



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:31 PM UTC

PDB ID : 7UI9 / pdb_00007ui9
EMDB ID : EMD-26542
Title : Core Mediator-PICearly (Copy A)
Authors : Gorbea Colon, J.J.; Chen, S.-F.; Tsai, K.L.; Murakami, K.
Deposited on : 2022-03-28
Resolution : 3.30 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:

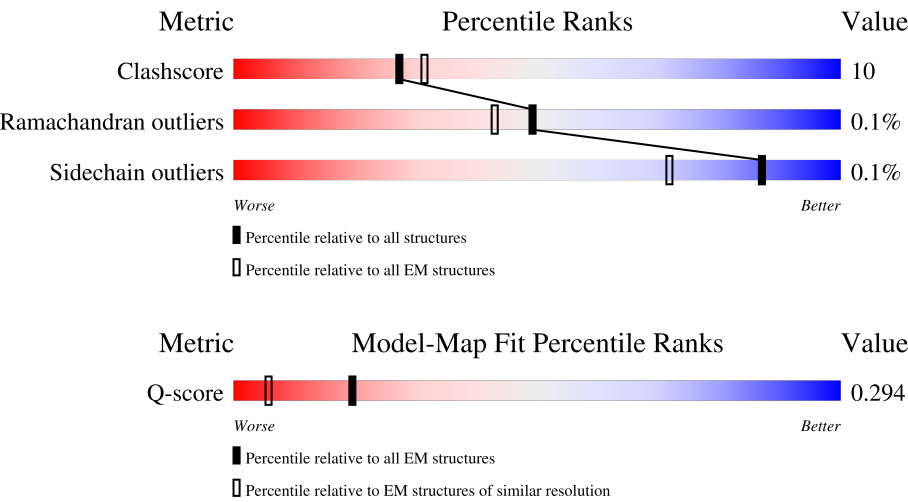
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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.



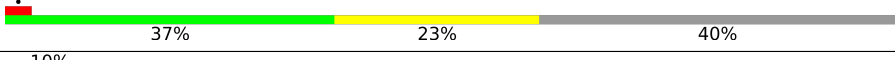
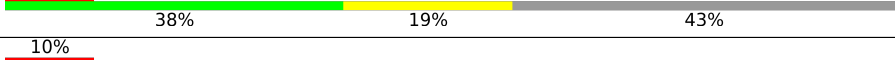
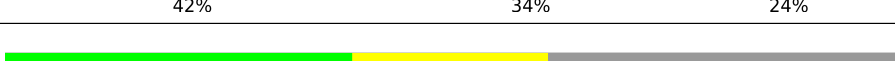
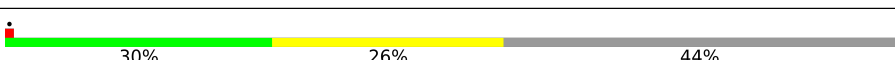
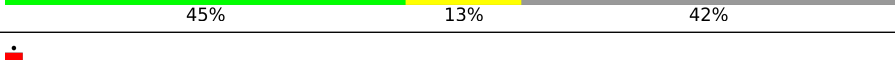
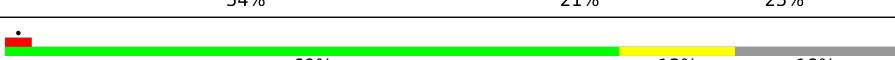
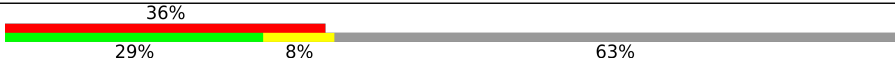
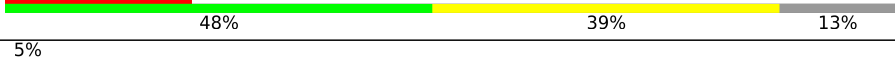
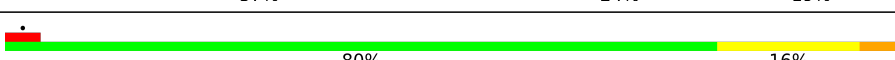
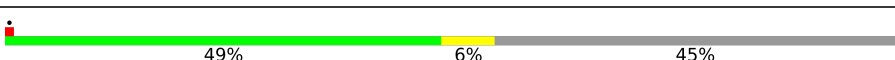
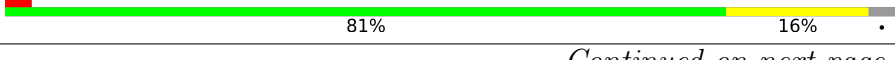
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	M	345	
2	P	735	
3	Q	400	
4	S	309	

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Mol	Chain	Length	Quality of chain
5	a	566	
6	d	284	
7	f	295	
8	g	222	
9	h	223	
10	i	149	
11	j	157	
12	k	115	
13	n	1082	
14	q	687	
15	r	307	
16	s	220	
17	t	210	
18	u	140	
19	v	120	
20	w	127	
21	z	25	
22	A	1453	
23	B	1224	
24	C	318	
25	D	221	
26	E	215	
27	F	155	
28	G	171	
29	H	146	

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Mol	Chain	Length	Quality of chain
30	I	122	
31	J	70	
32	K	120	
33	L	70	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 63137 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 Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	35	Total	C	N	O	S	0	0
			263	169	41	49	4		

- Molecule 2 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	103	Total	C	N	O	S	0	0
			861	554	142	162	3		

- Molecule 3 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	125	Total	C	N	O	S	0	0
			1033	644	189	195	5		

- Molecule 4 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	181	Total	C	N	O	S	0	0
			1436	893	256	279	8		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	365	Total	C	N	O	S	0	0
			3008	1932	478	588	10		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	171	Total	C	N	O	S	0	0
			1388	875	233	276	4		

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	169	Total	C	N	O	S	0	0
			1407	905	234	262	6		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	169	Total	C	N	O	S	0	0
			1409	903	238	263	5		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	136	Total	C	N	O	S	0	0
			1126	709	199	215	3		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	83	Total	C	N	O	S	0	0
			709	444	130	134	1		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	146	Total	C	N	O	S	0	0
			1173	725	206	239	3		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	108	Total	C	N	O	S	0	0
			876	546	149	177	4		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	625	Total	C	N	O	S	0	0
			5139	3318	884	913	24		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	515	Total	C	N	O	S	0	0
			4182	2674	707	788	13		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	253	Total	C	N	O	S	0	0
			1995	1271	331	383	10		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	81	Total	C	N	O	S	0	0
			657	415	109	132	1		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	210	Total	C	N	O	S	0	0
			1609	1016	270	317	6		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	122	Total	C	N	O	S	0	0
			978	611	163	199	5		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	109	Total	C	N	O	S	0	0
			869	540	143	180	6		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	103	Total	C	N	O	S	0	0
			871	575	135	155	6		

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	z	25	Total	C	N	O	0	0
			184	116	25	43		

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	1453	Total	C	N	O	S	0	0
			11425	7192	1995	2176	62		

- Molecule 23 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	1172	Total	C	N	O	S	0	0
			9336	5895	1637	1748	56		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	271	Total	C	N	O	S	0	0
			2133	1340	355	424	14		

- Molecule 25 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	D	169	Total	C	N	O	S	0	0
			1353	838	237	275	3		

- Molecule 26 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 27 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F	86	Total	C	N	O	S	0	0
			697	445	118	131	3		

- Molecule 28 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	H	141	Total	C	N	O	S	0	0
			1126	706	189	226	5		

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	116	Total	C	N	O	S	0	0
			943	580	171	181	11		

- Molecule 31 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 32 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	116	Total	C	N	O	S	0	0
			929	596	158	173	2		

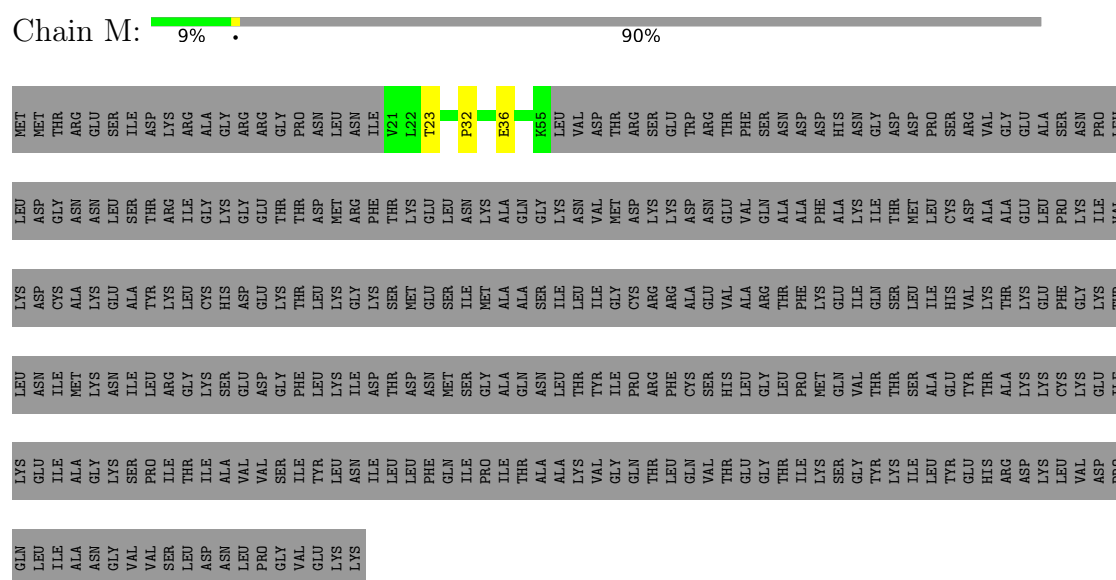
- Molecule 33 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	43	Total	C	N	O	S	0	0
			344	211	69	60	4		

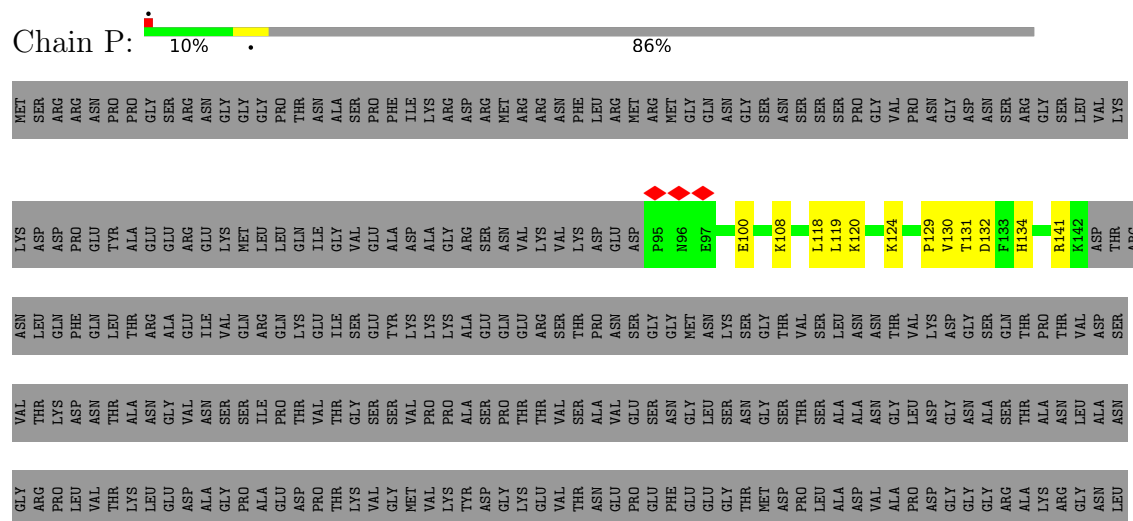
3 Residue-property plots

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: Transcription initiation factor IIB

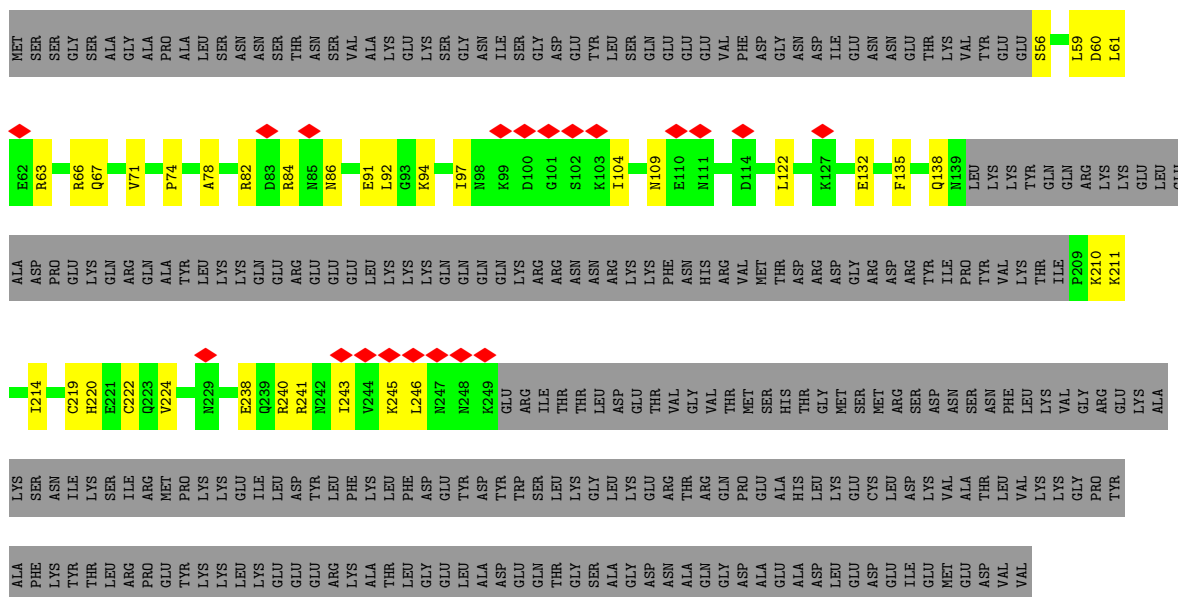


• Molecule 2: Transcription initiation factor IIF subunit alpha

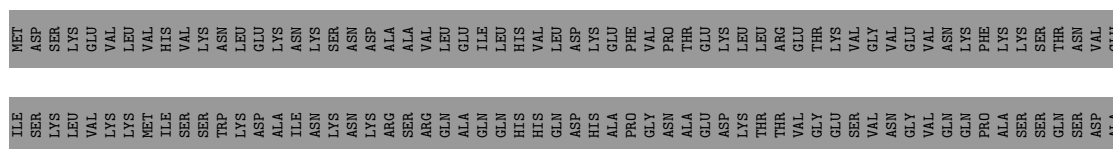


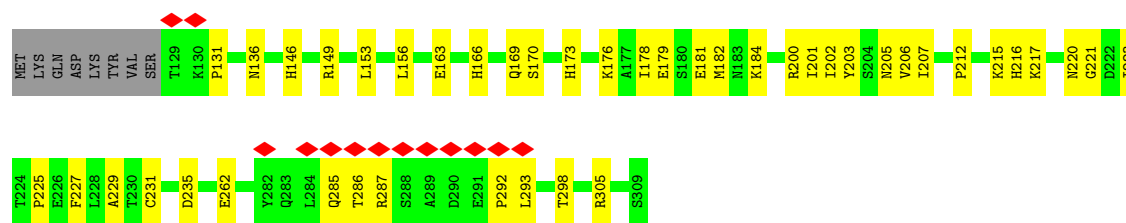


- Molecule 3: Transcription initiation factor IIF subunit beta

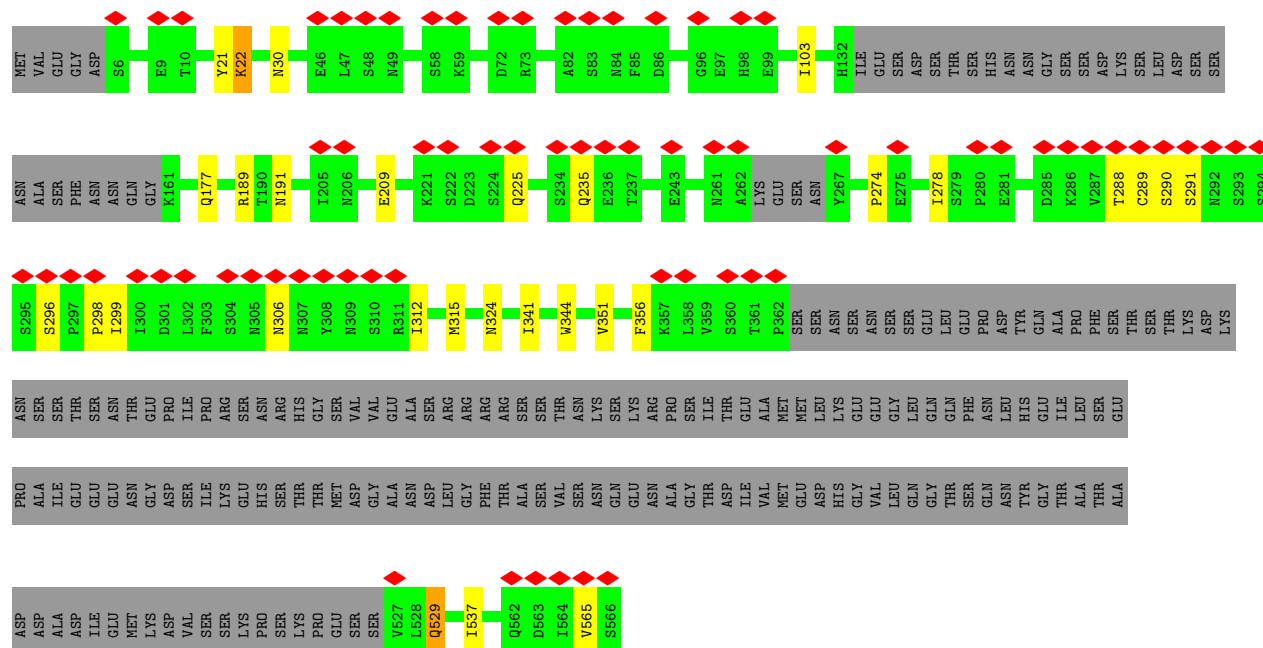


- Molecule 4: Transcription elongation factor S-II

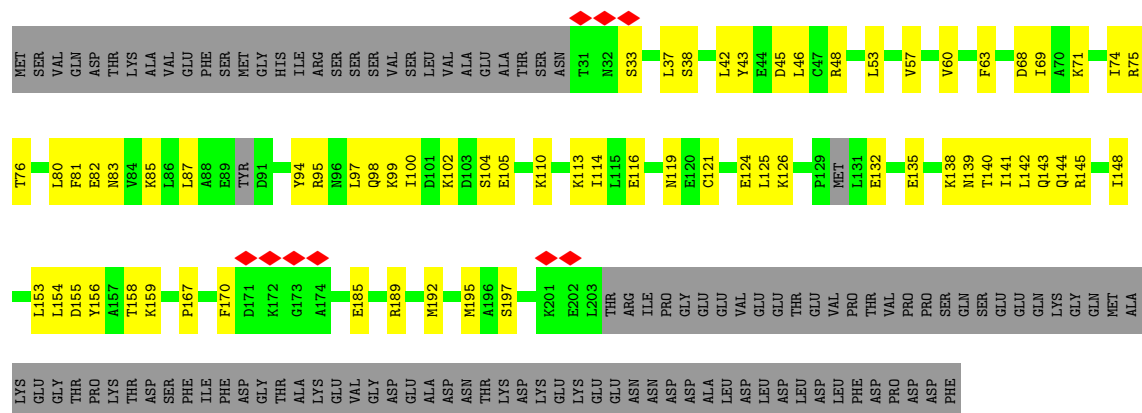




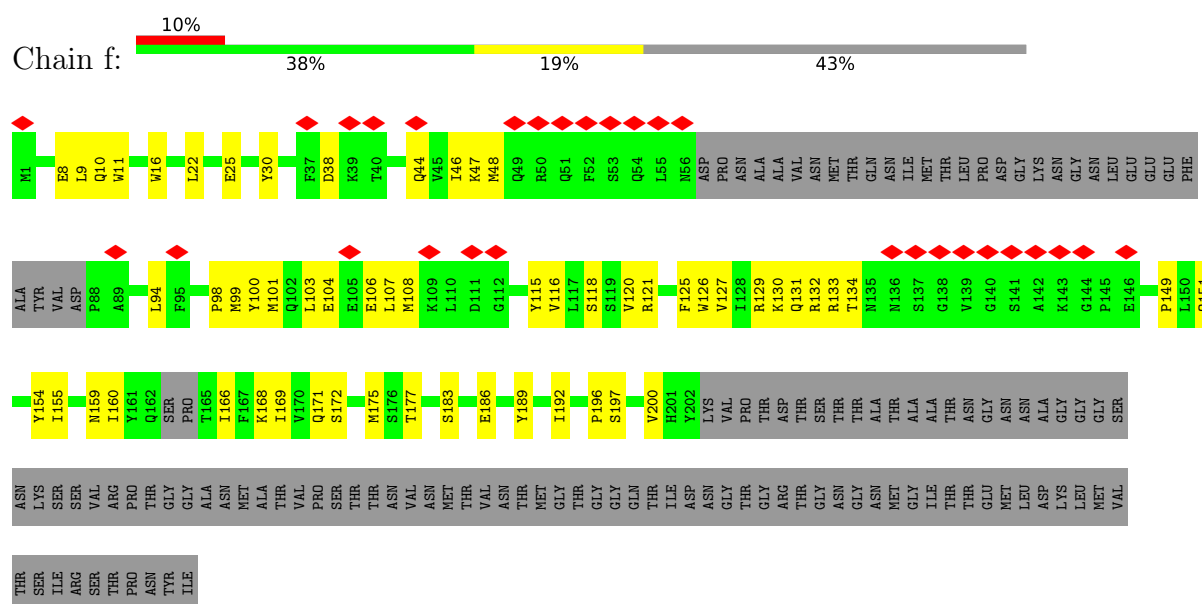
• Molecule 5: Mediator of RNA polymerase II transcription subunit 1



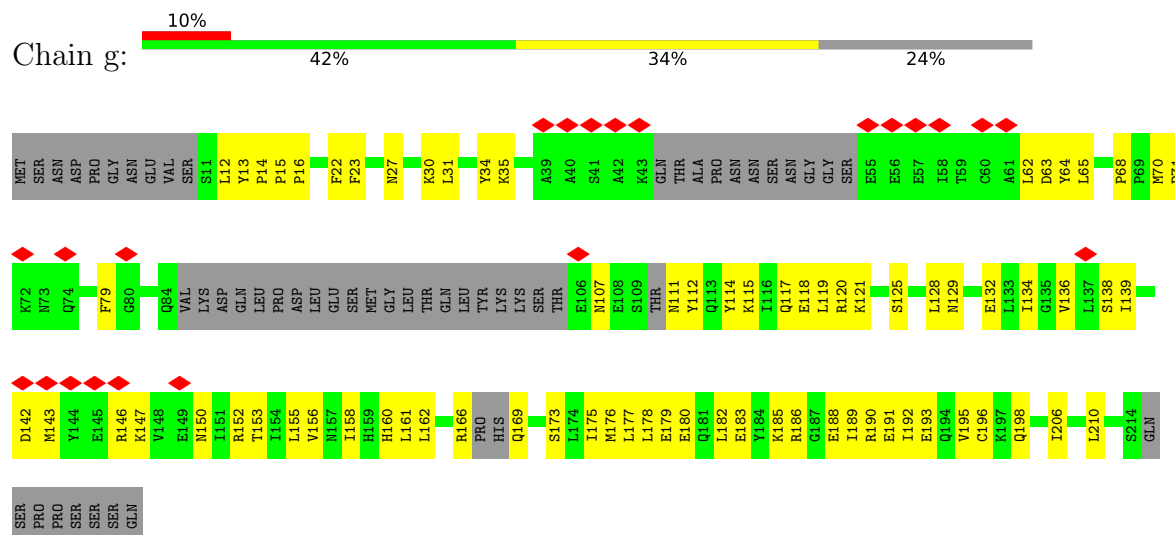
• Molecule 6: Mediator of RNA polymerase II transcription subunit 4



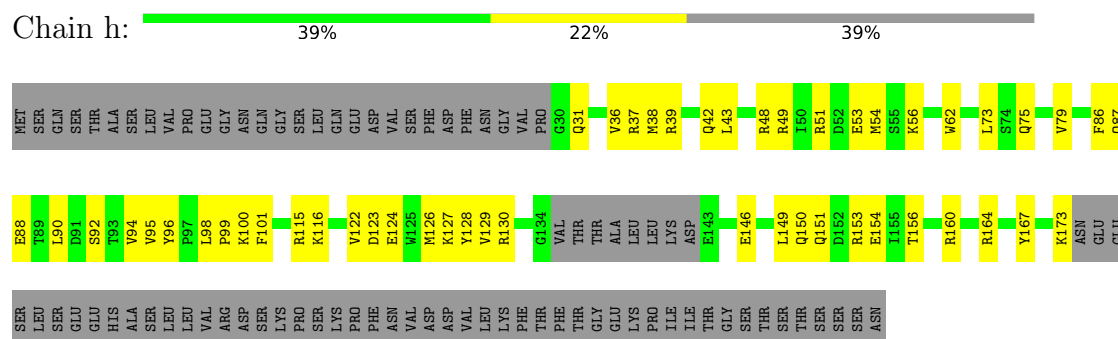
• Molecule 7: Mediator of RNA polymerase II transcription subunit 6



