



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:17 AM UTC

PDB ID : 5FJA / pdb_00005fja
EMDB ID : EMD-3180
Title : Cryo-EM structure of yeast RNA polymerase III at 4.7 Å
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.;
Hagen, W.J.; Sachse, C.; Muller, C.W.
Deposited on : 2015-10-06
Resolution : 4.65 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:

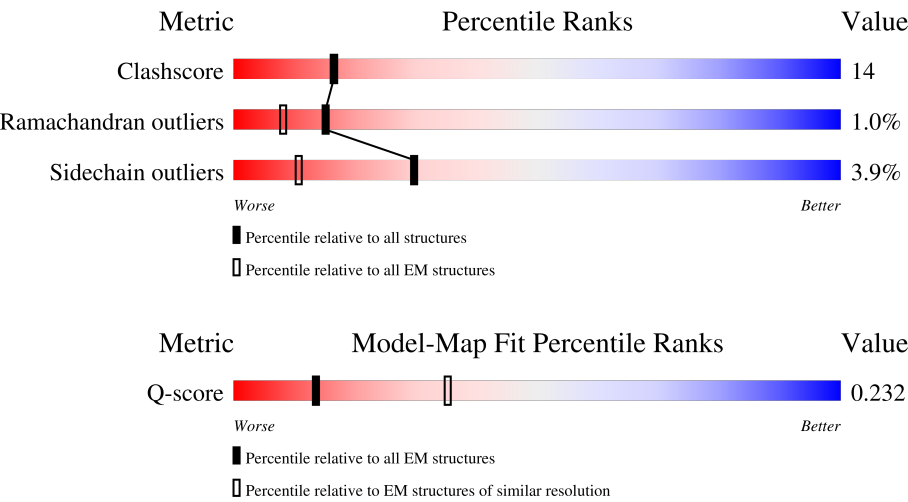
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.65 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	1989 (4.20 - 5.20)

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	1460	
2	B	1149	
3	C	335	
4	D	161	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	88	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38434 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 III SUBUNIT RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1403	Total	C	N	O	S	0	0
			11007	6941	1943	2065	58		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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 RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	182	Total	C	N	O	S	0	0
			1464	961	234	263	6		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	92	Total	C	N	O	S	0	0
			728	455	117	145	11		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	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 RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	89	Total	C	N	O	S	0	0
			738	474	115	146	3		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	47	Total	C	N	O	0	0
			310	195	57	58		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

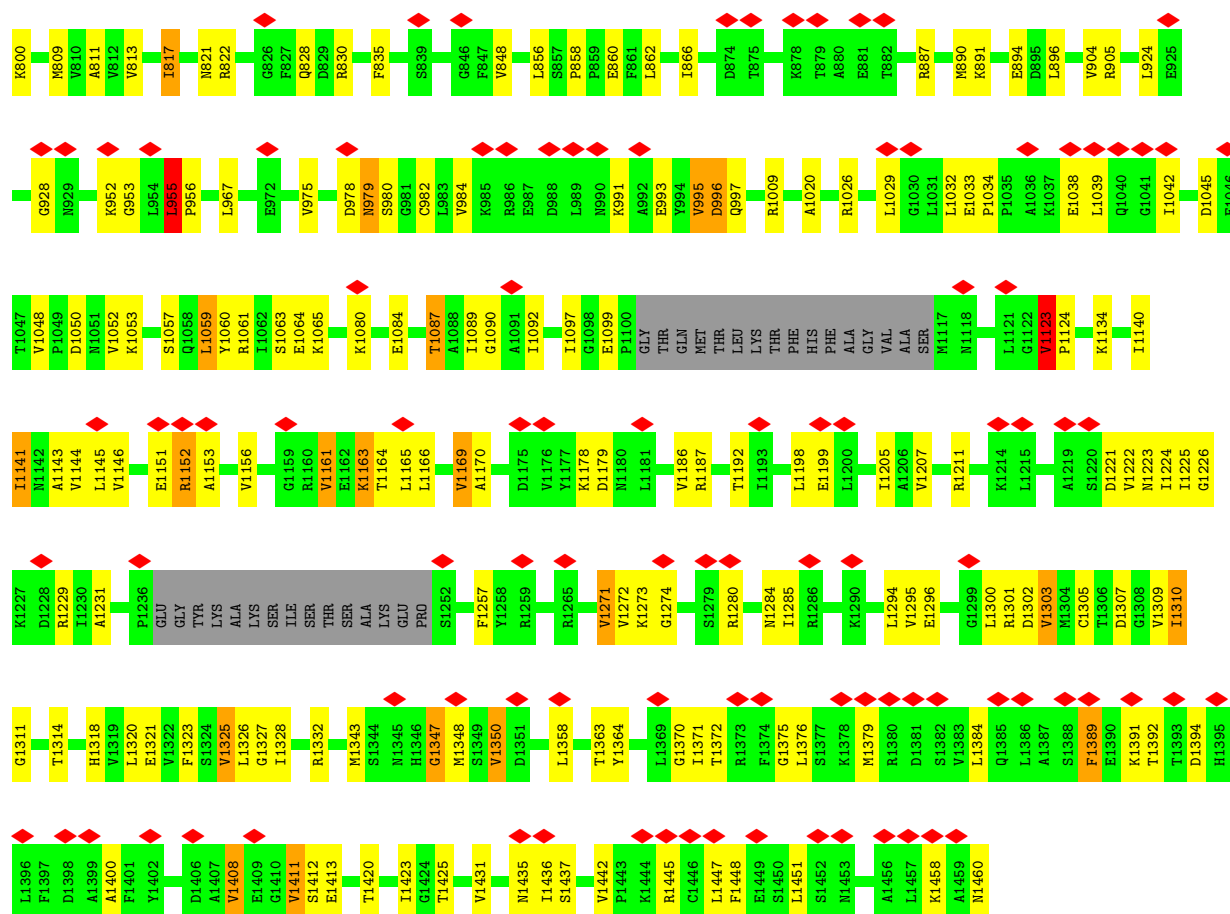
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	1	Total	Zn	0
			1	1	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

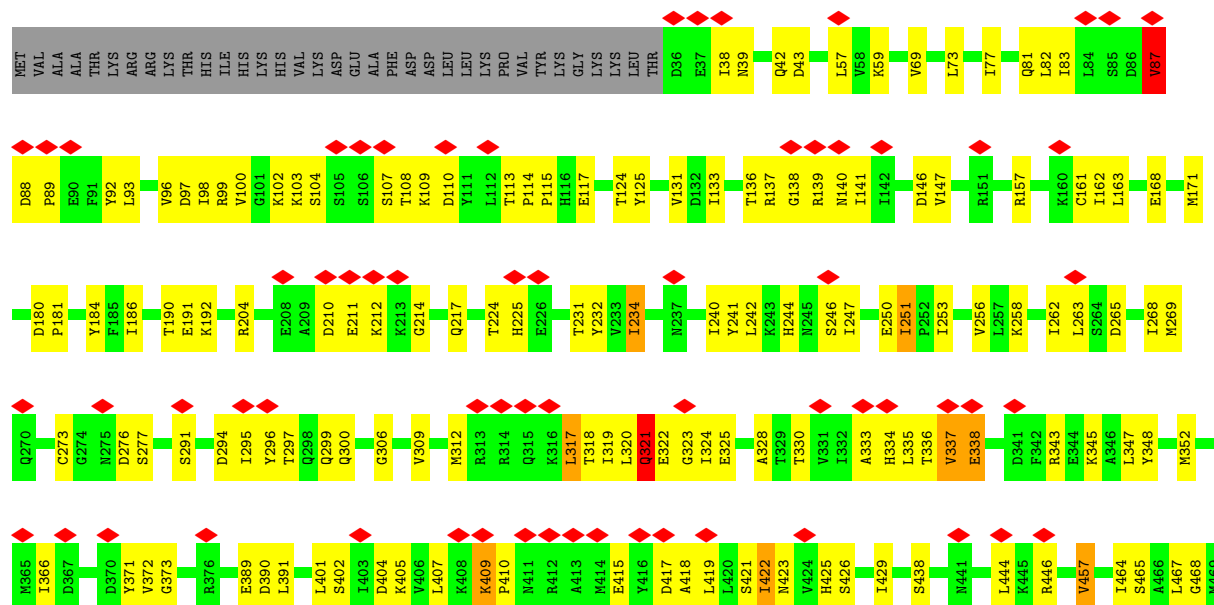
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

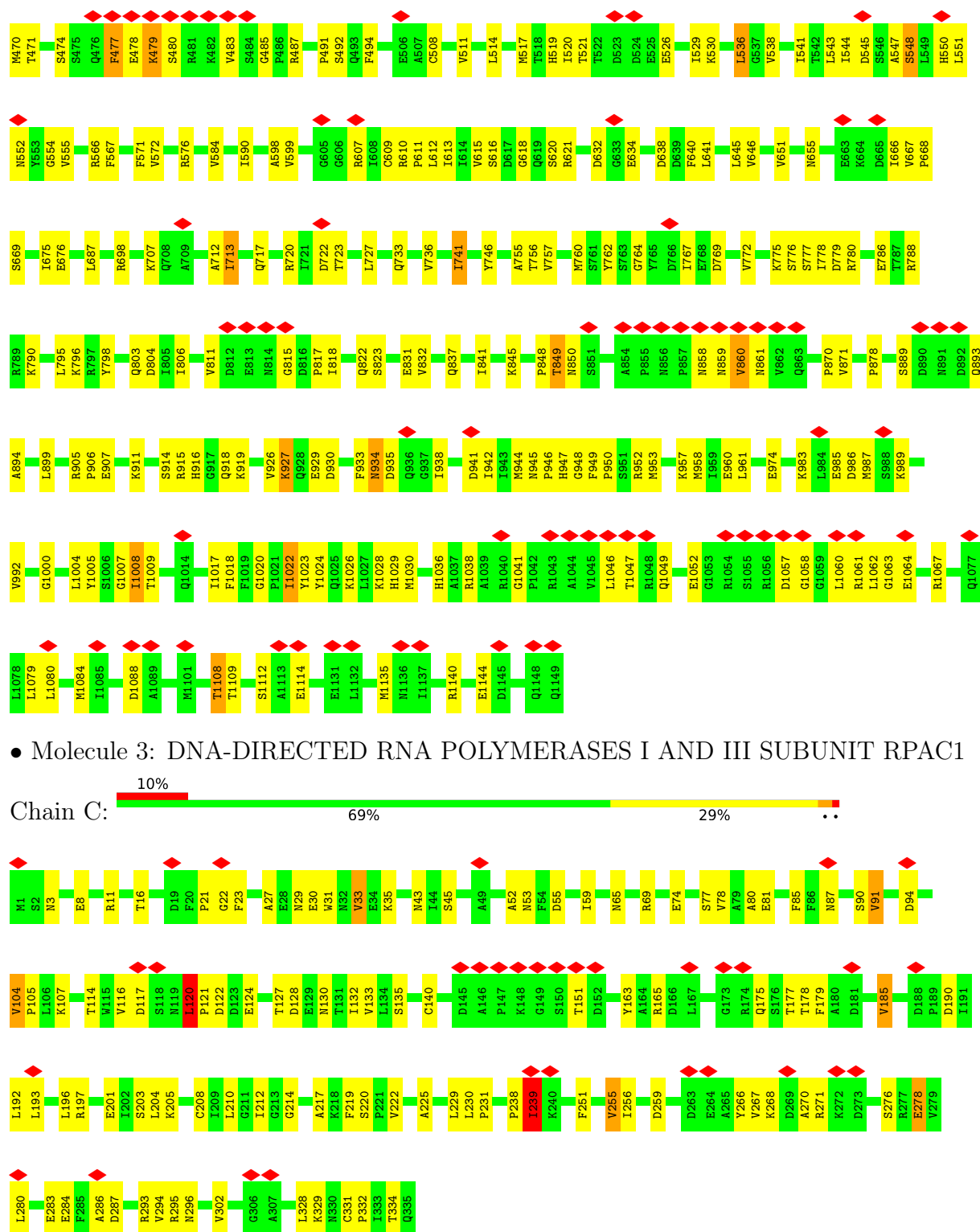
• Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1

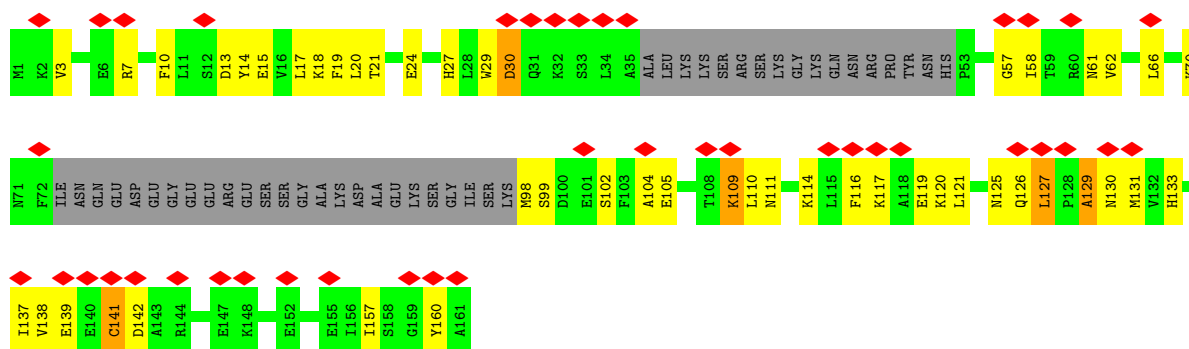




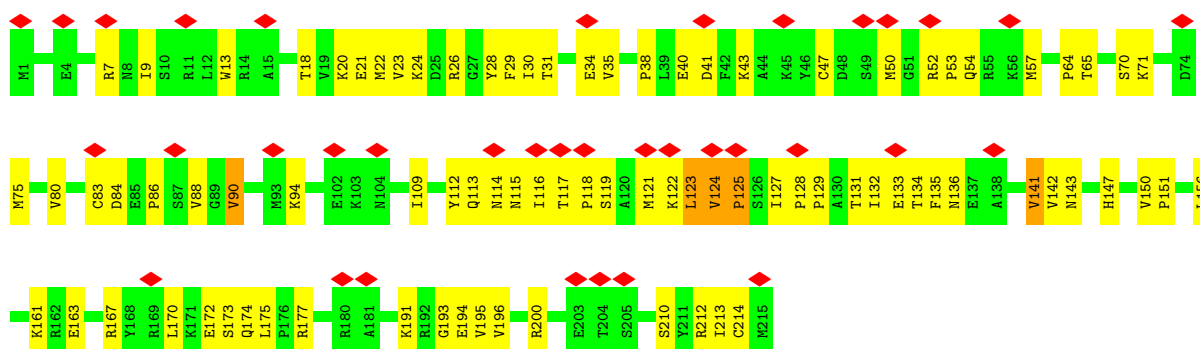
• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2



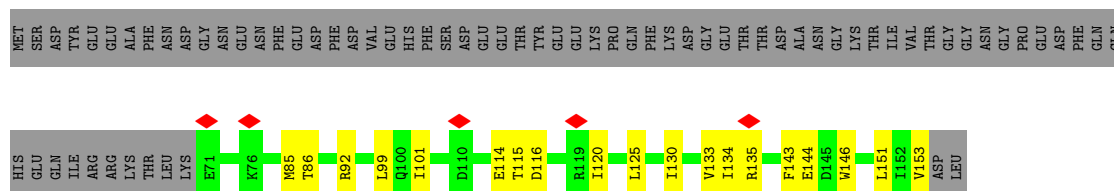




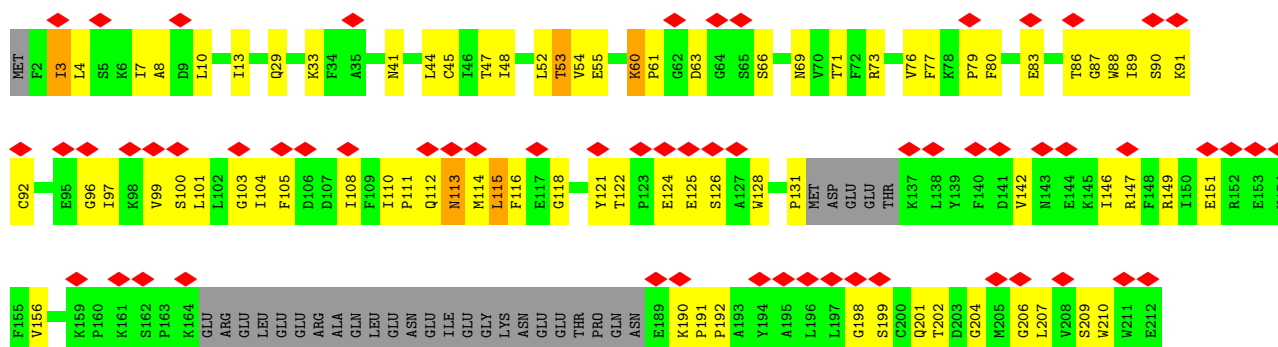
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



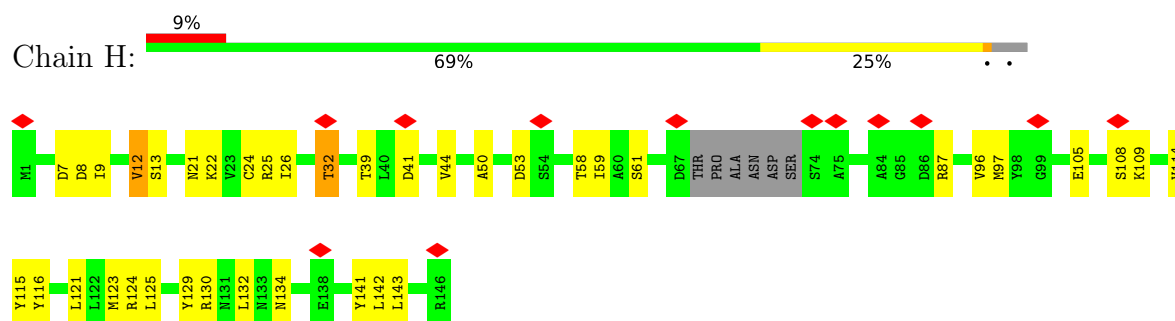
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



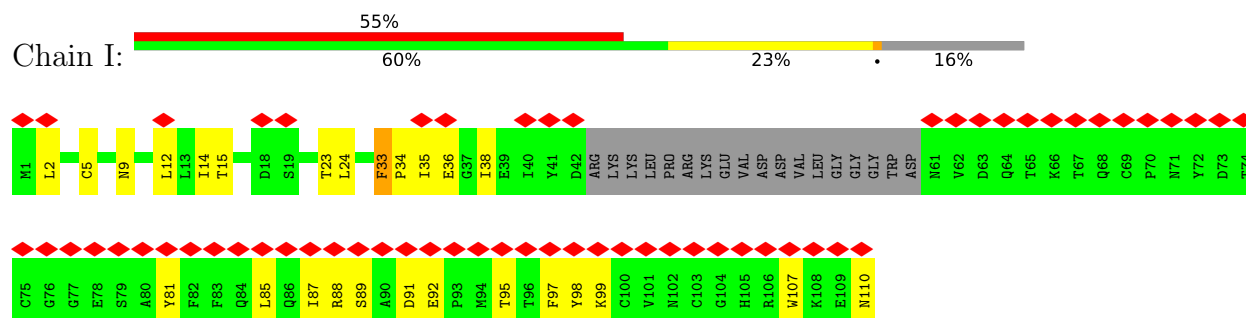
• Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8



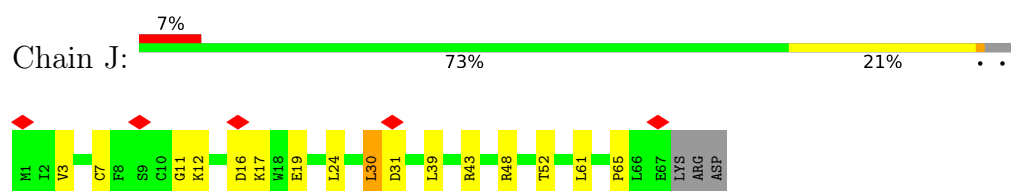
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



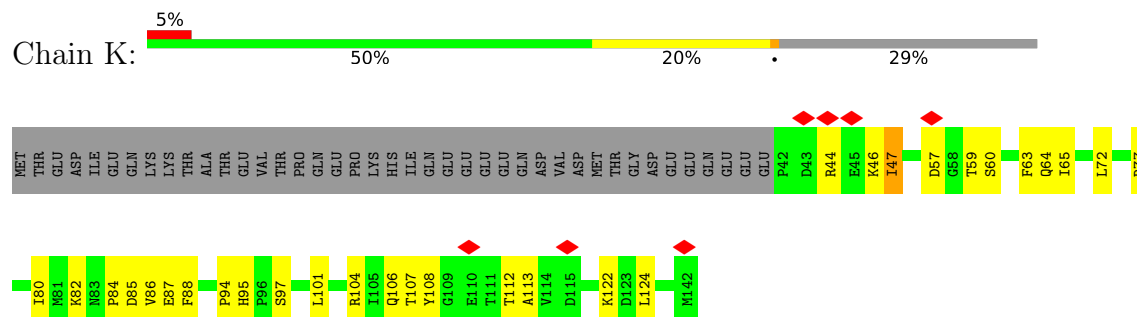
• Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10



