



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 5LMX / pdb_00005lmx
EMDB ID : EMD-4088
Title : Monomeric RNA polymerase I at 4.9 Å resolution
Authors : Torreira, E.; Louro, J.A.; Gil-Carton, D.; Gallego, O.; Calvo, O.; Fernandez-Tornero, C.
Deposited on : 2016-08-02
Resolution : 4.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

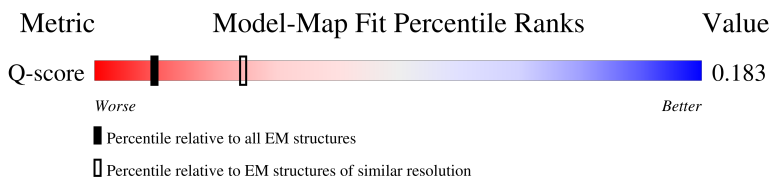
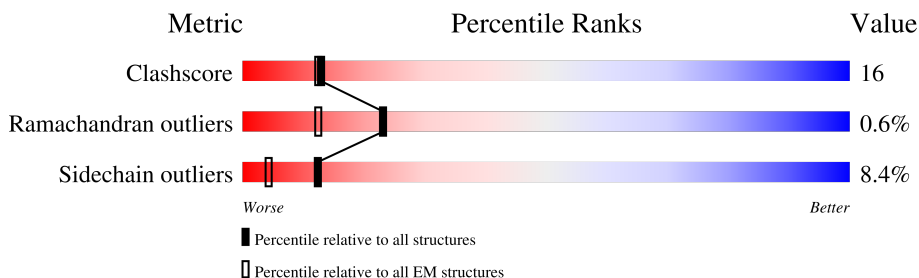
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1274 (4.40 - 5.40)

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

Mol	Chain	Length	Quality of chain
1	A	1664	29% 64% 19% • 15%
2	B	1203	30% 68% 22% • 7%
3	C	380	9% 56% 21% •• 20%
4	D	137	11% 7% 5% • 87%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ZN	L	101	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31118 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1420	Total	C	N	O	S	0	0
			11207	7087	1942	2118	60		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0
			8868	5618	1546	1656	48		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1,DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	18	Total	C	N	O	0	0
			133	84	23	26		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	89	Total	C	N	O	S	0	0
			706	465	113	123	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	134	Total	C	N	O	S	0	0
			1072	676	181	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	64	Total	C	N	O	S	0	0
			472	295	78	95	4		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

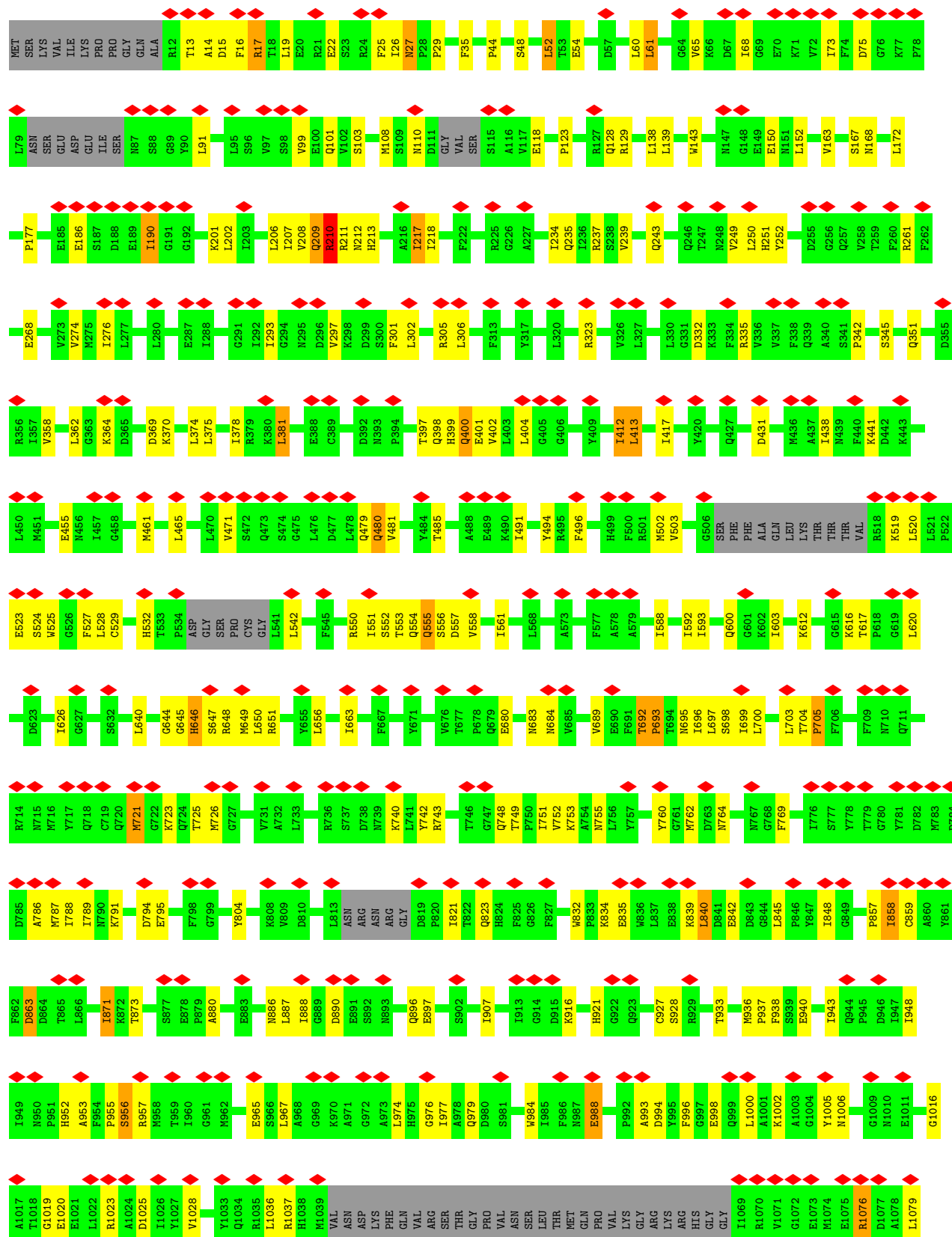
Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			831	528	137	166		

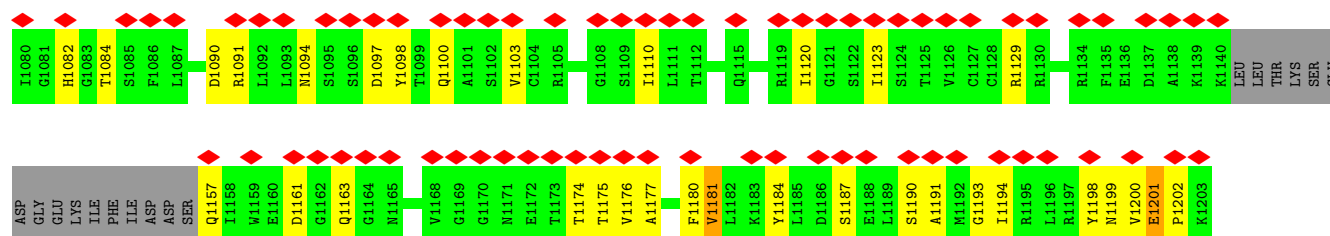
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	139	Total	C	N	O	S	0	0
			1103	706	179	214	4		

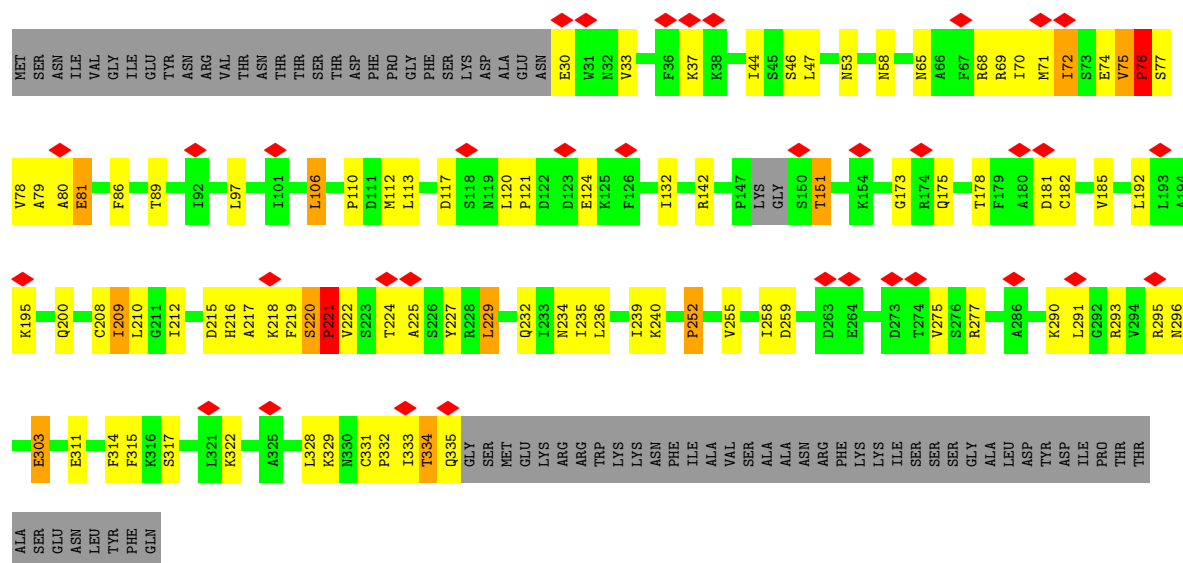
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	I	1	Total	Zn	0
			1	1	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	

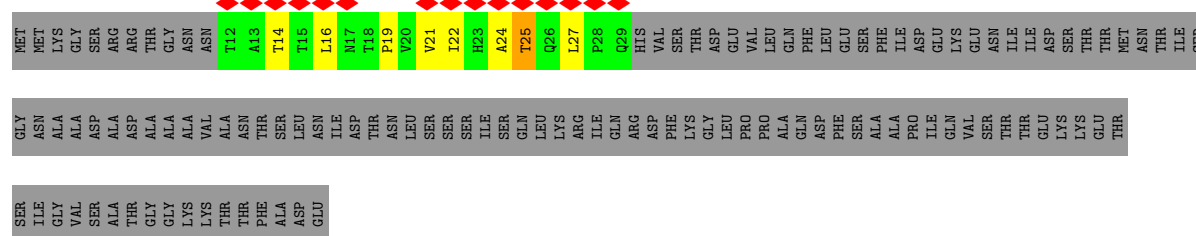




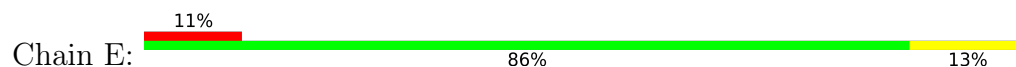
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1, DNA-directed RNA polymerases I and III subunit RPAC1

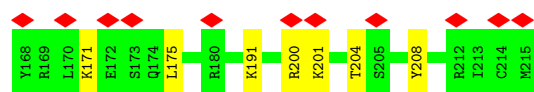


- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

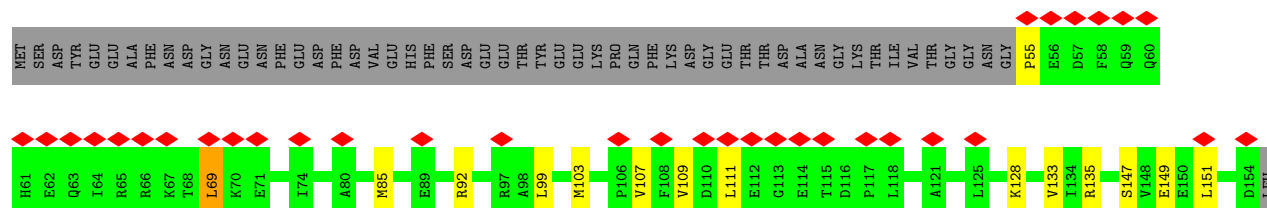


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

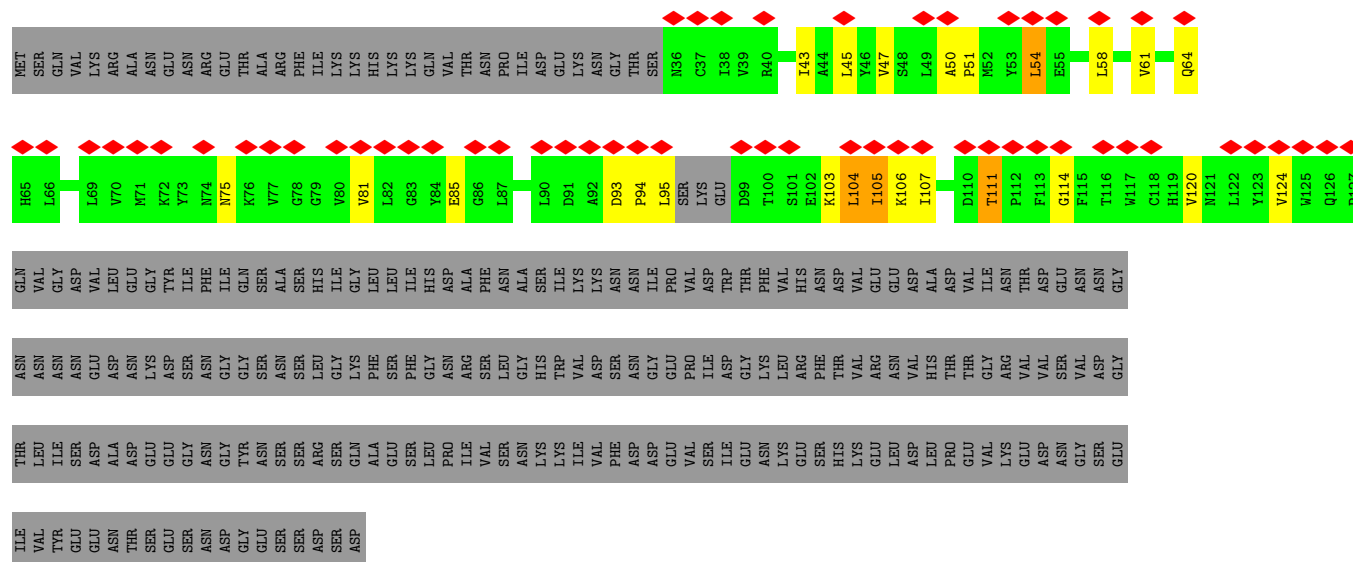




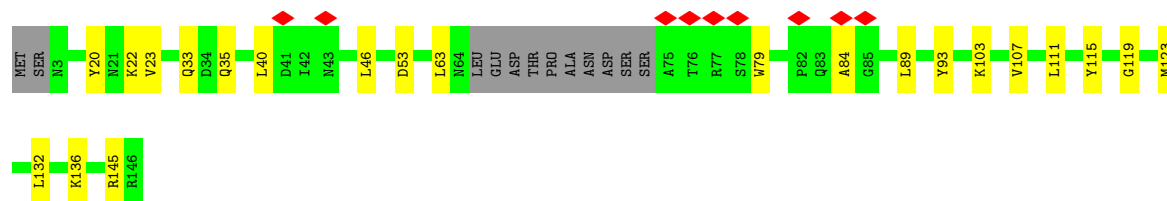
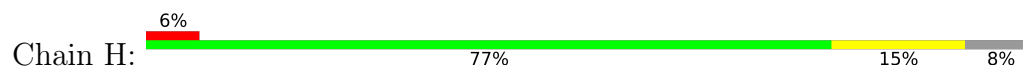
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



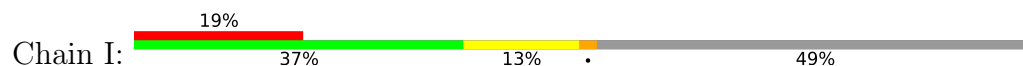
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

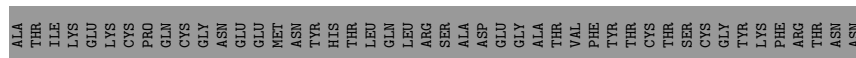


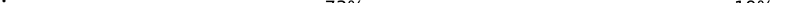
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

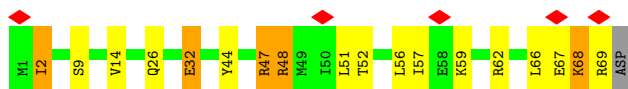


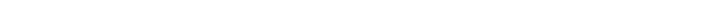
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