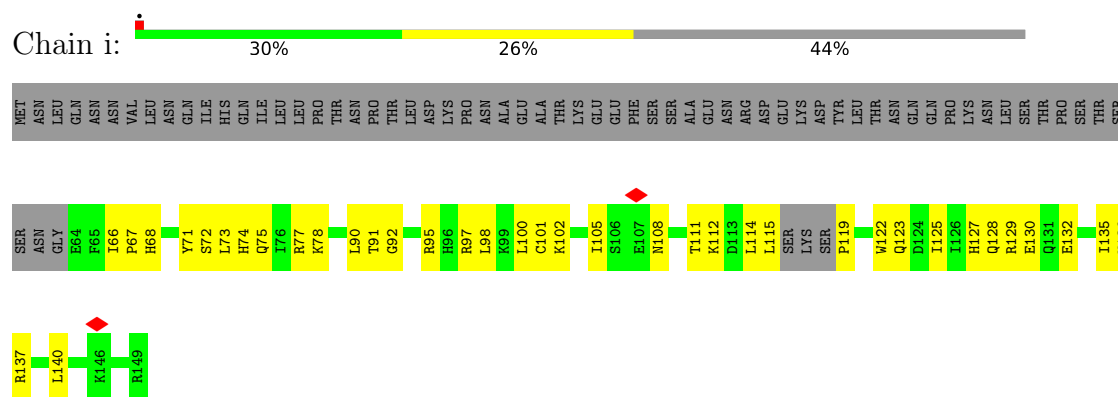
- Molecule 8: Mediator of RNA polymerase II transcription subunit 7



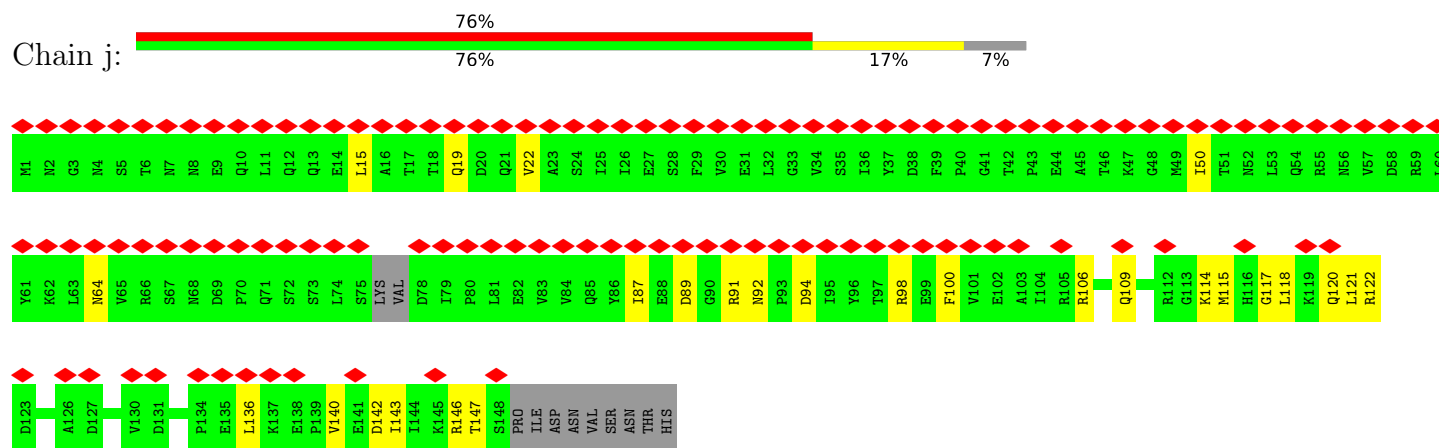
- Molecule 9: Mediator of RNA polymerase II transcription subunit 8



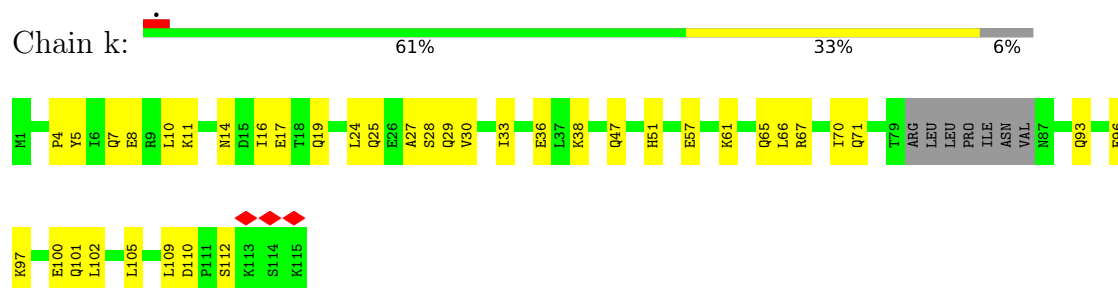
- Molecule 10: Mediator of RNA polymerase II transcription subunit 9



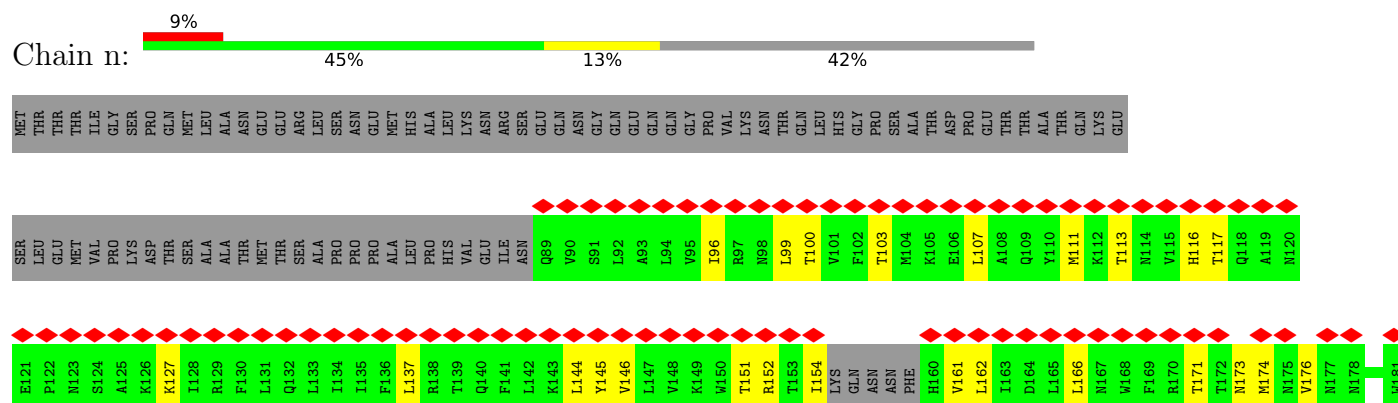
- Molecule 11: Mediator of RNA polymerase II transcription subunit 10

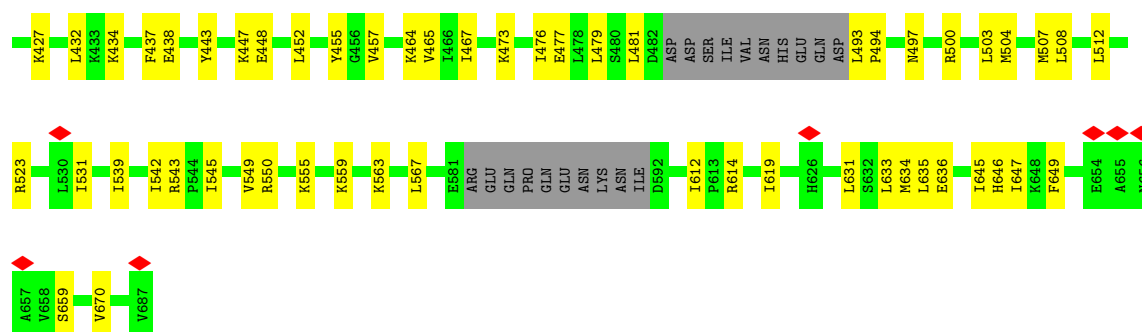


- Molecule 12: Mediator of RNA polymerase II transcription subunit 11

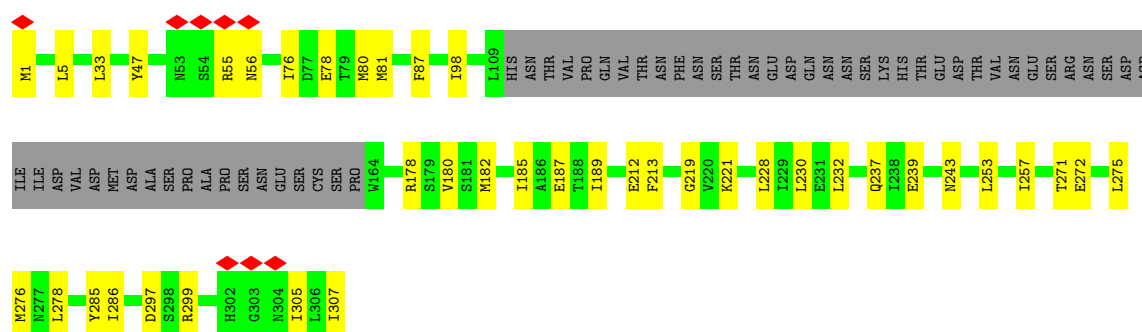


- Molecule 13: Mediator of RNA polymerase II transcription subunit 14

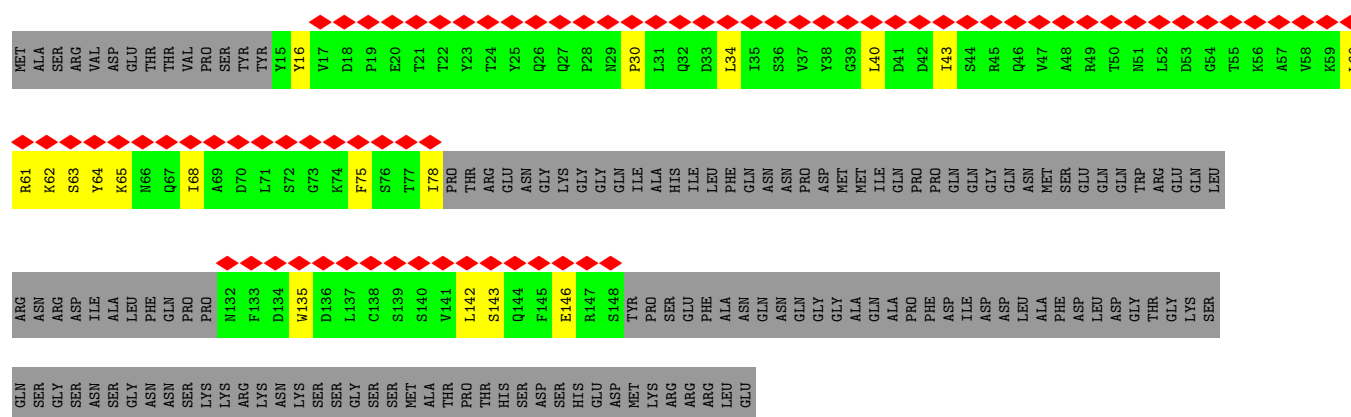




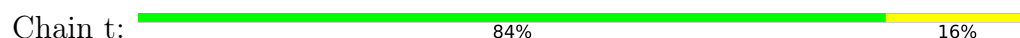
• Molecule 15: Mediator of RNA polymerase II transcription subunit 18

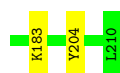


• Molecule 16: Mediator of RNA polymerase II transcription subunit 19

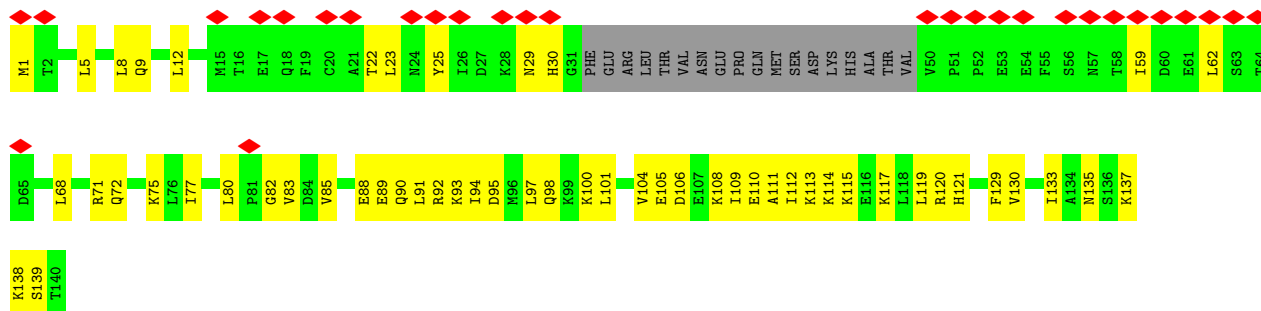


• Molecule 17: Mediator of RNA polymerase II transcription subunit 20

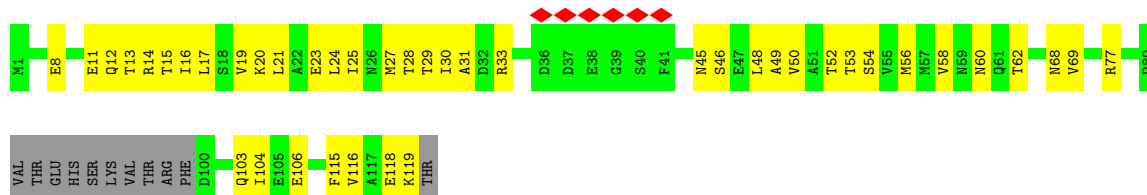




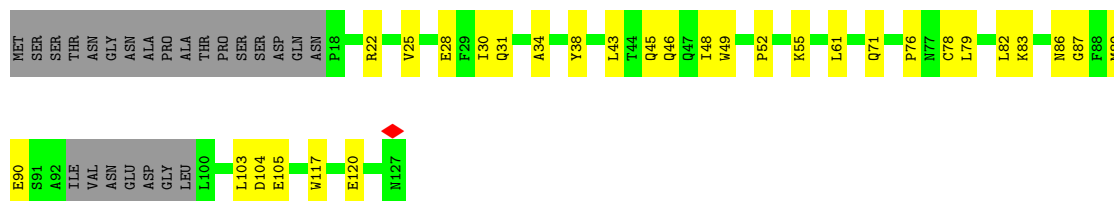
• Molecule 18: Mediator of RNA polymerase II transcription subunit 21



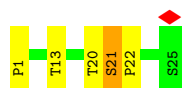
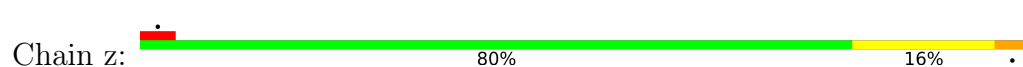
• Molecule 19: Mediator of RNA polymerase II transcription subunit 22



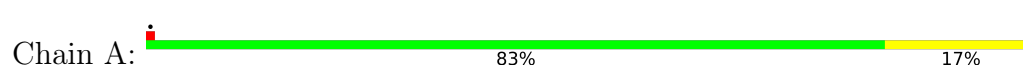
• Molecule 20: Mediator of RNA polymerase II transcription subunit 31

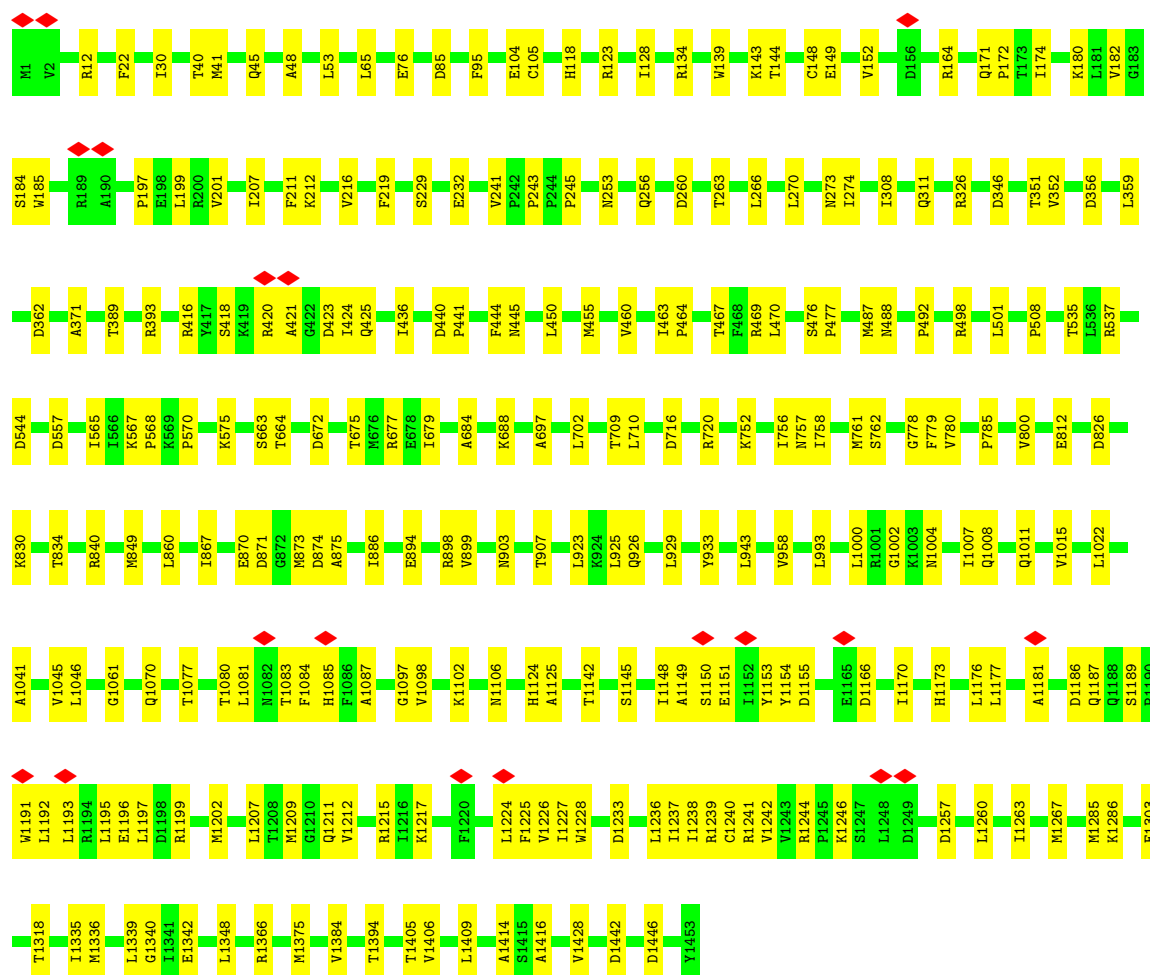


• Molecule 21: DNA-directed RNA polymerase II subunit RPB1



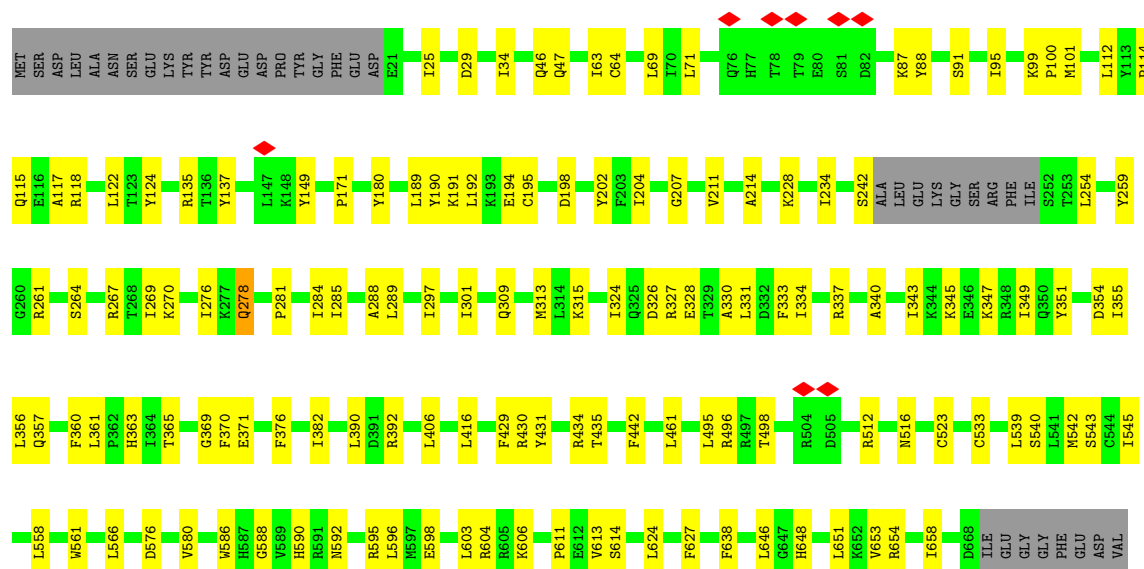
• Molecule 22: DNA-directed RNA polymerase II subunit RPB1

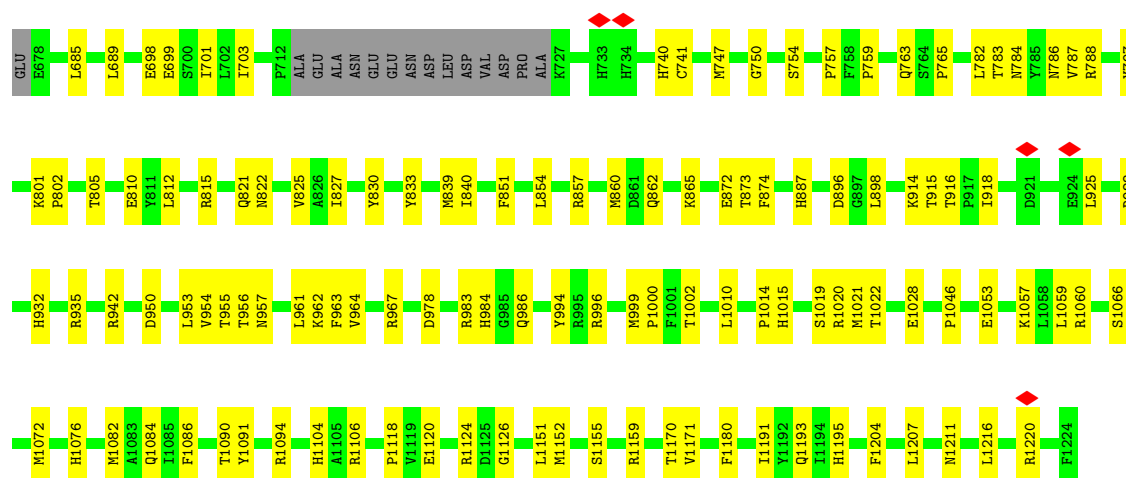




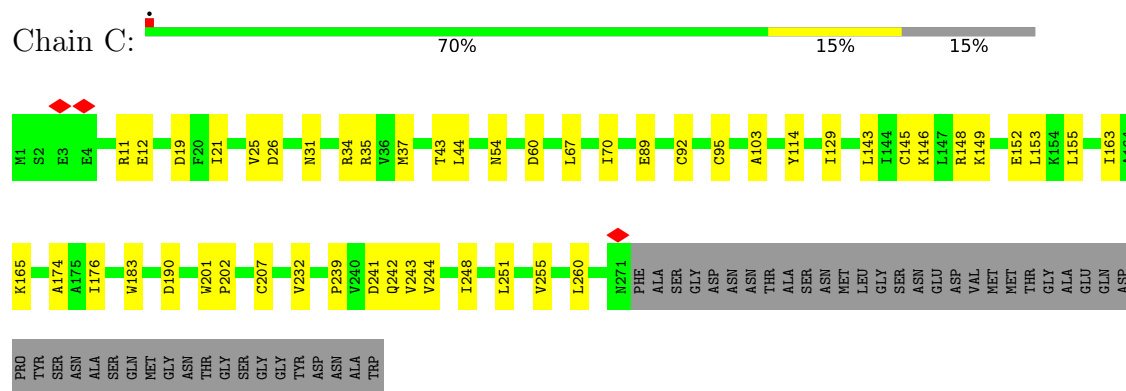
• Molecule 23: DNA-directed RNA polymerase II subunit RPB2

Chain B: 75% 21%

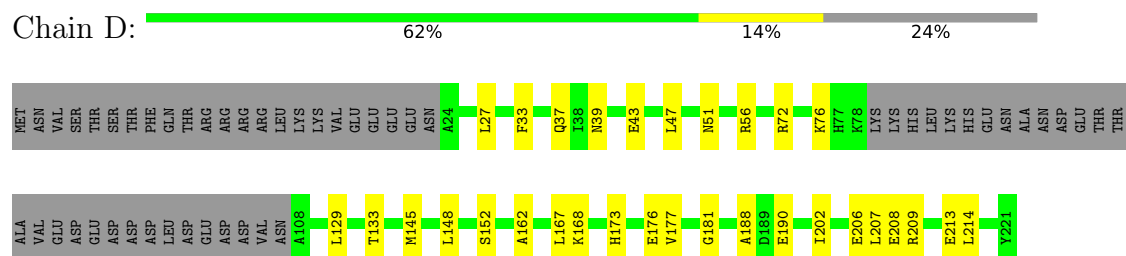




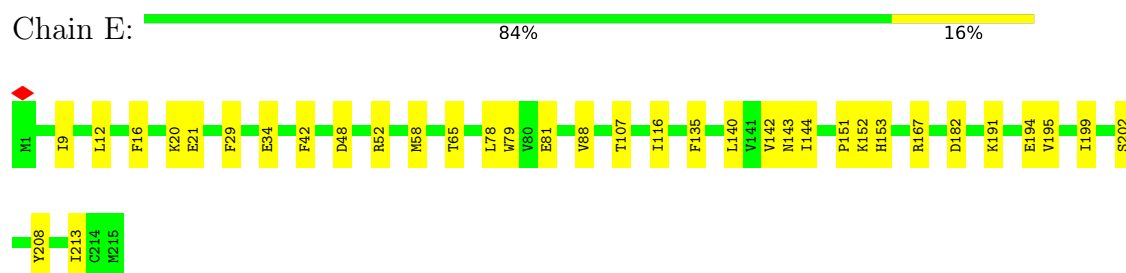
- Molecule 24: DNA-directed RNA polymerase II subunit RPB3



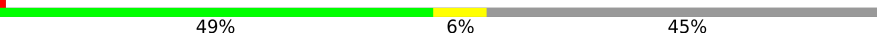
- Molecule 25: DNA-directed RNA polymerase II subunit RPB4



- Molecule 26: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 27: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 

