Full wwPDB EM Validation Report

Nov 19, 2022 – 05:14 PM EST

PDB ID	:	3J1N
EMDB ID	:	EMD-5407
Title	:	Cryo-EM map of a yeast minimal preinitiation complex interacting with the Mediator Head module
Authors	:	Asturias, F.J.; Imasaki, T.
Deposited on	:	2012-03-29
Resolution	:	16.00 Å(reported)
Based on initial model	:	1WCM

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

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

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

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

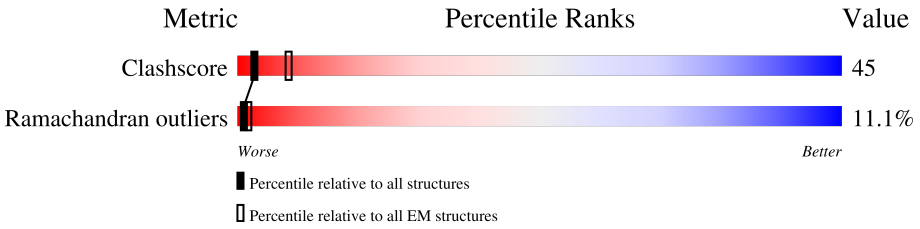
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 16.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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

Mol	Chain	Length	Quality of chain
1	A	1455	14% 60% 31% 6% •
2	B	1224	9% 62% 23% • 11%
3	C	268	32% 66% 29% 5% •
4	D	218	21% 55% 24% • 19%
5	E	215	26% 79% 18% •
6	F	84	63% 37%
7	G	171	22% 74% 23% •
8	H	146	57% 59% 28% • 9%
9	I	122	12% 75% 20% • •

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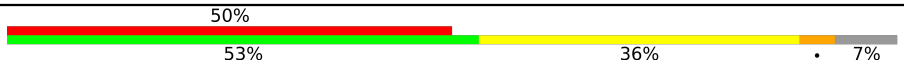
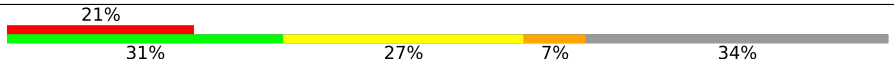
Mol	Chain	Length	Quality of chain
10	J	70	
11	K	120	
12	L	70	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19237 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	1412	Total 6964	C 4140	N 1412	O 1412	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	1094	Total 5397	C 3209	N 1094	O 1094	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	266	Total 1317	C 785	N 266	O 266	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	177	Total 878	C 524	N 177	O 177	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPABC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	214	Total 1062	C 634	N 214	O 214	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPABC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	84	Total 417	C 249	N 84	O 84	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	171	Total	C	N	O	0	0
			841	499	171	171		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPABC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	133	Total	C	N	O	0	0
			659	393	133	133		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	118	Total	C	N	O	0	0
			587	351	118	118		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPABC5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	65	Total	C	N	O	0	0
			321	191	65	65		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	114	Total	C	N	O	0	0
			565	337	114	114		

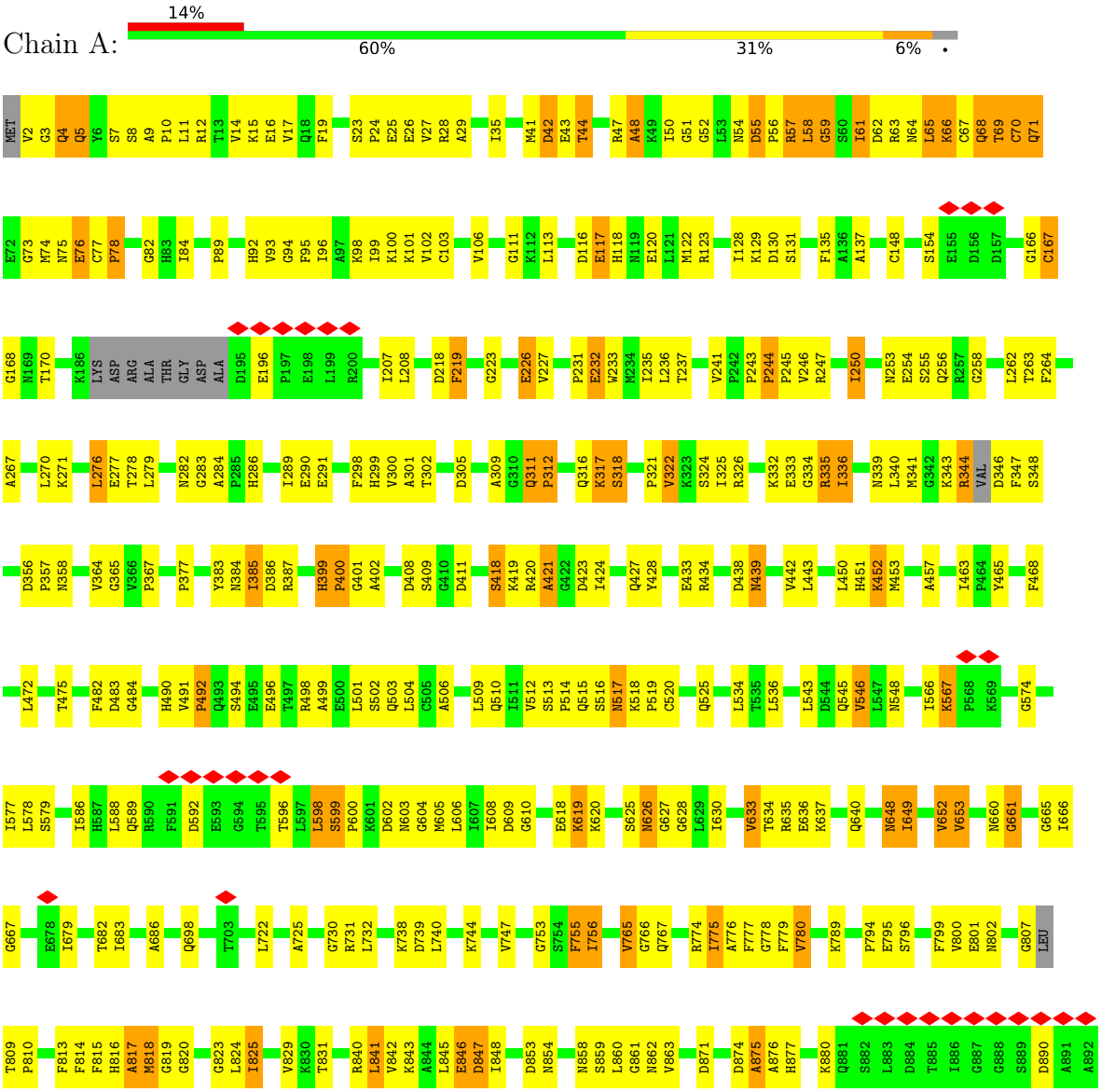
- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPABC4.

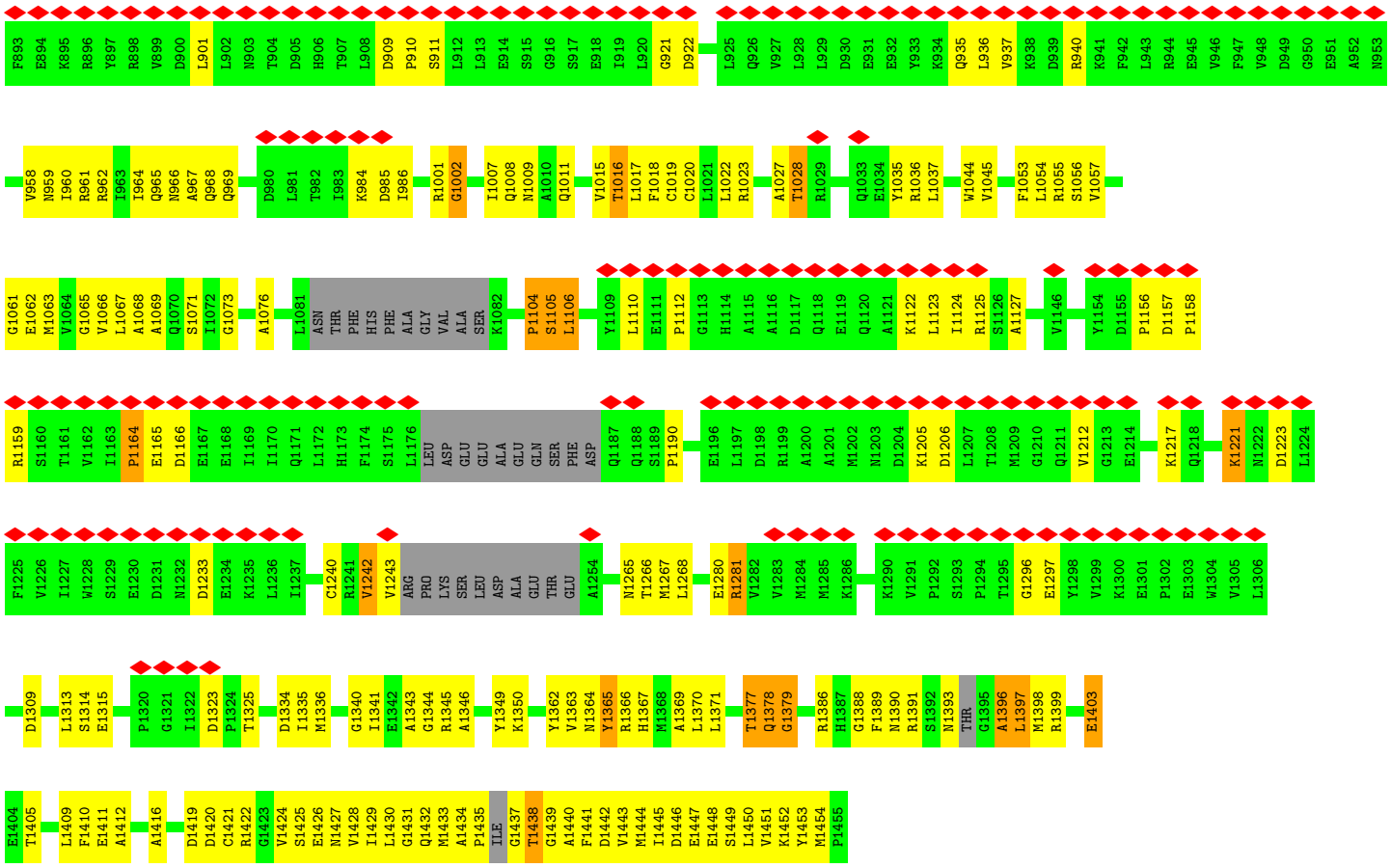
Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	46	Total	C	N	O	0	0
			229	137	46	46		

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.

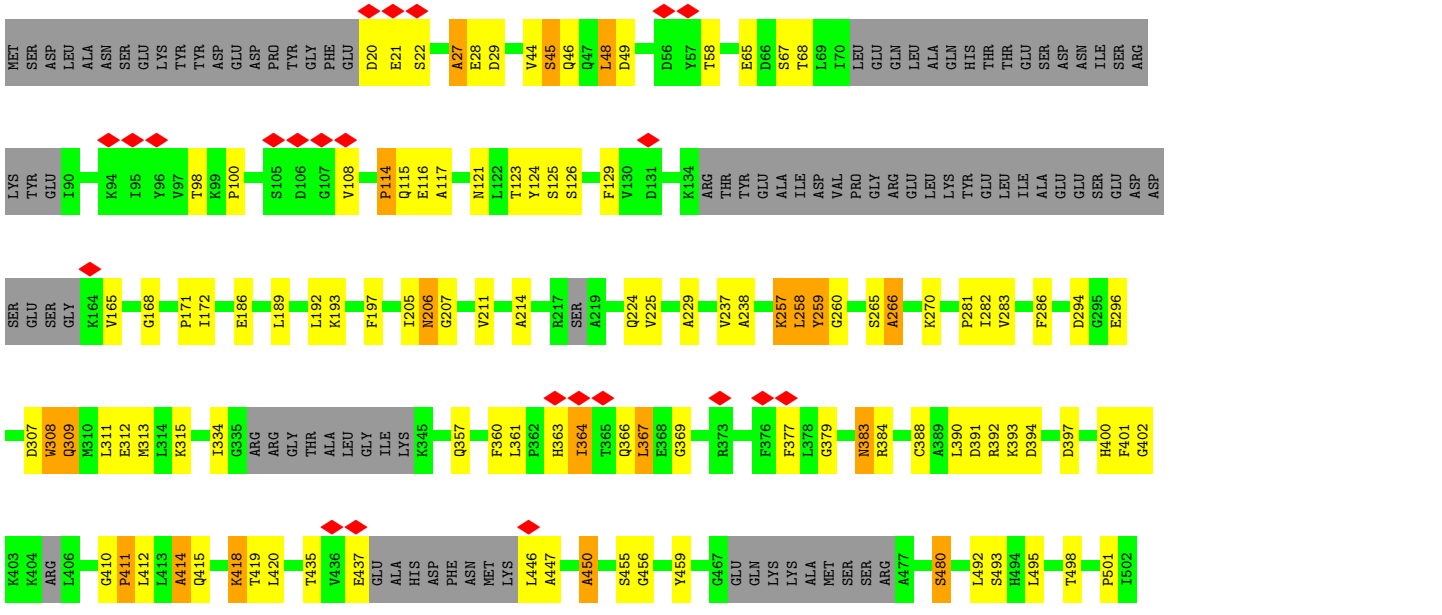
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

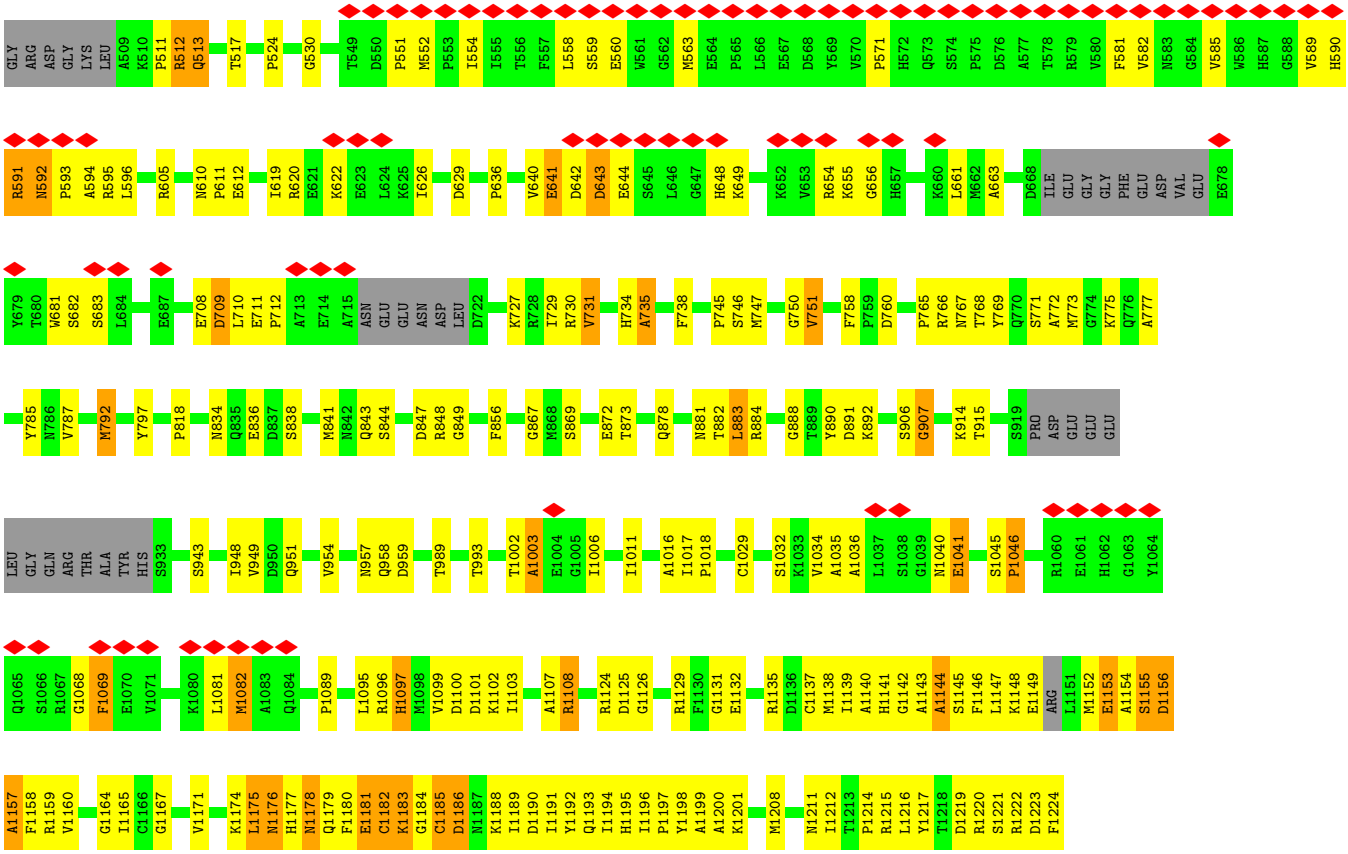




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

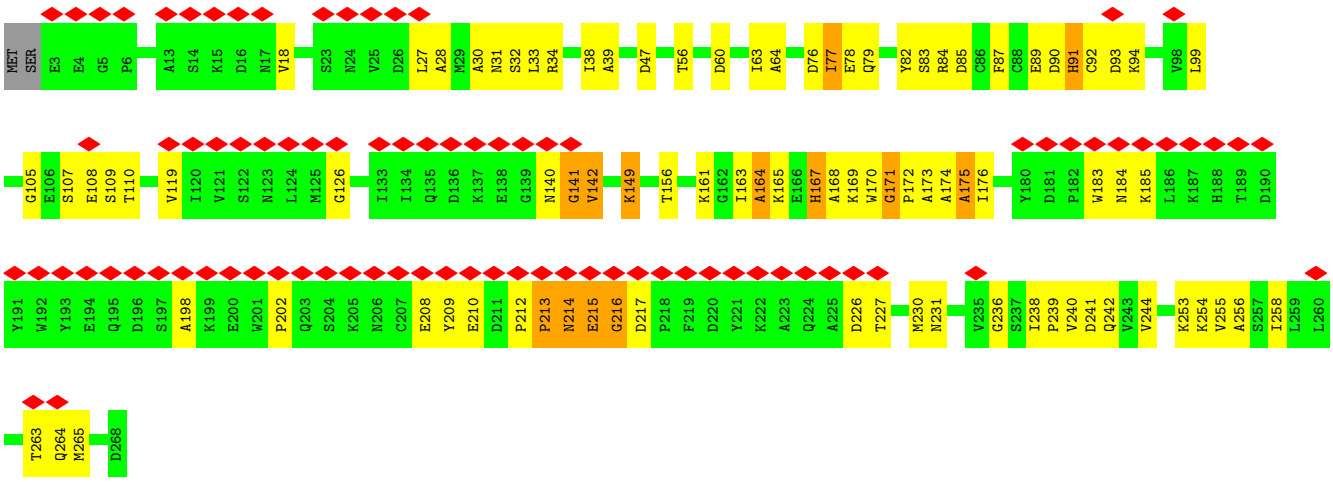
Chain B:





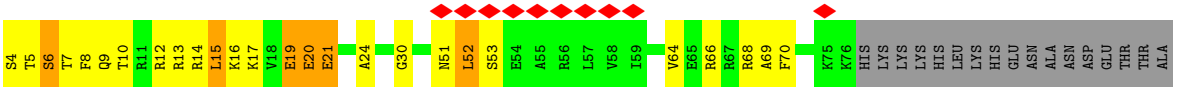
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