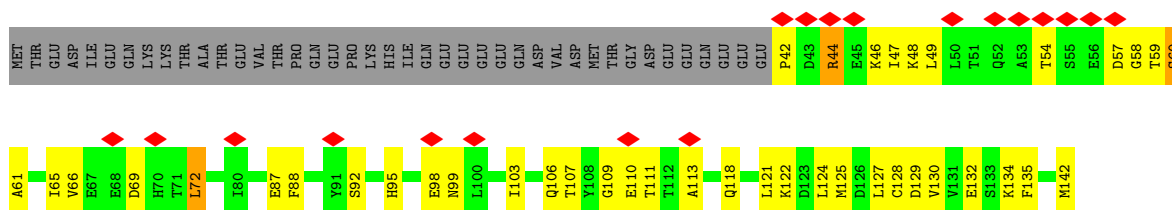




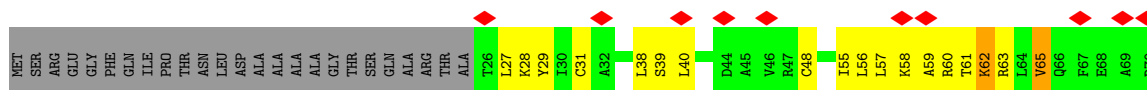
- Chain J:  7% 73% 19% 7%

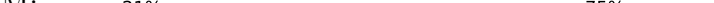


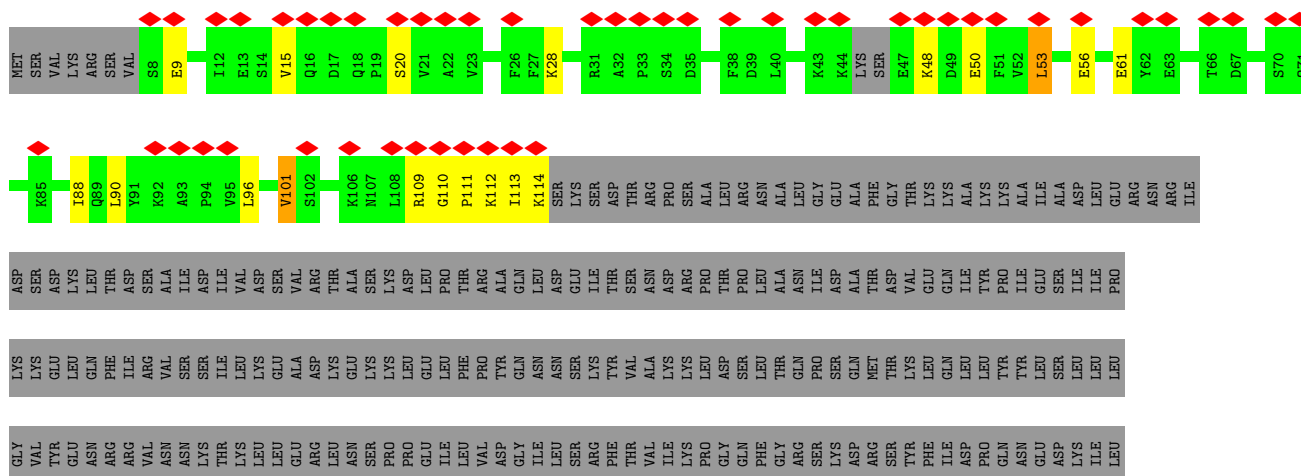
- Chain K:  13% 42% 27% 29%



- Chain L: 14% 39% 23% 36%



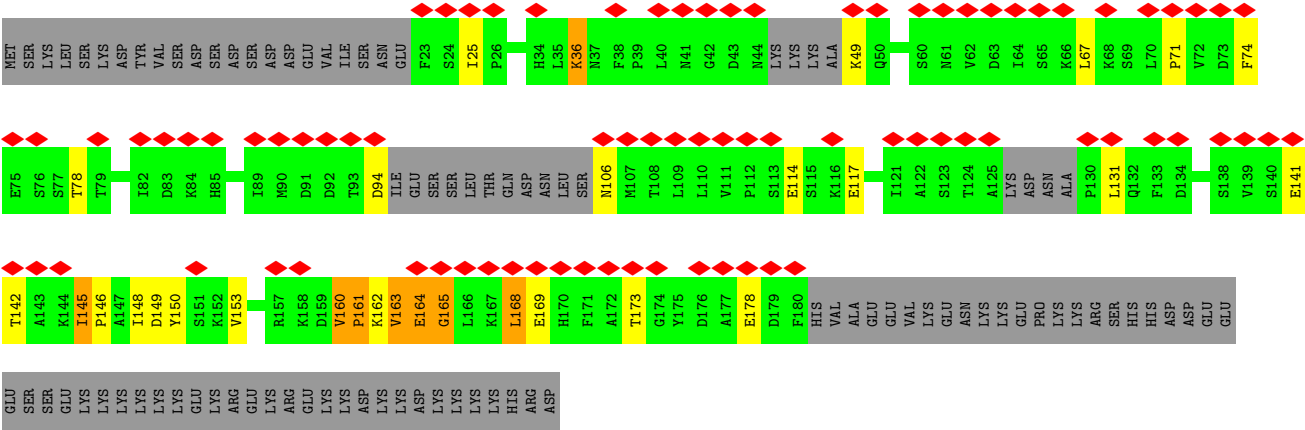
- Chain M: 



CYS
TYR
ILE
LEU
LYS
ALA
ILE
ILE
MET
HIS
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ASP
ASN
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ARG

● Molecule 14: DNA-directed RNA polymerase I subunit RPA34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.0	Depositor
Minimum defocus (nm)	1900.0	Depositor
Maximum defocus (nm)	4200.0	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	286.74, 286.74, 286.74	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.77, 1.77, 1.77	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.72	3/11408 (0.0%)	1.26	32/15405 (0.2%)
2	B	0.72	2/9062 (0.0%)	1.22	14/12249 (0.1%)
3	C	0.74	3/2469 (0.1%)	1.20	13/3347 (0.4%)
4	D	0.73	0/135	1.16	0/188
5	E	0.76	0/1795	1.20	6/2416 (0.2%)
6	F	0.73	0/838	1.22	0/1129
7	G	0.77	0/725	1.08	0/990
8	H	0.74	0/1090	1.00	0/1476
9	I	0.70	0/478	1.07	0/647
10	J	0.76	0/578	1.33	0/775
11	K	0.70	0/803	1.23	1/1083 (0.1%)
12	L	0.61	0/361	1.05	0/478
13	M	0.73	0/846	0.98	0/1136
14	N	0.75	2/1124 (0.2%)	1.03	4/1512 (0.3%)
All	All	0.73	10/31712 (0.0%)	1.21	70/42831 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	252	PRO	CA-C	5.48	1.54	1.51
1	A	1181	PRO	N-CD	5.38	1.55	1.47
2	B	693	PRO	N-CD	5.34	1.55	1.47
1	A	508	PRO	N-CD	5.06	1.54	1.47
3	C	221	PRO	N-CD	5.06	1.54	1.47
2	B	705	PRO	N-CD	5.06	1.54	1.47
14	N	146	PRO	N-CD	5.04	1.54	1.47
1	A	1502	PRO	N-CD	5.04	1.54	1.47
3	C	76	PRO	N-CD	5.03	1.54	1.47
14	N	161	PRO	N-CD	5.02	1.54	1.47