MET SER ASP TYR GLU GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY GLU THR THR ASP ALA ASN GLY LYS THR ILE VAL THR THR GLY ASN GLY PRO GLU ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU K70 K71 K72 T81 T82 T83 V133 I134 Y137 S142 F143 E144 D145 V146 L155

- Molecule 28: DNA-directed RNA polymerase II subunit RPB7

Chain G: 

M1 D6 H14 P15 F18 L26 C38 T39 G43 Y44 I45 L46 I66 R75 V78 F79 K80 P81 E85 H97 G98 M106 K107 V108 F109 V110 T111 K112 M115 A123 N126 P127 P128 S133 I137 T138 I139 K140 I143 I147

A159 I163 Y167 L168 I171

- Molecule 29: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

M1 D8 T9 V12 A28 C36 K37 V44 P48 D67 THR PRO ALA ASN ASP S73 S74 A75 T76 R77 Q83 A90 G99 T100 A101 Y102 K103 A113 V114 Y115 Y116 S117 F118 L122 L125 E126 M133 N146

- Molecule 30: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

M1 T2 T3 F4 R6 L14 D19 K20 E21 N22 N23 R24 F27 Y34 Y35 E36 V43 Y44 R45 I49 T55 A56 G57 C75 S80 Q90 R91 R92 T95 N116 LYS ARG THR GLN PHE SER

- Molecule 31: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 

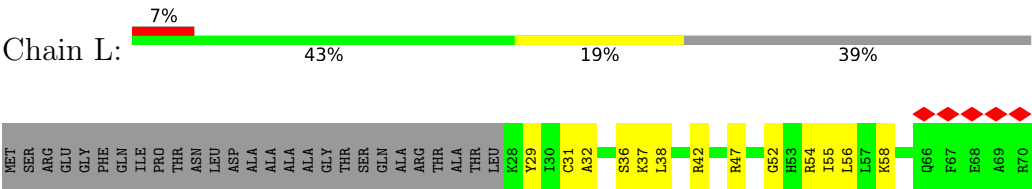
M1 I2 R6 C7 F8 K12 V13 K17 L36 S37 L41 C46 R47 R48 M49 I60 L51 R62 P65 L66 E67 K68 R69 D70

- Molecule 32: DNA-directed RNA polymerase II subunit RPB11

Chain K: 

M1 P4 L9 E14 L19 F35 H40 V56 T77 A100 N104 E108 Q112 A116 ASP ASP ALA PHE

- Molecule 33: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1102984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0125	Depositor
Map size ($\text{\AA}$)	496.8, 496.8, 496.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.14	0/267	0.27	0/362
2	P	0.11	0/886	0.24	0/1198
3	Q	0.10	0/1049	0.28	0/1413
4	S	0.13	0/1462	0.31	0/1973
5	a	0.67	0/3067	1.13	7/4148 (0.2%)
6	d	0.17	0/1405	0.51	0/1889
7	f	0.14	0/1440	0.35	0/1946
8	g	0.16	0/1434	0.41	1/1930 (0.1%)
9	h	0.16	0/1147	0.44	0/1552
10	i	0.21	0/720	0.53	0/965
11	j	0.12	0/1188	0.24	0/1604
12	k	0.16	0/885	0.44	0/1183
13	n	0.11	0/5226	0.28	0/7051
14	q	0.13	0/4245	0.33	0/5702
15	r	0.16	0/2030	0.33	0/2747
16	s	0.10	0/669	0.22	0/906
17	t	0.14	0/1635	0.32	0/2215
18	u	0.19	0/984	0.54	0/1317
19	v	0.17	0/873	0.46	0/1177
20	w	0.12	0/897	0.32	0/1219
21	z	0.15	0/194	0.36	0/270
22	A	0.17	0/11632	0.35	0/15735
23	B	0.17	0/9520	0.35	2/12839 (0.0%)
24	C	0.17	0/2171	0.35	0/2941
25	D	0.10	0/1365	0.21	0/1831
26	E	0.12	0/1796	0.27	0/2416
27	F	0.15	0/709	0.31	0/956
28	G	0.12	0/1368	0.30	0/1844
29	H	0.15	0/1144	0.32	0/1548
30	I	0.13	0/961	0.35	0/1294
31	J	0.18	0/587	0.45	0/786
32	K	0.18	0/947	0.35	0/1279
33	L	0.11	0/346	0.27	0/457
All	All	0.21	0/64249	0.42	10/86693 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	278	GLN	CA-C-N	5.82	132.65	121.54
23	B	278	GLN	C-N-CA	5.82	132.65	121.54
8	g	16	PRO	CA-N-CD	-5.58	104.19	112.00
5	a	298	PRO	CA-C-N	5.47	127.45	120.56
5	a	298	PRO	C-N-CA	5.47	127.45	120.56
5	a	529	GLN	OE1-CD-NE2	-5.46	117.14	122.60
5	a	324	ASN	OD1-CG-ND2	-5.10	117.50	122.60
5	a	22	LYS	CA-C-N	5.07	124.73	119.56
5	a	22	LYS	C-N-CA	5.07	124.73	119.56
5	a	225	GLN	OE1-CD-NE2	-5.01	117.59	122.60

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	M	263	0	273	2	0
2	P	861	0	819	22	0
3	Q	1033	0	1036	28	0
4	S	1436	0	1428	32	0
5	a	3008	0	2953	35	0
6	d	1388	0	1400	72	0
7	f	1407	0	1385	49	0
8	g	1409	0	1434	68	0
9	h	1126	0	1125	53	0
10	i	709	0	712	49	0
11	j	1173	0	1156	34	0
12	k	876	0	885	28	0
13	n	5139	0	5375	94	0
14	q	4182	0	4324	108	0
15	r	1995	0	2018	29	0
16	s	657	0	636	24	0
17	t	1609	0	1626	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	u	978	0	1005	53	0
19	v	869	0	881	44	0
20	w	871	0	857	21	0
21	z	184	0	163	6	0
22	A	11425	0	11482	210	0
23	B	9336	0	9341	211	0
24	C	2133	0	2096	37	0
25	D	1353	0	1352	23	0
26	E	1760	0	1788	23	0
27	F	697	0	720	7	0
28	G	1340	0	1357	23	0
29	H	1126	0	1094	14	0
30	I	943	0	906	17	0
31	J	578	0	593	30	0
32	K	929	0	939	11	0
33	L	344	0	367	11	0
All	All	63137	0	63526	1243	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 10.