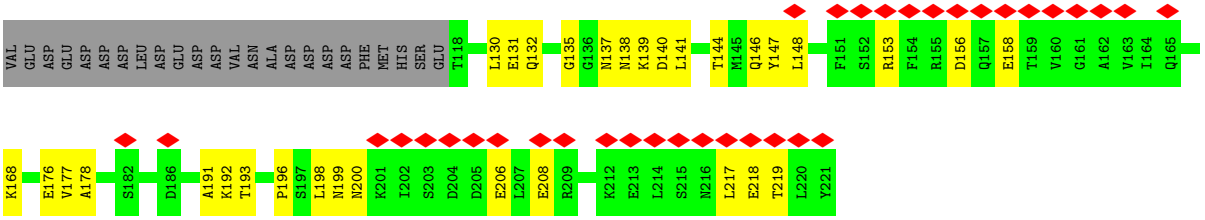
Chain C:



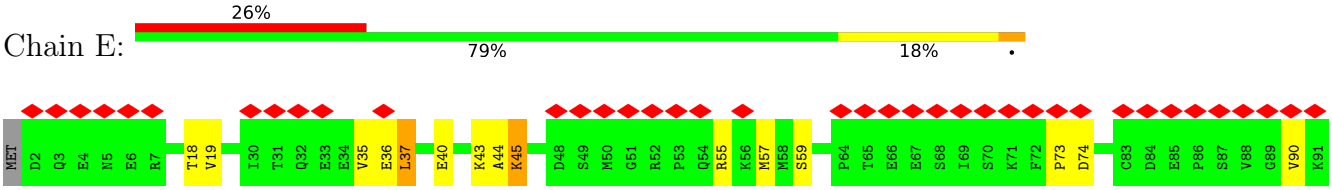
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:

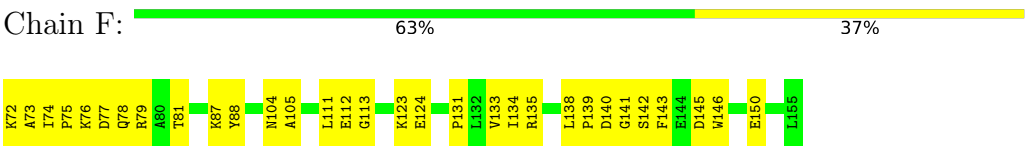




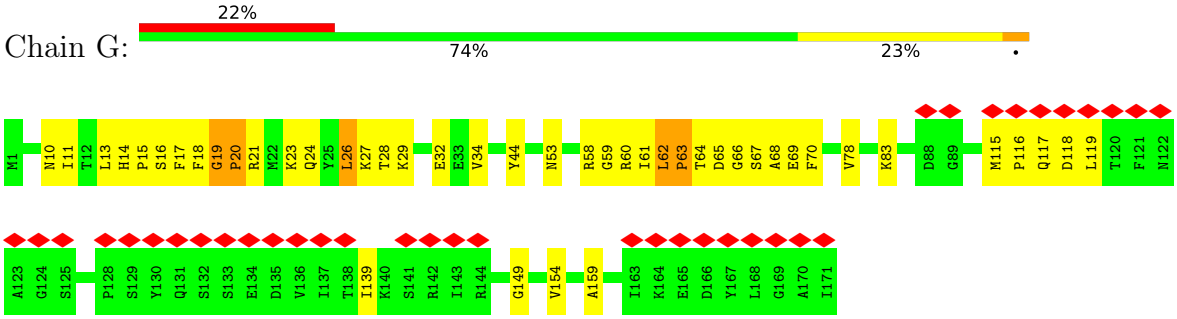
• Molecule 5: DNA-directed RNA polymerase II subunit RPABC1



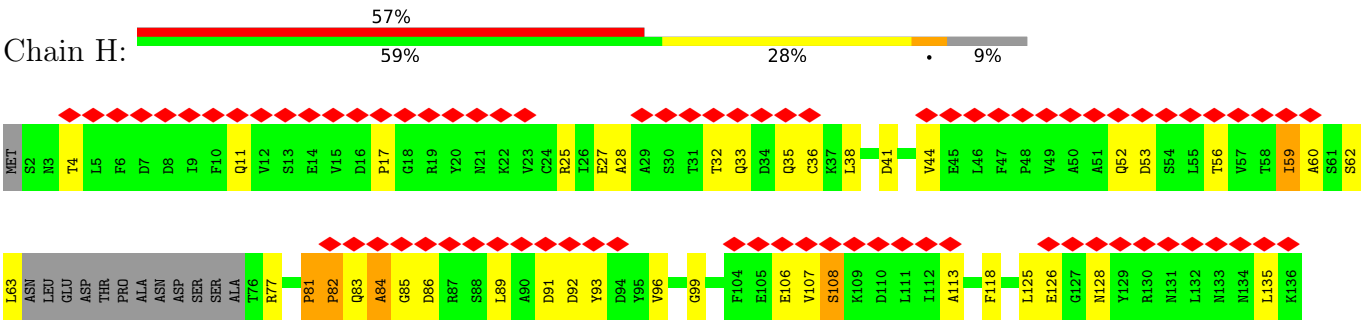
• Molecule 6: DNA-directed RNA polymerase II subunit RPABC2

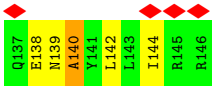


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

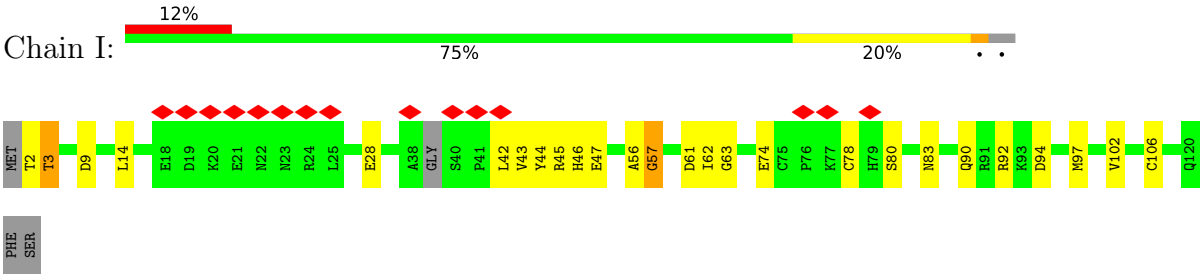


• Molecule 8: DNA-directed RNA polymerase II subunit RPABC3

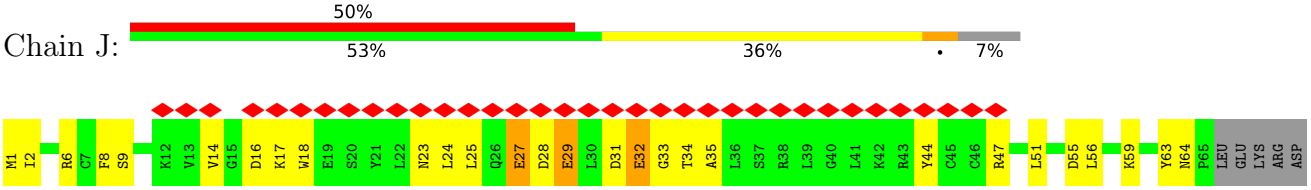




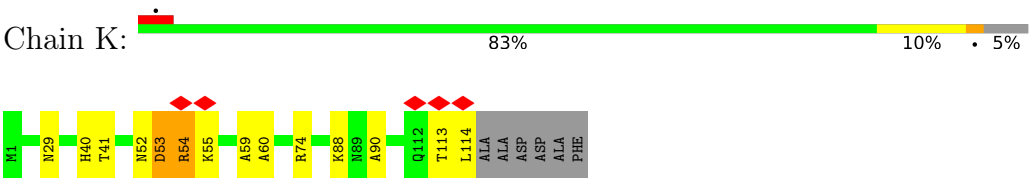
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



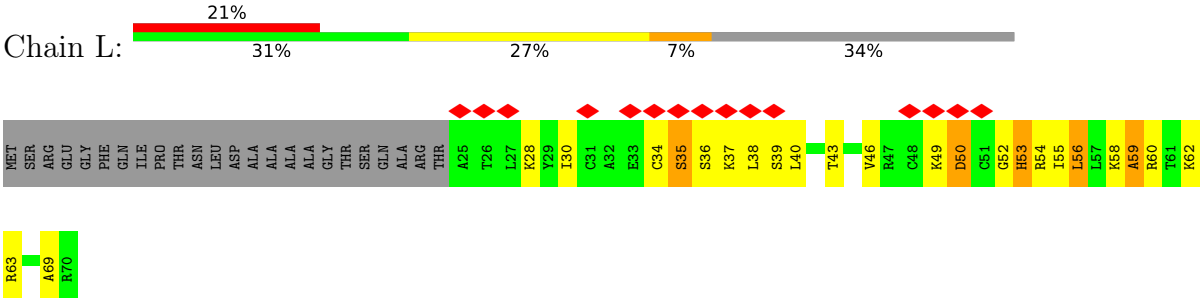
• Molecule 10: DNA-directed RNA polymerase II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



• Molecule 12: DNA-directed RNA polymerase II subunit RPABC4



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each CCD frame	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	50000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	32.476	Depositor
Minimum map value	-4.340	Depositor
Average map value	0.557	Depositor
Map value standard deviation	2.374	Depositor
Recommended contour level	3.25	Depositor
Map size (Å)	268.1, 268.1, 268.1	wwPDB
Map dimensions	70, 70, 70	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.83, 3.83, 3.83	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/6953	0.77	3/9659 (0.0%)
2	B	0.39	0/5384	0.74	1/7473 (0.0%)
3	C	0.44	0/1316	0.81	0/1833
4	D	0.36	0/876	0.75	1/1219 (0.1%)
5	E	0.34	0/1061	0.66	0/1479
6	F	0.48	0/416	0.80	0/579
7	G	0.45	0/840	0.80	0/1166
8	H	0.34	0/657	0.69	0/913
9	I	0.43	0/585	0.82	0/814
10	J	0.45	0/320	0.88	0/444
11	K	0.40	0/564	0.70	0/785
12	L	0.52	0/228	0.82	0/317
All	All	0.41	0/19200	0.76	5/26681 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1403	GLU	N-CA-C	5.38	125.52	111.00
2	B	1185	CYS	N-CA-C	-5.30	96.70	111.00
1	A	452	LYS	N-CA-C	-5.21	96.93	111.00
4	D	7	THR	N-CA-C	5.14	124.88	111.00
1	A	344	ARG	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6964	0	3039	671	0
2	B	5397	0	2399	433	0
3	C	1317	0	590	53	0
4	D	878	0	387	63	0
5	E	1062	0	453	43	0
6	F	417	0	180	123	0
7	G	841	0	354	181	0
8	H	659	0	296	30	0
9	I	587	0	235	31	0
10	J	321	0	137	15	0
11	K	565	0	260	6	0
12	L	229	0	107	12	0
All	All	19237	0	8437	1250	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 45.