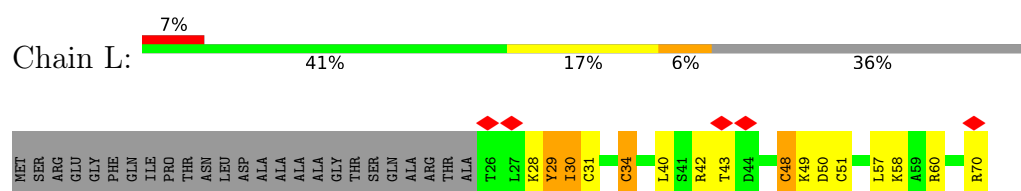
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



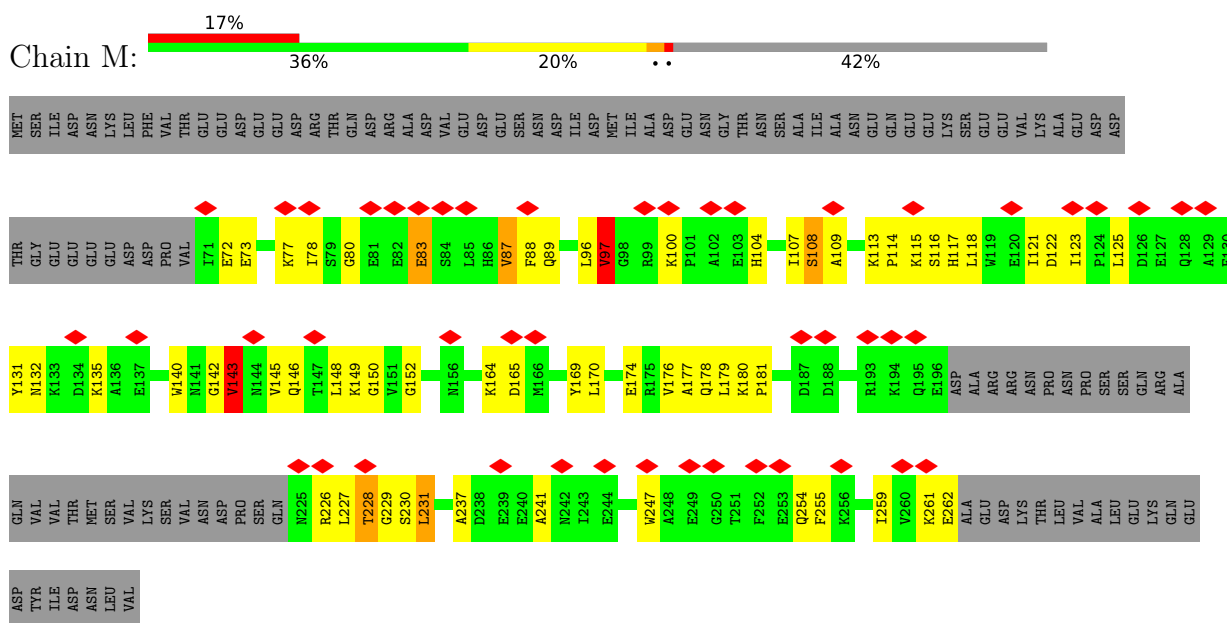
• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



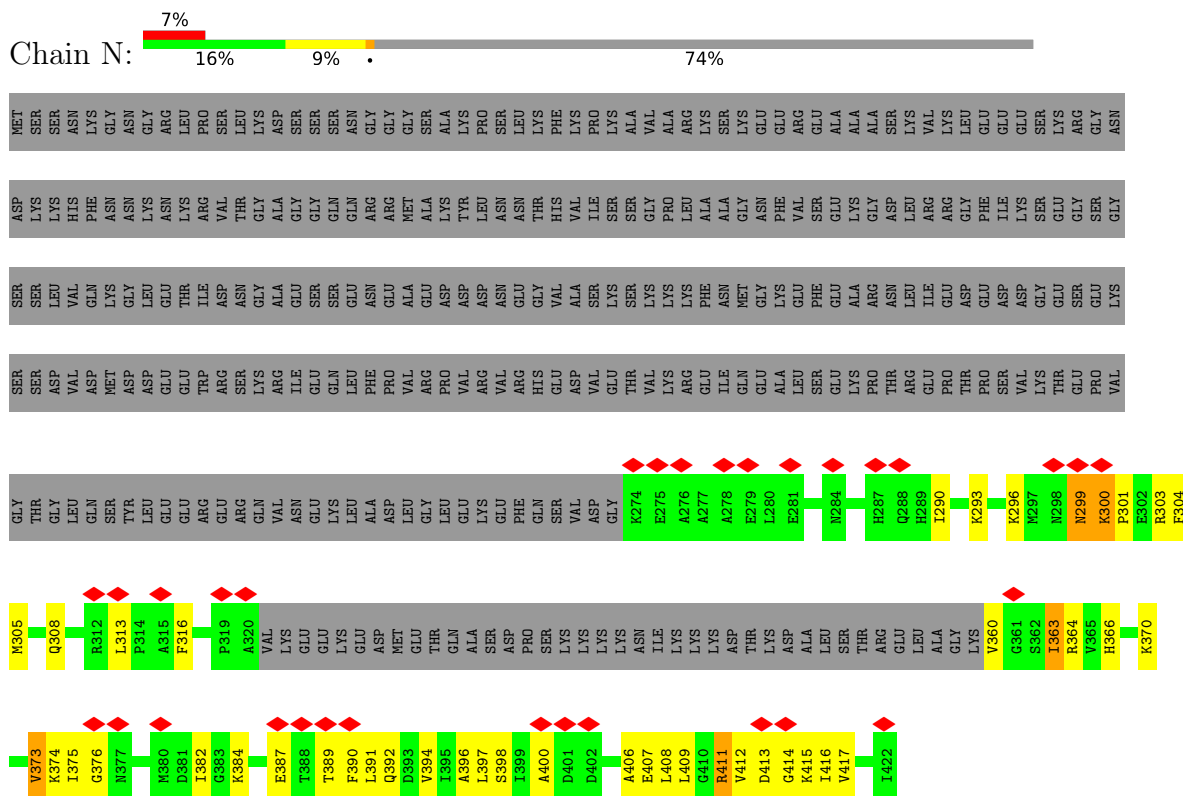
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



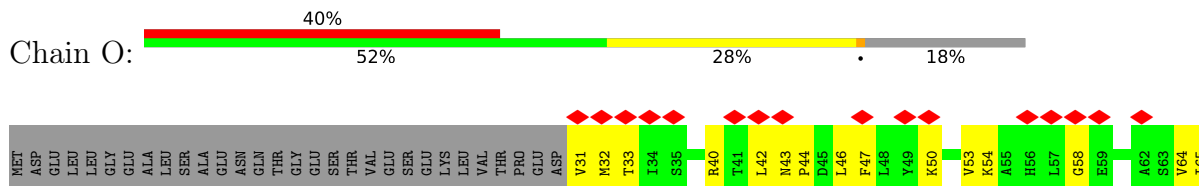
• Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5

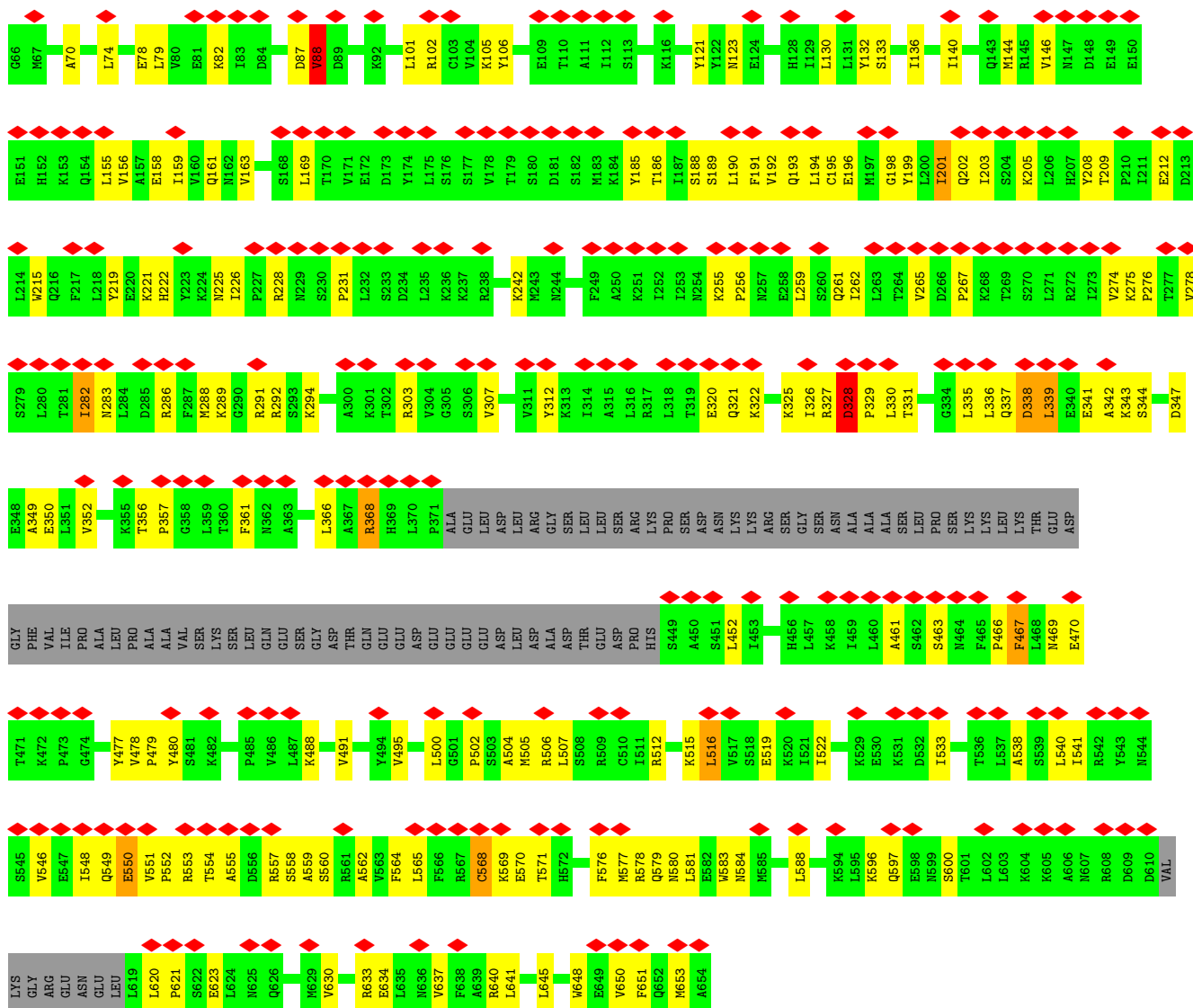


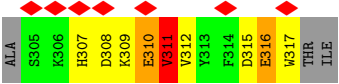
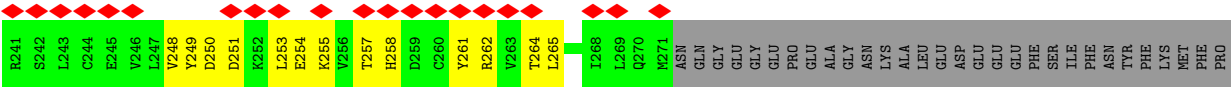
● Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4



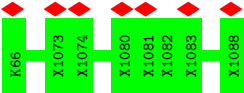
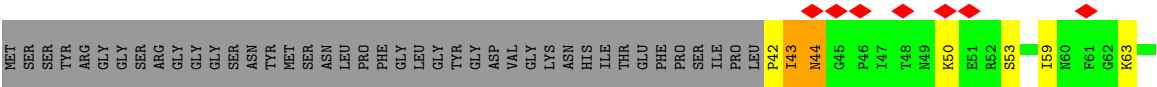
● Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3







• Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52423	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.297	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	320.86398, 320.86398, 320.86398	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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	0.30	0/11202	0.84	30/15130 (0.2%)
2	B	0.29	0/8943	0.81	20/12068 (0.2%)
3	C	0.31	0/2711	0.81	7/3676 (0.2%)
4	D	0.30	0/991	0.92	5/1328 (0.4%)
5	E	0.31	0/1795	0.76	1/2416 (0.0%)
6	F	0.29	0/683	0.75	0/923
7	G	0.32	0/1503	0.82	2/2040 (0.1%)
8	H	0.28	0/1138	0.75	1/1540 (0.1%)
9	I	0.26	0/745	0.78	3/1007 (0.3%)
10	J	0.26	0/558	0.70	0/750
11	K	0.29	0/803	0.78	1/1083 (0.1%)
12	L	0.26	0/360	0.74	1/478 (0.2%)
13	M	0.35	0/1369	0.90	7/1851 (0.4%)
14	N	0.35	0/855	0.95	2/1149 (0.2%)
15	O	0.30	0/4394	0.87	11/5928 (0.2%)
16	P	0.37	0/750	0.86	3/1017 (0.3%)
17	Q	0.39	0/219	0.84	1/294 (0.3%)
All	All	0.30	0/39019	0.83	95/52678 (0.2%)

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	300	LYS	CA-C-N	8.67	130.68	119.84
14	N	300	LYS	C-N-CA	8.67	130.68	119.84
1	A	858	PRO	CA-C-N	-7.89	109.97	119.84
1	A	858	PRO	C-N-CA	-7.89	109.97	119.84
15	O	551	VAL	CA-C-N	7.68	127.84	120.31
15	O	551	VAL	C-N-CA	7.68	127.84	120.31
15	O	568	CYS	CB-CA-C	-7.38	108.05	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	LEU	CA-C-N	6.99	126.47	118.85
1	A	955	LEU	C-N-CA	6.99	126.47	118.85
4	D	30	ASP	CB-CA-C	-6.89	108.61	116.54
2	B	634	GLU	N-CA-C	6.67	116.67	107.73
17	Q	44	ASN	CB-CA-C	-6.67	108.89	116.63
1	A	1442	VAL	N-CA-C	6.51	114.57	107.60
4	D	116	PHE	CB-CA-C	-6.38	109.23	116.63
4	D	141	CYS	CB-CA-C	-6.36	109.23	116.54
15	O	328	ASP	CA-C-N	-6.34	111.91	119.84
15	O	328	ASP	C-N-CA	-6.34	111.91	119.84
15	O	568	CYS	N-CA-C	6.33	117.93	108.31
1	A	1163	LYS	CB-CA-C	-6.27	107.57	116.34
2	B	815	GLY	N-CA-C	-6.25	106.60	114.16
15	O	199	TYR	CB-CA-C	-6.19	109.45	116.63
13	M	108	SER	CB-CA-C	-6.07	108.97	117.23
16	P	310	GLU	CB-CA-C	-6.06	109.60	116.63
2	B	276	ASP	N-CA-C	6.05	116.07	108.45
1	A	1033	GLU	CA-C-N	-6.04	114.16	120.38
1	A	1033	GLU	C-N-CA	-6.04	114.16	120.38
1	A	1152	ARG	CB-CA-C	-5.93	109.17	117.23
5	E	128	PRO	N-CA-C	5.88	117.88	110.70
15	O	559	ALA	N-CA-C	5.84	115.81	108.45
2	B	479	LYS	N-CA-C	5.83	116.62	108.00
9	I	33	PHE	CA-C-N	5.80	140.92	127.00
9	I	33	PHE	C-N-CA	5.80	140.92	127.00
2	B	780	ARG	N-CA-C	-5.79	106.22	113.28
1	A	1050	ASP	CB-CA-C	-5.76	109.40	117.23
13	M	174	GLU	CB-CA-C	-5.74	109.97	116.63
4	D	30	ASP	N-CA-C	5.73	117.02	108.31
2	B	168	GLU	CB-CA-C	-5.65	109.55	117.23
1	A	1123	VAL	CA-C-N	-5.63	113.87	119.56
1	A	1123	VAL	C-N-CA	-5.63	113.87	119.56
13	M	104	HIS	CA-C-N	5.62	125.61	120.21
13	M	104	HIS	C-N-CA	5.62	125.61	120.21
11	K	59	THR	CB-CA-C	-5.60	109.61	117.23
13	M	100	LYS	CA-C-N	5.58	125.20	119.56
13	M	100	LYS	C-N-CA	5.58	125.20	119.56
3	C	120	LEU	CA-C-N	5.58	125.89	119.92
3	C	120	LEU	C-N-CA	5.58	125.89	119.92
1	A	1034	PRO	CA-C-N	5.53	125.54	119.90
1	A	1034	PRO	C-N-CA	5.53	125.54	119.90
13	M	165	ASP	CB-CA-C	-5.52	110.23	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	122	ASP	CB-CA-C	-5.51	110.20	116.54
1	A	1163	LYS	N-CA-C	5.51	116.15	108.00
1	A	38	ASP	CB-CA-C	-5.49	109.26	115.79
2	B	479	LYS	CB-CA-C	-5.48	108.67	116.34
2	B	409	LYS	CA-C-N	5.44	124.90	119.24
2	B	409	LYS	C-N-CA	5.44	124.90	119.24
1	A	555	GLN	CB-CA-C	-5.43	109.84	117.23
3	C	220	SER	CA-C-N	5.42	124.76	118.85
3	C	220	SER	C-N-CA	5.42	124.76	118.85
1	A	448	ASP	CB-CA-C	-5.41	109.87	117.23
3	C	185	VAL	N-CA-C	5.38	113.60	109.19
15	O	43	ASN	N-CA-C	5.35	118.35	109.79
1	A	1179	ASP	CB-CA-C	-5.33	109.98	117.23
3	C	90	SER	N-CA-C	5.32	117.41	107.99
7	G	60	LYS	CA-C-N	5.32	125.38	119.32
7	G	60	LYS	C-N-CA	5.32	125.38	119.32
1	A	274	MET	CB-CA-C	-5.28	109.50	115.79
2	B	338	GLU	CB-CA-C	-5.28	110.05	117.23
1	A	952	LYS	CB-CA-C	-5.28	108.95	116.34
4	D	129	ALA	N-CA-C	5.26	119.28	112.86
2	B	764	GLY	N-CA-C	-5.26	107.28	114.64
1	A	979	ASN	CB-CA-C	-5.25	110.09	117.23
2	B	934	ASN	N-CA-C	5.24	115.75	108.00
1	A	160	LEU	N-CA-C	5.22	115.18	108.34
2	B	477	PHE	CB-CA-C	-5.22	110.14	117.23
16	P	316	GLU	CB-CA-C	-5.21	110.15	117.23
8	H	32	THR	CB-CA-C	-5.20	110.16	117.23
15	O	133	SER	CB-CA-C	-5.20	110.16	117.23
2	B	214	GLY	N-CA-C	5.18	117.02	110.38
2	B	277	SER	CB-CA-C	-5.18	109.08	116.34
12	L	29	TYR	CB-CA-C	-5.17	109.64	115.79
1	A	247	THR	N-CA-C	-5.13	106.61	112.92
1	A	1370	GLY	N-CA-C	5.13	117.53	110.56
15	O	467	PHE	N-CA-C	5.12	117.20	109.41
2	B	1041	GLY	CA-C-N	5.11	125.04	119.78
2	B	1041	GLY	C-N-CA	5.11	125.04	119.78
1	A	55	ASP	CA-C-N	5.10	125.14	119.32
1	A	55	ASP	C-N-CA	5.10	125.14	119.32
1	A	1347	GLY	N-CA-C	5.10	118.03	110.63
1	A	649	ASP	CB-CA-C	-5.09	110.31	117.23
2	B	548	SER	N-CA-C	5.09	116.97	108.99
2	B	676	GLU	CA-C-N	5.05	124.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	676	GLU	C-N-CA	5.05	124.71	119.56
1	A	236	SER	CB-CA-C	-5.04	110.78	116.63
16	P	251	ASP	CB-CA-C	-5.04	110.38	117.23
9	I	33	PHE	C-N-CD	-5.02	109.55	120.60

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	11007	0	11137	328	0
2	B	8788	0	8902	262	0
3	C	2655	0	2628	71	0
4	D	977	0	983	40	0
5	E	1759	0	1788	59	0
6	F	671	0	692	12	0
7	G	1464	0	1466	51	0
8	H	1120	0	1089	32	0
9	I	728	0	672	27	0
10	J	549	0	560	10	0
11	K	792	0	790	29	0
12	L	358	0	381	15	0
13	M	1338	0	1307	52	0
14	N	845	0	891	42	0
15	O	4329	0	4497	153	0
16	P	738	0	719	38	0
17	Q	310	0	248	8	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	38434	0	38750	1086	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 14.