All (1243) 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)
5:a:21:TYR:CE1	6:d:74:ILE:HG21	1.49	1.46
5:a:21:TYR:HE1	6:d:74:ILE:CG2	1.46	1.26
5:a:22:LYS:NZ	10:i:73:LEU:HD22	1.56	1.19
5:a:22:LYS:NZ	10:i:73:LEU:CD2	2.11	1.12
5:a:22:LYS:HD2	6:d:74:ILE:HD12	1.35	1.07
5:a:22:LYS:HZ3	10:i:73:LEU:HD22	0.93	1.05
5:a:21:TYR:CE1	6:d:74:ILE:CG2	2.31	0.98
23:B:115:GLN:HB3	31:J:69:ARG:HG2	1.42	0.98
5:a:22:LYS:HZ2	10:i:73:LEU:HD21	1.28	0.97
14:q:302:LEU:HG	14:q:306:HIS:HE1	1.29	0.97
5:a:22:LYS:HZ2	10:i:73:LEU:CD2	1.76	0.95
5:a:22:LYS:HD2	6:d:74:ILE:CD1	1.94	0.95
18:u:5:LEU:HG	18:u:9:GLN:HE22	1.41	0.85
22:A:185:TRP:O	22:A:197:PRO:HA	1.77	0.84
23:B:435:THR:HG21	23:B:442:PHE:HB3	1.61	0.83
9:h:42:GLN:HE21	25:D:162:ALA:HB2	1.44	0.82
3:Q:122:LEU:HD12	3:Q:222:CYS:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:302:LEU:HG	14:q:306:HIS:CE1	2.17	0.80
14:q:302:LEU:O	14:q:306:HIS:ND1	2.15	0.79
28:G:46:LEU:HD11	28:G:79:PHE:HB2	1.63	0.79
8:g:138:SER:HA	11:j:118:LEU:HD13	1.64	0.78
22:A:1193:LEU:HB3	22:A:1240:CYS:HB2	1.64	0.78
22:A:1217:LYS:HD2	22:A:1224:LEU:HD23	1.64	0.77
14:q:280:LYS:HB3	19:v:30:ILE:HG13	1.65	0.77
22:A:445:ASN:HD22	22:A:455:MET:HE2	1.50	0.76
22:A:849:MET:HE3	22:A:1061:GLY:HA2	1.68	0.76
22:A:800:VAL:HG22	22:A:812:GLU:HB2	1.67	0.75
22:A:346:ASP:OD1	23:B:1106:ARG:NH1	2.18	0.75
11:j:91:ARG:HB3	16:s:61:ARG:HB3	1.68	0.75
3:Q:238:GLU:HA	3:Q:241:ARG:HD2	1.69	0.74
23:B:118:ARG:NH1	23:B:207:GLY:O	2.20	0.74
23:B:276:ILE:HG12	23:B:334:ILE:HD12	1.70	0.74
23:B:788:ARG:NH1	31:J:70:ASP:OD1	2.21	0.74
6:d:97:LEU:HD13	6:d:100:ILE:HD11	1.70	0.73
7:f:25:GLU:HA	7:f:99:MET:HE1	1.70	0.73
10:i:73:LEU:HD23	10:i:77:ARG:HE	1.52	0.73
12:k:19:GLN:HE22	12:k:61:LYS:HG3	1.53	0.73
28:G:112:LYS:HA	28:G:115:MET:HE3	1.70	0.73
10:i:105:ILE:O	10:i:112:LYS:NZ	2.22	0.72
18:u:94:ILE:O	18:u:98:GLN:NE2	2.23	0.72
28:G:81:PRO:HD3	28:G:106:MET:HE1	1.72	0.72
9:h:146:GLU:HG3	9:h:150:GLN:HE22	1.55	0.72
15:r:1:MET:HA	15:r:185:ILE:O	1.89	0.72
6:d:53:LEU:HD22	10:i:98:LEU:HD12	1.69	0.72
10:i:123:GLN:O	10:i:127:HIS:ND1	2.22	0.72
5:a:22:LYS:NZ	10:i:73:LEU:HD21	1.93	0.72
10:i:105:ILE:HD12	10:i:115:LEU:HD11	1.69	0.71
3:Q:63:ARG:NH1	3:Q:214:ILE:O	2.20	0.71
23:B:496:ARG:NH2	23:B:540:SER:O	2.23	0.71
23:B:118:ARG:NE	31:J:70:ASP:OD2	2.23	0.71
23:B:114:PRO:HG2	31:J:69:ARG:HD3	1.71	0.71
10:i:92:GLY:HA2	10:i:95:ARG:HE	1.55	0.71
14:q:119:LEU:HD21	14:q:124:LEU:HD13	1.73	0.71
23:B:281:PRO:HD2	23:B:284:ILE:HD12	1.72	0.71
24:C:54:ASN:ND2	24:C:60:ASP:OD1	2.23	0.71
2:P:377:SER:OG	2:P:385:THR:OG1	2.08	0.71
23:B:651:LEU:O	23:B:654:ARG:NH2	2.24	0.70
31:J:37:SER:OG	31:J:47:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:298:THR:HG23	4:S:305:ARG:HG2	1.73	0.70
6:d:45:ASP:OD2	6:d:83:ASN:ND2	2.24	0.70
5:a:21:TYR:HE1	6:d:74:ILE:HG21	0.60	0.70
23:B:261:ARG:O	23:B:267:ARG:NH2	2.25	0.70
23:B:786:ASN:O	23:B:967:ARG:NH1	2.23	0.70
4:S:287:ARG:HA	22:A:1081:LEU:HD13	1.73	0.69
11:j:91:ARG:N	16:s:63:SER:OG	2.24	0.69
17:t:32:ARG:HD2	17:t:131:ILE:HD11	1.74	0.69
22:A:1084:PHE:O	22:A:1087:ALA:HB3	1.92	0.69
14:q:421:GLU:HG2	14:q:427:LYS:HD3	1.74	0.69
18:u:117:LYS:O	18:u:121:HIS:ND1	2.23	0.69
24:C:92:CYS:HB2	24:C:95:CYS:H	1.57	0.69
15:r:228:LEU:HD21	15:r:278:LEU:HD22	1.73	0.69
7:f:46:ILE:HD13	7:f:106:GLU:HG3	1.74	0.69
23:B:288:ALA:HA	23:B:327:ARG:HG3	1.73	0.69
23:B:703:ILE:HG22	23:B:740:HIS:HB2	1.74	0.69
22:A:41:MET:HA	22:A:48:ALA:HA	1.74	0.68
24:C:145:CYS:SG	24:C:146:LYS:N	2.64	0.68
13:n:484:LEU:HD22	13:n:491:GLU:HG2	1.75	0.68
19:v:11:GLU:HA	19:v:14:ARG:HG2	1.75	0.68
23:B:810:GLU:OE1	23:B:815:ARG:NH1	2.27	0.68
8:g:111:ASN:OD1	8:g:115:LYS:NZ	2.25	0.68
21:z:1:PRO:H3	25:D:168:LYS:HD2	1.58	0.68
23:B:189:LEU:HB3	23:B:194:GLU:HB2	1.74	0.68
8:g:23:PHE:HA	8:g:27:ASN:HD22	1.58	0.67
22:A:440:ASP:OD1	22:A:498:ARG:NH1	2.27	0.67
23:B:34:ILE:HG21	23:B:747:MET:HE3	1.76	0.67
19:v:12:GLN:HE22	19:v:16:ILE:HD11	1.58	0.67
30:I:92:ARG:HB3	30:I:95:THR:HG23	1.75	0.67
22:A:40:THR:HG22	22:A:53:LEU:HB2	1.75	0.67
31:J:13:VAL:O	31:J:17:LYS:NZ	2.28	0.67
8:g:166:ARG:O	8:g:169:GLN:N	2.28	0.67
23:B:604:ARG:NH1	23:B:613:VAL:O	2.28	0.67
2:P:130:VAL:HG23	2:P:131:THR:HG23	1.77	0.67
18:u:90:GLN:HA	18:u:93:LYS:HG2	1.76	0.67
22:A:535:THR:O	22:A:575:LYS:NZ	2.24	0.67
17:t:13:THR:HG1	17:t:16:THR:HG1	1.39	0.66
23:B:278:GLN:OE1	23:B:337:ARG:NH1	2.27	0.66
23:B:264:SER:O	23:B:267:ARG:NH1	2.27	0.66
26:E:78:LEU:HD13	26:E:107:THR:HG23	1.78	0.66
5:a:312:ILE:HD11	5:a:565:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:39:ASN:HB2	28:G:75:ARG:HH22	1.61	0.66
9:h:39:ARG:HH11	9:h:79:VAL:HG22	1.60	0.66
13:n:113:THR:O	13:n:117:THR:OG1	2.13	0.66
9:h:146:GLU:O	9:h:150:GLN:NE2	2.28	0.66
15:r:285:TYR:HB3	15:r:286:ILE:HD12	1.77	0.66
22:A:758:ILE:O	22:A:762:SER:OG	2.11	0.66
18:u:68:LEU:O	18:u:71:ARG:HG3	1.96	0.66
20:w:34:ALA:HB2	20:w:78:CYS:HB3	1.78	0.66
22:A:1260:LEU:HA	22:A:1263:ILE:HG12	1.77	0.65
2:P:132:ASP:O	2:P:359:ASN:ND2	2.29	0.65
22:A:830:LYS:HD3	22:A:1080:THR:HB	1.78	0.65
23:B:264:SER:OG	23:B:267:ARG:NH2	2.27	0.65
4:S:166:HIS:HE1	4:S:170:SER:HB3	1.60	0.65
22:A:393:ARG:NH1	22:A:421:ALA:O	2.27	0.65
23:B:822:ASN:O	31:J:48:ARG:NH1	2.29	0.65
2:P:129:PRO:HG2	3:Q:61:LEU:HD21	1.79	0.65
4:S:169:GLN:O	4:S:173:HIS:ND1	2.29	0.65
8:g:143:MET:HE2	8:g:146:ARG:HD2	1.77	0.65
13:n:290:THR:HB	13:n:297:LEU:HD23	1.79	0.65
22:A:779:PHE:HE2	22:A:785:PRO:HG3	1.62	0.65
23:B:872:GLU:HG3	23:B:916:THR:HG22	1.79	0.65
6:d:33:SER:O	6:d:37:LEU:HG	1.97	0.65
9:h:39:ARG:HD2	9:h:79:VAL:HA	1.79	0.65
23:B:984:HIS:NE2	23:B:1028:GLU:OE1	2.24	0.65
2:P:375:LEU:HB2	2:P:387:ILE:HB	1.78	0.65
7:f:100:TYR:HA	7:f:103:LEU:HD12	1.78	0.65
14:q:455:TYR:HB3	14:q:550:ARG:HH12	1.62	0.65
23:B:276:ILE:HG23	23:B:337:ARG:HE	1.62	0.65
6:d:167:PRO:HG2	6:d:170:PHE:HB2	1.78	0.64
23:B:763:GLN:HG2	23:B:765:PRO:HD2	1.78	0.64
23:B:994:TYR:HB2	23:B:999:MET:HE3	1.78	0.64
23:B:354:ASP:OD1	23:B:357:GLN:NE2	2.30	0.64
6:d:114:ILE:HG23	8:g:206:ILE:HD13	1.80	0.64
9:h:37:ARG:HG2	14:q:225:VAL:HG13	1.80	0.64
13:n:386:PHE:HE1	13:n:464:ILE:HG12	1.62	0.64
8:g:189:ILE:HG12	18:u:108:LYS:HE3	1.80	0.64
22:A:1102:LYS:O	22:A:1106:ASN:ND2	2.30	0.64
23:B:69:LEU:HD21	23:B:429:PHE:HB2	1.79	0.64
28:G:108:VAL:HG22	28:G:159:ALA:HB3	1.79	0.64
1:M:36:GLU:O	23:B:887:HIS:NE2	2.31	0.64
2:P:108:LYS:HD3	3:Q:84:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:184:SER:HB2	22:A:197:PRO:HB2	1.80	0.64
22:A:229:SER:OG	22:A:1414:ALA:O	2.14	0.64
3:Q:67:GLN:HB3	3:Q:219:CYS:HB3	1.79	0.63
9:h:51:ARG:HG3	14:q:215:MET:HE1	1.79	0.63
11:j:118:LEU:HD23	11:j:121:LEU:HD12	1.80	0.63
22:A:1154:TYR:HB2	30:I:43:VAL:HG22	1.80	0.63
23:B:986:GLN:OE1	23:B:1020:ARG:NH1	2.31	0.63
5:a:22:LYS:HB3	10:i:77:ARG:HD3	1.81	0.63
5:a:103:ILE:HD11	5:a:191:ASN:HB3	1.79	0.63
8:g:112:TYR:HA	8:g:115:LYS:HE2	1.81	0.63
14:q:397:ILE:HG22	14:q:399:SER:H	1.64	0.63
11:j:15:LEU:HD13	13:n:152:ARG:HA	1.80	0.62
12:k:67:ARG:NH1	12:k:71:GLN:OE1	2.32	0.62
13:n:414:ARG:NH1	13:n:415:TYR:O	2.32	0.62
22:A:352:VAL:HG23	22:A:467:THR:HG22	1.82	0.62
12:k:24:LEU:HD11	19:v:69:VAL:HG11	1.81	0.62
6:d:189:ARG:NH1	8:g:12:LEU:O	2.33	0.62
23:B:315:LYS:HB2	30:I:4:PHE:HZ	1.63	0.62
20:w:43:LEU:HB3	20:w:103:LEU:HD13	1.81	0.62
22:A:716:ASP:OD2	22:A:720:ARG:NH2	2.32	0.62
22:A:757:ASN:O	22:A:761:MET:HG3	1.99	0.62
4:S:153:LEU:HD21	4:S:179:GLU:HB3	1.82	0.62
6:d:185:GLU:OE2	6:d:189:ARG:NH1	2.33	0.62
23:B:63:ILE:HD13	23:B:95:ILE:HD11	1.82	0.62
9:h:98:LEU:HB2	9:h:101:PHE:HB2	1.82	0.62
9:h:73:LEU:HG	19:v:56:MET:SD	2.39	0.62
22:A:243:PRO:HB2	22:A:245:PRO:HD2	1.81	0.62
23:B:1152:MET:HE1	23:B:1195:HIS:HB3	1.80	0.61
4:S:163:GLU:O	4:S:215:LYS:NZ	2.30	0.61
23:B:91:SER:HB3	23:B:135:ARG:HH22	1.63	0.61
18:u:72:GLN:HG3	18:u:75:LYS:HE3	1.82	0.61
22:A:757:ASN:HD22	23:B:1021:MET:HE2	1.64	0.61
22:A:1207:LEU:HD11	22:A:1212:VAL:HG11	1.83	0.61
6:d:95:ARG:HB3	6:d:99:LYS:NZ	2.16	0.61
10:i:137:ARG:HH21	10:i:140:LEU:HD12	1.64	0.61
24:C:35:ARG:NH1	32:K:40:HIS:HB2	2.16	0.61
29:H:8:ASP:OD1	29:H:9:ILE:N	2.33	0.61
14:q:539:ILE:O	14:q:543:ARG:NH1	2.33	0.61
23:B:289:LEU:HD22	23:B:371:GLU:OE2	2.00	0.61
22:A:830:LYS:HB3	22:A:1080:THR:HG21	1.81	0.61
22:A:1339:LEU:HD23	26:E:144:ILE:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:177:LEU:HA	8:g:180:GLU:HG2	1.82	0.61
23:B:950:ASP:OD2	23:B:967:ARG:NH2	2.33	0.61
7:f:44:GLN:HG3	7:f:48:MET:HE1	1.81	0.61
19:v:25:ILE:O	19:v:29:THR:HG22	2.01	0.61
22:A:1083:THR:HG23	22:A:1097:GLY:HA3	1.81	0.61
7:f:129:ARG:HH12	7:f:149:PRO:HA	1.66	0.60
12:k:25:GLN:O	12:k:28:SER:OG	2.12	0.60
20:w:86:ASN:O	20:w:89:MET:HG3	2.00	0.60
22:A:1224:LEU:HD11	22:A:1240:CYS:HB3	1.83	0.60
23:B:898:LEU:O	33:L:58:LYS:NZ	2.34	0.60
23:B:1082:MET:HE2	24:C:190:ASP:HB2	1.82	0.60
7:f:189:TYR:HA	7:f:192:ILE:HD12	1.82	0.60
11:j:91:ARG:HB3	16:s:62:LYS:H	1.66	0.60
20:w:43:LEU:HD23	20:w:103:LEU:HB2	1.82	0.60
23:B:955:THR:HG22	33:L:55:ILE:HA	1.81	0.60
22:A:1211:GLN:HE22	22:A:1215:ARG:HH21	1.50	0.60
23:B:117:ALA:HA	23:B:122:LEU:HB2	1.81	0.60
7:f:177:THR:HG23	14:q:214:ALA:HB1	1.82	0.60
14:q:612:ILE:O	14:q:614:ARG:NH1	2.34	0.60
2:P:141:ARG:NH1	2:P:345:GLU:O	2.35	0.60
12:k:96:GLU:OE2	12:k:97:LYS:NZ	2.26	0.60
15:r:221:LYS:NZ	17:t:93:PHE:O	2.31	0.60
22:A:182:VAL:HG22	22:A:201:VAL:HG12	1.84	0.60
22:A:1195:LEU:HB3	22:A:1197:LEU:HD21	1.84	0.60
23:B:874:PHE:HD2	23:B:962:LYS:HD2	1.67	0.60
5:a:177:GLN:HE22	5:a:235:GLN:CG	2.14	0.60
15:r:56:ASN:OD1	22:A:416:ARG:NH2	2.35	0.60
8:g:155:LEU:HD23	8:g:158:ILE:HD12	1.84	0.59
22:A:1173:HIS:HA	22:A:1176:LEU:HB2	1.84	0.59
23:B:254:LEU:HD22	23:B:361:LEU:HD11	1.84	0.59
7:f:10:GLN:NE2	21:z:20:THR:OG1	2.35	0.59
13:n:498:VAL:HG22	13:n:516:LYS:HG2	1.83	0.59
18:u:101:LEU:HA	18:u:104:VAL:HG12	1.85	0.59
23:B:787:VAL:HG11	31:J:68:LYS:H	1.67	0.59
18:u:135:ASN:O	18:u:139:SER:OG	2.19	0.59
23:B:25:ILE:HG23	23:B:29:ASP:HB2	1.84	0.59
14:q:549:VAL:HG22	19:v:119:LYS:HD2	1.83	0.59
5:a:22:LYS:HZ3	10:i:73:LEU:CD2	1.78	0.59
22:A:1348:LEU:HD21	22:A:1375:MET:HE3	1.83	0.59
23:B:862:GLN:OE1	23:B:957:ASN:ND2	2.36	0.59
30:I:19:ASP:O	30:I:23:ASN:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:L:31:CYS:HB3	33:L:36:SER:H	1.67	0.59
8:g:128:LEU:HD13	11:j:136:LEU:HD12	1.83	0.59
13:n:734:GLN:NE2	13:n:805:GLU:OE2	2.35	0.59
20:w:76:PRO:O	20:w:79:LEU:HB2	2.02	0.59
23:B:1120:GLU:O	23:B:1124:ARG:NH2	2.36	0.59
31:J:41:LEU:HD22	31:J:46:CYS:HB3	1.85	0.59
22:A:149:GLU:O	22:A:164:ARG:NE	2.36	0.58
22:A:441:PRO:HG2	22:A:498:ARG:HG2	1.84	0.58
23:B:137:TYR:HB3	23:B:149:TYR:HB3	1.85	0.58
3:Q:104:ILE:HB	3:Q:122:LEU:HB2	1.84	0.58
6:d:97:LEU:HD12	10:i:125:ILE:HG22	1.85	0.58
10:i:101:CYS:O	10:i:105:ILE:HG12	2.02	0.58
15:r:257:ILE:HD12	15:r:271:THR:HG23	1.86	0.58
23:B:431:TYR:HA	23:B:434:ARG:HD2	1.85	0.58
23:B:1090:THR:HG22	23:B:1091:TYR:H	1.68	0.58
12:k:93:GLN:O	12:k:96:GLU:HG3	2.03	0.58
6:d:98:GLN:HB3	6:d:102:LYS:NZ	2.18	0.58
14:q:392:ARG:HG2	14:q:408:GLU:HG3	1.85	0.58
6:d:139:ASN:O	6:d:142:LEU:HG	2.04	0.58
17:t:28:ILE:HA	17:t:132:LEU:HD23	1.86	0.58
22:A:1191:TRP:CD1	22:A:1260:LEU:HD21	2.39	0.58
23:B:194:GLU:OE1	31:J:69:ARG:HB2	2.04	0.58
23:B:956:THR:OG1	33:L:54:ARG:NH2	2.36	0.58
18:u:110:GLU:HA	18:u:113:LYS:HG2	1.85	0.58
7:f:108:MET:SD	7:f:133:ARG:NH1	2.77	0.58
22:A:840:ARG:NH1	22:A:1384:VAL:O	2.30	0.58
22:A:1125:ALA:HB1	22:A:1303:GLU:HG3	1.84	0.58
24:C:163:ILE:HG13	24:C:165:LYS:H	1.68	0.58
11:j:117:GLY:O	11:j:121:LEU:HG	2.04	0.58
28:G:163:ILE:HG22	28:G:168:LEU:HD22	1.84	0.58
8:g:188:GLU:O	8:g:191:GLU:HG3	2.04	0.57
13:n:508:VAL:HG12	13:n:681:GLU:HB3	1.85	0.57
26:E:20:LYS:HE3	26:E:34:GLU:HG2	1.84	0.57
4:S:131:PRO:O	4:S:136:ASN:ND2	2.35	0.57
22:A:423:ASP:O	22:A:425:GLN:NE2	2.36	0.57
24:C:12:GLU:HB2	24:C:19:ASP:HB3	1.85	0.57
23:B:603:LEU:HA	23:B:606:LYS:HG2	1.85	0.57
12:k:24:LEU:HD21	19:v:69:VAL:HG21	1.86	0.57
13:n:772:ASP:O	13:n:776:SER:N	2.37	0.57
22:A:1209:MET:HE1	22:A:1236:LEU:HB3	1.87	0.57
22:A:1153:TYR:OH	30:I:45:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1226:VAL:HG12	22:A:1228:TRP:HD1	1.70	0.57
22:A:241:VAL:HG22	22:A:266:LEU:HD21	1.86	0.57
23:B:797:TYR:HE1	23:B:854:LEU:HG	1.69	0.57
23:B:896:ASP:OD2	33:L:29:TYR:OH	2.22	0.57
28:G:137:ILE:HG21	28:G:143:ILE:HD12	1.85	0.57
9:h:38:MET:HE3	25:D:213:GLU:HB3	1.87	0.57
22:A:993:LEU:HD22	22:A:1022:LEU:HD11	1.87	0.57
7:f:197:SER:HA	19:v:77:ARG:HH22	1.70	0.57
20:w:46:GLN:OE1	20:w:49:TRP:NE1	2.38	0.57
23:B:586:TRP:NE1	23:B:588:GLY:O	2.34	0.57
13:n:171:THR:HA	13:n:174:MET:SD	2.45	0.57
13:n:652:GLU:OE1	13:n:654:ARG:NH2	2.38	0.57
18:u:5:LEU:O	18:u:9:GLN:NE2	2.37	0.57
23:B:558:LEU:HD21	23:B:580:VAL:HG11	1.87	0.57
14:q:634:MET:SD	14:q:646:HIS:HB3	2.44	0.57
10:i:75:GLN:HG2	10:i:90:LEU:HD11	1.87	0.56
5:a:22:LYS:HD2	6:d:74:ILE:HD11	1.85	0.56
19:v:24:LEU:HD23	19:v:27:MET:HE2	1.86	0.56
23:B:34:ILE:HG12	23:B:542:MET:HE1	1.86	0.56
32:K:100:ALA:O	32:K:104:ASN:ND2	2.27	0.56
7:f:200:VAL:HB	9:h:62:TRP:CE3	2.41	0.56
9:h:156:THR:HG23	19:v:28:THR:HB	1.88	0.56
13:n:502:GLN:HB3	13:n:510:MET:HE3	1.86	0.56
13:n:661:GLN:OE1	13:n:666:ASN:ND2	2.35	0.56
23:B:333:PHE:HB3	23:B:337:ARG:HH22	1.69	0.56
26:E:21:GLU:OE1	26:E:143:ASN:ND2	2.39	0.56
25:D:167:LEU:HD21	25:D:214:LEU:HD11	1.87	0.56
10:i:68:HIS:HB3	10:i:97:ARG:HH11	1.69	0.56
22:A:118:HIS:O	22:A:123:ARG:NH2	2.38	0.56
23:B:827:ILE:HG22	23:B:1014:PRO:HG3	1.88	0.56
33:L:47:ARG:NH2	33:L:52:GLY:O	2.39	0.56
22:A:172:PRO:HG3	22:A:185:TRP:NE1	2.21	0.56
23:B:918:ILE:HD11	23:B:935:ARG:HB2	1.87	0.56
28:G:85:GLU:O	28:G:147:ILE:N	2.36	0.56
6:d:104:SER:OG	10:i:136:LYS:NZ	2.38	0.56
22:A:128:ILE:O	22:A:134:ARG:NH2	2.38	0.56
22:A:149:GLU:H	22:A:164:ARG:HH21	1.54	0.56
24:C:25:VAL:HG12	24:C:26:ASP:O	2.06	0.56
14:q:500:ARG:HD2	19:v:118:GLU:HG3	1.86	0.56
26:E:195:VAL:HG22	26:E:213:ILE:HG22	1.88	0.56
23:B:1002:THR:HG22	23:B:1072:MET:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:166:ILE:HG12	14:q:224:PHE:CE2	2.41	0.55
24:C:92:CYS:HB2	24:C:95:CYS:N	2.21	0.55
23:B:46:GLN:HG2	23:B:47:GLN:N	2.21	0.55
20:w:104:ASP:OD1	20:w:105:GLU:N	2.40	0.55
22:A:779:PHE:HB3	23:B:699:GLU:OE2	2.05	0.55
22:A:899:VAL:HG13	22:A:929:LEU:HD13	1.88	0.55
22:A:1239:ARG:HD3	22:A:1241:ARG:HH21	1.71	0.55
31:J:12:LYS:HG2	31:J:13:VAL:H	1.71	0.55
2:P:354:ASP:OD1	2:P:355:PHE:N	2.39	0.55
9:h:98:LEU:HD13	9:h:100:LYS:HE3	1.89	0.55
13:n:515:LEU:HD11	13:n:524:PHE:HB3	1.89	0.55
27:F:72:LYS:HB3	27:F:142:SER:HA	1.89	0.55
28:G:163:ILE:HA	28:G:168:LEU:HD13	1.88	0.55
7:f:196:PRO:O	19:v:77:ARG:NH2	2.39	0.55
13:n:263:PRO:HD2	13:n:266:LEU:HD12	1.88	0.55
20:w:30:ILE:HD11	20:w:61:LEU:HD22	1.89	0.55
27:F:144:GLU:HG2	27:F:146:TRP:HE1	1.71	0.55
6:d:45:ASP:HB3	6:d:80:LEU:HD23	1.89	0.55
20:w:83:LYS:O	20:w:86:ASN:HB2	2.06	0.55
14:q:633:LEU:HD22	14:q:647:ILE:HG12	1.89	0.55
23:B:376:PHE:HD2	23:B:566:LEU:HG	1.72	0.55
23:B:750:GLY:O	23:B:754:SER:OG	2.25	0.55
6:d:48:ARG:NH1	6:d:76:THR:HB	2.22	0.54
7:f:121:ARG:HH21	9:h:99:PRO:HA	1.72	0.54
17:t:43:ARG:HH22	24:C:89:GLU:HB2	1.71	0.54
23:B:954:VAL:HG12	23:B:964:VAL:HG12	1.89	0.54
2:P:100:GLU:HG3	3:Q:94:LYS:HD2	1.89	0.54
13:n:275:ARG:NH2	14:q:118:ASP:OD1	2.40	0.54
22:A:675:THR:O	22:A:679:ILE:HG12	2.07	0.54
23:B:862:GLN:HB3	23:B:963:PHE:HD1	1.72	0.54
11:j:106:ARG:NH2	11:j:109:GLN:OE1	2.37	0.54
9:h:43:LEU:HD22	9:h:79:VAL:HG21	1.89	0.54
13:n:530:THR:HG23	13:n:533:LEU:HD12	1.89	0.54
23:B:351:TYR:O	23:B:355:ILE:HG12	2.06	0.54
18:u:137:LYS:HD2	18:u:138:LYS:HE3	1.88	0.54
19:v:54:SER:O	19:v:58:VAL:HG23	2.06	0.54
22:A:76:GLU:OE2	23:B:1159:ARG:NH2	2.28	0.54
23:B:214:ALA:HB3	23:B:498:THR:HG22	1.90	0.54
4:S:149:ARG:NH2	4:S:179:GLU:OE1	2.41	0.54
4:S:292:PRO:HD3	23:B:1019:SER:HB3	1.88	0.54
8:g:14:PRO:HD2	20:w:38:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:507:MET:HG3	14:q:545:ILE:HD11	1.90	0.54
15:r:187:GLU:OE1	17:t:98:THR:OG1	2.22	0.54
22:A:1148:ILE:HG13	30:I:49:ILE:HD11	1.88	0.54
28:G:123:ALA:HA	28:G:128:PRO:HB3	1.89	0.54
8:g:150:ASN:O	8:g:153:THR:OG1	2.15	0.54
23:B:1204:PHE:HE2	23:B:1216:LEU:HD21	1.73	0.54
22:A:1193:LEU:HD22	22:A:1267:MET:HE1	1.90	0.54
23:B:611:PRO:HG3	23:B:685:LEU:HD21	1.89	0.54
23:B:1151:LEU:O	23:B:1155:SER:OG	2.26	0.54
24:C:165:LYS:HE2	32:K:9:LEU:HB3	1.89	0.54
23:B:228:LYS:HE3	23:B:234:ILE:HG21	1.90	0.54
26:E:48:ASP:OD1	26:E:52:ARG:N	2.40	0.54
14:q:222:LEU:HA	14:q:225:VAL:HG12	1.89	0.53
23:B:324:ILE:HG22	23:B:326:ASP:H	1.72	0.53
3:Q:245:LYS:HG3	3:Q:246:LEU:HD12	1.91	0.53
8:g:178:LEU:O	8:g:182:LEU:HD23	2.09	0.53
18:u:94:ILE:HG22	18:u:98:GLN:HE22	1.73	0.53
6:d:189:ARG:HH22	8:g:14:PRO:HD3	1.73	0.53
22:A:1217:LYS:HZ3	22:A:1226:VAL:HG23	1.73	0.53
6:d:132:GLU:O	6:d:135:GLU:HG3	2.09	0.53
8:g:119:LEU:HD13	8:g:161:LEU:HD23	1.89	0.53
4:S:181:GLU:HA	4:S:184:LYS:HG2	1.90	0.53
14:q:500:ARG:HE	19:v:115:PHE:HE1	1.56	0.53
18:u:110:GLU:HG3	18:u:113:LYS:NZ	2.24	0.53
19:v:56:MET:HE3	19:v:60:ASN:HD21	1.73	0.53
22:A:1149:ALA:HB1	22:A:1151:GLU:CD	2.34	0.53
24:C:244:VAL:O	24:C:248:ILE:HG13	2.08	0.53
30:I:55:THR:HG22	30:I:57:GLY:H	1.73	0.53
13:n:161:VAL:HB	16:s:43:ILE:HD12	1.90	0.53
15:r:178:ARG:HD2	15:r:182:MET:HE3	1.91	0.53
19:v:12:GLN:NE2	19:v:68:ASN:HB3	2.23	0.53
22:A:1080:THR:HG22	22:A:1098:VAL:HG21	1.90	0.53
22:A:1189:SER:HA	22:A:1244:ARG:HH22	1.72	0.53
22:A:1342:GLU:OE2	26:E:153:HIS:NE2	2.40	0.53
23:B:996:ARG:NH2	24:C:174:ALA:O	2.42	0.53
7:f:169:ILE:HG12	9:h:116:LYS:HB3	1.90	0.53
10:i:72:SER:HB3	10:i:90:LEU:HD21	1.91	0.53
23:B:328:GLU:N	23:B:328:GLU:OE1	2.42	0.53
29:H:36:CYS:HA	29:H:126:GLU:O	2.09	0.53
31:J:36:LEU:HD11	31:J:51:LEU:HD13	1.91	0.53
9:h:42:GLN:HG3	9:h:75:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:k:100:GLU:OE2	12:k:101:GLN:NE2	2.41	0.53
23:B:523:CYS:SG	23:B:750:GLY:N	2.75	0.53
23:B:1053:GLU:O	23:B:1057:LYS:HG2	2.09	0.53
9:h:42:GLN:NE2	25:D:162:ALA:HB2	2.20	0.53
14:q:392:ARG:NH1	14:q:477:GLU:OE1	2.41	0.53
14:q:394:PHE:HB3	14:q:403:TYR:HB3	1.91	0.53
22:A:544:ASP:N	22:A:544:ASP:OD1	2.41	0.53
22:A:1242:VAL:O	22:A:1244:ARG:NH1	2.42	0.53
25:D:206:GLU:OE1	25:D:209:ARG:NH2	2.33	0.53
33:L:31:CYS:SG	33:L:32:ALA:N	2.82	0.53
11:j:114:LYS:HZ1	13:n:176:VAL:HG11	1.74	0.53
12:k:97:LYS:O	12:k:100:GLU:HG3	2.09	0.53
23:B:787:VAL:HG21	31:J:68:LYS:H	1.74	0.53
25:D:168:LYS:HG3	25:D:177:VAL:HG11	1.91	0.53
8:g:162:LEU:HD22	8:g:166:ARG:HH22	1.74	0.52
10:i:74:HIS:HA	10:i:77:ARG:HG2	1.90	0.52
24:C:251:LEU:O	24:C:255:VAL:HG23	2.09	0.52
8:g:185:LYS:HE3	18:u:105:GLU:OE2	2.09	0.52
14:q:305:GLU:HA	14:q:308:TYR:CD1	2.44	0.52
18:u:111:ALA:HA	18:u:114:LYS:NZ	2.24	0.52
23:B:614:SER:OG	23:B:627:PHE:HB2	2.10	0.52
6:d:57:VAL:HA	6:d:60:VAL:HG22	1.91	0.52
23:B:646:LEU:HB3	23:B:648:HIS:CE1	2.44	0.52
13:n:489:PHE:HD2	13:n:499:LEU:HD13	1.74	0.52
14:q:199:GLN:HB2	14:q:203:ARG:HH21	1.74	0.52
18:u:112:ILE:HA	18:u:115:LYS:HE2	1.91	0.52
22:A:663:SER:OG	22:A:664:THR:N	2.42	0.52
22:A:697:ALA:HB2	22:A:702:LEU:HD13	1.91	0.52
23:B:115:GLN:OE1	31:J:67:GLU:HB3	2.10	0.52
23:B:865:LYS:HB2	23:B:961:LEU:HD21	1.91	0.52
23:B:978:ASP:OD2	23:B:1094:ARG:NH2	2.33	0.52
17:t:70:VAL:HG22	17:t:79:VAL:HG22	1.91	0.52
23:B:1084:GLN:HG2	24:C:201:TRP:CH2	2.44	0.52
6:d:110:LYS:HA	6:d:113:LYS:NZ	2.24	0.52
8:g:107:ASN:HB2	18:u:91:LEU:HB3	1.91	0.52
13:n:107:LEU:HD13	16:s:135:TRP:HH2	1.75	0.52
17:t:14:PRO:HB3	24:C:260:LEU:HD12	1.92	0.52
6:d:45:ASP:O	6:d:48:ARG:NH1	2.42	0.52
6:d:94:TYR:HB2	10:i:122:TRP:HE1	1.75	0.52
18:u:88:GLU:HA	18:u:91:LEU:HD12	1.92	0.52
22:A:860:LEU:HD21	22:A:1394:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:586:ILE:O	13:n:622:GLN:NE2	2.42	0.52
14:q:465:VAL:HG12	14:q:476:ILE:HB	1.90	0.52
23:B:1159:ARG:HD3	23:B:1193:GLN:HG3	1.92	0.52
9:h:151:GLN:O	9:h:154:GLU:HG3	2.09	0.52
14:q:123:GLU:HA	14:q:126:ASN:HD22	1.73	0.52
18:u:72:GLN:HA	18:u:75:LYS:HG2	1.90	0.52
23:B:784:ASN:O	31:J:68:LYS:HD2	2.10	0.52
23:B:788:ARG:HG3	31:J:68:LYS:HD3	1.92	0.52
22:A:1226:VAL:HG13	22:A:1238:ILE:HG23	1.91	0.52
5:a:312:ILE:HD11	5:a:565:VAL:CG2	2.40	0.51
14:q:207:MET:SD	14:q:208:LEU:HD12	2.50	0.51
22:A:356:ASP:HB3	22:A:359:LEU:HD12	1.92	0.51
8:g:139:ILE:HD12	11:j:147:THR:HB	1.92	0.51
8:g:125:SER:O	8:g:129:ASN:ND2	2.43	0.51
17:t:38:ASP:HB2	17:t:61:THR:HB	1.92	0.51
23:B:198:ASP:OD2	23:B:202:TYR:OH	2.27	0.51
23:B:330:ALA:O	23:B:334:ILE:HG12	2.10	0.51
28:G:6:ASP:OD1	28:G:75:ARG:NH1	2.43	0.51
2:P:108:LYS:NZ	3:Q:84:ARG:O	2.43	0.51
14:q:243:PRO:HA	14:q:246:ARG:HD2	1.92	0.51
14:q:211:ILE:HG13	14:q:215:MET:HE2	1.91	0.51
17:t:138:ARG:HB2	17:t:154:GLU:HG3	1.93	0.51
22:A:1285:MET:HE3	22:A:1286:LYS:H	1.76	0.51
23:B:192:LEU:HD22	31:J:69:ARG:NH2	2.25	0.51
24:C:35:ARG:HH12	32:K:40:HIS:HB2	1.75	0.51
3:Q:78:ALA:O	3:Q:82:ARG:HG2	2.09	0.51
8:g:186:ARG:NH1	18:u:104:VAL:HG11	2.26	0.51
21:z:21:SER:H	21:z:22:PRO:CD	2.24	0.51
22:A:420:ARG:HB3	22:A:424:ILE:HG13	1.93	0.51
23:B:202:TYR:OH	31:J:70:ASP:OXT	2.29	0.51
6:d:138:LYS:HE2	6:d:141:ILE:HD12	1.93	0.51
7:f:183:SER:O	7:f:186:GLU:HG3	2.11	0.51
22:A:1011:GLN:O	22:A:1015:VAL:HG12	2.10	0.51
28:G:97:HIS:O	28:G:112:LYS:N	2.38	0.51
30:I:14:LEU:HB3	30:I:27:PHE:HB3	1.91	0.51
13:n:705:ILE:HA	13:n:715:ASN:HD21	1.76	0.51
15:r:230:LEU:HD21	15:r:253:LEU:HD11	1.92	0.51
4:S:178:ILE:HG22	4:S:225:PRO:HB3	1.93	0.51
6:d:110:LYS:HA	6:d:113:LYS:HZ3	1.76	0.51
14:q:457:VAL:HG13	14:q:467:ILE:HG13	1.93	0.51
22:A:85:ASP:O	22:A:273:ASN:ND2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:r:232:LEU:HG	15:r:253:LEU:HD12	1.93	0.51
22:A:1335:ILE:HG23	22:A:1339:LEU:HD12	1.92	0.51
30:I:34:TYR:HE1	30:I:36:GLU:HB2	1.75	0.51
30:I:90:GLN:HE22	30:I:92:ARG:HB2	1.76	0.51
6:d:95:ARG:HB3	6:d:99:LYS:HZ1	1.76	0.50
7:f:121:ARG:NH2	9:h:98:LEU:O	2.44	0.50
8:g:193:GLU:HA	8:g:196:CYS:SG	2.51	0.50
13:n:111:MET:HE1	16:s:142:LEU:HD11	1.93	0.50
14:q:645:ILE:HD12	14:q:670:VAL:HG21	1.92	0.50
15:r:219:GLY:HA3	15:r:232:LEU:O	2.12	0.50
22:A:1342:GLU:CD	26:E:153:HIS:HE2	2.19	0.50
5:a:274:PRO:HD3	5:a:344:TRP:CZ2	2.47	0.50
14:q:464:LYS:NZ	14:q:477:GLU:OE2	2.35	0.50
22:A:41:MET:HE2	22:A:45:GLN:HA	1.93	0.50
23:B:297:ILE:O	23:B:301:ILE:HG12	2.11	0.50
28:G:39:THR:O	28:G:43:GLY:N	2.44	0.50
31:J:68:LYS:NZ	31:J:69:ARG:O	2.39	0.50
3:Q:74:PRO:HD3	3:Q:224:VAL:HB	1.92	0.50
4:S:212:PRO:O	4:S:215:LYS:HG3	2.12	0.50
6:d:126:LYS:HZ2	13:n:244:GLN:HG3	1.76	0.50
14:q:455:TYR:O	14:q:550:ARG:NH2	2.33	0.50
14:q:635:LEU:HD13	14:q:645:ILE:HG12	1.92	0.50
30:I:19:ASP:O	30:I:23:ASN:CA	2.60	0.50
5:a:22:LYS:HB3	10:i:77:ARG:CD	2.41	0.50
11:j:140:VAL:O	11:j:143:ILE:HB	2.11	0.50
23:B:345:LYS:O	23:B:349:ILE:HG12	2.11	0.50
22:A:1442:ASP:OD2	27:F:137:TYR:OH	2.24	0.50
29:H:74:SER:HA	29:H:77:ARG:HB2	1.93	0.50
30:I:19:ASP:O	30:I:23:ASN:HA	2.11	0.50
4:S:217:LYS:HB3	4:S:223:ILE:HG12	1.93	0.50
4:S:262:GLU:O	22:A:720:ARG:NH1	2.44	0.50
6:d:155:ASP:OD2	20:w:71:GLN:NE2	2.45	0.50
23:B:101:MET:HA	23:B:112:LEU:H	1.77	0.50
18:u:25:TYR:O	18:u:29:ASN:HB2	2.12	0.50
18:u:101:LEU:O	18:u:104:VAL:HG12	2.12	0.50
18:u:117:LYS:O	18:u:120:ARG:HD3	2.12	0.50
23:B:34:ILE:HG23	23:B:542:MET:HE3	1.93	0.50
3:Q:63:ARG:HB2	3:Q:66:ARG:HH22	1.77	0.50
6:d:68:ASP:OD1	6:d:69:ILE:N	2.45	0.50
11:j:19:GLN:HG3	13:n:145:TYR:CE1	2.46	0.50
12:k:25:GLN:HG3	12:k:29:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:n:371:HIS:NE2	13:n:436:GLU:O	2.38	0.50
18:u:22:THR:HG23	18:u:62:LEU:HD13	1.93	0.50
18:u:82:GLY:HA2	18:u:85:VAL:HB	1.93	0.50
19:v:21:LEU:HA	19:v:24:LEU:HD12	1.94	0.50
22:A:216:VAL:HA	22:A:219:PHE:HD2	1.76	0.50
23:B:124:TYR:HB2	23:B:204:ILE:HB	1.93	0.50
23:B:242:SER:HB3	23:B:363:HIS:HB3	1.94	0.49
23:B:825:VAL:HG22	23:B:1010:LEU:HD21	1.94	0.49
28:G:137:ILE:HD13	28:G:143:ILE:HD12	1.94	0.49
32:K:56:VAL:HG22	32:K:77:THR:HG22	1.94	0.49
3:Q:240:ARG:HA	3:Q:243:ILE:HD12	1.94	0.49
8:g:31:LEU:HD22	8:g:65:LEU:HD13	1.94	0.49
8:g:153:THR:OG1	16:s:16:TYR:OH	2.30	0.49
9:h:48:ARG:HD3	9:h:51:ARG:HH21	1.77	0.49
18:u:97:LEU:HG	18:u:100:LYS:HE3	1.93	0.49
23:B:192:LEU:HB3	31:J:69:ARG:CZ	2.42	0.49
23:B:365:THR:HG21	23:B:370:PHE:HB2	1.94	0.49
6:d:43:TYR:O	6:d:46:LEU:HG	2.12	0.49
12:k:102:LEU:HD23	19:v:104:ILE:HD12	1.95	0.49
14:q:266:LYS:O	14:q:270:ILE:HG12	2.12	0.49
14:q:493:LEU:HD12	14:q:494:PRO:HD2	1.94	0.49
18:u:59:ILE:HD13	18:u:62:LEU:HD12	1.93	0.49
22:A:1150:SER:HA	22:A:1195:LEU:HD23	1.94	0.49
22:A:1193:LEU:HD21	22:A:1195:LEU:HD21	1.94	0.49
23:B:1171:VAL:HG21	23:B:1191:ILE:HG12	1.94	0.49
4:S:200:ARG:HG3	22:A:1176:LEU:HD13	1.94	0.49
14:q:271:GLU:HA	14:q:274:ILE:HG22	1.93	0.49
23:B:269:ILE:HD13	23:B:382:ILE:HD11	1.95	0.49
6:d:114:ILE:HG21	8:g:206:ILE:HG21	1.93	0.49
13:n:113:THR:HA	13:n:116:HIS:NE2	2.28	0.49
20:w:22:ARG:HA	20:w:25:VAL:HG22	1.93	0.49
22:A:1149:ALA:HB3	22:A:1196:GLU:HB3	1.93	0.49
4:S:217:LYS:O	4:S:221:GLY:N	2.45	0.49
5:a:21:TYR:CZ	6:d:74:ILE:CG2	2.93	0.49
5:a:177:GLN:HE22	5:a:235:GLN:HG2	1.77	0.49
7:f:94:LEU:O	7:f:101:MET:HE3	2.12	0.49
8:g:34:TYR:OH	8:g:63:ASP:OD1	2.30	0.49
9:h:37:ARG:HH22	14:q:229:LEU:HD22	1.78	0.49
23:B:340:ALA:HB3	23:B:343:ILE:HD11	1.95	0.49
23:B:356:LEU:O	23:B:360:PHE:HB3	2.12	0.49
9:h:94:VAL:H	14:q:257:ASP:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:j:114:LYS:HG3	11:j:115:MET:HE2	1.94	0.49
23:B:603:LEU:HD23	23:B:606:LYS:HD3	1.95	0.49
8:g:210:LEU:HD13	10:i:140:LEU:HD22	1.94	0.49
11:j:98:ARG:HD3	16:s:60:LEU:HD12	1.95	0.49
18:u:88:GLU:HB2	18:u:92:ARG:HH12	1.78	0.49
22:A:362:ASP:HB3	22:A:508:PRO:HD3	1.95	0.49
22:A:780:VAL:HG12	23:B:699:GLU:OE2	2.12	0.49
22:A:1187:GLN:O	22:A:1244:ARG:NH1	2.46	0.49
22:A:1199:ARG:NH2	22:A:1233:ASP:O	2.46	0.49
3:Q:135:PHE:HA	3:Q:214:ILE:HA	1.94	0.49
13:n:654:ARG:HD2	13:n:670:LEU:HD11	1.95	0.49
22:A:1197:LEU:HD11	22:A:1238:ILE:HD12	1.93	0.49
24:C:103:ALA:O	24:C:152:GLU:HG3	2.13	0.49
26:E:152:LYS:HG3	26:E:199:ILE:HB	1.95	0.49
9:h:56:LYS:O	14:q:204:ARG:NH2	2.46	0.48
22:A:1155:ASP:HB2	22:A:1192:LEU:HB2	1.95	0.48
23:B:327:ARG:O	23:B:331:LEU:HG	2.12	0.48
5:a:351:VAL:HG12	5:a:537:ILE:HD12	1.95	0.48
6:d:45:ASP:HA	6:d:48:ARG:NE	2.28	0.48
9:h:160:ARG:O	9:h:164:ARG:HG2	2.14	0.48
12:k:7:GLN:O	12:k:10:LEU:HG	2.13	0.48
13:n:241:LEU:HD11	14:q:95:GLY:HA2	1.95	0.48
13:n:275:ARG:HE	13:n:300:VAL:HG11	1.78	0.48
19:v:115:PHE:HA	19:v:118:GLU:HG2	1.95	0.48
22:A:1191:TRP:HB2	22:A:1260:LEU:HD22	1.94	0.48
23:B:787:VAL:HG11	31:J:68:LYS:N	2.28	0.48
3:Q:56:SER:HA	3:Q:211:LYS:HB2	1.95	0.48
6:d:102:LYS:HA	6:d:105:GLU:CD	2.39	0.48
23:B:171:PRO:HG2	23:B:461:LEU:HD12	1.95	0.48
5:a:22:LYS:HD3	10:i:77:ARG:NE	2.29	0.48
6:d:63:PHE:HZ	29:H:133:ASN:HD21	1.61	0.48
8:g:134:ILE:HB	11:j:122:ARG:NH2	2.28	0.48
19:v:46:SER:OG	19:v:49:ALA:HB3	2.14	0.48
22:A:270:LEU:O	22:A:274:ILE:HG23	2.12	0.48
23:B:576:ASP:OD1	23:B:576:ASP:N	2.46	0.48
6:d:192:MET:HE1	8:g:79:PHE:H	1.78	0.48
9:h:92:SER:HA	14:q:259:ILE:HG22	1.94	0.48
11:j:94:ASP:HB3	16:s:60:LEU:HD22	1.95	0.48
13:n:103:THR:HG23	13:n:137:LEU:HD22	1.95	0.48
23:B:289:LEU:HD22	23:B:371:GLU:CD	2.39	0.48
23:B:561:TRP:HE1	23:B:595:ARG:HH22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:145:ARG:HH22	6:d:153:LEU:HD22	1.78	0.48
13:n:486:ARG:HH21	13:n:549:LEU:HD22	1.78	0.48
25:D:37:GLN:HE21	25:D:47:LEU:HD13	1.79	0.48
25:D:51:ASN:HD22	25:D:181:GLY:HA3	1.79	0.48
6:d:82:GLU:HA	6:d:85:LYS:HE2	1.96	0.48
7:f:100:TYR:O	7:f:103:LEU:HB2	2.14	0.48
13:n:812:LEU:HD22	13:n:832:LYS:HD3	1.94	0.48
14:q:219:SER:O	14:q:223:GLU:HG3	2.14	0.48
22:A:229:SER:HB2	22:A:1416:ALA:HB2	1.95	0.48
25:D:202:ILE:HD13	25:D:207:LEU:HD13	1.95	0.48
6:d:38:SER:HA	6:d:43:TYR:CD2	2.49	0.48
8:g:132:GLU:O	8:g:136:VAL:HG23	2.14	0.48
10:i:66:ILE:HB	10:i:67:PRO:HD3	1.95	0.48
14:q:309:TRP:CH2	19:v:77:ARG:HG3	2.48	0.48
23:B:334:ILE:HD13	23:B:337:ARG:HH21	1.78	0.48
32:K:112:GLN:O	32:K:116:ALA:N	2.46	0.48
8:g:190:ARG:HA	8:g:193:GLU:CD	2.38	0.48
11:j:91:ARG:HG2	16:s:61:ARG:HD3	1.95	0.48
14:q:265:THR:HG23	14:q:267:LYS:H	1.79	0.48
14:q:288:LYS:HD2	14:q:292:ARG:HH12	1.79	0.48
22:A:785:PRO:HB2	23:B:703:ILE:HD11	1.95	0.48
22:A:903:ASN:O	22:A:907:THR:HG23	2.14	0.48
23:B:195:CYS:SG	23:B:782:LEU:HD22	2.54	0.48
9:h:153:ARG:HG2	19:v:33:ARG:NH1	2.28	0.48
19:v:33:ARG:HA	19:v:33:ARG:HD3	1.66	0.48
29:H:99:GLY:HA3	29:H:118:PHE:HD1	1.78	0.48
7:f:155:ILE:HG13	7:f:160:ILE:HD13	1.96	0.47
12:k:30:VAL:HA	12:k:33:ILE:HG22	1.95	0.47
14:q:277:LYS:HE2	19:v:31:ALA:HB1	1.95	0.47
14:q:339:TYR:CE2	14:q:432:LEU:HB3	2.49	0.47
23:B:190:TYR:CE2	31:J:62:ARG:HD2	2.48	0.47
23:B:539:LEU:HB3	23:B:543:SER:OG	2.14	0.47
23:B:638:PHE:HE1	23:B:653:VAL:HG11	1.77	0.47
2:P:119:LEU:HB3	2:P:395:PHE:CE2	2.49	0.47
7:f:166:ILE:HD12	7:f:169:ILE:HD12	1.96	0.47
8:g:155:LEU:HA	8:g:158:ILE:HD12	1.95	0.47
19:v:15:THR:O	19:v:19:VAL:HG22	2.14	0.47
6:d:45:ASP:O	6:d:48:ARG:HD3	2.15	0.47
7:f:11:TRP:CE3	21:z:22:PRO:HB2	2.48	0.47
7:f:38:ASP:OD1	7:f:38:ASP:N	2.44	0.47
13:n:415:TYR:OH	13:n:442:TRP:NE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:r:5:LEU:HD23	15:r:180:VAL:HG21	1.96	0.47
22:A:420:ARG:HB3	22:A:423:ASP:HB2	1.95	0.47
22:A:450:LEU:O	22:A:1070:GLN:HG2	2.13	0.47
25:D:39:ASN:ND2	25:D:43:GLU:OE2	2.47	0.47
8:g:176:MET:HA	8:g:179:GLU:CD	2.39	0.47
10:i:97:ARG:O	10:i:100:LEU:HG	2.14	0.47
19:v:8:GLU:HA	19:v:11:GLU:CD	2.40	0.47
22:A:420:ARG:CB	22:A:424:ILE:HG13	2.44	0.47
23:B:118:ARG:HH11	23:B:118:ARG:HA	1.79	0.47
23:B:333:PHE:HD1	23:B:337:ARG:HH12	1.62	0.47
6:d:156:TYR:HA	6:d:159:LYS:HG2	1.96	0.47
7:f:16:TRP:CH2	7:f:30:TYR:HB2	2.49	0.47
8:g:27:ASN:HA	8:g:30:LYS:HG2	1.97	0.47
8:g:175:ILE:HG12	18:u:94:ILE:HD11	1.95	0.47
10:i:111:THR:O	10:i:115:LEU:N	2.38	0.47
13:n:800:ILE:HG12	13:n:812:LEU:HD21	1.96	0.47
15:r:237:GLN:NE2	15:r:239:GLU:OE2	2.44	0.47
22:A:1428:VAL:HG13	23:B:1151:LEU:HD11	1.97	0.47
5:a:22:LYS:CD	6:d:74:ILE:CD1	2.80	0.47
9:h:123:ASP:HA	9:h:126:MET:SD	2.53	0.47
11:j:117:GLY:O	11:j:120:GLN:HG2	2.14	0.47
14:q:413:ARG:HH12	14:q:481:LEU:HD21	1.79	0.47
22:A:1446:ASP:HB2	27:F:133:VAL:HG23	1.95	0.47
23:B:87:LYS:HB2	23:B:137:TYR:HB2	1.97	0.47
1:M:23:THR:HG22	1:M:32:PRO:HG3	1.95	0.47
