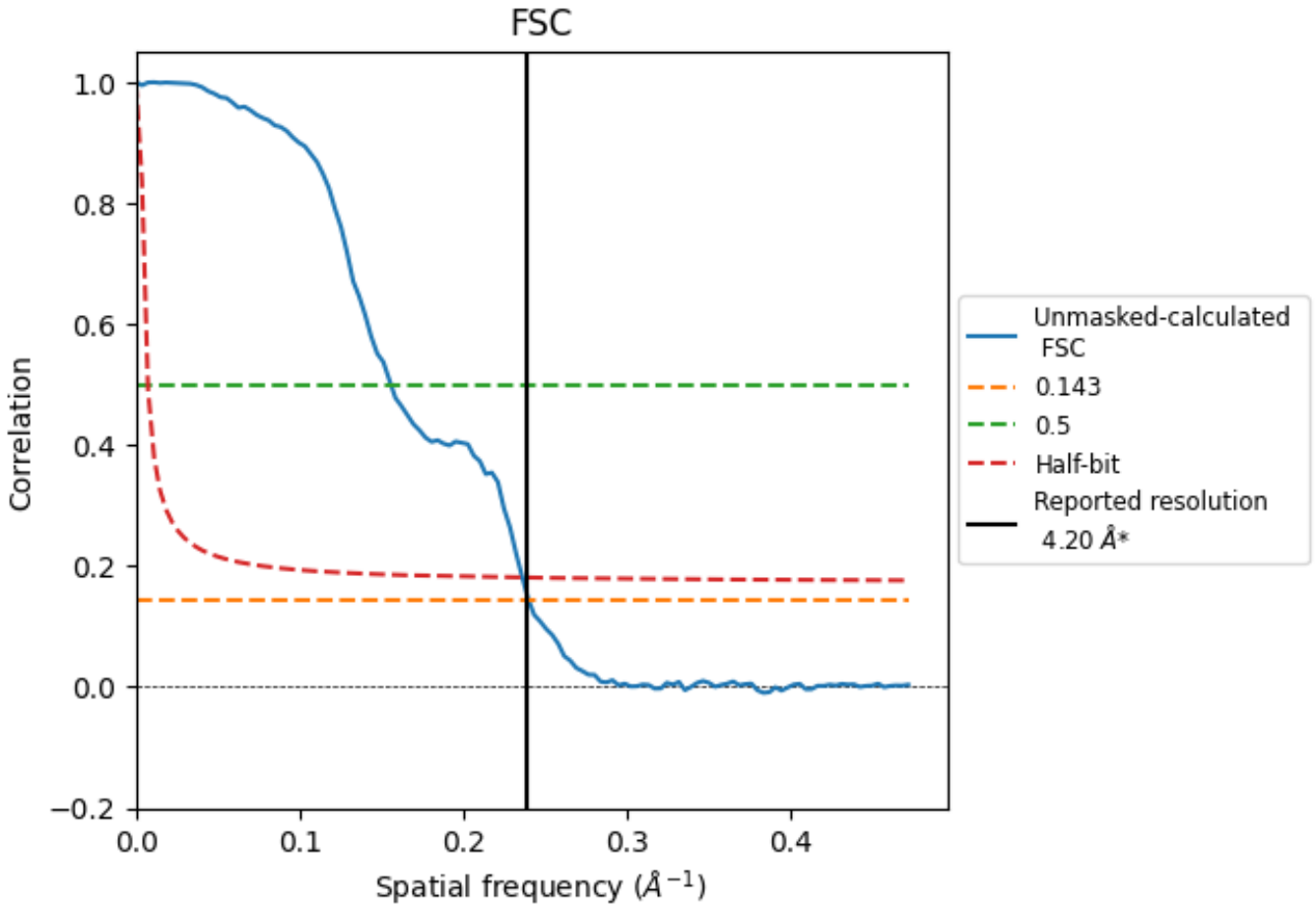


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

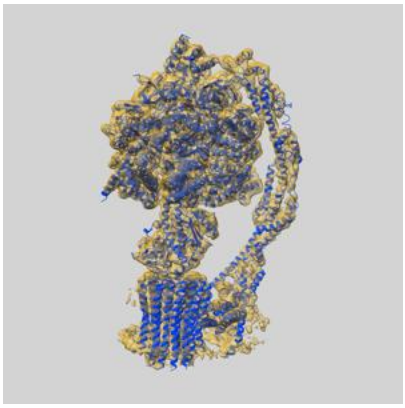
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.42	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

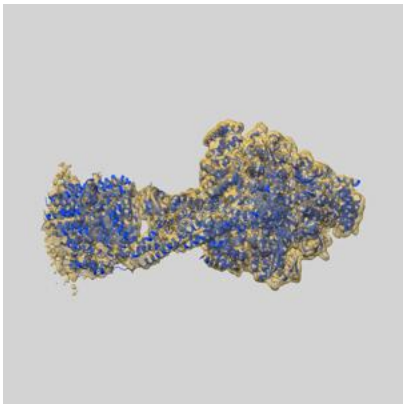
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29270 and PDB model 8FL8. Per-residue inclusion information can be found in section 3 on page 9.