All (1250) 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)
6:F:143:PHE:CB	7:G:68:ALA:CA	1.76	1.61
1:A:344:ARG:CA	2:B:1129:ARG:HA	1.27	1.60
6:F:143:PHE:CA	7:G:68:ALA:HB1	1.11	1.58
2:B:1148:LYS:HA	2:B:1200:ALA:CB	1.22	1.57
1:A:1444:MET:CB	7:G:10:ASN:CB	1.82	1.57
2:B:312:GLU:CB	9:I:46:HIS:CB	1.83	1.56
2:B:1148:LYS:CB	2:B:1200:ALA:HB3	1.16	1.55
2:B:1193:GLN:CB	7:G:65:ASP:CB	1.84	1.55
2:B:1148:LYS:CA	2:B:1200:ALA:HB3	1.02	1.49
1:A:509:LEU:CB	1:A:1062:GLU:HA	1.03	1.49
1:A:858:ASN:CB	1:A:1422:ARG:C	1.78	1.49
1:A:237:THR:CB	4:D:17:LYS:H	1.25	1.48
1:A:89:PRO:CB	4:D:16:LYS:CB	1.88	1.48
2:B:1148:LYS:CA	2:B:1200:ALA:CB	1.79	1.48
1:A:1444:MET:CB	7:G:10:ASN:CA	1.89	1.47
1:A:63:ARG:CB	1:A:411:ASP:HA	1.44	1.46
2:B:1222:ARG:CB	5:E:171:LYS:CA	1.94	1.44
2:B:1193:GLN:CB	7:G:65:ASP:CA	1.93	1.43
6:F:73:ALA:N	7:G:70:PHE:H	0.96	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLU:CA	1:A:1056:SER:CB	1.84	1.41
1:A:846:GLU:CB	2:B:1140:ALA:HB3	1.15	1.41
2:B:1193:GLN:CB	7:G:65:ASP:H	1.34	1.40
1:A:509:LEU:CB	1:A:1062:GLU:CA	1.99	1.40
1:A:609:ASP:H	1:A:962:ARG:CB	1.35	1.39
1:A:862:ASN:N	1:A:1420:ASP:CB	1.86	1.39
1:A:341:MET:O	2:B:1132:GLU:CA	1.70	1.38
1:A:63:ARG:O	1:A:411:ASP:CB	1.71	1.37
2:B:1193:GLN:CB	7:G:65:ASP:N	1.84	1.37
6:F:73:ALA:N	7:G:70:PHE:N	1.72	1.35
6:F:73:ALA:H	7:G:70:PHE:N	1.17	1.35
1:A:566:ILE:CB	8:H:81:PRO:CB	2.05	1.34
1:A:636:GLU:HA	1:A:1056:SER:CB	0.95	1.34
1:A:858:ASN:CB	1:A:1422:ARG:CA	2.03	1.34
1:A:846:GLU:CB	2:B:1140:ALA:CB	1.97	1.33
1:A:1425:SER:C	2:B:1139:ILE:CB	1.96	1.33
1:A:129:LYS:CB	5:E:192:ARG:O	1.76	1.33
1:A:453:MET:N	1:A:1066:VAL:CB	1.90	1.33
2:B:1191:ILE:O	7:G:67:SER:CB	1.77	1.33
2:B:1145:SER:CB	2:B:1195:HIS:C	1.98	1.32
1:A:609:ASP:N	1:A:962:ARG:CB	1.87	1.32
6:F:135:ARG:N	7:G:15:PRO:CB	1.93	1.31
1:A:766:GLY:HA3	1:A:820:GLY:N	1.46	1.30
6:F:142:SER:HA	7:G:69:GLU:O	1.19	1.28
6:F:138:LEU:CB	7:G:59:GLY:O	1.81	1.28
1:A:859:SER:O	1:A:1421:CYS:CB	1.80	1.28
1:A:859:SER:C	1:A:1421:CYS:CB	1.83	1.27
2:B:1185:CYS:C	4:D:4:SER:N	1.88	1.26
1:A:1427:ASN:CB	2:B:1142:GLY:H	1.47	1.26
1:A:846:GLU:CB	2:B:1137:CYS:HA	1.62	1.25
1:A:1429:ILE:C	2:B:1147:LEU:CB	2.04	1.25
6:F:142:SER:HA	7:G:69:GLU:C	1.57	1.25
1:A:1430:LEU:C	2:B:1143:ALA:O	1.74	1.25
1:A:630:ILE:O	1:A:876:ALA:CA	1.83	1.24
2:B:1223:ASP:HA	5:E:168:TYR:CB	1.67	1.23
1:A:846:GLU:N	2:B:1140:ALA:CB	1.93	1.23
1:A:1425:SER:O	2:B:1139:ILE:CB	1.87	1.22
2:B:1148:LYS:CB	2:B:1200:ALA:CB	2.03	1.22
1:A:1444:MET:CB	7:G:10:ASN:C	2.06	1.21
2:B:1149:GLU:C	2:B:1156:ASP:CB	2.08	1.21
6:F:143:PHE:CA	7:G:68:ALA:CB	1.79	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:CB	6:F:104:ASN:O	1.89	1.21
1:A:766:GLY:O	1:A:817:ALA:C	1.77	1.21
1:A:503:GLN:O	1:A:1061:GLY:HA2	1.35	1.20
6:F:142:SER:CA	7:G:69:GLU:O	1.87	1.20
6:F:72:LYS:N	7:G:70:PHE:N	1.88	1.20
1:A:452:LYS:CA	1:A:846:GLU:HA	1.70	1.19
1:A:515:GLN:CB	1:A:1069:ALA:HA	1.72	1.19
1:A:635:ARG:N	1:A:877:HIS:H	1.40	1.19
1:A:1431:GLY:HA3	2:B:1147:LEU:N	1.55	1.19
1:A:1444:MET:CB	6:F:72:LYS:HA	1.66	1.19
1:A:341:MET:HA	2:B:1135:ARG:CB	1.73	1.18
6:F:72:LYS:N	7:G:69:GLU:C	1.96	1.18
1:A:858:ASN:CB	1:A:1422:ARG:O	1.90	1.18
1:A:341:MET:O	2:B:1132:GLU:HA	1.23	1.18
2:B:1145:SER:CB	2:B:1195:HIS:O	1.91	1.18
1:A:518:LYS:CB	1:A:1364:ASN:N	2.07	1.18
1:A:810:PRO:CB	2:B:731:VAL:N	2.07	1.17
2:B:1192:TYR:HA	7:G:67:SER:CB	1.73	1.17
1:A:344:ARG:CA	2:B:1129:ARG:CA	2.23	1.17
1:A:1444:MET:CB	2:B:1165:ILE:N	2.07	1.17
1:A:63:ARG:O	1:A:411:ASP:CA	1.85	1.16
1:A:858:ASN:CB	1:A:1422:ARG:HA	1.72	1.16
1:A:766:GLY:CA	1:A:820:GLY:H	1.57	1.16
1:A:810:PRO:CB	2:B:731:VAL:HA	1.74	1.15
1:A:630:ILE:O	1:A:876:ALA:HA	0.98	1.15
1:A:237:THR:CB	4:D:17:LYS:N	2.08	1.15
2:B:1148:LYS:HA	2:B:1200:ALA:HB2	1.25	1.15
2:B:1192:TYR:CB	7:G:62:LEU:CB	2.23	1.15
1:A:810:PRO:CB	2:B:731:VAL:CA	2.25	1.14
2:B:1185:CYS:CA	4:D:4:SER:N	2.11	1.14
1:A:383:TYR:O	6:F:105:ALA:HB1	1.46	1.14
1:A:1427:ASN:CB	2:B:1142:GLY:N	2.10	1.14
1:A:443:LEU:H	2:B:1153:GLU:CB	1.60	1.14
1:A:846:GLU:N	2:B:1140:ALA:HB1	1.39	1.14
1:A:344:ARG:C	2:B:1129:ARG:HA	1.67	1.13
1:A:77:CYS:O	1:A:78:PRO:O	1.65	1.13
1:A:862:ASN:CB	1:A:1422:ARG:CB	2.27	1.13
1:A:1431:GLY:C	2:B:1143:ALA:O	1.87	1.13
1:A:490:HIS:O	2:B:1153:GLU:CB	1.84	1.12
6:F:135:ARG:CB	7:G:66:GLY:O	1.96	1.12
1:A:846:GLU:CB	2:B:1137:CYS:CA	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:GLU:CB	2:B:1137:CYS:O	1.98	1.12
2:B:1148:LYS:O	2:B:1198:TYR:C	1.81	1.12
1:A:11:LEU:HA	7:G:65:ASP:O	1.48	1.11
1:A:1431:GLY:N	2:B:1143:ALA:O	1.83	1.11
1:A:10:PRO:CB	7:G:67:SER:HA	1.80	1.11
2:B:1149:GLU:CB	2:B:1158:PHE:N	2.12	1.11
1:A:858:ASN:N	1:A:1422:ARG:HA	1.64	1.11
1:A:1452:LYS:CB	7:G:28:THR:CB	2.29	1.11
1:A:518:LYS:CB	1:A:1364:ASN:H	1.64	1.10
1:A:513:SER:O	1:A:1367:HIS:CB	1.99	1.10
1:A:450:LEU:O	1:A:842:VAL:N	1.68	1.09
1:A:767:GLN:HA	1:A:818:MET:CB	1.79	1.09
1:A:858:ASN:CA	1:A:1422:ARG:HA	1.81	1.09
1:A:1431:GLY:N	2:B:1147:LEU:CB	2.15	1.09
1:A:341:MET:O	2:B:1132:GLU:C	1.90	1.09
2:B:1193:GLN:N	7:G:62:LEU:CB	2.15	1.09
2:B:1219:ASP:CB	7:G:59:GLY:C	2.20	1.09
1:A:344:ARG:HA	2:B:1129:ARG:CA	1.80	1.09
1:A:845:LEU:C	2:B:1140:ALA:HB1	1.73	1.08
1:A:1428:VAL:HA	2:B:1138:MET:CB	1.84	1.08
1:A:777:PHE:O	2:B:400:HIS:CB	1.97	1.08
1:A:452:LYS:HA	1:A:846:GLU:CA	1.84	1.07
1:A:1444:MET:CB	2:B:1164:GLY:C	2.21	1.07
2:B:1193:GLN:CB	7:G:65:ASP:C	2.22	1.07
6:F:77:ASP:N	7:G:23:LYS:N	1.99	1.06
1:A:344:ARG:C	2:B:1129:ARG:CA	2.21	1.06
1:A:635:ARG:HA	1:A:874:ASP:N	1.42	1.06
1:A:383:TYR:O	6:F:105:ALA:CB	2.04	1.05
1:A:766:GLY:CA	1:A:820:GLY:N	2.17	1.05
1:A:1393:ASN:HA	1:A:1399:ARG:H	1.18	1.05
1:A:510:GLN:O	1:A:1067:LEU:CB	2.04	1.05
1:A:1448:GLU:CB	7:G:27:LYS:O	2.05	1.05
1:A:1430:LEU:C	2:B:1147:LEU:H	1.60	1.04
1:A:452:LYS:CB	1:A:1066:VAL:CB	2.34	1.04
1:A:858:ASN:H	1:A:1422:ARG:HA	1.20	1.04
1:A:862:ASN:CA	1:A:1420:ASP:CB	2.34	1.04
1:A:1431:GLY:CA	2:B:1147:LEU:N	2.20	1.04
2:B:1219:ASP:HA	6:F:138:LEU:C	1.77	1.04
2:B:1223:ASP:CA	5:E:168:TYR:CB	2.35	1.03
1:A:450:LEU:C	1:A:843:LYS:H	1.61	1.03
1:A:608:ILE:CA	1:A:962:ARG:CB	2.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:CB	7:G:10:ASN:HA	1.86	1.03
1:A:503:GLN:O	1:A:1061:GLY:CA	2.05	1.02
2:B:1146:PHE:N	2:B:1195:HIS:O	1.92	1.02
1:A:810:PRO:HA	2:B:729:ILE:O	1.60	1.02
1:A:1427:ASN:CB	2:B:1142:GLY:CA	2.35	1.02
2:B:1146:PHE:C	2:B:1197:PRO:N	2.11	1.02
1:A:23:SER:HA	4:D:13:ARG:CB	1.90	1.02
1:A:518:LYS:H	1:A:1367:HIS:CB	1.72	1.02
1:A:504:LEU:HA	1:A:1061:GLY:O	1.59	1.02
1:A:1427:ASN:CB	2:B:1142:GLY:HA2	1.89	1.02
1:A:452:LYS:HA	1:A:846:GLU:HA	1.02	1.01
1:A:452:LYS:CB	1:A:1066:VAL:CA	2.38	1.01
1:A:11:LEU:CB	7:G:65:ASP:C	2.19	1.01
9:I:3:THR:O	9:I:43:VAL:N	1.88	1.01
1:A:514:PRO:CB	1:A:1370:LEU:CB	2.39	1.01
2:B:401:PHE:C	2:B:517:THR:H	1.54	1.01
1:A:450:LEU:C	1:A:843:LYS:N	2.11	1.00
1:A:1431:GLY:CA	2:B:1143:ALA:O	2.09	1.00
1:A:452:LYS:CB	1:A:1066:VAL:N	2.25	1.00
1:A:515:GLN:CB	1:A:1069:ALA:CA	2.38	1.00
1:A:1430:LEU:N	2:B:1147:LEU:CB	2.24	1.00
6:F:138:LEU:H	7:G:60:ARG:HA	1.26	1.00
6:F:75:PRO:HA	7:G:26:LEU:H	1.23	0.99
6:F:143:PHE:N	7:G:68:ALA:HB1	1.76	0.99
1:A:766:GLY:O	1:A:815:PHE:O	1.78	0.99
1:A:341:MET:O	2:B:1132:GLU:O	1.78	0.99
1:A:341:MET:C	2:B:1132:GLU:HA	1.82	0.98
2:B:1219:ASP:CB	7:G:58:ARG:C	2.31	0.98
2:B:1148:LYS:HA	2:B:1200:ALA:CA	1.93	0.98
1:A:492:PRO:HA	2:B:1157:ALA:HB1	1.45	0.98
6:F:133:VAL:O	7:G:15:PRO:CB	2.12	0.98
1:A:63:ARG:CB	1:A:411:ASP:CA	2.41	0.98
2:B:1148:LYS:O	2:B:1199:ALA:N	1.96	0.97
6:F:72:LYS:C	7:G:70:PHE:H	1.52	0.97
1:A:10:PRO:CB	7:G:67:SER:CA	2.41	0.96
2:B:1192:TYR:C	7:G:62:LEU:CB	2.34	0.96
1:A:341:MET:CA	2:B:1135:ARG:CB	2.42	0.96
6:F:77:ASP:H	7:G:24:GLN:H	1.07	0.96
1:A:344:ARG:HA	2:B:1129:ARG:HA	0.99	0.96
2:B:1219:ASP:CB	6:F:138:LEU:CB	2.43	0.96
6:F:135:ARG:H	7:G:15:PRO:CB	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:MET:H	1:A:1066:VAL:CB	1.64	0.96
1:A:1429:ILE:O	2:B:1147:LEU:CB	2.12	0.96
2:B:1193:GLN:O	7:G:65:ASP:O	1.84	0.95
1:A:1430:LEU:C	2:B:1147:LEU:CB	2.34	0.95
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.47	0.95
1:A:862:ASN:H	1:A:1420:ASP:CB	1.75	0.95
1:A:516:SER:N	1:A:1367:HIS:C	2.16	0.94
1:A:1448:GLU:HA	7:G:32:GLU:H	1.31	0.94
1:A:518:LYS:N	1:A:1367:HIS:CB	2.28	0.94
6:F:145:ASP:CB	7:G:17:PHE:C	2.30	0.94
2:B:1223:ASP:CB	5:E:168:TYR:CB	2.45	0.94
1:A:1432:GLN:O	2:B:1138:MET:O	1.86	0.93
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.50	0.93
2:B:1149:GLU:O	2:B:1156:ASP:CB	2.17	0.93
1:A:387:ARG:N	6:F:104:ASN:CB	2.32	0.93
1:A:1444:MET:CB	7:G:11:ILE:N	2.31	0.92
2:B:1192:TYR:CB	7:G:67:SER:O	2.17	0.92
6:F:77:ASP:H	7:G:23:LYS:N	1.67	0.92
1:A:640:GLN:CB	6:F:87:LYS:CB	2.47	0.92
1:A:863:VAL:CB	2:B:1224:PHE:C	2.37	0.92
1:A:608:ILE:HA	1:A:962:ARG:CB	1.99	0.92
1:A:1432:GLN:O	2:B:1141:HIS:CB	2.11	0.92
6:F:72:LYS:N	7:G:69:GLU:CA	2.28	0.92
1:A:635:ARG:CA	1:A:874:ASP:N	2.30	0.92
1:A:608:ILE:C	1:A:962:ARG:CB	2.38	0.92
1:A:859:SER:C	1:A:1437:GLY:N	2.23	0.91
1:A:1444:MET:CB	6:F:72:LYS:CA	2.47	0.91
1:A:766:GLY:O	1:A:816:HIS:C	2.02	0.91
1:A:800:VAL:HA	1:A:814:PHE:HA	1.51	0.91
1:A:452:LYS:CB	1:A:846:GLU:HA	1.99	0.91
1:A:11:LEU:CA	7:G:65:ASP:O	2.09	0.91
1:A:1431:GLY:HA3	2:B:1147:LEU:H	1.36	0.91
1:A:1430:LEU:O	2:B:1143:ALA:O	1.89	0.91
1:A:55:ASP:C	1:A:57:ARG:H	1.72	0.90
1:A:1446:ASP:O	7:G:29:LYS:CB	2.19	0.90
1:A:1431:GLY:CA	2:B:1147:LEU:H	1.82	0.90
1:A:800:VAL:HA	1:A:814:PHE:CA	1.99	0.90
1:A:1442:ASP:HA	2:B:1216:LEU:O	1.72	0.90
1:A:63:ARG:CA	1:A:411:ASP:HA	2.01	0.90
1:A:11:LEU:CB	7:G:65:ASP:O	2.20	0.89
1:A:767:GLN:CA	1:A:818:MET:CB	2.44	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:THR:HA	8:H:60:ALA:HB2	1.52	0.89
1:A:235:ILE:C	4:D:16:LYS:H	1.76	0.89
6:F:138:LEU:N	7:G:60:ARG:HA	1.79	0.89
1:A:1427:ASN:N	2:B:1139:ILE:CA	2.30	0.88
1:A:1425:SER:CA	2:B:1139:ILE:CB	2.52	0.88
6:F:77:ASP:H	7:G:24:GLN:N	1.71	0.88
1:A:846:GLU:CB	2:B:1137:CYS:C	2.41	0.88
1:A:515:GLN:CB	1:A:1069:ALA:N	2.37	0.88
1:A:1428:VAL:HA	2:B:1138:MET:CA	1.95	0.87
2:B:1146:PHE:O	2:B:1197:PRO:N	2.06	0.87
1:A:766:GLY:C	1:A:815:PHE:O	2.12	0.87
1:A:635:ARG:HA	1:A:874:ASP:H	1.41	0.86
1:A:235:ILE:O	4:D:16:LYS:N	2.09	0.86
2:B:168:GLY:H	2:B:450:ALA:HB1	1.39	0.86
1:A:859:SER:O	1:A:1437:GLY:N	2.09	0.86
1:A:1427:ASN:C	2:B:1138:MET:O	2.14	0.86
1:A:1452:LYS:H	7:G:28:THR:CB	1.88	0.86
1:A:625:SER:HA	1:A:1362:TYR:O	1.75	0.85
1:A:1431:GLY:N	2:B:1147:LEU:H	1.75	0.85
6:F:77:ASP:N	7:G:24:GLN:H	1.74	0.85
2:B:1145:SER:CB	2:B:1196:ILE:N	2.34	0.85
3:C:164:ALA:HA	3:C:167:HIS:O	1.76	0.85
1:A:859:SER:CB	1:A:1426:GLU:CB	2.55	0.85
1:A:799:PHE:HA	1:A:818:MET:CB	2.06	0.84
1:A:1443:VAL:HA	7:G:69:GLU:O	1.76	0.84
6:F:146:TRP:CA	7:G:18:PHE:O	2.24	0.84
1:A:492:PRO:HA	2:B:1157:ALA:CB	2.08	0.84
1:A:496:GLU:C	7:G:63:PRO:O	2.16	0.84
3:C:47:ASP:HA	12:L:69:ALA:CB	2.06	0.84
1:A:443:LEU:N	2:B:1153:GLU:CB	2.41	0.84
6:F:134:ILE:C	7:G:15:PRO:CB	2.45	0.84
2:B:1149:GLU:CB	2:B:1157:ALA:C	2.46	0.84
6:F:75:PRO:N	7:G:26:LEU:CB	2.41	0.84
1:A:634:THR:O	1:A:874:ASP:CB	2.26	0.83
1:A:1393:ASN:HA	1:A:1399:ARG:N	1.92	0.83
1:A:1444:MET:O	6:F:72:LYS:C	2.16	0.83
1:A:1065:GLY:HA3	1:A:1435:PRO:C	1.99	0.83
1:A:1427:ASN:CB	2:B:1138:MET:O	2.27	0.83
2:B:1219:ASP:CB	7:G:58:ARG:O	2.27	0.83
2:B:1146:PHE:O	2:B:1197:PRO:CA	2.26	0.83
1:A:1430:LEU:CA	2:B:1147:LEU:CB	2.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:1435:PRO:C	2.17	0.82
2:B:1193:GLN:CA	7:G:65:ASP:H	1.92	0.82
1:A:766:GLY:HA3	1:A:819:GLY:C	1.94	0.82
1:A:123:ARG:CB	5:E:128:PRO:CB	2.56	0.82
2:B:1145:SER:CB	7:G:63:PRO:CB	2.58	0.82
1:A:514:PRO:HA	1:A:1367:HIS:HA	1.62	0.82
6:F:138:LEU:H	7:G:60:ARG:CA	1.91	0.82
1:A:635:ARG:N	1:A:877:HIS:N	2.25	0.82
2:B:1219:ASP:HA	6:F:138:LEU:CB	2.09	0.82
2:B:1219:ASP:CB	7:G:59:GLY:O	2.28	0.82
2:B:1149:GLU:O	2:B:1198:TYR:CB	2.26	0.81
2:B:401:PHE:C	2:B:517:THR:N	2.34	0.81
1:A:1431:GLY:HA3	2:B:1146:PHE:C	2.01	0.81
2:B:1185:CYS:HA	4:D:4:SER:N	1.94	0.81
2:B:1148:LYS:N	2:B:1197:PRO:N	2.20	0.81
2:B:1192:TYR:CA	7:G:67:SER:CB	2.58	0.81
2:B:312:GLU:H	9:I:46:HIS:HA	1.45	0.81
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.80
1:A:766:GLY:O	1:A:818:MET:N	2.13	0.80
6:F:73:ALA:N	7:G:70:PHE:CA	2.45	0.80
1:A:71:GLN:CB	1:A:408:ASP:CB	2.59	0.80
6:F:78:GLN:CB	7:G:23:LYS:CB	2.60	0.80
1:A:800:VAL:HA	1:A:814:PHE:O	1.81	0.80
6:F:146:TRP:CB	7:G:18:PHE:O	2.29	0.80
1:A:847:ASP:O	2:B:1141:HIS:C	2.20	0.80
2:B:1223:ASP:O	5:E:170:LEU:CB	2.29	0.80
6:F:142:SER:N	7:G:69:GLU:O	2.14	0.79
1:A:341:MET:C	2:B:1135:ARG:CB	2.51	0.79
1:A:1432:GLN:N	2:B:1143:ALA:O	2.05	0.79
2:B:1146:PHE:N	2:B:1195:HIS:C	2.35	0.79
1:A:766:GLY:O	1:A:817:ALA:N	2.16	0.78
2:B:1145:SER:CA	2:B:1195:HIS:O	2.30	0.78
1:A:452:LYS:CB	1:A:1066:VAL:H	1.94	0.78
1:A:810:PRO:CB	2:B:730:ARG:C	2.52	0.78
1:A:767:GLN:O	1:A:819:GLY:HA2	1.83	0.78
1:A:847:ASP:HA	2:B:1142:GLY:N	1.88	0.78
1:A:800:VAL:N	1:A:815:PHE:C	2.37	0.77
1:A:10:PRO:N	7:G:67:SER:CA	2.37	0.77
2:B:1219:ASP:HA	6:F:139:PRO:N	1.99	0.77
1:A:453:MET:CA	1:A:1066:VAL:CB	2.63	0.77
1:A:520:CYS:CB	1:A:1071:SER:N	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:H	1:A:877:HIS:H	1.31	0.77
1:A:626:ASN:H	1:A:1362:TYR:C	1.87	0.77
1:A:588:LEU:O	1:A:606:LEU:HA	1.85	0.77
2:B:401:PHE:O	2:B:517:THR:CB	2.33	0.76
1:A:630:ILE:C	1:A:876:ALA:HA	2.01	0.76
4:D:130:LEU:C	4:D:132:GLN:H	1.86	0.76
6:F:72:LYS:C	7:G:11:ILE:O	2.21	0.76
1:A:1430:LEU:C	2:B:1147:LEU:N	2.37	0.76
2:B:1148:LYS:HA	2:B:1200:ALA:N	2.00	0.76
2:B:1149:GLU:CB	2:B:1158:PHE:H	1.95	0.76
1:A:16:GLU:O	1:A:1441:PHE:N	2.11	0.76
1:A:633:VAL:C	1:A:877:HIS:CA	2.46	0.76
2:B:392:ARG:CA	9:I:90:GLN:CB	2.64	0.76
1:A:516:SER:N	1:A:1367:HIS:O	2.19	0.75
2:B:1159:ARG:CB	7:G:64:THR:CB	2.64	0.75
1:A:634:THR:C	1:A:877:HIS:H	1.87	0.75
1:A:1393:ASN:HA	1:A:1396:ALA:O	1.86	0.75
1:A:846:GLU:N	2:B:1140:ALA:HB2	2.01	0.75
2:B:1219:ASP:CA	6:F:138:LEU:CB	2.65	0.75
1:A:810:PRO:CA	2:B:729:ILE:O	2.33	0.75
2:B:1194:ILE:O	7:G:64:THR:CA	2.35	0.74
1:A:634:THR:C	1:A:874:ASP:CB	2.56	0.74
1:A:1449:SER:HA	7:G:28:THR:N	2.00	0.74
2:B:392:ARG:CB	9:I:90:GLN:CB	2.65	0.74
6:F:73:ALA:N	7:G:11:ILE:O	2.20	0.74
1:A:235:ILE:C	4:D:16:LYS:N	2.39	0.74
1:A:10:PRO:CB	7:G:66:GLY:O	2.36	0.74
1:A:1444:MET:CB	2:B:1165:ILE:CA	2.66	0.74
2:B:1193:GLN:CB	7:G:65:ASP:O	2.36	0.74
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.74
1:A:2:VAL:O	1:A:494:SER:C	2.17	0.73
2:B:411:PRO:O	2:B:414:ALA:HB3	1.88	0.73
1:A:386:ASP:C	6:F:104:ASN:CB	2.56	0.73
1:A:626:ASN:HA	1:A:1364:ASN:N	2.04	0.73
2:B:1219:ASP:CB	7:G:59:GLY:CA	2.66	0.73
6:F:75:PRO:HA	7:G:26:LEU:N	2.03	0.73
1:A:800:VAL:N	1:A:817:ALA:N	2.14	0.73
1:A:55:ASP:C	1:A:57:ARG:N	2.41	0.73
1:A:504:LEU:O	1:A:1063:MET:CB	2.36	0.73
1:A:1104:PRO:O	1:A:1105:SER:O	2.06	0.73
6:F:111:LEU:C	6:F:113:GLY:H	1.90	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:CA	7:G:64:THR:CB	2.67	0.73
1:A:450:LEU:CA	1:A:843:LYS:H	2.01	0.72
8:H:36:CYS:HA	8:H:126:GLU:O	1.89	0.72
2:B:642:ASP:O	2:B:644:GLU:N	2.22	0.72
1:A:386:ASP:CB	6:F:104:ASN:CB	2.67	0.72
4:D:130:LEU:O	4:D:132:GLN:N	2.22	0.72
2:B:1148:LYS:N	2:B:1200:ALA:CB	2.52	0.72
2:B:1224:PHE:CB	5:E:175:LEU:HA	2.19	0.72
1:A:862:ASN:CB	1:A:1420:ASP:CB	2.68	0.72
1:A:1427:ASN:N	2:B:1139:ILE:HA	1.64	0.72
2:B:1149:GLU:CB	2:B:1157:ALA:CA	2.68	0.72
2:B:1219:ASP:CB	7:G:59:GLY:N	2.52	0.72
6:F:73:ALA:N	7:G:70:PHE:CB	2.52	0.72
2:B:1192:TYR:HA	7:G:67:SER:C	2.10	0.72
1:A:452:LYS:C	1:A:1066:VAL:CB	2.58	0.71
1:A:608:ILE:CB	1:A:962:ARG:CB	2.67	0.71
1:A:89:PRO:CA	4:D:16:LYS:CB	2.69	0.71
2:B:1219:ASP:CA	6:F:138:LEU:C	2.54	0.71
2:B:1185:CYS:O	4:D:4:SER:N	2.23	0.71
1:A:1431:GLY:N	2:B:1147:LEU:N	2.34	0.70
1:A:513:SER:HA	1:A:1067:LEU:CB	2.19	0.70
1:A:862:ASN:O	1:A:1422:ARG:CB	2.38	0.70
4:D:5:THR:O	4:D:6:SER:O	2.07	0.70
1:A:302:THR:HA	1:A:305:ASP:O	1.91	0.70
1:A:509:LEU:CA	1:A:1062:GLU:HA	2.12	0.70
1:A:846:GLU:CB	2:B:1140:ALA:HB2	2.16	0.70
2:B:211:VAL:O	2:B:480:SER:HA	1.91	0.70
2:B:708:GLU:O	2:B:710:LEU:N	2.25	0.70
1:A:1445:ILE:N	2:B:1190:ASP:O	2.18	0.70
1:A:847:ASP:CA	2:B:1142:GLY:N	2.51	0.70
2:B:1222:ARG:CB	5:E:171:LYS:C	2.60	0.70
1:A:1430:LEU:O	2:B:1147:LEU:N	2.23	0.70
1:A:10:PRO:CB	7:G:15:PRO:N	2.55	0.70
2:B:1194:ILE:O	7:G:64:THR:N	2.03	0.70
1:A:9:ALA:HB3	7:G:65:ASP:CB	2.22	0.69
1:A:766:GLY:O	1:A:817:ALA:O	2.10	0.69
1:A:860:LEU:O	1:A:1419:ASP:O	2.10	0.69
1:A:92:HIS:O	1:A:94:GLY:N	2.24	0.69
1:A:766:GLY:N	1:A:820:GLY:H	1.89	0.69
2:B:1099:VAL:O	2:B:1101:ASP:N	2.24	0.69
6:F:133:VAL:C	7:G:15:PRO:CB	2.60	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:THR:HA	8:H:60:ALA:CB	2.23	0.69
1:A:800:VAL:H	1:A:817:ALA:N	1.89	0.69
2:B:393:LYS:HA	9:I:90:GLN:O	1.76	0.69
1:A:348:SER:CB	2:B:1154:ALA:O	2.39	0.69
1:A:862:ASN:N	1:A:1420:ASP:CA	2.55	0.69
1:A:233:TRP:O	4:D:13:ARG:O	1.93	0.69
1:A:635:ARG:O	1:A:1056:SER:CB	2.41	0.69
2:B:1148:LYS:HA	2:B:1200:ALA:H	1.57	0.69
1:A:626:ASN:N	1:A:1362:TYR:O	2.26	0.69
1:A:1430:LEU:O	2:B:1146:PHE:N	2.25	0.69
2:B:1192:TYR:CB	7:G:62:LEU:H	2.06	0.69
2:B:1193:GLN:O	7:G:62:LEU:C	2.31	0.69
1:A:514:PRO:CA	1:A:1367:HIS:HA	2.22	0.68
1:A:19:PHE:O	1:A:1416:ALA:HA	1.93	0.68
1:A:491:VAL:C	2:B:1153:GLU:HA	2.14	0.68
1:A:513:SER:O	1:A:1367:HIS:CA	2.41	0.68
1:A:860:LEU:O	1:A:1440:ALA:HB2	1.93	0.68
1:A:1448:GLU:HA	7:G:32:GLU:N	2.07	0.68
3:C:263:THR:C	3:C:265:MET:H	1.97	0.68
1:A:451:HIS:N	1:A:843:LYS:N	2.41	0.67
1:A:800:VAL:H	1:A:818:MET:N	1.92	0.67
2:B:1192:TYR:HA	7:G:67:SER:CA	2.25	0.67
1:A:630:ILE:O	1:A:876:ALA:C	2.31	0.67
2:B:1184:GLY:O	4:D:4:SER:CB	2.42	0.67
1:A:1431:GLY:O	2:B:1146:PHE:CB	2.43	0.67
1:A:68:GLN:C	1:A:70:CYS:H	1.96	0.67
1:A:633:VAL:O	1:A:877:HIS:CB	2.43	0.67
1:A:399:HIS:O	1:A:401:GLY:N	2.28	0.66
1:A:75:ASN:O	1:A:76:GLU:CB	2.43	0.66
1:A:518:LYS:HA	1:A:1364:ASN:CB	2.25	0.66
1:A:635:ARG:H	1:A:876:ALA:N	1.93	0.66
2:B:1191:ILE:C	7:G:67:SER:CB	2.63	0.66
2:B:1223:ASP:CB	5:E:164:LEU:O	2.44	0.66
4:D:176:GLU:C	4:D:178:ALA:H	1.98	0.66
1:A:69:THR:O	1:A:71:GLN:N	2.29	0.66
1:A:1431:GLY:H	2:B:1147:LEU:CB	2.08	0.66