8:g:188:GLU:O	8:g:192:ILE:HG13	2.15	0.47
9:h:54:MET:SD	14:q:211:ILE:HG21	2.54	0.47
10:i:71:TYR:O	10:i:75:GLN:OE1	2.32	0.47
11:j:87:ILE:C	16:s:63:SER:HB2	2.40	0.47
15:r:47:TYR:HB3	17:t:46:ILE:HG21	1.97	0.47
3:Q:97:ILE:HG12	3:Q:104:ILE:HD12	1.97	0.47
5:a:22:LYS:CD	6:d:74:ILE:HD11	2.45	0.47
5:a:299:ILE:HG12	5:a:356:PHE:CE2	2.49	0.47
13:n:151:THR:HA	13:n:154:ILE:HB	1.97	0.47
18:u:101:LEU:O	18:u:105:GLU:OE1	2.33	0.47
6:d:53:LEU:CD2	10:i:98:LEU:HD12	2.42	0.47
10:i:73:LEU:CD2	10:i:77:ARG:HE	2.22	0.47
15:r:98:ILE:HG22	15:r:243:ASN:HD22	1.80	0.47
22:A:923:LEU:O	22:A:926:GLN:HG3	2.15	0.47
22:A:1193:LEU:HD23	22:A:1240:CYS:SG	2.55	0.47
4:S:166:HIS:CE1	4:S:170:SER:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:154:TYR:OH	9:h:95:VAL:O	2.29	0.47
22:A:199:LEU:HD23	22:A:199:LEU:H	1.80	0.47
22:A:826:ASP:OD1	22:A:830:LYS:HD2	2.15	0.47
28:G:139:ILE:HG22	28:G:140:LYS:HG3	1.97	0.47
32:K:108:GLU:O	32:K:112:GLN:HG2	2.15	0.47
4:S:153:LEU:HD23	4:S:156:LEU:HD21	1.97	0.46
11:j:100:PHE:HE2	13:n:166:LEU:HG	1.80	0.46
14:q:206:ASP:O	14:q:209:GLU:HG3	2.15	0.46
22:A:1193:LEU:HD22	22:A:1267:MET:CE	2.45	0.46
23:B:561:TRP:NE1	23:B:595:ARG:HH12	2.13	0.46
23:B:561:TRP:CD1	23:B:595:ARG:HH12	2.34	0.46
6:d:125:LEU:HD22	18:u:119:LEU:HD13	1.97	0.46
8:g:147:LYS:O	8:g:150:ASN:HB2	2.15	0.46
10:i:72:SER:OG	10:i:97:ARG:NH1	2.36	0.46
13:n:517:ILE:HG12	13:n:524:PHE:CE1	2.50	0.46
14:q:503:LEU:O	14:q:507:MET:HG2	2.15	0.46
22:A:148:CYS:SG	22:A:164:ARG:NH2	2.88	0.46
23:B:99:LYS:HD3	23:B:180:TYR:CE1	2.51	0.46
4:S:203:TYR:CE1	4:S:207:ILE:HD11	2.51	0.46
6:d:42:LEU:HD12	6:d:45:ASP:HB2	1.95	0.46
8:g:70:MET:SD	8:g:71:PRO:HD2	2.55	0.46
11:j:22:VAL:HG11	13:n:145:TYR:HB2	1.96	0.46
13:n:250:ASN:ND2	13:n:274:GLY:H	2.13	0.46
22:A:867:ILE:HD11	22:A:1000:LEU:HD11	1.96	0.46
28:G:14:HIS:CG	28:G:15:PRO:HD2	2.50	0.46
13:n:304:LEU:HD11	13:n:343:LEU:HD11	1.97	0.46
14:q:105:ILE:O	14:q:108:ARG:HG3	2.15	0.46
18:u:85:VAL:HG13	18:u:89:GLU:OE2	2.15	0.46
22:A:1192:LEU:HD21	22:A:1239:ARG:HG2	1.98	0.46
22:A:1267:MET:HE2	22:A:1267:MET:HB3	1.55	0.46
23:B:1180:PHE:HB3	23:B:1191:ILE:HD13	1.97	0.46
25:D:129:LEU:O	25:D:133:THR:OG1	2.20	0.46
4:S:201:ILE:O	4:S:205:ASN:ND2	2.48	0.46
14:q:123:GLU:O	14:q:126:ASN:HB2	2.15	0.46
19:v:53:THR:O	19:v:56:MET:HB3	2.16	0.46
23:B:118:ARG:HG3	31:J:70:ASP:HB2	1.97	0.46
29:H:44:VAL:HG13	29:H:48:PRO:HA	1.98	0.46
2:P:119:LEU:HB3	2:P:395:PHE:HE2	1.81	0.46
8:g:23:PHE:CZ	8:g:64:TYR:HB2	2.51	0.46
13:n:803:VAL:HG12	13:n:806:GLU:H	1.80	0.46
20:w:52:PRO:HA	20:w:55:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:95:PHE:CE1	22:A:1414:ALA:HB2	2.50	0.46
22:A:440:ASP:H	22:A:460:VAL:HG22	1.81	0.46
23:B:309:GLN:O	23:B:313:MET:HG3	2.15	0.46
24:C:37:MET:HE1	24:C:232:VAL:HG21	1.98	0.46
8:g:23:PHE:CE1	8:g:65:LEU:HG	2.50	0.46
9:h:31:GLN:HG3	25:D:209:ARG:HG3	1.97	0.46
22:A:1195:LEU:HB2	22:A:1238:ILE:HB	1.98	0.46
23:B:195:CYS:SG	23:B:783:THR:HG22	2.55	0.46
23:B:874:PHE:O	33:L:42:ARG:NH2	2.47	0.46
4:S:231:CYS:SG	4:S:235:ASP:HB3	2.56	0.46
6:d:148:ILE:HD12	6:d:153:LEU:HD11	1.97	0.46
8:g:152:ARG:HD2	13:n:190:MET:HE3	1.98	0.46
8:g:173:SER:HA	8:g:176:MET:HG2	1.97	0.46
11:j:142:ASP:O	11:j:146:ARG:N	2.48	0.46
13:n:764:GLU:HA	13:n:785:LYS:HE3	1.98	0.46
14:q:234:GLU:O	14:q:238:MET:HG2	2.15	0.46
22:A:420:ARG:CB	22:A:423:ASP:HB2	2.46	0.46
26:E:29:PHE:HB2	26:E:65:THR:HG22	1.97	0.46
7:f:9:LEU:HD11	21:z:22:PRO:HG3	1.96	0.46
9:h:130:ARG:HG2	9:h:130:ARG:HH11	1.81	0.46
10:i:119:PRO:HA	10:i:122:TRP:HZ3	1.80	0.46
13:n:772:ASP:OD2	13:n:775:ASN:ND2	2.49	0.46
18:u:105:GLU:O	18:u:109:ILE:HG13	2.15	0.46
22:A:30:ILE:HD12	23:B:1170:THR:HG21	1.96	0.46
4:S:286:THR:HB	22:A:1081:LEU:O	2.16	0.46
10:i:125:ILE:O	10:i:128:GLN:HG2	2.16	0.46
22:A:840:ARG:HG2	22:A:1384:VAL:HG12	1.98	0.46
22:A:1177:LEU:HD11	22:A:1227:ILE:HD11	1.98	0.46
6:d:195:MET:SD	6:d:195:MET:N	2.89	0.45
9:h:96:TYR:HE1	14:q:255:ASN:HB3	1.80	0.45
13:n:253:VAL:HG11	13:n:276:ILE:HB	1.97	0.45
22:A:308:ILE:HG23	22:A:311:GLN:HB2	1.98	0.45
22:A:993:LEU:HD13	22:A:1046:LEU:HD22	1.98	0.45
22:A:1166:ASP:O	22:A:1170:ILE:HG13	2.17	0.45
23:B:953:LEU:HD11	33:L:55:ILE:HG23	1.98	0.45
2:P:120:LYS:HZ1	3:Q:132:GLU:HA	1.80	0.45
5:a:278:ILE:HD11	5:a:341:ILE:HG12	1.98	0.45
14:q:407:GLY:HA3	14:q:497:ASN:HB2	1.98	0.45
22:A:253:ASN:H	22:A:256:GLN:HB2	1.81	0.45
25:D:33:PHE:CE1	28:G:80:LYS:HD3	2.51	0.45
2:P:118:LEU:HB2	2:P:392:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:142:ASP:OD1	8:g:142:ASP:N	2.48	0.45
13:n:146:VAL:HG21	16:s:64:TYR:CD2	2.51	0.45
13:n:161:VAL:HG13	16:s:40:LEU:HB3	1.98	0.45
19:v:116:VAL:HG22	19:v:119:LYS:HZ3	1.81	0.45
24:C:148:ARG:HG2	24:C:149:LYS:H	1.80	0.45
6:d:82:GLU:HA	6:d:85:LYS:HZ1	1.79	0.45
8:g:173:SER:HA	8:g:176:MET:HE3	1.98	0.45
9:h:167:TYR:OH	9:h:173:LYS:NZ	2.50	0.45
14:q:228:LEU:O	14:q:231:SER:OG	2.33	0.45
15:r:297:ASP:OD1	15:r:299:ARG:HG3	2.17	0.45
22:A:567:LYS:NZ	29:H:90:ALA:O	2.43	0.45
22:A:664:THR:HB	23:B:1014:PRO:HB3	1.99	0.45
31:J:8:PHE:CD2	31:J:49:MET:HE1	2.51	0.45
9:h:124:GLU:HB2	9:h:128:TYR:CZ	2.52	0.45
22:A:371:ALA:HA	22:A:436:ILE:HD11	1.98	0.45
8:g:210:LEU:HB2	10:i:140:LEU:HD13	1.99	0.45
13:n:146:VAL:HG21	16:s:64:TYR:HD2	1.81	0.45
13:n:395:PHE:HA	13:n:399:ASN:HD22	1.82	0.45
14:q:280:LYS:HD3	19:v:30:ILE:O	2.17	0.45
15:r:305:ILE:HG22	15:r:307:ILE:HG13	1.99	0.45
22:A:1342:GLU:CD	22:A:1342:GLU:H	2.24	0.45
23:B:190:TYR:CD2	31:J:62:ARG:HD2	2.51	0.45
24:C:239:PRO:O	24:C:243:VAL:HG23	2.17	0.45
6:d:43:TYR:N	10:i:115:LEU:O	2.50	0.45
13:n:526:PHE:HB2	13:n:529:PRO:HB3	1.99	0.45
14:q:277:LYS:CE	19:v:31:ALA:HB1	2.47	0.45
15:r:212:GLU:HG2	15:r:213:PHE:HD2	1.82	0.45
22:A:444:PHE:HE2	22:A:470:LEU:HD11	1.82	0.45
22:A:1225:PHE:CG	22:A:1226:VAL:N	2.84	0.45
24:C:114:TYR:HA	24:C:143:LEU:HA	1.99	0.45
26:E:135:PHE:HB3	26:E:140:LEU:HD21	1.99	0.45
29:H:12:VAL:HG12	29:H:28:ALA:HB2	1.98	0.45
8:g:22:PHE:O	8:g:27:ASN:ND2	2.49	0.45
8:g:118:GLU:O	8:g:121:LYS:HG3	2.17	0.45
9:h:156:THR:OG1	19:v:28:THR:O	2.27	0.45
12:k:16:ILE:HD11	12:k:65:GLN:HB3	1.99	0.45
13:n:99:LEU:HD23	13:n:144:LEU:HD22	1.99	0.45
13:n:187:LEU:HG	18:u:23:LEU:HD11	1.97	0.45
15:r:272:GLU:O	15:r:276:MET:HG2	2.16	0.45
18:u:117:LYS:C	18:u:121:HIS:HD1	2.20	0.45
22:A:216:VAL:HA	22:A:219:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1342:GLU:HG3	26:E:151:PRO:HD2	1.99	0.45
23:B:71:LEU:HD23	23:B:88:TYR:HD2	1.81	0.45
23:B:592:ASN:OD1	23:B:595:ARG:HG2	2.17	0.45
25:D:188:ALA:HB2	25:D:208:GLU:HG3	1.98	0.45
30:I:21:GLU:HG2	30:I:22:ASN:OD1	2.16	0.45
12:k:14:ASN:HA	12:k:17:GLU:CD	2.42	0.45
14:q:264:PRO:HB3	14:q:269:TYR:OH	2.17	0.45
14:q:649:PHE:O	14:q:659:SER:OG	2.28	0.45
18:u:80:LEU:HB2	18:u:83:VAL:HB	1.99	0.45
22:A:834:THR:HG21	22:A:1077:THR:HA	1.98	0.45
23:B:115:GLN:CB	31:J:69:ARG:HG2	2.31	0.45
23:B:1076:HIS:O	24:C:31:ASN:ND2	2.47	0.45
2:P:367:ALA:HB3	23:B:369:GLY:HA3	1.97	0.45
4:S:176:LYS:O	4:S:179:GLU:HG3	2.16	0.45
9:h:123:ASP:O	9:h:127:LYS:HG2	2.17	0.45
14:q:394:PHE:HB2	14:q:473:LYS:HB3	1.99	0.45
22:A:143:LYS:HG3	22:A:144:THR:HG23	1.99	0.45
29:H:103:LYS:HB3	29:H:115:TYR:CD1	2.52	0.45
11:j:87:ILE:HA	16:s:63:SER:HA	1.98	0.44
11:j:89:ASP:HB3	11:j:91:ARG:HH21	1.82	0.44
13:n:660:SER:HB2	13:n:665:TRP:CZ3	2.51	0.44
15:r:80:MET:HE3	15:r:80:MET:HA	1.99	0.44
22:A:216:VAL:O	22:A:219:PHE:HB2	2.16	0.44
22:A:886:ILE:HG12	22:A:943:LEU:HB3	1.99	0.44
22:A:1226:VAL:CG1	22:A:1238:ILE:HG23	2.48	0.44
23:B:122:LEU:O	23:B:207:GLY:N	2.51	0.44
13:n:718:CYS:HB3	13:n:728:LEU:HD11	1.99	0.44
14:q:523:ARG:HE	14:q:531:ILE:HD13	1.81	0.44
19:v:48:LEU:O	19:v:52:THR:HG23	2.18	0.44
22:A:326:ARG:HG3	22:A:1406:VAL:HG21	1.99	0.44
29:H:83:GLN:OE1	29:H:83:GLN:HA	2.17	0.44
9:h:37:ARG:HG3	14:q:226:SER:HA	1.98	0.44
12:k:27:ALA:HA	12:k:30:VAL:HG12	1.98	0.44
14:q:123:GLU:O	14:q:127:GLU:OE1	2.35	0.44
18:u:8:LEU:HD23	18:u:12:LEU:HD23	1.99	0.44
20:w:82:LEU:O	20:w:86:ASN:N	2.46	0.44
22:A:684:ALA:O	22:A:688:LYS:HG2	2.17	0.44
22:A:1041:ALA:O	22:A:1045:VAL:HG23	2.18	0.44
22:A:1209:MET:SD	22:A:1238:ILE:HD11	2.58	0.44
24:C:183:TRP:CZ2	24:C:207:CYS:HB3	2.52	0.44
5:a:22:LYS:CD	10:i:73:LEU:HD21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:348:TYR:CZ	14:q:350:HIS:HB2	2.53	0.44
15:r:1:MET:HE3	15:r:1:MET:HB3	1.84	0.44
17:t:143:PHE:HZ	24:C:260:LEU:HD22	1.82	0.44
18:u:129:PHE:CZ	18:u:133:ILE:HD11	2.52	0.44
22:A:1226:VAL:HG12	22:A:1228:TRP:CD1	2.51	0.44
23:B:191:LYS:HA	23:B:191:LYS:HD3	1.75	0.44
3:Q:60:ASP:OD2	3:Q:211:LYS:NZ	2.49	0.44
7:f:120:VAL:HG22	7:f:126:TRP:HD1	1.83	0.44
7:f:132:ARG:NH1	7:f:134:THR:HG23	2.32	0.44
12:k:38:LYS:HG2	14:q:284:LEU:HD23	1.98	0.44
13:n:822:ILE:HA	13:n:825:TYR:HD2	1.83	0.44
22:A:180:LYS:HD2	22:A:180:LYS:HA	1.73	0.44
22:A:389:THR:O	22:A:393:ARG:HG2	2.17	0.44
23:B:234:ILE:HG23	23:B:259:TYR:HE1	1.82	0.44
23:B:430:ARG:HE	23:B:434:ARG:NH2	2.15	0.44
25:D:72:ARG:HH11	25:D:76:LYS:HD2	1.83	0.44
31:J:68:LYS:HG2	31:J:69:ARG:N	2.32	0.44
3:Q:86:ASN:HB3	3:Q:92:LEU:HD11	2.00	0.44
8:g:195:VAL:O	8:g:198:GLN:HG3	2.17	0.44
12:k:66:LEU:O	12:k:70:ILE:HG13	2.17	0.44
12:k:110:ASP:OD2	12:k:112:SER:OG	2.31	0.44
18:u:68:LEU:O	18:u:72:GLN:OE1	2.36	0.44
25:D:173:HIS:HB3	25:D:176:GLU:HG3	1.99	0.44
11:j:50:ILE:HD11	16:s:143:SER:HB3	2.00	0.44
15:r:76:ILE:HG23	15:r:80:MET:HB2	1.99	0.44
22:A:104:GLU:HG2	22:A:174:ILE:HD12	1.99	0.44
22:A:1224:LEU:HA	22:A:1242:VAL:HA	1.99	0.44
24:C:67:LEU:HD23	24:C:70:ILE:HD12	1.99	0.44
6:d:121:CYS:O	6:d:124:GLU:HG3	2.17	0.44
8:g:68:PRO:HD3	20:w:22:ARG:HH22	1.82	0.44
9:h:87:GLN:HG3	9:h:88:GLU:N	2.33	0.44
13:n:346:PRO:HB2	13:n:350:LYS:HZ1	1.83	0.44
17:t:63:HIS:CE1	17:t:67:ARG:HH12	2.36	0.44
22:A:1340:GLY:HA2	26:E:182:ASP:OD1	2.18	0.44
24:C:11:ARG:NH2	24:C:21:ILE:HD11	2.33	0.44
24:C:143:LEU:HG	31:J:2:ILE:HD11	1.98	0.44
8:g:186:ARG:HH12	18:u:104:VAL:HG11	1.83	0.44
9:h:49:ARG:HG3	9:h:53:GLU:OE2	2.18	0.44
12:k:47:GLN:O	12:k:51:HIS:ND1	2.33	0.44
13:n:251:LEU:HD11	18:u:130:VAL:HG21	1.98	0.44
22:A:1428:VAL:HG13	23:B:1151:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:176:ILE:HG22	24:C:232:VAL:HA	1.98	0.44
30:I:19:ASP:OD2	30:I:24:ARG:NH1	2.51	0.44
5:a:177:GLN:HE22	5:a:235:GLN:CB	2.31	0.43
14:q:270:ILE:HG13	14:q:271:GLU:N	2.33	0.43
14:q:300:SER:O	14:q:303:GLN:HG3	2.17	0.43
14:q:301:ILE:O	14:q:305:GLU:OE1	2.36	0.43
15:r:81:MET:SD	15:r:81:MET:N	2.91	0.43
17:t:24:LEU:O	17:t:28:ILE:HG13	2.17	0.43
3:Q:138:GLN:N	3:Q:138:GLN:OE1	2.51	0.43
6:d:81:PHE:CD2	6:d:85:LYS:NZ	2.86	0.43
14:q:500:ARG:O	14:q:504:MET:HG2	2.18	0.43
23:B:595:ARG:O	23:B:598:GLU:HG2	2.18	0.43
25:D:168:LYS:HG2	25:D:177:VAL:HG21	2.00	0.43
9:h:48:ARG:NH2	14:q:215:MET:HB3	2.33	0.43
14:q:283:SER:O	14:q:287:SER:OG	2.33	0.43
17:t:57:MET:HE2	17:t:57:MET:HB3	1.93	0.43
22:A:492:PRO:HG3	22:A:501:LEU:HD12	2.00	0.43
22:A:567:LYS:HG2	22:A:568:PRO:HA	1.99	0.43
26:E:16:PHE:CE2	26:E:20:LYS:HE2	2.53	0.43
28:G:38:CYS:HA	28:G:44:TYR:HA	1.99	0.43
14:q:443:TYR:O	14:q:447:LYS:HG2	2.18	0.43
16:s:30:PRO:HA	16:s:34:LEU:HD11	2.00	0.43
19:v:103:GLN:HA	19:v:106:GLU:CD	2.43	0.43
22:A:65:LEU:HG	23:B:925:LEU:HD23	1.99	0.43
22:A:873:MET:HB2	22:A:1366:ARG:HH21	1.82	0.43
22:A:894:GLU:O	22:A:898:ARG:HB3	2.18	0.43
23:B:872:GLU:HG2	23:B:914:LYS:HE2	2.01	0.43
29:H:37:LYS:HG3	29:H:126:GLU:HB3	2.00	0.43
2:P:120:LYS:NZ	3:Q:132:GLU:HA	2.33	0.43
5:a:30:ASN:O	10:i:78:LYS:NZ	2.51	0.43
8:g:120:ARG:CZ	18:u:77:ILE:HG21	2.48	0.43
9:h:37:ARG:HH12	14:q:229:LEU:HB3	1.83	0.43
13:n:173:ASN:C	13:n:173:ASN:HD22	2.27	0.43
13:n:539:LYS:O	13:n:542:ARG:NH1	2.51	0.43
13:n:629:LEU:HB2	13:n:632:TRP:CD1	2.53	0.43
13:n:741:ASN:HD22	13:n:774:SER:HG	1.58	0.43
14:q:614:ARG:HG3	14:q:636:GLU:HG3	1.99	0.43
22:A:22:PHE:HB2	23:B:1211:ASN:OD1	2.18	0.43
22:A:1150:SER:HB2	22:A:1193:LEU:HD11	1.99	0.43
22:A:1195:LEU:HB3	22:A:1197:LEU:CD2	2.49	0.43
22:A:1318:THR:HG22	26:E:142:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:313:MET:SD	23:B:390:LEU:HD21	2.59	0.43
23:B:390:LEU:HD12	23:B:392:ARG:HH12	1.83	0.43
2:P:124:LYS:HD2	30:I:8:ARG:HH21	1.83	0.43
2:P:346:GLU:OE2	2:P:391:LYS:NZ	2.43	0.43
4:S:293:LEU:HD12	22:A:756:ILE:HG21	2.01	0.43
14:q:619:ILE:HD12	14:q:631:LEU:HD23	2.00	0.43
17:t:183:LYS:HA	17:t:183:LYS:HD3	1.84	0.43
23:B:234:ILE:HG12	23:B:259:TYR:CZ	2.54	0.43
7:f:121:ARG:CG	7:f:125:PHE:HB3	2.49	0.43
10:i:108:ASN:HB3	10:i:111:THR:HG22	2.00	0.43
11:j:121:LEU:HD21	18:u:59:ILE:HG13	2.00	0.43
13:n:480:ARG:NH1	13:n:484:LEU:HD11	2.34	0.43
13:n:486:ARG:NH2	13:n:549:LEU:HD22	2.34	0.43
14:q:311:LYS:NZ	14:q:364:GLN:HG2	2.34	0.43
14:q:555:LYS:HE2	14:q:559:LYS:HE3	2.00	0.43
18:u:94:ILE:CG2	18:u:98:GLN:HE22	2.30	0.43
19:v:103:GLN:HA	19:v:106:GLU:OE2	2.19	0.43
20:w:87:GLY:HA2	20:w:90:GLU:OE2	2.18	0.43
22:A:677:ARG:HA	22:A:677:ARG:NE	2.33	0.43
24:C:43:THR:HG22	24:C:44:LEU:N	2.34	0.43
7:f:8:GLU:HB3	9:h:115:ARG:HH22	1.84	0.43
7:f:103:LEU:O	7:f:107:LEU:HB2	2.19	0.43
7:f:115:TYR:CE1	7:f:130:LYS:HD3	2.54	0.43
8:g:31:LEU:HG	8:g:35:LYS:NZ	2.33	0.43
11:j:92:ASN:H	16:s:61:ARG:CB	2.32	0.43
13:n:257:ILE:HG21	13:n:276:ILE:HD13	2.00	0.43
19:v:12:GLN:HE21	19:v:68:ASN:HB3	1.83	0.43
23:B:698:GLU:HA	23:B:701:ILE:HG12	2.00	0.43
32:K:14:GLU:OE1	32:K:14:GLU:HA	2.18	0.43
7:f:11:TRP:H	7:f:160:ILE:HG22	1.84	0.43
8:g:30:LYS:HD2	8:g:62:LEU:HD11	2.01	0.43
14:q:125:GLN:OE1	14:q:129:LYS:NZ	2.49	0.43
22:A:1257:ASP:HA	22:A:1260:LEU:HG	2.00	0.43
23:B:512:ARG:NH1	23:B:533:CYS:O	2.51	0.43
28:G:26:LEU:HD13	28:G:56:ILE:HD11	2.00	0.43
6:d:71:LYS:HA	6:d:74:ILE:HG22	2.01	0.43
6:d:85:LYS:HE2	6:d:85:LYS:HB2	1.80	0.43
11:j:121:LEU:HD22	18:u:59:ILE:HG21	2.00	0.43
12:k:33:ILE:HG13	12:k:36:GLU:OE2	2.19	0.43
13:n:266:LEU:HB3	13:n:278:PHE:CE2	2.54	0.43
14:q:119:LEU:HD12	14:q:120:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:1226:VAL:HG22	22:A:1240:CYS:HA	2.00	0.43
23:B:63:ILE:HG13	23:B:64:CYS:N	2.32	0.43
23:B:561:TRP:HE1	23:B:595:ARG:HH12	1.67	0.43
23:B:1090:THR:HG22	23:B:1091:TYR:N	2.32	0.43
7:f:192:ILE:HG23	7:f:200:VAL:HG13	2.01	0.42
17:t:10:GLU:HG3	17:t:11:ARG:HG2	2.01	0.42
22:A:149:GLU:N	22:A:164:ARG:HH21	2.16	0.42
24:C:43:THR:HG22	24:C:44:LEU:H	1.83	0.42
24:C:44:LEU:HD22	24:C:129:ILE:HG12	2.01	0.42
28:G:98:GLY:HA3	28:G:110:VAL:O	2.18	0.42
3:Q:210:LYS:HD3	3:Q:210:LYS:HA	1.80	0.42
4:S:285:GLN:HB2	4:S:293:LEU:HD22	2.01	0.42
8:g:128:LEU:HG	11:j:143:ILE:HD11	2.00	0.42
14:q:301:ILE:O	14:q:304:ASN:HB2	2.19	0.42
20:w:45:GLN:HB2	20:w:48:ILE:HD12	2.00	0.42
23:B:328:GLU:HG3	23:B:349:ILE:HD12	2.01	0.42
25:D:190:GLU:HA	28:G:167:TYR:CD2	2.54	0.42
27:F:144:GLU:HG2	27:F:146:TRP:NE1	2.33	0.42
6:d:37:LEU:HD13	10:i:112:LYS:HD2	2.01	0.42
7:f:121:ARG:HG3	7:f:125:PHE:HB3	2.02	0.42
11:j:64:ASN:HB2	13:n:100:THR:HG21	2.00	0.42
11:j:118:LEU:HA	11:j:121:LEU:HD12	2.00	0.42
12:k:57:GLU:O	12:k:61:LYS:HG2	2.19	0.42
13:n:96:ILE:HG12	13:n:144:LEU:HD21	2.01	0.42
13:n:741:ASN:ND2	13:n:774:SER:OG	2.31	0.42
14:q:279:TRP:O	14:q:282:GLN:HB3	2.19	0.42
22:A:351:THR:HG22	22:A:352:VAL:N	2.34	0.42
22:A:672:ASP:N	22:A:672:ASP:OD1	2.52	0.42
23:B:590:HIS:CE1	23:B:596:LEU:HD13	2.54	0.42
23:B:653:VAL:HG12	23:B:689:LEU:HD23	2.01	0.42
3:Q:219:CYS:SG	3:Q:220:HIS:N	2.92	0.42
6:d:71:LYS:HA	6:d:71:LYS:HD2	1.79	0.42
6:d:87:LEU:HD11	10:i:114:LEU:HB3	2.00	0.42
7:f:116:VAL:HG13	7:f:129:ARG:HB3	2.00	0.42
12:k:7:GLN:O	12:k:11:LYS:HG2	2.19	0.42
13:n:127:LYS:HE2	16:s:146:GLU:HG2	2.00	0.42
14:q:348:TYR:CE2	14:q:350:HIS:HB2	2.54	0.42
15:r:189:ILE:HD12	17:t:87:ILE:HG12	2.01	0.42
16:s:65:LYS:O	16:s:68:ILE:HG12	2.18	0.42
22:A:444:PHE:CE2	22:A:487:MET:HE2	2.54	0.42
22:A:537:ARG:HH21	29:H:122:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:894:GLU:OE1	22:A:933:TYR:OH	2.23	0.42
23:B:211:VAL:HG21	23:B:495:LEU:HD23	2.02	0.42
23:B:365:THR:HG21	23:B:370:PHE:CB	2.48	0.42
23:B:801:LYS:HE2	23:B:815:ARG:HB3	2.01	0.42
29:H:113:ALA:HA	29:H:125:LEU:O	2.20	0.42
32:K:19:LEU:HD22	32:K:35:PHE:CD1	2.55	0.42
2:P:120:LYS:O	2:P:395:PHE:N	2.46	0.42
10:i:132:GLU:HA	10:i:135:ILE:HG22	2.01	0.42
12:k:102:LEU:CD2	19:v:104:ILE:HD12	2.50	0.42
13:n:255:ILE:O	13:n:259:LEU:HG	2.20	0.42
14:q:309:TRP:HH2	19:v:77:ARG:HG3	1.84	0.42
14:q:452:LEU:HD21	14:q:543:ARG:HE	1.84	0.42
22:A:212:LYS:HG3	22:A:232:GLU:OE1	2.19	0.42
22:A:557:ASP:OD1	22:A:557:ASP:N	2.53	0.42
22:A:1148:ILE:HG22	22:A:1196:GLU:O	2.20	0.42
23:B:406:LEU:HD12	23:B:545:ILE:HD11	2.02	0.42
23:B:787:VAL:HG22	31:J:65:PRO:C	2.44	0.42
23:B:821:GLN:HB2	23:B:851:PHE:CE1	2.55	0.42
23:B:1104:HIS:NE2	23:B:1126:GLY:O	2.46	0.42
2:P:376:LEU:HD11	3:Q:71:VAL:HG12	2.00	0.42
4:S:286:THR:HG21	22:A:1085:HIS:NE2	2.34	0.42
8:g:136:VAL:HG21	8:g:147:LYS:HD2	2.02	0.42
11:j:114:LYS:HB2	18:u:30:HIS:HB2	2.01	0.42
13:n:162:LEU:O	13:n:166:LEU:HB2	2.19	0.42
15:r:33:LEU:HD13	15:r:87:PHE:HA	2.02	0.42
23:B:754:SER:HB2	23:B:812:LEU:HD11	2.02	0.42
23:B:827:ILE:HD12	23:B:1086:PHE:HD2	1.84	0.42
26:E:9:ILE:HG23	26:E:42:PHE:HE2	1.85	0.42
7:f:22:LEU:HB3	7:f:126:TRP:CH2	2.54	0.42
7:f:159:ASN:OD1	7:f:160:ILE:N	2.53	0.42
9:h:129:VAL:HG11	14:q:282:GLN:CD	2.44	0.42
13:n:795:ILE:HG22	13:n:795:ILE:O	2.20	0.42
14:q:448:GLU:OE2	14:q:542:ILE:N	2.48	0.42
15:r:78:GLU:O	15:r:81:MET:HE1	2.20	0.42
23:B:189:LEU:O	23:B:194:GLU:N	2.31	0.42
23:B:354:ASP:HA	23:B:357:GLN:NE2	2.34	0.42
23:B:1204:PHE:CE2	23:B:1216:LEU:HD21	2.52	0.42
4:S:202:ILE:O	4:S:206:VAL:HG23	2.20	0.42
6:d:144:GLN:O	6:d:148:ILE:HG12	2.20	0.42
6:d:192:MET:HA	6:d:195:MET:HE2	2.01	0.42
8:g:143:MET:O	8:g:146:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:169:GLN:HE21	18:u:5:LEU:HD22	1.83	0.42
8:g:189:ILE:O	8:g:193:GLU:OE1	2.37	0.42
9:h:86:PHE:O	9:h:90:LEU:HG	2.20	0.42
13:n:286:ILE:HD13	13:n:302:LEU:HD12	2.01	0.42
22:A:12:ARG:NH2	23:B:1220:ARG:HB2	2.34	0.42
23:B:580:VAL:HG22	23:B:624:LEU:HD12	2.01	0.42
23:B:873:THR:OG1	23:B:915:THR:OG1	2.26	0.42
14:q:437:PHE:CE1	14:q:512:LEU:HD23	2.55	0.42
22:A:445:ASN:OD1	22:A:488:ASN:HB2	2.19	0.42
23:B:757:PRO:HG3	23:B:983:ARG:NH2	2.34	0.42
23:B:860:MET:HE2	23:B:963:PHE:CE1	2.54	0.42
26:E:88:VAL:HB	26:E:116:ILE:HG12	2.02	0.42
6:d:139:ASN:O	6:d:143:GLN:OE1	2.37	0.42
10:i:91:THR:O	10:i:95:ARG:HG3	2.19	0.42
12:k:105:LEU:O	12:k:109:LEU:N	2.50	0.42
13:n:503:LEU:HD11	13:n:557:LYS:HA	2.02	0.42
13:n:564:VAL:O	13:n:568:MET:HG2	2.19	0.42
15:r:98:ILE:HG22	15:r:243:ASN:ND2	2.35	0.42
22:A:1186:ASP:HB2	22:A:1246:LYS:HE2	2.02	0.42
22:A:1187:GLN:NE2	22:A:1244:ARG:O	2.43	0.42
23:B:860:MET:HE2	23:B:963:PHE:HE1	1.85	0.42
23:B:1020:ARG:HB3	23:B:1022:THR:HG23	2.01	0.42
6:d:71:LYS:O	6:d:75:ARG:HG2	2.20	0.41
7:f:118:SER:HB3	7:f:127:VAL:HG23	2.02	0.41
13:n:241:LEU:HA	13:n:244:GLN:NE2	2.35	0.41
13:n:714:ARG:H	13:n:751:SER:HB2	1.84	0.41
13:n:718:CYS:SG	13:n:746:THR:HG23	2.59	0.41
13:n:821:ILE:O	13:n:821:ILE:HG22	2.20	0.41
14:q:238:MET:HE1	14:q:251:PRO:HG2	2.02	0.41
14:q:298:LEU:O	14:q:302:LEU:HB2	2.20	0.41
14:q:563:LYS:HA	14:q:567:LEU:HB2	2.02	0.41
18:u:111:ALA:HA	18:u:114:LYS:HZ3	1.84	0.41
22:A:418:SER:C	22:A:420:ARG:H	2.28	0.41
22:A:1004:ASN:O	22:A:1008:GLN:HG2	2.20	0.41
22:A:1015:VAL:HG22	22:A:1015:VAL:O	2.20	0.41
22:A:1177:LEU:HD13	22:A:1181:ALA:HB1	2.01	0.41
22:A:1202:MET:HE2	22:A:1202:MET:HB2	1.82	0.41
23:B:390:LEU:HD23	23:B:390:LEU:HA	1.79	0.41
23:B:918:ILE:HB	23:B:928:ARG:NH2	2.35	0.41
24:C:241:ASP:N	24:C:241:ASP:OD1	2.51	0.41
2:P:119:LEU:HD22	2:P:395:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:116:GLU:OE1	13:n:293:ARG:HD3	2.19	0.41
7:f:130:LYS:HB3	7:f:151:GLN:O	2.19	0.41
22:A:870:GLU:OE1	26:E:202:SER:OG	2.26	0.41
22:A:1142:THR:O	22:A:1145:SER:OG	2.34	0.41
24:C:34:ARG:HB2	24:C:176:ILE:CD1	2.49	0.41
25:D:27:LEU:HD23	25:D:27:LEU:HA	1.94	0.41
26:E:79:TRP:HE1	26:E:81:GLU:HB2	1.84	0.41
28:G:46:LEU:HG	28:G:78:VAL:HA	2.02	0.41
6:d:197:SER:HB2	8:g:15:PRO:HG2	2.02	0.41
7:f:196:PRO:CD	14:q:305:GLU:HG2	2.51	0.41
14:q:227:LEU:HB3	14:q:253:SER:HB2	2.02	0.41
17:t:159:GLU:CD	17:t:161:GLY:H	2.28	0.41
22:A:326:ARG:HG3	22:A:1406:VAL:HG11	2.03	0.41
22:A:778:GLY:HA3	23:B:516:ASN:HB2	2.03	0.41
22:A:1233:ASP:OD1	22:A:1233:ASP:N	2.53	0.41
22:A:1405:THR:OG1	22:A:1406:VAL:N	2.53	0.41
23:B:416:LEU:HD12	23:B:416:LEU:HA	1.88	0.41
27:F:93:ILE:HD11	27:F:134:ILE:HD11	2.01	0.41
6:d:98:GLN:HB3	6:d:102:LYS:HZ3	1.85	0.41
7:f:129:ARG:NH1	7:f:131:GLN:HB3	2.34	0.41
7:f:172:SER:O	7:f:175:MET:HG3	2.20	0.41
14:q:381:PHE:CZ	14:q:385:VAL:HG21	2.56	0.41
19:v:46:SER:O	19:v:50:VAL:HG23	2.20	0.41
22:A:476:SER:HB2	22:A:477:PRO:HD3	2.02	0.41
22:A:830:LYS:CD	22:A:1080:THR:HB	2.48	0.41
22:A:1192:LEU:HD11	22:A:1239:ARG:HA	2.02	0.41
23:B:928:ARG:NE	23:B:932:HIS:O	2.50	0.41
31:J:6:ARG:HG2	31:J:13:VAL:HG22	2.02	0.41
5:a:315:MET:SD	5:a:529:GLN:NE2	2.93	0.41
7:f:47:LYS:HD2	7:f:47:LYS:HA	1.78	0.41
8:g:156:VAL:HG12	8:g:160:HIS:CE1	2.55	0.41
12:k:4:PRO:O	12:k:7:GLN:N	2.54	0.41
12:k:5:TYR:HA	12:k:8:GLU:OE2	2.21	0.41
13:n:767:MET:SD	13:n:780:LEU:HD11	2.61	0.41
14:q:504:MET:O	14:q:508:LEU:HG	2.19	0.41
17:t:152:LEU:HD21	17:t:204:TYR:CE2	2.56	0.41
22:A:464:PRO:HB3	32:K:4:PRO:HD3	2.02	0.41
22:A:1207:LEU:HD12	22:A:1207:LEU:HA	1.85	0.41
22:A:1336:MET:HA	22:A:1340:GLY:O	2.21	0.41
23:B:759:PRO:HD2	23:B:1046:PRO:HB3	2.02	0.41
32:K:19:LEU:HD22	32:K:35:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:134:HIS:HB2	2:P:354:ASP:OD1	2.21	0.41
4:S:153:LEU:HD21	4:S:179:GLU:CB	2.50	0.41
5:a:189:ARG:HH21	5:a:209:GLU:CD	2.28	0.41
6:d:119:ASN:OD1	13:n:293:ARG:NH2	2.53	0.41
8:g:114:TYR:O	8:g:117:GLN:HG3	2.21	0.41
20:w:117:TRP:O	20:w:120:GLU:HG2	2.21	0.41
22:A:393:ARG:HD3	22:A:421:ALA:O	2.20	0.41
22:A:709:THR:HG22	22:A:710:LEU:N	2.36	0.41
22:A:874:ASP:OD1	22:A:875:ALA:N	2.54	0.41
23:B:234:ILE:HG12	23:B:259:TYR:CE1	2.56	0.41
23:B:833:TYR:HB2	23:B:840:ILE:HD11	2.01	0.41
13:n:479:ILE:O	13:n:483:LEU:HG	2.20	0.41
14:q:130:GLN:O	14:q:133:SER:OG	2.38	0.41
22:A:925:LEU:O	22:A:929:LEU:HG	2.20	0.41
22:A:1177:LEU:HD23	22:A:1177:LEU:HA	1.91	0.41
23:B:830:TYR:CZ	23:B:1000:PRO:HD3	2.56	0.41
28:G:15:PRO:HA	28:G:18:PHE:CE2	2.56	0.41
3:Q:59:LEU:HD23	3:Q:61:LEU:HD11	2.03	0.41
3:Q:63:ARG:HB2	3:Q:66:ARG:NH2	2.36	0.41
4:S:216:HIS:O	4:S:220:ASN:N	2.45	0.41
8:g:180:GLU:O	8:g:183:GLU:HG3	2.21	0.41
9:h:153:ARG:HG2	19:v:33:ARG:CZ	2.51	0.41
10:i:98:LEU:O	10:i:102:LYS:HG2	2.19	0.41
13:n:716:LYS:HB3	13:n:746:THR:OG1	2.20	0.41
14:q:254:LEU:HD23	14:q:254:LEU:HA	1.88	0.41
14:q:275:LEU:HD12	14:q:275:LEU:HA	1.91	0.41
16:s:75:PHE:HB3	16:s:78:ILE:HD11	2.02	0.41
23:B:29:ASP:HB3	23:B:658:ILE:HG13	2.01	0.41
24:C:153:LEU:HD11	24:C:155:LEU:HD23	2.03	0.41
24:C:239:PRO:HB2	24:C:242:GLN:HG2	2.01	0.41
33:L:37:LYS:O	33:L:38:LEU:HD23	2.20	0.41
3:Q:91:GLU:HG2	3:Q:109:ASN:HD21	1.85	0.41
4:S:146:HIS:ND1	4:S:149:ARG:HG3	2.36	0.41
4:S:227:PHE:O	4:S:231:CYS:HB2	2.21	0.41
7:f:168:LYS:O	7:f:171:GLN:HG3	2.21	0.41
9:h:42:GLN:HG3	9:h:75:GLN:HE22	1.86	0.41
13:n:299:PHE:HB2	13:n:352:ILE:HG21	2.03	0.41
13:n:689:MET:O	13:n:693:ARG:HG3	2.21	0.41
13:n:753:LEU:HB3	13:n:756:SER:HB3	2.03	0.41
14:q:276:ASN:HA	14:q:279:TRP:HE3	1.86	0.41
14:q:434:LYS:O	14:q:438:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:r:275:LEU:HD23	15:r:275:LEU:HA	1.88	0.41
18:u:106:ASP:O	18:u:110:GLU:OE1	2.39	0.41
18:u:110:GLU:HG3	18:u:113:LYS:HZ3	1.83	0.41
22:A:260:ASP:O	22:A:263:THR:HG22	2.21	0.41
22:A:463:ILE:HD13	22:A:469:ARG:HG2	2.03	0.41
22:A:871:ASP:OD1	22:A:871:ASP:N	2.52	0.41
22:A:1002:GLY:H	22:A:1007:ILE:HG21	1.86	0.41
23:B:281:PRO:O	23:B:285:ILE:HG12	2.21	0.41
23:B:651:LEU:HD21	23:B:741:CYS:SG	2.61	0.41
23:B:857:ARG:HD3	23:B:942:ARG:NH1	2.36	0.41
29:H:101:ALA:HB2	29:H:116:TYR:CZ	2.56	0.41
5:a:299:ILE:HG23	5:a:356:PHE:CZ	2.55	0.41
6:d:140:THR:HA	6:d:143:GLN:NE2	2.36	0.41
7:f:8:GLU:HB3	9:h:115:ARG:HH12	1.86	0.41
8:g:107:ASN:HB3	18:u:95:ASP:HB2	2.03	0.41
9:h:149:LEU:O	9:h:153:ARG:HG3	2.21	0.41
9:h:149:LEU:HG	14:q:277:LYS:NZ	2.36	0.41
10:i:119:PRO:HA	10:i:122:TRP:CZ3	2.55	0.41
14:q:388:PHE:CZ	14:q:479:LEU:HB2	2.56	0.41
17:t:25:SER:HA	17:t:28:ILE:HD12	2.02	0.41
22:A:207:ILE:HG22	22:A:211:PHE:CE1	2.56	0.41
23:B:118:ARG:HA	23:B:118:ARG:HD2	1.72	0.41
30:I:2:THR:OG1	30:I:43:VAL:O	2.33	0.41
8:g:150:ASN:O	16:s:16:TYR:OH	2.38	0.40
17:t:125:ASP:OD1	17:t:126:ALA:N	2.53	0.40
17:t:143:PHE:HD1	17:t:148:PHE:HA	1.86	0.40
19:v:58:VAL:O	19:v:62:THR:HG23	2.21	0.40
20:w:28:GLU:O	20:w:31:GLN:HG3	2.20	0.40
22:A:171:GLN:HA	22:A:172:PRO:HD3	1.92	0.40
23:B:347:LYS:HA	23:B:347:LYS:HD3	1.60	0.40
26:E:167:ARG:HD3	26:E:167:ARG:HA	1.83	0.40
26:E:191:LYS:N	26:E:194:GLU:OE1	2.42	0.40
30:I:75:CYS:HB3	30:I:80:SER:H	1.85	0.40
7:f:100:TYR:O	7:f:104:GLU:OE1	2.38	0.40
7:f:169:ILE:HG12	9:h:116:LYS:CB	2.51	0.40
10:i:72:SER:HA	10:i:75:GLN:CD	2.45	0.40
10:i:129:ARG:O	10:i:132:GLU:HG2	2.20	0.40
13:n:495:ASN:HB3	13:n:498:VAL:HB	2.03	0.40
18:u:1:MET:SD	18:u:1:MET:N	2.85	0.40
19:v:45:ASN:C	19:v:45:ASN:HD22	2.28	0.40
22:A:105:CYS:SG	22:A:139:TRP:HA	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:565:ILE:O	22:A:570:PRO:HA	2.20	0.40
23:B:954:VAL:HG23	33:L:56:LEU:HB2	2.02	0.40
23:B:1106:ARG:NH1	23:B:1118:PRO:HB3	2.34	0.40
25:D:148:LEU:O	25:D:152:SER:OG	2.29	0.40
26:E:12:LEU:HD21	26:E:58:MET:HE1	2.03	0.40
6:d:154:LEU:O	6:d:158:THR:HG23	2.21	0.40
8:g:13:TYR:HD2	20:w:38:TYR:CD1	2.40	0.40
9:h:122:VAL:HG12	9:h:126:MET:HE1	2.02	0.40
10:i:127:HIS:O	10:i:130:GLU:HG3	2.21	0.40
13:n:161:VAL:HG13	16:s:40:LEU:HD22	2.03	0.40
13:n:287:GLN:O	13:n:300:VAL:HB	2.20	0.40
13:n:782:ALA:HB3	13:n:810:PHE:CZ	2.56	0.40
22:A:118:HIS:CG	22:A:152:VAL:HG11	2.56	0.40
22:A:1166:ASP:OD1	22:A:1237:ILE:HG21	2.21	0.40
7:f:98:PRO:O	7:f:101:MET:HB2	2.22	0.40
12:k:4:PRO:O	12:k:7:GLN:HB2	2.21	0.40
22:A:752:LYS:HG2	23:B:1015:HIS:O	2.21	0.40
22:A:873:MET:HB2	22:A:1366:ARG:NH2	2.36	0.40
23:B:100:PRO:O	23:B:180:TYR:OH	2.28	0.40
23:B:802:PRO:HG2	23:B:805:THR:HG22	2.03	0.40
23:B:1060:ARG:NH1	24:C:202:PRO:HG3	2.37	0.40
4:S:182:MET:HE1	4:S:229:ALA:HA	2.03	0.40
9:h:36:VAL:HA	9:h:39:ARG:NH2	2.36	0.40
11:j:87:ILE:O	16:s:63:SER:HB2	2.22	0.40
14:q:93:ILE:O	14:q:97:MET:HG2	2.22	0.40
15:r:55:ARG:NH1	23:B:887:HIS:O	2.49	0.40
19:v:13:THR:O	19:v:17:LEU:HG	2.22	0.40
19:v:20:LYS:O	19:v:23:GLU:HG3	2.22	0.40
20:w:104:ASP:HB2	21:z:13:THR:O	2.22	0.40
22:A:870:GLU:HG2	26:E:208:TYR:CD2	2.57	0.40
22:A:1409:LEU:HD13	23:B:1207:LEU:HD21	2.04	0.40
23:B:259:TYR:HB2	23:B:270:LYS:HZ1	1.86	0.40
23:B:461:LEU:HA	23:B:461:LEU:HD23	1.89	0.40
23:B:839:MET:HE2	23:B:839:MET:HB3	1.88	0.40
23:B:1059:LEU:HD22	23:B:1066:SER:HA	2.02	0.40
25:D:56:ARG:HG3	25:D:145:MET:HE1	2.03	0.40
27:F:81:THR:HG22	27:F:82:THR:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	M	33/345 (10%)	33 (100%)	0	0	100	100
2	P	99/735 (14%)	98 (99%)	1 (1%)	0	100	100
3	Q	121/400 (30%)	121 (100%)	0	0	100	100
4	S	179/309 (58%)	177 (99%)	2 (1%)	0	100	100
5	a	357/566 (63%)	343 (96%)	11 (3%)	3 (1%)	16	45
6	d	165/284 (58%)	164 (99%)	1 (1%)	0	100	100
7	f	163/295 (55%)	161 (99%)	2 (1%)	0	100	100
8	g	159/222 (72%)	159 (100%)	0	0	100	100
9	h	132/223 (59%)	129 (98%)	3 (2%)	0	100	100
10	i	79/149 (53%)	79 (100%)	0	0	100	100
11	j	142/157 (90%)	137 (96%)	5 (4%)	0	100	100
12	k	104/115 (90%)	104 (100%)	0	0	100	100
13	n	611/1082 (56%)	607 (99%)	4 (1%)	0	100	100
14	q	505/687 (74%)	500 (99%)	5 (1%)	0	100	100
15	r	249/307 (81%)	244 (98%)	5 (2%)	0	100	100
16	s	77/220 (35%)	76 (99%)	1 (1%)	0	100	100
17	t	208/210 (99%)	206 (99%)	2 (1%)	0	100	100
18	u	116/140 (83%)	115 (99%)	1 (1%)	0	100	100
19	v	105/120 (88%)	105 (100%)	0	0	100	100
20	w	99/127 (78%)	97 (98%)	2 (2%)	0	100	100
21	z	23/25 (92%)	21 (91%)	1 (4%)	1 (4%)	2	14
22	A	1451/1453 (100%)	1407 (97%)	43 (3%)	1 (0%)	48	75
23	B	1164/1224 (95%)	1132 (97%)	32 (3%)	0	100	100
24	C	269/318 (85%)	261 (97%)	8 (3%)	0	100	100
25	D	165/221 (75%)	163 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	E	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
27	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
28	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
29	H	137/146 (94%)	133 (97%)	4 (3%)	0	100	100
30	I	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
31	J	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
32	K	114/120 (95%)	112 (98%)	2 (2%)	0	100	100
33	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	7715/11003 (70%)	7560 (98%)	150 (2%)	5 (0%)	49	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	z	21	SER
5	a	291	SER
5	a	306	ASN
5	a	289	CYS
22	A	958	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	M	32/299 (11%)	32 (100%)	0	100	100
2	P	95/641 (15%)	95 (100%)	0	100	100
3	Q	119/363 (33%)	119 (100%)	0	100	100
4	S	158/274 (58%)	158 (100%)	0	100	100
5	a	350/528 (66%)	347 (99%)	3 (1%)	70	78
6	d	158/258 (61%)	158 (100%)	0	100	100
7	f	158/259 (61%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	g	160/208 (77%)	160 (100%)	0	100	100
9	h	128/207 (62%)	128 (100%)	0	100	100
10	i	82/144 (57%)	82 (100%)	0	100	100
11	j	134/145 (92%)	134 (100%)	0	100	100
12	k	101/108 (94%)	101 (100%)	0	100	100
13	n	591/1001 (59%)	591 (100%)	0	100	100
14	q	482/642 (75%)	482 (100%)	0	100	100
15	r	228/280 (81%)	228 (100%)	0	100	100
16	s	75/195 (38%)	75 (100%)	0	100	100
17	t	178/178 (100%)	178 (100%)	0	100	100
18	u	115/132 (87%)	115 (100%)	0	100	100
19	v	101/112 (90%)	101 (100%)	0	100	100
20	w	97/117 (83%)	97 (100%)	0	100	100
21	z	25/25 (100%)	25 (100%)	0	100	100
22	A	1268/1268 (100%)	1267 (100%)	1 (0%)	88	90
23	B	1018/1061 (96%)	1018 (100%)	0	100	100
24	C	239/274 (87%)	239 (100%)	0	100	100
25	D	150/200 (75%)	150 (100%)	0	100	100
26	E	197/197 (100%)	197 (100%)	0	100	100
27	F	76/137 (56%)	76 (100%)	0	100	100
28	G	152/152 (100%)	152 (100%)	0	100	100
29	H	124/128 (97%)	124 (100%)	0	100	100
30	I	110/116 (95%)	110 (100%)	0	100	100
31	J	65/65 (100%)	65 (100%)	0	100	100
32	K	99/102 (97%)	99 (100%)	0	100	100
33	L	38/57 (67%)	38 (100%)	0	100	100
All	All	7103/9873 (72%)	7099 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	a	288	THR
5	a	290	SER