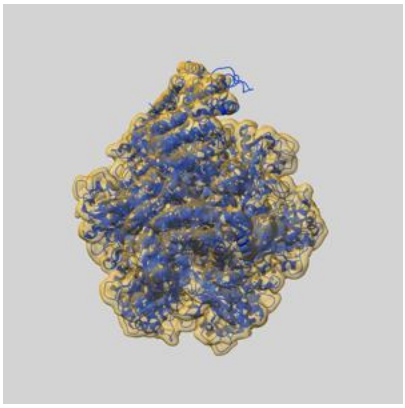
9.1 Map-model overlay



X



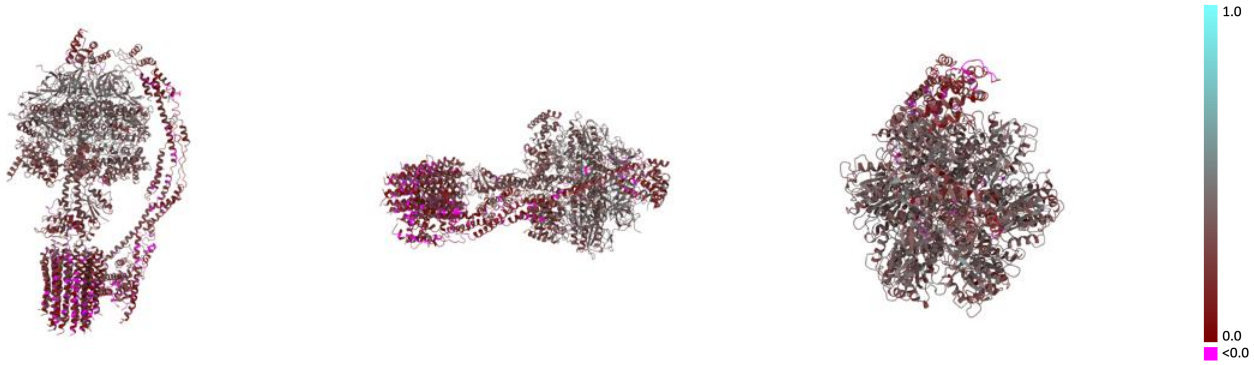
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

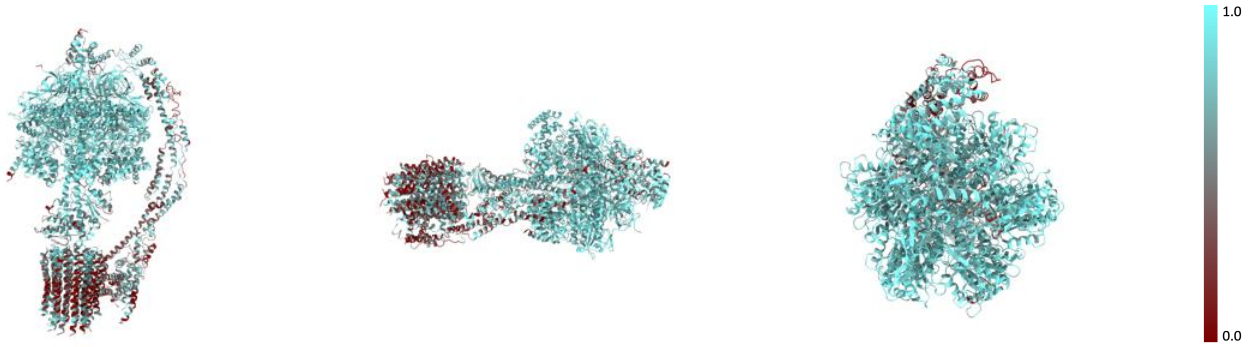
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