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	670	ILE	N-CA-C	7.63	118.13	111.56
3	C	173	GLY	CA-C-N	6.79	129.68	120.38
3	C	173	GLY	C-N-CA	6.79	129.68	120.38
1	A	1218	GLY	CA-C-N	6.63	124.42	120.24
1	A	1218	GLY	C-N-CA	6.63	124.42	120.24
3	C	151	THR	CA-C-N	6.13	129.40	120.51
3	C	151	THR	C-N-CA	6.13	129.40	120.51
2	B	1006	ASN	CA-C-N	5.89	128.45	120.38
2	B	1006	ASN	C-N-CA	5.89	128.45	120.38
3	C	121	PRO	CA-C-N	5.83	128.89	120.38
3	C	121	PRO	C-N-CA	5.83	128.89	120.38
1	A	365	THR	CA-C-N	5.81	128.34	120.38
1	A	365	THR	C-N-CA	5.81	128.34	120.38
1	A	1225	ILE	CA-C-N	5.78	127.84	120.56
1	A	1225	ILE	C-N-CA	5.78	127.84	120.56
1	A	1629	ASN	CA-C-N	5.65	128.87	120.90
1	A	1629	ASN	C-N-CA	5.65	128.87	120.90
1	A	1035	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	27	ASN	CA-CB-CG	5.61	118.21	112.60
3	C	124	GLU	CA-C-N	5.61	128.06	120.65
3	C	124	GLU	C-N-CA	5.61	128.06	120.65
2	B	167	SER	CA-C-N	5.60	128.05	120.38
2	B	167	SER	C-N-CA	5.60	128.05	120.38
2	B	751	ILE	N-CA-C	-5.47	105.39	110.53
2	B	692	THR	CA-C-N	-5.46	113.01	119.84
2	B	692	THR	C-N-CA	-5.46	113.01	119.84
1	A	1180	ASN	CA-C-N	-5.46	113.01	119.84
1	A	1180	ASN	C-N-CA	-5.46	113.01	119.84
11	K	69	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	627	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	1524	VAL	CA-C-N	5.32	128.78	121.33
1	A	1524	VAL	C-N-CA	5.32	128.78	121.33
1	A	852	ASP	CA-C-N	5.30	127.65	120.38
1	A	852	ASP	C-N-CA	5.30	127.65	120.38
1	A	1136	VAL	N-CA-CB	-5.28	103.56	112.44
1	A	691	GLN	CA-C-N	5.27	127.29	120.44
1	A	691	GLN	C-N-CA	5.27	127.29	120.44
2	B	863	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	340	HIS	CA-C-N	5.21	127.26	120.28
1	A	340	HIS	C-N-CA	5.21	127.26	120.28
2	B	834	LYS	CA-C-N	5.21	131.48	121.54
2	B	834	LYS	C-N-CA	5.21	131.48	121.54
3	C	220	SER	CA-C-N	-5.20	113.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	220	SER	C-N-CA	-5.20	113.34	119.84
1	A	1501	ILE	CA-C-N	-5.20	113.34	119.84
1	A	1501	ILE	C-N-CA	-5.20	113.34	119.84
14	N	160	VAL	CA-C-N	-5.18	113.36	119.84
14	N	160	VAL	C-N-CA	-5.18	113.36	119.84
3	C	75	VAL	CA-C-N	-5.17	113.38	119.84
3	C	75	VAL	C-N-CA	-5.17	113.38	119.84
2	B	704	THR	CA-C-N	-5.17	113.38	119.84
2	B	704	THR	C-N-CA	-5.17	113.38	119.84
14	N	145	ILE	CA-C-N	-5.17	113.38	119.84
14	N	145	ILE	C-N-CA	-5.17	113.38	119.84
2	B	75	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	507	TYR	CA-C-N	-5.16	113.39	119.84
1	A	507	TYR	C-N-CA	-5.16	113.39	119.84
1	A	670	ILE	CA-C-O	-5.12	115.81	120.73
1	A	39	ASP	CA-CB-CG	5.10	117.70	112.60
5	E	21	GLU	CA-C-N	5.10	127.07	120.44
5	E	21	GLU	C-N-CA	5.10	127.07	120.44
5	E	17	ARG	CA-C-N	5.08	127.08	120.28
5	E	17	ARG	C-N-CA	5.08	127.08	120.28
3	C	215	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	1554	GLY	CA-C-N	5.03	127.35	120.46
1	A	1554	GLY	C-N-CA	5.03	127.35	120.46
1	A	994	GLU	CA-C-N	5.00	126.95	120.44
1	A	994	GLU	C-N-CA	5.00	126.95	120.44
5	E	116	ILE	CA-C-N	5.00	127.34	120.39
5	E	116	ILE	C-N-CA	5.00	127.34	120.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11207	0	11249	530	0
2	B	8868	0	8734	476	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2418	0	2401	147	0
4	D	133	0	138	5	0
5	E	1759	0	1788	13	0
6	F	823	0	841	28	0
7	G	706	0	721	58	0
8	H	1072	0	1042	15	0
9	I	472	0	473	9	0
10	J	569	0	585	58	0
11	K	792	0	790	94	0
12	L	359	0	384	17	0
13	M	831	0	820	19	0
14	N	1103	0	1106	27	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	2	0
All	All	31118	0	31072	1026	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 (1026) 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)
2:B:697:LEU:HD11	2:B:984:TRP:CH2	1.23	1.65
2:B:697:LEU:HD11	2:B:984:TRP:CZ3	1.31	1.59
1:A:5:LYS:CB	2:B:1100:GLN:NE2	1.67	1.57
1:A:1660:VAL:CG2	7:G:105:ILE:HG23	1.10	1.56
3:C:37:LYS:HG3	11:K:134:LYS:CE	1.33	1.55
1:A:824:THR:CG2	2:B:1023:ARG:HD3	1.30	1.55
1:A:9:SER:HB3	2:B:1200:VAL:CG1	1.05	1.52
1:A:49:LEU:HD22	1:A:390:LEU:CD1	1.42	1.48
1:A:49:LEU:CD2	1:A:390:LEU:HD11	1.42	1.47
1:A:1660:VAL:HG21	7:G:105:ILE:CG2	1.02	1.47
1:A:35:PRO:CD	1:A:394:LEU:HD12	1.48	1.42
1:A:826:PHE:HA	2:B:1023:ARG:NH2	1.27	1.42
2:B:683:ASN:OD1	14:N:150:TYR:CE2	1.72	1.42
1:A:35:PRO:CD	1:A:394:LEU:CD1	1.97	1.41
1:A:367:PHE:CE1	2:B:1184:TYR:HA	1.57	1.38
2:B:697:LEU:CD1	2:B:984:TRP:CZ3	2.03	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:CB	2:B:1200:VAL:CG1	2.00	1.37
1:A:11:ILE:HD13	2:B:1198:TYR:CD1	1.57	1.36
1:A:49:LEU:CD2	1:A:390:LEU:CD1	2.00	1.36
3:C:37:LYS:CG	11:K:134:LYS:CE	2.01	1.36
2:B:342:PRO:O	13:M:112:LYS:CE	1.74	1.36
2:B:974:LEU:HD21	10:J:44:TYR:CD1	1.60	1.35
2:B:401:GLU:CD	2:B:647:SER:OG	1.67	1.35
1:A:1662:ASN:ND2	7:G:58:LEU:H	1.18	1.35
1:A:34:ASN:O	1:A:390:LEU:CD2	1.75	1.33
1:A:9:SER:HA	2:B:1201:GLU:O	1.22	1.33
3:C:142:ARG:HH21	10:J:67:GLU:CD	1.38	1.31
1:A:1:MET:HG2	2:B:1098:TYR:CE2	1.65	1.31
1:A:5:LYS:HB3	2:B:1100:GLN:NE2	1.01	1.31
2:B:494:TYR:CE1	2:B:762:MET:SD	2.25	1.30
2:B:342:PRO:O	13:M:112:LYS:HE3	1.14	1.27
1:A:1003:ARG:NH2	2:B:520:LEU:HD22	1.50	1.27
1:A:1659:LYS:CE	6:F:133:VAL:HG21	1.64	1.26
1:A:11:ILE:CG1	2:B:1198:TYR:HB3	1.65	1.25
3:C:37:LYS:CG	11:K:134:LYS:HE2	1.64	1.25
1:A:1662:ASN:HD22	7:G:58:LEU:N	1.35	1.24
1:A:824:THR:HG22	2:B:1023:ARG:CD	1.65	1.23
1:A:826:PHE:CA	2:B:1023:ARG:NH2	2.01	1.23
2:B:683:ASN:OD1	14:N:150:TYR:CZ	1.91	1.23
2:B:697:LEU:CD1	2:B:984:TRP:CH2	2.19	1.23
1:A:35:PRO:HD3	1:A:394:LEU:CD1	1.61	1.22
1:A:11:ILE:HA	2:B:1199:ASN:O	1.35	1.22
1:A:363:PRO:CG	2:B:1191:ALA:HB2	1.69	1.21
1:A:1660:VAL:HG22	7:G:105:ILE:N	1.57	1.19
1:A:76:GLN:NE2	2:B:1190:SER:HB3	1.55	1.18
2:B:494:TYR:CZ	2:B:762:MET:SD	2.36	1.17
1:A:35:PRO:CG	1:A:394:LEU:HD12	1.73	1.16
1:A:824:THR:CG2	2:B:1023:ARG:CD	2.21	1.15
1:A:34:ASN:C	1:A:390:LEU:HD22	1.70	1.15
1:A:49:LEU:HG	1:A:386:LEU:HB3	1.28	1.15
1:A:363:PRO:HG3	2:B:1191:ALA:CB	1.75	1.15
1:A:825:ALA:O	2:B:1023:ARG:NH2	1.79	1.15
1:A:1660:VAL:CG2	7:G:105:ILE:CG2	1.85	1.15
1:A:368:ARG:HG3	1:A:382:GLN:OE1	1.48	1.13
1:A:1048:PHE:HB2	5:E:208:TYR:OH	1.47	1.13
1:A:1003:ARG:HH12	2:B:520:LEU:CB	1.60	1.13
2:B:974:LEU:HD23	10:J:44:TYR:HB3	1.21	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:HD2	1:A:394:LEU:CD1	1.77	1.13
2:B:974:LEU:CD2	10:J:44:TYR:CD1	2.32	1.12
1:A:34:ASN:O	1:A:390:LEU:HD22	0.96	1.12
1:A:825:ALA:O	2:B:1023:ARG:NE	1.83	1.12
1:A:1260:LYS:HG3	1:A:1500:GLN:HB2	1.18	1.11
1:A:83:VAL:HG21	1:A:427:PHE:CE2	1.84	1.11
3:C:53:ASN:ND2	14:N:173:THR:HB	1.63	1.11
1:A:1660:VAL:HG21	7:G:105:ILE:HG21	1.28	1.11
3:C:37:LYS:HG3	11:K:134:LYS:HE3	1.15	1.11
1:A:5:LYS:HB3	2:B:1100:GLN:CD	1.75	1.10
1:A:83:VAL:HG21	1:A:427:PHE:CZ	1.86	1.10
1:A:825:ALA:O	2:B:1023:ARG:CZ	1.96	1.10
3:C:75:VAL:CG1	3:C:221:PRO:HG3	1.81	1.10
3:C:33:VAL:HG22	11:K:130:VAL:HG21	1.30	1.10
2:B:697:LEU:CD1	2:B:984:TRP:HZ3	1.50	1.10
1:A:368:ARG:CG	1:A:382:GLN:OE1	1.99	1.10
2:B:397:THR:HB	2:B:523:GLU:CB	1.80	1.10
2:B:207:ILE:HD13	2:B:402:VAL:HG22	1.33	1.10
3:C:37:LYS:CG	11:K:134:LYS:HE3	1.72	1.10
3:C:70:ILE:HG23	3:C:74:GLU:HG3	1.32	1.10
1:A:826:PHE:CA	2:B:1023:ARG:HH21	1.62	1.09
1:A:988:SER:C	2:B:988:GLU:OE1	1.83	1.09
9:I:6:SER:HA	9:I:45:LEU:HD13	1.18	1.09
1:A:1003:ARG:HH12	2:B:520:LEU:HB2	1.11	1.08
2:B:401:GLU:CG	2:B:647:SER:OG	2.01	1.08
1:A:934:LYS:NZ	2:B:956:SER:OG	1.87	1.07
3:C:314:PHE:CE2	11:K:135:PHE:CE1	2.42	1.07
1:A:35:PRO:CD	1:A:394:LEU:HD11	1.78	1.07
1:A:11:ILE:CD1	2:B:1198:TYR:CD1	2.38	1.06
3:C:333:ILE:HG23	11:K:47:ILE:HG12	1.35	1.06
1:A:9:SER:HB3	2:B:1200:VAL:HG13	1.14	1.05
1:A:1003:ARG:NH2	2:B:520:LEU:CD2	2.19	1.05
1:A:5:LYS:HB2	2:B:1100:GLN:NE2	1.68	1.05
1:A:11:ILE:HG12	2:B:1198:TYR:CB	1.87	1.04
1:A:363:PRO:HG3	2:B:1191:ALA:HB2	1.09	1.04
2:B:26:ILE:HA	10:J:62:ARG:HD2	1.33	1.04
3:C:314:PHE:CD2	11:K:135:PHE:CZ	2.45	1.04
1:A:1659:LYS:HD2	6:F:133:VAL:HG23	1.40	1.03
1:A:1663:ALA:CA	7:G:103:LYS:HD2	1.88	1.03
1:A:49:LEU:CD2	1:A:390:LEU:HD12	1.89	1.03
3:C:333:ILE:HA	11:K:47:ILE:CG2	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HB3	2:B:1200:VAL:HG11	1.34	1.02
2:B:345:SER:CB	13:M:111:PRO:O	2.07	1.02
2:B:697:LEU:HD12	2:B:984:TRP:HZ3	1.21	1.02
2:B:345:SER:HB2	13:M:111:PRO:O	1.57	1.02
2:B:401:GLU:OE1	2:B:647:SER:CB	2.08	1.02
3:C:322:LYS:HE3	11:K:129:ASP:OD1	1.57	1.02
1:A:1003:ARG:NH1	2:B:520:LEU:CB	2.23	1.01
3:C:37:LYS:HG3	11:K:134:LYS:HE2	1.02	1.01
3:C:222:VAL:HG23	3:C:303:GLU:O	1.58	1.01
3:C:328:LEU:CD1	11:K:72:LEU:HD11	1.91	1.01
1:A:10:GLU:O	2:B:1200:VAL:HA	1.59	1.01
1:A:759:TYR:OH	1:A:930:LEU:HD22	1.57	1.01
3:C:75:VAL:HG12	3:C:221:PRO:HG3	1.38	1.01
3:C:76:PRO:HB3	3:C:212:ILE:HG22	1.39	1.01
3:C:314:PHE:HE2	11:K:135:PHE:CE1	1.75	1.01
1:A:76:GLN:HE22	2:B:1190:SER:HB3	1.16	1.00
3:C:328:LEU:CD1	11:K:72:LEU:CD1	2.38	1.00
1:A:7:VAL:CG1	2:B:1176:VAL:HA	1.91	1.00
1:A:759:TYR:OH	1:A:930:LEU:CD2	2.10	1.00
1:A:934:LYS:NZ	2:B:956:SER:CB	2.24	1.00
1:A:1659:LYS:HE3	6:F:133:VAL:HG21	1.41	1.00
1:A:1660:VAL:HG23	7:G:105:ILE:HG23	1.39	1.00
1:A:1:MET:N	2:B:1098:TYR:CG	2.30	1.00
1:A:367:PHE:HD1	2:B:1184:TYR:HD1	1.03	0.99
12:L:48:CYS:SG	15:L:101:ZN:ZN	1.51	0.99
2:B:397:THR:HB	2:B:523:GLU:HB3	1.01	0.99
12:L:28:LYS:HB2	12:L:59:ALA:HB3	1.42	0.99
3:C:142:ARG:NH2	10:J:67:GLU:OE2	1.95	0.99
1:A:63:SER:O	2:B:1163:GLN:OE1	1.81	0.98
1:A:7:VAL:HG11	2:B:1176:VAL:HA	1.43	0.98
1:A:1663:ALA:HA	7:G:103:LYS:HD2	1.00	0.98
2:B:397:THR:CB	2:B:523:GLU:HB3	1.92	0.98
1:A:689:ARG:NH2	11:K:87:GLU:O	1.97	0.98
1:A:1501:ILE:HG13	1:A:1502:PRO:CD	1.93	0.98
3:C:70:ILE:HG23	3:C:74:GLU:CG	1.92	0.98
1:A:1603:MET:HE1	1:A:1615:TYR:CD2	1.97	0.98
2:B:25:PHE:CE1	2:B:764:ASN:OD1	2.16	0.98
1:A:1:MET:HA	2:B:1098:TYR:CD2	1.99	0.98
1:A:1663:ALA:HA	7:G:103:LYS:CD	1.94	0.98
1:A:1660:VAL:H	7:G:104:LEU:HA	1.26	0.97
1:A:11:ILE:CD1	2:B:1198:TYR:HB3	1.92	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:CG1	3:C:221:PRO:CG	2.42	0.97
1:A:9:SER:HB3	2:B:1200:VAL:HG12	1.01	0.97
2:B:211:ARG:HH22	2:B:243:GLN:NE2	1.61	0.97
1:A:1659:LYS:NZ	6:F:133:VAL:HG21	1.78	0.97
2:B:974:LEU:CD2	10:J:44:TYR:HB3	1.93	0.97
1:A:1:MET:HA	2:B:1098:TYR:CD1	2.00	0.97
1:A:1657:LEU:CD1	6:F:135:ARG:HD2	1.94	0.97
2:B:25:PHE:CZ	2:B:764:ASN:OD1	2.18	0.96
1:A:11:ILE:HG12	2:B:1198:TYR:HB3	0.99	0.96
3:C:142:ARG:NH2	10:J:67:GLU:CD	2.22	0.96
1:A:1660:VAL:CG2	7:G:105:ILE:CB	2.34	0.96
2:B:401:GLU:OE1	2:B:647:SER:HB3	1.62	0.96
1:A:1:MET:HA	2:B:1098:TYR:CG	2.00	0.96
1:A:1:MET:CA	2:B:1098:TYR:CG	2.49	0.96
1:A:9:SER:CA	2:B:1201:GLU:O	2.13	0.96
1:A:1654:PHE:HE2	6:F:92:ARG:HH11	1.09	0.96
1:A:367:PHE:CD1	2:B:1184:TYR:HD1	1.82	0.95
1:A:824:THR:HG23	2:B:1023:ARG:HD3	1.48	0.95
1:A:200:GLY:O	5:E:171:LYS:NZ	2.00	0.95
2:B:401:GLU:OE1	2:B:647:SER:OG	1.84	0.95
1:A:989:GLY:N	2:B:988:GLU:OE1	1.99	0.95
1:A:367:PHE:HE1	2:B:1184:TYR:HA	1.18	0.94
3:C:334:THR:HG21	11:K:44:ARG:HB3	1.47	0.94
1:A:1660:VAL:HG21	7:G:105:ILE:CB	1.89	0.94
1:A:1660:VAL:HG22	7:G:105:ILE:HG23	1.49	0.94
1:A:1662:ASN:ND2	7:G:58:LEU:N	2.02	0.94
1:A:8:GLY:O	2:B:1202:PRO:HD3	1.68	0.94
2:B:527:PHE:CE2	2:B:651:ARG:HD3	2.04	0.93
3:C:142:ARG:NH2	10:J:67:GLU:OE1	2.02	0.93
1:A:1003:ARG:HH22	2:B:520:LEU:HD22	1.09	0.93
1:A:76:GLN:NE2	2:B:1190:SER:CB	2.31	0.93
3:C:37:LYS:HG2	11:K:134:LYS:CE	1.97	0.93
1:A:1316:VAL:HG21	1:A:1498:ILE:HG23	1.50	0.93
4:D:24:ALA:O	6:F:55:PRO:HA	1.69	0.92
2:B:211:ARG:HD3	2:B:239:VAL:HG21	1.48	0.92
3:C:53:ASN:ND2	14:N:173:THR:CB	2.31	0.92
1:A:1:MET:CG	2:B:1098:TYR:CE2	2.52	0.92
2:B:494:TYR:OH	2:B:762:MET:SD	2.28	0.92
2:B:26:ILE:HA	10:J:62:ARG:CD	1.99	0.92
1:A:12:THR:HG21	2:B:1201:GLU:OE2	1.70	0.91
2:B:974:LEU:CD2	10:J:44:TYR:HD1	1.78	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:CA	2:B:1199:ASN:O	2.16	0.91
1:A:1003:ARG:NH1	2:B:520:LEU:HB3	1.83	0.91
2:B:209:GLN:HG2	2:B:210:ARG:H	1.35	0.91
1:A:1:MET:HA	2:B:1098:TYR:CE2	2.05	0.91
1:A:1657:LEU:HD13	6:F:135:ARG:HD2	1.50	0.91
3:C:33:VAL:CG2	11:K:130:VAL:HG21	2.00	0.91
1:A:1603:MET:HE1	1:A:1615:TYR:CG	2.06	0.91
14:N:149:ASP:O	14:N:153:VAL:HG12	1.69	0.91
1:A:1:MET:CA	2:B:1098:TYR:CD2	2.54	0.90
2:B:529:CYS:SG	2:B:698:SER:HB2	2.10	0.90
1:A:13:SER:O	2:B:1199:ASN:OD1	1.89	0.90
1:A:1659:LYS:HD2	6:F:133:VAL:CG2	2.01	0.90
1:A:363:PRO:CG	2:B:1191:ALA:CB	2.42	0.89
1:A:1003:ARG:NH1	2:B:520:LEU:HB2	1.86	0.89
1:A:367:PHE:CE1	2:B:1184:TYR:CA	2.53	0.89
1:A:759:TYR:HD1	1:A:920:PHE:CD2	1.90	0.89
11:K:59:THR:O	11:K:113:ALA:HB2	1.72	0.89
1:A:35:PRO:HD3	1:A:394:LEU:HD11	1.40	0.89
1:A:34:ASN:O	1:A:390:LEU:CG	2.20	0.89
1:A:1659:LYS:CE	6:F:133:VAL:CG2	2.51	0.89
2:B:14:ALA:HB3	2:B:755:ASN:HD21	1.37	0.89
1:A:824:THR:HG22	2:B:1023:ARG:HD3	0.89	0.88
1:A:1:MET:HA	2:B:1098:TYR:CE1	2.08	0.88
1:A:1260:LYS:HG3	1:A:1500:GLN:CB	2.04	0.88
1:A:934:LYS:NZ	2:B:956:SER:HB2	1.87	0.88
2:B:211:ARG:NH2	2:B:243:GLN:HE22	1.72	0.88
1:A:1659:LYS:NZ	6:F:133:VAL:CG2	2.37	0.88
1:A:1654:PHE:CE2	6:F:92:ARG:NH1	2.42	0.87
1:A:1003:ARG:HH22	2:B:520:LEU:CD2	1.81	0.87
2:B:99:VAL:HG21	2:B:417:ILE:HD11	1.55	0.87
3:C:314:PHE:HD2	11:K:135:PHE:CZ	1.91	0.87
1:A:11:ILE:HD13	2:B:1198:TYR:HD1	0.96	0.87
2:B:525:TRP:CZ2	2:B:696:ILE:HG21	2.10	0.87
3:C:53:ASN:HD21	14:N:173:THR:CB	1.88	0.87
1:A:35:PRO:HG2	1:A:394:LEU:HD12	1.55	0.87
1:A:49:LEU:CG	1:A:386:LEU:HB3	2.04	0.87
2:B:401:GLU:CD	2:B:647:SER:CB	2.47	0.87
1:A:367:PHE:HD1	2:B:1184:TYR:CD1	1.93	0.87
3:C:328:LEU:HD12	11:K:72:LEU:CD1	2.04	0.87
2:B:974:LEU:HD23	10:J:44:TYR:CB	2.04	0.87
1:A:825:ALA:C	2:B:1023:ARG:HH21	1.81	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ARG:HG2	1:A:382:GLN:OE1	1.76	0.86
14:N:163:VAL:HG12	14:N:164:GLU:H	1.41	0.86
1:A:35:PRO:HD2	1:A:394:LEU:HD11	1.47	0.86
1:A:834:ARG:HH22	2:B:994:ASP:CG	1.83	0.86
2:B:209:GLN:HG2	2:B:210:ARG:N	1.91	0.86
3:C:37:LYS:O	11:K:134:LYS:NZ	2.07	0.86
3:C:315:PHE:CE1	11:K:135:PHE:HD2	1.94	0.86
3:C:333:ILE:HA	11:K:47:ILE:HG23	1.54	0.86
1:A:1:MET:HG2	2:B:1098:TYR:HE2	1.35	0.85
1:A:1659:LYS:HG2	7:G:104:LEU:HB3	1.58	0.85
2:B:398:GLN:HG3	2:B:399:HIS:CE1	2.11	0.85
2:B:697:LEU:HD11	2:B:984:TRP:HH2	1.13	0.85
1:A:1:MET:HA	2:B:1098:TYR:CZ	2.10	0.85
1:A:718:THR:HG21	8:H:119:GLY:HA3	1.56	0.85
2:B:404:LEU:HD21	2:B:551:ILE:HD13	1.57	0.85
1:A:1:MET:CB	2:B:1098:TYR:CD2	2.59	0.85
9:I:6:SER:HA	9:I:45:LEU:CD1	2.05	0.85
1:A:8:GLY:O	2:B:1202:PRO:CD	2.25	0.85
1:A:76:GLN:HE22	2:B:1190:SER:CB	1.87	0.85
3:C:314:PHE:CE2	11:K:135:PHE:CZ	2.65	0.85
2:B:26:ILE:HG23	10:J:62:ARG:HH11	1.42	0.84
3:C:328:LEU:CD1	11:K:72:LEU:HD13	2.07	0.84
3:C:335:GLN:HB3	11:K:49:LEU:H	1.40	0.84
1:A:9:SER:CB	2:B:1200:VAL:HG12	1.83	0.84
2:B:128:GLN:HB3	12:L:55:ILE:HD13	1.59	0.84
1:A:1:MET:HE3	2:B:1094:ASN:ND2	1.91	0.84
1:A:49:LEU:HG	1:A:386:LEU:CB	2.07	0.84
2:B:14:ALA:CB	2:B:755:ASN:ND2	2.41	0.84
9:I:6:SER:CA	9:I:45:LEU:HD13	2.04	0.84
1:A:1:MET:CB	2:B:1094:ASN:OD1	2.26	0.84
2:B:494:TYR:HE1	2:B:762:MET:SD	2.00	0.84
1:A:1501:ILE:HG13	1:A:1502:PRO:HD2	1.58	0.83
12:L:48:CYS:HG	15:L:101:ZN:ZN	0.87	0.83
3:C:333:ILE:HA	11:K:47:ILE:HG21	1.59	0.83
3:C:333:ILE:HG23	11:K:47:ILE:CG1	2.07	0.83
3:C:335:GLN:O	11:K:49:LEU:HB3	1.77	0.83
1:A:1606:SER:OG	1:A:1611:MET:HE1	1.78	0.82
2:B:208:VAL:O	2:B:401:GLU:N	2.09	0.82
2:B:211:ARG:HH22	2:B:243:GLN:HE22	0.87	0.82
1:A:654:ASP:O	1:A:656:GLN:N	2.12	0.82
1:A:824:THR:HA	2:B:1023:ARG:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1654:PHE:HE2	6:F:92:ARG:NH1	1.77	0.82
1:A:7:VAL:HG21	2:B:1177:ALA:N	1.94	0.82
2:B:527:PHE:CZ	2:B:651:ARG:HD3	2.15	0.82
2:B:401:GLU:CB	2:B:647:SER:OG	2.27	0.81
1:A:722:PRO:HG2	8:H:46:LEU:HD13	1.61	0.81
1:A:722:PRO:CG	8:H:46:LEU:HD13	2.11	0.81
3:C:75:VAL:HG12	3:C:221:PRO:CG	2.10	0.81
14:N:162:LYS:N	14:N:162:LYS:HD2	1.96	0.81
1:A:651:ALA:O	1:A:652:ASN:O	1.97	0.80
3:C:37:LYS:CA	11:K:134:LYS:HE3	2.11	0.80
2:B:211:ARG:HD3	2:B:239:VAL:CG2	2.10	0.80
3:C:33:VAL:HG22	11:K:130:VAL:CG2	2.12	0.80
2:B:401:GLU:HB2	2:B:647:SER:OG	1.81	0.80
1:A:1:MET:N	2:B:1098:TYR:CB	2.45	0.80
1:A:7:VAL:HG21	2:B:1177:ALA:H	1.46	0.80
1:A:489:ASN:HB3	11:K:95:HIS:HD2	1.46	0.80
2:B:494:TYR:CZ	2:B:762:MET:CE	2.65	0.80
2:B:26:ILE:CA	10:J:62:ARG:HD2	2.12	0.79
1:A:1660:VAL:HG22	7:G:105:ILE:CB	2.08	0.79
1:A:722:PRO:HD2	8:H:46:LEU:HD13	1.63	0.79
2:B:398:GLN:HG3	2:B:399:HIS:ND1	1.98	0.78
2:B:525:TRP:CH2	2:B:696:ILE:HG21	2.19	0.78
1:A:367:PHE:CD1	2:B:1184:TYR:CD1	2.70	0.77
1:A:826:PHE:HA	2:B:1023:ARG:HH22	0.97	0.77
1:A:9:SER:CB	2:B:1200:VAL:HG13	1.89	0.77
1:A:489:ASN:CB	11:K:95:HIS:HD2	1.97	0.77
1:A:1600:ARG:HD2	1:A:1616:GLU:OE2	1.84	0.77
1:A:1659:LYS:CD	6:F:133:VAL:CG2	2.63	0.77
2:B:527:PHE:CE1	2:B:651:ARG:HB3	2.18	0.77
3:C:222:VAL:CG2	3:C:303:GLU:O	2.30	0.77
1:A:832:ASP:C	1:A:833:LEU:HD12	2.09	0.77
2:B:14:ALA:HB1	2:B:755:ASN:ND2	2.00	0.77
2:B:974:LEU:HD21	10:J:44:TYR:HD1	1.07	0.77