All (1086) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:HG2	1:A:600:PRO:CD	1.32	1.57
1:A:599:LYS:CG	1:A:600:PRO:HD2	1.25	1.56
1:A:599:LYS:CG	1:A:600:PRO:CD	1.99	1.11
1:A:599:LYS:HG3	1:A:600:PRO:HD2	1.47	0.93
3:C:251:PHE:HB3	3:C:255:VAL:HG11	1.51	0.92
1:A:599:LYS:HG3	1:A:600:PRO:CD	1.96	0.90
1:A:602:TYR:O	1:A:603:LEU:O	1.91	0.89
5:E:127:ILE:HG22	5:E:129:PRO:HD2	1.53	0.89
1:A:615:LYS:NZ	1:A:620:SER:O	2.05	0.88
3:C:16:THR:O	3:C:295:ARG:NH1	2.07	0.87
15:O:488:LYS:NZ	15:O:650:VAL:O	2.09	0.85
2:B:192:LYS:NZ	2:B:438:SER:O	2.09	0.84
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.51	0.84
2:B:373:GLY:HA2	2:B:607:ARG:HH22	1.43	0.83
1:A:1163:LYS:HZ1	1:A:1280:ARG:HA	1.41	0.83
2:B:139:ARG:HE	2:B:141:ILE:HD11	1.44	0.83
1:A:232:LYS:NZ	16:P:316:GLU:OE1	2.12	0.82
2:B:319:ILE:HG12	13:M:231:LEU:HD21	1.59	0.82
2:B:312:MET:HB3	2:B:317:LEU:HD21	1.59	0.80
1:A:599:LYS:O	1:A:602:TYR:CE2	2.34	0.79
1:A:413:ARG:NH1	1:A:456:LEU:O	2.16	0.79
1:A:43:GLU:HB2	1:A:48:PRO:HD2	1.62	0.79
1:A:599:LYS:HG2	1:A:600:PRO:N	1.97	0.78
2:B:823:SER:OG	2:B:831:GLU:OE2	2.02	0.78
1:A:905:ARG:HH22	5:E:170:LEU:HD21	1.50	0.77
5:E:124:VAL:HG13	5:E:125:PRO:HD3	1.67	0.77
15:O:190:LEU:HG	15:O:193:GLN:HB3	1.67	0.76
1:A:154:CYS:HB2	1:A:160:LEU:HB3	1.68	0.75
2:B:321:GLN:NE2	2:B:322:GLU:OE1	2.20	0.75
2:B:247:ILE:HG21	2:B:251:ILE:HD11	1.69	0.74
12:L:48:CYS:SG	12:L:51:CYS:HB2	2.17	0.74
1:A:160:LEU:HD21	15:O:339:LEU:HG	1.70	0.74
2:B:1007:GLY:O	3:C:69:ARG:NH1	2.21	0.73
7:G:207:LEU:HD23	7:G:209:SER:H	1.51	0.73
7:G:146:ILE:HG23	7:G:206:GLY:HA2	1.69	0.73
13:M:87:VAL:HA	14:N:396:ALA:HA	1.71	0.73
14:N:299:ASN:C	14:N:301:PRO:HD3	2.14	0.72
3:C:270:ALA:HB3	3:C:271:ARG:HH11	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:CG	1:A:154:CYS:SG	2.72	0.72
11:K:65:ILE:HB	11:K:101:LEU:HB3	1.71	0.72
14:N:303:ARG:HD3	14:N:411:ARG:HD3	1.69	0.71
14:N:301:PRO:O	14:N:303:ARG:HG2	1.91	0.71
1:A:756:CYS:SG	1:A:757:ASN:N	2.56	0.71
1:A:550:ILE:HG23	1:A:551:ILE:HG23	1.72	0.70
10:J:12:LYS:HE3	10:J:43:ARG:NH2	2.06	0.70
15:O:488:LYS:NZ	15:O:651:PHE:HA	2.07	0.70
1:A:598:MET:HE1	8:H:141:TYR:CE1	2.27	0.70
2:B:322:GLU:O	2:B:325:GLU:OE1	2.10	0.69
2:B:778:ILE:HD11	2:B:906:PRO:HG2	1.74	0.69
1:A:182:THR:HG22	1:A:185:TRP:HE1	1.56	0.69
1:A:436:ARG:HD3	1:A:459:GLY:HA3	1.75	0.69
2:B:419:LEU:O	2:B:423:ASN:ND2	2.25	0.69
1:A:1020:ALA:HB2	1:A:1032:LEU:HD11	1.74	0.69
1:A:1425:THR:C	6:F:92:ARG:HH21	2.01	0.69
16:P:229:GLN:H	16:P:233:VAL:HG12	1.58	0.69
1:A:602:TYR:O	1:A:603:LEU:C	2.34	0.69
2:B:234:ILE:HB	2:B:240:ILE:HG22	1.75	0.69
1:A:476:ARG:HG2	1:A:478:PRO:HD2	1.73	0.69
2:B:698:ARG:HH21	2:B:952:ARG:HG2	1.56	0.69
4:D:141:CYS:SG	4:D:142:ASP:N	2.65	0.69
15:O:620:LEU:HD23	15:O:623:GLU:HB2	1.74	0.69
3:C:31:TRP:H	11:K:82:LYS:HE2	1.56	0.68
2:B:373:GLY:HA2	2:B:607:ARG:NH2	2.08	0.68
4:D:110:LEU:HB3	4:D:120:LYS:HZ2	1.59	0.68
1:A:247:THR:HG23	1:A:249:PRO:HD3	1.76	0.68
1:A:601:TYR:CD1	3:C:23:PHE:CE2	2.82	0.68
13:M:113:LYS:HD3	13:M:241:ALA:HB2	1.73	0.68
15:O:507:LEU:HD13	15:O:540:LEU:HD22	1.75	0.68
15:O:549:GLN:HG2	15:O:565:LEU:HD13	1.75	0.68
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.76	0.68
13:M:247:TRP:HE1	14:N:408:LEU:HB2	1.58	0.67
1:A:599:LYS:HG3	1:A:600:PRO:HD3	1.73	0.67
4:D:127:LEU:HB2	4:D:133:HIS:HB3	1.76	0.67
1:A:573:ARG:HH21	11:K:87:GLU:HB3	1.60	0.67
7:G:147:ARG:NH2	7:G:204:GLY:O	2.22	0.67
12:L:29:TYR:HE2	12:L:40:LEU:HB2	1.59	0.67
1:A:1164:THR:HB	1:A:1271:VAL:HA	1.76	0.67
15:O:341:GLU:HG2	15:O:344:SER:HB2	1.75	0.67
9:I:81:TYR:HB2	9:I:99:LYS:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:CG	1:A:600:PRO:HD3	2.19	0.66
1:A:107:CYS:CB	1:A:110:CYS:SG	2.84	0.66
2:B:914:SER:OG	2:B:957:LYS:NZ	2.21	0.66
15:O:322:LYS:HB3	15:O:361:PHE:HE1	1.58	0.66
4:D:117:LYS:NZ	4:D:121:LEU:HD22	2.10	0.66
1:A:887:ARG:HH12	1:A:1389:PHE:HD1	1.43	0.66
2:B:81:GLN:HG2	2:B:82:LEU:HG	1.78	0.66
1:A:663:VAL:HG23	1:A:665:ASP:OD2	1.95	0.66
7:G:96:GLY:HA3	7:G:111:PRO:HA	1.77	0.66
8:H:24:CYS:SG	8:H:25:ARG:N	2.69	0.66
1:A:40:PHE:HZ	1:A:282:GLU:HB3	1.61	0.65
1:A:599:LYS:O	1:A:602:TYR:CD2	2.49	0.65
1:A:1435:ASN:O	1:A:1435:ASN:ND2	2.28	0.65
2:B:1067:ARG:NH1	2:B:1079:LEU:HD22	2.12	0.65
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.77	0.65
2:B:698:ARG:HE	2:B:952:ARG:HB3	1.61	0.65
2:B:760:MET:HE3	2:B:762:TYR:HB2	1.77	0.65
11:K:47:ILE:HG12	11:K:65:ILE:HG12	1.78	0.65
1:A:476:ARG:NH1	1:A:509:ASN:O	2.29	0.65
5:E:88:VAL:HG23	5:E:117:THR:HG22	1.79	0.65
13:M:148:LEU:HG	13:M:181:PRO:HB3	1.78	0.65
15:O:105:LYS:HB3	15:O:121:TYR:HB2	1.79	0.64
1:A:356:ARG:HH22	2:B:1046:LEU:HD11	1.60	0.64
1:A:482:ARG:HH12	1:A:924:LEU:HD11	1.60	0.64
5:E:90:VAL:HG13	5:E:122:LYS:NZ	2.12	0.64
8:H:58:THR:HB	8:H:143:LEU:HB3	1.80	0.64
15:O:40:ARG:O	16:P:317:TRP:NE1	2.30	0.64
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.78	0.64
1:A:297:SER:HA	1:A:300:LYS:HB3	1.80	0.64
7:G:104:ILE:HG23	7:G:105:PHE:H	1.62	0.64
15:O:466:PRO:HG2	15:O:467:PHE:HD1	1.62	0.64
8:H:97:MET:HB2	8:H:142:LEU:HB3	1.80	0.64
2:B:796:LYS:NZ	2:B:798:TYR:OH	2.31	0.64
1:A:799:SER:OG	1:A:800:LYS:N	2.31	0.64
15:O:327:ARG:NH1	15:O:330:LEU:HD22	2.12	0.64
9:I:24:LEU:HG	9:I:33:PHE:HB3	1.80	0.63
13:M:77:LYS:HE3	13:M:262:GLU:HB3	1.78	0.63
1:A:393:ALA:HA	1:A:491:LYS:HB2	1.81	0.63
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.80	0.63
12:L:42:ARG:HG3	12:L:43:THR:HG23	1.81	0.63
3:C:328:LEU:HA	11:K:46:LYS:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:PRO:HD3	5:E:113:GLN:HG2	1.81	0.63
2:B:757:VAL:HG23	2:B:942:ILE:HB	1.80	0.63
15:O:303:ARG:HD2	15:O:467:PHE:HE1	1.64	0.63
1:A:67:CYS:SG	1:A:69:THR:OG1	2.57	0.62
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.80	0.62
3:C:270:ALA:HB3	3:C:271:ARG:NH1	2.14	0.62
16:P:236:THR:HG22	16:P:237:PRO:HD2	1.81	0.62
2:B:103:LYS:NZ	2:B:146:ASP:HB2	2.14	0.62
15:O:185:TYR:HA	15:O:188:SER:HB2	1.80	0.62
1:A:62:SER:HB3	1:A:65:LEU:HG	1.82	0.62
1:A:272:VAL:HG23	1:A:281:ASN:HB3	1.81	0.62
2:B:87:VAL:HG11	2:B:407:LEU:HB3	1.80	0.62
2:B:755:ALA:HA	10:J:48:ARG:NH1	2.15	0.62
1:A:1372:THR:O	1:A:1376:LEU:N	2.33	0.62
2:B:832:VAL:HB	12:L:60:ARG:HA	1.82	0.62
5:E:122:LYS:HG3	5:E:123:LEU:H	1.65	0.62
15:O:286:ARG:NH2	15:O:321:GLN:O	2.32	0.62
2:B:554:GLY:H	2:B:598:ALA:HA	1.65	0.61
4:D:130:ASN:O	4:D:133:HIS:ND1	2.33	0.61
1:A:1064:GLU:OE1	1:A:1065:LYS:N	2.33	0.61
14:N:363:ILE:HG12	14:N:373:VAL:HG13	1.80	0.61
2:B:389:GLU:OE2	2:B:446:ARG:NH2	2.33	0.61
2:B:948:GLY:HA2	2:B:952:ARG:NH1	2.15	0.61
1:A:712:ILE:HG23	1:A:790:ALA:HB3	1.82	0.61
2:B:253:ILE:HD12	2:B:256:VAL:HB	1.82	0.61
1:A:1311:GLY:O	5:E:147:HIS:NE2	2.33	0.61
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.83	0.60
14:N:363:ILE:HG23	14:N:373:VAL:HG22	1.83	0.60
15:O:555:ALA:HB1	15:O:558:SER:HB2	1.83	0.60
9:I:33:PHE:CD2	9:I:34:PRO:HA	2.36	0.60
15:O:198:GLY:HA3	15:O:286:ARG:HG2	1.82	0.60
1:A:598:MET:O	1:A:599:LYS:HB2	2.01	0.60
1:A:252:ARG:O	1:A:254:GLU:N	2.29	0.60
1:A:1169:VAL:HG13	1:A:1192:THR:HB	1.84	0.60
5:E:200:ARG:NH1	5:E:210:SER:OG	2.34	0.60
15:O:552:PRO:HA	15:O:562:ALA:HB1	1.83	0.60
1:A:631:LYS:NZ	1:A:797:CYS:O	2.34	0.60
4:D:24:GLU:OE2	4:D:30:ASP:HB2	2.02	0.60
4:D:127:LEU:HD11	4:D:137:ILE:HD13	1.84	0.60
7:G:89:ILE:HA	7:G:99:VAL:HA	1.84	0.60
2:B:779:ASP:OD2	3:C:217:ALA:N	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HD2	1:A:54:LEU:HB3	1.83	0.59
2:B:775:LYS:HA	2:B:778:ILE:HG22	1.84	0.59
1:A:220:ASP:OD1	1:A:220:ASP:N	2.34	0.59
1:A:574:ALA:O	11:K:77:ARG:NH2	2.35	0.59
1:A:25:ASP:O	1:A:29:GLN:N	2.34	0.59
1:A:674:LYS:HZ3	1:A:928:GLY:HA2	1.66	0.59
1:A:372:ARG:HG2	2:B:1049:GLN:HB2	1.83	0.59
1:A:486:LEU:HD23	1:A:537:VAL:HG22	1.83	0.59
2:B:258:LYS:O	2:B:297:THR:OG1	2.17	0.59
2:B:926:VAL:HG11	2:B:930:ASP:HB2	1.83	0.59
1:A:112:ALA:HA	1:A:234:ILE:HD11	1.83	0.59
1:A:225:LEU:O	1:A:229:ASN:ND2	2.35	0.59
1:A:1048:VAL:HG11	1:A:1053:LYS:HB2	1.84	0.59
9:I:87:ILE:HG23	9:I:88:ARG:HG3	1.83	0.59
12:L:48:CYS:CB	12:L:51:CYS:HB2	2.30	0.59
1:A:235:LYS:HZ1	15:O:44:PRO:HG2	1.67	0.59
1:A:235:LYS:NZ	15:O:44:PRO:HG2	2.18	0.59
1:A:310:ASN:ND2	15:O:562:ALA:O	2.34	0.59
2:B:258:LYS:NZ	2:B:295:ILE:HG13	2.17	0.59
1:A:353:PHE:HE2	2:B:1135:MET:HB2	1.67	0.59
1:A:1161:VAL:HG11	1:A:1303:VAL:HG23	1.85	0.59
2:B:258:LYS:HZ3	2:B:295:ILE:HG13	1.68	0.59
5:E:83:CYS:SG	5:E:84:ASP:N	2.76	0.58
7:G:45:CYS:HA	7:G:76:VAL:HA	1.84	0.58
15:O:633:ARG:HE	16:P:307:HIS:HB2	1.68	0.58
5:E:112:TYR:HB2	5:E:136:ASN:HA	1.85	0.58
16:P:218:THR:HB	16:P:221:ILE:HB	1.84	0.58
2:B:616:SER:HB2	2:B:621:ARG:HH21	1.69	0.58
4:D:129:ALA:HB2	4:D:157:ILE:HG23	1.86	0.58
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.86	0.58
16:P:216:SER:HB3	16:P:222:LEU:HD11	1.84	0.58
1:A:598:MET:HB2	8:H:96:VAL:HG23	1.86	0.58
1:A:1045:ASP:HB2	1:A:1053:LYS:NZ	2.19	0.58
1:A:600:PRO:O	1:A:601:TYR:HB2	2.03	0.58
11:K:65:ILE:HD12	11:K:101:LEU:HD23	1.85	0.58
15:O:31:VAL:HG12	15:O:32:MET:HG3	1.84	0.58
16:P:179:LEU:O	16:P:183:TRP:NE1	2.37	0.58
1:A:127:LEU:HD11	1:A:140:ILE:HG21	1.84	0.58
2:B:487:ARG:HH21	2:B:508:CYS:HB3	1.68	0.58
15:O:188:SER:HA	15:O:191:PHE:HB2	1.86	0.58
1:A:1436:ILE:HG13	1:A:1437:SER:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HD11	2:B:253:ILE:HD13	1.85	0.58
2:B:299:GLN:HG3	2:B:300:GLN:H	1.68	0.58
2:B:720:ARG:NH2	2:B:722:ASP:OD2	2.29	0.58
1:A:225:LEU:HD23	1:A:226:LYS:NZ	2.18	0.57
1:A:473:LEU:HA	1:A:487:SER:HA	1.86	0.57
3:C:45:SER:HB2	3:C:53:ASN:HB3	1.87	0.57
7:G:113:ASN:OD1	7:G:113:ASN:N	2.37	0.57
13:M:96:LEU:O	13:M:97:VAL:HG12	2.04	0.57
2:B:137:ARG:HD2	2:B:415:GLU:HB2	1.86	0.57
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.38	0.57
1:A:1141:ILE:N	1:A:1295:VAL:O	2.38	0.57
2:B:137:ARG:HH11	2:B:139:ARG:HB2	1.68	0.57
2:B:543:LEU:HG	13:M:176:VAL:HG11	1.86	0.57
7:G:190:LYS:C	7:G:192:PRO:HD3	2.29	0.57
14:N:305:MET:HG2	14:N:414:GLY:H	1.70	0.57
1:A:412:ASN:HB3	1:A:416:LEU:HD13	1.87	0.57
15:O:488:LYS:HZ3	15:O:651:PHE:HA	1.69	0.57
1:A:995:VAL:HG12	1:A:997:GLN:H	1.69	0.57
10:J:7:CYS:SG	10:J:11:GLY:N	2.76	0.57
11:K:85:ASP:O	11:K:107:THR:OG1	2.20	0.57
1:A:953:GLY:HA2	1:A:1063:SER:HB2	1.87	0.57
1:A:1152:ARG:HB2	9:I:85:LEU:HD12	1.87	0.57
1:A:1343:MET:HE3	1:A:1350:VAL:HG21	1.87	0.57
2:B:39:ASN:HB3	2:B:42:GLN:HG3	1.87	0.57
9:I:23:THR:HA	9:I:34:PRO:HD3	1.87	0.57
11:K:46:LYS:O	11:K:47:ILE:C	2.48	0.57
15:O:477:TYR:HH	15:O:480:TYR:HH	1.50	0.57
15:O:583:TRP:HE1	16:P:315:ASP:HB3	1.69	0.57
1:A:598:MET:CB	8:H:96:VAL:HG23	2.36	0.56
15:O:286:ARG:NH1	15:O:320:GLU:O	2.38	0.56
15:O:540:LEU:HD21	15:O:546:VAL:HG11	1.87	0.56
1:A:358:LYS:HE2	1:A:1392:THR:HG21	1.87	0.56
1:A:1084:GLU:HB2	6:F:86:THR:HG23	1.86	0.56
1:A:1144:VAL:HG23	1:A:1310:ILE:HG23	1.87	0.56
2:B:1112:SER:HB2	2:B:1114:GLU:HG2	1.87	0.56
3:C:229:LEU:O	3:C:293:ARG:NH2	2.35	0.56
4:D:109:LYS:NZ	4:D:109:LYS:HB3	2.20	0.56
15:O:158:GLU:OE1	15:O:161:GLN:NE2	2.38	0.56
2:B:59:LYS:NZ	2:B:520:ILE:HG13	2.21	0.56
7:G:91:LYS:HG2	7:G:92:CYS:H	1.71	0.56
1:A:317:ASP:OD1	1:A:320:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:MET:O	1:A:540:ASN:ND2	2.38	0.56
2:B:157:ARG:NH2	2:B:180:ASP:OD1	2.38	0.56
2:B:244:HIS:HD1	2:B:246:SER:HG	1.54	0.56
2:B:572:VAL:HG12	2:B:576:ARG:HH12	1.71	0.56
2:B:618:GLY:HA2	2:B:668:PRO:HB3	1.87	0.56
2:B:483:VAL:HG12	2:B:485:GLY:H	1.70	0.56
3:C:80:ALA:HA	3:C:208:CYS:HA	1.87	0.56
11:K:107:THR:OG1	11:K:108:TYR:N	2.38	0.56
16:P:248:VAL:HG23	16:P:255:LYS:HE2	1.87	0.56
1:A:1364:TYR:OH	1:A:1379:MET:SD	2.64	0.56
2:B:57:LEU:HD22	2:B:467:LEU:HD11	1.87	0.56
16:P:174:PHE:O	16:P:175:ILE:HG12	2.06	0.56
5:E:28:TYR:HA	5:E:64:PRO:HA	1.88	0.56
5:E:161:LYS:NZ	5:E:193:GLY:O	2.36	0.56
7:G:3:ILE:HG13	7:G:76:VAL:HG23	1.87	0.56
2:B:161:CYS:SG	2:B:162:ILE:N	2.79	0.56
15:O:506:ARG:HA	16:P:249:TYR:HD2	1.71	0.56
1:A:712:ILE:HD12	2:B:949:PHE:HD2	1.71	0.55
2:B:860:VAL:HG13	2:B:861:ASN:H	1.70	0.55
13:M:164:LYS:HG3	14:N:300:LYS:HE3	1.88	0.55
14:N:304:PHE:O	14:N:413:ASP:N	2.32	0.55
2:B:296:TYR:O	2:B:300:GLN:NE2	2.32	0.55
2:B:548:SER:HB3	2:B:550:HIS:H	1.71	0.55
5:E:38:PRO:HB2	5:E:40:GLU:HG2	1.88	0.55
2:B:319:ILE:HG12	13:M:231:LEU:CD2	2.35	0.55
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.41	0.55
15:O:328:ASP:OD1	15:O:328:ASP:N	2.39	0.55
11:K:80:ILE:HG22	11:K:86:VAL:HG11	1.87	0.55
13:M:108:SER:OG	13:M:109:ALA:N	2.39	0.55
2:B:1061:ARG:NH1	2:B:1063:GLY:HA2	2.21	0.55
7:G:156:VAL:HG11	7:G:190:LYS:HZ3	1.71	0.55
1:A:991:LYS:HG3	1:A:993:GLU:HG2	1.89	0.55
2:B:294:ASP:HB3	2:B:300:GLN:HG3	1.88	0.55
1:A:896:LEU:HB3	1:A:1090:GLY:HA3	1.89	0.55
8:H:50:ALA:N	8:H:53:ASP:OD2	2.40	0.55
2:B:115:PRO:HG3	2:B:163:LEU:HD11	1.89	0.55
5:E:90:VAL:HG13	5:E:122:LYS:HZ3	1.72	0.55
5:E:109:ILE:HG22	5:E:133:GLU:HB3	1.87	0.55
2:B:333:ALA:C	2:B:335:LEU:H	2.14	0.55
7:G:207:LEU:HD22	7:G:210:TRP:CD1	2.42	0.54
13:M:132:ASN:OD1	13:M:132:ASN:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:553:ARG:HB3	15:O:562:ALA:HA	1.89	0.54
1:A:100:ILE:HG13	1:A:166:LYS:HD3	1.88	0.54
5:E:156:LEU:HD11	5:E:195:VAL:HB	1.89	0.54
7:G:13:ILE:HG13	7:G:66:SER:HB3	1.89	0.54
15:O:347:ASP:HA	15:O:350:GLU:HB2	1.89	0.54
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.39	0.54
9:I:5:CYS:HB2	9:I:12:LEU:HD21	1.89	0.54
15:O:78:GLU:HG2	15:O:82:LYS:HZ1	1.72	0.54
1:A:1323:PHE:HA	1:A:1327:GLY:HA2	1.89	0.54
7:G:118:GLY:HA3	7:G:131:PRO:HD3	1.89	0.54
15:O:338:ASP:OD1	15:O:339:LEU:N	2.39	0.54
1:A:413:ARG:NH1	1:A:456:LEU:HB3	2.22	0.54
2:B:974:GLU:OE2	2:B:987:MET:HE1	2.07	0.54
14:N:389:THR:OG1	14:N:390:PHE:N	2.40	0.54
16:P:310:GLU:O	16:P:311:VAL:HG12	2.07	0.54
1:A:599:LYS:HG2	1:A:600:PRO:HD2	0.57	0.54
2:B:775:LYS:HB3	2:B:927:LYS:HA	1.88	0.54
8:H:39:THR:N	8:H:124:ARG:O	2.39	0.54
12:L:50:ASP:OD1	12:L:51:CYS:N	2.40	0.54
14:N:366:HIS:HB3	14:N:370:LYS:HB2	1.90	0.54
15:O:633:ARG:NH2	16:P:308:ASP:O	2.41	0.54
3:C:140:CYS:HB2	3:C:196:LEU:HD13	1.89	0.54
13:M:116:SER:O	13:M:117:HIS:ND1	2.40	0.54
15:O:338:ASP:HB3	15:O:342:ALA:N	2.23	0.54
1:A:179:ILE:HD12	15:O:557:ARG:HE	1.71	0.54
1:A:598:MET:HE1	8:H:141:TYR:HE1	1.72	0.54
2:B:712:ALA:O	2:B:717:GLN:NE2	2.41	0.54
7:G:87:GLY:O	7:G:146:ILE:N	2.28	0.54
1:A:109:ASN:ND2	1:A:154:CYS:SG	2.81	0.54
1:A:235:LYS:HG3	15:O:44:PRO:HB2	1.88	0.54
1:A:356:ARG:NH2	2:B:1046:LEU:HD11	2.23	0.54
1:A:714:ILE:HD13	2:B:958:MET:HE3	1.89	0.54
1:A:1163:LYS:NZ	1:A:1280:ARG:HA	2.19	0.54
1:A:1332:ARG:HB2	1:A:1363:THR:HG21	1.88	0.54
2:B:1004:LEU:HD12	2:B:1017:ILE:HD12	1.89	0.54
15:O:228:ARG:HH12	15:O:231:PRO:HD3	1.73	0.54
15:O:640:ARG:NH1	17:Q:42:PRO:O	2.36	0.54
1:A:1145:LEU:HG	1:A:1309:VAL:HG12	1.89	0.54
2:B:817:PRO:HD2	2:B:822:GLN:HA	1.89	0.54
7:G:44:LEU:O	7:G:77:PHE:N	2.40	0.54
13:M:247:TRP:HD1	14:N:406:ALA:HB1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:TYR:O	1:A:604:TRP:N	2.37	0.53
15:O:163:VAL:HA	15:O:169:LEU:HD13	1.90	0.53
1:A:828:GLN:HB3	2:B:655:ASN:HD21	1.73	0.53
2:B:372:VAL:O	2:B:607:ARG:NH1	2.40	0.53
7:G:88:TRP:O	7:G:100:SER:N	2.35	0.53
15:O:185:TYR:O	15:O:189:SER:N	2.42	0.53
1:A:15:GLY:H	1:A:1408:VAL:HG12	1.73	0.53
1:A:582:MET:HE3	1:A:703:ARG:HB2	1.89	0.53
1:A:631:LYS:HD2	1:A:797:CYS:HA	1.90	0.53
2:B:519:HIS:O	2:B:609:CYS:N	2.40	0.53
3:C:94:ASP:N	3:C:94:ASP:OD1	2.39	0.53
6:F:92:ARG:NH1	7:G:61:PRO:HB3	2.24	0.53
13:M:118:LEU:HG	13:M:149:LYS:HZ2	1.72	0.53
15:O:163:VAL:HG22	15:O:169:LEU:HD22	1.89	0.53
16:P:254:GLU:HB2	16:P:262:ARG:HB2	1.90	0.53
1:A:46:ARG:HG3	1:A:48:PRO:HG3	1.89	0.53
2:B:269:MET:HE1	9:I:2:LEU:HD21	1.90	0.53
15:O:322:LYS:HB3	15:O:361:PHE:CE1	2.42	0.53
15:O:470:GLU:HB2	15:O:479:PRO:HD3	1.91	0.53
1:A:601:TYR:CD1	3:C:23:PHE:HE2	2.26	0.53
2:B:59:LYS:HZ1	2:B:520:ILE:HG13	1.71	0.53
2:B:474:SER:HA	2:B:511:VAL:HG12	1.90	0.53
7:G:60:LYS:HZ2	7:G:63:ASP:HB2	1.74	0.53
15:O:512:ARG:HH22	15:O:568:CYS:HA	1.74	0.53
2:B:687:LEU:O	2:B:915:ARG:NH2	2.42	0.53
15:O:516:LEU:O	15:O:565:LEU:HD23	2.09	0.53
16:P:223:GLU:O	16:P:227:ALA:N	2.24	0.53
12:L:30:ILE:N	12:L:57:LEU:O	2.42	0.53
1:A:1420:THR:HG22	2:B:1080:LEU:HD21	1.91	0.53
2:B:521:THR:OG1	2:B:609:CYS:SG	2.66	0.53
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.74	0.53
9:I:12:LEU:HB3	9:I:24:LEU:HD13	1.90	0.53
1:A:378:ARG:HE	1:A:516:GLU:HB3	1.73	0.53
10:J:12:LYS:HE3	10:J:43:ARG:HH22	1.73	0.53
1:A:905:ARG:NH2	5:E:170:LEU:HD21	2.22	0.53
1:A:978:ASP:HB2	1:A:984:VAL:HB	1.91	0.53
1:A:1384:LEU:HD12	1:A:1413:GLU:OE2	2.08	0.53
15:O:538:ALA:HA	15:O:541:ILE:HG22	1.91	0.53
1:A:402:LEU:HD23	1:A:466:LEU:HD22	1.91	0.52
2:B:163:LEU:HD22	2:B:171:MET:HE1	1.91	0.52
2:B:322:GLU:HG2	2:B:323:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:GLU:HB3	3:C:11:ARG:HG2	1.91	0.52