6:F:73:ALA:HB3	7:G:11:ILE:CB	2.27	0.65
1:A:1391:ARG:O	1:A:1399:ARG:HA	1.96	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.65
4:D:176:GLU:O	4:D:178:ALA:N	2.26	0.65
1:A:69:THR:C	1:A:71:GLN:H	1.98	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ASN:N	1:A:1420:ASP:C	2.45	0.65
2:B:1045:SER:O	2:B:1046:PRO:O	2.14	0.65
6:F:135:ARG:CA	7:G:15:PRO:CB	2.75	0.65
1:A:1424:VAL:O	2:B:1140:ALA:N	2.23	0.65
1:A:1393:ASN:O	1:A:1397:LEU:N	2.21	0.64
1:A:862:ASN:H	1:A:1420:ASP:C	2.01	0.64
2:B:357:GLN:O	2:B:366:GLN:HA	1.97	0.64
1:A:344:ARG:C	2:B:1129:ARG:C	2.56	0.64
1:A:346:ASP:O	2:B:1155:SER:O	2.16	0.64
2:B:1195:HIS:N	7:G:63:PRO:CB	2.54	0.64
2:B:642:ASP:HA	2:B:649:LYS:HA	1.77	0.64
6:F:135:ARG:CB	7:G:66:GLY:C	2.28	0.64
1:A:861:GLY:C	1:A:1420:ASP:CB	2.62	0.64
1:A:50:ILE:O	1:A:52:GLY:N	2.28	0.64
1:A:340:LEU:O	2:B:1135:ARG:CB	2.45	0.64
1:A:1430:LEU:O	2:B:1145:SER:C	2.36	0.64
1:A:1431:GLY:HA3	2:B:1146:PHE:CB	2.28	0.64
3:C:168:ALA:O	3:C:170:TRP:N	2.30	0.64
1:A:514:PRO:CA	1:A:1370:LEU:CB	2.76	0.63
1:A:766:GLY:O	1:A:817:ALA:CA	2.47	0.63
2:B:1145:SER:C	2:B:1195:HIS:O	2.28	0.63
2:B:847:ASP:C	2:B:849:GLY:H	1.99	0.63
6:F:77:ASP:H	7:G:23:LYS:CA	2.12	0.63
9:I:3:THR:O	9:I:42:LEU:C	2.37	0.63
1:A:858:ASN:H	1:A:1422:ARG:CA	2.05	0.63
8:H:89:LEU:C	8:H:91:ASP:H	2.02	0.63
2:B:1184:GLY:O	4:D:4:SER:N	2.32	0.63
1:A:4:GLN:O	1:A:5:GLN:O	2.17	0.63
2:B:121:ASN:HA	2:B:207:GLY:CA	2.29	0.63
3:C:99:LEU:HA	3:C:119:VAL:O	1.98	0.63
1:A:227:VAL:O	4:D:10:THR:HA	1.96	0.63
1:A:383:TYR:O	6:F:105:ALA:HB2	1.98	0.62
4:D:191:ALA:O	4:D:193:THR:N	2.32	0.62
1:A:1007:ILE:C	1:A:1009:ASN:H	2.02	0.62
2:B:205:ILE:O	2:B:207:GLY:N	2.32	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.81	0.62
2:B:1192:TYR:CA	7:G:62:LEU:CB	2.77	0.62
2:B:1222:ARG:CB	5:E:171:LYS:H	1.27	0.62
1:A:235:ILE:O	4:D:15:LEU:C	2.26	0.62
1:A:722:LEU:O	1:A:725:ALA:HB3	1.99	0.62
6:F:142:SER:CB	7:G:70:PHE:HA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:862:ASN:HA	1:A:1420:ASP:CB	2.27	0.62
4:D:198:LEU:O	4:D:200:ASN:N	2.33	0.62
1:A:10:PRO:N	7:G:67:SER:HA	2.13	0.62
1:A:778:GLY:C	2:B:402:GLY:H	2.03	0.62
1:A:1452:LYS:N	7:G:28:THR:CB	2.61	0.61
1:A:1393:ASN:CA	1:A:1399:ARG:H	2.06	0.61
1:A:453:MET:H	1:A:1066:VAL:CA	2.13	0.61
1:A:1450:LEU:CB	2:B:1189:ILE:CB	2.77	0.61
1:A:384:ASN:O	1:A:386:ASP:N	2.34	0.61
1:A:520:CYS:CB	1:A:1071:SER:H	2.11	0.61
2:B:745:PRO:O	2:B:747:MET:N	2.33	0.61
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.29	0.61
2:B:1148:LYS:N	2:B:1200:ALA:HB3	2.02	0.61
1:A:492:PRO:N	2:B:1153:GLU:HA	2.15	0.61
6:F:143:PHE:CB	7:G:68:ALA:HB3	1.09	0.60
9:I:2:THR:O	9:I:3:THR:C	2.39	0.60
1:A:1444:MET:CA	2:B:1165:ILE:N	2.60	0.60
6:F:73:ALA:HB2	7:G:11:ILE:O	2.01	0.60
2:B:1190:ASP:CB	6:F:73:ALA:HB2	2.31	0.60
3:C:208:GLU:O	3:C:210:GLU:N	2.34	0.60
1:A:1431:GLY:N	2:B:1147:LEU:CA	2.64	0.60
1:A:341:MET:O	2:B:1132:GLU:N	2.34	0.60
1:A:626:ASN:N	1:A:1362:TYR:C	2.54	0.60
1:A:520:CYS:HA	1:A:1071:SER:HA	1.84	0.60
1:A:1065:GLY:CA	1:A:1435:PRO:C	2.70	0.60
8:H:91:ASP:C	8:H:93:TYR:H	2.06	0.60
1:A:237:THR:CB	4:D:16:LYS:HA	2.31	0.60
1:A:1430:LEU:C	2:B:1143:ALA:C	2.60	0.59
2:B:1148:LYS:CB	2:B:1201:LYS:N	2.64	0.59
1:A:862:ASN:CA	1:A:1422:ARG:CB	2.80	0.59
2:B:265:SER:O	2:B:266:ALA:HB3	2.02	0.59
2:B:1180:PHE:O	2:B:1181:GLU:O	2.20	0.59
3:C:254:LYS:O	3:C:256:ALA:N	2.35	0.59
1:A:1017:LEU:CB	5:E:205:SER:HA	2.33	0.59
1:A:492:PRO:CA	2:B:1157:ALA:HB1	2.29	0.59
4:D:156:ASP:C	4:D:158:GLU:H	2.03	0.59
5:E:157:SER:C	5:E:159:ASP:H	2.03	0.59
1:A:1313:LEU:O	1:A:1315:GLU:N	2.35	0.59
6:F:72:LYS:N	7:G:69:GLU:HA	2.17	0.59
2:B:446:LEU:O	2:B:447:ALA:HB3	2.02	0.59
2:B:189:LEU:O	2:B:192:LEU:N	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:O	1:A:385:ILE:C	2.41	0.59
2:B:1099:VAL:C	2:B:1101:ASP:H	2.07	0.59
1:A:637:LYS:C	1:A:1055:ARG:O	2.41	0.58
1:A:69:THR:C	1:A:71:GLN:N	2.55	0.58
1:A:262:LEU:O	1:A:264:PHE:N	2.37	0.58
1:A:698:GLN:HA	9:I:97:MET:O	2.04	0.58
4:D:130:LEU:C	4:D:132:GLN:N	2.54	0.58
2:B:1219:ASP:HA	6:F:138:LEU:CA	2.33	0.58
1:A:665:GLY:O	1:A:667:GLY:N	2.36	0.58
1:A:135:PHE:C	1:A:137:ALA:H	2.06	0.58
1:A:801:GLU:HA	1:A:816:HIS:CB	2.33	0.58
1:A:515:GLN:CB	1:A:1068:ALA:C	2.71	0.58
10:J:23:ASN:C	10:J:25:LEU:H	2.05	0.58
1:A:35:ILE:HA	1:A:52:GLY:O	2.04	0.58
2:B:283:VAL:O	2:B:286:PHE:N	2.37	0.58
2:B:1193:GLN:C	7:G:65:ASP:O	2.41	0.58
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.85	0.58
1:A:848:ILE:O	1:A:1434:ALA:O	2.22	0.57
1:A:513:SER:CA	1:A:1067:LEU:CB	2.81	0.57
3:C:31:ASN:O	3:C:32:SER:C	2.42	0.57
1:A:800:VAL:N	1:A:818:MET:H	2.02	0.57
9:I:14:LEU:HA	9:I:28:GLU:O	2.04	0.57
1:A:61:ILE:O	1:A:63:ARG:N	2.38	0.57
1:A:289:ILE:C	1:A:291:GLU:H	2.07	0.57
6:F:72:LYS:O	7:G:11:ILE:N	2.33	0.57
6:F:135:ARG:HA	7:G:15:PRO:HA	1.86	0.57
2:B:224:GLN:O	2:B:238:ALA:HA	2.04	0.57
2:B:1192:TYR:CB	7:G:62:LEU:N	2.66	0.57
1:A:15:LYS:N	1:A:1440:ALA:N	2.47	0.57
1:A:496:GLU:O	7:G:63:PRO:O	2.22	0.57
2:B:957:ASN:O	2:B:959:ASP:N	2.37	0.57
2:B:1159:ARG:C	7:G:64:THR:CB	2.73	0.57
10:J:1:MET:H2	10:J:56:LEU:N	2.02	0.57
1:A:859:SER:N	1:A:1421:CYS:C	2.55	0.57
2:B:1192:TYR:CA	7:G:67:SER:O	2.52	0.57
1:A:50:ILE:C	1:A:52:GLY:H	2.06	0.57
2:B:745:PRO:C	2:B:747:MET:H	2.09	0.57
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.57
1:A:14:VAL:CB	2:B:1144:ALA:CB	2.83	0.56
1:A:1393:ASN:CA	1:A:1399:ARG:N	2.65	0.56
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:TYR:O	1:A:1037:LEU:N	2.37	0.56
1:A:1396:ALA:O	1:A:1398:MET:N	2.38	0.56
2:B:1146:PHE:O	2:B:1197:PRO:CB	2.54	0.56
6:F:111:LEU:C	6:F:113:GLY:N	2.55	0.56
9:I:3:THR:HA	9:I:45:ARG:N	2.21	0.56
1:A:513:SER:O	1:A:1367:HIS:HA	2.04	0.56
1:A:1445:ILE:CB	2:B:1189:ILE:N	2.68	0.56
1:A:321:PRO:O	1:A:322:VAL:CB	2.53	0.56
1:A:634:THR:C	1:A:877:HIS:N	2.58	0.56
4:D:68:ARG:C	4:D:70:PHE:H	2.09	0.56
1:A:387:ARG:N	6:F:104:ASN:CA	2.66	0.56
2:B:401:PHE:O	2:B:517:THR:N	2.34	0.56
2:B:1217:TYR:C	6:F:140:ASP:C	2.53	0.56
9:I:74:GLU:HA	9:I:80:SER:O	2.06	0.56
12:L:36:SER:O	12:L:37:LYS:C	2.44	0.56
1:A:774:ARG:O	1:A:775:ILE:C	2.43	0.56
2:B:393:LYS:CA	9:I:90:GLN:O	2.40	0.56
1:A:514:PRO:O	1:A:1370:LEU:CB	2.53	0.56
6:F:143:PHE:CB	7:G:68:ALA:C	2.70	0.56
2:B:114:PRO:O	2:B:116:GLU:N	2.38	0.56
2:B:1148:LYS:CA	2:B:1200:ALA:H	2.18	0.56
2:B:1148:LYS:O	2:B:1200:ALA:N	2.39	0.56
1:A:502:SER:O	6:F:88:TYR:CB	2.54	0.55
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.89	0.55
3:C:174:ALA:O	3:C:175:ALA:HB2	2.05	0.55
1:A:630:ILE:O	1:A:876:ALA:O	2.24	0.55
2:B:392:ARG:C	9:I:90:GLN:CB	2.51	0.55
1:A:450:LEU:O	1:A:843:LYS:N	2.40	0.55
1:A:847:ASP:CA	2:B:1142:GLY:H	2.18	0.55
2:B:1148:LYS:CA	2:B:1200:ALA:CA	2.69	0.55
6:F:72:LYS:C	7:G:11:ILE:H	2.10	0.55
1:A:625:SER:CA	1:A:1362:TYR:O	2.50	0.55
1:A:637:LYS:HA	1:A:1055:ARG:CB	2.37	0.55
1:A:730:GLY:O	1:A:732:LEU:N	2.40	0.55
1:A:1431:GLY:HA3	2:B:1146:PHE:CA	2.37	0.55
2:B:1034:VAL:C	2:B:1036:ALA:H	2.10	0.55
1:A:520:CYS:CB	1:A:1071:SER:CA	2.85	0.55
2:B:129:PHE:HA	2:B:165:VAL:O	2.06	0.55
4:D:51:ASN:O	4:D:52:LEU:O	2.25	0.55
6:F:134:ILE:CA	7:G:15:PRO:CB	2.85	0.55
6:F:143:PHE:C	7:G:68:ALA:CB	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CB	2:B:1217:TYR:C	2.75	0.55
6:F:77:ASP:C	6:F:79:ARG:H	2.10	0.55
1:A:16:GLU:N	6:F:139:PRO:O	2.40	0.55
5:E:35:VAL:C	5:E:37:LEU:H	2.10	0.55
1:A:452:LYS:H	1:A:1066:VAL:HA	1.71	0.54
1:A:800:VAL:N	1:A:818:MET:N	2.55	0.54
5:E:157:SER:C	5:E:159:ASP:N	2.60	0.54
1:A:1377:THR:O	1:A:1379:GLY:N	2.41	0.54
2:B:1192:TYR:HA	7:G:67:SER:O	2.06	0.54
6:F:75:PRO:CA	7:G:26:LEU:CB	2.85	0.54
1:A:1393:ASN:CA	1:A:1396:ALA:O	2.54	0.54
1:A:1437:GLY:O	1:A:1439:GLY:N	2.23	0.54
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.54
2:B:1147:LEU:N	2:B:1197:PRO:N	2.56	0.54
4:D:156:ASP:C	4:D:158:GLU:N	2.60	0.54
6:F:73:ALA:CB	7:G:11:ILE:CB	2.86	0.54
6:F:143:PHE:CB	7:G:68:ALA:HA	2.17	0.54
1:A:71:GLN:C	1:A:73:GLY:H	2.09	0.54
10:J:44:TYR:HA	10:J:47:ARG:CB	2.37	0.54
1:A:518:LYS:CB	1:A:1363:VAL:C	2.73	0.54
1:A:847:ASP:O	2:B:1142:GLY:N	2.41	0.54
1:A:1428:VAL:CB	2:B:1139:ILE:CB	2.86	0.54
2:B:847:ASP:C	2:B:849:GLY:N	2.61	0.54
2:B:1146:PHE:CA	2:B:1196:ILE:CA	2.61	0.54
2:B:1159:ARG:HA	7:G:64:THR:CB	2.38	0.54
1:A:92:HIS:O	1:A:95:PHE:N	2.34	0.54
3:C:263:THR:C	3:C:265:MET:N	2.61	0.54
4:D:191:ALA:C	4:D:193:THR:H	2.12	0.54
2:B:1068:GLY:O	2:B:1069:PHE:O	2.27	0.53
4:D:24:ALA:HA	7:G:83:LYS:O	2.08	0.53
6:F:142:SER:O	7:G:60:ARG:C	2.45	0.53
1:A:9:ALA:O	7:G:66:GLY:N	2.39	0.53
1:A:262:LEU:C	1:A:264:PHE:H	2.11	0.53
1:A:809:THR:CA	2:B:729:ILE:CB	2.86	0.53
2:B:1220:ARG:HA	6:F:140:ASP:CB	2.37	0.53
1:A:98:LYS:O	1:A:99:ILE:C	2.45	0.53
2:B:363:HIS:O	2:B:364:ILE:CB	2.56	0.53
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.53
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.56	0.53
1:A:453:MET:CB	1:A:1066:VAL:CB	2.86	0.53
1:A:517:ASN:O	1:A:1365:TYR:C	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.90	0.53
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.53
1:A:47:ARG:O	1:A:48:ALA:HB2	2.08	0.53
2:B:312:GLU:H	9:I:46:HIS:CA	2.17	0.53
2:B:1148:LYS:CA	2:B:1200:ALA:HB2	1.96	0.53
1:A:244:PRO:O	1:A:247:ARG:N	2.41	0.53
1:A:311:GLN:O	1:A:312:PRO:C	2.47	0.53
2:B:872:GLU:HA	2:B:915:THR:O	2.08	0.53
1:A:17:VAL:CA	1:A:1439:GLY:O	2.56	0.53
2:B:281:PRO:O	2:B:283:VAL:N	2.41	0.53
2:B:1194:ILE:O	7:G:64:THR:CB	2.57	0.53
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.53
1:A:1007:ILE:O	1:A:1009:ASN:N	2.41	0.53
1:A:341:MET:C	2:B:1132:GLU:CA	2.57	0.53
1:A:207:ILE:O	1:A:208:LEU:C	2.48	0.52
1:A:438:ASP:O	1:A:439:ASN:CB	2.57	0.52
1:A:618:GLU:O	1:A:620:LYS:N	2.42	0.52
1:A:635:ARG:H	1:A:875:ALA:C	2.11	0.52
8:H:113:ALA:HB1	8:H:125:LEU:O	2.09	0.52
1:A:77:CYS:O	1:A:78:PRO:C	2.40	0.52
1:A:765:VAL:O	1:A:820:GLY:CA	2.57	0.52
1:A:848:ILE:O	1:A:1434:ALA:C	2.46	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
1:A:817:ALA:O	1:A:819:GLY:N	2.41	0.52
2:B:1102:LYS:O	2:B:1103:ILE:C	2.47	0.52
2:B:1160:VAL:N	7:G:64:THR:CB	2.73	0.52
2:B:1193:GLN:O	7:G:63:PRO:N	2.36	0.52
6:F:135:ARG:CA	7:G:15:PRO:HA	2.39	0.52
6:F:143:PHE:C	7:G:68:ALA:HB3	2.30	0.52
1:A:299:HIS:C	1:A:301:ALA:H	2.11	0.52
1:A:1323:ASP:C	1:A:1325:THR:H	2.12	0.52
2:B:1186:ASP:N	4:D:4:SER:N	2.54	0.52
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.52
1:A:545:GLN:O	1:A:546:VAL:C	2.46	0.52
1:A:589:GLN:O	1:A:880:LYS:CB	2.58	0.52
1:A:766:GLY:C	1:A:820:GLY:H	2.12	0.52
2:B:492:LEU:O	2:B:495:LEU:N	2.40	0.52
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.52
1:A:356:ASP:O	1:A:358:ASN:N	2.42	0.52
1:A:509:LEU:CB	1:A:1063:MET:H	2.23	0.52
1:A:1164:PRO:O	1:A:1166:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:ASN:N	2:B:1139:ILE:CB	2.72	0.52
2:B:311:LEU:O	2:B:312:GLU:C	2.48	0.52
3:C:76:ASP:O	3:C:77:ILE:C	2.48	0.52
6:F:146:TRP:HA	7:G:19:GLY:N	2.08	0.52
7:G:117:GLN:O	7:G:119:LEU:N	2.43	0.52
10:J:27:GLU:C	10:J:29:GLU:H	2.13	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
1:A:1007:ILE:C	1:A:1009:ASN:N	2.62	0.52
2:B:1220:ARG:CA	6:F:140:ASP:CB	2.87	0.52
1:A:386:ASP:CB	6:F:104:ASN:C	2.76	0.52
1:A:840:ARG:O	1:A:841:LEU:C	2.47	0.52
1:A:452:LYS:HA	1:A:846:GLU:CB	2.40	0.51
1:A:845:LEU:O	1:A:846:GLU:C	2.49	0.51
3:C:27:LEU:O	3:C:28:ALA:C	2.47	0.51
4:D:176:GLU:C	4:D:178:ALA:N	2.63	0.51
1:A:367:PRO:HA	1:A:463:ILE:O	2.10	0.51
1:A:514:PRO:O	1:A:1371:LEU:N	2.39	0.51
1:A:800:VAL:CA	1:A:814:PHE:O	1.68	0.51
1:A:1393:ASN:O	1:A:1396:ALA:C	2.48	0.51
3:C:263:THR:O	3:C:265:MET:N	2.43	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.64	0.51
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.51
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.51
3:C:39:ALA:HA	3:C:164:ALA:CB	2.31	0.51
1:A:2:VAL:HA	1:A:492:PRO:O	2.10	0.51
1:A:236:LEU:O	4:D:16:LYS:CA	2.56	0.51
1:A:482:PHE:C	1:A:484:GLY:H	2.13	0.51
1:A:63:ARG:CA	1:A:411:ASP:CA	2.76	0.51
2:B:377:PHE:C	2:B:379:GLY:N	2.62	0.51
2:B:765:PRO:O	2:B:768:THR:N	2.44	0.51
3:C:239:PRO:O	3:C:241:ASP:N	2.43	0.51
10:J:23:ASN:C	10:J:25:LEU:N	2.64	0.51
1:A:418:SER:O	1:A:420:ARG:N	2.43	0.51
1:A:516:SER:H	1:A:1367:HIS:CA	2.24	0.51
1:A:817:ALA:O	1:A:818:MET:C	2.48	0.51
2:B:394:ASP:HA	9:I:92:ARG:C	2.30	0.51
8:H:27:GLU:HA	8:H:38:LEU:O	2.11	0.51
1:A:496:GLU:O	2:B:1195:HIS:CB	2.52	0.51
1:A:82:GLY:O	1:A:241:VAL:N	2.42	0.51
2:B:1107:ALA:O	2:B:1108:ARG:O	2.28	0.51
2:B:1149:GLU:CB	2:B:1157:ALA:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1193:GLN:C	7:G:62:LEU:CB	2.80	0.51
2:B:1222:ARG:CB	5:E:171:LYS:N	0.66	0.51
1:A:450:LEU:HA	1:A:843:LYS:H	1.75	0.50
1:A:829:VAL:C	1:A:831:THR:H	2.14	0.50
1:A:1017:LEU:CB	5:E:206:GLY:H	2.23	0.50
1:A:1157:ASP:C	1:A:1159:ARG:H	2.14	0.50
1:A:1334:ASP:O	1:A:1336:MET:N	2.43	0.50
1:A:1442:ASP:HA	2:B:1216:LEU:C	2.29	0.50
2:B:642:ASP:CB	2:B:649:LYS:HA	2.41	0.50
2:B:773:MET:C	2:B:775:LYS:H	2.13	0.50
10:J:32:GLU:O	10:J:34:THR:N	2.45	0.50
1:A:365:GLY:O	1:A:468:PHE:HA	2.10	0.50
3:C:215:GLU:O	3:C:216:GLY:C	2.50	0.50
1:A:58:LEU:O	1:A:59:GLY:O	2.30	0.50
1:A:317:LYS:O	1:A:318:SER:CB	2.60	0.50
1:A:845:LEU:O	2:B:1140:ALA:HB1	2.08	0.50
2:B:552:MET:C	2:B:554:ILE:H	2.15	0.50
2:B:1148:LYS:CA	2:B:1197:PRO:N	2.72	0.50
5:E:128:PRO:HA	5:E:129:PRO:C	2.32	0.50
1:A:823:GLY:O	1:A:825:ILE:N	2.44	0.50
2:B:1221:SER:O	5:E:165:LEU:O	2.30	0.50
3:C:140:ASN:O	3:C:141:GLY:O	2.30	0.50
1:A:626:ASN:O	1:A:628:GLY:N	2.44	0.50
1:A:802:ASN:H	1:A:813:PHE:CB	2.24	0.50
1:A:861:GLY:C	1:A:1420:ASP:CA	2.74	0.50
3:C:213:PRO:O	3:C:214:ASN:CB	2.60	0.50
1:A:1445:ILE:N	7:G:10:ASN:O	2.44	0.50
3:C:163:ILE:O	3:C:165:LYS:N	2.45	0.50
8:H:84:ALA:C	8:H:86:ASP:H	2.15	0.50
1:A:802:ASN:N	1:A:813:PHE:CB	2.70	0.50
2:B:642:ASP:CA	2:B:649:LYS:HA	2.42	0.50
6:F:146:TRP:HA	7:G:18:PHE:O	1.93	0.50
10:J:27:GLU:O	10:J:29:GLU:N	2.45	0.50
1:A:316:GLN:O	1:A:317:LYS:C	2.50	0.50
1:A:442:VAL:O	1:A:457:ALA:HA	2.12	0.50
2:B:773:MET:C	2:B:775:LYS:N	2.65	0.50
1:A:12:ARG:C	7:G:61:ILE:O	2.50	0.49
1:A:23:SER:O	1:A:24:PRO:C	2.48	0.49
2:B:1174:LYS:O	2:B:1176:ASN:N	2.44	0.49
3:C:168:ALA:C	3:C:170:TRP:H	2.16	0.49
3:C:254:LYS:C	3:C:256:ALA:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:O	1:A:70:CYS:N	2.43	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.49
1:A:738:LYS:C	1:A:740:LEU:H	2.15	0.49
1:A:909:ASP:O	1:A:911:SER:N	2.45	0.49
2:B:890:TYR:O	2:B:892:LYS:N	2.45	0.49
1:A:116:ASP:O	1:A:118:HIS:N	2.45	0.49
1:A:341:MET:O	2:B:1135:ARG:CB	2.60	0.49
1:A:635:ARG:N	1:A:876:ALA:N	2.59	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
3:C:142:VAL:H	10:J:16:ASP:CB	2.24	0.49
7:G:117:GLN:C	7:G:119:LEU:H	2.15	0.49
2:B:1148:LYS:N	2:B:1200:ALA:HB2	2.24	0.49
3:C:90:ASP:O	3:C:91:HIS:CB	2.60	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.43	0.49
1:A:509:LEU:CB	1:A:1063:MET:N	2.75	0.49
1:A:244:PRO:O	1:A:246:VAL:N	2.46	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
2:B:1040:ASN:O	2:B:1041:GLU:C	2.50	0.49
9:I:2:THR:O	9:I:44:TYR:N	2.44	0.49
3:C:77:ILE:O	3:C:79:GLN:N	2.46	0.49
4:D:64:VAL:C	4:D:66:ARG:H	2.14	0.49
1:A:332:LYS:O	1:A:334:GLY:N	2.46	0.49
1:A:1053:PHE:C	1:A:1055:ARG:H	2.15	0.49
1:A:1388:GLY:O	1:A:1390:ASN:N	2.46	0.49
2:B:558:LEU:C	2:B:560:GLU:H	2.16	0.49
1:A:452:LYS:CB	1:A:1066:VAL:HA	2.34	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.45	0.49
1:A:809:THR:HA	2:B:729:ILE:CB	2.43	0.49
2:B:1193:GLN:C	7:G:65:ASP:H	2.15	0.49
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.49
1:A:262:LEU:C	1:A:264:PHE:N	2.66	0.49
1:A:586:ILE:C	1:A:959:ASN:CB	2.80	0.49
3:C:107:SER:C	3:C:109:SER:H	2.17	0.49
6:F:77:ASP:HA	7:G:21:ARG:HA	1.95	0.49
12:L:49:LYS:O	12:L:50:ASP:CB	2.60	0.49
1:A:794:PRO:C	1:A:796:SER:H	2.15	0.48
1:A:1001:ARG:O	1:A:1002:GLY:O	2.31	0.48
1:A:1424:VAL:HA	2:B:1140:ALA:HA	1.94	0.48
2:B:954:VAL:O	12:L:55:ILE:O	2.31	0.48
6:F:72:LYS:O	7:G:11:ILE:CB	2.61	0.48
1:A:232:GLU:O	4:D:14:ARG:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ARG:O	1:A:421:ALA:C	2.51	0.48
1:A:1433:MET:N	2:B:1143:ALA:HB2	2.03	0.48
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.48
2:B:125:SER:HA	2:B:172:ILE:H	1.78	0.48
1:A:68:GLN:C	1:A:70:CYS:N	2.65	0.48
1:A:299:HIS:O	1:A:301:ALA:N	2.46	0.48
2:B:1193:GLN:CA	7:G:62:LEU:CB	2.90	0.48
6:F:76:LYS:O	7:G:20:PRO:O	2.30	0.48
8:H:82:PRO:O	8:H:84:ALA:N	2.35	0.48
1:A:387:ARG:CA	6:F:104:ASN:CB	2.88	0.48
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.48
5:E:55:ARG:C	5:E:57:MET:H	2.17	0.48
1:A:766:GLY:C	1:A:820:GLY:N	2.67	0.48
1:A:1431:GLY:CA	2:B:1147:LEU:CA	2.91	0.48
2:B:1034:VAL:O	2:B:1036:ALA:N	2.46	0.48
5:E:161:LYS:C	5:E:163:GLU:H	2.17	0.48
6:F:141:GLY:C	7:G:69:GLU:O	2.51	0.48
1:A:254:GLU:O	1:A:256:GLN:N	2.47	0.48
1:A:299:HIS:C	1:A:301:ALA:N	2.67	0.48
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.13	0.48
2:B:98:THR:O	2:B:126:SER:CB	2.62	0.48
2:B:847:ASP:O	2:B:849:GLY:N	2.47	0.48
2:B:1184:GLY:C	4:D:4:SER:N	2.67	0.48
12:L:52:GLY:O	12:L:53:HIS:C	2.52	0.48
1:A:277:GLU:C	1:A:279:LEU:H	2.17	0.48
2:B:205:ILE:O	2:B:206:ASN:C	2.52	0.48
4:D:20:GLU:O	4:D:21:GLU:O	2.32	0.48
8:H:84:ALA:C	8:H:86:ASP:N	2.67	0.48
1:A:960:ILE:O	1:A:961:ARG:C	2.50	0.48
1:A:1265:ASN:C	1:A:1267:MET:N	2.67	0.48
1:A:1451:VAL:C	1:A:1453:TYR:H	2.16	0.48
2:B:391:ASP:CB	9:I:94:ASP:CB	2.91	0.48
10:J:32:GLU:O	10:J:35:ALA:N	2.46	0.48
1:A:166:GLY:O	1:A:167:CYS:CB	2.62	0.48
1:A:237:THR:CB	4:D:16:LYS:CA	2.92	0.48
2:B:27:ALA:O	2:B:29:ASP:N	2.47	0.48
3:C:168:ALA:C	3:C:170:TRP:N	2.64	0.48
4:D:64:VAL:C	4:D:66:ARG:N	2.67	0.48
6:F:145:ASP:CB	7:G:14:HIS:O	2.62	0.48
8:H:138:GLU:O	8:H:139:ASN:C	2.52	0.48
6:F:73:ALA:CB	7:G:11:ILE:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:VAL:CA	1:A:814:PHE:CA	2.71	0.47
1:A:1445:ILE:CB	2:B:1189:ILE:H	2.26	0.47
2:B:1148:LYS:CB	2:B:1201:LYS:H	2.27	0.47
1:A:1369:ALA:O	1:A:1370:LEU:C	2.52	0.47
2:B:1148:LYS:CB	2:B:1200:ALA:CA	2.86	0.47
3:C:242:GLN:C	3:C:244:VAL:H	2.18	0.47
2:B:360:PHE:O	2:B:361:LEU:C	2.51	0.47
2:B:383:ASN:O	2:B:384:ARG:C	2.53	0.47