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Mol	Chain	Res	Type
5	a	296	SER
22	A	1124	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	359	ASN
4	S	166	HIS
4	S	169	GLN
4	S	304	ASN
5	a	30	ASN
5	a	106	ASN
5	a	177	GLN
5	a	235	GLN
5	a	250	ASN
5	a	292	ASN
5	a	529	GLN
6	d	144	GLN
7	f	10	GLN
8	g	129	ASN
8	g	169	GLN
8	g	194	GLN
9	h	150	GLN
12	k	14	ASN
12	k	19	GLN
12	k	101	GLN
13	n	114	ASN
13	n	173	ASN
13	n	250	ASN
13	n	399	ASN
13	n	502	GLN
13	n	541	ASN
13	n	715	ASN
14	q	360	ASN
14	q	365	ASN
15	r	243	ASN
18	u	9	GLN
18	u	98	GLN
19	v	4	GLN
19	v	43	GLN
20	w	119	ASN
22	A	169	ASN

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Mol	Chain	Res	Type
22	A	471	ASN
22	A	490	HIS
22	A	510	GLN
22	A	589	GLN
22	A	742	ASN
22	A	760	GLN
22	A	1211	GLN
22	A	1232	ASN
22	A	1427	ASN
23	B	60	GLN
23	B	357	GLN
23	B	821	GLN
25	D	138	ASN
25	D	179	GLN
27	F	100	GLN
28	G	122	ASN
28	G	131	GLN
29	H	133	ASN
29	H	137	GLN
30	I	89	GLN
31	J	23	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	q	1
18	u	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	318:ASN	C	319:LYS	N	5.82
1	u	80:LEU	C	81:PRO	N	3.18