1:A:1:MET:HB3	2:B:1094:ASN:CG	2.10	0.77
1:A:1260:LYS:NZ	1:A:1262:LEU:HD11	1.98	0.77
1:A:1:MET:H1	2:B:1098:TYR:CB	1.98	0.76
2:B:14:ALA:CB	2:B:755:ASN:HD21	1.99	0.76
1:A:367:PHE:HE1	2:B:1184:TYR:CA	1.96	0.76
3:C:328:LEU:HD12	11:K:72:LEU:HD11	1.62	0.76
9:I:5:GLY:O	9:I:45:LEU:HD22	1.85	0.75
1:A:1660:VAL:HG22	7:G:105:ILE:CA	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:CB	2:B:1200:VAL:HG11	2.00	0.75
2:B:494:TYR:OH	2:B:762:MET:CG	2.35	0.74
1:A:1:MET:CA	2:B:1098:TYR:CD1	2.68	0.74
1:A:1260:LYS:CG	1:A:1500:GLN:HB2	2.10	0.74
1:A:1659:LYS:CD	6:F:133:VAL:HG21	2.17	0.74
3:C:75:VAL:HG11	3:C:221:PRO:CG	2.15	0.74
1:A:1:MET:HG3	2:B:1094:ASN:OD1	1.87	0.74
3:C:37:LYS:HA	11:K:134:LYS:HE3	1.69	0.74
1:A:11:ILE:CD1	2:B:1198:TYR:CB	2.66	0.74
1:A:11:ILE:CD1	2:B:1198:TYR:CG	2.71	0.74
1:A:1657:LEU:CG	7:G:106:LYS:HG3	2.17	0.74
1:A:19:LEU:HD12	2:B:1193:GLY:C	2.12	0.74
14:N:168:LEU:O	14:N:169:GLU:HG3	1.88	0.73
1:A:49:LEU:HD21	1:A:390:LEU:CD1	2.12	0.73
3:C:328:LEU:HD11	11:K:72:LEU:HD13	1.71	0.73
1:A:7:VAL:HG13	2:B:1175:THR:O	1.87	0.73
1:A:722:PRO:CD	8:H:46:LEU:HD13	2.18	0.73
2:B:209:GLN:C	2:B:400:GLN:HA	2.13	0.73
1:A:363:PRO:HG2	2:B:1191:ALA:HB2	1.67	0.73
1:A:824:THR:HG23	2:B:1023:ARG:CG	2.18	0.72
3:C:328:LEU:HD13	11:K:72:LEU:HD11	1.71	0.72
1:A:1048:PHE:CB	5:E:208:TYR:OH	2.32	0.72
1:A:1606:SER:CB	1:A:1611:MET:HE1	2.19	0.72
2:B:44:PRO:CB	2:B:551:ILE:HD12	2.20	0.72
3:C:75:VAL:CB	3:C:221:PRO:HG3	2.19	0.72
1:A:1:MET:CE	2:B:1094:ASN:HD21	2.02	0.72
2:B:209:GLN:HA	2:B:400:GLN:HA	1.71	0.72
1:A:35:PRO:HD3	1:A:394:LEU:CG	2.18	0.72
2:B:1005:TYR:HH	10:J:44:TYR:HE1	1.37	0.72
1:A:7:VAL:HG13	2:B:1176:VAL:HA	1.71	0.72
1:A:759:TYR:HB3	1:A:920:PHE:CE2	2.25	0.72
1:A:759:TYR:OH	1:A:930:LEU:HD21	1.90	0.72
3:C:37:LYS:CB	11:K:134:LYS:HE3	2.19	0.71
1:A:759:TYR:HB3	1:A:920:PHE:HE2	1.55	0.71
2:B:14:ALA:O	2:B:755:ASN:OD1	2.08	0.71
1:A:1179:ILE:HG13	1:A:1180:ASN:N	2.04	0.71
1:A:826:PHE:CB	2:B:1023:ARG:NH2	2.52	0.71
1:A:988:SER:O	2:B:988:GLU:CA	2.39	0.71
2:B:342:PRO:O	13:M:112:LYS:HE2	1.83	0.71
1:A:1179:ILE:HG13	1:A:1180:ASN:H	1.55	0.71
3:C:328:LEU:HB3	11:K:121:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CE1	1:A:383:ASN:OD1	2.37	0.71
1:A:759:TYR:CD1	1:A:920:PHE:CD2	2.76	0.71
1:A:63:SER:O	2:B:1163:GLN:CD	2.33	0.71
1:A:489:ASN:CB	11:K:95:HIS:CD2	2.74	0.70
1:A:759:TYR:CZ	1:A:930:LEU:HD22	2.26	0.70
1:A:1660:VAL:N	7:G:104:LEU:HA	2.05	0.70
3:C:71:MET:HG3	3:C:317:SER:HB3	1.73	0.70
1:A:597:LYS:HB2	2:B:1082:HIS:CE1	2.27	0.70
1:A:993:GLN:NE2	2:B:680:GLU:OE2	2.24	0.70
2:B:345:SER:CA	13:M:111:PRO:O	2.39	0.70
3:C:70:ILE:HG23	3:C:74:GLU:CB	2.22	0.70
3:C:71:MET:SD	3:C:314:PHE:HA	2.31	0.70
1:A:76:GLN:HE21	2:B:1190:SER:HB3	1.53	0.69
1:A:1260:LYS:HZ2	1:A:1262:LEU:HD11	1.57	0.69
1:A:818:THR:O	1:A:821:ILE:HG22	1.92	0.69
3:C:335:GLN:O	11:K:49:LEU:CB	2.40	0.69
1:A:34:ASN:C	1:A:390:LEU:CD2	2.49	0.69
1:A:1663:ALA:CB	7:G:103:LYS:NZ	2.56	0.69
2:B:401:GLU:HB2	2:B:647:SER:O	1.91	0.69
1:A:826:PHE:N	2:B:1023:ARG:HH21	1.88	0.69
2:B:397:THR:CB	2:B:523:GLU:CB	2.60	0.69
1:A:1:MET:HB2	2:B:1094:ASN:HA	1.75	0.69
1:A:1023:LEU:HB3	1:A:1190:SER:HB3	1.74	0.69
1:A:1:MET:N	2:B:1098:TYR:HB3	2.07	0.68
1:A:10:GLU:O	2:B:1199:ASN:O	2.11	0.68
1:A:759:TYR:CE1	1:A:930:LEU:HD13	2.29	0.68
2:B:44:PRO:CG	2:B:551:ILE:HD12	2.22	0.68
2:B:342:PRO:O	13:M:112:LYS:CD	2.42	0.68
3:C:44:ILE:HD13	11:K:142:MET:SD	2.34	0.68
3:C:71:MET:HG3	3:C:317:SER:CB	2.24	0.68
2:B:974:LEU:CD2	10:J:44:TYR:CG	2.76	0.68
1:A:1:MET:HB2	2:B:1098:TYR:CD2	2.29	0.68
2:B:208:VAL:HG23	2:B:401:GLU:CG	2.24	0.68
1:A:11:ILE:HD13	2:B:1198:TYR:CG	2.25	0.68
1:A:1:MET:CG	2:B:1094:ASN:OD1	2.42	0.67
1:A:49:LEU:HD23	1:A:390:LEU:HD12	1.75	0.67
1:A:367:PHE:CZ	2:B:1187:SER:HB2	2.01	0.67
3:C:229:LEU:HB3	3:C:293:ARG:HG2	1.76	0.67
1:A:64:THR:HG23	2:B:1129:ARG:NH1	2.10	0.67
1:A:693:GLN:HB3	11:K:88:PHE:CE2	2.29	0.67
1:A:1:MET:CE	2:B:1094:ASN:ND2	2.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:THR:HG23	2:B:1023:ARG:CD	2.12	0.67
12:L:28:LYS:NZ	12:L:60:ARG:O	2.18	0.67
3:C:221:PRO:HD2	3:C:222:VAL:H	1.59	0.67
2:B:697:LEU:CD1	2:B:984:TRP:HH2	1.84	0.67
2:B:210:ARG:N	2:B:400:GLN:HA	2.10	0.67
2:B:404:LEU:HD21	2:B:551:ILE:HG21	1.76	0.67
1:A:826:PHE:CB	2:B:1023:ARG:HH21	2.07	0.67
14:N:162:LYS:HD2	14:N:162:LYS:H	1.58	0.67
2:B:555:GLN:HB3	2:B:644:GLY:O	1.94	0.66
2:B:1005:TYR:CZ	10:J:44:TYR:HE1	2.13	0.66
3:C:329:LYS:NZ	11:K:125:MET:CE	2.54	0.66
11:K:54:THR:HG23	11:K:61:ALA:HB2	1.75	0.66
1:A:34:ASN:O	1:A:390:LEU:CD1	2.43	0.66
1:A:1622:LEU:HD21	2:B:1194:ILE:HD13	1.78	0.66
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.77	0.66
3:C:53:ASN:HD22	14:N:173:THR:HB	1.58	0.66
1:A:35:PRO:HD2	1:A:394:LEU:HD12	1.49	0.66
1:A:1038:ILE:HB	1:A:1047:GLN:HB2	1.78	0.66
2:B:44:PRO:HB3	2:B:551:ILE:HD12	1.76	0.66
1:A:83:VAL:HG11	1:A:427:PHE:HZ	1.61	0.66
1:A:1504:ILE:HG22	1:A:1505:ASP:N	2.11	0.66
1:A:34:ASN:O	1:A:390:LEU:HD13	1.96	0.66
1:A:1622:LEU:HD21	2:B:1194:ILE:CD1	2.26	0.66
2:B:25:PHE:CZ	10:J:59:LYS:HE2	2.29	0.66
1:A:988:SER:O	2:B:988:GLU:CB	2.44	0.66
2:B:210:ARG:NH2	2:B:648:ARG:HA	2.11	0.66
1:A:825:ALA:C	2:B:1023:ARG:NH2	2.46	0.65
2:B:345:SER:HA	13:M:111:PRO:O	1.96	0.65
2:B:1019:GLY:HA3	3:C:65:ASN:ND2	2.11	0.65
1:A:824:THR:HG22	2:B:1023:ARG:NE	2.12	0.65
1:A:1660:VAL:HG22	7:G:104:LEU:C	2.20	0.65
1:A:1657:LEU:CB	7:G:106:LYS:HG3	2.27	0.65
1:A:10:GLU:C	2:B:1200:VAL:HA	2.22	0.65
1:A:581:ILE:HD11	1:A:605:VAL:HG21	1.78	0.65
1:A:655:SER:O	1:A:656:GLN:NE2	2.30	0.64
1:A:1659:LYS:HA	7:G:104:LEU:CB	2.27	0.64
2:B:209:GLN:CA	2:B:400:GLN:HA	2.28	0.64
2:B:210:ARG:O	2:B:237:ARG:NH1	2.31	0.64
1:A:1:MET:CB	2:B:1094:ASN:CG	2.69	0.64
1:A:1659:LYS:HZ2	6:F:133:VAL:CG2	2.08	0.64
2:B:886:ASN:OD1	12:L:57:LEU:HD23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:H	2:B:1201:GLU:H	1.45	0.64
1:A:1260:LYS:HG2	1:A:1261:VAL:N	2.11	0.64
1:A:1663:ALA:HB1	7:G:103:LYS:NZ	2.13	0.64
1:A:697:TYR:CE2	11:K:92:SER:HB2	2.33	0.64
2:B:25:PHE:HE2	10:J:56:LEU:HD23	1.63	0.64
1:A:19:LEU:HD12	2:B:1193:GLY:O	1.98	0.64
2:B:399:HIS:O	2:B:400:GLN:HB3	1.96	0.64
2:B:190:ILE:HD13	2:B:190:ILE:H	1.63	0.64
2:B:404:LEU:CD2	2:B:551:ILE:HD13	2.26	0.64
2:B:699:ILE:HG23	2:B:760:TYR:CE2	2.32	0.64
1:A:1034:TYR:HA	1:A:1181:PRO:HG2	1.80	0.63
2:B:974:LEU:CD2	10:J:44:TYR:CB	2.69	0.63
2:B:974:LEU:CG	10:J:44:TYR:HB3	2.29	0.63
2:B:1016:GLY:O	3:C:69:ARG:NH2	2.30	0.63
3:C:315:PHE:CE1	11:K:135:PHE:CD2	2.81	0.63
1:A:368:ARG:HE	1:A:386:LEU:HD11	1.62	0.63
1:A:913:PRO:HB3	1:A:926:GLN:HE22	1.63	0.63
2:B:208:VAL:HG23	2:B:401:GLU:HG3	1.81	0.63
2:B:494:TYR:OH	2:B:762:MET:HG3	1.99	0.63
2:B:697:LEU:HD21	2:B:984:TRP:HH2	1.64	0.63
1:A:367:PHE:CZ	2:B:1187:SER:CB	2.55	0.63
2:B:211:ARG:CD	2:B:239:VAL:HG21	2.28	0.63
1:A:1:MET:N	2:B:1098:TYR:CD1	2.60	0.63
1:A:1608:SER:HB2	1:A:1636:SER:HB3	1.80	0.63
3:C:79:ALA:HA	3:C:106:LEU:HD11	1.79	0.63
2:B:998:GLU:O	2:B:1002:LYS:HG2	1.99	0.63
1:A:1:MET:HB2	2:B:1094:ASN:OD1	1.99	0.62
3:C:75:VAL:HG11	3:C:221:PRO:HG2	1.80	0.62
1:A:1663:ALA:HB1	7:G:103:LYS:HZ3	1.63	0.62
2:B:210:ARG:HH12	2:B:648:ARG:HG2	1.64	0.62
1:A:713:VAL:H	1:A:738:ASN:HD21	1.47	0.62
2:B:16:PHE:HB3	2:B:753:LYS:NZ	2.14	0.62
11:K:59:THR:HG22	11:K:107:THR:OG1	2.00	0.62
1:A:37:VAL:HG13	1:A:387:SER:OG	1.99	0.62
14:N:160:VAL:HG12	14:N:161:PRO:HD2	1.82	0.62
1:A:824:THR:HG21	2:B:1023:ARG:HD3	1.64	0.62
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.33	0.62
3:C:142:ARG:CZ	10:J:67:GLU:OE2	2.48	0.62
4:D:24:ALA:O	6:F:55:PRO:CA	2.46	0.62
1:A:833:LEU:HD12	1:A:833:LEU:N	2.15	0.62
3:C:329:LYS:NZ	11:K:125:MET:HE2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:CG2	10:J:62:ARG:HH11	2.12	0.62
14:N:160:VAL:HG12	14:N:161:PRO:CD	2.30	0.62
3:C:71:MET:C	3:C:72:ILE:HG13	2.24	0.62
1:A:701:ARG:H	1:A:706:HIS:HD2	1.46	0.61
1:A:988:SER:O	2:B:988:GLU:HA	1.99	0.61
3:C:335:GLN:HB3	11:K:49:LEU:N	2.14	0.61
1:A:363:PRO:HG3	2:B:1191:ALA:CA	2.30	0.61
2:B:335:ARG:NH2	13:M:114:LYS:C	2.58	0.61
2:B:558:VAL:HA	2:B:561:ILE:HD12	1.80	0.61
1:A:1608:SER:CB	1:A:1636:SER:HB3	2.29	0.61
2:B:25:PHE:HE2	10:J:56:LEU:CD2	2.14	0.61
3:C:79:ALA:HA	3:C:106:LEU:CD1	2.29	0.61
3:C:322:LYS:CE	11:K:129:ASP:OD1	2.43	0.61
1:A:1:MET:HG2	2:B:1098:TYR:CD2	2.33	0.61
1:A:368:ARG:HE	1:A:386:LEU:CD1	2.13	0.61
2:B:494:TYR:CZ	2:B:762:MET:HE3	2.36	0.61
2:B:527:PHE:CZ	2:B:651:ARG:CG	2.84	0.61
3:C:335:GLN:HB2	11:K:48:LYS:HG2	1.82	0.61
1:A:1600:ARG:HG3	1:A:1615:TYR:HE2	1.66	0.61
3:C:76:PRO:HB3	3:C:212:ILE:CG2	2.24	0.61
3:C:329:LYS:HD2	11:K:122:LYS:HA	1.82	0.61
1:A:9:SER:C	2:B:1200:VAL:HG13	2.26	0.61
1:A:1659:LYS:HA	7:G:104:LEU:HB2	1.83	0.61
2:B:494:TYR:HE2	2:B:703:LEU:HD13	1.64	0.61
1:A:1657:LEU:HD11	6:F:135:ARG:HD2	1.79	0.60
2:B:211:ARG:HG3	2:B:211:ARG:O	2.00	0.60
1:A:1003:ARG:CZ	2:B:520:LEU:HB3	2.31	0.60
2:B:683:ASN:OD1	14:N:150:TYR:OH	2.18	0.60
3:C:44:ILE:CD1	11:K:142:MET:SD	2.88	0.60
2:B:527:PHE:CZ	2:B:651:ARG:HG2	2.37	0.60
14:N:149:ASP:O	14:N:153:VAL:CG1	2.48	0.60
3:C:275:VAL:HG21	3:C:293:ARG:HH21	1.66	0.60
1:A:697:TYR:CD2	11:K:92:SER:HB2	2.37	0.60
3:C:334:THR:H	11:K:47:ILE:HG23	1.67	0.60
1:A:1600:ARG:CD	1:A:1616:GLU:OE2	2.49	0.60
2:B:494:TYR:CE1	2:B:762:MET:CE	2.84	0.60
2:B:527:PHE:HE1	2:B:650:LEU:C	2.10	0.60
2:B:128:GLN:CB	12:L:55:ILE:HD13	2.30	0.60
1:A:507:TYR:HE1	1:A:639:GLN:HA	1.68	0.59
3:C:334:THR:CB	11:K:47:ILE:O	2.49	0.59
1:A:785:GLN:HB3	1:A:793:ILE:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1556:GLU:OE2	5:E:200:ARG:NH1	2.35	0.59
1:A:1503:HIS:C	1:A:1504:ILE:HG13	2.26	0.59
3:C:37:LYS:HG2	11:K:134:LYS:NZ	2.16	0.59
13:M:61:GLU:HB3	13:M:101:VAL:HG23	1.84	0.59
2:B:52:LEU:HG	2:B:61:LEU:HD13	1.84	0.59
2:B:683:ASN:OD1	14:N:150:TYR:HE2	1.69	0.59
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.82	0.59
10:J:48:ARG:O	10:J:52:THR:HB	2.01	0.59
2:B:527:PHE:CZ	2:B:651:ARG:CD	2.85	0.59
3:C:332:PRO:O	11:K:47:ILE:CG2	2.50	0.59
3:C:75:VAL:HB	3:C:221:PRO:HG3	1.84	0.59
5:E:147:HIS:HD2	5:E:149:LEU:H	1.50	0.59
12:L:28:LYS:HB2	12:L:59:ALA:CB	2.26	0.59
1:A:83:VAL:CG2	1:A:427:PHE:CE2	2.75	0.59
1:A:1659:LYS:CG	7:G:104:LEU:HB3	2.32	0.59
3:C:71:MET:O	3:C:222:VAL:HG11	2.03	0.58
1:A:506:THR:HA	1:A:580:HIS:HA	1.85	0.58
1:A:35:PRO:O	1:A:387:SER:HA	2.02	0.58
1:A:507:TYR:CD2	1:A:508:PRO:HD2	2.38	0.58
2:B:412:ILE:HG23	2:B:461:MET:HE1	1.85	0.58
3:C:142:ARG:NE	10:J:67:GLU:OE2	2.37	0.58
1:A:934:LYS:HZ3	2:B:956:SER:HB2	1.67	0.58
1:A:527:PRO:HG2	1:A:547:ILE:HA	1.85	0.58
1:A:727:THR:HG22	1:A:730:GLN:HG3	1.85	0.58
1:A:1003:ARG:CZ	2:B:520:LEU:CB	2.80	0.58
2:B:839:LYS:HG3	2:B:857:PRO:HD2	1.86	0.58
2:B:974:LEU:HG	10:J:44:TYR:CG	2.39	0.58
1:A:32:ILE:HG22	1:A:390:LEU:HD21	1.84	0.58
1:A:332:GLN:HE22	1:A:350:VAL:H	1.52	0.58
1:A:1502:PRO:O	1:A:1503:HIS:HB2	2.03	0.58
2:B:400:GLN:O	2:B:649:MET:CE	2.51	0.58
3:C:332:PRO:HG2	11:K:42:PRO:HB2	1.85	0.58
2:B:656:LEU:HD23	14:N:148:ILE:HD13	1.86	0.57
2:B:210:ARG:NH1	2:B:648:ARG:HG2	2.18	0.57
2:B:938:PHE:CZ	3:C:68:ARG:CZ	2.87	0.57
3:C:328:LEU:HD11	11:K:72:LEU:CD1	2.29	0.57
1:A:952:LEU:HD21	1:A:1000:MET:HB3	1.85	0.57
2:B:398:GLN:CG	2:B:399:HIS:CE1	2.86	0.57
2:B:974:LEU:HA	10:J:44:TYR:HB3	1.84	0.57
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.86	0.57
1:A:1662:ASN:HD21	7:G:58:LEU:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1662:ASN:ND2	7:G:58:LEU:CB	2.67	0.57
1:A:1662:ASN:ND2	7:G:58:LEU:HB2	2.20	0.57
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.86	0.57
1:A:1610:PHE:CD2	1:A:1632:GLU:HG2	2.40	0.57
1:A:1:MET:HE2	2:B:1094:ASN:HD21	1.68	0.57
2:B:840:LEU:HD21	2:B:857:PRO:HB2	1.87	0.57
1:A:10:GLU:O	2:B:1200:VAL:CA	2.46	0.56
1:A:579:ARG:NH1	1:A:580:HIS:O	2.38	0.56
2:B:26:ILE:O	10:J:62:ARG:NE	2.38	0.56
3:C:70:ILE:CG2	3:C:74:GLU:HG3	2.21	0.56
3:C:78:VAL:HG22	3:C:210:LEU:CD1	2.36	0.56
1:A:367:PHE:CZ	2:B:1187:SER:HB3	2.39	0.56
1:A:1501:ILE:HG13	1:A:1502:PRO:N	2.21	0.56
1:A:1663:ALA:CB	7:G:103:LYS:HZ2	2.19	0.56
1:A:1:MET:CG	2:B:1098:TYR:CD2	2.86	0.56
1:A:502:ALA:O	1:A:580:HIS:HB3	2.05	0.56
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.86	0.56
1:A:507:TYR:CE2	1:A:508:PRO:HD2	2.40	0.56
1:A:1662:ASN:OD1	7:G:58:LEU:HD12	2.05	0.56
3:C:78:VAL:HG22	3:C:210:LEU:HD12	1.87	0.56
1:A:824:THR:HG23	2:B:1023:ARG:HG3	1.87	0.56
1:A:826:PHE:HB2	2:B:1023:ARG:NH2	2.21	0.56
1:A:502:ALA:HA	1:A:581:ILE:CG2	2.36	0.56
1:A:1605:THR:HG22	1:A:1605:THR:O	2.04	0.56
2:B:207:ILE:HG12	2:B:503:VAL:HG22	1.88	0.56
1:A:363:PRO:HG2	2:B:1191:ALA:CB	2.28	0.55
2:B:791:LYS:O	2:B:795:GLU:HG2	2.06	0.55
1:A:361:VAL:CG2	2:B:1190:SER:O	2.54	0.55
1:A:367:PHE:CZ	2:B:1184:TYR:HA	2.32	0.55
1:A:722:PRO:HG3	8:H:46:LEU:HB3	1.87	0.55
1:A:1501:ILE:HG23	1:A:1504:ILE:HB	1.88	0.55
3:C:78:VAL:O	3:C:79:ALA:HB2	2.05	0.55
1:A:586:VAL:HG21	1:A:648:LEU:HG	1.87	0.55
1:A:1606:SER:HB3	1:A:1611:MET:HE1	1.89	0.55
2:B:699:ILE:HD13	2:B:760:TYR:CZ	2.41	0.55
3:C:200:GLN:HG3	10:J:66:LEU:HD13	1.87	0.55
3:C:221:PRO:CD	3:C:222:VAL:H	2.19	0.55
2:B:697:LEU:CD2	2:B:984:TRP:HH2	2.19	0.55
1:A:476:VAL:HG12	2:B:1091:ARG:O	2.06	0.55
1:A:361:VAL:HG21	2:B:1190:SER:O	2.06	0.55
1:A:1501:ILE:CG2	1:A:1504:ILE:HB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:LYS:HA	11:K:66:VAL:HG22	1.88	0.55
1:A:586:VAL:CG2	1:A:648:LEU:HG	2.37	0.55
3:C:33:VAL:CG2	11:K:130:VAL:CG2	2.79	0.55
13:M:9:GLU:HG2	14:N:71:PRO:HB3	1.89	0.55
2:B:555:GLN:HG2	2:B:645:GLY:HA2	1.89	0.55
1:A:64:THR:O	2:B:1161:ASP:HB2	2.07	0.54
1:A:934:LYS:HZ2	2:B:956:SER:HB2	1.69	0.54
3:C:232:GLN:HE21	3:C:234:ASN:HD21	1.55	0.54
3:C:334:THR:O	11:K:48:LYS:HA	2.08	0.54
1:A:1:MET:H2	2:B:1098:TYR:HB3	1.72	0.54
1:A:63:SER:O	2:B:1163:GLN:HG3	2.07	0.54
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.07	0.54
1:A:695:TYR:HE1	1:A:820:TYR:HA	1.71	0.54
1:A:1658:ALA:H	7:G:107:ILE:H	1.55	0.54
1:A:834:ARG:NH2	2:B:994:ASP:OD2	2.36	0.54
2:B:721:MET:HG3	2:B:1036:LEU:HD21	1.88	0.54
2:B:525:TRP:CZ2	2:B:696:ILE:CG2	2.86	0.54
2:B:699:ILE:HG12	2:B:760:TYR:OH	2.08	0.54
2:B:787:MET:HE3	2:B:927:CYS:HA	1.90	0.54
2:B:943:ILE:HG23	10:J:9:SER:HB3	1.90	0.54
10:J:2:ILE:HG23	10:J:57:ILE:HG21	1.90	0.54
2:B:938:PHE:CE1	3:C:68:ARG:NH2	2.76	0.54
1:A:701:ARG:H	1:A:706:HIS:CD2	2.24	0.53
2:B:857:PRO:HB3	2:B:871:ILE:HD13	1.89	0.53
11:K:54:THR:HG23	11:K:61:ALA:CB	2.38	0.53
1:A:49:LEU:HD23	1:A:390:LEU:CD1	2.22	0.53
1:A:438:ILE:HA	1:A:456:VAL:HG22	1.89	0.53
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.90	0.53
3:C:333:ILE:CA	11:K:47:ILE:HG23	2.35	0.53
1:A:366:ARG:NH2	2:B:1180:PHE:CE2	2.76	0.53
1:A:1062:HIS:HA	1:A:1065:GLN:HB2	1.90	0.53
2:B:748:GLN:HB2	2:B:769:PHE:HA	1.89	0.53
13:M:28:LYS:HD2	14:N:106:ASN:HB2	1.91	0.53
7:G:81:VAL:HA	7:G:124:VAL:HG12	1.90	0.53
2:B:323:ARG:HH22	2:B:351:GLN:HE22	1.56	0.53
2:B:211:ARG:O	2:B:212:ASN:HB2	2.08	0.53
3:C:335:GLN:OE1	11:K:49:LEU:O	2.27	0.53
1:A:11:ILE:HD11	2:B:1198:TYR:CG	2.43	0.53
3:C:58:ASN:HA	3:C:296:ASN:HB3	1.90	0.53
3:C:71:MET:CG	3:C:317:SER:HB3	2.39	0.53
1:A:1:MET:CA	2:B:1098:TYR:CE2	2.83	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:OG	2:B:1174:THR:HG21	2.09	0.53
3:C:328:LEU:HD12	11:K:72:LEU:HD13	1.81	0.52
2:B:16:PHE:HB3	2:B:753:LYS:HZ1	1.72	0.52
1:A:5:LYS:O	2:B:1100:GLN:NE2	2.42	0.52
1:A:1658:ALA:H	7:G:106:LYS:HA	1.74	0.52
2:B:555:GLN:O	2:B:556:SER:HB3	2.09	0.52
1:A:1055:ILE:HD13	1:A:1063:MET:HE1	1.90	0.52
2:B:1019:GLY:HA3	3:C:65:ASN:HD21	1.74	0.52
1:A:8:GLY:O	2:B:1202:PRO:HD2	2.06	0.52
1:A:646:GLU:OE1	2:B:1084:THR:OG1	2.27	0.52
1:A:1056:ASP:HB3	1:A:1059:LYS:HD3	1.91	0.52
5:E:131:THR:HG21	5:E:191:LYS:HE2	1.91	0.52
1:A:502:ALA:HA	1:A:581:ILE:HG22	1.90	0.52
1:A:833:LEU:HD23	1:A:943:ILE:CG2	2.40	0.52
7:G:50:ALA:H	7:G:64:GLN:HE22	1.56	0.52
1:A:697:TYR:CE2	11:K:92:SER:CB	2.93	0.52
2:B:979:GLN:HG2	2:B:996:PHE:HE1	1.73	0.52
2:B:26:ILE:CG2	10:J:62:ARG:NH1	2.73	0.52
2:B:646:HIS:CD2	2:B:646:HIS:H	2.28	0.52
1:A:1:MET:CB	2:B:1094:ASN:HA	2.40	0.52
2:B:208:VAL:HG23	2:B:401:GLU:HG2	1.92	0.52
2:B:749:THR:HG22	10:J:52:THR:O	2.10	0.52
3:C:216:HIS:HD2	3:C:218:LYS:H	1.58	0.52
1:A:489:ASN:HB2	11:K:95:HIS:CD2	2.44	0.51
2:B:726:MET:HG3	2:B:742:TYR:HB3	1.93	0.51
1:A:722:PRO:HD2	8:H:46:LEU:CD1	2.37	0.51
2:B:91:LEU:CD2	2:B:342:PRO:HG2	2.40	0.51
6:F:69:LEU:HB3	7:G:94:PRO:HG3	1.92	0.51
1:A:934:LYS:HG2	2:B:955:PRO:HB2	1.92	0.51
1:A:1504:ILE:HA	1:A:1523:GLY:HA3	1.91	0.51
2:B:974:LEU:HA	10:J:44:TYR:CB	2.40	0.51
1:A:759:TYR:CD1	1:A:920:PHE:CE2	2.98	0.51
2:B:974:LEU:HG	10:J:44:TYR:CB	2.40	0.51
1:A:720:PHE:CE2	8:H:79:TRP:CD1	2.98	0.51
1:A:1229:ALA:CB	1:A:1597:ALA:HB2	2.41	0.51
2:B:25:PHE:CE1	10:J:59:LYS:HE2	2.45	0.51
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.91	0.51
1:A:1003:ARG:NH2	2:B:520:LEU:CB	2.74	0.51