3:C:183:TRP:O	3:C:185:LYS:N	2.48	0.47
3:C:254:LYS:C	3:C:256:ALA:N	2.67	0.47
7:G:44:TYR:O	7:G:78:VAL:HA	2.14	0.47
8:H:4:THR:CA	8:H:60:ALA:HB2	2.34	0.47
1:A:730:GLY:C	1:A:732:LEU:H	2.18	0.47
1:A:766:GLY:C	1:A:817:ALA:O	2.52	0.47
10:J:16:ASP:O	10:J:18:TRP:N	2.47	0.47
1:A:921:GLY:O	1:A:922:ASP:C	2.53	0.47
6:F:135:ARG:CA	7:G:15:PRO:CA	2.92	0.47
8:H:91:ASP:O	8:H:93:TYR:N	2.46	0.47
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.95	0.47
9:I:61:ASP:O	9:I:63:GLY:N	2.48	0.47
1:A:42:ASP:O	1:A:44:THR:N	2.45	0.47
1:A:496:GLU:O	1:A:499:ALA:HB3	2.15	0.47
1:A:847:ASP:HA	2:B:1142:GLY:H	1.58	0.47
1:A:1340:GLY:O	1:A:1343:ALA:N	2.43	0.47
2:B:192:LEU:O	2:B:193:LYS:CB	2.62	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.47	0.47
2:B:1208:MET:O	2:B:1211:ASN:N	2.40	0.47
6:F:77:ASP:C	6:F:79:ARG:N	2.67	0.47
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.48	0.47
1:A:636:GLU:CB	1:A:877:HIS:O	2.62	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.68	0.47
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.47
2:B:1192:TYR:CB	7:G:62:LEU:CA	2.90	0.47
3:C:242:GLN:C	3:C:244:VAL:N	2.68	0.47
1:A:648:ASN:O	1:A:649:ILE:C	2.53	0.47
2:B:20:ASP:O	2:B:22:SER:N	2.45	0.47
2:B:225:VAL:HA	2:B:237:VAL:O	2.14	0.47
5:E:35:VAL:O	5:E:37:LEU:N	2.48	0.47
5:E:55:ARG:C	5:E:57:MET:N	2.69	0.47
1:A:279:LEU:O	1:A:284:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:THR:O	1:A:1378:GLN:C	2.54	0.47
2:B:455:SER:O	2:B:456:GLY:C	2.52	0.47
3:C:253:LYS:O	3:C:256:ALA:HB3	2.15	0.47
1:A:730:GLY:C	1:A:732:LEU:N	2.67	0.46
2:B:1146:PHE:O	2:B:1197:PRO:HA	2.12	0.46
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.46
6:F:135:ARG:N	7:G:15:PRO:CA	2.74	0.46
8:H:33:GLN:C	8:H:35:GLN:H	2.18	0.46
1:A:237:THR:CA	4:D:16:LYS:HA	2.45	0.46
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.46
10:J:23:ASN:O	10:J:25:LEU:N	2.49	0.46
1:A:8:SER:O	7:G:14:HIS:CB	2.63	0.46
1:A:298:PHE:O	1:A:301:ALA:HB3	2.15	0.46
1:A:402:ALA:HB1	1:A:433:GLU:O	2.15	0.46
1:A:1122:LYS:O	1:A:1124:ILE:N	2.49	0.46
2:B:1152:MET:O	2:B:1154:ALA:N	2.49	0.46
6:F:72:LYS:C	7:G:70:PHE:CB	2.82	0.46
8:H:82:PRO:C	8:H:84:ALA:H	2.17	0.46
1:A:335:ARG:O	1:A:336:ILE:C	2.52	0.46
1:A:95:PHE:O	1:A:96:ILE:C	2.53	0.46
1:A:452:LYS:CA	1:A:1066:VAL:CB	2.92	0.46
1:A:452:LYS:N	1:A:1066:VAL:HA	2.30	0.46
1:A:859:SER:CB	2:B:1139:ILE:O	2.62	0.46
2:B:1174:LYS:O	2:B:1175:LEU:C	2.53	0.46
3:C:47:ASP:CA	12:L:69:ALA:CB	2.87	0.46
9:I:56:ALA:O	9:I:57:GLY:O	2.34	0.46
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.46
2:B:681:TRP:O	2:B:683:SER:N	2.49	0.46
11:K:113:THR:O	11:K:114:LEU:CB	2.62	0.46
1:A:43:GLU:O	1:A:44:THR:CB	2.64	0.46
1:A:984:LYS:O	1:A:985:ASP:C	2.54	0.46
1:A:1428:VAL:O	2:B:1147:LEU:CB	2.64	0.46
4:D:19:GLU:O	4:D:21:GLU:N	2.49	0.46
1:A:577:ILE:C	1:A:579:SER:N	2.65	0.46
1:A:600:PRO:C	1:A:602:ASP:H	2.19	0.46
1:A:1019:CYS:O	1:A:1022:LEU:N	2.48	0.46
2:B:843:GLN:O	2:B:844:SER:C	2.54	0.46
2:B:873:THR:O	2:B:914:LYS:HA	2.16	0.46
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.98	0.46
5:E:129:PRO:O	5:E:130:ALA:O	2.34	0.46
8:H:62:SER:O	8:H:63:LEU:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:C	1:A:73:GLY:N	2.69	0.46
1:A:347:PHE:H	2:B:1107:ALA:HA	1.80	0.46
3:C:256:ALA:C	3:C:258:ILE:H	2.19	0.46
5:E:157:SER:O	5:E:159:ASP:N	2.48	0.46
6:F:138:LEU:N	7:G:59:GLY:O	2.49	0.46
7:G:13:LEU:O	7:G:67:SER:HA	2.15	0.46
1:A:26:GLU:O	1:A:27:VAL:C	2.54	0.45
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.46	0.45
1:A:1446:ASP:CB	7:G:11:ILE:CB	2.64	0.45
2:B:1148:LYS:CB	2:B:1200:ALA:HB1	2.29	0.45
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.45
4:D:206:GLU:C	4:D:208:GLU:N	2.68	0.45
6:F:111:LEU:O	6:F:113:GLY:N	2.48	0.45
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.45
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.45
1:A:17:VAL:HA	2:B:1215:ARG:O	2.15	0.45
1:A:250:ILE:O	1:A:258:GLY:HA3	2.16	0.45
1:A:289:ILE:O	1:A:291:GLU:N	2.50	0.45
2:B:123:THR:O	2:B:125:SER:N	2.47	0.45
2:B:168:GLY:N	2:B:450:ALA:HB1	2.19	0.45
2:B:838:SER:CB	2:B:989:THR:O	2.64	0.45
5:E:161:LYS:O	5:E:163:GLU:N	2.49	0.45
8:H:25:ARG:HA	8:H:41:ASP:HA	1.98	0.45
1:A:28:ARG:O	1:A:29:ALA:C	2.55	0.45
1:A:635:ARG:H	1:A:877:HIS:N	2.00	0.45
1:A:755:PHE:O	1:A:756:ILE:C	2.55	0.45
1:A:853:ASP:O	1:A:854:ASN:CB	2.64	0.45
1:A:1019:CYS:O	1:A:1023:ARG:N	2.45	0.45
1:A:1280:GLU:O	1:A:1281:ARG:C	2.55	0.45
2:B:654:ARG:O	2:B:656:GLY:N	2.48	0.45
2:B:1193:GLN:C	7:G:62:LEU:C	2.69	0.45
1:A:509:LEU:CB	1:A:1062:GLU:CB	2.88	0.45
2:B:307:ASP:O	2:B:309:GLN:N	2.50	0.45
2:B:410:GLY:O	2:B:412:LEU:N	2.50	0.45
3:C:82:TYR:O	3:C:83:SER:C	2.54	0.45
1:A:1265:ASN:O	1:A:1267:MET:N	2.50	0.45
2:B:1182:CYS:O	2:B:1183:LYS:C	2.54	0.45
1:A:10:PRO:HA	7:G:15:PRO:CB	2.46	0.45
1:A:1265:ASN:O	1:A:1268:LEU:N	2.41	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.45
4:D:138:ASN:C	4:D:140:ASP:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:ASN:O	5:E:115:ASN:CB	2.65	0.45
1:A:243:PRO:O	1:A:244:PRO:C	2.55	0.45
1:A:1053:PHE:C	1:A:1055:ARG:N	2.70	0.45
1:A:1420:ASP:CB	5:E:174:GLN:CB	2.95	0.45
1:A:1427:ASN:CA	2:B:1138:MET:O	2.64	0.45
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.17	0.45
7:G:117:GLN:C	7:G:119:LEU:N	2.69	0.45
1:A:236:LEU:N	4:D:16:LYS:N	2.60	0.45
1:A:384:ASN:HA	6:F:105:ALA:HB2	1.99	0.45
1:A:1451:VAL:C	1:A:1453:TYR:N	2.70	0.45
2:B:114:PRO:O	2:B:117:ALA:N	2.48	0.45
2:B:511:PRO:O	2:B:512:ARG:C	2.54	0.45
2:B:769:TYR:O	2:B:772:ALA:N	2.50	0.45
2:B:1220:ARG:CB	6:F:139:PRO:CB	2.95	0.45
1:A:71:GLN:O	1:A:73:GLY:N	2.38	0.45
1:A:498:ARG:O	1:A:501:LEU:N	2.47	0.45
1:A:767:GLN:HA	1:A:815:PHE:O	2.17	0.45
1:A:776:ALA:HB1	2:B:397:ASP:CB	2.47	0.45
1:A:859:SER:CA	1:A:1437:GLY:N	2.80	0.45
2:B:785:TYR:C	2:B:787:VAL:H	2.19	0.45
2:B:882:THR:O	2:B:883:LEU:CB	2.65	0.45
8:H:11:GLN:O	8:H:28:ALA:HB1	2.17	0.45
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:1197:PRO:O	2:B:1200:ALA:N	2.48	0.44
5:E:18:THR:O	5:E:19:VAL:C	2.55	0.44
1:A:845:LEU:O	1:A:1434:ALA:C	2.56	0.44
1:A:1015:VAL:O	1:A:1018:PHE:N	2.49	0.44
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.16	0.44
1:A:1430:LEU:C	2:B:1147:LEU:CA	2.85	0.44
2:B:258:LEU:O	2:B:259:TYR:O	2.35	0.44
2:B:785:TYR:C	2:B:787:VAL:N	2.71	0.44
2:B:1146:PHE:C	2:B:1196:ILE:C	2.75	0.44
3:C:63:ILE:O	3:C:64:ALA:C	2.55	0.44
1:A:860:LEU:CB	1:A:1422:ARG:H	2.30	0.44
1:A:1393:ASN:O	1:A:1397:LEU:CB	2.52	0.44
2:B:661:LEU:C	2:B:663:ALA:H	2.19	0.44
3:C:83:SER:O	3:C:85:ASP:N	2.51	0.44
1:A:3:GLY:O	1:A:377:PRO:O	2.10	0.44
1:A:766:GLY:N	1:A:816:HIS:CA	2.51	0.44
1:A:1053:PHE:O	1:A:1055:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:PHE:HA	2:B:585:VAL:O	2.17	0.44
3:C:27:LEU:O	3:C:30:ALA:N	2.50	0.44
11:K:53:ASP:O	11:K:55:LYS:N	2.50	0.44
1:A:135:PHE:C	1:A:137:ALA:N	2.70	0.44
1:A:1122:LYS:O	1:A:1125:ARG:N	2.51	0.44
2:B:1081:LEU:O	2:B:1082:MET:C	2.55	0.44
4:D:135:GLY:C	4:D:137:ASN:H	2.21	0.44
1:A:452:LYS:CB	1:A:846:GLU:CA	2.85	0.44
3:C:105:GLY:HA3	3:C:149:LYS:O	2.17	0.44
6:F:143:PHE:CB	7:G:68:ALA:HB2	0.92	0.44
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.44
1:A:966:ASN:O	1:A:967:ALA:C	2.56	0.44
2:B:1177:HIS:O	2:B:1179:GLN:N	2.50	0.44
1:A:120:GLU:C	1:A:122:MET:N	2.70	0.44
1:A:800:VAL:N	1:A:815:PHE:O	2.50	0.44
1:A:901:LEU:O	1:A:921:GLY:N	2.48	0.44
1:A:1442:ASP:C	6:F:141:GLY:HA3	2.38	0.44
2:B:661:LEU:C	2:B:663:ALA:N	2.71	0.44
2:B:1145:SER:CB	2:B:1195:HIS:N	2.81	0.44
7:G:15:PRO:O	7:G:16:SER:C	2.55	0.44
1:A:626:ASN:C	1:A:628:GLY:H	2.21	0.44
2:B:312:GLU:CA	9:I:46:HIS:CB	2.84	0.44
3:C:77:ILE:C	3:C:79:GLN:H	2.20	0.44
4:D:68:ARG:C	4:D:70:PHE:N	2.70	0.44
9:I:3:THR:H	9:I:45:ARG:CB	2.30	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.00	0.43
1:A:282:ASN:O	1:A:284:ALA:N	2.51	0.43
12:L:58:LYS:O	12:L:59:ALA:O	2.34	0.43
1:A:9:ALA:HB1	7:G:67:SER:CB	2.48	0.43
1:A:95:PHE:O	1:A:98:LYS:N	2.49	0.43
1:A:309:ALA:C	1:A:311:GLN:H	2.21	0.43
1:A:514:PRO:C	1:A:1370:LEU:CB	2.87	0.43
2:B:418:LYS:O	2:B:420:LEU:N	2.51	0.43
2:B:619:ILE:O	2:B:622:LYS:N	2.50	0.43
5:E:35:VAL:C	5:E:37:LEU:N	2.72	0.43
1:A:874:ASP:O	1:A:876:ALA:N	2.50	0.43
2:B:765:PRO:O	2:B:767:ASN:N	2.51	0.43
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.43
7:G:66:GLY:O	7:G:67:SER:C	2.56	0.43
8:H:91:ASP:C	8:H:93:TYR:N	2.72	0.43
1:A:324:SER:O	1:A:325:ILE:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:O	1:A:326:ARG:C	2.55	0.43
1:A:636:GLU:CB	1:A:877:HIS:C	2.83	0.43
1:A:935:GLN:C	1:A:937:VAL:N	2.72	0.43
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.43
2:B:552:MET:C	2:B:554:ILE:N	2.72	0.43
6:F:135:ARG:CB	7:G:15:PRO:CB	2.95	0.43
8:H:11:GLN:HA	8:H:53:ASP:O	2.18	0.43
1:A:10:PRO:O	7:G:65:ASP:C	2.55	0.43
1:A:41:MET:O	1:A:42:ASP:C	2.56	0.43
1:A:1105:SER:O	1:A:1106:LEU:CB	2.67	0.43
2:B:388:CYS:HA	9:I:92:ARG:HA	2.00	0.43
2:B:730:ARG:O	2:B:731:VAL:O	2.36	0.43
4:D:146:GLN:O	4:D:147:TYR:C	2.57	0.43
2:B:394:ASP:N	9:I:92:ARG:O	2.51	0.43
3:C:92:CYS:O	3:C:94:LYS:N	2.52	0.43
1:A:387:ARG:HA	6:F:104:ASN:CB	2.48	0.43
1:A:858:ASN:CA	1:A:1422:ARG:CA	2.61	0.43
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.43
1:A:450:LEU:HA	1:A:843:LYS:CB	2.49	0.43
1:A:496:GLU:C	7:G:63:PRO:C	2.76	0.43
1:A:67:CYS:O	1:A:68:GLN:CB	2.67	0.43
1:A:73:GLY:O	1:A:75:ASN:N	2.52	0.43
1:A:513:SER:N	1:A:1067:LEU:CB	2.82	0.43
1:A:807:GLY:HA2	2:B:760:ASP:O	2.19	0.43
1:A:1015:VAL:O	1:A:1016:THR:C	2.57	0.43
2:B:446:LEU:O	2:B:447:ALA:CB	2.66	0.43
2:B:582:VAL:HA	2:B:626:ILE:O	2.19	0.43
2:B:1032:SER:O	2:B:1036:ALA:HB2	2.19	0.43
2:B:1034:VAL:C	2:B:1036:ALA:N	2.72	0.43
6:F:72:LYS:HA	7:G:10:ASN:HA	2.00	0.43
6:F:77:ASP:N	7:G:23:LYS:CA	2.72	0.43
1:A:652:VAL:O	1:A:653:VAL:C	2.56	0.43
2:B:593:PRO:O	2:B:596:LEU:N	2.52	0.43
1:A:823:GLY:C	1:A:825:ILE:N	2.72	0.42
2:B:394:ASP:N	9:I:92:ARG:C	2.73	0.42
6:F:138:LEU:N	7:G:61:ILE:N	2.66	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.42
2:B:1029:CYS:HA	2:B:1089:PRO:O	2.19	0.42
3:C:170:TRP:O	3:C:171:GLY:C	2.57	0.42
4:D:53:SER:CB	4:D:153:ARG:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3:THR:N	9:I:45:ARG:CB	2.82	0.42
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.42
1:A:226:GLU:CB	4:D:9:GLN:CB	2.97	0.42
1:A:660:ASN:O	1:A:661:GLY:O	2.37	0.42
1:A:679:ILE:O	1:A:682:THR:N	2.52	0.42
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.84	0.42
1:A:1447:GLU:O	7:G:29:LYS:CB	2.47	0.42
1:A:1452:LYS:CA	7:G:28:THR:CB	2.97	0.42
2:B:257:LYS:N	2:B:270:LYS:O	2.52	0.42
2:B:312:GLU:O	2:B:315:LYS:N	2.50	0.42
4:D:206:GLU:C	4:D:208:GLU:H	2.23	0.42
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.01	0.42
2:B:394:ASP:HA	9:I:92:ARG:O	2.20	0.42
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.42
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.42
5:E:205:SER:O	5:E:206:GLY:C	2.58	0.42
6:F:72:LYS:O	6:F:73:ALA:HB3	2.20	0.42
6:F:74:ILE:C	7:G:26:LEU:CB	2.87	0.42
1:A:116:ASP:O	1:A:117:GLU:C	2.57	0.42
1:A:277:GLU:O	1:A:279:LEU:N	2.52	0.42
4:D:206:GLU:O	4:D:208:GLU:N	2.53	0.42
2:B:654:ARG:C	2:B:656:GLY:H	2.23	0.42
2:B:1148:LYS:CA	2:B:1200:ALA:N	2.73	0.42
5:E:127:ILE:O	5:E:130:ALA:HB3	2.20	0.42
1:A:65:LEU:O	1:A:66:LYS:C	2.57	0.42
1:A:100:LYS:O	1:A:102:VAL:N	2.52	0.42
1:A:335:ARG:HA	1:A:339:ASN:CB	2.50	0.42
1:A:1428:VAL:CA	2:B:1138:MET:CB	2.75	0.42
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.49	0.42
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	2.00	0.42
1:A:341:MET:O	2:B:1131:GLY:O	2.38	0.42
1:A:608:ILE:C	1:A:610:GLY:N	2.72	0.42
1:A:817:ALA:O	1:A:820:GLY:N	2.53	0.42
1:A:1334:ASP:C	1:A:1336:MET:H	2.23	0.42
1:A:1449:SER:N	7:G:27:LYS:C	2.73	0.42
2:B:307:ASP:O	2:B:308:TRP:C	2.58	0.42
2:B:366:GLN:O	2:B:367:LEU:O	2.38	0.42
2:B:414:ALA:O	2:B:415:GLN:C	2.57	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.20	0.42
6:F:77:ASP:CA	7:G:21:ARG:HA	2.48	0.42
7:G:149:GLY:O	7:G:159:ALA:HB1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.42
1:A:472:LEU:O	1:A:475:THR:CB	2.68	0.42
1:A:1217:LYS:O	1:A:1221:LYS:N	2.52	0.42
2:B:610:ASN:O	2:B:612:GLU:N	2.53	0.42
2:B:1178:ASN:O	2:B:1179:GLN:C	2.56	0.42
2:B:1182:CYS:O	2:B:1183:LYS:O	2.37	0.42
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.42
1:A:845:LEU:O	1:A:1434:ALA:O	2.38	0.42
1:A:1449:SER:CA	7:G:28:THR:N	2.77	0.42
2:B:593:PRO:O	2:B:595:ARG:N	2.53	0.42
2:B:1208:MET:HA	2:B:1212:ILE:O	2.20	0.42
3:C:208:GLU:C	3:C:210:GLU:H	2.22	0.42
3:C:226:ASP:O	3:C:227:THR:CB	2.66	0.42
4:D:51:ASN:O	4:D:52:LEU:C	2.57	0.42
4:D:144:THR:O	4:D:148:LEU:CB	2.68	0.42
1:A:450:LEU:CA	1:A:843:LYS:N	2.74	0.41
1:A:1157:ASP:O	1:A:1159:ARG:N	2.53	0.41
2:B:1149:GLU:CB	2:B:1158:PHE:CB	2.98	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.53	0.41
6:F:72:LYS:HA	7:G:11:ILE:H	1.85	0.41
1:A:7:SER:C	1:A:9:ALA:H	2.23	0.41
1:A:277:GLU:C	1:A:279:LEU:N	2.74	0.41
2:B:769:TYR:C	2:B:771:SER:N	2.73	0.41
9:I:61:ASP:C	9:I:63:GLY:N	2.73	0.41
10:J:31:ASP:O	10:J:32:GLU:C	2.58	0.41
1:A:509:LEU:CB	1:A:1062:GLU:C	2.82	0.41
1:A:577:ILE:O	1:A:578:LEU:C	2.56	0.41
1:A:633:VAL:O	1:A:877:HIS:CA	2.67	0.41
1:A:1410:PHE:C	1:A:1412:ALA:H	2.23	0.41
2:B:1124:ARG:O	2:B:1125:ASP:CB	2.68	0.41
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.41
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.41
5:E:43:LYS:O	5:E:45:LYS:N	2.48	0.41
5:E:98:ILE:O	5:E:100:ILE:N	2.54	0.41
5:E:117:THR:O	5:E:120:ALA:N	2.44	0.41
5:E:201:LYS:HA	5:E:206:GLY:O	2.19	0.41
1:A:264:PHE:O	1:A:267:ALA:HB3	2.20	0.41
1:A:1027:ALA:O	1:A:1028:THR:C	2.59	0.41
2:B:1099:VAL:C	2:B:1101:ASP:N	2.70	0.41
9:I:83:ASN:HA	9:I:102:VAL:O	2.20	0.41
1:A:744:LYS:O	1:A:747:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.41
4:D:51:ASN:C	4:D:52:LEU:O	2.59	0.41
6:F:123:LYS:O	6:F:124:GLU:C	2.58	0.41
6:F:138:LEU:CA	7:G:59:GLY:O	2.61	0.41
8:H:56:THR:O	8:H:144:ILE:HA	2.21	0.41
1:A:70:CYS:O	1:A:71:GLN:C	2.59	0.41
1:A:935:GLN:O	1:A:936:LEU:C	2.59	0.41
1:A:1334:ASP:C	1:A:1336:MET:N	2.74	0.41
2:B:214:ALA:HB3	2:B:498:THR:HA	2.01	0.41
2:B:552:MET:O	2:B:554:ILE:N	2.53	0.41
2:B:708:GLU:O	2:B:709:ASP:C	2.58	0.41
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.41
1:A:231:PRO:C	1:A:233:TRP:N	2.73	0.41
1:A:343:LYS:O	2:B:1129:ARG:CB	2.65	0.41
1:A:427:GLN:O	1:A:428:TYR:C	2.56	0.41
1:A:1420:ASP:CB	5:E:174:GLN:HA	2.50	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.41
5:E:98:ILE:O	5:E:99:HIS:C	2.59	0.41
6:F:143:PHE:CA	7:G:68:ALA:HB3	1.96	0.41
1:A:11:LEU:N	6:F:135:ARG:CB	2.71	0.41
1:A:226:GLU:CB	4:D:9:GLN:HA	2.50	0.41
1:A:276:LEU:O	1:A:279:LEU:N	2.47	0.41
1:A:356:ASP:C	1:A:358:ASN:H	2.24	0.41
1:A:859:SER:HA	1:A:1437:GLY:N	2.36	0.41
1:A:964:ILE:O	1:A:965:GLN:C	2.59	0.41
2:B:48:LEU:O	2:B:49:ASP:C	2.59	0.41
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.41
2:B:1068:GLY:O	2:B:1069:PHE:C	2.59	0.41
1:A:14:VAL:CB	2:B:1144:ALA:HB3	2.50	0.41
1:A:341:MET:O	2:B:1131:GLY:C	2.59	0.41
1:A:514:PRO:C	1:A:516:SER:N	2.75	0.41
1:A:566:ILE:O	1:A:567:LYS:O	2.39	0.41
1:A:635:ARG:CB	1:A:874:ASP:N	2.84	0.41
1:A:801:GLU:CA	1:A:816:HIS:CB	2.98	0.41
1:A:874:ASP:O	1:A:875:ALA:C	2.59	0.41
1:A:1044:TRP:O	1:A:1045:VAL:C	2.59	0.41
1:A:1265:ASN:C	1:A:1267:MET:H	2.23	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.23	0.41
2:B:492:LEU:O	2:B:493:SER:C	2.59	0.41
2:B:511:PRO:O	2:B:513:GLN:N	2.54	0.41
3:C:92:CYS:C	3:C:94:LYS:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:PRO:C	4:D:198:LEU:H	2.23	0.41
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.41
1:A:332:LYS:C	1:A:334:GLY:H	2.25	0.41
1:A:399:HIS:O	1:A:400:PRO:C	2.58	0.41
1:A:482:PHE:O	1:A:484:GLY:N	2.53	0.41
1:A:1125:ARG:C	1:A:1127:ALA:H	2.24	0.41
1:A:1242:VAL:O	1:A:1243:VAL:CB	2.69	0.41
2:B:838:SER:CA	2:B:989:THR:O	2.69	0.41
2:B:1185:CYS:N	4:D:4:SER:N	2.63	0.41
8:H:106:GLU:O	8:H:108:SER:N	2.48	0.41
1:A:512:VAL:C	1:A:1067:LEU:CB	2.89	0.40
1:A:589:GLN:N	1:A:880:LYS:O	2.53	0.40
1:A:809:THR:O	1:A:810:PRO:C	2.59	0.40
1:A:596:THR:C	1:A:598:LEU:N	2.74	0.40
1:A:618:GLU:O	1:A:619:LYS:C	2.60	0.40
1:A:779:PHE:O	1:A:780:VAL:C	2.59	0.40
1:A:1019:CYS:O	1:A:1020:CYS:C	2.60	0.40
1:A:1349:TYR:O	1:A:1350:LYS:C	2.60	0.40
1:A:1438:THR:CB	2:B:1144:ALA:HB3	2.51	0.40
2:B:294:ASP:O	2:B:296:GLU:N	2.48	0.40
1:A:289:ILE:C	1:A:291:GLU:N	2.73	0.40
1:A:1205:LYS:O	1:A:1206:ASP:C	2.59	0.40
1:A:1442:ASP:O	6:F:141:GLY:HA3	2.20	0.40
2:B:392:ARG:HA	9:I:90:GLN:CB	2.47	0.40
2:B:641:GLU:C	2:B:643:ASP:H	2.25	0.40
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.40
2:B:948:ILE:C	2:B:949:VAL:O	2.56	0.40
2:B:1145:SER:CB	2:B:1195:HIS:CA	2.93	0.40
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.40
10:J:34:THR:O	10:J:35:ALA:C	2.59	0.40
12:L:62:LYS:O	12:L:63:ARG:C	2.59	0.40
1:A:23:SER:O	1:A:25:GLU:N	2.55	0.40
1:A:270:LEU:O	1:A:271:LYS:C	2.60	0.40
1:A:334:GLY:O	1:A:335:ARG:C	2.60	0.40
1:A:603:ASN:O	1:A:604:GLY:C	2.60	0.40
1:A:1313:LEU:C	1:A:1315:GLU:H	2.24	0.40
2:B:1135:ARG:O	2:B:1138:MET:N	2.54	0.40
2:B:1192:TYR:CA	7:G:67:SER:C	2.85	0.40
4:D:138:ASN:O	4:D:141:LEU:N	2.54	0.40
1:A:683:ILE:O	1:A:686:ALA:HB3	2.21	0.40
2:B:435:THR:C	2:B:437:GLU:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ALA:C	4:D:193:THR:N	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1390/1455 (96%)	938 (68%)	290 (21%)	162 (12%)	0 6
2	B	1068/1224 (87%)	727 (68%)	220 (21%)	121 (11%)	0 7
3	C	264/268 (98%)	159 (60%)	66 (25%)	39 (15%)	0 3
4	D	173/218 (79%)	122 (70%)	34 (20%)	17 (10%)	0 10
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1 14
6	F	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	2 20
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1 14
8	H	129/146 (88%)	84 (65%)	30 (23%)	15 (12%)	0 6
9	I	114/122 (93%)	77 (68%)	30 (26%)	7 (6%)	1 17
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0 1
11	K	112/120 (93%)	89 (80%)	18 (16%)	5 (4%)	2 22
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0 1
All	All	3820/4163 (92%)	2595 (68%)	801 (21%)	424 (11%)	1 7