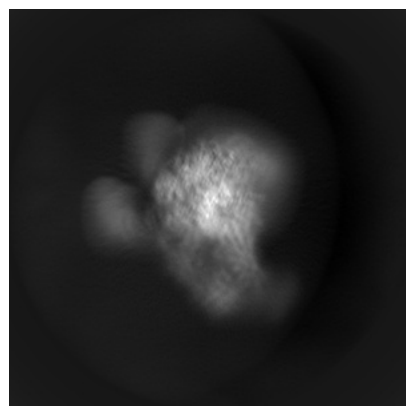
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26542. These allow visual inspection of the internal detail of the map and identification of artifacts.

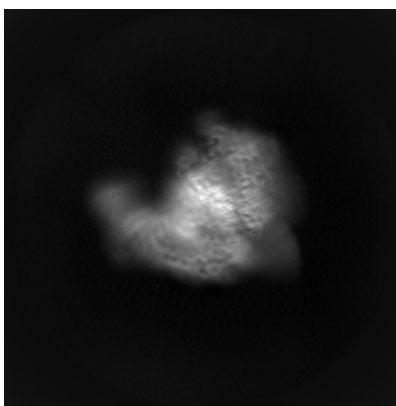
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

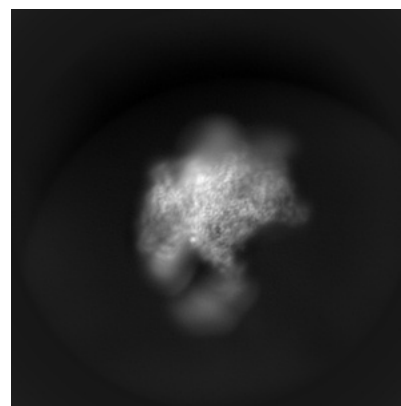
6.1.1 Primary map



X

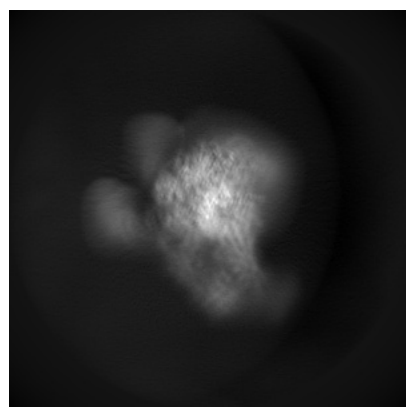


Y

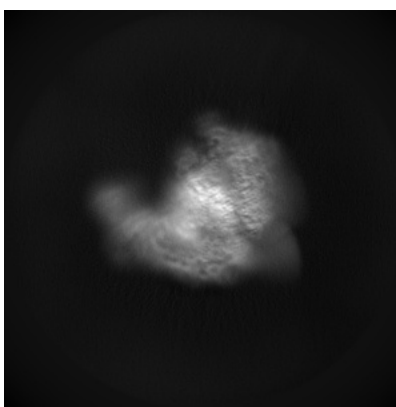


Z

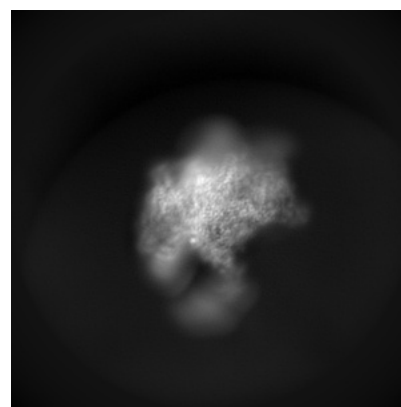
6.1.2 Raw map



X



Y

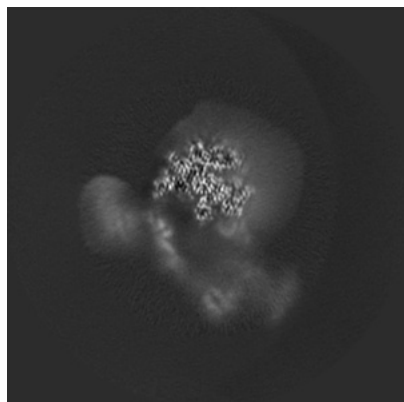


Z

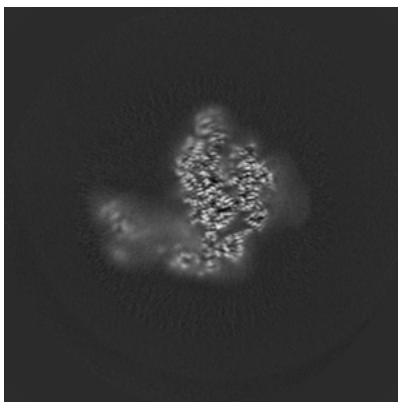
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

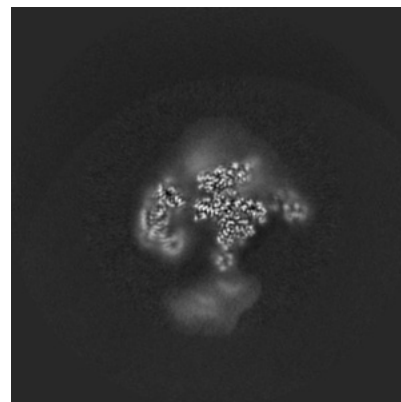
6.2.1 Primary map



X Index: 180

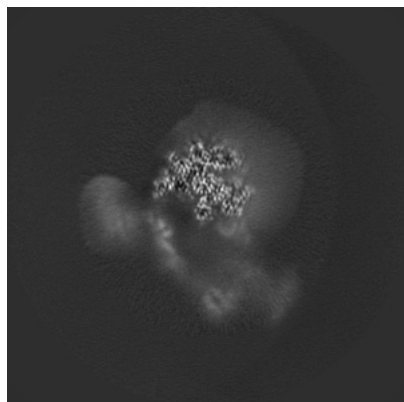


Y Index: 180

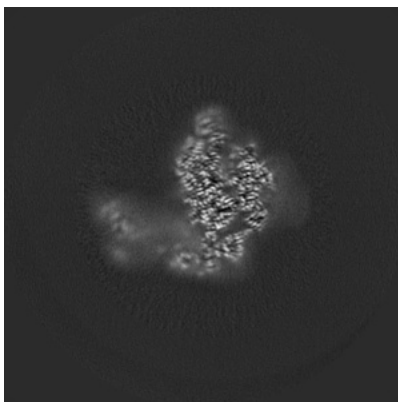


Z Index: 180

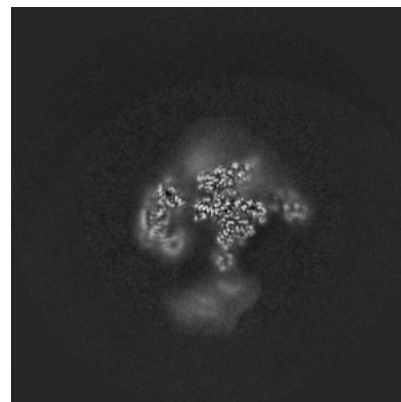
6.2.2 Raw map



X Index: 180



Y Index: 180

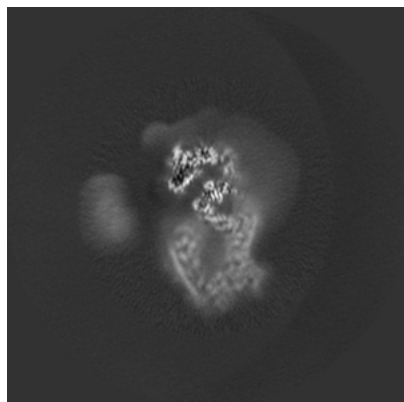


Z Index: 180

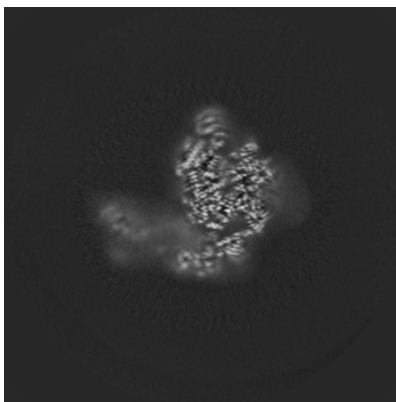
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

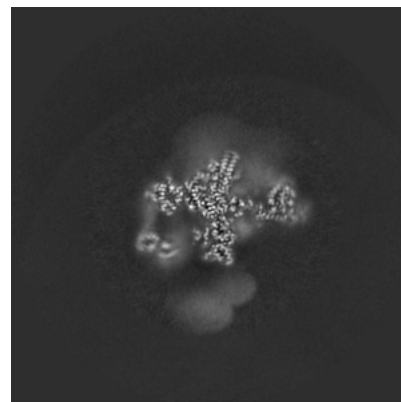
6.3.1 Primary map



X Index: 166

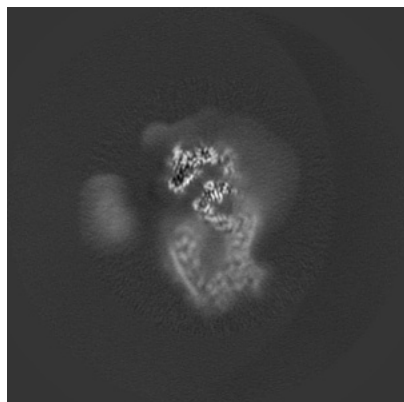


Y Index: 178

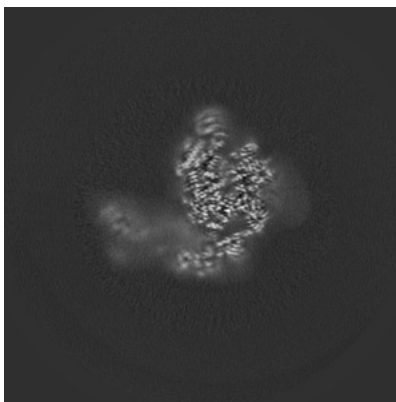


Z Index: 193

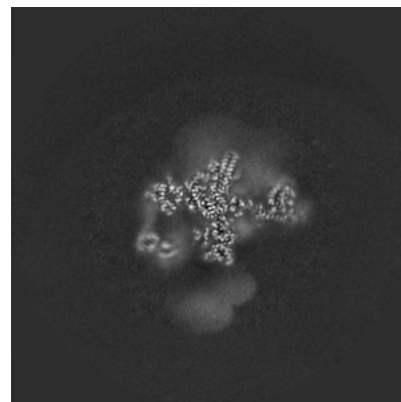
6.3.2 Raw map



X Index: 166



Y Index: 178

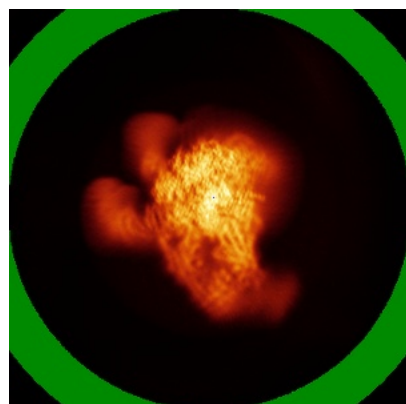


Z Index: 193

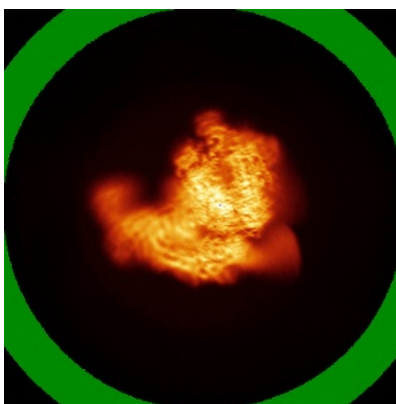
The images above show the largest variance slices of the map in three orthogonal directions.