2:B:526:GLU:O	2:B:529:ILE:HG22	2.09	0.52
15:O:292:ARG:HE	15:O:326:ILE:HD11	1.74	0.52
1:A:219:MET:O	15:O:550:GLU:HG3	2.09	0.52
1:A:626:LEU:HD21	1:A:675:HIS:HB2	1.91	0.52
2:B:543:LEU:HD21	13:M:176:VAL:HG21	1.92	0.52
3:C:197:ARG:HH11	10:J:61:LEU:HD13	1.74	0.52
7:G:101:LEU:HD22	7:G:104:ILE:HG22	1.92	0.52
14:N:290:ILE:HG13	14:N:293:LYS:HE2	1.91	0.52
15:O:366:LEU:HD23	15:O:452:LEU:HD13	1.92	0.52
2:B:465:SER:OG	2:B:707:LYS:O	2.28	0.52
4:D:125:ASN:OD1	4:D:126:GLN:N	2.41	0.52
9:I:15:THR:HG23	9:I:23:THR:HG23	1.91	0.52
1:A:192:PRO:HB3	15:O:343:LYS:NZ	2.24	0.52
5:E:141:VAL:HG23	5:E:142:VAL:H	1.75	0.52
1:A:165:LYS:NZ	1:A:184:ARG:HH22	2.06	0.52
1:A:269:ARG:HD2	1:A:283:ASP:OD2	2.10	0.52
4:D:57:GLY:O	4:D:61:ASN:ND2	2.43	0.52
5:E:31:THR:HG22	5:E:34:GLU:HG2	1.92	0.52
8:H:114:VAL:HG21	8:H:130:ARG:HH11	1.75	0.52
13:M:152:GLY:HA2	13:M:177:ALA:HA	1.92	0.52
1:A:1045:ASP:HB2	1:A:1053:LYS:HZ3	1.73	0.52
1:A:1221:ASP:OD1	1:A:1222:VAL:N	2.43	0.52
2:B:404:ASP:HA	2:B:407:LEU:HB2	1.91	0.52
15:O:192:VAL:HG12	15:O:274:VAL:HG13	1.92	0.52
1:A:22:SER:O	1:A:24:ALA:N	2.43	0.52
3:C:334:THR:OG1	11:K:44:ARG:NH1	2.42	0.52
15:O:500:LEU:HD23	15:O:504:ALA:HB2	1.92	0.52
1:A:541:LEU:HG	1:A:551:ILE:HD11	1.92	0.52
2:B:723:THR:HA	2:B:790:LYS:HG2	1.92	0.52
1:A:1223:ASN:HB3	1:A:1231:ALA:HB3	1.92	0.52
12:L:28:LYS:HG3	12:L:29:TYR:HD2	1.74	0.52
1:A:645:MET:HE1	8:H:124:ARG:HB2	1.92	0.51
1:A:1372:THR:HG23	1:A:1375:GLY:H	1.75	0.51
2:B:343:ARG:NH2	2:B:544:ILE:O	2.44	0.51
9:I:33:PHE:CG	9:I:34:PRO:HA	2.44	0.51
15:O:502:PRO:HA	15:O:505:MET:HE2	1.92	0.51
15:O:620:LEU:HD12	15:O:621:PRO:HD2	1.92	0.51
16:P:223:GLU:HG2	16:P:240:ILE:HA	1.92	0.51
17:Q:43:ILE:HG23	17:Q:44:ASN:H	1.74	0.51
1:A:182:THR:HG22	1:A:185:TRP:NE1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ARG:HG2	2:B:138:GLY:H	1.76	0.51
5:E:86:PRO:HA	5:E:113:GLN:HB3	1.91	0.51
9:I:23:THR:OG1	9:I:24:LEU:N	2.44	0.51
15:O:488:LYS:HZ1	15:O:651:PHE:HA	1.75	0.51
2:B:69:VAL:HA	2:B:73:LEU:HD23	1.92	0.51
8:H:8:ASP:OD1	8:H:9:ILE:N	2.43	0.51
11:K:95:HIS:ND1	11:K:97:SER:OG	2.44	0.51
1:A:132:VAL:HG11	1:A:137:ARG:HH12	1.76	0.51
1:A:1153:ALA:HA	1:A:1156:VAL:HB	1.92	0.51
5:E:50:MET:HG2	5:E:52:ARG:NH1	2.24	0.51
1:A:305:LYS:HG3	1:A:306:GLY:H	1.76	0.51
3:C:22:GLY:H	3:C:27:ALA:HB3	1.75	0.51
5:E:112:TYR:HE2	5:E:134:THR:HB	1.76	0.51
16:P:186:ILE:HG23	16:P:253:LEU:HD21	1.92	0.51
1:A:1284:ASN:OD1	1:A:1285:ILE:N	2.43	0.51
1:A:1408:VAL:HG23	1:A:1413:GLU:HG3	1.93	0.51
7:G:115:LEU:HD23	7:G:116:PHE:H	1.74	0.51
8:H:61:SER:HA	8:H:141:TYR:HD2	1.76	0.51
2:B:38:ILE:HD11	2:B:43:ASP:OD2	2.11	0.51
4:D:98:MET:SD	4:D:160:TYR:OH	2.68	0.51
15:O:553:ARG:HD2	15:O:554:THR:HG23	1.93	0.51
1:A:674:LYS:NZ	1:A:928:GLY:HA2	2.25	0.51
2:B:258:LYS:HB3	2:B:297:THR:HA	1.91	0.51
11:K:112:THR:HG22	11:K:113:ALA:H	1.76	0.51
1:A:252:ARG:HH22	15:O:46:LEU:HD22	1.76	0.51
1:A:538:LYS:HB3	1:A:687:PRO:HB2	1.92	0.51
5:E:13:TRP:HH2	9:I:91:ASP:HB3	1.76	0.51
12:L:49:LYS:N	12:L:51:CYS:SG	2.84	0.51
13:M:80:GLY:HA3	13:M:261:LYS:HE2	1.91	0.51
2:B:769:ASP:OD1	2:B:952:ARG:NH2	2.44	0.51
3:C:31:TRP:HE3	11:K:82:LYS:HD3	1.76	0.51
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.93	0.51
4:D:130:ASN:HB3	4:D:133:HIS:CE1	2.46	0.51
5:E:54:GLN:HG3	5:E:57:MET:HE2	1.92	0.51
15:O:106:TYR:HB3	15:O:208:TYR:HE2	1.76	0.50
5:E:21:GLU:HB3	5:E:35:VAL:HG21	1.93	0.50
15:O:221:LYS:O	15:O:225:ASN:ND2	2.45	0.50
1:A:393:ALA:HB1	1:A:493:ARG:HG3	1.94	0.50
15:O:337:GLN:O	15:O:338:ASP:HB2	2.10	0.50
1:A:235:LYS:HD2	1:A:252:ARG:HH11	1.76	0.50
1:A:830:ARG:NH2	1:A:835:PHE:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:SER:HA	2:B:405:LYS:HZ3	1.75	0.50
2:B:667:VAL:O	2:B:669:SER:N	2.42	0.50
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.26	0.50
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.94	0.50
4:D:110:LEU:HB3	4:D:120:LYS:NZ	2.26	0.50
7:G:10:LEU:HD12	7:G:69:ASN:HB3	1.94	0.50
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.92	0.50
3:C:81:GLU:OE2	3:C:219:PHE:HZ	1.95	0.50
4:D:17:LEU:HB2	4:D:66:LEU:HD23	1.92	0.50
1:A:862:LEU:HD21	2:B:491:PRO:HA	1.93	0.50
10:J:30:LEU:HD22	10:J:31:ASP:H	1.76	0.50
17:Q:50:LYS:O	17:Q:53:SER:OG	2.29	0.50
1:A:113:ILE:HD13	1:A:120:LYS:HE2	1.93	0.50
2:B:319:ILE:O	2:B:319:ILE:HG13	2.11	0.50
16:P:312:VAL:HG11	17:Q:42:PRO:HB3	1.92	0.50
1:A:34:VAL:HG23	1:A:35:SER:H	1.76	0.50
3:C:163:TYR:HD2	3:C:165:ARG:NH1	2.10	0.50
7:G:112:GLN:HG2	7:G:115:LEU:HD13	1.93	0.50
1:A:252:ARG:HH22	15:O:46:LEU:CD2	2.25	0.50
1:A:1425:THR:HG22	6:F:92:ARG:NH2	2.27	0.50
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.94	0.50
2:B:914:SER:HB3	2:B:918:GLN:HB2	1.93	0.50
1:A:653:ILE:HG23	1:A:660:LEU:HB2	1.94	0.49
2:B:638:ASP:HA	2:B:641:LEU:HD13	1.93	0.49
13:M:142:GLY:O	13:M:143:VAL:HG12	2.12	0.49
1:A:980:SER:HB3	5:E:163:GLU:HG2	1.93	0.49
1:A:1347:GLY:O	1:A:1348:MET:HG2	2.12	0.49
2:B:140:ASN:O	2:B:140:ASN:ND2	2.45	0.49
2:B:1000:GLY:HA3	2:B:1018:PHE:HD1	1.77	0.49
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.94	0.49
8:H:130:ARG:O	8:H:134:ASN:ND2	2.37	0.49
15:O:132:TYR:HE1	15:O:645:LEU:HD21	1.77	0.49
3:C:197:ARG:NH1	10:J:61:LEU:HD13	2.27	0.49
2:B:59:LYS:HE2	2:B:519:HIS:HA	1.94	0.49
2:B:536:LEU:HD22	2:B:571:PHE:HD1	1.77	0.49
1:A:524:THR:HG23	1:A:527:ALA:H	1.77	0.49
1:A:1451:LEU:HD11	4:D:104:ALA:HA	1.93	0.49
2:B:210:ASP:OD1	2:B:211:GLU:N	2.46	0.49
13:M:113:LYS:NZ	13:M:237:ALA:HB1	2.26	0.49
1:A:126:GLU:OE2	1:A:136:ARG:NH2	2.32	0.49
7:G:122:THR:OG1	7:G:126:SER:OG	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:TYR:CE2	12:L:40:LEU:HB2	2.44	0.49
1:A:121:ARG:NH2	15:O:212:GLU:OE1	2.46	0.49
1:A:408:VAL:HG23	1:A:412:ASN:HB2	1.95	0.49
2:B:391:LEU:HD23	2:B:429:ILE:HA	1.94	0.49
4:D:117:LYS:HZ3	4:D:121:LEU:HD22	1.77	0.49
5:E:213:ILE:HG12	5:E:214:CYS:H	1.77	0.49
1:A:383:PRO:HB3	1:A:502:GLU:HG2	1.95	0.49
1:A:1084:GLU:O	1:A:1087:THR:OG1	2.27	0.49
1:A:1318:HIS:HD2	1:A:1321:GLU:HB3	1.77	0.49
13:M:228:THR:HG22	13:M:229:GLY:H	1.78	0.49
1:A:355:GLN:O	1:A:359:GLY:N	2.29	0.49
1:A:1020:ALA:HA	1:A:1032:LEU:HD21	1.95	0.49
3:C:201:GLU:OE2	3:C:203:SER:HB2	2.12	0.49
4:D:119:GLU:HG3	4:D:138:VAL:HB	1.95	0.49
6:F:115:THR:HG22	6:F:116:ASP:H	1.78	0.49
7:G:110:ILE:HG22	7:G:198:GLY:H	1.77	0.49
7:G:149:ARG:O	7:G:198:GLY:HA3	2.13	0.49
2:B:796:LYS:HZ3	2:B:798:TYR:HE1	1.60	0.48
7:G:80:PHE:CE2	7:G:83:GLU:HB2	2.48	0.48
14:N:409:LEU:HD12	14:N:409:LEU:H	1.77	0.48
1:A:1145:LEU:HD23	1:A:1146:VAL:HG23	1.95	0.48
12:L:31:CYS:HB3	12:L:34:CYS:HB2	1.95	0.48
15:O:343:LYS:O	15:O:347:ASP:N	2.34	0.48
1:A:706:GLY:HA2	2:B:762:TYR:HA	1.95	0.48
1:A:1273:LYS:HG2	1:A:1274:GLY:H	1.78	0.48
2:B:517:MET:HE2	2:B:611:PRO:HG2	1.94	0.48
2:B:775:LYS:HE3	2:B:927:LYS:HA	1.95	0.48
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.95	0.48
1:A:235:LYS:HZ2	15:O:44:PRO:HD2	1.78	0.48
2:B:989:LYS:HA	2:B:992:VAL:HG12	1.95	0.48
3:C:21:PRO:HA	3:C:27:ALA:HB1	1.95	0.48
13:M:118:LEU:HA	13:M:150:GLY:O	2.13	0.48
16:P:264:THR:HG23	16:P:265:LEU:H	1.78	0.48
1:A:226:LYS:HE2	15:O:548:ILE:HG13	1.95	0.48
6:F:134:ILE:N	6:F:146:TRP:O	2.46	0.48
15:O:50:LYS:HA	15:O:53:VAL:HG12	1.94	0.48
1:A:127:LEU:HD22	1:A:240:GLU:OE2	2.12	0.48
1:A:1302:ASP:OD1	1:A:1303:VAL:N	2.46	0.48
2:B:330:THR:O	2:B:333:ALA:HB2	2.14	0.48
2:B:804:ASP:OD1	2:B:804:ASP:N	2.47	0.48
4:D:17:LEU:O	4:D:21:THR:OG1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:83:GLU:HB2	14:N:400:ALA:HB2	1.94	0.48
15:O:578:ARG:HG2	15:O:648:TRP:HZ3	1.77	0.48
3:C:30:GLU:HG3	11:K:84:PRO:HD3	1.96	0.48
5:E:143:ASN:N	5:E:143:ASN:OD1	2.46	0.48
6:F:85:MET:HG2	6:F:153:VAL:HG11	1.96	0.48
6:F:114:GLU:OE2	6:F:120:ILE:HG22	2.14	0.48
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.79	0.48
8:H:87:ARG:HH11	8:H:87:ARG:HB2	1.78	0.48
11:K:47:ILE:HG23	11:K:63:PHE:HB3	1.96	0.48
12:L:29:TYR:HA	12:L:58:LYS:HA	1.96	0.48
15:O:242:LYS:NZ	15:O:341:GLU:OE2	2.44	0.48
15:O:495:VAL:HG11	15:O:577:MET:HE3	1.95	0.48
1:A:165:LYS:HZ2	1:A:184:ARG:HH22	1.62	0.48
1:A:645:MET:HE1	8:H:124:ARG:HD2	1.96	0.48
1:A:1134:LYS:HA	1:A:1320:LEU:HD23	1.96	0.48
4:D:20:LEU:HD12	4:D:62:VAL:HG11	1.95	0.48
7:G:8:ALA:HA	7:G:71:THR:HA	1.96	0.48
7:G:89:ILE:HG12	7:G:90:SER:H	1.77	0.48
7:G:104:ILE:HG13	7:G:105:PHE:CD2	2.49	0.48
7:G:121:TYR:HB2	7:G:128:TRP:CZ3	2.49	0.48
15:O:570:GLU:HG2	15:O:571:THR:H	1.77	0.48
15:O:580:ASN:O	15:O:584:ASN:ND2	2.47	0.48
16:P:223:GLU:HB3	16:P:240:ILE:HD13	1.95	0.48
1:A:601:TYR:O	1:A:602:TYR:HB2	2.14	0.48
2:B:321:GLN:O	2:B:322:GLU:C	2.57	0.48
3:C:74:GLU:HA	3:C:212:ILE:HD11	1.94	0.48
3:C:127:THR:HG22	3:C:128:ASP:H	1.79	0.48
15:O:54:LYS:HA	15:O:58:GLY:HA2	1.96	0.48
15:O:255:LYS:HB3	15:O:256:PRO:HD3	1.96	0.48
1:A:809:MET:HE1	2:B:950:PRO:HA	1.95	0.47
1:A:1411:VAL:HG13	1:A:1412:SER:H	1.79	0.47
2:B:727:LEU:HD11	2:B:788:ARG:HE	1.78	0.47
5:E:24:LYS:HB2	5:E:30:ILE:HD11	1.96	0.47
1:A:107:CYS:HB2	1:A:110:CYS:SG	2.53	0.47
1:A:890:MET:O	1:A:894:GLU:N	2.47	0.47
2:B:88:ASP:CG	2:B:89:PRO:HD2	2.40	0.47
2:B:102:LYS:NZ	2:B:107:SER:HA	2.28	0.47
2:B:184:TYR:HB2	2:B:191:GLU:OE2	2.13	0.47
2:B:269:MET:O	2:B:273:CYS:HB3	2.14	0.47
3:C:284:GLU:HA	3:C:287:ASP:OD2	2.14	0.47
15:O:477:TYR:OH	15:O:480:TYR:OH	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:N	1:A:502:GLU:OE2	2.48	0.47
3:C:43:ASN:HB2	3:C:55:ASP:HB3	1.95	0.47
11:K:60:SER:HB3	11:K:104:ARG:NH2	2.30	0.47
13:M:123:ILE:C	13:M:145:VAL:HG23	2.39	0.47
1:A:1038:GLU:HG3	1:A:1039:LEU:H	1.80	0.47
5:E:118:PRO:HA	5:E:121:MET:HB2	1.95	0.47
7:G:114:MET:O	7:G:201:GLN:HB3	2.14	0.47
14:N:305:MET:HE3	14:N:414:GLY:HA3	1.95	0.47
15:O:329:PRO:C	15:O:331:THR:H	2.23	0.47
1:A:303:LEU:HD22	15:O:538:ALA:HB1	1.97	0.47
1:A:669:LEU:HD21	1:A:697:MET:HE3	1.97	0.47
2:B:103:LYS:HZ2	2:B:146:ASP:HB2	1.78	0.47
2:B:423:ASN:O	2:B:426:SER:OG	2.22	0.47
3:C:107:LYS:HB3	3:C:185:VAL:HG23	1.97	0.47
1:A:180:HIS:NE2	1:A:220:ASP:OD2	2.48	0.47
2:B:1022:ILE:HG22	2:B:1023:TYR:H	1.78	0.47
2:B:1061:ARG:NH1	2:B:1062:LEU:O	2.48	0.47
3:C:29:ASN:HA	3:C:35:LYS:NZ	2.30	0.47
15:O:265:VAL:HG12	15:O:267:PRO:HD3	1.95	0.47
1:A:14:LYS:NZ	2:B:1144:GLU:OE1	2.43	0.47
1:A:349:PRO:O	1:A:351:ARG:NH1	2.48	0.47
1:A:598:MET:HA	1:A:602:TYR:CD1	2.50	0.47
2:B:336:THR:HG21	2:B:348:TYR:CE1	2.50	0.47
2:B:615:VAL:HG12	2:B:620:SER:HA	1.97	0.47
2:B:733:GLN:HB2	10:J:52:THR:HG21	1.97	0.47
4:D:117:LYS:HZ1	4:D:121:LEU:HD22	1.80	0.47
4:D:139:GLU:C	4:D:141:CYS:H	2.23	0.47
7:G:89:ILE:HG12	7:G:90:SER:N	2.30	0.47
8:H:87:ARG:HB2	8:H:87:ARG:NH1	2.30	0.47
13:M:89:GLN:HB3	14:N:394:VAL:HG22	1.97	0.47
15:O:259:LEU:HD21	15:O:261:GLN:HB2	1.95	0.47
1:A:444:LEU:HD21	1:A:449:ARG:HG2	1.96	0.47
1:A:1143:ALA:HA	1:A:1314:THR:HG22	1.96	0.47
1:A:1325:VAL:HG23	1:A:1326:LEU:H	1.80	0.47
2:B:832:VAL:HG12	12:L:60:ARG:HG3	1.96	0.47
2:B:849:THR:HG23	2:B:850:ASN:H	1.79	0.47
5:E:20:LYS:HB3	5:E:35:VAL:HG23	1.96	0.47
1:A:444:LEU:HD11	1:A:449:ARG:H	1.79	0.47
1:A:556:ASP:OD1	2:B:947:HIS:NE2	2.45	0.47
1:A:630:ASN:ND2	1:A:650:GLY:O	2.48	0.47
1:A:766:ILE:HG21	1:A:822:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ARG:HB2	2:B:204:ARG:NH1	2.30	0.47
2:B:983:LYS:HG3	2:B:985:GLU:H	1.80	0.47
15:O:191:PHE:O	15:O:194:LEU:HB2	2.14	0.47
1:A:308:SER:N	1:A:311:ASN:HD21	2.12	0.47
1:A:395:PRO:HG2	1:A:398:VAL:HG22	1.96	0.47
1:A:1123:VAL:HG13	1:A:1124:PRO:HD3	1.97	0.47
1:A:1207:VAL:O	1:A:1211:ARG:HG2	2.15	0.47
1:A:1225:ILE:HG23	1:A:1226:GLY:H	1.80	0.47
4:D:126:GLN:OE1	7:G:86:THR:OG1	2.32	0.47
5:E:170:LEU:HB3	5:E:174:GLN:NE2	2.30	0.47
5:E:173:SER:C	5:E:175:LEU:H	2.23	0.47
15:O:641:LEU:O	15:O:645:LEU:HB2	2.15	0.47
1:A:541:LEU:HD22	1:A:682:LEU:HD22	1.97	0.46
2:B:103:LYS:HZ3	2:B:146:ASP:HB2	1.79	0.46
2:B:371:TYR:HB2	2:B:492:SER:OG	2.15	0.46
2:B:934:ASN:OD1	2:B:935:ASP:N	2.47	0.46
2:B:992:VAL:HG23	3:C:278:GLU:HG2	1.96	0.46
5:E:86:PRO:HB3	5:E:114:ASN:HB2	1.97	0.46
15:O:286:ARG:HA	15:O:289:LYS:HB2	1.97	0.46
1:A:132:VAL:HG21	1:A:137:ARG:HH22	1.79	0.46
1:A:213:ARG:O	1:A:213:ARG:NH1	2.49	0.46
2:B:837:GLN:HA	2:B:878:PRO:HB3	1.97	0.46
13:M:122:ASP:HB3	13:M:145:VAL:HG21	1.97	0.46
15:O:282:ILE:HG22	15:O:283:ASN:H	1.81	0.46
1:A:90:VAL:HG13	1:A:258:TRP:HB2	1.97	0.46
1:A:393:ALA:HB3	1:A:499:ARG:HG3	1.96	0.46
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.31	0.46
13:M:72:GLU:O	14:N:364:ARG:HG2	2.16	0.46
15:O:312:TYR:HE1	15:O:478:VAL:HG21	1.80	0.46
1:A:602:TYR:C	1:A:603:LEU:O	2.57	0.46
2:B:92:TYR:CZ	2:B:136:THR:HG21	2.50	0.46
2:B:244:HIS:ND1	2:B:246:SER:OG	2.44	0.46
2:B:390:ASP:OD2	2:B:444:LEU:HG	2.16	0.46
2:B:1038:ARG:HH11	2:B:1057:ASP:CG	2.23	0.46
3:C:120:LEU:HB2	3:C:124:GLU:HB3	1.98	0.46
13:M:255:PHE:O	13:M:259:ILE:HG12	2.15	0.46
15:O:195:CYS:SG	15:O:196:GLU:N	2.88	0.46
2:B:108:THR:OG1	2:B:109:LYS:N	2.48	0.46
2:B:698:ARG:HH21	2:B:952:ARG:CG	2.28	0.46
7:G:89:ILE:HG23	7:G:142:VAL:HG12	1.97	0.46
1:A:163:VAL:HG22	1:A:164:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:H	15:O:550:GLU:HB3	1.81	0.46
1:A:389:ILE:HD11	1:A:691:ALA:HB1	1.97	0.46
1:A:600:PRO:O	1:A:601:TYR:CB	2.64	0.46
2:B:211:GLU:HG3	2:B:212:LYS:HD2	1.98	0.46
2:B:736:VAL:HG21	2:B:960:GLU:HG3	1.97	0.46
7:G:60:LYS:NZ	7:G:63:ASP:HB2	2.29	0.46
14:N:316:PHE:HE1	14:N:360:VAL:HA	1.81	0.46
15:O:101:LEU:HD21	15:O:130:LEU:HD11	1.98	0.46
15:O:326:ILE:HG23	15:O:653:MET:HE1	1.96	0.46
16:P:221:ILE:HA	16:P:224:PHE:HB2	1.98	0.46
1:A:133:ASP:OD1	1:A:134:ASN:N	2.49	0.46
1:A:311:ASN:OD1	1:A:312:MET:N	2.43	0.46
1:A:371:LYS:NZ	2:B:1052:GLU:OE1	2.44	0.46
1:A:629:LYS:HB3	1:A:633:PHE:HE2	1.80	0.46
1:A:967:LEU:HD11	1:A:1009:ARG:HD3	1.98	0.46
1:A:1057:SER:O	1:A:1061:ARG:NH1	2.49	0.46
1:A:1097:ILE:HD13	1:A:1358:LEU:HD22	1.97	0.46
2:B:741:ILE:HB	2:B:746:TYR:HB3	1.98	0.46
15:O:47:PHE:HA	15:O:50:LYS:NZ	2.31	0.46
15:O:203:ILE:HG13	15:O:203:ILE:O	2.16	0.46
15:O:640:ARG:NH1	17:Q:44:ASN:OD1	2.49	0.46
16:P:235:LEU:HD12	16:P:236:THR:H	1.80	0.46
1:A:110:CYS:HB3	1:A:157:CYS:CB	2.46	0.46
2:B:181:PRO:HB2	2:B:470:MET:HE1	1.97	0.46
2:B:312:MET:HB3	2:B:317:LEU:CD2	2.38	0.46
3:C:116:VAL:HG22	3:C:117:ASP:H	1.80	0.46
14:N:375:ILE:HG22	14:N:376:GLY:H	1.80	0.46
2:B:566:ARG:HG3	2:B:567:PHE:H	1.81	0.46
5:E:18:THR:OG1	5:E:141:VAL:O	2.34	0.46
14:N:392:GLN:HB3	14:N:394:VAL:HG23	1.98	0.46
15:O:190:LEU:HD23	15:O:194:LEU:HG	1.96	0.46
1:A:578:GLN:O	1:A:582:MET:N	2.48	0.46
1:A:1152:ARG:HH11	9:I:85:LEU:HB2	1.81	0.46
1:A:1187:ARG:HG2	1:A:1229:ARG:HG3	1.98	0.46
2:B:464:ILE:O	2:B:468:GLY:N	2.48	0.46
2:B:916:HIS:CD2	2:B:957:LYS:HB2	2.51	0.46
1:A:47:ALA:N	1:A:48:PRO:HD3	2.31	0.45
1:A:376:SER:HB2	2:B:1060:LEU:HD12	1.98	0.45
1:A:387:LEU:HD21	1:A:393:ALA:HB2	1.99	0.45
1:A:862:LEU:HD22	2:B:494:PHE:HB2	1.96	0.45
8:H:21:ASN:OD1	8:H:22:LYS:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HG3	1:A:56:PRO:HD3	1.98	0.45
2:B:217:GLN:HG2	2:B:232:TYR:CD2	2.52	0.45
5:E:191:LYS:HB2	5:E:194:GLU:OE2	2.16	0.45
8:H:41:ASP:HB2	8:H:121:LEU:HB3	1.99	0.45
9:I:5:CYS:O	9:I:9:ASN:HA	2.16	0.45
16:P:257:THR:OG1	16:P:258:HIS:N	2.49	0.45
2:B:103:LYS:HG2	2:B:104:SER:H	1.81	0.45
2:B:934:ASN:HA	2:B:1005:TYR:CD2	2.51	0.45
15:O:583:TRP:NE1	16:P:315:ASP:HB3	2.30	0.45
1:A:21:LEU:HB3	1:A:25:ASP:OD2	2.16	0.45
1:A:326:TYR:CD2	1:A:327:ILE:HG23	2.52	0.45
1:A:1307:ASP:OD1	9:I:88:ARG:HG2	2.16	0.45
2:B:929:GLU:HB3	3:C:69:ARG:HG2	1.98	0.45
4:D:7:ARG:HE	4:D:10:PHE:HE1	1.64	0.45
15:O:288:MET:HG3	15:O:291:ARG:NH2	2.31	0.45
1:A:113:ILE:HG12	1:A:115:LEU:H	1.82	0.45
2:B:110:ASP:OD1	2:B:110:ASP:N	2.49	0.45
15:O:541:ILE:HD11	15:O:548:ILE:HG12	1.99	0.45
1:A:308:SER:OG	1:A:309:ILE:N	2.48	0.45
1:A:666:LYS:O	1:A:667:SER:HB3	2.17	0.45
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.50	0.45
3:C:175:GLN:O	3:C:178:THR:HG23	2.17	0.45
5:E:70:SER:OG	5:E:71:LYS:N	2.48	0.45
15:O:634:GLU:O	15:O:637:VAL:HG12	2.16	0.45
16:P:215:TYR:CZ	16:P:262:ARG:HD3	2.51	0.45
5:E:172:GLU:HG2	5:E:173:SER:H	1.81	0.45
7:G:47:THR:OG1	7:G:48:ILE:N	2.49	0.45
15:O:87:ASP:O	15:O:88:VAL:HG12	2.17	0.45
15:O:140:ILE:O	15:O:144:MET:HB2	2.17	0.45
2:B:124:THR:OG1	2:B:125:TYR:N	2.49	0.45
2:B:613:ILE:HG12	2:B:646:VAL:HG12	1.98	0.45
2:B:640:PHE:HB3	2:B:645:LEU:HB2	1.99	0.45
6:F:143:PHE:O	6:F:144:GLU:HB2	2.16	0.45
8:H:96:VAL:HG12	8:H:143:LEU:HA	1.99	0.45
9:I:95:THR:HA	9:I:110:ASN:HA	1.97	0.45
15:O:325:LYS:HD3	15:O:480:TYR:CD1	2.51	0.45
16:P:309:LYS:HB3	16:P:310:GLU:HG3	1.98	0.45
1:A:1445:ARG:HB3	1:A:1448:PHE:HD2	1.82	0.45
2:B:347:LEU:HD13	2:B:541:ILE:HD11	1.98	0.45
2:B:477:PHE:HB3	2:B:478:GLU:H	1.58	0.45
2:B:552:ASN:HB2	2:B:566:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:LEU:HB3	3:C:293:ARG:CZ	2.47	0.45
