Full wwPDB EM Validation Report

Oct 27, 2024 – 08:35 AM EDT

PDB ID	:	8TQW
EMDB ID	:	EMD-41565
Title	:	Structure of human transcriptional Mediator complex
Authors	:	Chen, S.F.; Chao, T.C.; Kim, H.J.; Tang, H.C.; Khadka, S.; Li, T.; Murakami, K.; Boyer, T.G.; Tsai, K.L.
Deposited on	:	2023-08-08
Resolution	:	8.20 Å(reported)

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

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

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

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

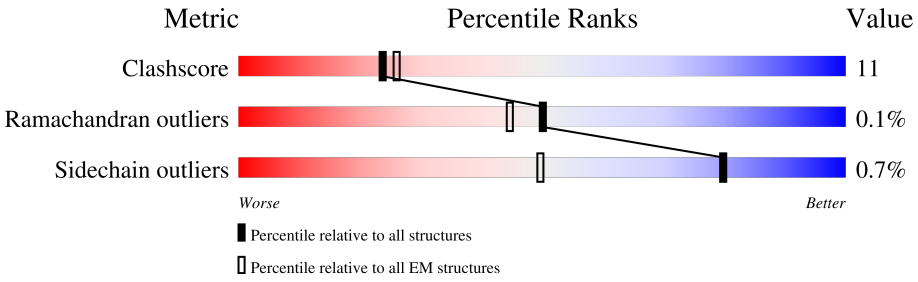
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 8.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	311	68% 18% · 14%
2	1	178	33% 22% · 44%
3	2	200	48% 10% 42%
4	3	178	52% 16% 31%
5	4	131	57% 29% 14%
6	A	1581	19% 11% 70%
7	B	20	65% 35%
8	D	270	36% 21% · 41%

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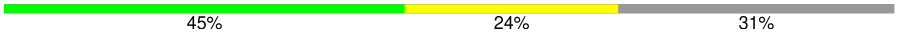
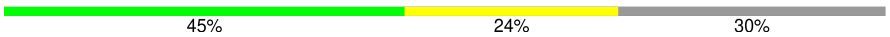
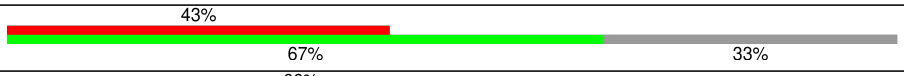
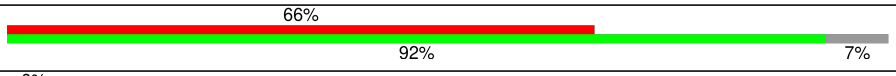
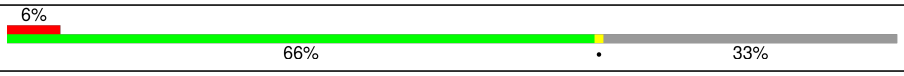
Mol	Chain	Length	Quality of chain
9	F	246	
10	G	233	
11	H	268	
12	I	146	
13	J	135	
14	K	117	
15	N	1454	
16	O	788	
17	P	877	
18	Q	651	
19	R	208	
20	S	244	
21	T	212	
22	U	144	
23	V	200	
24	W	1368	
25	X	989	
26	a	464	
27	b	283	
28	c	2177	
29	d	2174	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83816 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 Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	267	Total	C	N	O	S	0	0
			2159	1373	384	390	12		

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	99	Total	C	N	O	S	0	0
			817	511	143	160	3		

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	122	Total	C	N	O	S	0	0
			1022	639	187	189	7		

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	113	Total	C	N	O	S	0	0
			986	642	171	168	5		

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	467	Total	C	N	O	S	0	0
			3578	2278	613	663	24		

- Molecule 7 is a protein called Unknown Chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	158	Total	C	N	O	S	0	0
			1268	791	228	243	6		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	166	Total	C	N	O	S	0	0
			1363	882	234	242	5		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	161	Total	C	N	O	S	0	0
			1348	856	239	243	10		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	181	Total	C	N	O	S	0	0
			1422	888	250	280	4		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	73	Total	C	N	O	S	0	0
			605	382	107	110	6		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	122	Total	C	N	O	S	0	0
			840	527	151	159	3		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	112	Total	C	N	O	S	0	0
			879	537	163	175	4		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	1017	Total	C	N	O	S	0	0
			7772	4958	1365	1407	42		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	157	Total	C	N	O	S	0	0
			1226	783	213	223	7		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	753	Total	C	N	O	S	0	0
			5875	3742	1008	1077	48		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	546	Total	C	N	O	S	0	0
			4319	2732	773	794	20		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	191	Total	C	N	O	S	0	0
			1532	971	270	276	15		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	75	Total	C	N	O	S	0	0
			517	328	87	100	2		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	193	Total	C	N	O	S	0	0
			1499	955	247	280	17		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	121	Total	C	N	O	S	0	0
			918	570	153	190	5		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	130	Total	C	N	O	S	0	0
			1063	656	181	222	4		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	1334	Total	C	N	O	S	0	0
			10774	6967	1827	1909	71		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	897	Total	C	N	O	S	0	0
			7061	4524	1190	1293	54		

- Molecule 26 is a protein called Cyclin-dependent kinase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	313	Total	C	N	O	S	0	0
			2561	1663	439	442	17		

- Molecule 27 is a protein called Cyclin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	262	Total	C	N	O	S	1	0
			2196	1442	358	379	17		

- Molecule 28 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	1452	Total	C	N	O	S	0	0
			11499	7270	2009	2147	73		

- Molecule 29 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	969	Total	C	N	O	S	0	0
			7714	4945	1310	1393	66		

- Molecule 30 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

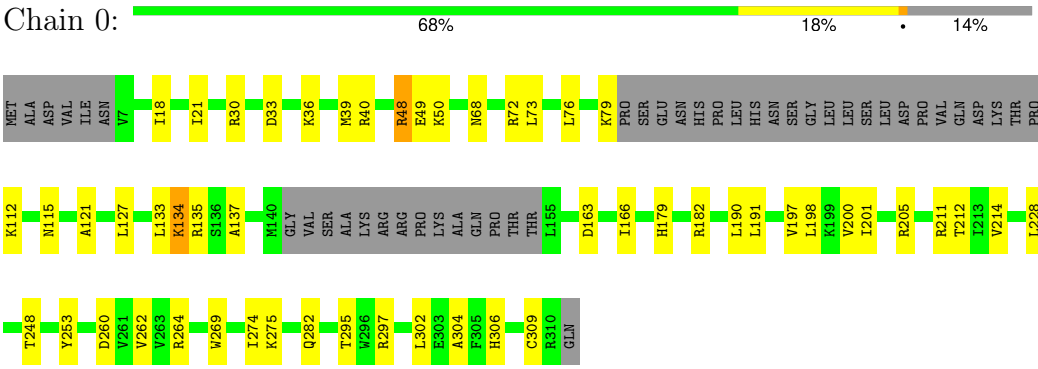
Mol	Chain	Residues	Atoms		AltConf
30	0	1	Total	Zn	0
			1	1	
30	P	1	Total	Zn	0
			1	1	
30	c	1	Total	Zn	0
			1	1	
30	d	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

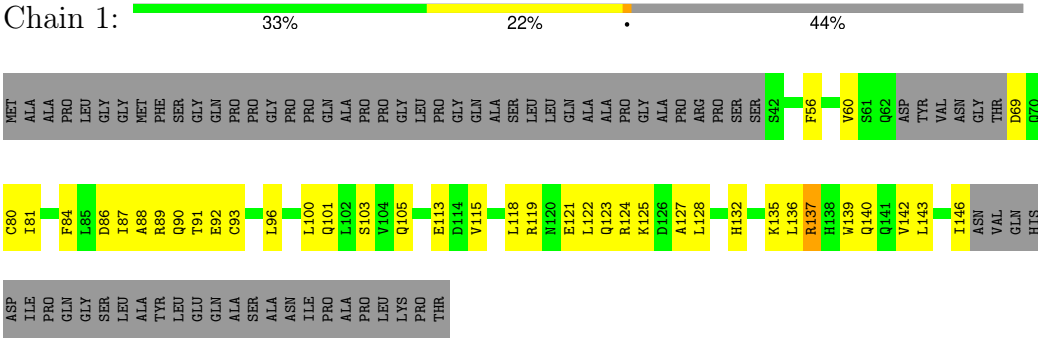
• Molecule 1: Mediator of RNA polymerase II transcription subunit 27

Chain 0:



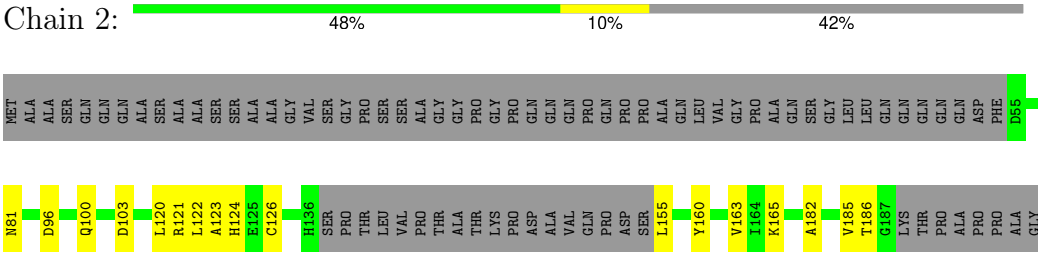
• Molecule 2: Mediator of RNA polymerase II transcription subunit 28

Chain 1:



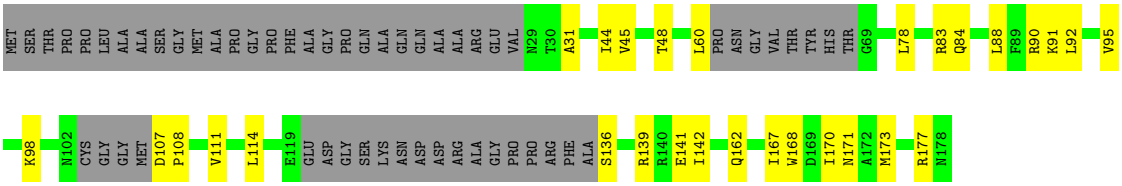
• Molecule 3: Mediator of RNA polymerase II transcription subunit 29

Chain 2:



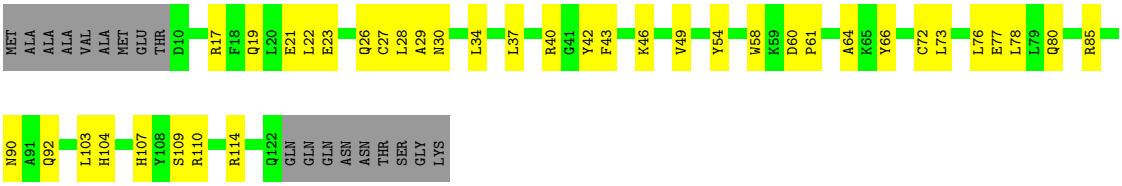
• Molecule 4: Mediator of RNA polymerase II transcription subunit 30

Chain 3:



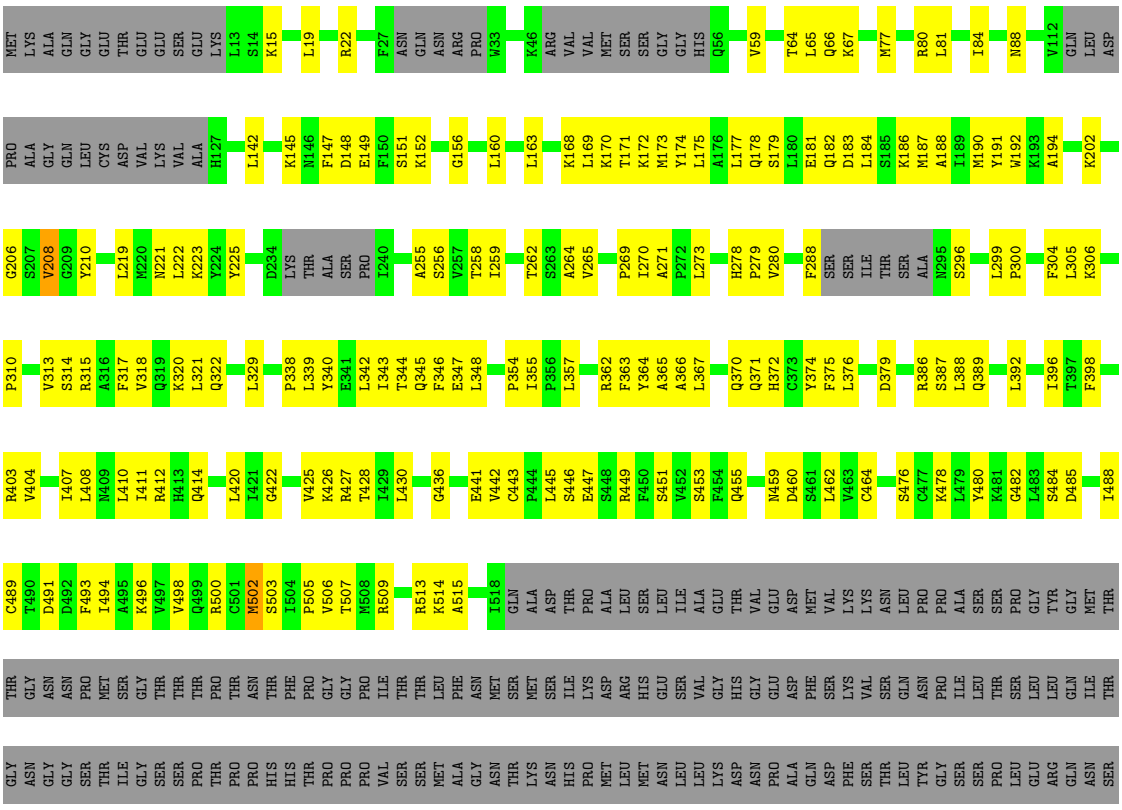
• Molecule 5: Mediator of RNA polymerase II transcription subunit 31

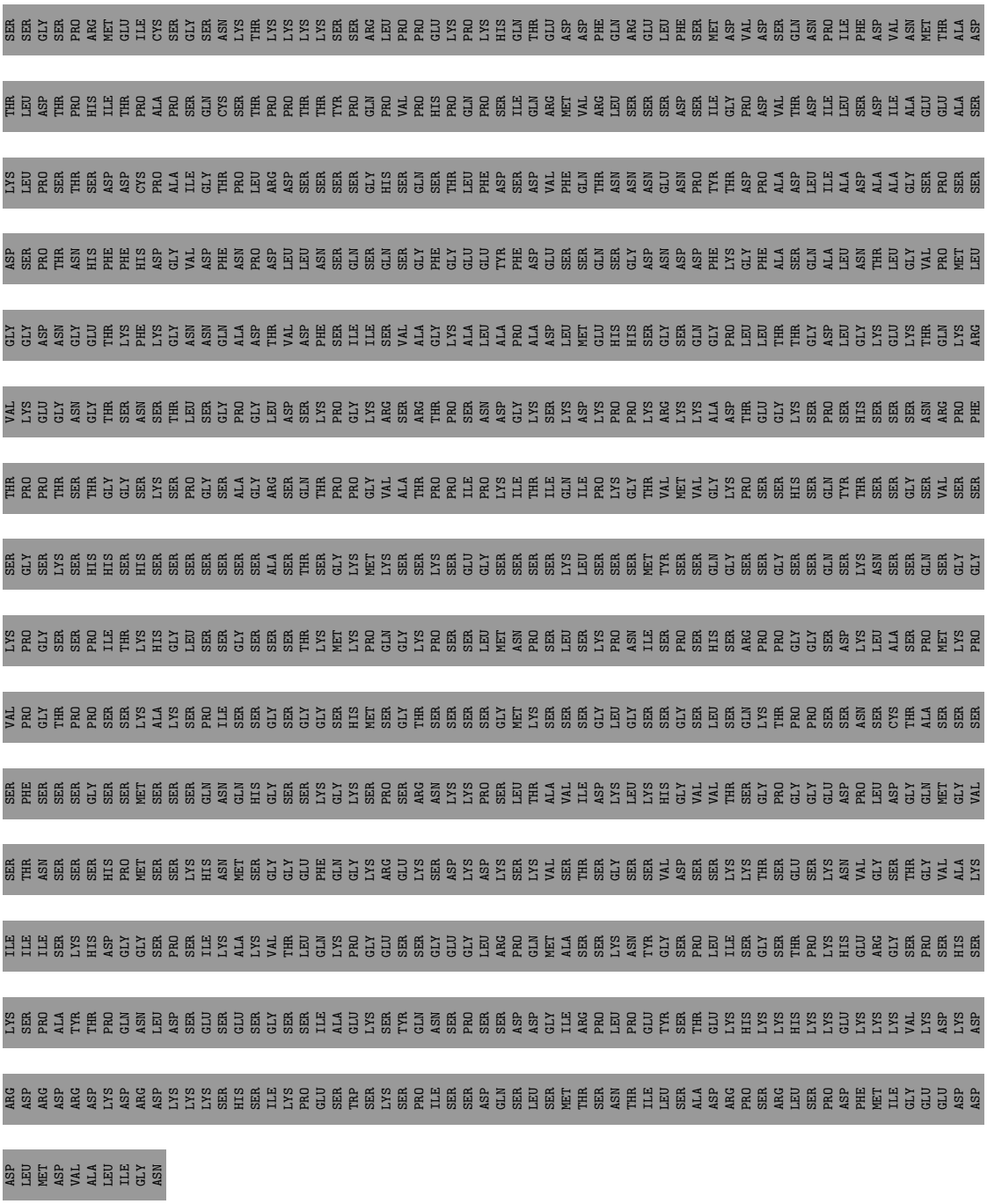
Chain 4:



• Molecule 6: Mediator of RNA polymerase II transcription subunit 1

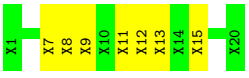
Chain A:





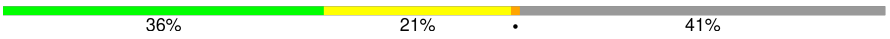
• Molecule 7: Unknown Chain

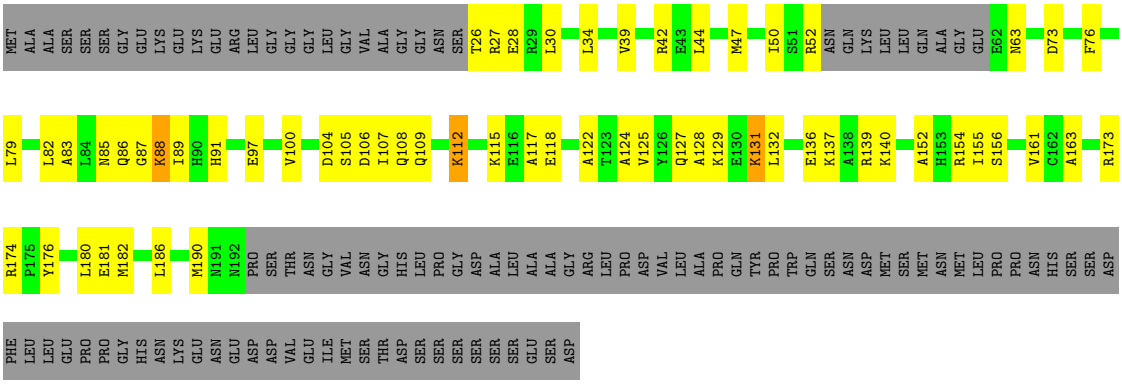
Chain B:



• Molecule 8: Mediator of RNA polymerase II transcription subunit 4

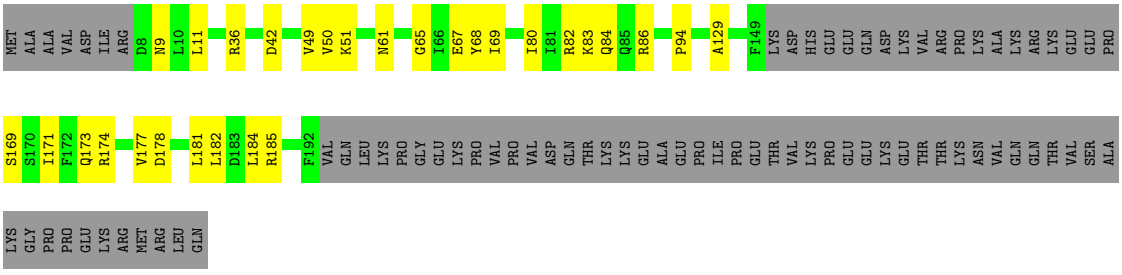
Chain D:





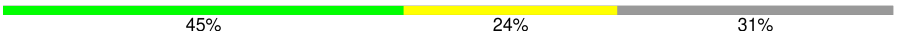
• Molecule 9: Mediator of RNA polymerase II transcription subunit 6

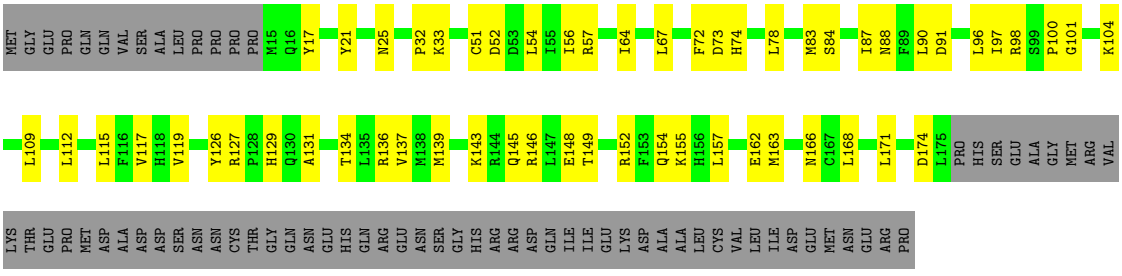
Chain F:



• Molecule 10: Mediator of RNA polymerase II transcription subunit 7

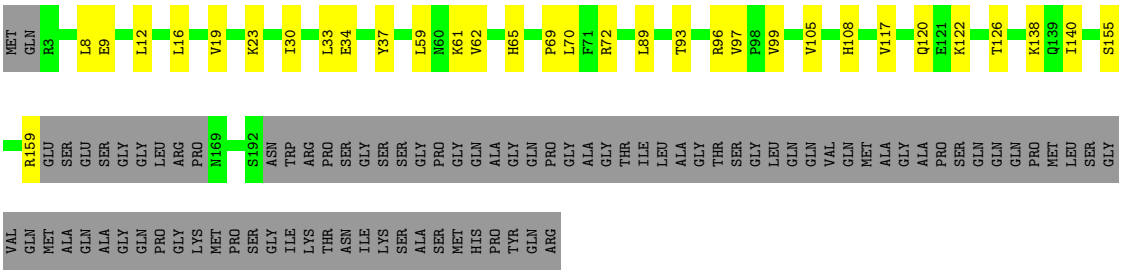
Chain G:





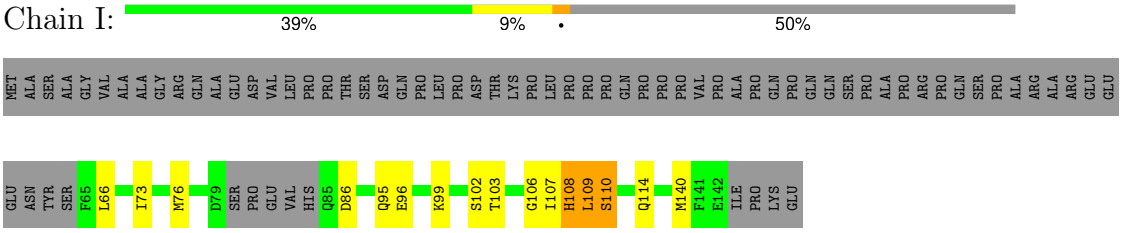
• Molecule 11: Mediator of RNA polymerase II transcription subunit 8

Chain H:



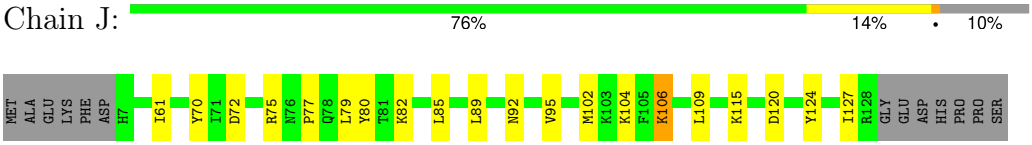
• Molecule 12: Mediator of RNA polymerase II transcription subunit 9

Chain I:



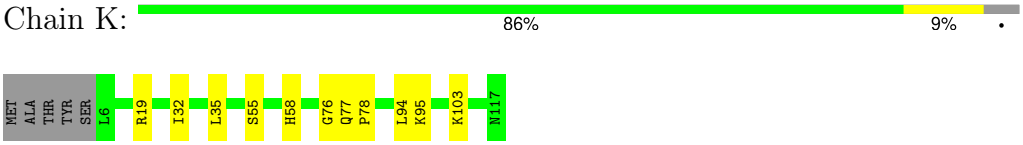
• Molecule 13: Mediator of RNA polymerase II transcription subunit 10

Chain J:



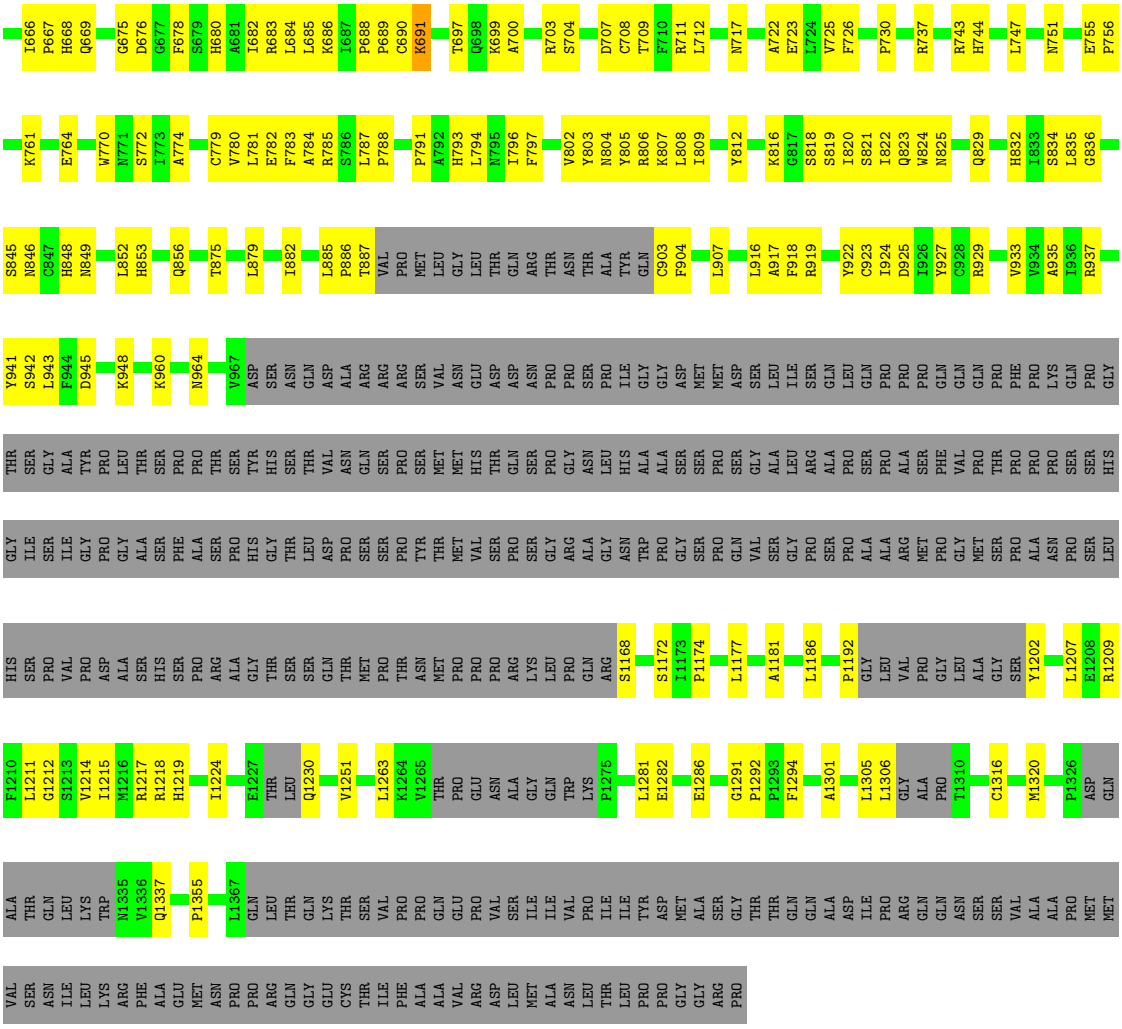
• Molecule 14: Mediator of RNA polymerase II transcription subunit 11

Chain K:



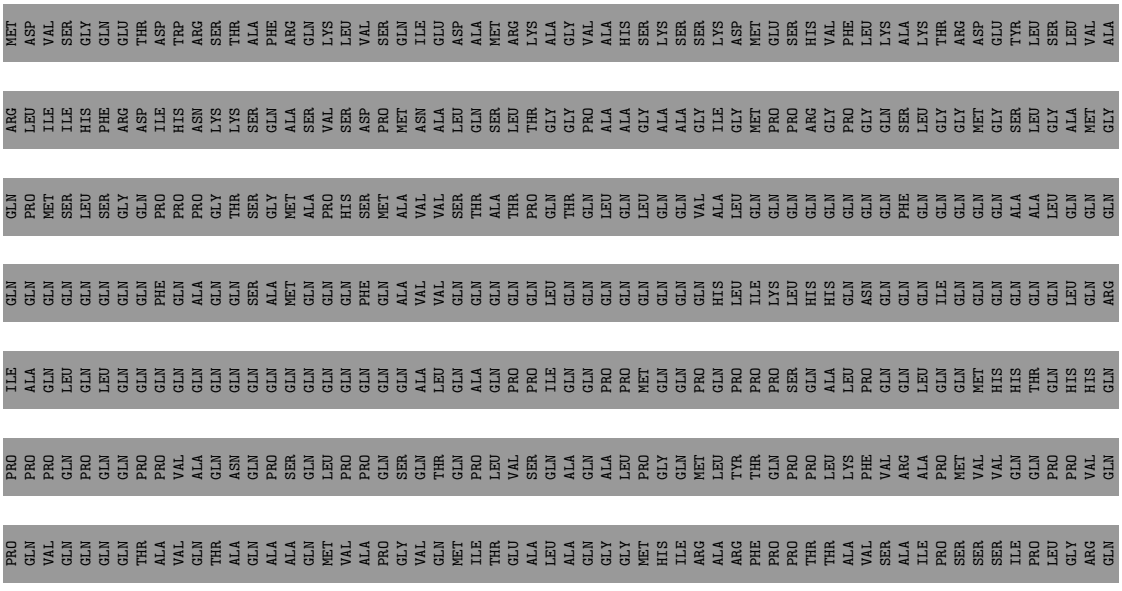
• Molecule 15: Mediator of RNA polymerase II transcription subunit 14

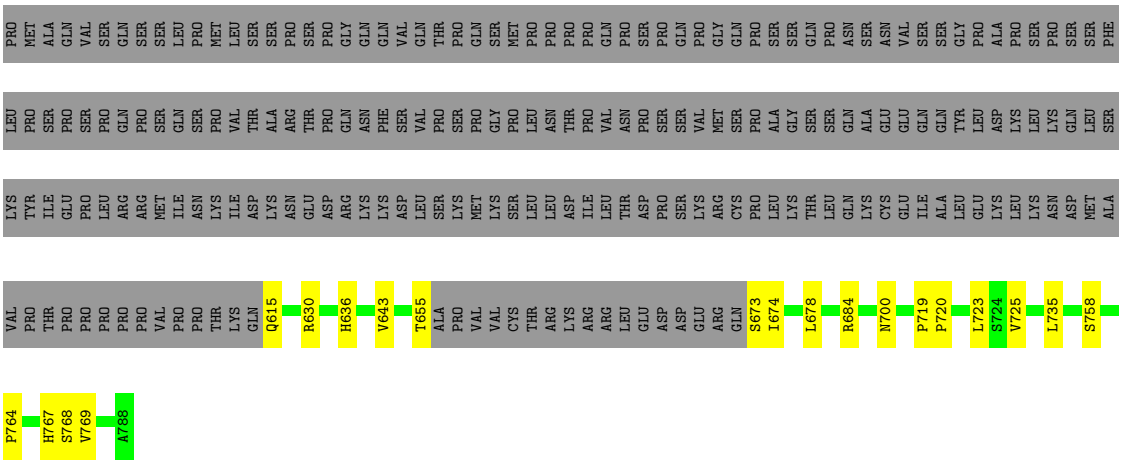
Chain N:



• Molecule 16: Mediator of RNA polymerase II transcription subunit 15

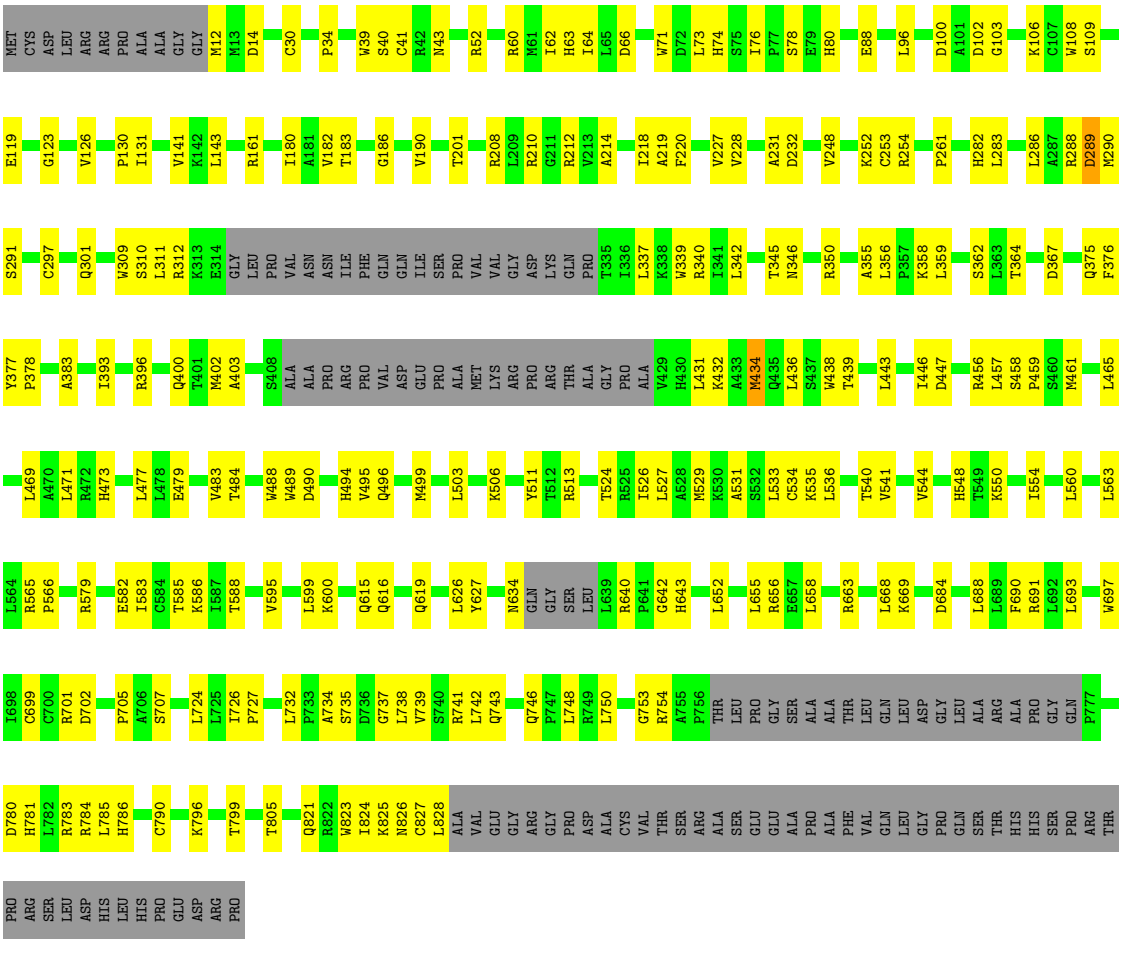
Chain O:





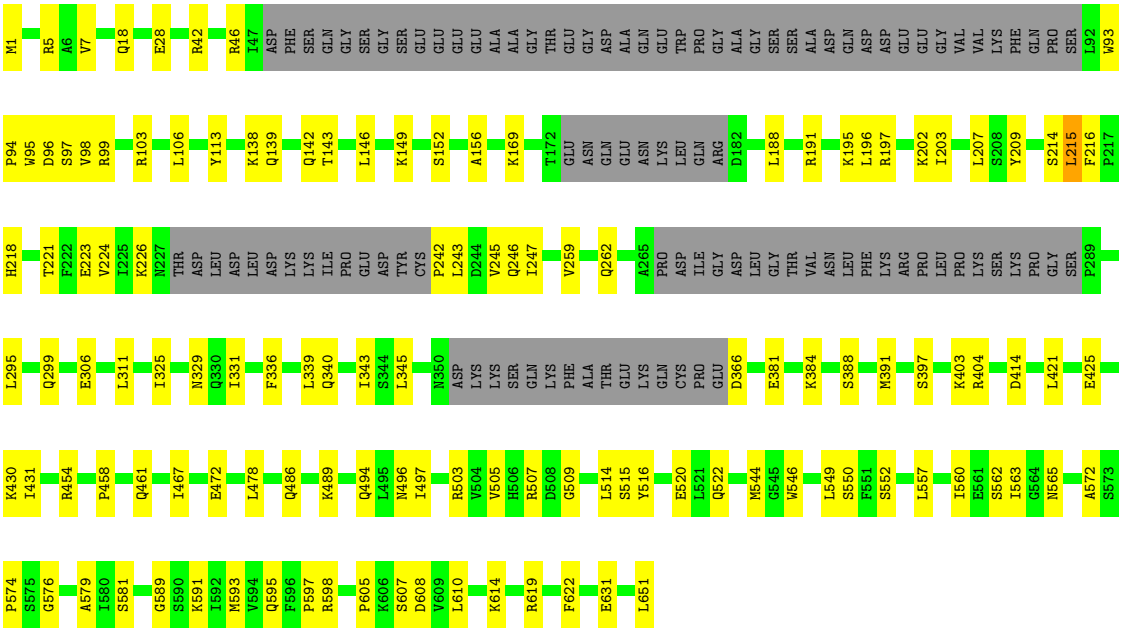
• Molecule 17: Mediator of RNA polymerase II transcription subunit 16

Chain P:



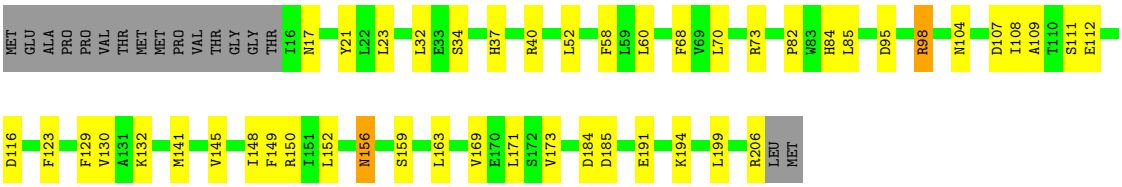
• Molecule 18: Mediator of RNA polymerase II transcription subunit 17

Chain Q:



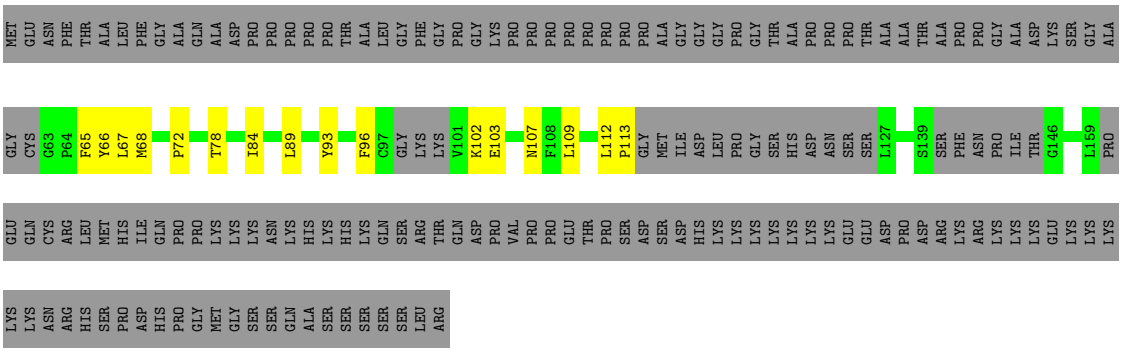
• Molecule 19: Mediator of RNA polymerase II transcription subunit 18

Chain R:



• Molecule 20: Mediator of RNA polymerase II transcription subunit 19

Chain S:

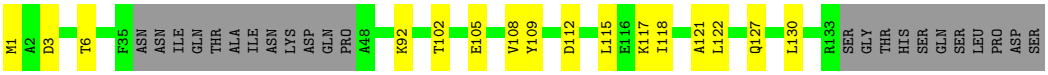


• Molecule 21: Mediator of RNA polymerase II transcription subunit 20

Chain T:

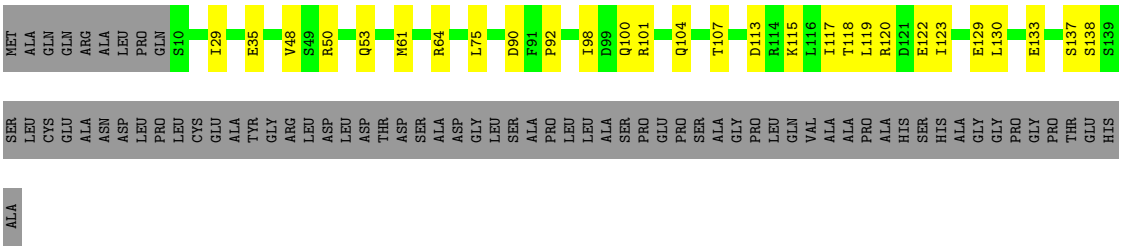
• Molecule 22: Mediator of RNA polymerase II transcription subunit 21

Chain U:



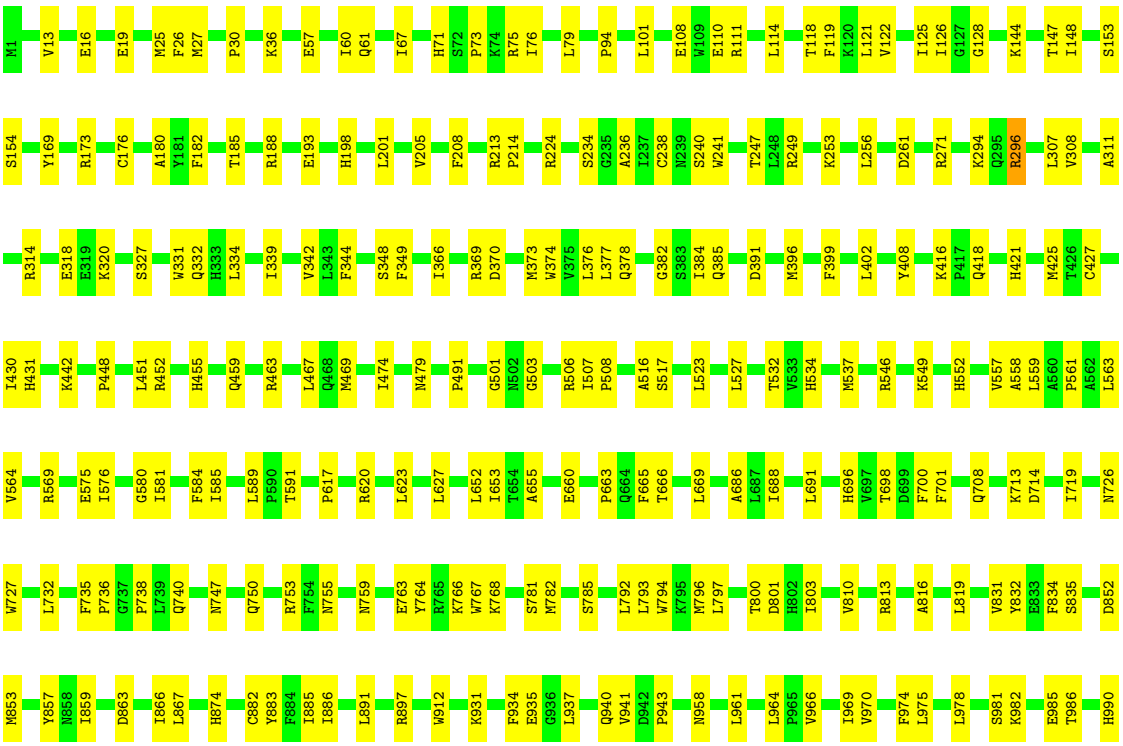
• Molecule 23: Mediator of RNA polymerase II transcription subunit 22

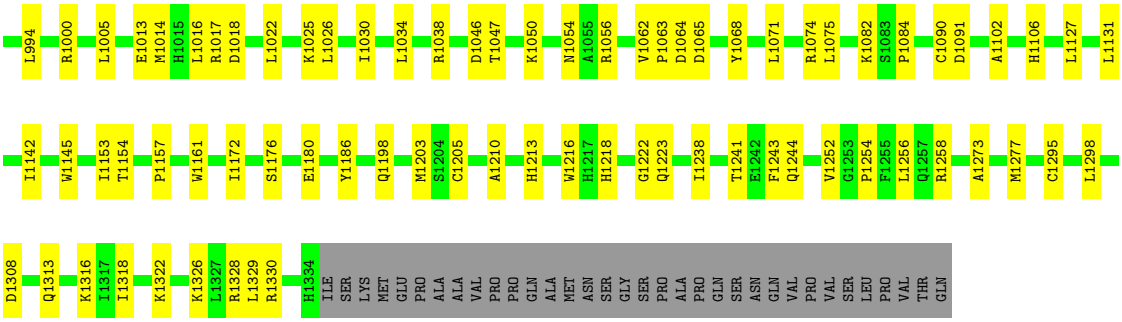
Chain V:



• Molecule 24: Mediator of RNA polymerase II transcription subunit 23

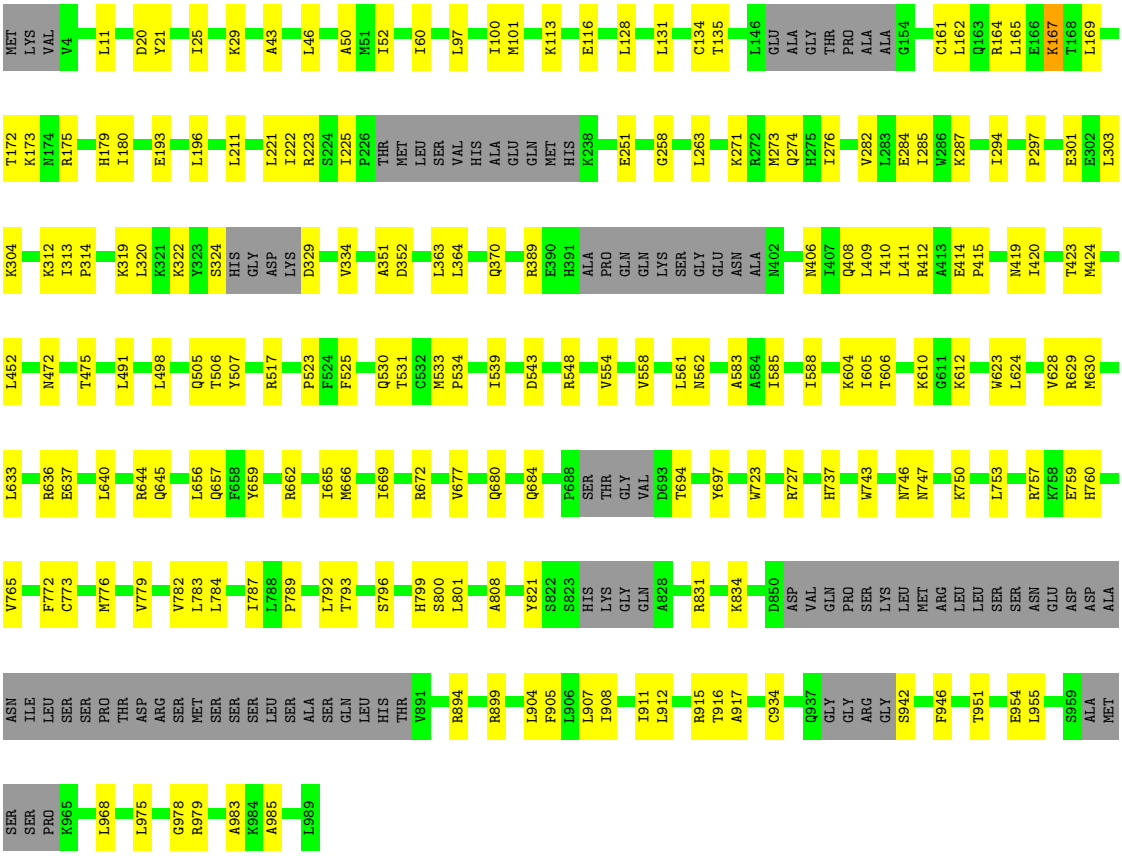
Chain W:





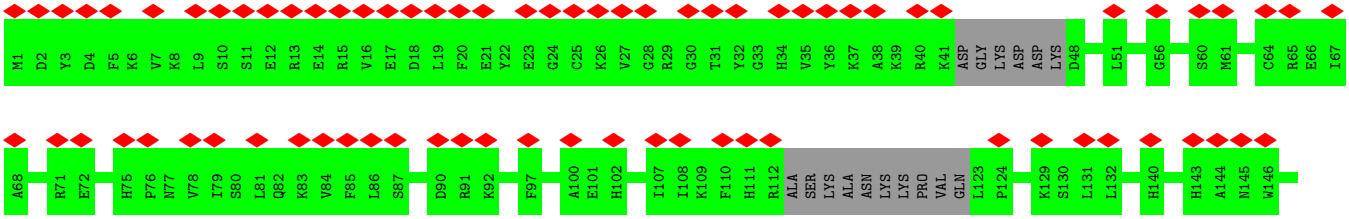
• Molecule 25: Mediator of RNA polymerase II transcription subunit 24

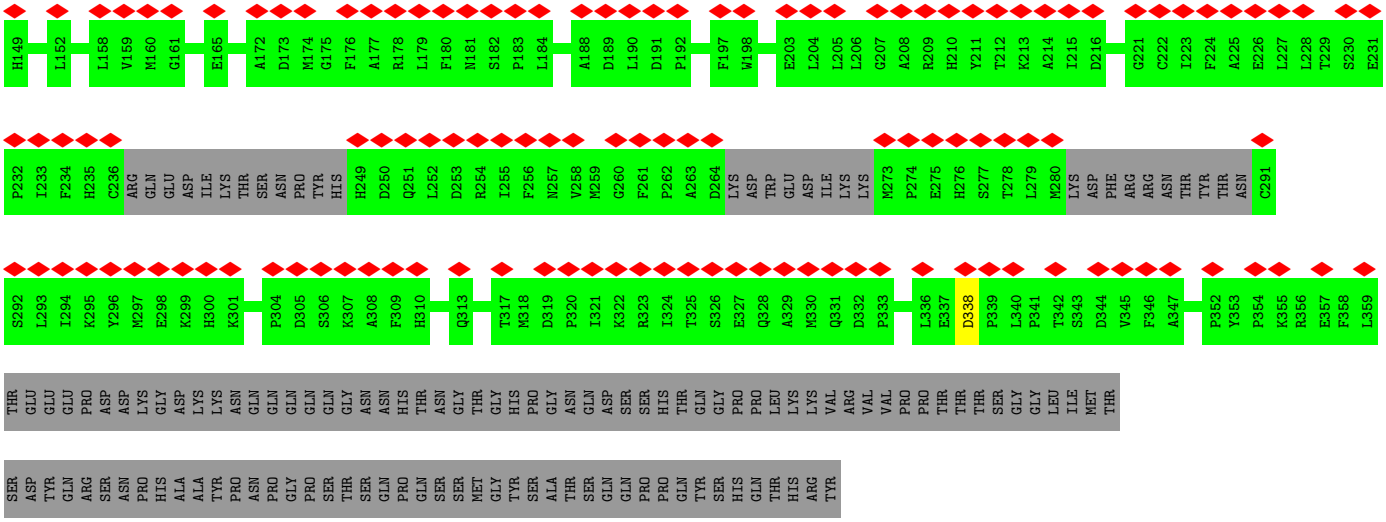
Chain X:



• Molecule 26: Cyclin-dependent kinase 8

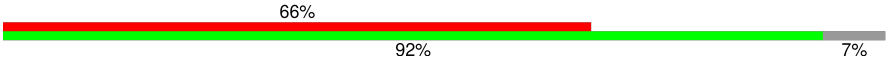
Chain a:

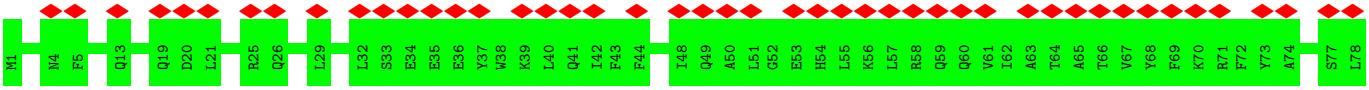


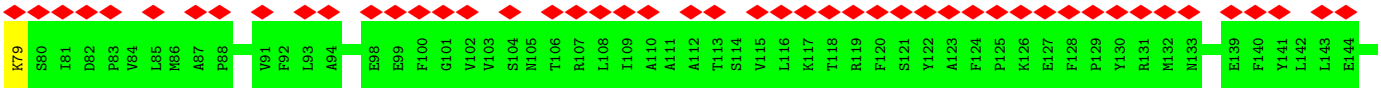


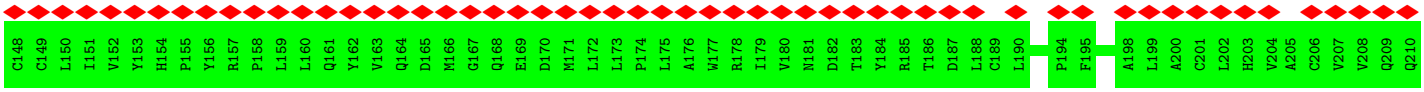
- Molecule 27: Cyclin-C

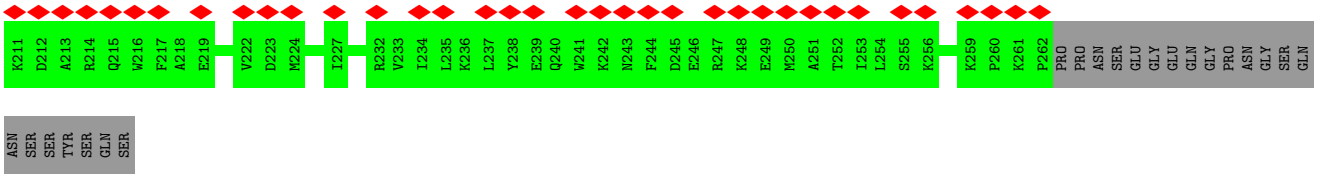
Chain b:





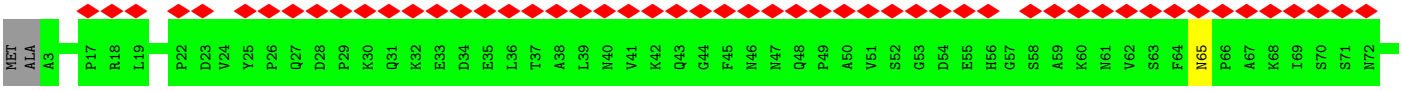


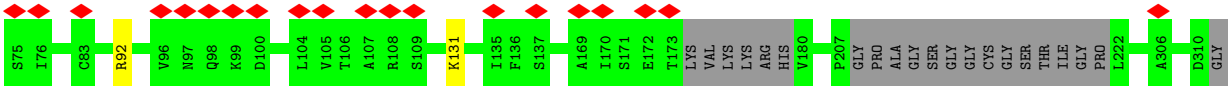


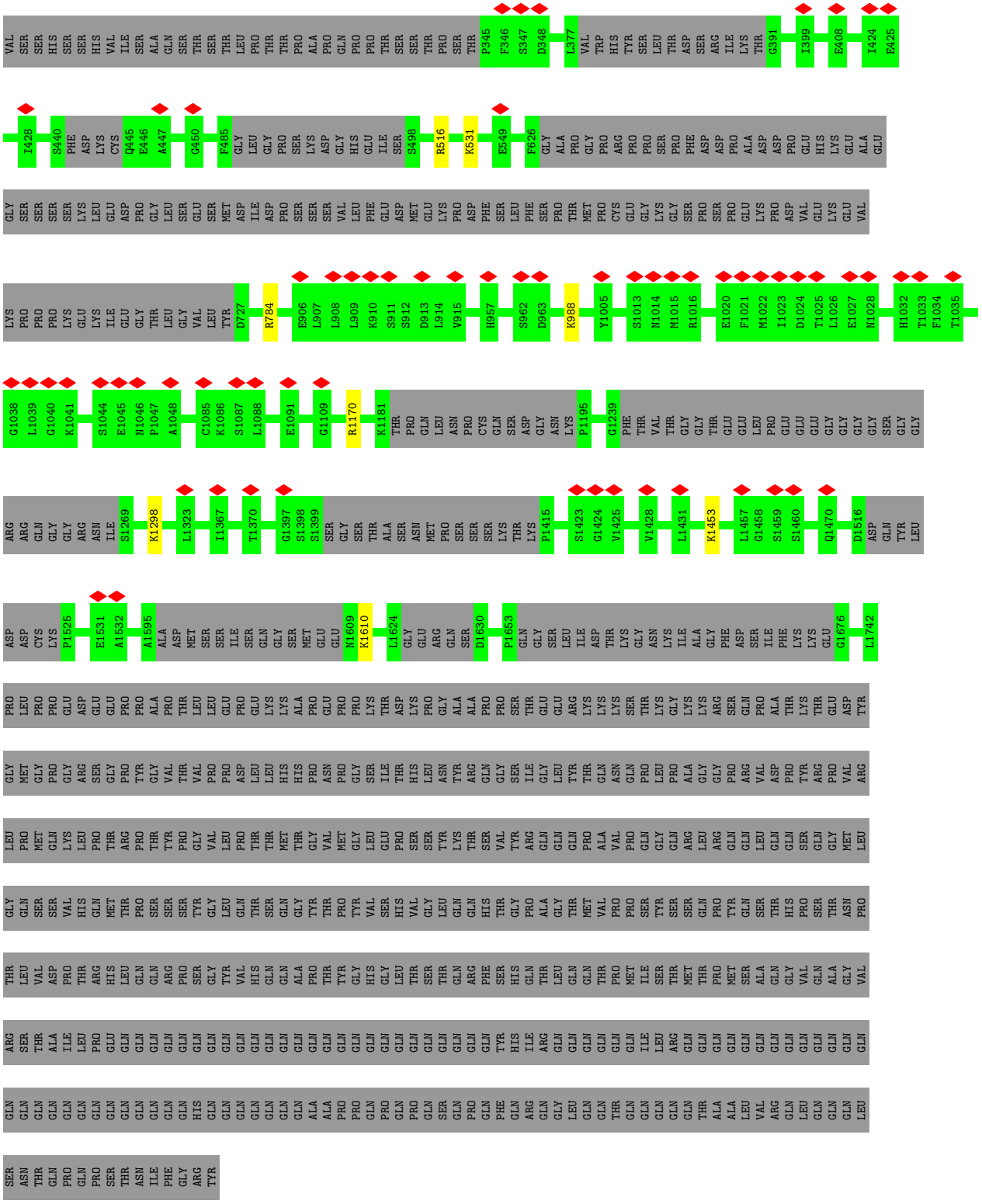


- Molecule 28: Mediator of RNA polymerase II transcription subunit 12

Chain c:

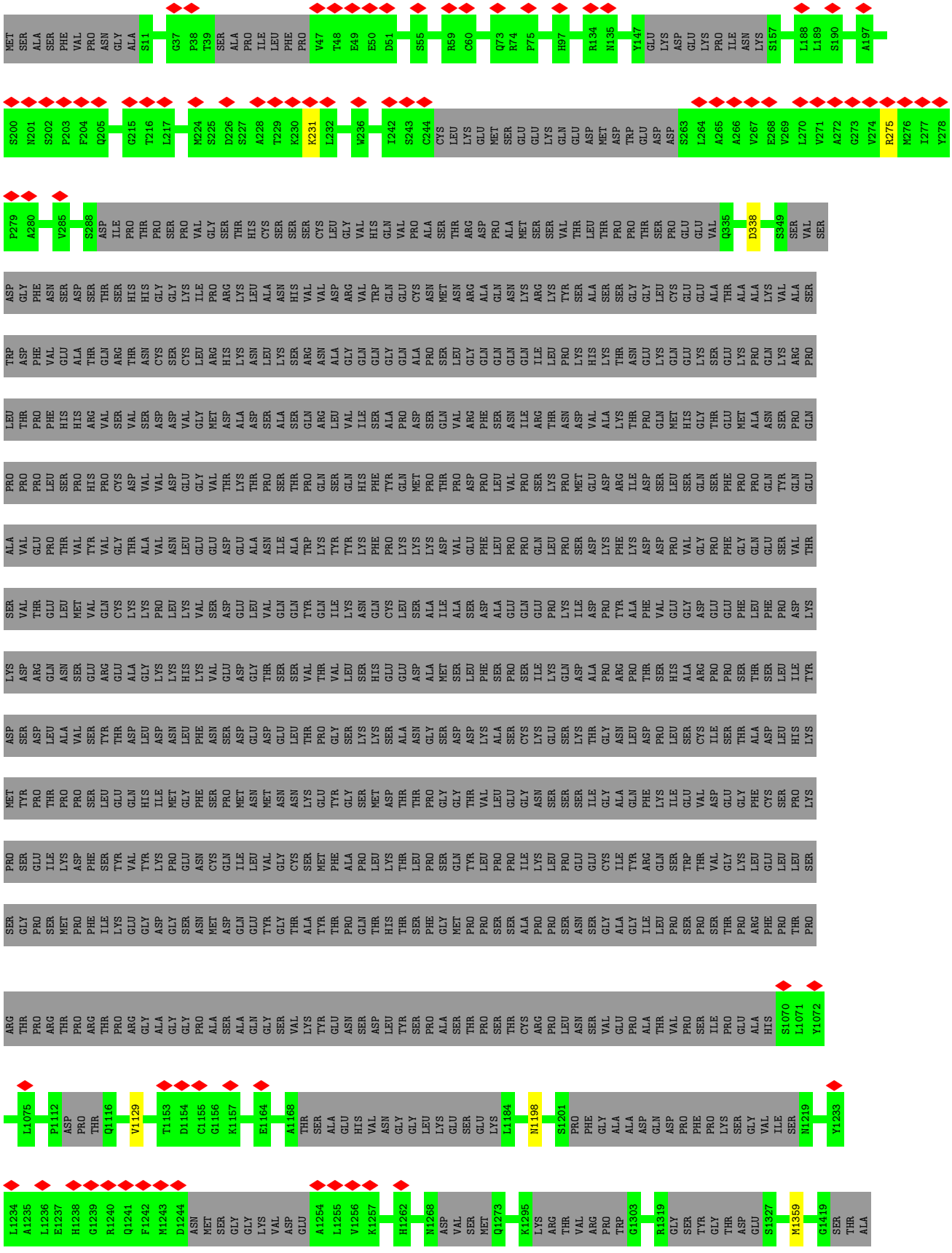


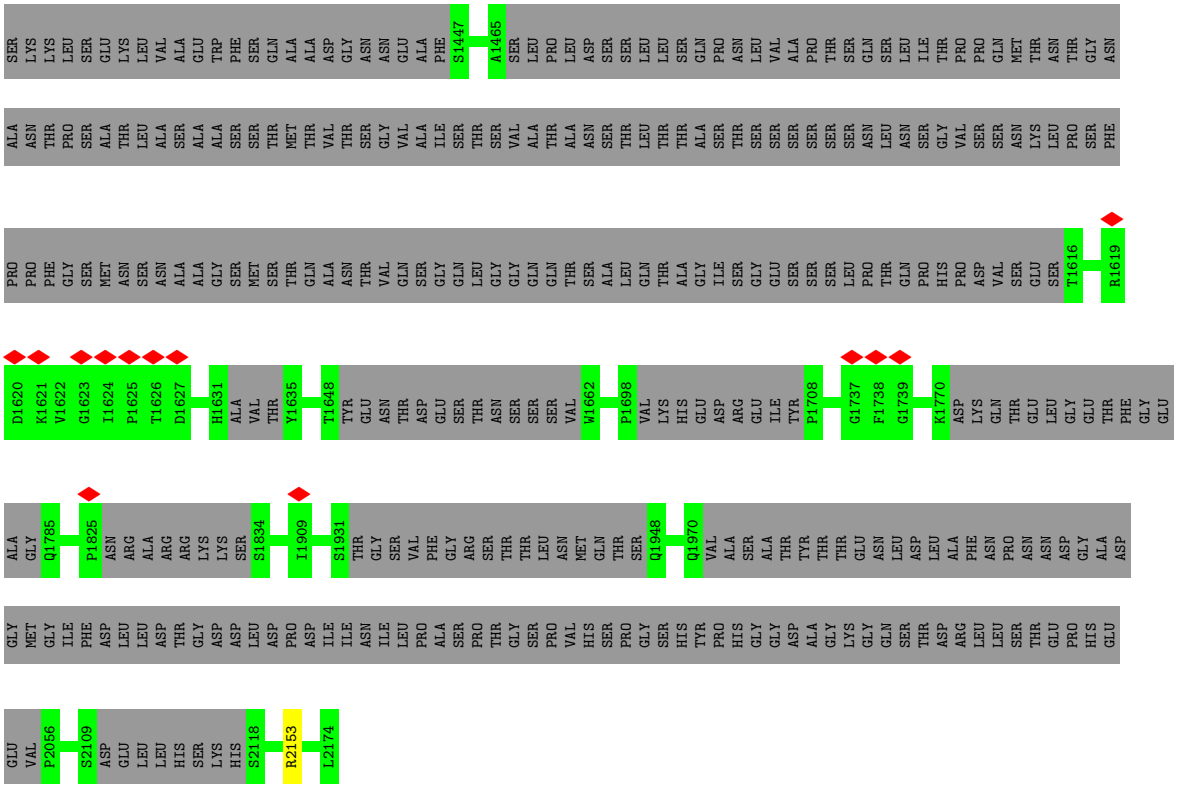




• Molecule 29: Mediator of RNA polymerase II transcription subunit 13

Chain d:


MET SER ALA SER PHE VAL PRO ASN GLY ALA S11 G37 P38 T39 SER ALA PRO ILE LEU PHE PRO V47 T48 E49 E50 D51 S55 R59 C60 Q73 R74 P75 H97 R134 N135 Y147 GLU LYS ASP GLU LYS PRO ILE ASN LYS S157 L188 L189 S190 A197
S200 N201 S202 P203 F204 Q205 G215 T216 L217 M224 S225 D226 S227 A228 T229 K230 K231 L232 W236 I242 S243 C244 CYS LEU LYS GLU MET SER GLU GLU LYS GLN GLU ASP MET ASP TRP GLU ASP S263 L264 A265 A266 V267 E268 V269 L270 V271 A272 G273 V274 R275 M276 I277 Y278
P279 A280 V285 S288 ASP ILE PRO THR PRO SER PRO VAL GLY SER THR HIS CYS SER SER SER CYS LEU GLY VAL HIS GLN VAL PRO ALA SER THR ARG ASP PRO ALA MET SER SER VAL THR LEU THR PRO PRO THR SER PRO GLU GLU VAL Q335 D338 S349 SER VAL SER
ASP GLY PHE ASN SER ASP SER THR SER HIS HIS GLY GLY LYS ILE PRO ARG LYS LEU ALA ASN HIS VAL VAL ASP ARG VAL TRP GLN GLU CYS ASN MET ASN ARG ALA GLN ASN LYS ARG LYS TYR SER ALA SER SER GLY GLY LEU CYS GLU GLU ALA THR ALA ALA LYS VAL ALA SER
TRP ASP PHE VAL GLU ALA THR GLN ARG THR ASN CYS SER CYS LEU ARG HIS LYS ASN LEU LEU LYS SER ARG ASN ALA GLY GLN GLN GLY GLN ALA PRO SER LEU GLY GLN GLN GLN ILE LEU PRO LYS HIS LYS THR ASN GLU LYS GLN GLU LYS SER GLU LYS PRO GLN LYS ARG PRO
LEU THR PRO PHE HIS HIS ARG VAL SER VAL SER ASP SER ASP VAL GLY MET ASP ALA ASP SER ALA SER GLN ARG LEU VAL ILE SER ALA PRO ASP SER GLN VAL ARG PHE SER ASN ILE ARG THR ASN ASP VAL ALA LYS THR PRO GLN MET HIS GLY THR GLU MET ALA ASN SER PRO GLN
PRO PRO PRO LEU SER PRO HIS PRO CYS ASP VAL VAL ASP GLU GLY VAL THR LYS THR PRO SER THR PRO GLN SER GLN HIS PHE TYR GLN MET PRO THR PRO ASP PRO LEU VAL PRO SER LYS PRO MET GLU ASP ARG ILE ASP SER LEU SER GLN SER PHE PRO PRO GLN TYR GLN GLU
ALA VAL GLU PRO THR VAL TYR VAL GLY THR ALA VAL ASN LEU GLU GLU ASP GLU ALA ASN ILE ALA TRP LYS TYR TYR TYR LYS PHE PRO LYS LYS ASP VAL GLU PHE LEU PRO PRO PRO GLN LEU LEU PRO SER ASP LYS PHE LYS ASP ASP PRO VAL GLY PRO PHE GLY GLN GLU SER VAL THR
SER VAL THR GLU LEU MET VAL GLN CYS LYS LYS PRO LEU LYS VAL SER ASP GLU LEU VAL GLN GLN GLN GLU CYS LEU SER ALA ILE ALA SER ASP ALA GLU GLU GLN GLU PRO LYS ILE ASP PRO TYR ALA PHE VAL GLU GLY ASP GLU GLU PHE LEU PHE PRO ASP LYS
LYS ASP ARG GLN ASN SER GLU ARG GLU GLY LYS LYS HIS LYS VAL GLU ASP GLY THR SER SER VAL THR VAL LEU SER HIS GLU GLU GLU ASP ALA MET SER LEU PHE SER PRO SER ILE LYS GLN ASP ALA PRO ARG PRO THR SER HIS ALA ARG PRO PRO SER THR SER LEU ILE TYR
ASP SER ASP LEU ALA VAL SER TYR THR ASP LEU LEU ASP ASN LEU PHE ASN SER ASP GLU ASP GLU LEU THR PRO GLY SER LYS LYS SER ALA ASN GLY SER ASP ASP LYS ALA ALA SER CYS LYS GLU SER LYS THR GLY ASN LEU ASP PRO LEU HIS SER CYS ILE SER THR ALA ASP LEU HIS LYS
MET TYR PRO THR PRO PRO SER LEU GLU GLN HIS ILE MET GLY PHE SER PRO MET ASN MET ASN ASN LYS GLU TYR GLY SER MET ASP THR THR PRO GLY GLY THR VAL LEU GLU GLU GLY ASN GLY SER SER SER ILE GLY ALA GLN PHE LYS ILE GLU VAL ASP GLU GLY PHE CYS SER PRO LYS
PRO SER GLU ILE LYS ASP PHE SER TYR VAL TYR LYS PRO GLU ASN CYS GLN ILE LEU VAL GLY CYS SER MET PHE ALA PRO LEU LYS THR LEU PRO SER GLN TYR LEU PRO PRO ILE LYS LEU PRO GLU GLU CYS ILE TYR ARG GLN SER TRP THR VAL GLY LYS LEU GLU LEU LEU SER
SER GLY PRO SER MET PRO PHE ILE LYS GLU GLY ASP GLY SER ASN MET ASP GLN GLU TYR GLY THR ALA TYR THR PRO GLN THR HIS THR SER PHE GLY MET PRO PRO SER SER ALA PRO PRO SER ASN SER GLY ALA GLY ILE LEU PRO SER PRO SER THR PRO ARG PHE PRO THR PRO
ARG THR PRO ARG THR PRO ARG THR PRO ARG GLY GLY ALA GLY GLY PRO ALA SER ALA GLN GLY GLY SER VAL LYS TYR GLU ASN SER ASP LEU TYR SER PRO ALA SER THR PRO SER THR CYS ARG PRO LEU ASN SER VAL GLU PRO ALA THR VAL PRO SER ILE PRO GLU ALA HIS S1070 L1071 Y1072
L1075 P1112 ASP PRO THR Q1116 V1129 T1153 D1154 C1155 G1156 K1157 E1164 A1168 THR SER ALA GLU HIS VAL ASN GLY GLY LEU LYS GLU SER GLU LYS L1184 N1198 S1201 PRO PHE GLY ALA ALA ASP GLN ASP PRO PHE PRO LYS SER GLY VAL ILE SER N1219 Y1233
L1234 A1235 L1236 E1237 H1238 G1239 R1240 Q1241 F1242 M1243 D1244 ASN MET SER GLY GLY LYS VAL ASP GLU A1254 L1255 V1256 K1257 H1262 N1268 ASP VAL SER MET Q1273 K1295 LYS ARG THR VAL ARG PRO TRP G1303 R1319 GLY SER TYR GLY THR ASP GLU S1327 M1359 G1419 SER THR ALA


SER LYS LYS LEU SER GLU LYS LEU VAL ALA GLU TRP PHE SER GLN ALA ALA ASP GLY ASN ASN GLU ALA PHE S1447 A1465 SER LEU PRO LEU ASP SER SER LEU LEU SER GLN PRO ASN LEU VAL ALA PRO THR SER GLN SER LEU ILE THR PRO PRO GLN MET THR ASN THR GLY ASN
ALA ASN THR PRO SER ALA THR LEU ALA SER ALA ALA SER SER THR MET THR VAL THR SER GLY VAL ALA ILE SER THR SER VAL ALA THR ALA ASN SER THR LEU THR THR ALA SER THR SER SER SER SER SER ASN LEU ASN SER GLY VAL SER SER ASN LYS LEU PRO SER PHE
PRO PRO PHE GLY SER MET ASN SER ASN ALA ALA GLY SER MET SER THR GLN ALA ASN THR VAL GLN SER GLY GLN LEU GLY GLY GLN GLN GLN THR SER ALA LEU GLN THR ALA GLY ILE SER GLY GLU SER SER LEU PRO THR GLN PRO HIS PRO ASP VAL SER GLU SER T1616 R1619
D1620 K1621 V1622 G1623 I1624 P1625 T1626 D1627 H1631 ALA VAL THR Y1635 T1648 TYR GLU ASN THR ASP GLU SER THR ASN SER SER SER VAL W1662 P1698 VAL LYS HIS GLU ASP ARG GLU ILE TYR P1708 G1737 F1738 G1739 K1770 ASP LYS GLN THR GLU LEU GLY GLU THR PHE GLY GLU
ALA GLY Q1785 P1825 ASN ARG ALA ARG ARG LYS LYS SER S1834 I1909 S1931 THR GLY SER VAL PHE GLY ARG SER THR THR LEU ASN MET GLN THR SER Q1948 Q1970 VAL ALA SER ALA THR TYR THR THR GLU ASN LEU ASP LEU ALA PHE ASN PRO ASN ASN ASP GLY ALA ASP
GLY MET GLY ILE PHE ASP LEU LEU ASP THR GLY ASP ASP LEU ASP PRO ASP ILE ILE ASN ILE LEU PRO ALA SER PRO THR GLY SER PRO VAL HIS SER PRO GLY SER HIS TYR PRO HIS GLY GLY ASP ALA GLY LYS GLY GLN SER THR ASP ARG LEU LEU SER THR GLU PRO HIS GLU
GLU VAL P2056 S2109 ASP GLU LEU LEU HIS SER LYS HIS S2118 R2153 L2174

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	727.04004, 727.04004, 727.04004	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.272, 2.272, 2.272	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.26	0/2201	0.58	0/2972
2	1	0.35	0/825	0.60	0/1107
3	2	0.26	0/911	0.49	0/1229
4	3	0.25	0/1029	0.61	0/1378
5	4	0.29	0/1013	0.55	0/1364
6	A	0.34	0/3653	0.60	0/4961
8	D	0.29	0/1281	0.61	0/1718
9	F	0.29	0/1400	0.61	0/1902
10	G	0.30	0/1374	0.61	0/1847
11	H	0.26	0/1441	0.59	0/1946
12	I	0.28	0/612	0.68	0/815
13	J	0.28	0/849	0.52	0/1150
14	K	0.25	0/885	0.59	0/1190
15	N	0.32	0/7923	0.60	0/10761
16	O	0.26	0/1261	0.61	0/1731
17	P	0.26	0/6001	0.61	0/8151
18	Q	0.26	0/4400	0.56	0/5941
19	R	0.26	0/1562	0.59	0/2101
20	S	0.28	0/524	0.55	0/709
21	T	0.28	0/1530	0.57	0/2066
22	U	0.26	0/927	0.53	0/1257
23	V	0.25	0/1072	0.54	0/1440
24	W	0.26	0/11056	0.52	0/15023
25	X	0.26	0/7191	0.55	0/9728
26	a	0.27	0/2627	0.56	0/3542
27	b	0.27	0/2253	0.56	0/3051
28	c	0.27	0/11719	0.57	0/15850
29	d	0.26	0/7895	0.56	0/10703
All	All	0.27	0/85415	0.57	0/115633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2159	0	2176	37	0
2	1	817	0	818	71	0
3	2	899	0	908	14	0
4	3	1022	0	1054	27	0
5	4	986	0	965	28	0
6	A	3578	0	3522	146	0
7	B	100	0	23	4	0
8	D	1268	0	1305	60	0
9	F	1363	0	1344	22	0
10	G	1348	0	1373	74	0
11	H	1422	0	1440	23	0
12	I	605	0	628	33	0
13	J	840	0	718	34	0
14	K	879	0	886	7	0
15	N	7772	0	7557	349	0
16	O	1226	0	1217	21	0
17	P	5875	0	5968	145	0
18	Q	4319	0	4403	118	0
19	R	1532	0	1542	29	0
20	S	517	0	432	24	0
21	T	1499	0	1484	35	0
22	U	918	0	905	12	0
23	V	1063	0	1051	48	0
24	W	10774	0	10838	194	0
25	X	7061	0	7223	128	0
26	a	2561	0	2578	0	0
27	b	2196	0	2233	0	0
28	c	11499	0	11504	0	0
29	d	7714	0	7627	0	0
30	0	1	0	0	0	0
30	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	1	0	0	0	0
30	d	1	0	0	0	0
All	All	83816	0	83722	1451	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 11.