1:A:1263:LEU:HD22	1:A:1267:ILE:HD11	1.92	0.51
1:A:10:GLU:H	2:B:1201:GLU:N	2.07	0.51
1:A:1660:VAL:HG22	7:G:105:ILE:H	1.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:LEU:HD22	7:G:94:PRO:HD3	1.92	0.51
3:C:86:PHE:HA	12:L:63:ARG:O	2.11	0.51
13:M:53:LEU:HB2	13:M:96:LEU:HD22	1.93	0.51
1:A:827:THR:OG1	1:A:828:CYS:N	2.42	0.51
2:B:207:ILE:CD1	2:B:402:VAL:HG22	2.24	0.51
2:B:293:ILE:HG12	2:B:302:LEU:HD23	1.91	0.51
1:A:507:TYR:O	1:A:578:TYR:HA	2.11	0.50
1:A:1049:MET:SD	1:A:1052:GLY:HA2	2.51	0.50
14:N:141:GLU:O	14:N:142:THR:HG23	2.10	0.50
2:B:123:PRO:HG2	2:B:172:LEU:HD11	1.92	0.50
2:B:699:ILE:HD13	2:B:760:TYR:CE1	2.46	0.50
3:C:78:VAL:HG12	3:C:79:ALA:N	2.27	0.50
3:C:314:PHE:HE2	11:K:135:PHE:CD1	2.23	0.50
4:D:25:THR:O	6:F:55:PRO:O	2.29	0.50
1:A:1039:ARG:HD2	1:A:1045:LEU:HA	1.94	0.50
1:A:1239:THR:HB	1:A:1542:THR:HB	1.92	0.50
1:A:1608:SER:CB	1:A:1636:SER:CB	2.90	0.50
2:B:25:PHE:HE1	2:B:764:ASN:OD1	1.85	0.50
2:B:400:GLN:O	2:B:649:MET:HE3	2.12	0.50
12:L:60:ARG:HG2	12:L:61:THR:H	1.77	0.50
1:A:11:ILE:HD11	2:B:1198:TYR:HB3	1.89	0.50
1:A:35:PRO:HD3	1:A:394:LEU:HG	1.92	0.50
2:B:974:LEU:HD23	10:J:44:TYR:CD1	2.40	0.50
1:A:34:ASN:O	1:A:390:LEU:CB	2.55	0.50
2:B:44:PRO:HB3	2:B:551:ILE:CD1	2.41	0.50
2:B:211:ARG:NH2	2:B:243:GLN:NE2	2.44	0.50
3:C:110:PRO:C	3:C:112:MET:H	2.20	0.50
1:A:5:LYS:HB3	2:B:1100:GLN:OE1	2.09	0.50
1:A:1501:ILE:HG12	1:A:1504:ILE:HD12	1.94	0.50
2:B:700:LEU:HA	2:B:703:LEU:HD12	1.94	0.50
1:A:940:VAL:HG13	1:A:944:MET:HE3	1.93	0.50
2:B:110:ASN:HB3	2:B:118:GLU:HG2	1.94	0.50
2:B:209:GLN:O	2:B:401:GLU:HG2	2.12	0.50
1:A:1003:ARG:HH21	2:B:520:LEU:HD22	1.62	0.49
1:A:1003:ARG:HH22	2:B:520:LEU:CB	2.25	0.49
1:A:1663:ALA:HB2	7:G:103:LYS:HZ2	1.77	0.49
2:B:26:ILE:HG23	10:J:62:ARG:NH1	2.20	0.49
7:G:51:PRO:HA	7:G:54:LEU:HD13	1.95	0.49
3:C:334:THR:HB	11:K:47:ILE:O	2.11	0.49
2:B:823:GLN:HG2	2:B:863:ASP:HB3	1.94	0.49
3:C:335:GLN:HB2	11:K:48:LYS:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:O	2:B:1163:GLN:CG	2.61	0.49
1:A:1038:ILE:HD12	1:A:1185:VAL:HG21	1.94	0.49
1:A:1613:MET:HE3	1:A:1622:LEU:HB2	1.94	0.49
2:B:974:LEU:CG	10:J:44:TYR:CB	2.91	0.49
3:C:334:THR:CG2	11:K:44:ARG:HB3	2.32	0.49
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.94	0.49
1:A:601:MET:HB3	1:A:653:THR:HG22	1.95	0.49
1:A:1503:HIS:O	1:A:1504:ILE:HG13	2.13	0.49
1:A:32:ILE:CG2	1:A:390:LEU:HD21	2.42	0.49
1:A:833:LEU:HD23	1:A:943:ILE:HG23	1.94	0.49
1:A:918:LYS:HE2	1:A:922:CYS:HB3	1.94	0.49
1:A:1500:GLN:NE2	1:A:1501:ILE:O	2.45	0.49
1:A:1659:LYS:HZ1	6:F:133:VAL:HG21	1.74	0.49
12:L:60:ARG:NH2	12:L:65:VAL:HG21	2.28	0.49
1:A:64:THR:CG2	2:B:1129:ARG:NH1	2.76	0.49
2:B:398:GLN:CD	2:B:399:HIS:CE1	2.91	0.49
14:N:163:VAL:HG12	14:N:164:GLU:N	2.18	0.49
1:A:19:LEU:HD12	2:B:1193:GLY:CA	2.42	0.49
1:A:861:VAL:HG21	1:A:892:LEU:HA	1.94	0.49
1:A:1504:ILE:HG22	1:A:1505:ASP:H	1.76	0.49
12:L:62:LYS:HB2	12:L:62:LYS:NZ	2.28	0.49
1:A:934:LYS:HZ1	2:B:956:SER:CB	1.94	0.49
2:B:705:PRO:HG2	2:B:921:HIS:CE1	2.47	0.49
2:B:976:GLY:HA2	10:J:51:LEU:CD2	2.43	0.49
1:A:504:LYS:O	1:A:506:THR:N	2.45	0.48
1:A:1504:ILE:CG2	1:A:1505:ASP:N	2.76	0.48
3:C:113:LEU:HD11	3:C:132:ILE:HD12	1.94	0.48
9:I:42:PHE:CD1	9:I:42:PHE:N	2.81	0.48
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.93	0.48
2:B:916:LYS:HB3	2:B:1036:LEU:HD12	1.95	0.48
3:C:334:THR:OG1	11:K:47:ILE:O	2.30	0.48
1:A:718:THR:CG2	8:H:119:GLY:HA3	2.36	0.48
1:A:952:LEU:HD23	1:A:1004:GLU:HG3	1.95	0.48
2:B:740:LYS:HA	2:B:804:TYR:O	2.13	0.48
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.96	0.48
6:F:69:LEU:HB3	7:G:94:PRO:CG	2.43	0.48
2:B:26:ILE:O	10:J:62:ARG:CZ	2.61	0.48
2:B:556:SER:C	2:B:558:VAL:H	2.20	0.48
1:A:1609:SER:HB2	1:A:1630:GLU:OE2	2.13	0.48
13:M:109:ARG:HG3	13:M:110:GLY:H	1.77	0.48
1:A:507:TYR:CE1	1:A:639:GLN:HA	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:ARG:NH2	2:B:520:LEU:HD23	2.23	0.48
1:A:1196:PRO:HB2	1:A:1575:ILE:HG21	1.96	0.48
1:A:9:SER:O	2:B:1176:VAL:HG12	2.13	0.48
1:A:518:GLU:OE2	1:A:582:LYS:NZ	2.43	0.48
7:G:47:VAL:HG21	7:G:61:VAL:HG13	1.96	0.48
1:A:836:THR:HG23	1:A:839:GLY:H	1.78	0.48
11:K:95:HIS:HB3	11:K:98:GLU:HG2	1.96	0.48
8:H:103:LYS:HB3	8:H:115:TYR:HB2	1.96	0.48
1:A:5:LYS:HB2	2:B:1100:GLN:HE21	1.72	0.47
1:A:5:LYS:HD3	2:B:1100:GLN:CD	2.39	0.47
1:A:727:THR:H	1:A:730:GLN:HE21	1.61	0.47
2:B:1005:TYR:OH	10:J:44:TYR:HE1	1.95	0.47
1:A:49:LEU:CD2	1:A:386:LEU:HB3	2.44	0.47
1:A:934:LYS:HZ3	2:B:956:SER:CB	2.18	0.47
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.95	0.47
3:C:314:PHE:HD2	11:K:135:PHE:CE2	2.31	0.47
3:C:333:ILE:CG2	11:K:47:ILE:HG12	2.25	0.47
1:A:1003:ARG:CZ	2:B:520:LEU:HB2	2.44	0.47
2:B:699:ILE:CD1	2:B:760:TYR:OH	2.62	0.47
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.96	0.47
1:A:862:THR:OG1	1:A:878:ARG:HB3	2.15	0.47
1:A:879:LEU:HA	1:A:882:ILE:HD12	1.97	0.47
1:A:1659:LYS:NZ	6:F:133:VAL:HG22	2.25	0.47
2:B:375:LEU:HA	2:B:378:ILE:HD12	1.96	0.47
2:B:554:GLN:HG3	2:B:646:HIS:CE1	2.48	0.47
5:E:56:LYS:HE2	5:E:84:ASP:H	1.80	0.47
8:H:107:VAL:O	8:H:111:LEU:HB2	2.15	0.47
1:A:37:VAL:HG12	1:A:49:LEU:HB2	1.95	0.47
1:A:538:ASN:HA	1:A:575:LYS:HG2	1.96	0.47
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.96	0.47
2:B:527:PHE:HZ	2:B:651:ARG:HG2	1.77	0.47
2:B:697:LEU:CG	2:B:984:TRP:HH2	2.27	0.47
1:A:9:SER:CA	2:B:1200:VAL:HG13	2.44	0.47
1:A:126:GLN:HB3	1:A:343:PRO:HD3	1.96	0.47
1:A:506:THR:HB	1:A:579:ARG:O	2.14	0.47
1:A:1640:ARG:HH11	1:A:1648:ASN:HB3	1.78	0.47
2:B:362:LEU:HD22	2:B:369:ASP:HB3	1.97	0.47
2:B:494:TYR:CE2	2:B:703:LEU:HD13	2.47	0.47
14:N:150:TYR:HA	14:N:153:VAL:HG12	1.96	0.47
1:A:652:ASN:HD22	1:A:654:ASP:HB2	1.80	0.47
3:C:229:LEU:HD23	3:C:293:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:4:GLU:HG2	5:E:7:ARG:HH12	1.80	0.47
1:A:826:PHE:CA	2:B:1023:ARG:HH22	1.88	0.47
1:A:1658:ALA:H	7:G:107:ILE:N	2.12	0.47
1:A:536:ILE:HD11	1:A:575:LYS:HD3	1.96	0.47
3:C:70:ILE:CG2	3:C:74:GLU:HB2	2.44	0.47
2:B:880:ALA:HB2	2:B:907:ILE:HG13	1.97	0.46
9:I:48:VAL:HG13	9:I:48:VAL:O	2.15	0.46
11:K:59:THR:CG2	11:K:107:THR:OG1	2.61	0.46
1:A:1660:VAL:H	7:G:104:LEU:CA	2.11	0.46
2:B:25:PHE:HZ	2:B:764:ASN:OD1	1.88	0.46
11:K:59:THR:HG22	11:K:111:THR:O	2.16	0.46
3:C:75:VAL:HB	3:C:221:PRO:CG	2.46	0.46
3:C:81:GLU:HG3	3:C:209:ILE:HG22	1.97	0.46
3:C:334:THR:HG21	11:K:44:ARG:CB	2.32	0.46
1:A:32:ILE:HG21	1:A:49:LEU:HD13	1.96	0.46
14:N:164:GLU:HG2	14:N:165:GLY:N	2.30	0.46
1:A:1641:ILE:HD13	2:B:1076:ARG:HH11	1.81	0.46
1:A:1662:ASN:HD22	7:G:58:LEU:H	0.54	0.46
2:B:397:THR:OG1	2:B:523:GLU:HB2	2.15	0.46
1:A:11:ILE:HD11	2:B:1198:TYR:CB	2.46	0.46
1:A:651:ALA:C	1:A:652:ASN:O	2.59	0.46
1:A:3:ILE:O	7:G:111:THR:CG2	2.64	0.46
1:A:1275:THR:HG23	1:A:1289:SER:HB2	1.97	0.46
2:B:65:VAL:HA	2:B:68:ILE:HG12	1.97	0.46
1:A:827:THR:HG21	2:B:1025:ASP:O	2.15	0.46
1:A:1657:LEU:HA	7:G:106:LYS:HG3	1.97	0.46
1:A:1112:PRO:HD2	1:A:1115:LYS:HB2	1.97	0.45
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.99	0.45
2:B:335:ARG:NH2	13:M:113:ILE:O	2.50	0.45
2:B:721:MET:O	2:B:725:THR:HG23	2.16	0.45
12:L:60:ARG:HG2	12:L:61:THR:N	2.31	0.45
1:A:1:MET:CB	2:B:1098:TYR:CE2	2.91	0.45
1:A:1003:ARG:HH22	2:B:520:LEU:HB2	1.82	0.45
2:B:1005:TYR:CE2	10:J:44:TYR:CE1	3.05	0.45
2:B:494:TYR:CE2	2:B:762:MET:HE3	2.50	0.45
14:N:162:LYS:H	14:N:162:LYS:CD	2.29	0.45
1:A:506:THR:CA	1:A:579:ARG:O	2.64	0.45
1:A:693:GLN:CD	11:K:88:PHE:CD2	2.94	0.45
1:A:824:THR:CA	2:B:1023:ARG:HB2	2.40	0.45
1:A:828:CYS:SG	1:A:829:GLY:N	2.89	0.45
14:N:160:VAL:CG1	14:N:161:PRO:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:HB2	1:A:391:THR:CG2	2.47	0.45
1:A:700:ILE:HD11	1:A:735:VAL:HA	1.97	0.45
1:A:1498:ILE:O	1:A:1499:ARG:HB2	2.16	0.45
2:B:553:THR:O	2:B:554:GLN:HB2	2.17	0.45
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.99	0.45
1:A:1657:LEU:HG	7:G:106:LYS:HG3	1.93	0.45
1:A:537:GLN:HB2	1:A:578:TYR:HE1	1.81	0.45
3:C:236:LEU:HD11	3:C:290:LYS:HG3	1.98	0.45
9:I:39:LYS:O	9:I:40:SER:HB2	2.15	0.45
1:A:35:PRO:HG2	1:A:391:THR:HA	1.34	0.45
1:A:1659:LYS:HZ2	6:F:133:VAL:HG22	1.80	0.45
2:B:400:GLN:HG3	2:B:649:MET:HE1	1.98	0.45
3:C:217:ALA:C	3:C:219:PHE:H	2.23	0.45
3:C:229:LEU:HD21	3:C:295:ARG:HA	1.99	0.45
12:L:28:LYS:CB	12:L:59:ALA:HB3	2.30	0.45
1:A:9:SER:HA	2:B:1201:GLU:C	2.21	0.45
1:A:507:TYR:CG	1:A:508:PRO:CD	3.00	0.45
1:A:672:ASP:OD1	2:B:952:HIS:CE1	2.70	0.45
1:A:833:LEU:N	1:A:833:LEU:CD1	2.79	0.45
1:A:1003:ARG:HH22	2:B:520:LEU:CG	2.29	0.45
1:A:1053:ASP:HB3	1:A:1137:SER:HB3	1.99	0.45
1:A:1604:GLU:C	1:A:1606:SER:H	2.25	0.45
2:B:397:THR:CB	2:B:523:GLU:HB2	2.44	0.45
3:C:71:MET:O	3:C:222:VAL:CG1	2.64	0.45
3:C:75:VAL:HG12	3:C:221:PRO:CB	2.46	0.45
1:A:35:PRO:HB2	1:A:391:THR:HG23	1.98	0.44
2:B:398:GLN:O	2:B:399:HIS:CG	2.70	0.44
2:B:556:SER:O	2:B:558:VAL:N	2.50	0.44
2:B:1097:ASP:OD2	2:B:1181:VAL:HG22	2.17	0.44
3:C:33:VAL:HG21	11:K:127:LEU:HA	1.98	0.44
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.53	0.44
9:I:27:ASN:HA	9:I:38:PRO:HD3	1.99	0.44
2:B:693:PRO:O	2:B:696:ILE:HG12	2.18	0.44
1:A:692:TYR:O	1:A:696:ILE:HG12	2.17	0.44
1:A:11:ILE:HA	2:B:1199:ASN:C	2.30	0.44
1:A:19:LEU:HD12	2:B:1193:GLY:HA2	2.00	0.44
1:A:1288:ARG:HB2	1:A:1476:LEU:HB2	1.98	0.44
2:B:555:GLN:HB3	2:B:644:GLY:C	2.41	0.44
1:A:988:SER:O	2:B:988:GLU:HB2	2.17	0.44
1:A:1258:ILE:O	1:A:1258:ILE:HG22	2.18	0.44
2:B:210:ARG:NH2	2:B:649:MET:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:GLN:CG	10:J:66:LEU:HD13	2.48	0.44
1:A:1029:GLY:HA3	1:A:1041:ALA:HB2	1.99	0.44
2:B:398:GLN:O	2:B:399:HIS:CD2	2.71	0.44
2:B:401:GLU:HG3	2:B:402:VAL:N	2.32	0.44
1:A:1038:ILE:HD11	1:A:1050:TYR:HB2	1.99	0.44
2:B:689:VAL:HG13	2:B:689:VAL:O	2.17	0.44
2:B:845:LEU:HB2	12:L:58:LYS:HE2	2.00	0.44
3:C:72:ILE:HG22	3:C:72:ILE:O	2.17	0.44
5:E:120:ALA:HA	5:E:123:LEU:HD12	2.00	0.44
1:A:655:SER:O	1:A:656:GLN:HG2	2.18	0.44
1:A:826:PHE:HB2	2:B:1023:ARG:HH21	1.77	0.44
1:A:1113:HIS:HB3	5:E:201:LYS:NZ	2.33	0.44
3:C:72:ILE:HD11	3:C:225:ALA:HB3	1.98	0.44
1:A:1:MET:H2	2:B:1098:TYR:CB	2.20	0.43
1:A:476:VAL:CG1	2:B:1091:ARG:O	2.66	0.43
1:A:506:THR:CB	1:A:579:ARG:O	2.65	0.43
1:A:385:LEU:HD13	1:A:437:PHE:HA	2.00	0.43
1:A:1603:MET:CE	1:A:1615:TYR:CD2	2.86	0.43
2:B:953:ALA:O	2:B:957:ARG:HG2	2.19	0.43
5:E:141:VAL:HG12	5:E:142:VAL:HG23	2.00	0.43
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.99	0.43
1:A:233:CYS:HB3	1:A:236:CYS:O	2.18	0.43
1:A:387:SER:HA	1:A:390:LEU:HD12	2.01	0.43
1:A:1658:ALA:N	7:G:107:ILE:H	2.16	0.43
2:B:26:ILE:O	10:J:62:ARG:CD	2.66	0.43
13:M:9:GLU:HA	14:N:71:PRO:HA	2.00	0.43
1:A:83:VAL:HG11	1:A:427:PHE:CZ	2.49	0.43
1:A:683:LYS:HD2	8:H:20:TYR:OH	2.17	0.43
1:A:1659:LYS:HA	7:G:104:LEU:HB3	2.01	0.43
1:A:862:THR:HG21	1:A:875:LEU:HD12	1.99	0.43
2:B:129:ARG:HG2	2:B:890:ASP:CG	2.44	0.43
2:B:529:CYS:SG	2:B:698:SER:CB	2.97	0.43
1:A:10:GLU:N	2:B:1200:VAL:HG13	2.34	0.43
1:A:885:ASP:HB3	1:A:888:LYS:HB2	2.01	0.43
1:A:1113:HIS:CB	5:E:201:LYS:NZ	2.82	0.43
1:A:1260:LYS:HZ1	1:A:1262:LEU:HD11	1.81	0.43
1:A:1481:GLU:HB2	1:A:1482:LYS:H	1.72	0.43
2:B:25:PHE:CE2	10:J:56:LEU:HD23	2.49	0.43
2:B:26:ILE:CA	10:J:62:ARG:CD	2.85	0.43
2:B:207:ILE:HD13	2:B:402:VAL:CG2	2.23	0.43
2:B:251:HIS:HE1	2:B:261:ARG:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:SER:C	2:B:558:VAL:N	2.77	0.43
1:A:396:ILE:HG12	1:A:426:ALA:HB1	2.01	0.43
1:A:739:VAL:HG11	1:A:812:VAL:HG21	2.00	0.43
1:A:759:TYR:HH	1:A:930:LEU:HD21	1.82	0.43
1:A:830:MET:C	1:A:832:ASP:N	2.77	0.43
2:B:25:PHE:HD2	10:J:59:LYS:HB2	1.32	0.43
3:C:80:ALA:HA	3:C:208:CYS:HA	2.00	0.43
3:C:333:ILE:CD1	11:K:118:GLN:HE21	2.31	0.43
3:C:44:ILE:HD12	11:K:142:MET:SD	2.59	0.42
3:C:221:PRO:CD	3:C:222:VAL:N	2.82	0.42
1:A:49:LEU:HD22	1:A:390:LEU:HD11	0.56	0.42
2:B:249:VAL:HB	2:B:261:ARG:HB3	2.00	0.42
2:B:974:LEU:CG	10:J:44:TYR:CG	3.02	0.42
6:F:107:VAL:HG12	6:F:109:VAL:H	1.84	0.42
4:D:19:PRO:HG2	4:D:22:ILE:HD11	2.01	0.42
1:A:657:TYR:O	1:A:665:PRO:HA	2.19	0.42
2:B:301:PHE:O	2:B:305:ARG:HG2	2.19	0.42
3:C:71:MET:O	3:C:72:ILE:HG13	2.19	0.42
11:K:46:LYS:O	11:K:65:ILE:HA	2.20	0.42
1:A:591:ARG:HB2	1:A:633:MET:HG2	2.02	0.42
1:A:966:LEU:HB2	1:A:969:PHE:HD2	1.84	0.42
10:J:32:GLU:H	10:J:32:GLU:HG2	1.53	0.42
2:B:61:LEU:HD21	2:B:413:LEU:HD13	2.02	0.42
2:B:561:ILE:HG12	2:B:620:LEU:HD12	2.01	0.42
1:A:399:LEU:HD11	1:A:422:ARG:HB3	2.02	0.42
2:B:612:LYS:HD3	2:B:626:ILE:HD11	2.01	0.42
4:D:24:ALA:HA	7:G:43:ILE:HG22	2.02	0.42
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.01	0.42
2:B:480:GLN:CD	2:B:480:GLN:H	2.27	0.42
3:C:252:PRO:HD2	3:C:255:VAL:HG21	2.02	0.42
12:L:29:TYR:HD2	12:L:39:SER:HA	1.85	0.42
1:A:536:ILE:HG23	1:A:544:VAL:HB	2.02	0.42
1:A:970:LYS:HG2	1:A:971:PRO:HD2	2.02	0.42
2:B:44:PRO:O	2:B:48:SER:HB2	2.20	0.42
2:B:209:GLN:CG	2:B:210:ARG:N	2.73	0.42
2:B:217:ILE:HD11	2:B:235:GLN:HB2	2.02	0.42
2:B:699:ILE:CD1	2:B:760:TYR:CZ	3.01	0.42
1:A:1238:MET:HB2	1:A:1521:THR:HB	2.01	0.41
2:B:26:ILE:HA	10:J:62:ARG:HD3	1.92	0.41
2:B:201:LYS:HD3	2:B:465:LEU:O	2.20	0.41
2:B:210:ARG:HH22	2:B:648:ARG:CA	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:MET:HB2	6:F:151:LEU:HB3	2.01	0.41
1:A:880:GLN:HE21	1:A:880:GLN:HB2	1.69	0.41
2:B:14:ALA:HB1	2:B:755:ASN:CG	2.44	0.41
2:B:212:ASN:O	2:B:213:HIS:HB2	2.20	0.41
9:I:52:ALA:HB3	9:I:55:ALA:HB2	2.02	0.41
11:K:60:SER:HB3	11:K:106:GLN:HG2	2.02	0.41
1:A:11:ILE:HG12	2:B:1198:TYR:CA	2.47	0.41
1:A:1459:LYS:HB2	1:A:1473:LYS:HB2	2.02	0.41
2:B:25:PHE:CE2	10:J:56:LEU:CD2	3.00	0.41
2:B:788:ILE:HB	2:B:948:ILE:HB	2.02	0.41
2:B:858:ILE:HD12	2:B:858:ILE:HA	1.97	0.41
2:B:936:MET:HG3	2:B:937:PRO:HD2	2.01	0.41
1:A:830:MET:SD	2:B:993:ALA:CB	3.09	0.41
5:E:6:GLU:HA	5:E:9:ILE:HD12	2.02	0.41
12:L:31:CYS:HA	12:L:56:LEU:HD23	2.03	0.41
1:A:492:THR:HB	1:A:667:ARG:HH22	1.85	0.41
3:C:335:GLN:C	11:K:49:LEU:HB3	2.44	0.41
1:A:533:ALA:HA	1:A:579:ARG:HA	2.03	0.41
3:C:335:GLN:CB	11:K:48:LYS:HG2	2.50	0.41
8:H:93:TYR:HA	8:H:145:ARG:HG3	2.03	0.41
13:M:20:SER:HB3	14:N:36:LYS:HB2	2.02	0.41
1:A:7:VAL:HG11	2:B:1176:VAL:CA	2.31	0.41
1:A:363:PRO:CG	2:B:1191:ALA:HB1	2.44	0.41
1:A:507:TYR:N	1:A:579:ARG:O	2.54	0.41
1:A:1550:LEU:HD12	1:A:1555:VAL:HA	2.02	0.41
10:J:68:LYS:HD3	10:J:69:ARG:HD2	2.03	0.41
2:B:16:PHE:HB3	2:B:753:LYS:HZ3	1.84	0.41
2:B:17:ARG:H	2:B:17:ARG:HG2	1.64	0.41
2:B:342:PRO:O	13:M:112:LYS:HD2	2.17	0.41
3:C:77:SER:OG	3:C:78:VAL:N	2.52	0.41
13:M:15:VAL:HG12	13:M:90:LEU:HB2	2.03	0.41
1:A:3:ILE:O	7:G:111:THR:HG21	2.20	0.41
1:A:124:LEU:HD21	1:A:189:VAL:HA	2.01	0.41
1:A:1663:ALA:CB	7:G:103:LYS:HZ3	2.25	0.41
2:B:190:ILE:HD11	2:B:496:PHE:HE2	1.85	0.41
2:B:1079:LEU:O	2:B:1084:THR:HG22	2.21	0.41
2:B:1084:THR:HG23	2:B:1084:THR:O	2.21	0.41
3:C:175:GLN:HB3	3:C:178:THR:HG22	2.03	0.41
1:A:582:LYS:HB3	1:A:583:ASN:H	1.69	0.41
1:A:912:VAL:HA	1:A:913:PRO:HA	1.92	0.41
1:A:1229:ALA:HB2	1:A:1597:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PRO:HB2	2:B:177:PRO:HG2	2.03	0.41
2:B:600:GLN:HA	2:B:603:ILE:HD12	2.03	0.41
2:B:1005:TYR:CE2	10:J:44:TYR:HE1	2.37	0.41
7:G:45:LEU:HD11	7:G:120:VAL:HG12	2.02	0.41
1:A:539:GLU:H	1:A:539:GLU:CD	2.30	0.40
2:B:210:ARG:NH2	2:B:648:ARG:CA	2.82	0.40
1:A:361:VAL:HG22	2:B:1190:SER:O	2.21	0.40
1:A:368:ARG:HG2	1:A:382:GLN:CD	2.45	0.40
1:A:368:ARG:NE	1:A:386:LEU:HD11	2.33	0.40
1:A:507:TYR:CD2	1:A:508:PRO:CD	3.04	0.40
1:A:990:ILE:HD12	1:A:995:TYR:HA	2.03	0.40
3:C:65:ASN:HA	3:C:227:TYR:HE2	1.86	0.40
3:C:322:LYS:HB2	11:K:128:CYS:HB3	2.03	0.40
1:A:12:THR:N	2:B:1199:ASN:O	2.54	0.40
1:A:76:GLN:HE21	2:B:1190:SER:CB	2.20	0.40
1:A:857:ALA:HB2	1:A:899:LYS:HD2	2.03	0.40
1:A:1272:VAL:HG11	1:A:1485:MET:HB3	2.03	0.40
2:B:693:PRO:C	2:B:695:ASN:H	2.30	0.40
2:B:974:LEU:CG	10:J:44:TYR:CD1	3.03	0.40
1:A:98:LEU:HD13	1:A:320:VAL:HG13	2.03	0.40
1:A:1503:HIS:HB3	1:A:1524:VAL:O	2.21	0.40
2:B:358:VAL:HG13	2:B:370:LYS:HD3	2.03	0.40
2:B:650:LEU:HB3	2:B:663:ILE:HG23	2.04	0.40
2:B:699:ILE:CG2	2:B:760:TYR:CE2	3.04	0.40
7:G:107:ILE:HA	7:G:114:GLY:HA2	2.03	0.40
11:K:109:GLY:O	11:K:110:GLU:HG2	2.21	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	1394/1664 (84%)	1309 (94%)	76 (6%)	9 (1%)	21	58
2	B	1099/1203 (91%)	1020 (93%)	73 (7%)	6 (0%)	24	63
3	C	300/380 (79%)	273 (91%)	24 (8%)	3 (1%)	12	47
4	D	16/137 (12%)	14 (88%)	2 (12%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	85/326 (26%)	80 (94%)	5 (6%)	0	100	100
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	16	52
9	I	62/125 (50%)	53 (86%)	8 (13%)	1 (2%)	7	37
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	99/142 (70%)	91 (92%)	6 (6%)	2 (2%)	6	31
12	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	114 (87%)	15 (12%)	2 (2%)	8	38
All	All	3838/5281 (73%)	3564 (93%)	250 (6%)	24 (1%)	23	58