9:I:89:SER:HB3	9:I:92:GLU:HB2	1.99	0.45
13:M:78:ILE:HG22	13:M:170:LEU:HD22	1.98	0.45
14:N:308:GLN:HB2	14:N:417:VAL:HG12	1.99	0.45
2:B:337:VAL:HG21	2:B:345:LYS:HA	1.99	0.45
15:O:40:ARG:HA	16:P:317:TRP:HE1	1.81	0.45
2:B:401:LEU:HA	2:B:404:ASP:OD2	2.17	0.44
2:B:915:ARG:HD2	2:B:1023:TYR:HD2	1.83	0.44
3:C:280:LEU:HA	3:C:286:ALA:HB2	1.99	0.44
13:M:135:LYS:HE3	13:M:140:TRP:HH2	1.81	0.44
2:B:83:ILE:HG13	2:B:93:LEU:HB3	1.99	0.44
2:B:262:ILE:HD13	13:M:180:LYS:NZ	2.32	0.44
2:B:889:SER:OG	2:B:893:GLN:HG2	2.17	0.44
4:D:138:VAL:HG13	4:D:141:CYS:HA	1.99	0.44
14:N:290:ILE:HD13	14:N:384:LYS:HE3	1.99	0.44
15:O:596:LYS:O	15:O:600:SER:N	2.50	0.44
2:B:291:SER:HA	2:B:295:ILE:HB	1.99	0.44
5:E:150:VAL:HA	5:E:151:PRO:HD3	1.79	0.44
9:I:98:TYR:HB2	9:I:107:TRP:HE3	1.83	0.44
13:M:114:PRO:O	13:M:116:SER:N	2.50	0.44
15:O:291:ARG:HA	15:O:294:LYS:HD3	2.00	0.44
1:A:62:SER:H	1:A:65:LEU:HD12	1.83	0.44
1:A:107:CYS:SG	1:A:109:ASN:ND2	2.90	0.44
1:A:563:LEU:HD13	1:A:708:ARG:NH1	2.32	0.44
1:A:1436:ILE:HG21	7:G:54:VAL:HG13	2.00	0.44
7:G:52:LEU:O	7:G:53:THR:HG22	2.17	0.44
1:A:22:SER:C	1:A:24:ALA:H	2.26	0.44
1:A:1151:GLU:HG3	1:A:1152:ARG:H	1.83	0.44
1:A:1431:VAL:HG21	6:F:135:ARG:CZ	2.48	0.44
7:G:55:GLU:OE1	7:G:55:GLU:N	2.51	0.44
9:I:35:ILE:HD12	9:I:35:ILE:HA	1.88	0.44
1:A:143:LYS:HA	1:A:146:ASP:OD2	2.17	0.44
1:A:723:LEU:HD21	1:A:811:ALA:HA	2.00	0.44
1:A:799:SER:HG	1:A:800:LYS:H	1.63	0.44
1:A:1166:LEU:O	1:A:1170:ALA:HB2	2.18	0.44
1:A:1447:LEU:HD13	4:D:15:GLU:OE2	2.18	0.44
3:C:178:THR:HB	3:C:179:PHE:H	1.49	0.44
13:M:122:ASP:HB3	13:M:145:VAL:CG2	2.48	0.44
1:A:114:LEU:HD11	1:A:148:CYS:HB2	2.00	0.44
2:B:217:GLN:NE2	2:B:352:MET:HG2	2.33	0.44
2:B:727:LEU:HB2	2:B:786:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:262:ILE:HG12	15:O:278:VAL:HG21	2.00	0.44
1:A:18:PHE:HB3	1:A:1400:ALA:HA	2.00	0.44
1:A:371:LYS:HD3	1:A:371:LYS:HA	1.86	0.44
2:B:57:LEU:HD13	2:B:467:LEU:HD21	2.00	0.44
14:N:300:LYS:N	14:N:301:PRO:HD3	2.32	0.44
15:O:581:LEU:HD13	15:O:648:TRP:CD2	2.53	0.44
1:A:93:ILE:HG23	1:A:94:GLY:H	1.83	0.44
1:A:862:LEU:O	1:A:866:ILE:HG12	2.18	0.44
1:A:1059:LEU:HD21	8:H:105:GLU:HA	2.00	0.44
2:B:334:HIS:NE2	2:B:352:MET:SD	2.75	0.44
2:B:803:GLN:HG2	2:B:804:ASP:H	1.83	0.44
5:E:115:ASN:OD1	5:E:116:ILE:N	2.50	0.44
12:L:28:LYS:HG3	12:L:29:TYR:CD2	2.51	0.44
1:A:545:LYS:HG3	1:A:546:SER:H	1.83	0.43
1:A:1059:LEU:HD22	1:A:1060:TYR:CE2	2.53	0.43
2:B:265:ASP:O	2:B:268:ILE:N	2.39	0.43
2:B:572:VAL:HA	2:B:590:ILE:HD13	1.98	0.43
2:B:804:ASP:HB3	2:B:848:PRO:HD3	1.99	0.43
2:B:1063:GLY:O	2:B:1067:ARG:N	2.51	0.43
13:M:116:SER:C	13:M:117:HIS:CG	2.95	0.43
1:A:314:GLU:HB3	15:O:560:SER:HB3	2.01	0.43
1:A:475:ASN:HB3	1:A:518:ASN:HB2	2.00	0.43
2:B:1038:ARG:NH1	2:B:1057:ASP:OD2	2.51	0.43
8:H:130:ARG:NH1	8:H:134:ASN:OD1	2.51	0.43
13:M:149:LYS:O	13:M:179:LEU:HD12	2.17	0.43
16:P:235:LEU:HB2	16:P:236:THR:OG1	2.18	0.43
1:A:996:ASP:O	1:A:997:GLN:HG2	2.19	0.43
3:C:177:THR:HG23	3:C:178:THR:H	1.83	0.43
11:K:46:LYS:O	11:K:47:ILE:O	2.37	0.43
15:O:132:TYR:CE1	15:O:645:LEU:HD21	2.54	0.43
15:O:570:GLU:H	15:O:570:GLU:CD	2.27	0.43
1:A:235:LYS:HZ2	15:O:44:PRO:CD	2.31	0.43
1:A:1199:GLU:HG2	5:E:7:ARG:NH2	2.34	0.43
2:B:756:THR:HG23	2:B:941:ASP:H	1.83	0.43
2:B:934:ASN:ND2	2:B:1004:LEU:HD22	2.33	0.43
4:D:102:SER:HA	4:D:105:GLU:HB2	2.01	0.43
1:A:617:ASN:O	1:A:620:SER:OG	2.34	0.43
1:A:1364:TYR:HA	5:E:212:ARG:HH12	1.84	0.43
2:B:790:LYS:HA	2:B:899:LEU:HA	2.00	0.43
13:M:123:ILE:O	13:M:146:GLN:N	2.49	0.43
13:M:149:LYS:HG2	13:M:150:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:394:VAL:O	14:N:412:VAL:HB	2.18	0.43
15:O:570:GLU:HG2	15:O:571:THR:N	2.34	0.43
1:A:192:PRO:HB3	15:O:343:LYS:HZ2	1.83	0.43
1:A:817:ILE:HG13	1:A:821:ASN:O	2.19	0.43
1:A:1038:GLU:HB3	1:A:1042:ILE:HD11	2.01	0.43
2:B:244:HIS:HB3	2:B:247:ILE:HG22	2.01	0.43
2:B:330:THR:HG21	13:M:230:SER:HB3	1.99	0.43
5:E:40:GLU:HG3	5:E:41:ASP:H	1.84	0.43
7:G:151:GLU:HB3	7:G:198:GLY:HA2	1.99	0.43
9:I:35:ILE:HG13	9:I:36:GLU:H	1.84	0.43
14:N:296:LYS:HA	14:N:296:LYS:HD3	1.83	0.43
1:A:200:GLU:HA	15:O:515:LYS:HE3	2.00	0.43
1:A:1420:THR:HA	2:B:1080:LEU:HD11	2.01	0.43
2:B:1061:ARG:HH12	2:B:1063:GLY:HA2	1.82	0.43
2:B:1067:ARG:HH22	2:B:1079:LEU:HB3	1.84	0.43
5:E:43:LYS:O	5:E:47:CYS:HB2	2.19	0.43
1:A:809:MET:HE2	2:B:953:MET:HA	2.01	0.43
2:B:306:GLY:HA3	2:B:325:GLU:OE2	2.18	0.43
2:B:337:VAL:HG23	2:B:345:LYS:NZ	2.33	0.43
2:B:722:ASP:OD1	2:B:723:THR:N	2.49	0.43
2:B:905:ARG:O	2:B:907:GLU:N	2.51	0.43
5:E:90:VAL:HG12	5:E:94:LYS:HG2	2.00	0.43
5:E:177:ARG:O	5:E:212:ARG:NH2	2.52	0.43
7:G:124:GLU:O	7:G:125:GLU:HB3	2.18	0.43
11:K:47:ILE:HA	11:K:64:GLN:O	2.18	0.43
16:P:249:TYR:CG	16:P:250:ASP:N	2.86	0.43
1:A:38:ASP:HB3	1:A:39:LEU:HD12	2.01	0.43
1:A:349:PRO:C	1:A:351:ARG:H	2.26	0.43
1:A:599:LYS:O	1:A:602:TYR:CZ	2.72	0.43
1:A:627:ASP:OD1	1:A:627:ASP:N	2.52	0.43
2:B:98:ILE:HG13	2:B:131:VAL:HG12	2.01	0.43
2:B:417:ASP:O	2:B:421:SER:HB2	2.18	0.43
3:C:230:LEU:HA	3:C:231:PRO:HD3	1.82	0.43
5:E:22:MET:HE1	5:E:135:PHE:HE2	1.84	0.43
8:H:12:VAL:HG12	8:H:13:SER:H	1.83	0.43
15:O:328:ASP:CG	15:O:329:PRO:HD3	2.44	0.43
1:A:29:GLN:HG3	2:B:1109:THR:HB	1.99	0.43
1:A:183:PHE:CD2	1:A:184:ARG:HG3	2.54	0.43
2:B:102:LYS:HZ3	2:B:107:SER:HA	1.84	0.43
9:I:24:LEU:HD21	9:I:33:PHE:HD2	1.84	0.43
13:M:121:ILE:O	13:M:148:LEU:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:132:ASN:OD1	13:M:132:ASN:C	2.61	0.43
14:N:366:HIS:N	14:N:370:LYS:O	2.52	0.43
15:O:144:MET:HE1	15:O:196:GLU:OE2	2.18	0.43
15:O:597:GLN:HA	15:O:600:SER:HB2	2.01	0.43
17:Q:42:PRO:HB2	17:Q:43:ILE:H	1.64	0.43
1:A:468:ASP:OD1	1:A:469:GLY:N	2.52	0.42
1:A:614:ILE:HD13	1:A:624:ILE:HD12	2.01	0.42
1:A:766:ILE:HD13	1:A:822:ARG:NH1	2.34	0.42
2:B:545:ASP:CG	14:N:391:LEU:HD22	2.43	0.42
4:D:61:ASN:HB3	7:G:103:GLY:O	2.18	0.42
5:E:173:SER:OG	5:E:174:GLN:N	2.48	0.42
13:M:88:PHE:HD2	14:N:397:LEU:HD13	1.84	0.42
13:M:121:ILE:HB	13:M:179:LEU:HD11	2.01	0.42
15:O:576:PHE:O	15:O:579:GLN:HG2	2.18	0.42
1:A:955:LEU:HA	1:A:956:PRO:HD2	1.82	0.42
1:A:1145:LEU:O	1:A:1310:ILE:HG22	2.19	0.42
1:A:1391:LYS:HD2	1:A:1391:LYS:HA	1.69	0.42
7:G:199:SER:HB3	7:G:201:GLN:OE1	2.19	0.42
15:O:205:LYS:HA	15:O:205:LYS:HD2	1.86	0.42
15:O:286:ARG:HA	15:O:286:ARG:HD3	1.87	0.42
1:A:397:ARG:HH11	1:A:496:ARG:HE	1.67	0.42
3:C:3:ASN:HD21	3:C:296:ASN:HB2	1.83	0.42
5:E:117:THR:OG1	5:E:118:PRO:HD2	2.19	0.42
7:G:97:ILE:HG22	7:G:128:TRP:NE1	2.33	0.42
15:O:275:LYS:HA	15:O:276:PRO:HD3	1.90	0.42
1:A:115:LEU:HD22	1:A:144:ILE:HD11	2.02	0.42
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.86	0.42
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.87	0.42
1:A:979:ASN:O	5:E:167:ARG:NH2	2.52	0.42
1:A:1064:GLU:HB3	1:A:1065:LYS:H	1.46	0.42
3:C:52:ALA:HB3	3:C:302:VAL:HG12	2.00	0.42
3:C:135:SER:HA	3:C:205:LYS:HA	2.02	0.42
3:C:255:VAL:O	3:C:268:LYS:HB2	2.19	0.42
3:C:276:SER:HB3	3:C:278:GLU:OE2	2.18	0.42
5:E:20:LYS:O	5:E:23:VAL:HG12	2.20	0.42
15:O:356:THR:HB	15:O:357:PRO:HD3	2.02	0.42
15:O:564:PHE:C	15:O:565:LEU:HD12	2.44	0.42
1:A:1140:ILE:HG22	1:A:1296:GLU:HG3	2.01	0.42
2:B:529:ILE:HG23	2:B:530:LYS:N	2.34	0.42
2:B:776:SER:HA	2:B:779:ASP:HB3	2.01	0.42
3:C:85:PHE:CE1	3:C:204:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:GLU:OE2	8:H:115:TYR:OH	2.22	0.42
14:N:398:SER:HB3	14:N:407:GLU:HB3	2.01	0.42
15:O:156:VAL:HA	15:O:159:ILE:HG12	2.00	0.42
15:O:325:LYS:HD2	15:O:325:LYS:HA	1.79	0.42
1:A:238:ASP:OD1	1:A:238:ASP:N	2.53	0.42
1:A:558:ILE:HG21	1:A:798:GLY:HA3	2.00	0.42
1:A:978:ASP:N	1:A:982:CYS:O	2.48	0.42
1:A:1300:LEU:O	1:A:1303:VAL:HG12	2.19	0.42
2:B:775:LYS:C	2:B:777:SER:H	2.28	0.42
3:C:332:PRO:HG2	11:K:44:ARG:NE	2.35	0.42
5:E:117:THR:HG23	5:E:119:SER:H	1.84	0.42
13:M:254:GLN:CD	14:N:409:LEU:HD23	2.44	0.42
14:N:299:ASN:O	14:N:301:PRO:HD3	2.18	0.42
14:N:389:THR:O	14:N:390:PHE:CG	2.72	0.42
15:O:491:VAL:HG11	15:O:650:VAL:HG11	2.02	0.42
1:A:29:GLN:HA	2:B:1108:THR:HG22	2.01	0.42
1:A:565:SER:HB3	1:A:663:VAL:HG12	2.01	0.42
1:A:1460:ASN:HB3	4:D:114:LYS:HG3	2.02	0.42
2:B:77:ILE:HD13	2:B:98:ILE:HB	2.01	0.42
2:B:180:ASP:HA	2:B:181:PRO:HD3	1.90	0.42
2:B:717:GLN:OE1	2:B:727:LEU:HD22	2.19	0.42
2:B:831:GLU:OE1	2:B:831:GLU:N	2.48	0.42
2:B:1008:ILE:HG13	2:B:1009:THR:H	1.84	0.42
15:O:201:ILE:HG22	15:O:202:GLN:H	1.84	0.42
15:O:549:GLN:HG3	15:O:550:GLU:H	1.85	0.42
1:A:953:GLY:HA3	1:A:1061:ARG:HD2	2.02	0.42
1:A:1165:LEU:HD13	1:A:1198:LEU:HD21	2.01	0.42
2:B:192:LYS:HA	2:B:457:VAL:HA	2.01	0.42
4:D:27:HIS:C	4:D:29:TRP:H	2.27	0.42
6:F:101:ILE:HG13	6:F:120:ILE:HD11	2.02	0.42
13:M:77:LYS:NZ	13:M:169:TYR:CE1	2.88	0.42
13:M:114:PRO:C	13:M:116:SER:H	2.26	0.42
13:M:226:ARG:HB3	13:M:227:LEU:H	1.46	0.42
15:O:155:LEU:O	15:O:159:ILE:HG12	2.20	0.42
16:P:308:ASP:OD1	16:P:308:ASP:N	2.53	0.42
1:A:482:ARG:HH11	1:A:544:PRO:HB3	1.85	0.42
1:A:620:SER:HA	1:A:621:PRO:HD3	1.86	0.42
1:A:856:LEU:HD12	1:A:860:GLU:HB3	2.01	0.42
3:C:329:LYS:NZ	11:K:122:LYS:HB2	2.34	0.42
17:Q:59:ILE:HG22	17:Q:63:LYS:HE3	2.01	0.42
1:A:153:ARG:HA	1:A:160:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:HA	15:O:550:GLU:CB	2.50	0.42
2:B:325:GLU:HA	2:B:328:ALA:HB3	2.01	0.42
2:B:422:ILE:HA	2:B:425:HIS:HB3	2.01	0.42
2:B:756:THR:OG1	2:B:757:VAL:N	2.53	0.42
2:B:1008:ILE:O	3:C:65:ASN:ND2	2.53	0.42
7:G:44:LEU:HD23	7:G:104:ILE:HD11	2.01	0.42
15:O:519:GLU:HA	15:O:522:ILE:HB	2.01	0.42
15:O:533:ILE:HD13	15:O:533:ILE:HA	1.92	0.42
1:A:530:GLU:OE2	1:A:534:LEU:HD13	2.21	0.41
2:B:320:LEU:HD23	2:B:324:ILE:HD12	2.02	0.41
2:B:911:LYS:HD3	2:B:919:LYS:NZ	2.35	0.41
3:C:331:CYS:SG	11:K:46:LYS:HB2	2.60	0.41
4:D:70:LYS:HG3	4:D:98:MET:SD	2.60	0.41
5:E:29:PHE:HB2	5:E:65:THR:HB	2.01	0.41
1:A:712:ILE:HG22	1:A:713:GLY:H	1.84	0.41
1:A:891:LYS:HE3	2:B:1064:GLU:OE2	2.20	0.41
2:B:471:THR:HG22	2:B:514:LEU:HB2	2.02	0.41
2:B:536:LEU:HD22	2:B:571:PHE:CD1	2.56	0.41
2:B:934:ASN:HB3	2:B:1004:LEU:HA	2.02	0.41
2:B:944:MET:HE1	2:B:957:LYS:HE2	2.01	0.41
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.84	0.41
3:C:33:VAL:C	3:C:35:LYS:H	2.28	0.41
3:C:104:VAL:HA	3:C:105:PRO:HD3	1.86	0.41
14:N:415:LYS:NZ	14:N:417:VAL:HG13	2.35	0.41
15:O:579:GLN:HB2	16:P:317:TRP:C	2.45	0.41
1:A:244:ILE:HG12	1:A:253:PRO:HG3	2.03	0.41
2:B:113:THR:HA	2:B:114:PRO:HD3	1.88	0.41
2:B:190:THR:OG1	2:B:191:GLU:N	2.54	0.41
2:B:224:THR:OG1	2:B:225:HIS:N	2.50	0.41
5:E:131:THR:OG1	5:E:132:ILE:N	2.49	0.41
7:G:115:LEU:HD23	7:G:116:PHE:N	2.36	0.41
1:A:634:VAL:HA	1:A:635:PRO:HD3	1.82	0.41
2:B:841:ILE:HG21	2:B:870:PRO:HB2	2.03	0.41
2:B:983:LYS:HB3	2:B:986:ASP:OD2	2.20	0.41
3:C:21:PRO:HD2	11:K:82:LYS:HA	2.02	0.41
15:O:105:LYS:N	15:O:123:ASN:HB2	2.36	0.41
15:O:132:TYR:HB3	15:O:136:ILE:HG13	2.03	0.41
1:A:21:LEU:HD23	2:B:1140:ARG:NH2	2.35	0.41
1:A:153:ARG:CZ	15:O:336:LEU:HD13	2.50	0.41
2:B:99:ARG:HH21	2:B:103:LYS:HG3	1.84	0.41
2:B:240:ILE:HG13	2:B:253:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:ASN:HB2	2:B:566:ARG:HH11	1.85	0.41
15:O:102:ARG:O	15:O:123:ASN:ND2	2.46	0.41
1:A:21:LEU:HD22	1:A:25:ASP:OD2	2.21	0.41
1:A:1152:ARG:HH21	9:I:97:PHE:HB2	1.86	0.41
1:A:1301:ARG:O	1:A:1305:CYS:N	2.46	0.41
1:A:1391:LYS:HE2	1:A:1394:ASP:OD2	2.20	0.41
3:C:259:ASP:HB2	3:C:266:TYR:HE1	1.86	0.41
5:E:47:CYS:HA	5:E:53:PRO:HA	2.01	0.41
8:H:58:THR:O	8:H:143:LEU:N	2.48	0.41
13:M:108:SER:O	13:M:122:ASP:HB2	2.20	0.41
1:A:1026:ARG:NH2	1:A:1052:VAL:HG13	2.36	0.41
1:A:1064:GLU:OE1	1:A:1065:LYS:HG3	2.20	0.41
2:B:933:PHE:O	2:B:934:ASN:ND2	2.53	0.41
2:B:1080:LEU:O	2:B:1084:MET:HB3	2.21	0.41
4:D:14:TYR:OH	4:D:99:SER:O	2.33	0.41
15:O:53:VAL:HG21	15:O:65:ILE:HD12	2.02	0.41
15:O:219:TYR:O	15:O:222:HIS:HB2	2.20	0.41
16:P:315:ASP:O	16:P:317:TRP:HD1	2.03	0.41
1:A:34:VAL:HG21	1:A:84:LEU:HG	2.02	0.41
1:A:40:PHE:HB2	1:A:42:LEU:HG	2.02	0.41
1:A:643:ASN:HB2	1:A:651:PHE:CE2	2.56	0.41
1:A:1178:LYS:HE2	9:I:36:GLU:HB3	2.03	0.41
2:B:99:ARG:NH2	2:B:103:LYS:HG3	2.35	0.41
2:B:263:LEU:HD12	2:B:297:THR:HG22	2.01	0.41
2:B:547:ALA:HB2	14:N:391:LEU:HD13	2.03	0.41
2:B:795:LEU:HD23	2:B:845:LYS:HZ3	1.86	0.41
3:C:132:ILE:O	3:C:208:CYS:HB2	2.21	0.41
3:C:192:LEU:HD11	10:J:19:GLU:HG2	2.02	0.41
13:M:121:ILE:HD13	13:M:121:ILE:HA	1.93	0.41
15:O:349:ALA:O	15:O:352:VAL:HG12	2.21	0.41
15:O:463:SER:HB3	16:P:262:ARG:HH12	1.85	0.41
1:A:386:ASN:ND2	11:K:94:PRO:O	2.54	0.41
1:A:431:ASN:HD21	1:A:465:HIS:CD2	2.39	0.41
1:A:1080:LYS:HD3	1:A:1080:LYS:HA	1.95	0.41
1:A:1152:ARG:HD2	9:I:85:LEU:HB2	2.01	0.41
1:A:1458:LYS:HB2	4:D:111:ASN:HB3	2.02	0.41
2:B:337:VAL:HG23	2:B:338:GLU:H	1.84	0.41
2:B:409:LYS:HA	2:B:410:PRO:HD3	1.86	0.41
2:B:418:ALA:O	2:B:422:ILE:HG12	2.20	0.41
2:B:914:SER:C	2:B:916:HIS:H	2.29	0.41
2:B:961:LEU:HD23	2:B:1020:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1038:ARG:NH1	2:B:1057:ASP:CG	2.79	0.41
3:C:77:SER:O	3:C:210:LEU:HD12	2.21	0.41
3:C:328:LEU:HD22	11:K:72:LEU:HD21	2.03	0.41
13:M:73:GLU:C	14:N:364:ARG:HE	2.29	0.41
14:N:373:VAL:HG12	14:N:374:LYS:H	1.85	0.41
15:O:368:ARG:HD2	15:O:368:ARG:HA	1.89	0.41
16:P:230:VAL:C	16:P:232:ASN:H	2.28	0.41
16:P:255:LYS:HD2	16:P:255:LYS:N	2.36	0.41
1:A:236:SER:HB2	15:O:70:ALA:HA	2.03	0.41
2:B:529:ILE:HG23	2:B:530:LYS:H	1.86	0.41
3:C:114:THR:OG1	3:C:130:ASN:OD1	2.39	0.41
3:C:120:LEU:HA	3:C:121:PRO:HD2	1.90	0.41
4:D:58:ILE:H	4:D:58:ILE:HG13	1.70	0.41
13:M:108:SER:HB2	13:M:247:TRP:HB3	2.02	0.41
13:M:150:GLY:HA3	13:M:178:GLN:O	2.21	0.41
14:N:303:ARG:HD3	14:N:411:ARG:HH11	1.86	0.41
17:Q:43:ILE:HG23	17:Q:44:ASN:N	2.35	0.41
1:A:1026:ARG:NH1	8:H:129:TYR:OH	2.54	0.40
2:B:113:THR:OG1	2:B:117:GLU:OE1	2.22	0.40
2:B:225:HIS:HA	2:B:446:ARG:HH11	1.85	0.40
2:B:945:ASN:HA	2:B:946:PRO:HD3	1.84	0.40
3:C:11:ARG:HH12	8:H:21:ASN:CB	2.34	0.40
3:C:283:GLU:O	3:C:286:ALA:N	2.53	0.40
5:E:122:LYS:HG3	5:E:123:LEU:N	2.33	0.40
7:G:29:GLN:O	7:G:33:LYS:HG2	2.21	0.40
15:O:461:ALA:HA	15:O:469:ASN:ND2	2.36	0.40
15:O:500:LEU:HD12	15:O:500:LEU:HA	1.90	0.40
2:B:858:ASN:OD1	2:B:859:ASN:N	2.54	0.40
3:C:331:CYS:HB3	11:K:46:LYS:HD3	2.03	0.40
4:D:19:PHE:HD1	4:D:19:PHE:HA	1.75	0.40
7:G:4:LEU:HD23	7:G:73:ARG:HH21	1.86	0.40
8:H:108:SER:OG	8:H:109:LYS:N	2.53	0.40
11:K:65:ILE:O	11:K:101:LEU:N	2.55	0.40
14:N:374:LYS:HE2	14:N:374:LYS:HB3	1.94	0.40
15:O:588:LEU:HG	15:O:637:VAL:HG22	2.02	0.40
1:A:598:MET:HE1	8:H:141:TYR:CD1	2.56	0.40
2:B:610:ARG:HA	2:B:611:PRO:HD3	1.77	0.40
2:B:1036:HIS:NE2	2:B:1058:GLY:HA3	2.36	0.40
3:C:238:PRO:O	3:C:239:ILE:HG13	2.22	0.40
4:D:130:ASN:CG	4:D:131:MET:HG2	2.46	0.40
15:O:215:TRP:O	15:O:219:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:357:PRO:HA	15:O:361:PHE:CD2	2.56	0.40
1:A:76:SER:OG	1:A:77:CYS:N	2.54	0.40
1:A:161:ASN:ND2	1:A:162:GLY:O	2.55	0.40
1:A:284:ASP:O	1:A:288:LYS:HG2	2.22	0.40
1:A:355:GLN:OE1	1:A:355:GLN:N	2.54	0.40
2:B:97:ASP:OD2	2:B:99:ARG:NH1	2.42	0.40
2:B:318:THR:HG22	2:B:318:THR:O	2.20	0.40
2:B:479:LYS:HB3	2:B:480:SER:H	1.63	0.40
2:B:944:MET:SD	2:B:1024:TYR:OH	2.80	0.40
13:M:131:TYR:OH	13:M:143:VAL:HG23	2.22	0.40
14:N:364:ARG:HA	14:N:364:ARG:HD3	1.85	0.40
14:N:387:GLU:H	14:N:387:GLU:CD	2.30	0.40
15:O:74:LEU:HD21	15:O:79:LEU:HG	2.03	0.40
15:O:208:TYR:O	15:O:209:THR:OG1	2.38	0.40
16:P:229:GLN:C	16:P:231:ALA:H	2.30	0.40
16:P:253:LEU:HB3	16:P:261:TYR:HB3	2.03	0.40
1:A:742:ILE:HD12	1:A:742:ILE:HA	1.92	0.40
1:A:1089:ILE:HD13	1:A:1092:ILE:HD12	2.03	0.40
1:A:1145:LEU:HD21	1:A:1153:ALA:HB1	2.04	0.40
2:B:241:TYR:CG	2:B:250:GLU:HB2	2.57	0.40
3:C:212:ILE:HG12	3:C:214:GLY:H	1.86	0.40
4:D:13:ASP:OD2	4:D:66:LEU:HG	2.21	0.40
15:O:568:CYS:HB3	15:O:569:LYS:H	1.58	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	1393/1460 (95%)	1147 (82%)	233 (17%)	13 (1%)	14	49
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	333/335 (99%)	282 (85%)	47 (14%)	4 (1%)	10	42
4	D	113/161 (70%)	80 (71%)	33 (29%)	0	100	100
5	E	213/215 (99%)	170 (80%)	41 (19%)	2 (1%)	14	49
6	F	81/155 (52%)	74 (91%)	7 (9%)	0	100	100
7	G	176/212 (83%)	149 (85%)	25 (14%)	2 (1%)	11	45
8	H	136/146 (93%)	117 (86%)	19 (14%)	0	100	100
9	I	88/110 (80%)	75 (85%)	13 (15%)	0	100	100
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	8	38
11	K	99/142 (70%)	83 (84%)	15 (15%)	1 (1%)	12	47
12	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
13	M	160/282 (57%)	138 (86%)	18 (11%)	4 (2%)	4	26
14	N	106/422 (25%)	80 (76%)	24 (23%)	2 (2%)	6	32
15	O	533/654 (82%)	436 (82%)	93 (17%)	4 (1%)	16	53
16	P	83/317 (26%)	54 (65%)	26 (31%)	3 (4%)	2	20
17	Q	26/88 (30%)	22 (85%)	3 (12%)	1 (4%)	2	19
All	All	4760/5988 (80%)	3936 (83%)	778 (16%)	46 (1%)	15	47