All (424) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	55	ASP
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	76	GLU
1	A	78	PRO
1	A	93	VAL
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	335	ARG
1	A	385	ILE
1	A	418	SER
1	A	423	ASP
1	A	424	ILE
1	A	536	LEU
1	A	567	LYS
1	A	619	LYS
1	A	626	ASN
1	A	666	ILE
1	A	775	ILE
1	A	968	GLN
1	A	1002	GLY
1	A	1036	ARG
1	A	1105	SER
1	A	1112	PRO
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1366	ARG
1	A	1378	GLN
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1438	THR
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	206	ASN
2	B	258	LEU
2	B	259	TYR
2	B	334	ILE
2	B	367	LEU
2	B	629	ASP
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	746	SER
2	B	751	VAL
2	B	881	ASN
2	B	891	ASP
2	B	907	GLY
2	B	958	GLN
2	B	1006	ILE
2	B	1046	PRO
2	B	1069	PHE
2	B	1100	ASP
2	B	1108	ARG
2	B	1156	ASP
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
3	C	56	THR
3	C	78	GLU
3	C	91	HIS
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	202	PRO

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Mol	Chain	Res	Type
3	C	209	TYR
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	231	ASN
3	C	240	VAL
4	D	6	SER
4	D	8	PHE
4	D	12	ARG
4	D	19	GLU
4	D	20	GLU
4	D	21	GLU
4	D	52	LEU
4	D	131	GLU
4	D	177	VAL
4	D	192	LYS
4	D	199	ASN
5	E	106	GLN
5	E	130	ALA
7	G	62	LEU
7	G	63	PRO
7	G	139	ILE
8	H	81	PRO
8	H	128	ASN
8	H	140	ALA
9	I	3	THR
9	I	9	ASP
9	I	106	CYS
10	J	2	ILE
10	J	6	ARG
10	J	8	PHE
10	J	9	SER
10	J	17	LYS
10	J	28	ASP
10	J	32	GLU
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
1	A	4	GLN
1	A	42	ASP
1	A	44	THR