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ASN
1	A	655	SER
1	A	505	LEU
1	A	654	ASP
1	A	1499	ARG
2	B	210	ARG
2	B	557	ASP
11	K	57	ASP
14	N	165	GLY
1	A	237	GLY
2	B	532	HIS
3	C	72	ILE
3	C	221	PRO
1	A	478	TYR
2	B	209	GLN
2	B	400	GLN
2	B	552	SER
1	A	508	PRO
1	A	580	HIS

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Mol	Chain	Res	Type
3	C	76	PRO
8	H	84	ALA
9	I	26	SER
11	K	58	GLY
14	N	163	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1250/1465 (85%)	1170 (94%)	80 (6%)	16	38
2	B	973/1053 (92%)	872 (90%)	101 (10%)	7	22
3	C	269/334 (80%)	241 (90%)	28 (10%)	7	22
4	D	16/116 (14%)	11 (69%)	5 (31%)	0	2
5	E	197/197 (100%)	187 (95%)	10 (5%)	21	43
6	F	90/137 (66%)	85 (94%)	5 (6%)	19	41
7	G	80/291 (28%)	72 (90%)	8 (10%)	7	24
8	H	116/128 (91%)	108 (93%)	8 (7%)	14	36
9	I	56/110 (51%)	48 (86%)	8 (14%)	3	14
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	21
11	K	91/130 (70%)	84 (92%)	7 (8%)	12	32
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	17
13	M	94/371 (25%)	88 (94%)	6 (6%)	16	38
14	N	128/220 (58%)	114 (89%)	14 (11%)	6	21
All	All	3464/4674 (74%)	3172 (92%)	292 (8%)	12	30