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ILE
1	A	587	ILE
1	A	603	LEU
1	A	632	VAL
1	A	1371	ILE
2	B	321	GLN
11	K	47	ILE
13	M	97	VAL
13	M	107	ILE
15	O	88	VAL
15	O	146	VAL
16	P	175	ILE
16	P	230	VAL
16	P	311	VAL
1	A	599	LYS
3	C	239	ILE
13	M	143	VAL

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Mol	Chain	Res	Type
1	A	307	ILE
1	A	975	VAL
2	B	811	VAL
2	B	927	LYS
3	C	255	VAL
1	A	995	VAL
1	A	1328	ILE
2	B	87	VAL
2	B	632	ASP
2	B	651	VAL
2	B	713	ILE
2	B	767	ILE
3	C	91	VAL
14	N	299	ASN
14	N	411	ARG
15	O	368	ARG
17	Q	43	ILE
1	A	23	ALA
1	A	1389	PHE
7	G	191	PRO
15	O	338	ASP
1	A	667	SER
3	C	87	ASN
13	M	115	LYS
5	E	90	VAL
10	J	65	PRO
7	G	79	PRO
2	B	584	VAL
5	E	125	PRO

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	1217/1257 (97%)	1170 (96%)	47 (4%)	28	49
2	B	975/1006 (97%)	938 (96%)	37 (4%)	29	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	296/296 (100%)	284 (96%)	12 (4%)	27	49
4	D	110/145 (76%)	108 (98%)	2 (2%)	51	67
5	E	197/197 (100%)	190 (96%)	7 (4%)	31	52
6	F	73/137 (53%)	70 (96%)	3 (4%)	27	49
7	G	162/190 (85%)	155 (96%)	7 (4%)	26	47
8	H	123/128 (96%)	116 (94%)	7 (6%)	18	40
9	I	83/98 (85%)	82 (99%)	1 (1%)	63	73
10	J	62/65 (95%)	58 (94%)	4 (6%)	15	37
11	K	91/130 (70%)	89 (98%)	2 (2%)	45	64
12	L	40/57 (70%)	37 (92%)	3 (8%)	12	33
13	M	142/249 (57%)	135 (95%)	7 (5%)	22	44
14	N	92/360 (26%)	87 (95%)	5 (5%)	20	42
15	O	495/593 (84%)	480 (97%)	15 (3%)	36	57
16	P	86/285 (30%)	79 (92%)	7 (8%)	11	31
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4268/5249 (81%)	4102 (96%)	166 (4%)	30	49