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Mol	Chain	Res	Type
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	101	LYS
1	A	111	GLY
1	A	113	LEU
1	A	244	PRO
1	A	263	THR
1	A	290	GLU
1	A	312	PRO
1	A	318	SER
1	A	333	GLU
1	A	336	ILE
1	A	364	VAL
1	A	409	SER
1	A	421	ALA
1	A	483	ASP
1	A	661	GLY
1	A	753	GLY
1	A	765	VAL
1	A	780	VAL
1	A	789	LYS
1	A	818	MET
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	875	ALA
1	A	986	ILE
1	A	1008	GLN
1	A	1016	THR
1	A	1106	LEU
1	A	1110	LEU
1	A	1123	LEU
1	A	1165	GLU
1	A	1212	VAL
1	A	1221	LYS
1	A	1233	ASP
1	A	1335	ILE
1	A	1377	THR
1	A	1386	ARG
1	A	1389	PHE

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Mol	Chain	Res	Type
2	B	21	GLU
2	B	28	GLU
2	B	45	SER
2	B	46	GLN
2	B	114	PRO
2	B	229	ALA
2	B	260	GLY
2	B	266	ALA
2	B	282	ILE
2	B	308	TRP
2	B	513	GLN
2	B	559	SER
2	B	641	GLU
2	B	655	LYS
2	B	869	SER
2	B	888	GLY
2	B	1003	ALA
2	B	1035	ALA
2	B	1041	GLU
2	B	1126	GLY
2	B	1153	GLU
2	B	1155	SER
2	B	1157	ALA
2	B	1167	GLY
2	B	1176	ASN
2	B	1178	ASN
3	C	84	ARG
3	C	87	PHE
3	C	110	THR
3	C	142	VAL
3	C	164	ALA
3	C	169	LYS
3	C	175	ALA
3	C	216	GLY
3	C	255	VAL
3	C	264	GLN
4	D	15	LEU
4	D	218	GLU
5	E	36	GLU
5	E	44	ALA
5	E	59	SER
5	E	73	PRO

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Mol	Chain	Res	Type
5	E	74	ASP
5	E	192	ARG
5	E	206	GLY
6	F	81	THR
7	G	118	ASP
7	G	154	VAL
8	H	32	THR
8	H	59	ILE
8	H	82	PRO
8	H	84	ALA
8	H	92	ASP
8	H	107	VAL
9	I	57	GLY
9	I	62	ILE
10	J	14	VAL
10	J	29	GLU
10	J	33	GLY
11	K	53	ASP
12	L	35	SER
1	A	58	LEU
1	A	71	GLN
1	A	117	GLU
1	A	131	SER
1	A	170	THR
1	A	219	PHE
1	A	223	GLY
1	A	232	GLU
1	A	253	ASN
1	A	278	THR
1	A	317	LYS
1	A	357	PRO
1	A	399	HIS
1	A	419	LYS
1	A	439	ASN
1	A	465	TYR
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	605	MET
1	A	731	ARG
1	A	817	ALA
1	A	940	ARG

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Mol	Chain	Res	Type
1	A	1164	PRO
1	A	1309	ASP
1	A	1411	GLU
2	B	58	THR
2	B	383	ASN
2	B	450	ALA
2	B	459	TYR
2	B	512	ARG
2	B	571	PRO
2	B	590	HIS
2	B	591	ARG
2	B	605	ARG
2	B	648	HIS
2	B	682	SER
2	B	711	GLU
2	B	738	PHE
2	B	792	MET
2	B	797	TYR
2	B	848	ARG
2	B	878	GLN
2	B	884	ARG
2	B	943	SER
2	B	1017	ILE
2	B	1082	MET
3	C	60	ASP
3	C	89	GLU
3	C	93	ASP
3	C	167	HIS
5	E	115	ASN
7	G	53	ASN
8	H	17	PRO
8	H	77	ARG
8	H	108	SER
8	H	135	LEU
9	I	78	CYS
10	J	24	LEU
10	J	51	LEU
10	J	55	ASP
11	K	54	ARG
11	K	88	LYS
12	L	40	LEU
12	L	54	ARG

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Mol	Chain	Res	Type
1	A	69	THR
1	A	276	LEU
1	A	283	GLY
1	A	400	PRO
1	A	756	ILE
1	A	795	GLU
1	A	910	PRO
1	A	958	VAL
1	A	1011	GLN
1	A	1028	THR
1	A	1104	PRO
1	A	1240	CYS
1	A	1242	VAL
1	A	1297	GLU
2	B	67	SER
2	B	68	THR
2	B	100	PRO
2	B	124	TYR
2	B	257	LYS
2	B	369	GLY
2	B	419	THR
2	B	594	ALA
2	B	620	ARG
2	B	735	ALA
2	B	883	LEU
2	B	951	GLN
2	B	1011	ILE
2	B	1097	HIS
2	B	1144	ALA
3	C	77	ILE
3	C	198	ALA
4	D	30	GLY
7	G	19	GLY
7	G	26	LEU
8	H	44	VAL
8	H	52	GLN
9	I	47	GLU
10	J	27	GLU
11	K	29	ASN
12	L	43	THR
12	L	56	LEU
12	L	60	ARG

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	84	ILE
1	A	128	ILE
1	A	226	GLU
1	A	598	LEU
1	A	599	SER
1	A	633	VAL
1	A	648	ASN
1	A	649	ILE
1	A	739	ASP
1	A	755	PHE
1	A	841	LEU
1	A	871	ASP
1	A	969	GLN
1	A	1054	LEU
1	A	1266	THR
2	B	27	ALA
2	B	48	LEU
2	B	65	GLU
2	B	197	PHE
2	B	309	GLN
2	B	414	ALA
2	B	418	LYS
2	B	530	GLY
2	B	636	PRO
2	B	758	PHE
2	B	766	ARG
2	B	867	GLY
2	B	1016	ALA
3	C	108	GLU
4	D	168	LYS
5	E	40	GLU
5	E	45	LYS
6	F	112	GLU
6	F	150	GLU
7	G	34	VAL
7	G	115	MET
1	A	245	PRO
1	A	492	PRO
1	A	525	GLN
1	A	1057	VAL
1	A	1158	PRO

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Mol	Chain	Res	Type
1	A	1396	ALA
2	B	313	MET
2	B	364	ILE
2	B	480	SER
2	B	611	PRO
2	B	836	GLU
2	B	1214	PRO
3	C	18	VAL
3	C	176	ILE
3	C	230	MET
4	D	69	ALA
4	D	139	LYS
5	E	158	SER
10	J	63	TYR
11	K	90	ALA
12	L	28	LYS
12	L	46	VAL
1	A	196	GLU
1	A	300	VAL
1	A	627	GLY
2	B	712	PRO
3	C	172	PRO
3	C	212	PRO
1	A	652	VAL
1	A	653	VAL
2	B	501	PRO
5	E	37	LEU
1	A	546	VAL
1	A	825	ILE
1	A	1379	GLY
1	A	1454	MET
2	B	411	PRO
2	B	551	PRO
2	B	1018	PRO
3	C	171	GLY
2	B	524	PRO
2	B	818	PRO
3	C	126	GLY
6	F	131	PRO
7	G	20	PRO
7	G	116	PRO
2	B	592	ASN

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Mol	Chain	Res	Type
5	E	129	PRO

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1274:ARG	C	1275:GLY	N	10.90

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1131:THR	C	1142:THR	N	8.08

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5407. These allow visual inspection of the internal detail of the map and identification of artifacts.