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

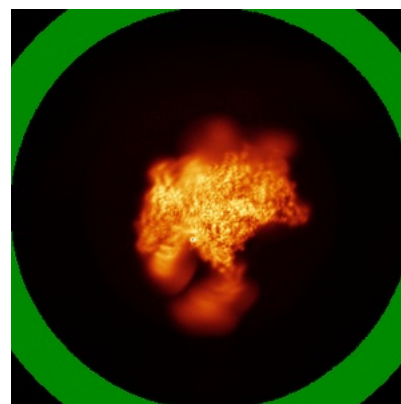
6.4.1 Primary map



X

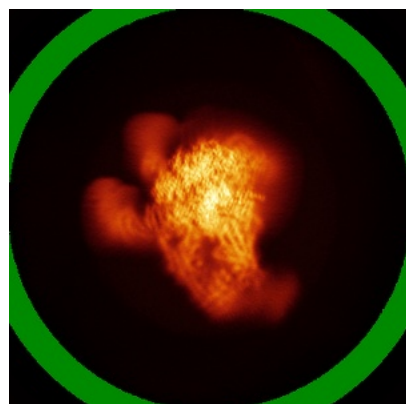


Y

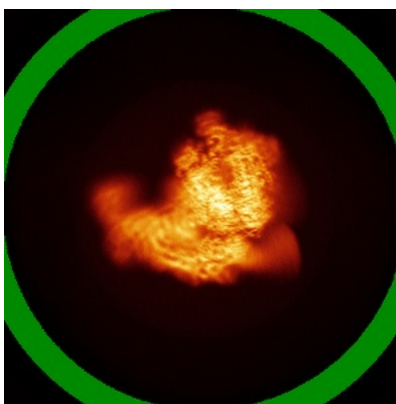


Z

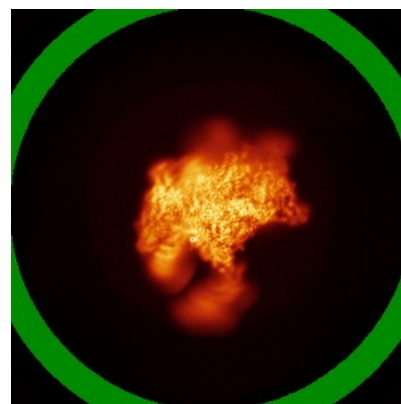
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

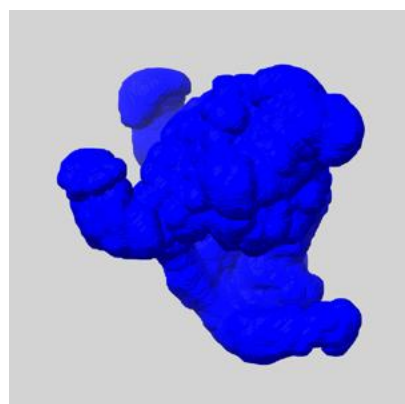
6.6 Mask visualisation [i](#)

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

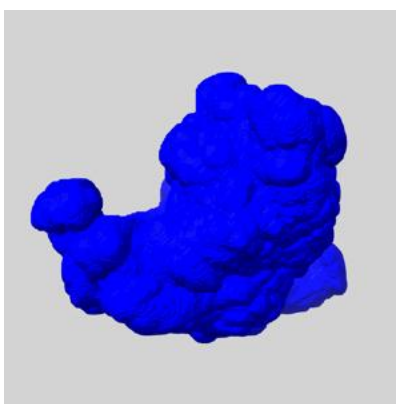
A mask typically either:

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

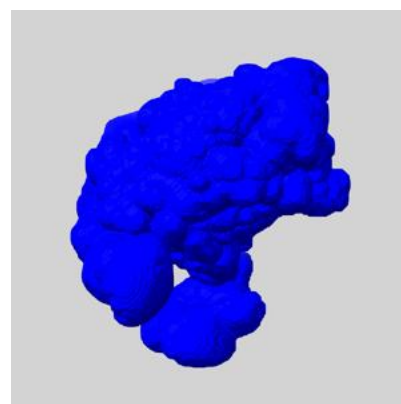
6.6.1 emd_26542_msk_1.map [i](#)



X



Y

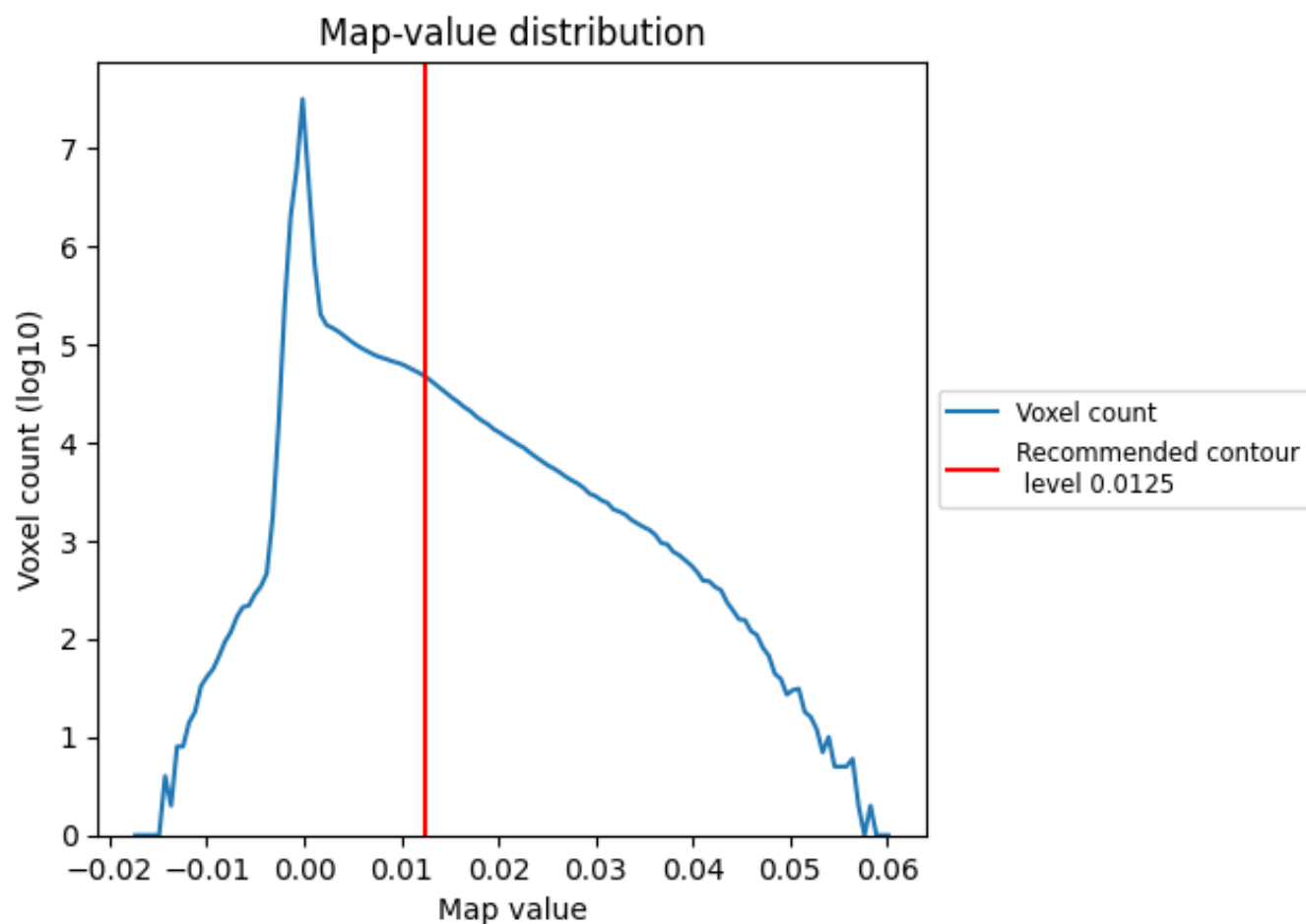


Z

7 Map analysis [i](#)

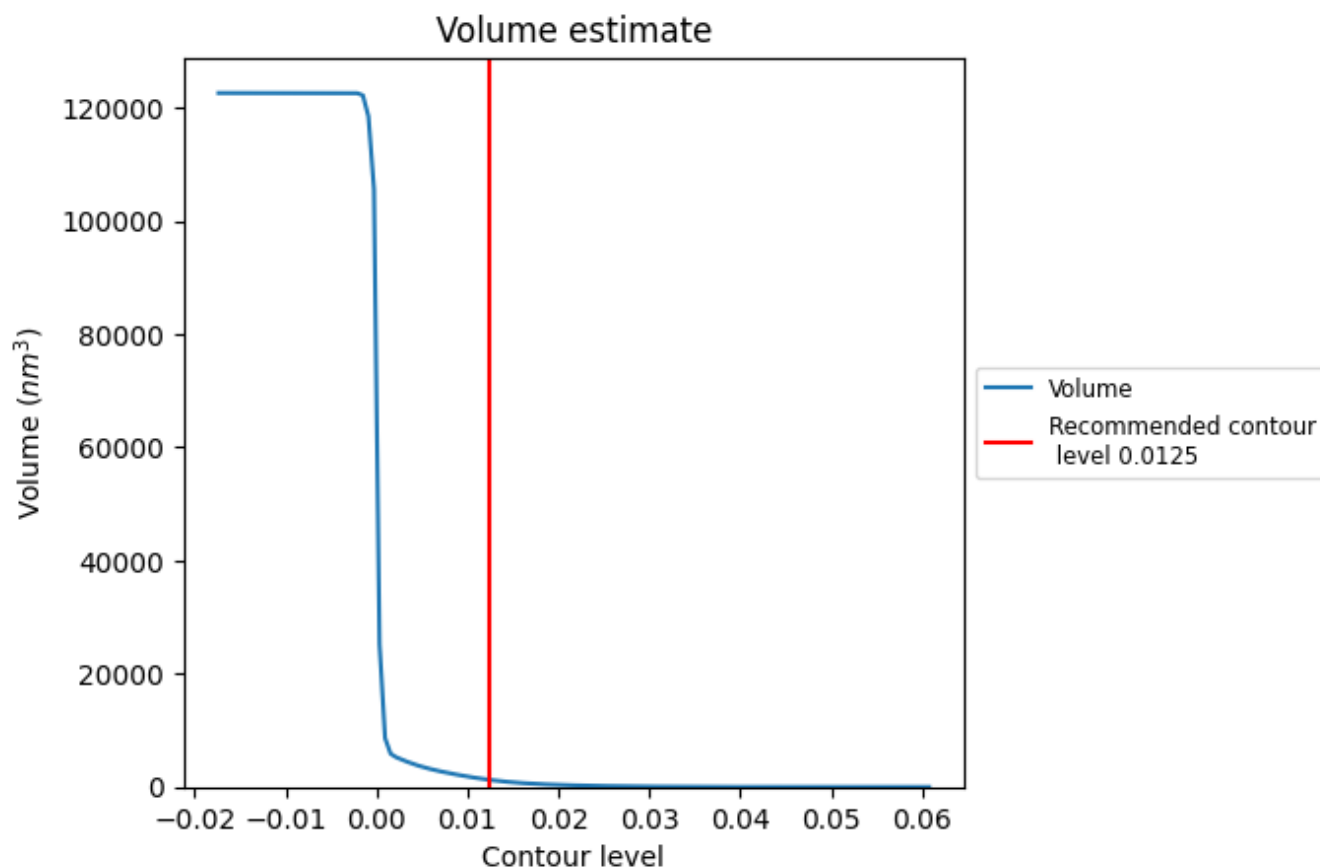
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

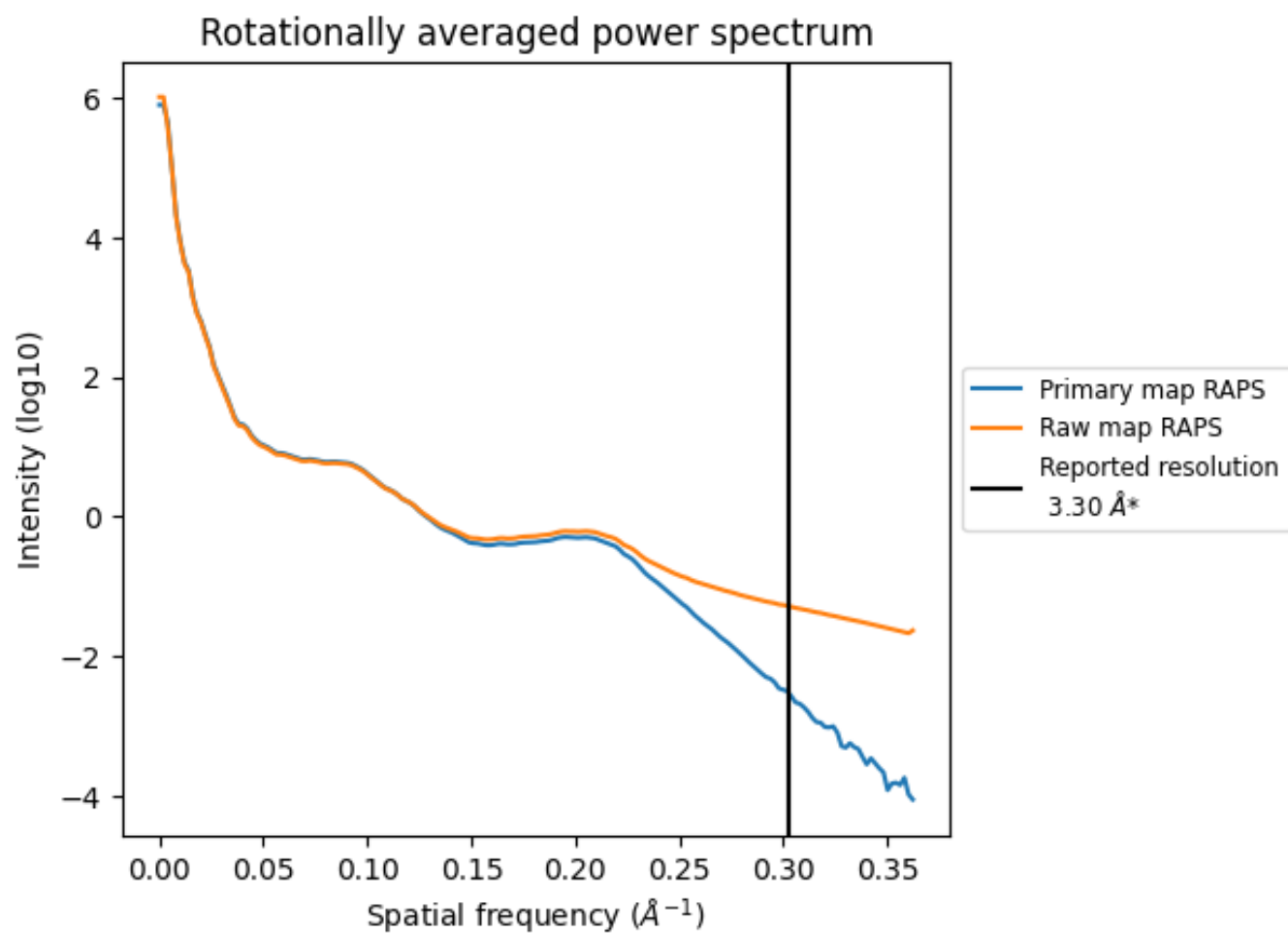
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1241 nm³; this corresponds to an approximate mass of 1121 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 ⓘ

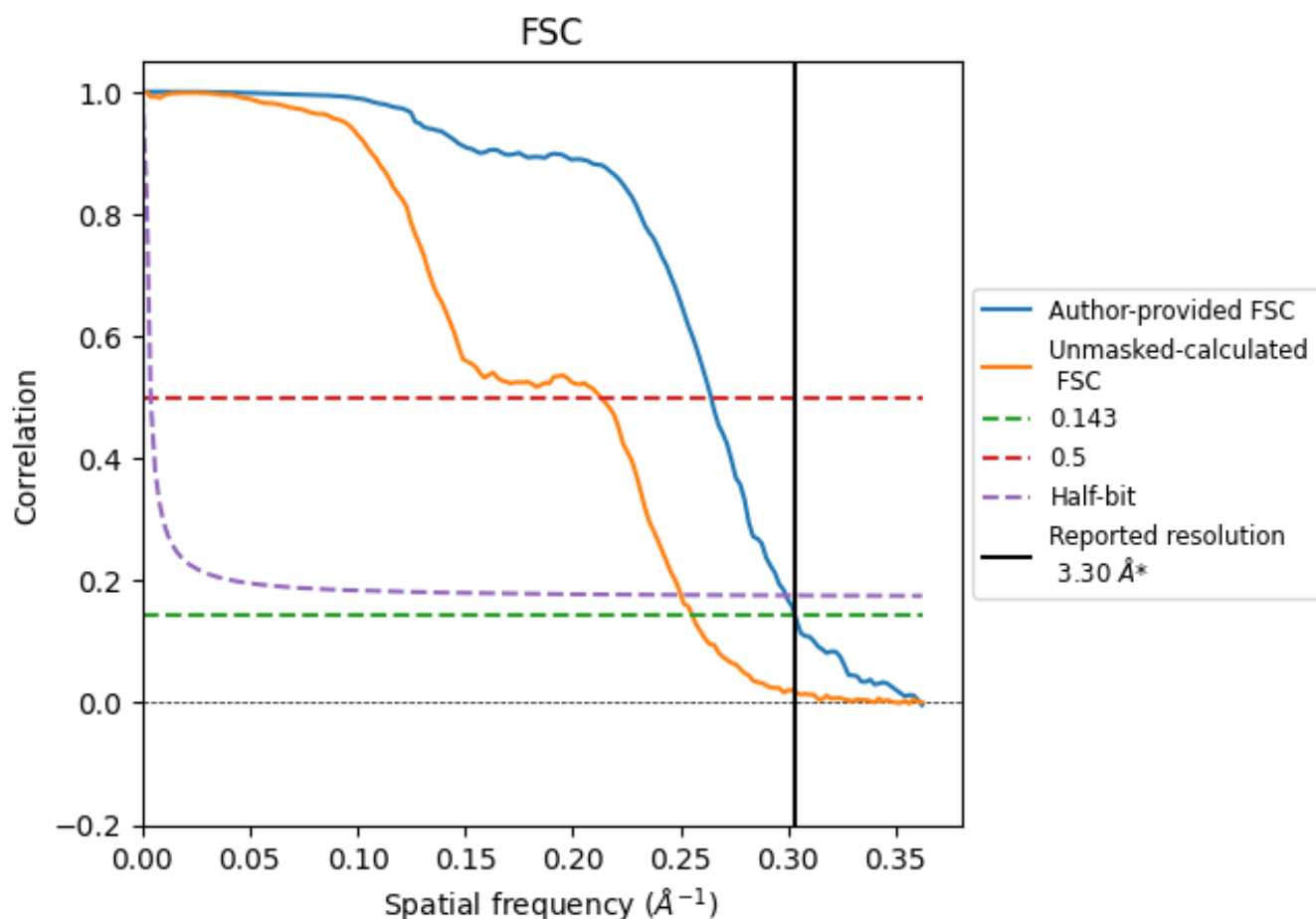


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

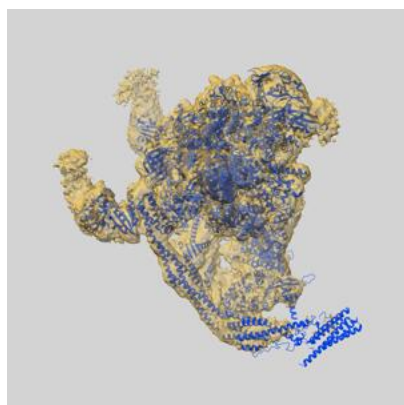
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.79	3.34
Unmasked-calculated*	3.91	4.70	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.3 by more than 10 %

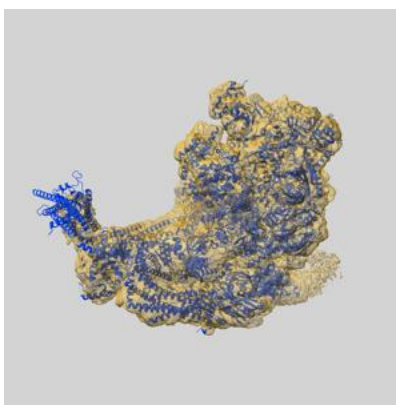
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26542 and PDB model 7UI9. Per-residue inclusion information can be found in section 3 on page 10.

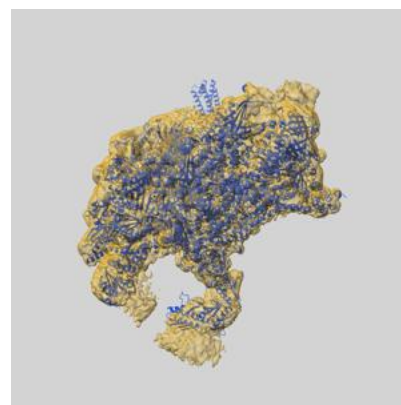
9.1 Map-model overlay [i](#)



X



Y



Z

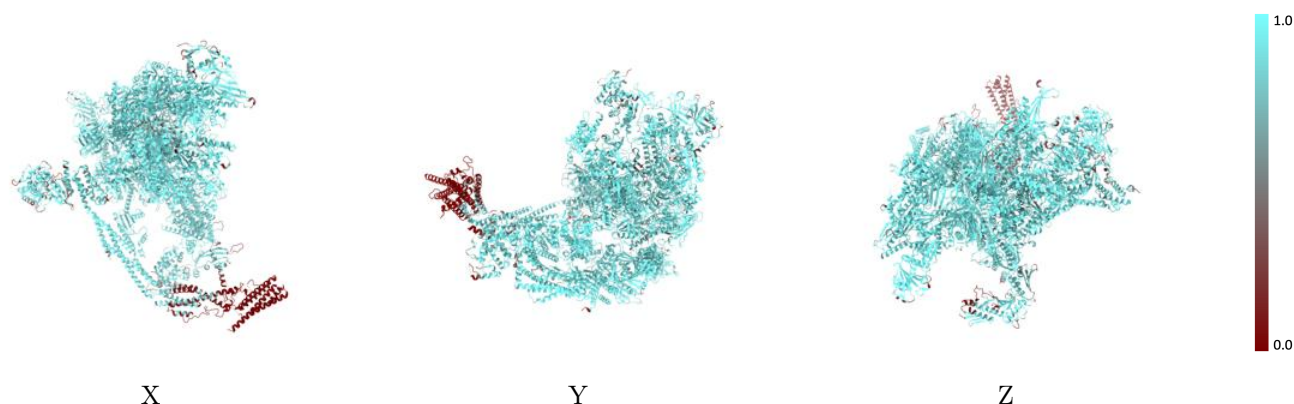
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



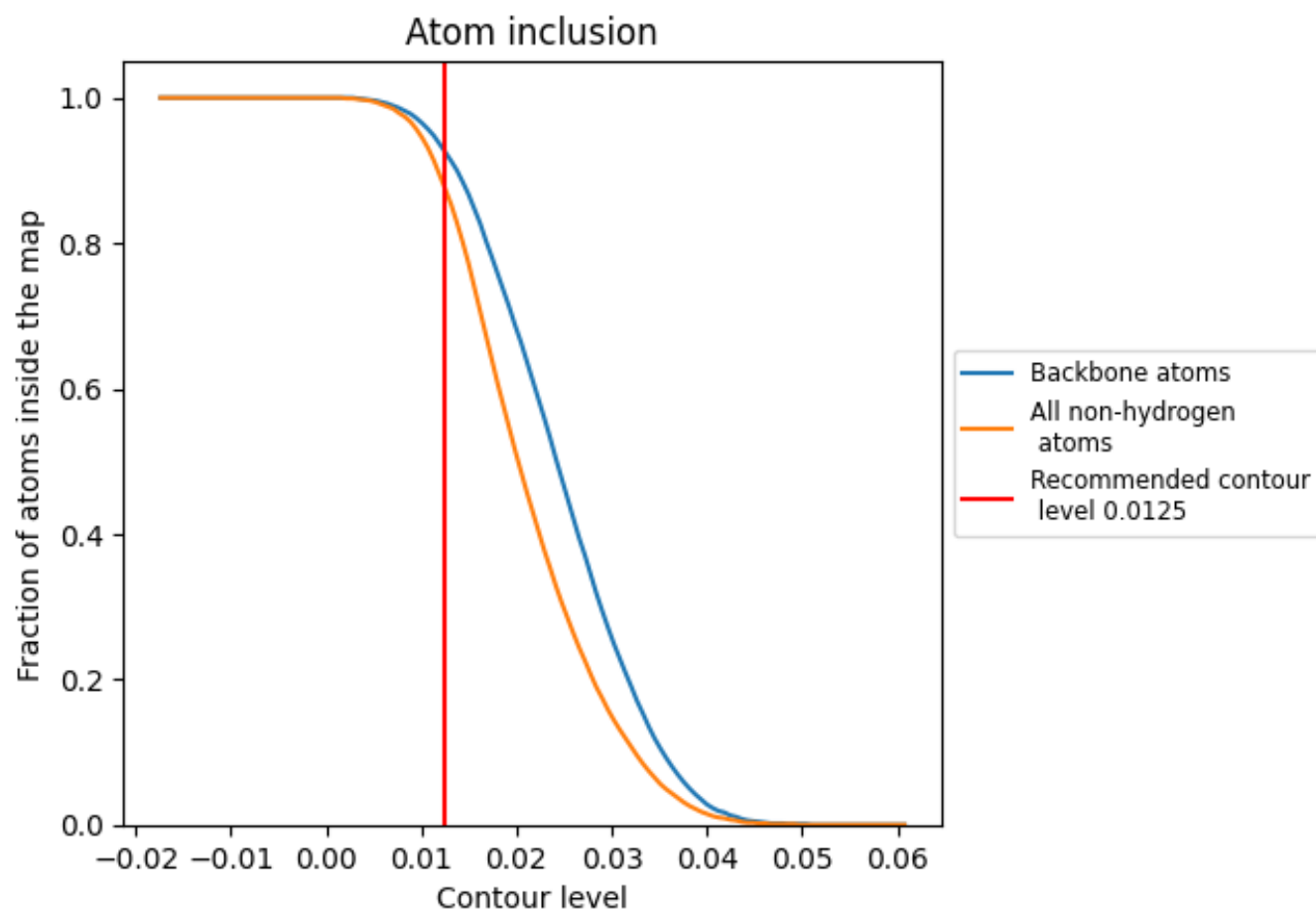
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.2940
A	 0.9300	 0.3960
B	 0.9450	 0.3960
C	 0.9390	 0.4190
D	 0.9840	 0.1810
E	 0.9660	 0.3800
F	 0.9350	 0.4230
G	 0.9730	 0.2730
H	 0.8940	 0.4240
I	 0.9190	 0.3600
J	 0.9090	 0.3550
K	 0.9260	 0.4140
L	 0.8400	 0.3210
M	 0.9730	 0.4370
P	 0.8710	 0.2170
Q	 0.7460	 0.1730
S	 0.8020	 0.2400
a	 0.7470	 0.1030
d	 0.8760	 0.1560
f	 0.7750	 0.1640
g	 0.7730	 0.1470
h	 0.9840	 0.2170
i	 0.8920	 0.1800
j	 0.1590	 0.0540
k	 0.9480	 0.2530
n	 0.8220	 0.1790
q	 0.9320	 0.2370
r	 0.9400	 0.4050
s	 0.0230	 0.0530
t	 0.9430	 0.4020
u	 0.6940	 0.1490
v	 0.9220	 0.2140
w	 0.9330	 0.1760
z	 0.9560	 0.1970