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	34	VAL
1	A	104	GLN
1	A	109	ASN
1	A	160	LEU
1	A	164	VAL
1	A	220	ASP
1	A	222	LEU
1	A	247	THR
1	A	255	THR
1	A	304	ASP
1	A	381	ILE
1	A	390	ASP
1	A	408	VAL
1	A	409	THR
1	A	500	LEU
1	A	506	THR

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Mol	Chain	Res	Type
1	A	542	LEU
1	A	712	ILE
1	A	747	LYS
1	A	813	VAL
1	A	817	ILE
1	A	848	VAL
1	A	904	VAL
1	A	955	LEU
1	A	996	ASP
1	A	1029	LEU
1	A	1059	LEU
1	A	1087	THR
1	A	1099	GLU
1	A	1123	VAL
1	A	1141	ILE
1	A	1161	VAL
1	A	1169	VAL
1	A	1186	VAL
1	A	1205	ILE
1	A	1224	ILE
1	A	1271	VAL
1	A	1272	VAL
1	A	1294	LEU
1	A	1303	VAL
1	A	1310	ILE
1	A	1325	VAL
1	A	1350	VAL
1	A	1408	VAL
1	A	1411	VAL
1	A	1423	ILE
2	B	87	VAL
2	B	96	VAL
2	B	100	VAL
2	B	133	ILE
2	B	147	VAL
2	B	186	ILE
2	B	231	THR
2	B	234	ILE
2	B	251	ILE
2	B	309	VAL
2	B	317	LEU
2	B	321	GLN

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Mol	Chain	Res	Type
2	B	337	VAL
2	B	366	ILE
2	B	422	ILE
2	B	457	VAL
2	B	536	LEU
2	B	538	VAL
2	B	551	LEU
2	B	555	VAL
2	B	599	VAL
2	B	612	LEU
2	B	666	ILE
2	B	675	ILE
2	B	713	ILE
2	B	741	ILE
2	B	772	VAL
2	B	806	ILE
2	B	818	ILE
2	B	849	THR
2	B	860	VAL
2	B	871	VAL
2	B	938	ILE
2	B	1008	ILE
2	B	1022	ILE
2	B	1047	THR
2	B	1108	THR
3	C	33	VAL
3	C	59	ILE
3	C	78	VAL
3	C	91	VAL
3	C	104	VAL
3	C	120	LEU
3	C	133	VAL
3	C	151	THR
3	C	193	LEU
3	C	239	ILE
3	C	278	GLU
3	C	294	VAL
4	D	109	LYS
4	D	127	LEU
5	E	9	ILE
5	E	75	MET
5	E	80	VAL

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Mol	Chain	Res	Type
5	E	123	LEU
5	E	124	VAL
5	E	141	VAL
5	E	196	VAL
6	F	99	LEU
6	F	133	VAL
6	F	151	LEU
7	G	3	ILE
7	G	41	ASN
7	G	53	THR
7	G	108	ILE
7	G	113	ASN
7	G	115	LEU
7	G	202	THR
8	H	12	VAL
8	H	26	ILE
8	H	32	THR
8	H	44	VAL
8	H	59	ILE
8	H	125	LEU
8	H	132	LEU
9	I	38	ILE
10	J	3	VAL
10	J	16	ASP
10	J	24	LEU
10	J	30	LEU
11	K	57	ASP
11	K	124	LEU
12	L	30	ILE
12	L	34	CYS
12	L	48	CYS
13	M	83	GLU
13	M	87	VAL
13	M	97	VAL
13	M	125	LEU
13	M	143	VAL
13	M	228	THR
13	M	231	LEU
14	N	313	LEU
14	N	363	ILE
14	N	373	VAL
14	N	382	ILE

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Mol	Chain	Res	Type
14	N	416	ILE
15	O	33	THR
15	O	42	LEU
15	O	64	VAL
15	O	88	VAL
15	O	186	THR
15	O	201	ILE
15	O	226	ILE
15	O	282	ILE
15	O	307	VAL
15	O	328	ASP
15	O	335	LEU
15	O	339	LEU
15	O	516	LEU
15	O	550	GLU
15	O	630	VAL
16	P	175	ILE
16	P	180	THR
16	P	221	ILE
16	P	235	LEU
16	P	236	THR
16	P	240	ILE
16	P	311	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	431	ASN
1	A	518	ASN
1	A	625	ASN
1	A	934	ASN
1	A	1174	GLN
1	A	1197	GLN
1	A	1233	ASN
1	A	1354	HIS
2	B	519	HIS
2	B	626	HIS
2	B	865	GLN
2	B	902	GLN
2	B	1025	GLN
3	C	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	126	GLN
5	E	5	ASN
5	E	54	GLN
5	E	153	HIS
9	I	61	ASN
14	N	287	HIS
15	O	207	HIS
15	O	244	ASN
15	O	298	ASN
15	O	346	GLN
15	O	607	ASN
16	P	176	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	69:PRO	C	1070:UNK	N	10.21

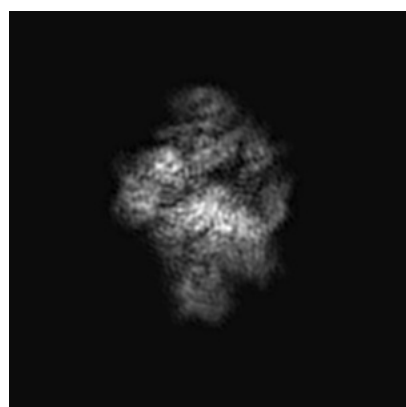
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3180. These allow visual inspection of the internal detail of the map and identification of artifacts.

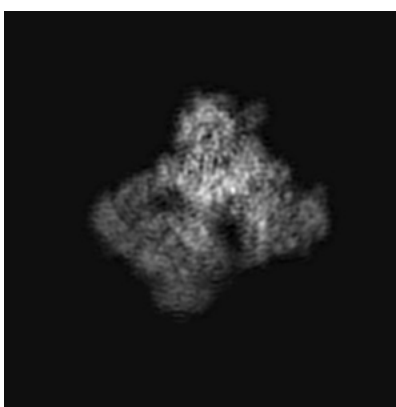
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

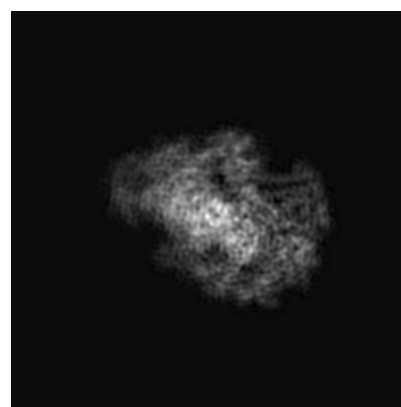
6.1.1 Primary map



X



Y

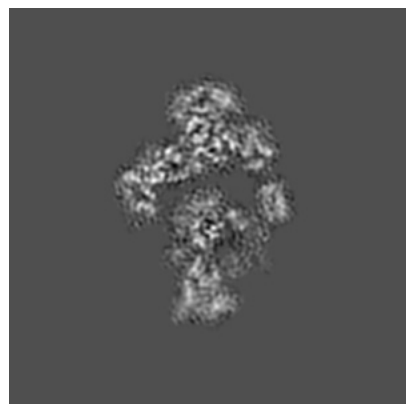


Z

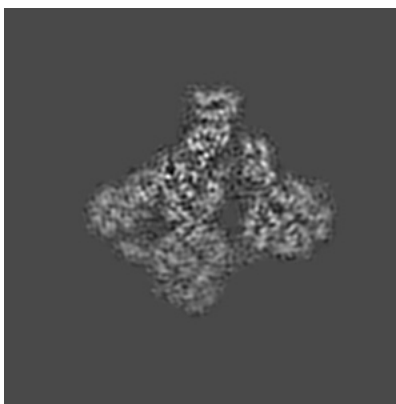
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

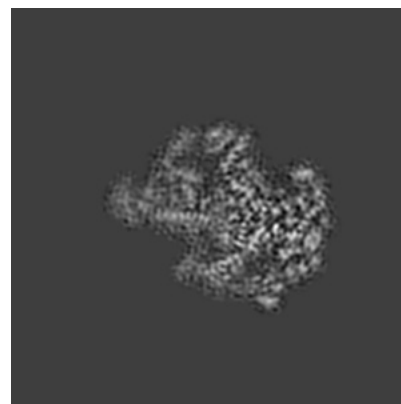
6.2.1 Primary map



X Index: 148



Y Index: 148

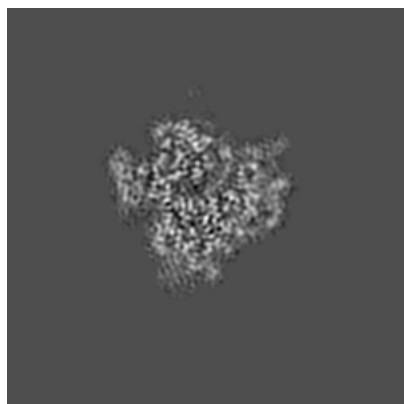


Z Index: 148

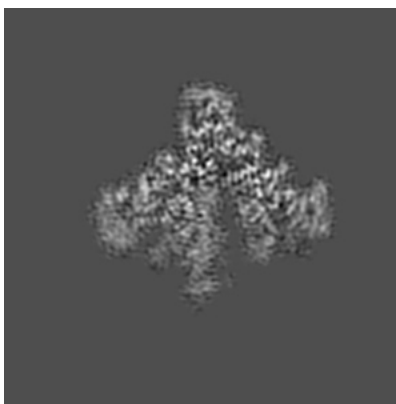
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

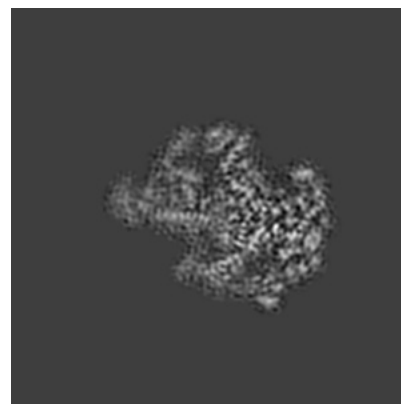
6.3.1 Primary map



X Index: 172



Y Index: 139

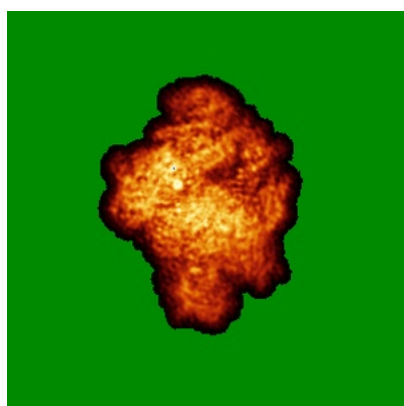


Z Index: 148

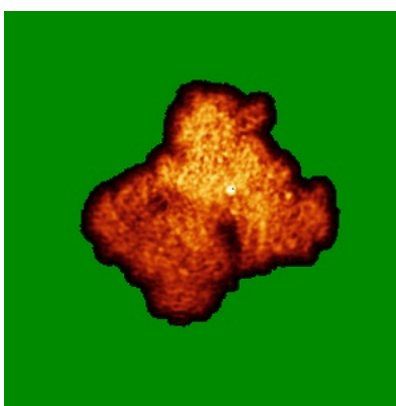
The images above show the largest variance slices of the map in three orthogonal directions.