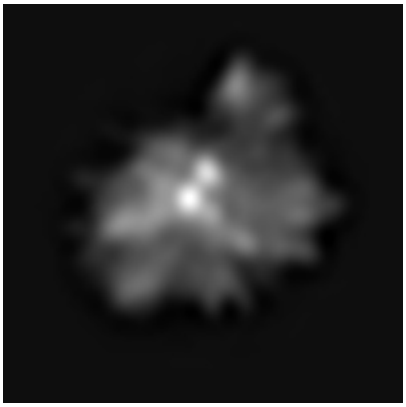
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

X

Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 35

Y Index: 35

Z Index: 35

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: 41

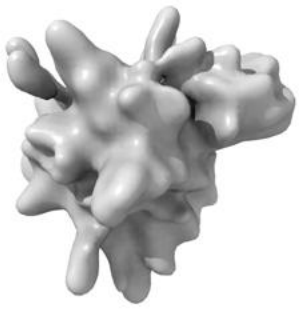
Y Index: 35

Z Index: 40

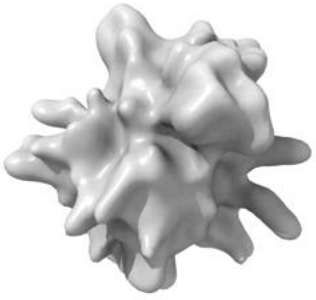
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

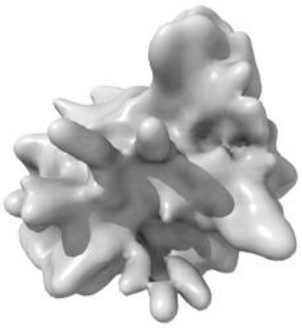
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

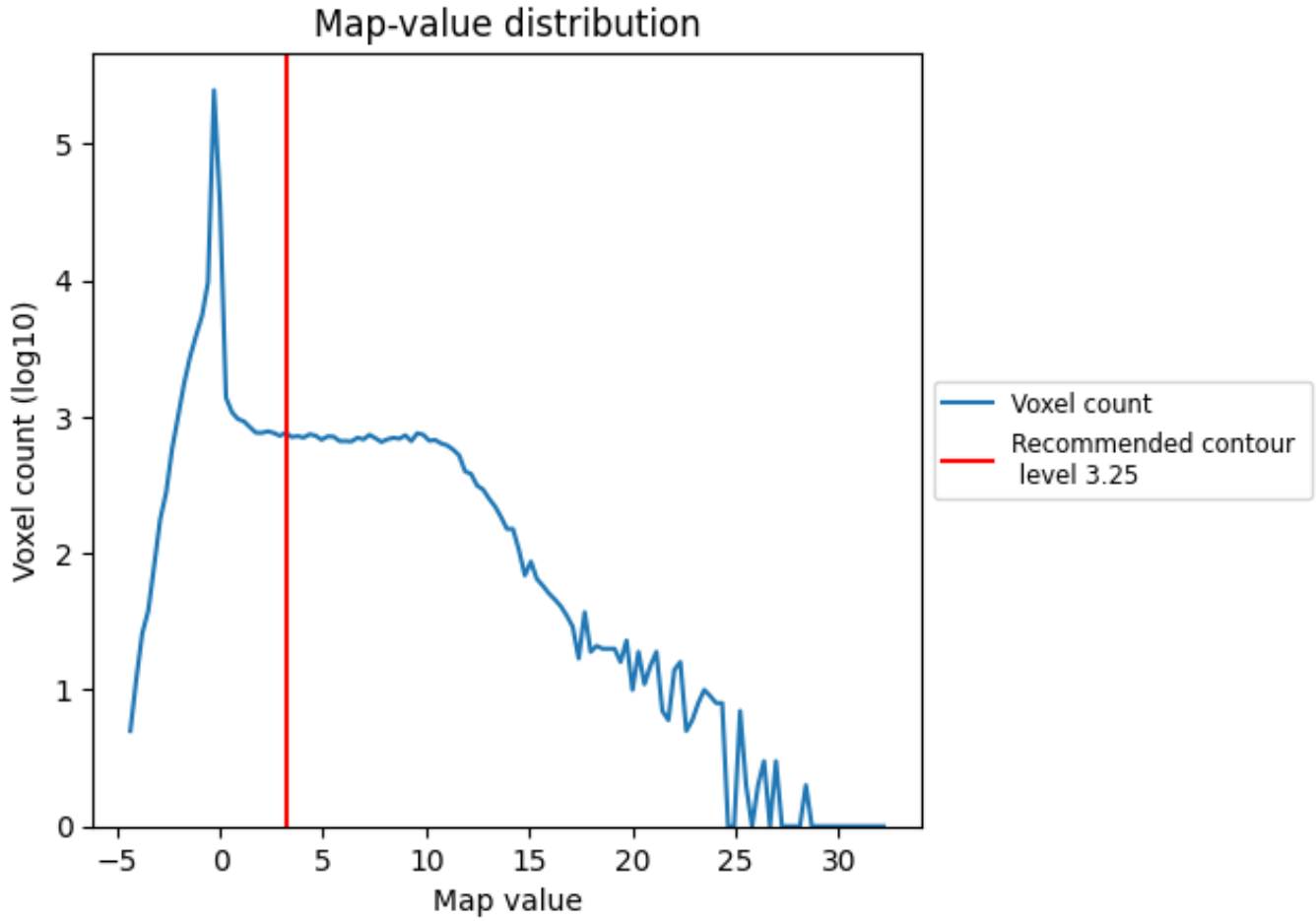
6.5 Mask visualisation (i)

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

7 Map analysis

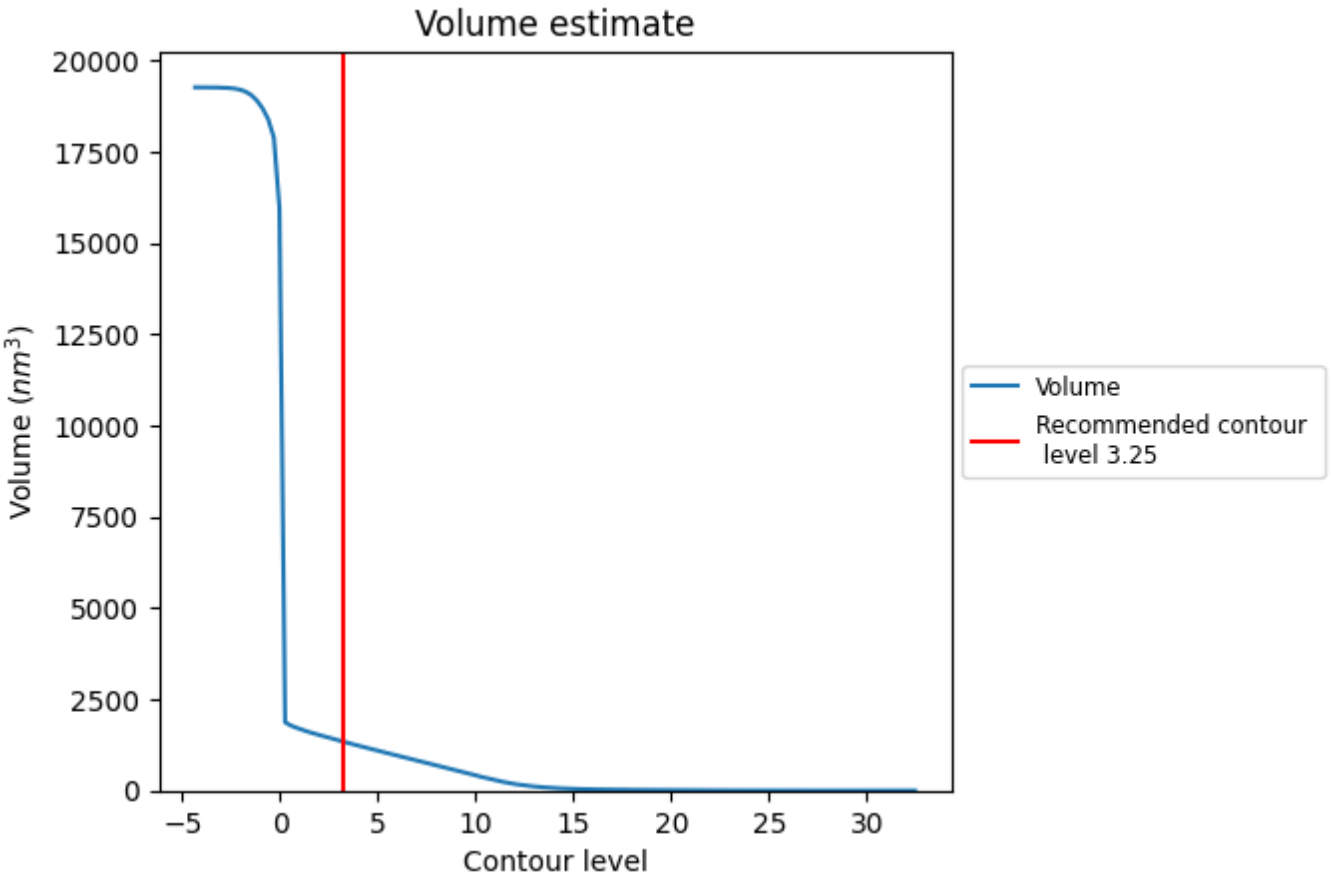
This section contains the results of statistical analysis of the map.

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.

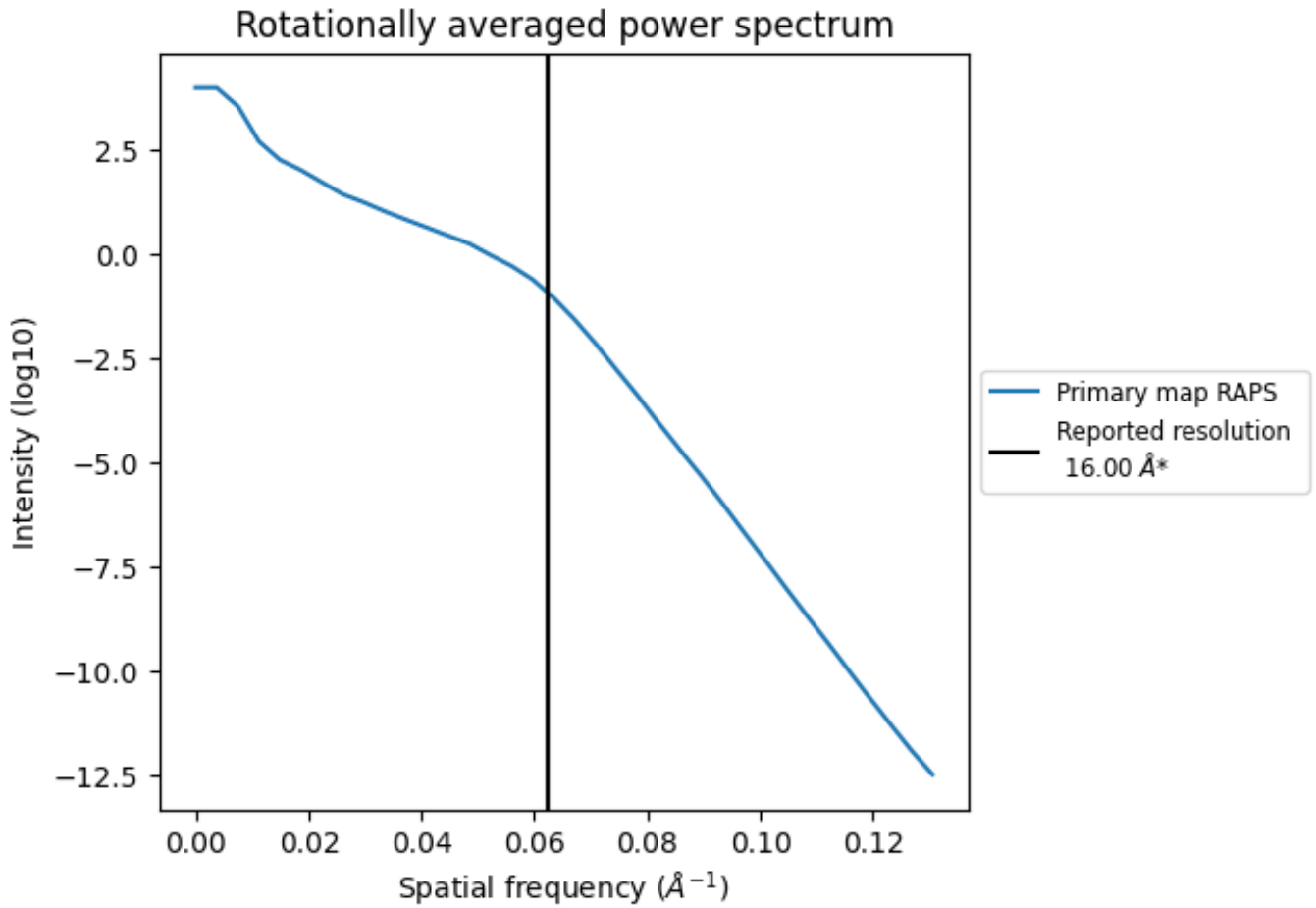
7.2 Volume estimate



The volume at the recommended contour level is 1339 nm^3; this corresponds to an approximate mass of 1210 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 0.062 $Å^{-1}$

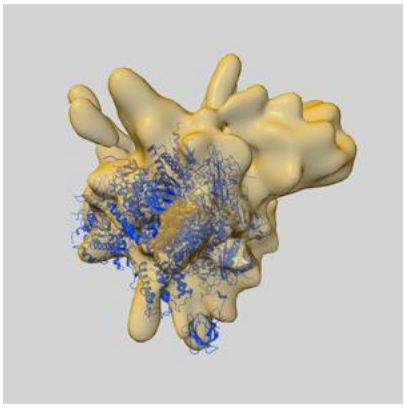
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

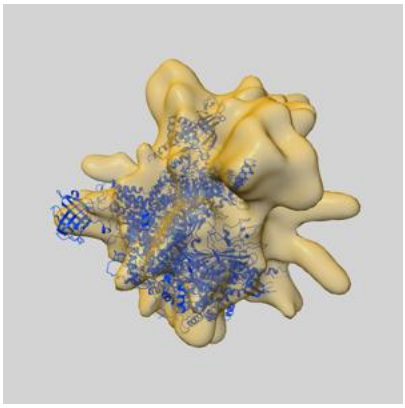
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5407 and PDB model 3J1N. Per-residue inclusion information can be found in section 3 on page 6.

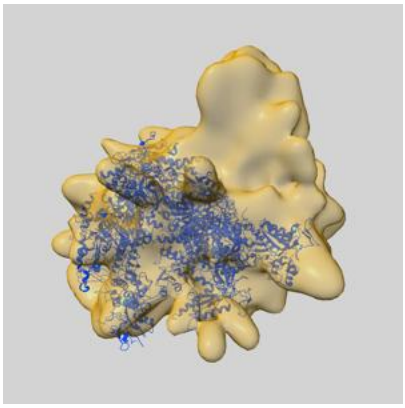
9.1 Map-model overlay



X



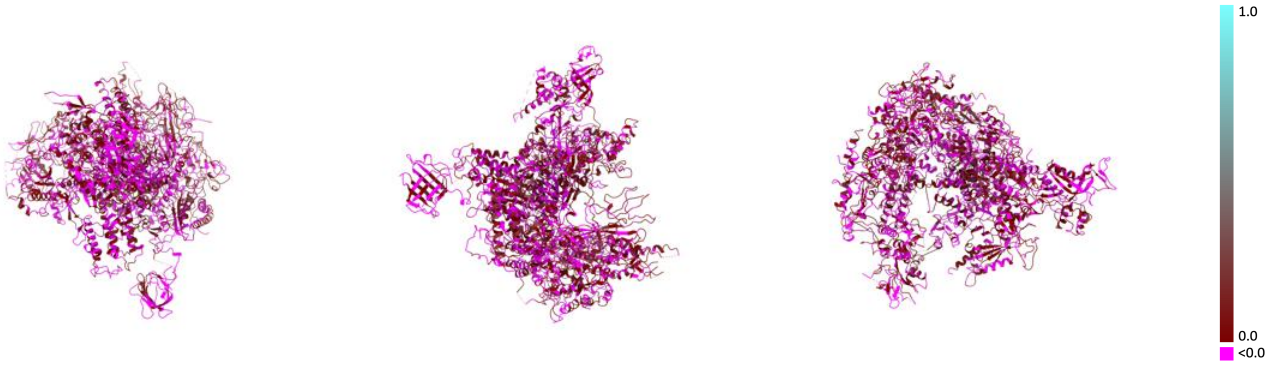
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.25 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.

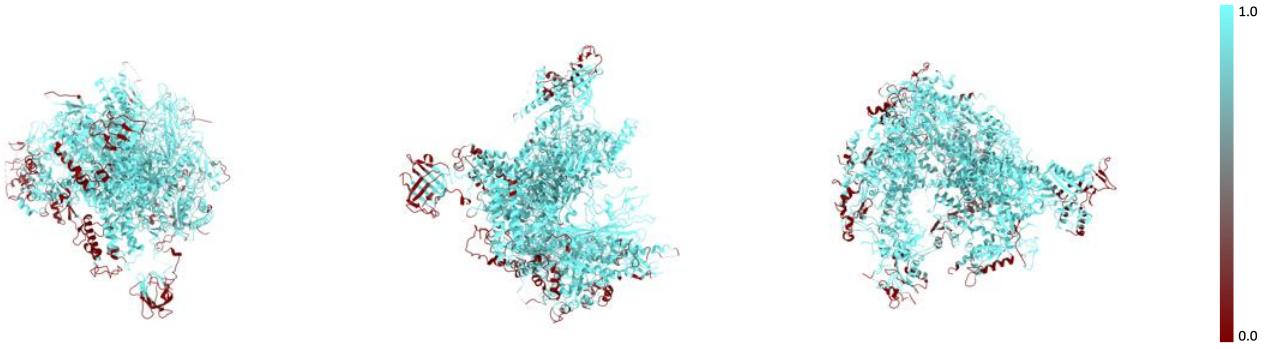
9.2 Q-score mapped to coordinate model (i)



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.

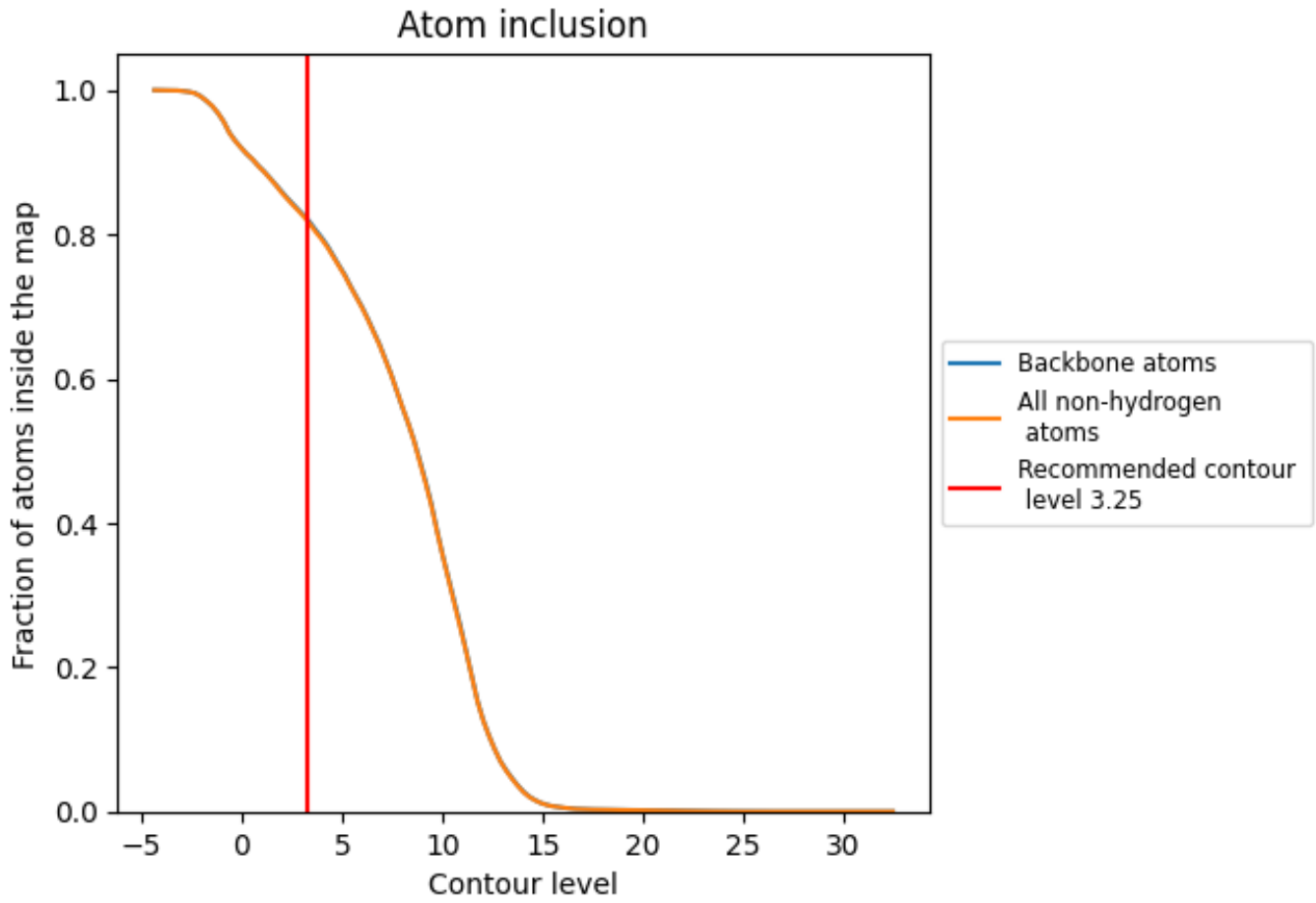
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.25).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (3.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8199	0.0150
A	0.8527	0.0170
B	0.8988	0.0240
C	0.6697	0.0100
D	0.7483	0.0150
E	0.7411	0.0060
F	1.0000	0.0350
G	0.7776	-0.0200
H	0.3763	-0.0470
I	0.8620	0.0560
J	0.4579	-0.0390
K	0.9504	0.0370
L	0.6507	-0.0100