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	94	LEU
1	A	103	LEU
1	A	113	VAL
1	A	129	LEU
1	A	136	LEU
1	A	177	LEU
1	A	195	LYS
1	A	199	ASP
1	A	211	THR
1	A	227	LEU
1	A	250	LYS
1	A	251	ILE
1	A	270	ILE
1	A	322	ASN
1	A	325	ASP
1	A	345	LEU
1	A	361	VAL
1	A	398	ASP
1	A	399	LEU
1	A	403	LEU
1	A	413	LEU
1	A	423	LEU
1	A	518	GLU
1	A	536	ILE
1	A	539	GLU
1	A	562	LEU
1	A	572	THR
1	A	587	VAL
1	A	621	THR
1	A	632	GLU
1	A	684	ASP
1	A	715	LEU
1	A	727	THR
1	A	743	ASP
1	A	747	ILE
1	A	831	ASP
1	A	840	ASN
1	A	844	THR
1	A	862	THR
1	A	878	ARG
1	A	952	LEU

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Mol	Chain	Res	Type
1	A	957	VAL
1	A	960	MET
1	A	1004	GLU
1	A	1059	LYS
1	A	1065	GLN
1	A	1086	ILE
1	A	1136	VAL
1	A	1164	LYS
1	A	1169	LEU
1	A	1171	GLN
1	A	1175	MET
1	A	1179	ILE
1	A	1183	GLU
1	A	1190	SER
1	A	1193	VAL
1	A	1217	LEU
1	A	1227	MET
1	A	1240	LEU
1	A	1242	ILE
1	A	1252	ASP
1	A	1263	LEU
1	A	1273	THR
1	A	1313	LEU
1	A	1474	LEU
1	A	1475	GLU
1	A	1481	GLU
1	A	1505	ASP
1	A	1531	ASP
1	A	1533	GLU
1	A	1550	LEU
1	A	1552	THR
1	A	1592	GLN
1	A	1610	PHE
1	A	1628	ASP
1	A	1629	ASN
1	A	1649	VAL
2	B	13	THR
2	B	15	ASP
2	B	17	ARG
2	B	19	LEU
2	B	22	GLU
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	35	PHE
2	B	52	LEU
2	B	54	GLU
2	B	60	LEU
2	B	61	LEU
2	B	73	ILE
2	B	101	GLN
2	B	108	MET
2	B	139	LEU
2	B	150	GLU
2	B	163	VAL
2	B	168	ASN
2	B	186	GLU
2	B	190	ILE
2	B	202	LEU
2	B	206	LEU
2	B	210	ARG
2	B	217	ILE
2	B	218	ILE
2	B	234	ILE
2	B	250	LEU
2	B	268	GLU
2	B	274	VAL
2	B	276	ILE
2	B	297	VAL
2	B	306	LEU
2	B	332	ASP
2	B	364	LYS
2	B	374	LEU
2	B	381	LEU
2	B	412	ILE
2	B	413	LEU
2	B	431	ASP
2	B	438	ILE
2	B	441	LYS
2	B	455	GLU
2	B	471	VAL
2	B	479	GLN
2	B	480	GLN
2	B	481	VAL
2	B	485	THR
2	B	491	ILE

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Mol	Chain	Res	Type
2	B	502	MET
2	B	519	LYS
2	B	542	LEU
2	B	550	ARG
2	B	555	GLN
2	B	588	ILE
2	B	592	ILE
2	B	593	ILE
2	B	616	LYS
2	B	617	THR
2	B	640	LEU
2	B	646	HIS
2	B	684	ASN
2	B	692	THR
2	B	721	MET
2	B	723	LYS
2	B	743	ARG
2	B	752	VAL
2	B	789	ILE
2	B	794	ASP
2	B	821	ILE
2	B	832	TRP
2	B	835	GLU
2	B	840	LEU
2	B	842	GLU
2	B	848	ILE
2	B	858	ILE
2	B	859	CYS
2	B	871	ILE
2	B	873	THR
2	B	887	LEU
2	B	888	ILE
2	B	896	GLN
2	B	897	GLU
2	B	933	THR
2	B	940	GLU
2	B	956	SER
2	B	965	GLU
2	B	967	LEU
2	B	977	ILE
2	B	988	GLU
2	B	1000	LEU

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Mol	Chain	Res	Type
2	B	1020	GLU
2	B	1028	VAL
2	B	1037	ARG
2	B	1076	ARG
2	B	1103	VAL
2	B	1110	ILE
2	B	1120	ILE
2	B	1123	ILE
2	B	1157	GLN
2	B	1181	VAL
2	B	1201	GLU
3	C	30	GLU
3	C	46	SER
3	C	47	LEU
3	C	81	GLU
3	C	89	THR
3	C	97	LEU
3	C	106	LEU
3	C	117	ASP
3	C	120	LEU
3	C	151	THR
3	C	181	ASP
3	C	182	CYS
3	C	185	VAL
3	C	209	ILE
3	C	220	SER
3	C	224	THR
3	C	229	LEU
3	C	235	ILE
3	C	239	ILE
3	C	240	LYS
3	C	258	ILE
3	C	259	ASP
3	C	277	ARG
3	C	291	LEU
3	C	303	GLU
3	C	311	GLU
3	C	331	CYS
3	C	334	THR
4	D	14	THR
4	D	16	LEU
4	D	21	VAL

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Mol	Chain	Res	Type
4	D	25	THR
4	D	27	LEU
5	E	37	LEU
5	E	84	ASP
5	E	106	GLN
5	E	122	LYS
5	E	127	ILE
5	E	154	ILE
5	E	163	GLU
5	E	167	ARG
5	E	175	LEU
5	E	204	THR
6	F	69	LEU
6	F	99	LEU
6	F	103	MET
6	F	111	LEU
6	F	147	SER
7	G	54	LEU
7	G	75	ASN
7	G	85	GLU
7	G	93	ASP
7	G	95	LEU
7	G	104	LEU
7	G	105	ILE
7	G	111	THR
8	H	22	LYS
8	H	23	VAL
8	H	33	GLN
8	H	53	ASP
8	H	63	LEU
8	H	89	LEU
8	H	132	LEU
8	H	136	LYS
9	I	3	VAL
9	I	17	LEU
9	I	27	ASN
9	I	42	PHE
9	I	50	THR
9	I	51	THR
9	I	53	ASP
9	I	60	LEU
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	14	VAL
10	J	26	GLN
10	J	32	GLU
10	J	47	ARG
10	J	48	ARG
10	J	68	LYS
11	K	44	ARG
11	K	60	SER
11	K	72	LEU
11	K	99	ASN
11	K	103	ILE
11	K	124	LEU
11	K	132	GLU
12	L	27	LEU
12	L	38	LEU
12	L	40	LEU
12	L	62	LYS
12	L	65	VAL
13	M	48	LYS
13	M	50	GLU
13	M	53	LEU
13	M	56	GLU
13	M	88	ILE
13	M	101	VAL
14	N	25	ILE
14	N	36	LYS
14	N	49	LYS
14	N	67	LEU
14	N	74	PHE
14	N	78	THR
14	N	94	ASP
14	N	114	GLU
14	N	117	GLU
14	N	131	LEU
14	N	145	ILE
14	N	164	GLU
14	N	168	LEU
14	N	178	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	76	GLN
1	A	263	ASN
1	A	332	GLN
1	A	431	GLN
1	A	435	ASN
1	A	538	ASN
1	A	583	ASN
1	A	590	ASN
1	A	592	GLN
1	A	610	ASN
1	A	639	GLN
1	A	671	GLN
1	A	693	GLN
1	A	694	GLN
1	A	706	HIS
1	A	730	GLN
1	A	738	ASN
1	A	753	ASN
1	A	798	HIS
1	A	887	ASN
1	A	926	GLN
1	A	949	GLN
1	A	998	HIS
1	A	1026	GLN
1	A	1171	GLN
1	A	1180	ASN
1	A	1293	HIS
1	A	1319	ASN
1	A	1320	GLN
1	A	1323	HIS
1	A	1440	ASN
1	A	1567	ASN
1	A	1592	GLN
1	A	1599	ASN
1	A	1647	ASN
1	A	1662	ASN
2	B	146	ASN
2	B	151	ASN
2	B	166	GLN
2	B	212	ASN
2	B	213	HIS
2	B	235	GLN

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Mol	Chain	Res	Type
2	B	243	GLN
2	B	251	HIS
2	B	328	GLN
2	B	351	GLN
2	B	361	HIS
2	B	399	HIS
2	B	400	GLN
2	B	480	GLN
2	B	646	HIS
2	B	683	ASN
2	B	695	ASN
2	B	755	ASN
2	B	875	HIS
2	B	975	HIS
2	B	999	GLN
2	B	1094	ASN
3	C	58	ASN
3	C	99	HIS
3	C	232	GLN
3	C	248	GLN
4	D	23	HIS
5	E	5	ASN
5	E	147	HIS
5	E	179	GLN
6	F	100	GLN
7	G	64	GLN
7	G	65	HIS
8	H	11	GLN
8	H	33	GLN
8	H	35	GLN
8	H	64	ASN
8	H	131	ASN
9	I	19	ASN
9	I	21	ASN
9	I	27	ASN
11	K	106	GLN
11	K	118	GLN
13	M	16	GLN
13	M	71	GLN
14	N	52	GLN
14	N	132	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

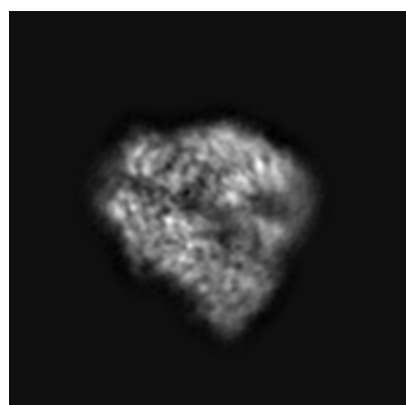
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4088. These allow visual inspection of the internal detail of the map and identification of artifacts.

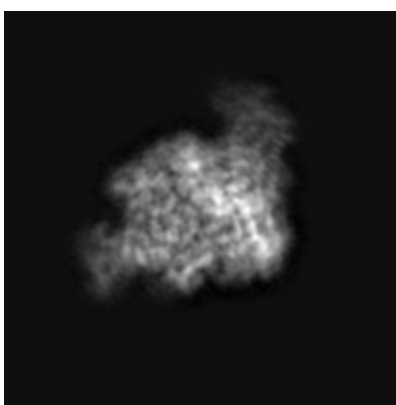
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

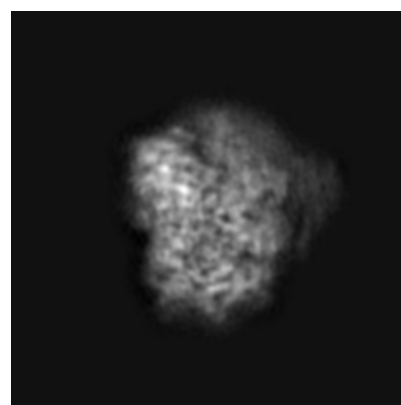
6.1.1 Primary map



X



Y

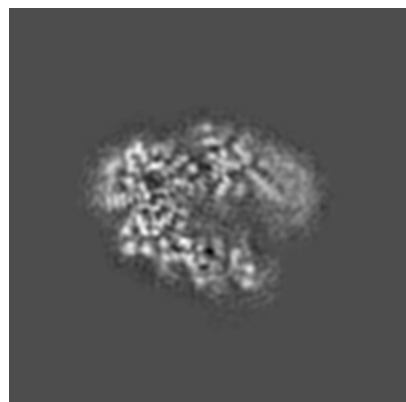


Z

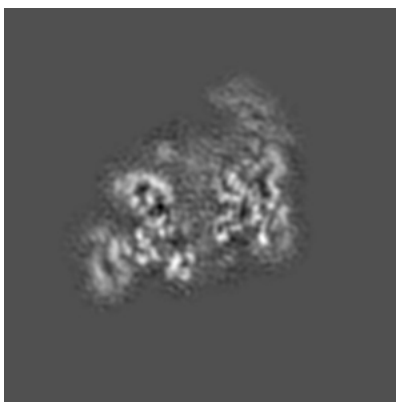
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

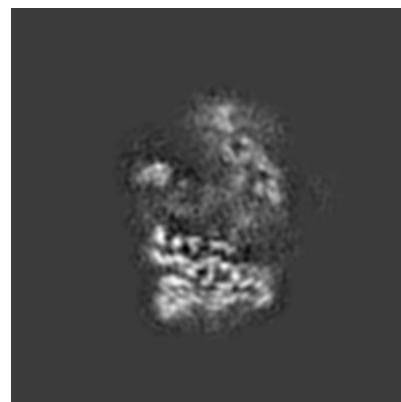
6.2.1 Primary map



X Index: 81



Y Index: 81

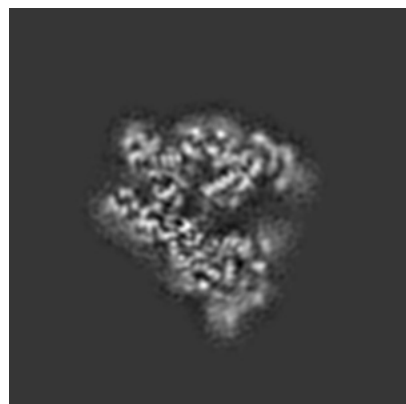


Z Index: 81

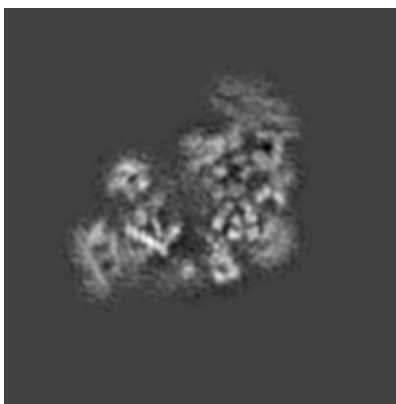
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

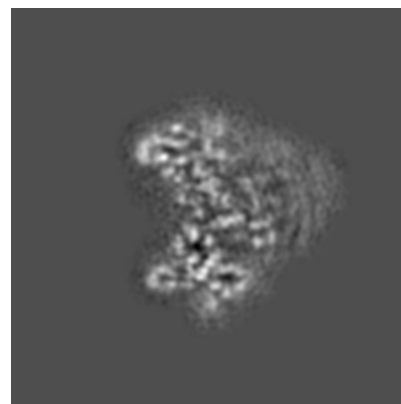
6.3.1 Primary map



X Index: 69



Y Index: 89



Z Index: 98

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

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

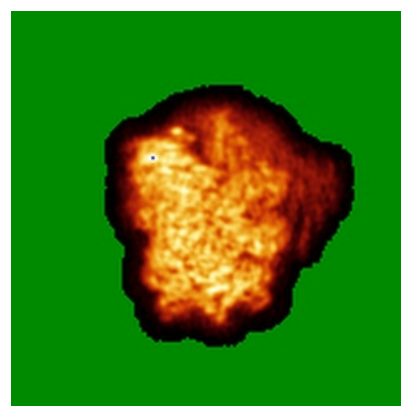
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