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

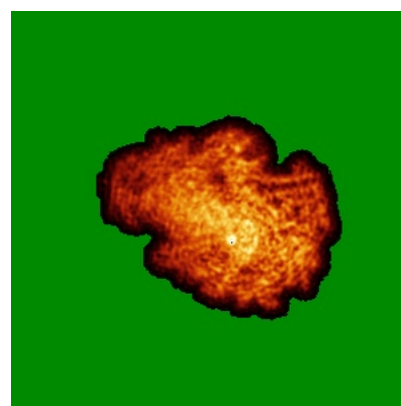
6.4.1 Primary map



X



Y

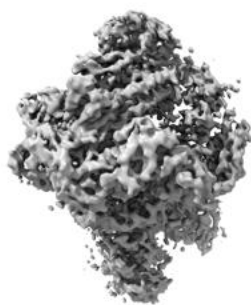


Z

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 [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

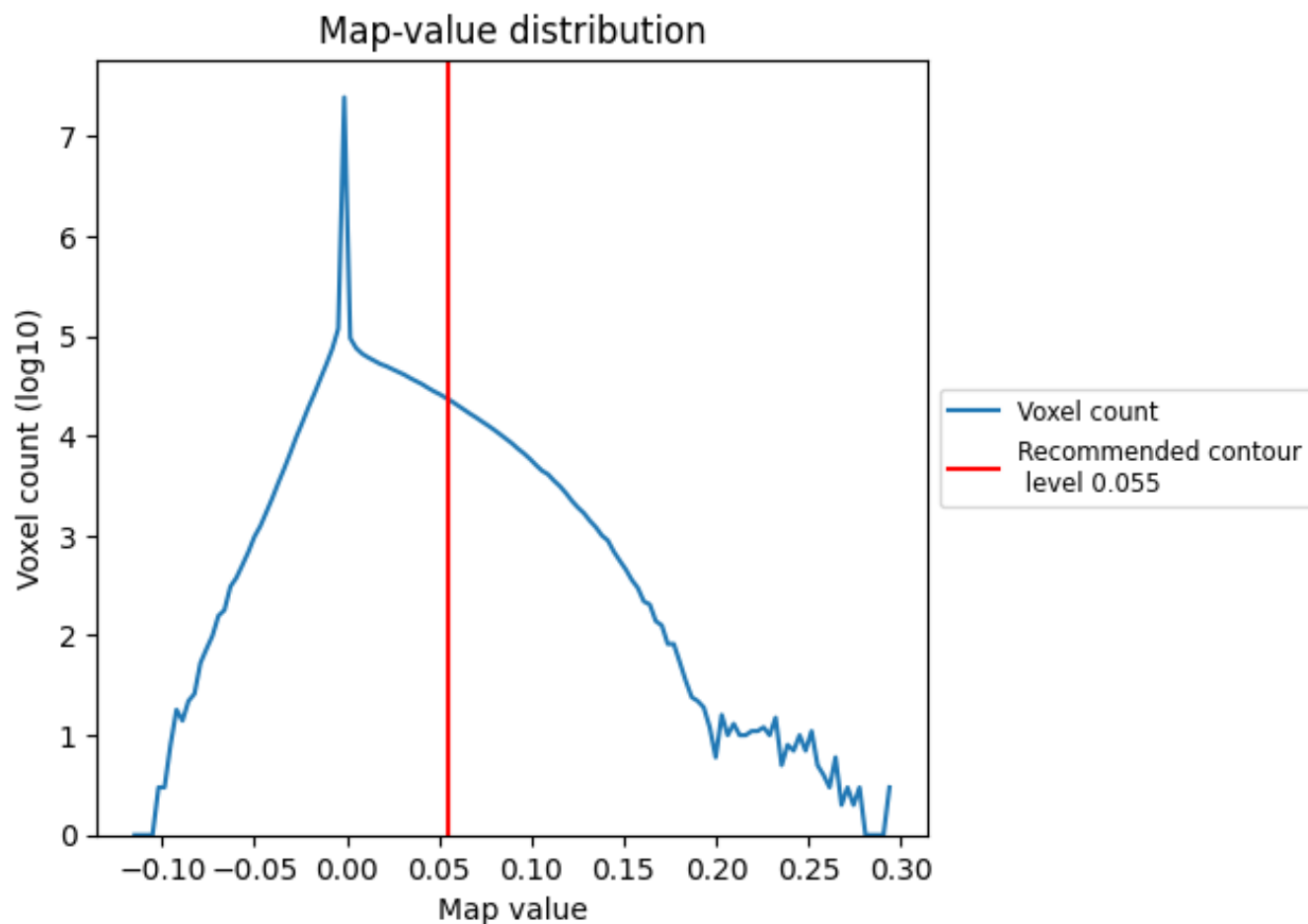
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

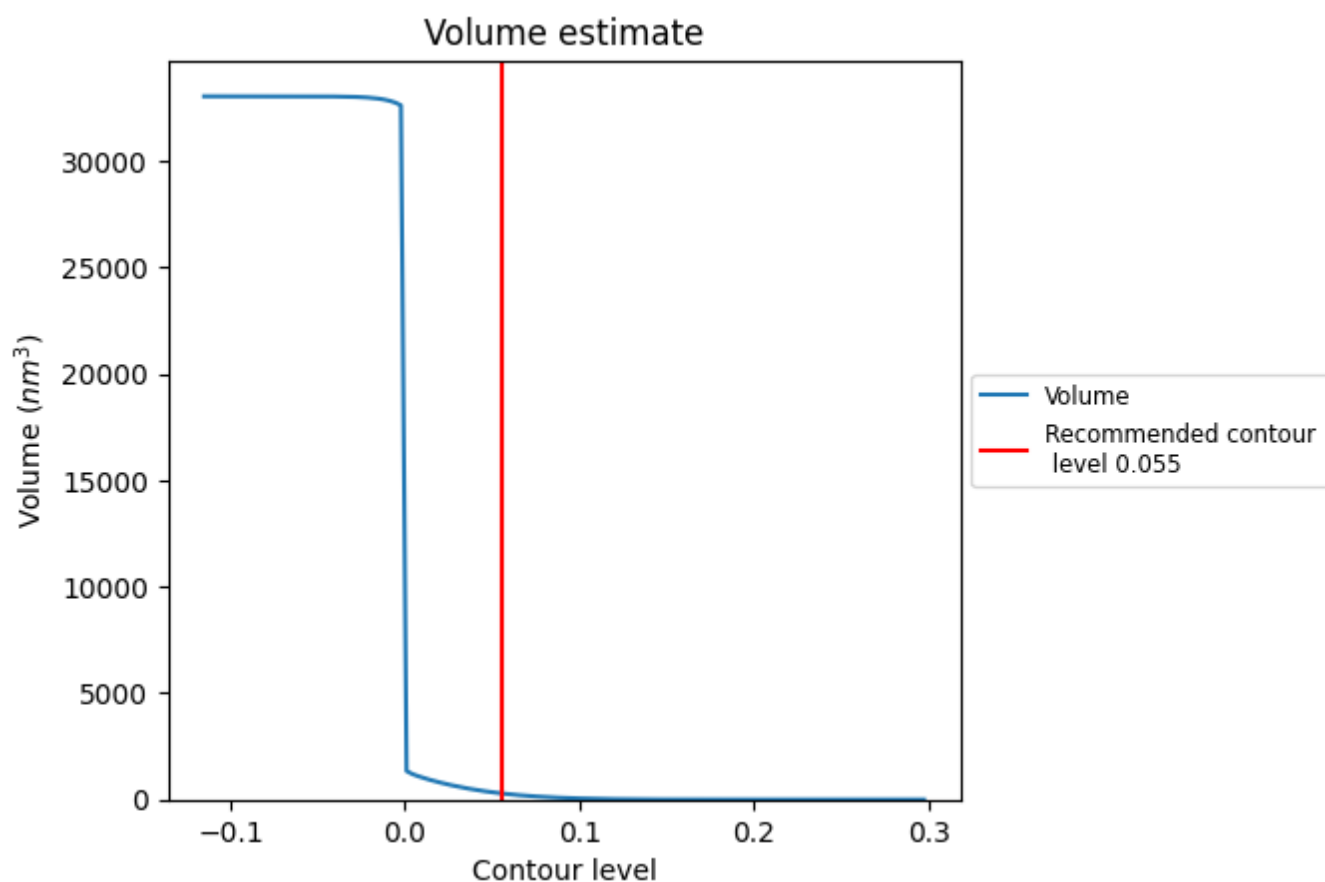
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

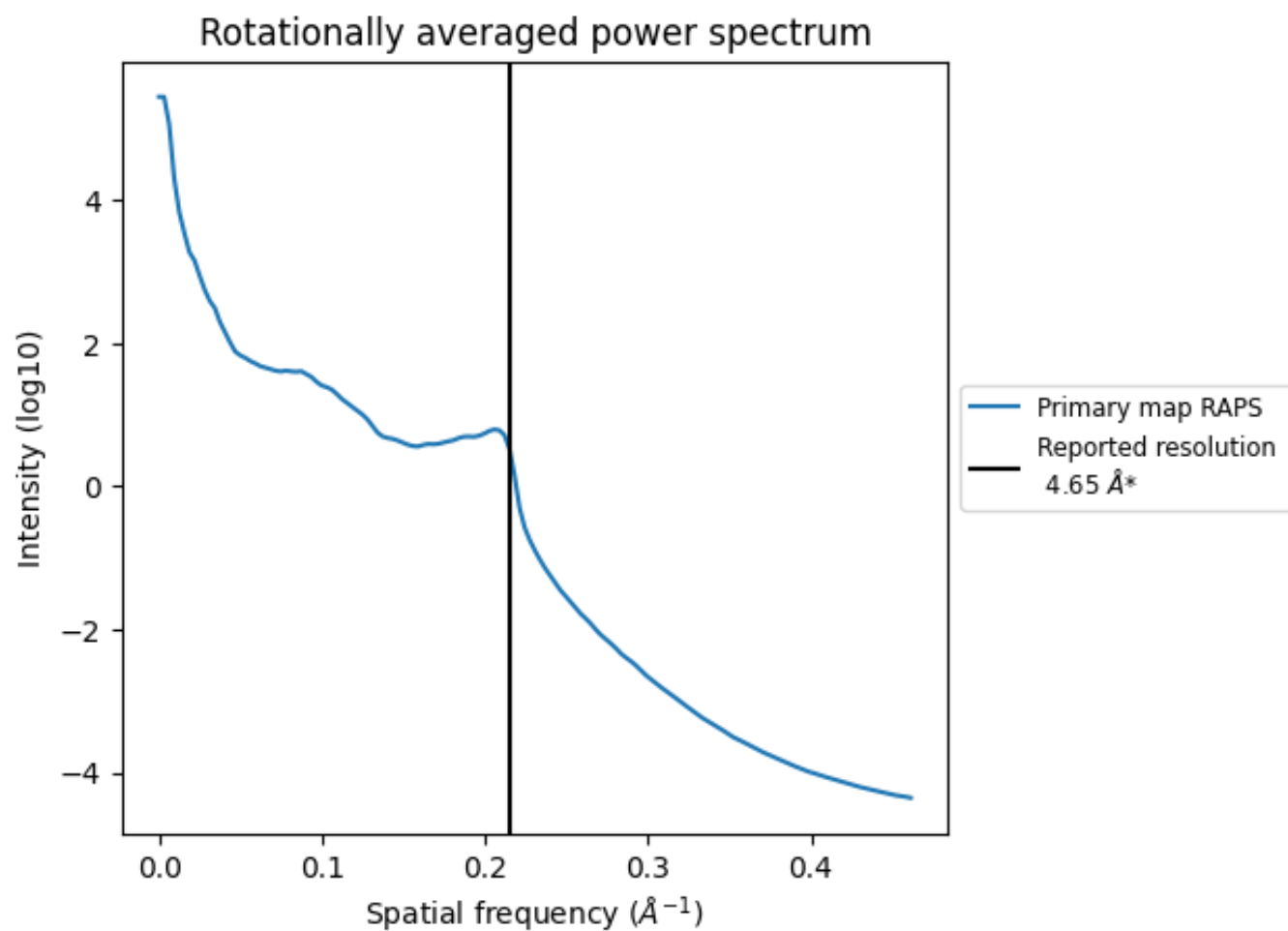
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293 nm³; this corresponds to an approximate mass of 264 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 ⓘ

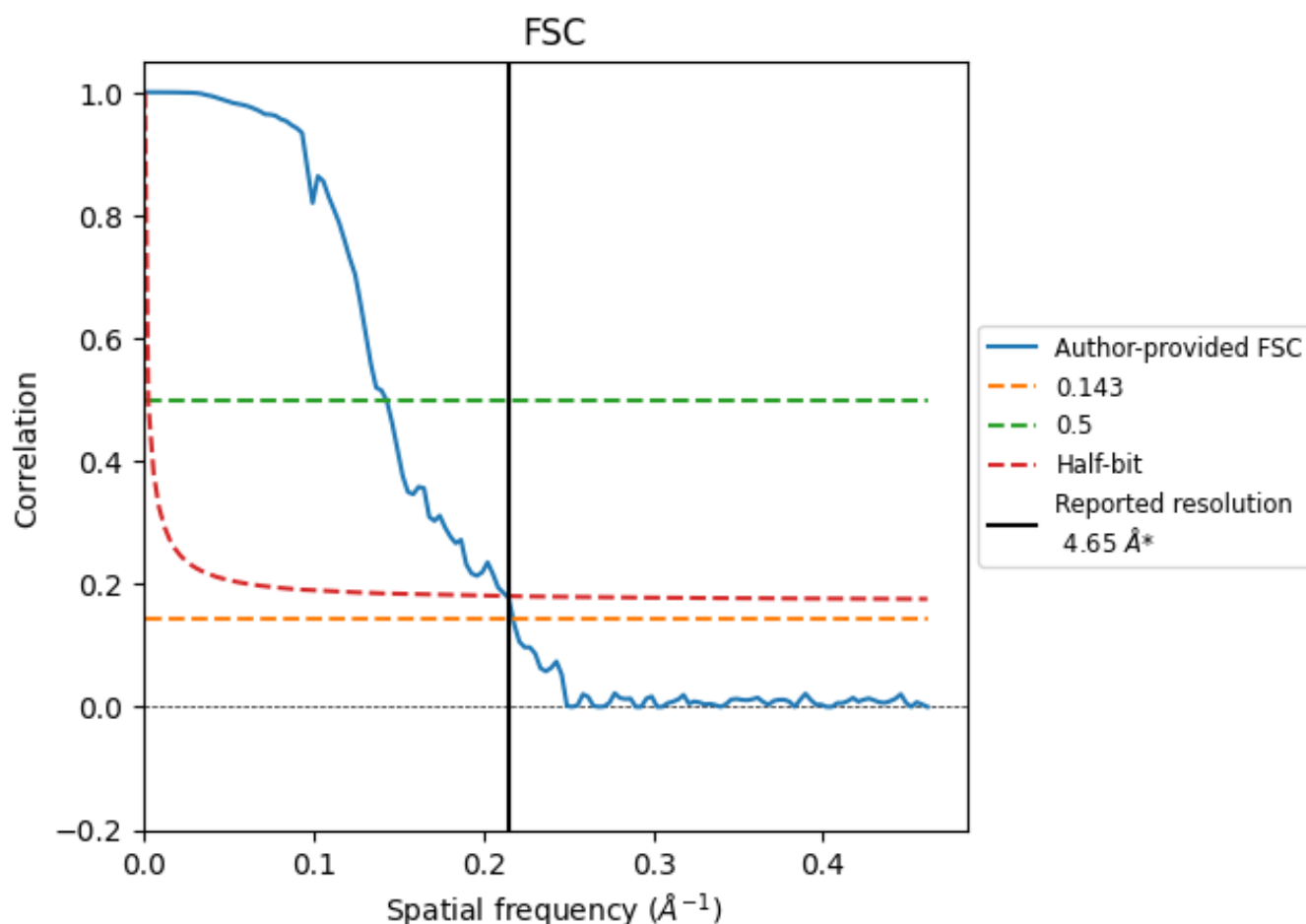


*Reported resolution corresponds to spatial frequency of 0.215 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.215 Å⁻¹

8.2 Resolution estimates [i](#)

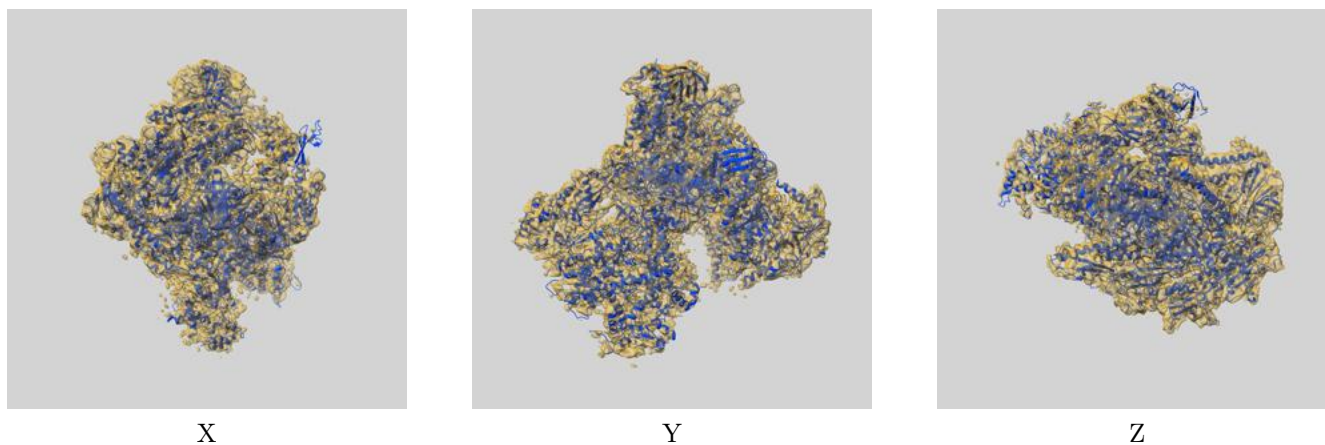
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	4.60	7.00	4.67
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3180 and PDB model 5FJA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



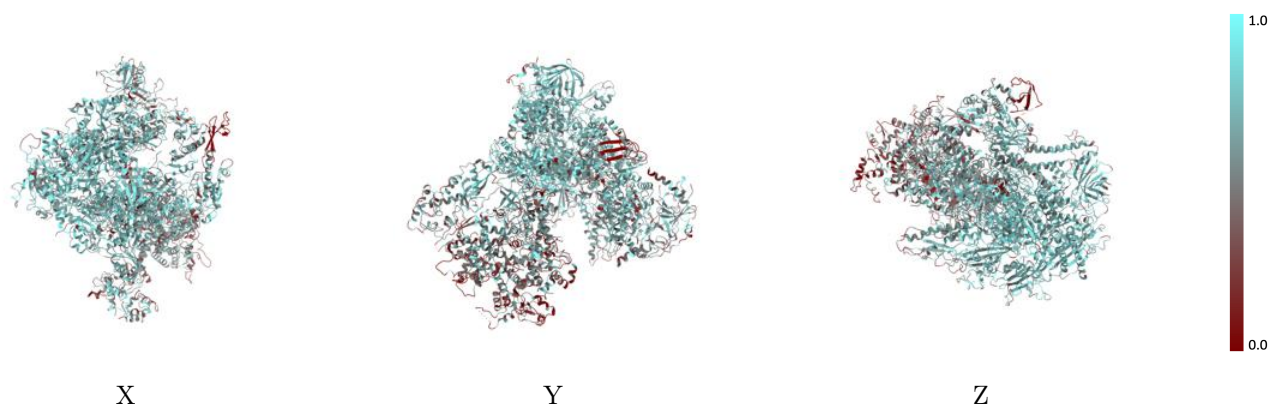
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



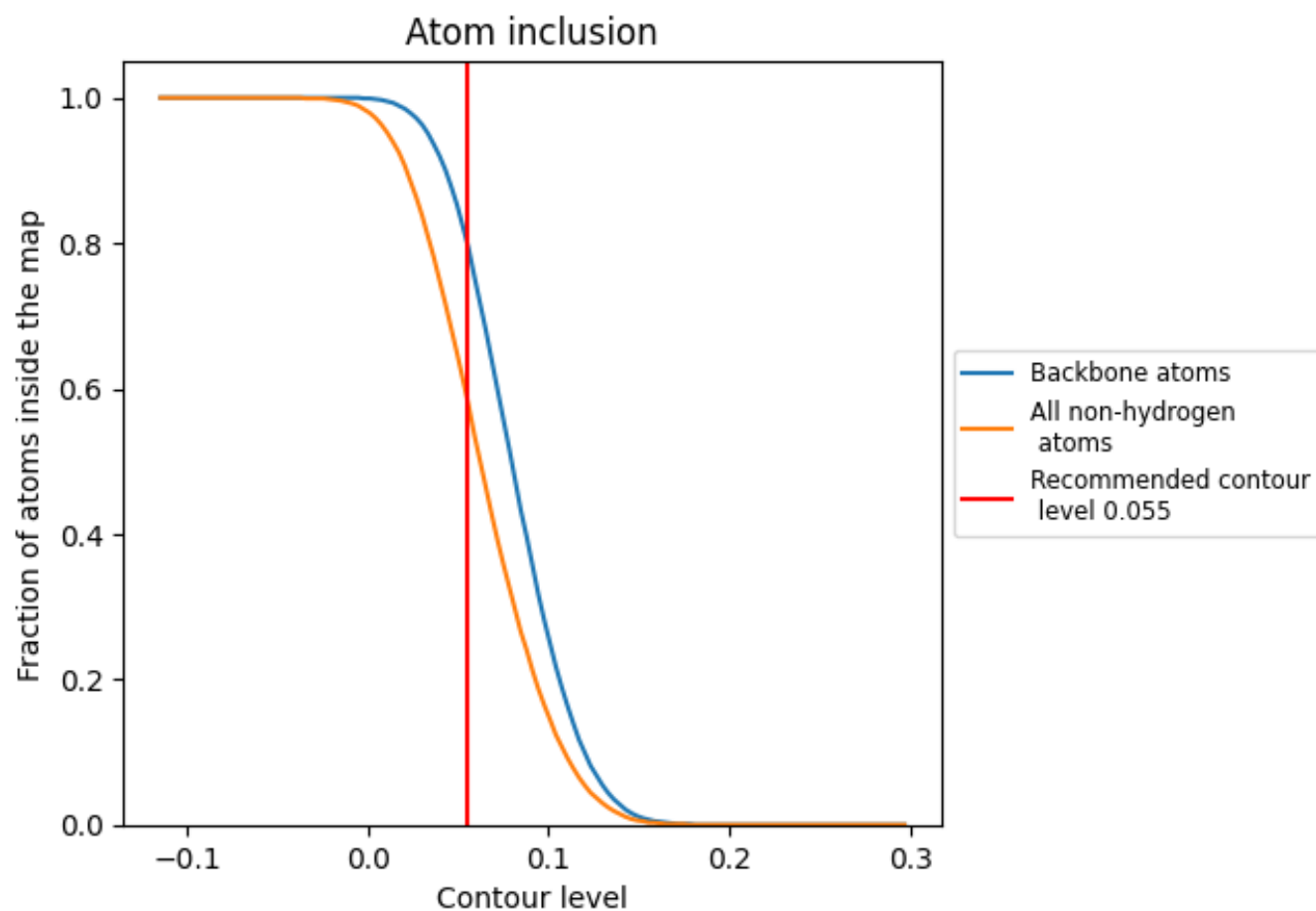
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 58% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5840	 0.2320
A	 0.6120	 0.2500
B	 0.6400	 0.2750
C	 0.6960	 0.2760
D	 0.5270	 0.1430
E	 0.6290	 0.2150
F	 0.6890	 0.3090
G	 0.5030	 0.1640
H	 0.6740	 0.2640
I	 0.2440	 0.1160
J	 0.7380	 0.2930
K	 0.6860	 0.2850
L	 0.6530	 0.2690
M	 0.5070	 0.2030
N	 0.5460	 0.2050
O	 0.4090	 0.1410
P	 0.2860	 0.0760
Q	 0.5600	 0.1880