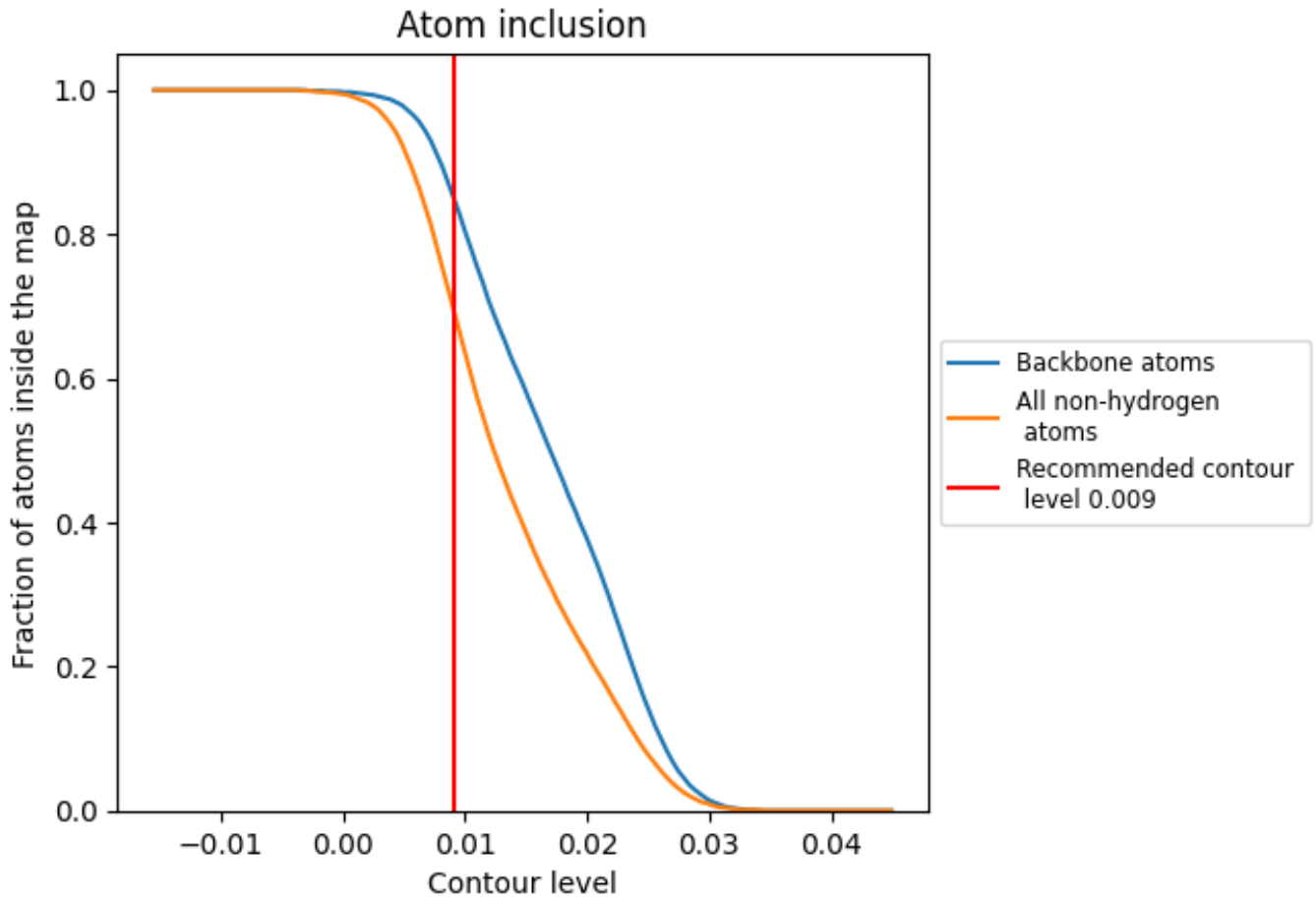
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.2850
6	0.4010	0.1340
7	0.4540	0.1510
8	0.5390	0.0860
A	0.8240	0.3550
B	0.8050	0.3450
C	0.8360	0.3640
D	0.8100	0.3450
E	0.8250	0.3780
F	0.8260	0.3740
G	0.7630	0.2950
H	0.6100	0.2140
I	0.6550	0.2100
J	0.3430	0.1180
K	0.4230	0.1730
L	0.5240	0.1590
M	0.5660	0.1700
N	0.4640	0.1400
O	0.3600	0.1330
P	0.3900	0.1510
Q	0.5600	0.1950
R	0.4420	0.1630
S	0.3700	0.1280
T	0.3380	0.1130
U	0.4520	0.1470
X	0.4880	0.1570
Y	0.7320	0.2550
Z	0.5160	0.1840