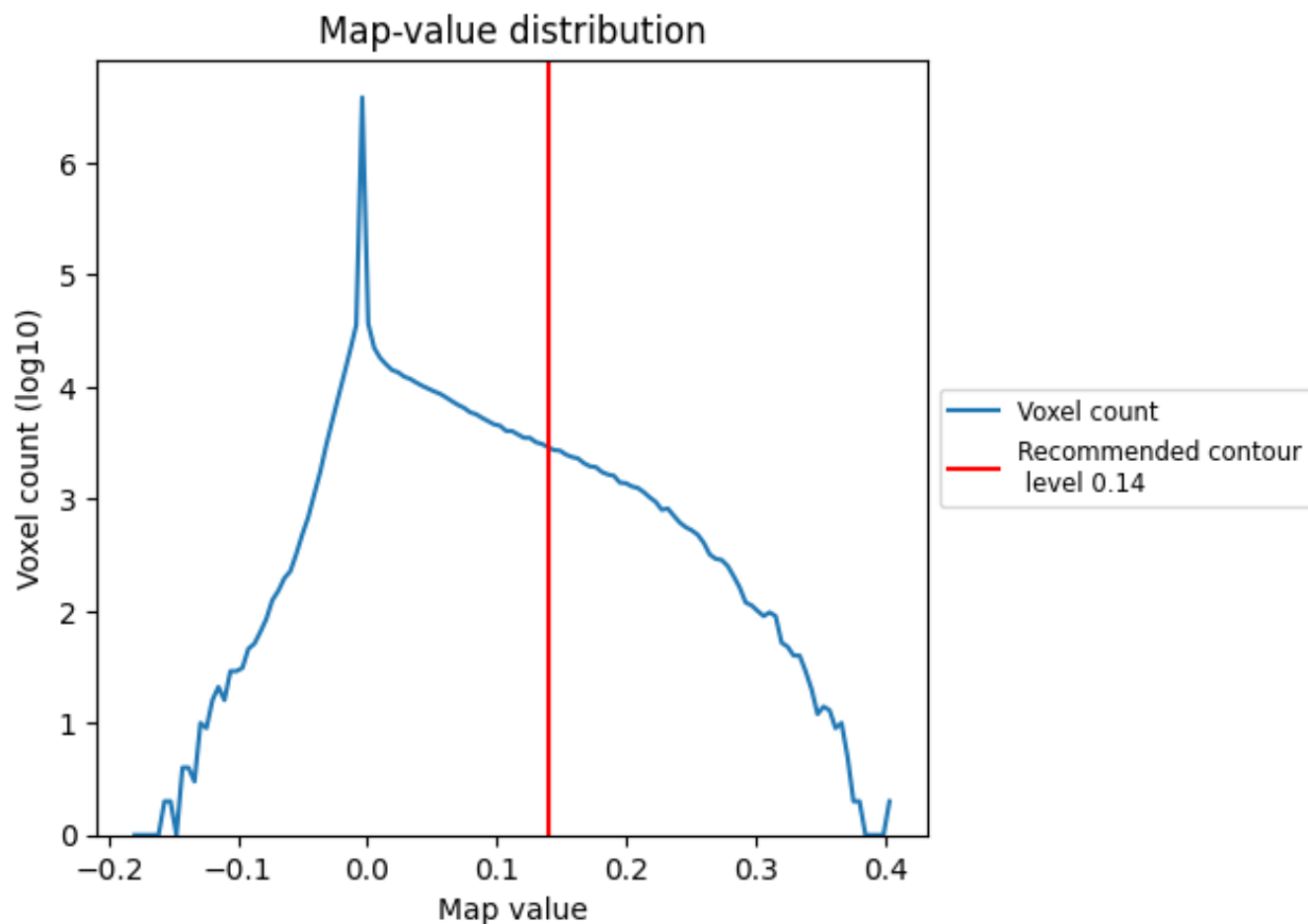
6.6 Mask visualisation

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

7 Map analysis [i](#)

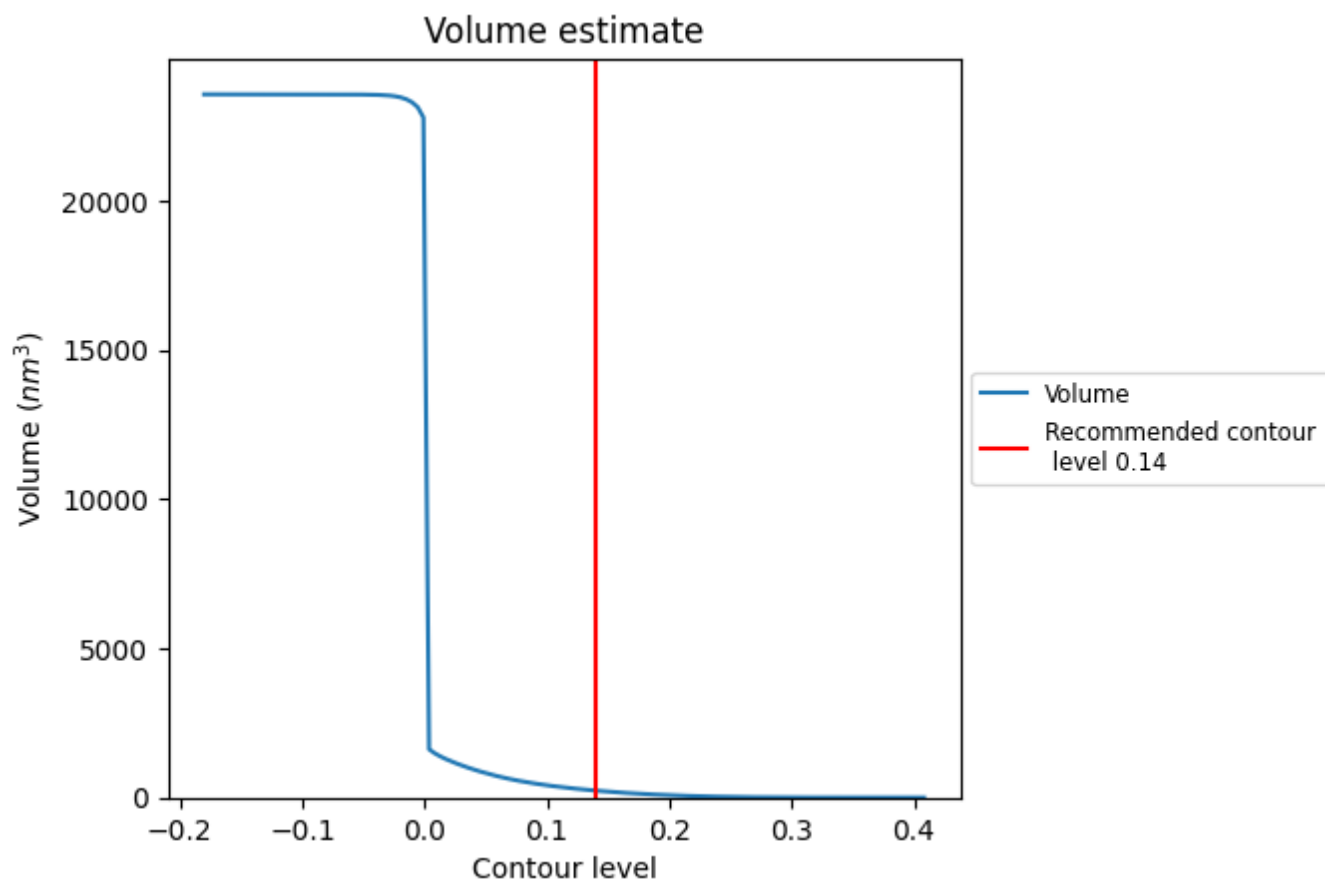
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

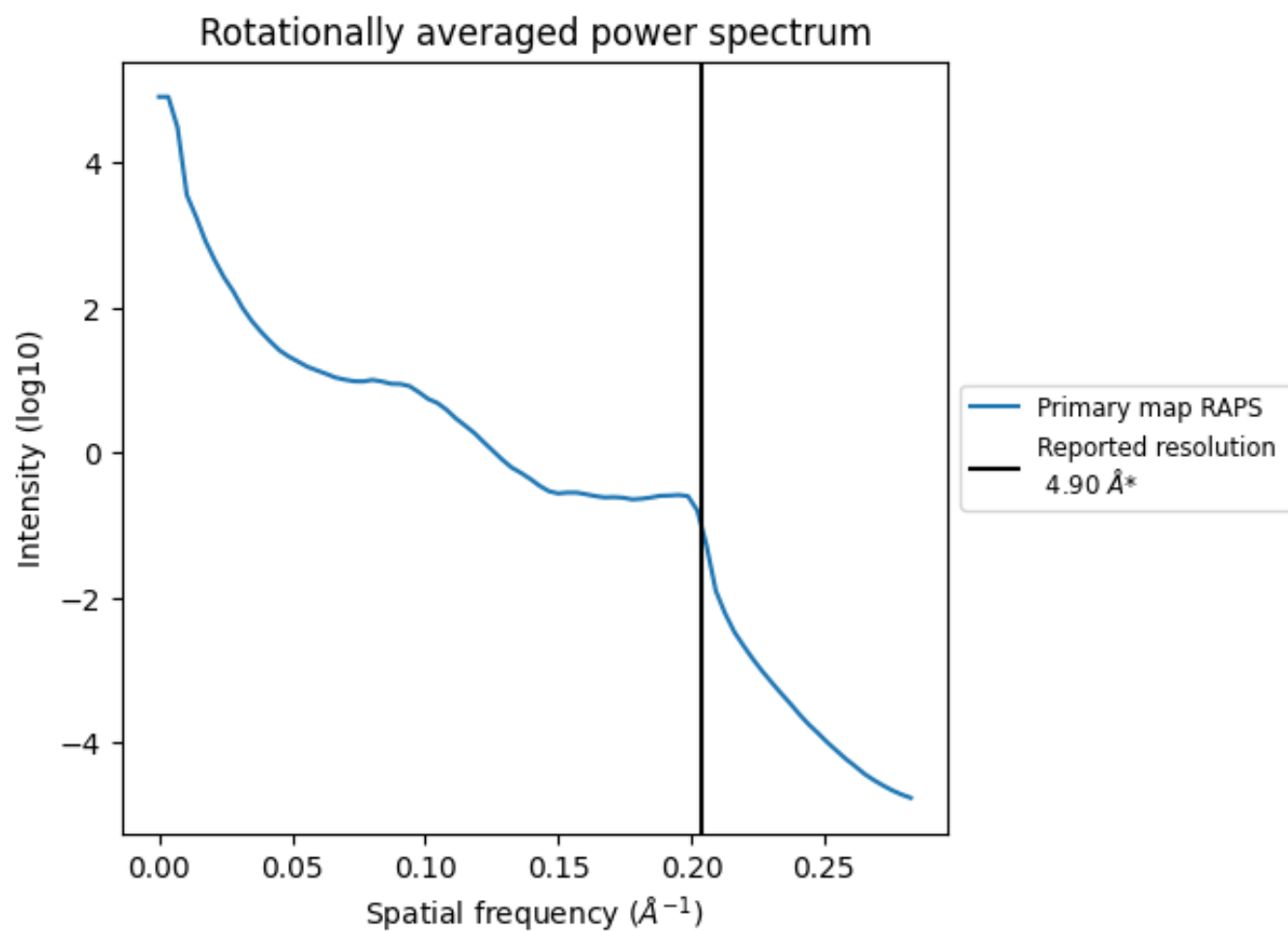
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 233 nm³; this corresponds to an approximate mass of 210 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

8 Fourier-Shell correlation

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

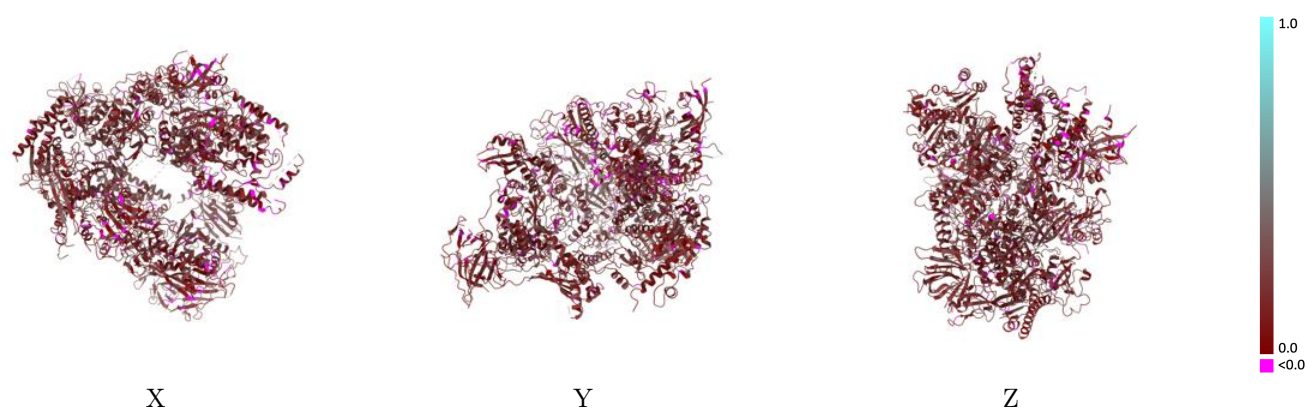
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4088 and PDB model 5LMX. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

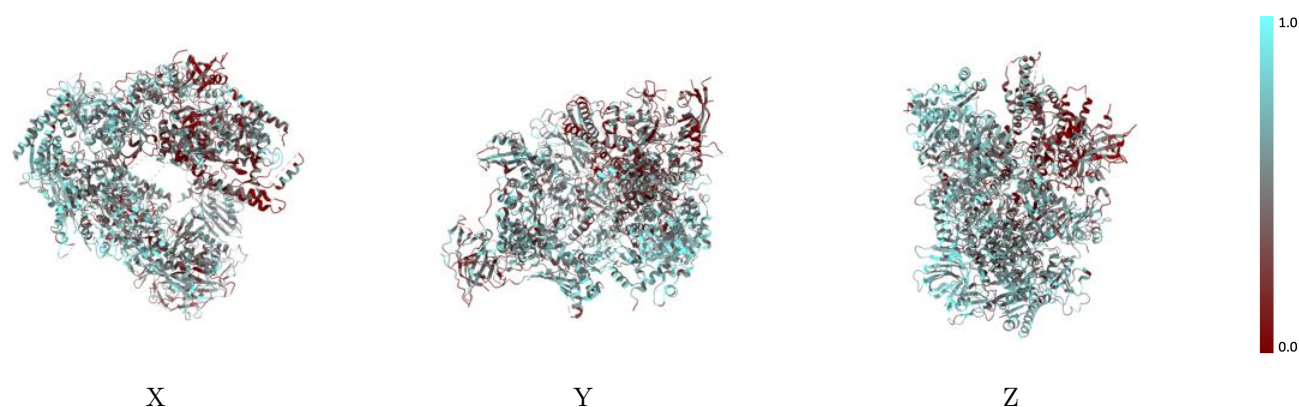
This section was not generated.

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



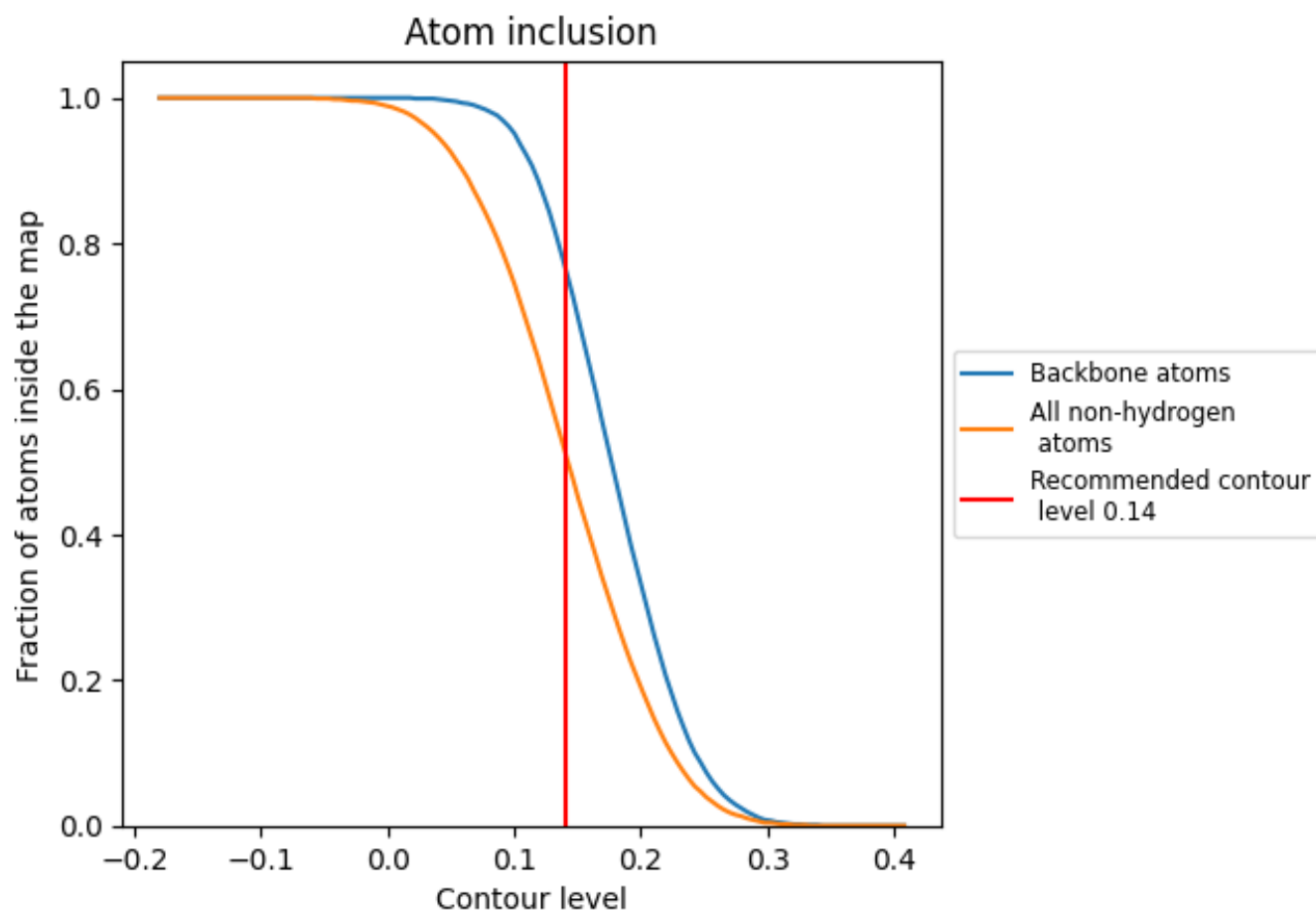
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 51% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5130	0.1830
A	0.4850	0.1820
B	0.5160	0.1770
C	0.6410	0.2020
D	0.1200	0.2100
E	0.6560	0.1840
F	0.4830	0.1910
G	0.2710	0.1830
H	0.6790	0.2120
I	0.4890	0.1950
J	0.6160	0.1980
K	0.5900	0.1840
L	0.5620	0.1250
M	0.4040	0.1460
N	0.3160	0.1800