All (1451) 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)
15:N:375:ASP:CB	15:N:376:PRO:HD3	1.67	1.22
2:1:115:VAL:HG22	4:3:142:ILE:HD11	1.29	1.14
12:I:109:LEU:CD2	12:I:114:GLN:HE21	1.60	1.14
12:I:140:MET:O	22:U:117:LYS:HD3	1.44	1.14
10:G:104:LYS:HD3	20:S:72:PRO:HG3	1.19	1.13
10:G:98:ARG:O	20:S:78:THR:HG22	1.47	1.12
10:G:104:LYS:CD	20:S:72:PRO:HG3	1.78	1.11
8:D:86:GLN:OE1	12:I:106:GLY:HA2	1.51	1.11
15:N:375:ASP:HB3	15:N:376:PRO:HD3	1.25	1.11
6:A:22:ARG:CB	8:D:39:VAL:HB	1.80	1.11
15:N:149:LEU:HD12	15:N:150:PRO:HD2	1.15	1.09
15:N:375:ASP:HB2	15:N:376:PRO:CD	1.82	1.09
15:N:308:LEU:HD13	15:N:370:LEU:HD11	1.30	1.09
8:D:86:GLN:CD	12:I:106:GLY:HA2	1.72	1.09
15:N:375:ASP:CB	15:N:376:PRO:CD	2.29	1.09
6:A:278:HIS:ND1	6:A:279:PRO:HD2	1.69	1.07
18:Q:216:PHE:HE1	18:Q:218:HIS:CB	1.68	1.07
15:N:374:HIS:CE1	15:N:379:PRO:HG2	1.88	1.06
10:G:90:LEU:CD2	13:J:109:LEU:HD13	1.87	1.03
18:Q:216:PHE:CE1	18:Q:218:HIS:HB3	1.94	1.03
10:G:90:LEU:HD21	13:J:109:LEU:HD13	1.36	1.03
2:1:128:LEU:HD13	23:V:133:GLU:CB	1.88	1.03
18:Q:216:PHE:CE1	18:Q:218:HIS:CB	2.42	1.02
10:G:97:ILE:HG13	13:J:102:MET:SD	2.00	1.00
15:N:358:THR:HG23	15:N:375:ASP:OD2	1.61	0.99
21:T:187:ALA:O	21:T:191:VAL:HG23	1.61	0.99
2:1:89:ARG:HD3	18:Q:544:MET:HG2	1.44	0.99
2:1:128:LEU:HD13	23:V:133:GLU:HB2	1.03	0.99
18:Q:215:LEU:HD23	18:Q:215:LEU:H	1.27	0.98
8:D:30:LEU:HD13	12:I:99:LYS:HB3	1.41	0.98
10:G:101:GLY:HA2	15:N:128:LEU:CD2	1.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:274:GLN:HE21	25:X:276:ILE:HD11	1.31	0.96
25:X:274:GLN:NE2	25:X:276:ILE:HD11	1.82	0.95
15:N:308:LEU:HD13	15:N:370:LEU:CD1	1.96	0.94
10:G:90:LEU:HD21	13:J:109:LEU:CD1	1.96	0.94
15:N:703:ARG:NH2	18:Q:614:LYS:HG3	1.82	0.94
15:N:643:HIS:CD2	18:Q:560:ILE:HG12	2.02	0.94
15:N:149:LEU:CD1	15:N:150:PRO:HD2	1.97	0.94
2:1:128:LEU:CD1	23:V:133:GLU:HB2	1.95	0.93
15:N:374:HIS:HB2	15:N:378:LEU:HD23	1.50	0.93
12:I:109:LEU:HD21	12:I:114:GLN:HE21	1.31	0.92
3:2:155:LEU:N	3:2:160:TYR:HH	1.68	0.92
10:G:90:LEU:CD2	13:J:109:LEU:CD1	2.48	0.92
15:N:374:HIS:CG	15:N:379:PRO:HD3	2.04	0.92
10:G:104:LYS:HD3	20:S:72:PRO:CG	1.98	0.91
2:1:115:VAL:CG2	4:3:142:ILE:HD11	2.00	0.90
15:N:374:HIS:CG	15:N:379:PRO:CD	2.56	0.89
20:S:109:LEU:O	20:S:113:PRO:CD	2.20	0.89
2:1:101:GLN:CG	4:3:114:LEU:HD21	2.03	0.89
23:V:119:LEU:O	23:V:123:ILE:HG12	1.73	0.89
10:G:101:GLY:HA2	15:N:128:LEU:HD23	1.55	0.88
15:N:375:ASP:HB2	15:N:376:PRO:HD3	1.46	0.88
2:1:101:GLN:HG3	4:3:114:LEU:HD21	1.55	0.87
15:N:149:LEU:HD12	15:N:150:PRO:CD	2.02	0.87
2:1:125:LYS:HE2	23:V:137:SER:HB2	1.58	0.86
18:Q:216:PHE:CE1	18:Q:218:HIS:HB2	2.10	0.86
2:1:125:LYS:HE2	23:V:137:SER:CB	2.06	0.85
6:A:278:HIS:CE1	6:A:279:PRO:HD2	2.12	0.85
2:1:135:LYS:HG2	2:1:139:TRP:HZ3	1.42	0.84
18:Q:472:GLU:HA	18:Q:497:ILE:O	1.78	0.83
10:G:131:ALA:HB1	15:N:154:ILE:HD11	1.60	0.82
15:N:374:HIS:CE1	15:N:379:PRO:CG	2.61	0.82
2:1:146:ILE:HG12	23:V:115:LYS:HE3	1.62	0.82
17:P:402:MET:SD	17:P:461:MET:HE2	2.19	0.82
12:I:109:LEU:CD2	12:I:114:GLN:NE2	2.42	0.81
18:Q:216:PHE:HE1	18:Q:218:HIS:HB3	1.35	0.81
6:A:278:HIS:CG	6:A:279:PRO:HD2	2.15	0.81
2:1:146:ILE:HD11	23:V:115:LYS:HD2	1.64	0.80
15:N:375:ASP:HB2	15:N:376:PRO:HD2	1.64	0.80
15:N:382:ASP:HB2	15:N:386:VAL:H	1.46	0.79
8:D:109:GLN:HE22	10:G:174:ASP:HB3	1.47	0.79
15:N:372:ILE:H	15:N:372:ILE:HD13	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:139:TRP:HZ2	23:V:122:GLU:HB3	1.50	0.77
15:N:361:ILE:HB	15:N:370:LEU:HD23	1.67	0.77
8:D:30:LEU:HD13	12:I:99:LYS:CB	2.15	0.77
15:N:145:VAL:O	15:N:148:ARG:HG2	1.85	0.77
15:N:374:HIS:CD2	15:N:379:PRO:HD2	2.19	0.77
20:S:109:LEU:O	20:S:113:PRO:CG	2.33	0.76
18:Q:216:PHE:CD1	18:Q:218:HIS:HB3	2.19	0.76
10:G:90:LEU:HD21	13:J:109:LEU:CB	2.15	0.76
8:D:83:ALA:HB1	12:I:102:SER:HB3	1.65	0.76
15:N:361:ILE:HD12	15:N:370:LEU:HD23	1.67	0.76
10:G:90:LEU:HD21	13:J:109:LEU:HB3	1.68	0.75
1:0:127:LEU:HD23	2:1:74:ARG:HG3	1.66	0.75
2:1:143:LEU:HD21	23:V:119:LEU:HG	1.67	0.75
10:G:96:LEU:HB3	15:N:129:PHE:CE1	2.21	0.75
15:N:703:ARG:HH22	18:Q:614:LYS:HG3	1.49	0.75
15:N:361:ILE:HB	15:N:370:LEU:CD2	2.16	0.75
15:N:453:HIS:HB2	15:N:466:MET:HB2	1.68	0.75
11:H:19:VAL:HG21	18:Q:113:TYR:HB2	1.68	0.75
18:Q:215:LEU:H	18:Q:215:LEU:CD2	1.98	0.74
15:N:374:HIS:ND1	15:N:379:PRO:CD	2.49	0.74
6:A:459:ASN:ND2	6:A:484:SER:O	2.20	0.74
12:I:140:MET:O	22:U:117:LYS:CD	2.31	0.74
25:X:585:ILE:HD11	25:X:623:TRP:HB3	1.69	0.74
3:2:121:ARG:HH12	15:N:907:LEU:HD21	1.52	0.73
8:D:86:GLN:OE1	12:I:106:GLY:CA	2.33	0.73
13:J:127:ILE:HG13	20:S:65:PHE:CE1	2.22	0.73
6:A:347:GLU:HG3	6:A:422:GLY:HA3	1.68	0.73
6:A:22:ARG:CB	8:D:39:VAL:CB	2.62	0.73
15:N:591:PHE:CD1	24:W:25:MET:HE2	2.24	0.72
24:W:396:MET:O	24:W:399:PHE:HB3	1.88	0.72
5:4:43:PHE:HB2	5:4:85:ARG:HB3	1.72	0.72
15:N:372:ILE:HD13	15:N:372:ILE:N	2.04	0.72
6:A:149:GLU:HG3	6:A:152:LYS:HD2	1.70	0.72
15:N:737:ARG:HH21	15:N:743:ARG:HH11	1.37	0.72
17:P:640:ARG:HG2	17:P:642:GLY:H	1.54	0.72
15:N:916:LEU:HB2	15:N:924:ILE:HB	1.71	0.72
1:0:306:HIS:H	1:0:309:CYS:HB2	1.54	0.72
21:T:46:TYR:HB2	21:T:63:MET:HB2	1.72	0.71
25:X:644:ARG:HH21	25:X:684:GLN:H	1.39	0.71
15:N:823:GLN:NE2	15:N:832:HIS:O	2.23	0.71
25:X:772:PHE:HB3	25:X:779:VAL:HG21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:139:TRP:CZ2	23:V:122:GLU:HB3	2.25	0.71
15:N:371:GLN:OE1	15:N:373:PHE:HE2	1.73	0.71
6:A:455:GLN:NE2	6:A:460:ASP:OD1	2.24	0.70
12:I:109:LEU:HD23	12:I:114:GLN:HE21	1.52	0.70
15:N:245:TRP:O	15:N:279:GLN:NE2	2.25	0.70
15:N:135:ARG:HD2	15:N:135:ARG:C	2.13	0.70
25:X:792:LEU:HD22	25:X:911:ILE:HD11	1.73	0.69
10:G:90:LEU:HD23	13:J:109:LEU:HD13	1.72	0.69
6:A:208:VAL:HG12	6:A:222:LEU:HD13	1.74	0.69
6:A:460:ASP:OD2	25:X:11:LEU:HD11	1.92	0.69
10:G:96:LEU:HB3	15:N:129:PHE:HE1	1.56	0.69
6:A:77:MET:SD	6:A:145:LYS:NZ	2.66	0.69
17:P:403:ALA:HB2	17:P:461:MET:HE1	1.74	0.69
5:4:17:ARG:NH2	5:4:54:TYR:OH	2.26	0.69
5:4:28:LEU:HG	5:4:34:LEU:HD21	1.75	0.69
15:N:374:HIS:CG	15:N:379:PRO:HD2	2.28	0.69
20:S:109:LEU:O	20:S:113:PRO:HG2	1.92	0.69
15:N:374:HIS:ND1	15:N:379:PRO:HD3	2.06	0.69
15:N:530:ILE:HB	15:N:588:LEU:HD21	1.74	0.69
24:W:931:LYS:HB3	24:W:935:GLU:HB2	1.75	0.68
13:J:82:LYS:HG2	20:S:96:PHE:HB3	1.74	0.68
21:T:186:PRO:O	21:T:190:MET:HG2	1.93	0.68
6:A:278:HIS:CG	6:A:279:PRO:CD	2.76	0.68
8:D:76:PHE:HA	8:D:79:LEU:HD13	1.75	0.68
18:Q:215:LEU:HD23	18:Q:215:LEU:N	2.07	0.68
8:D:152:ALA:CB	15:N:154:ILE:HA	2.24	0.68
15:N:853:HIS:O	15:N:856:GLN:NE2	2.24	0.68
8:D:152:ALA:HB2	15:N:154:ILE:HA	1.76	0.68
15:N:358:THR:HG23	15:N:375:ASP:CG	2.14	0.67
15:N:684:LEU:HB2	15:N:708:CYS:HB3	1.76	0.67
19:R:130:VAL:HB	19:R:149:PHE:HB2	1.77	0.67
15:N:676:ASP:OD2	18:Q:593:MET:HB2	1.93	0.67
6:A:181:GLU:HA	6:A:184:LEU:HD12	1.76	0.67
21:T:79:PHE:HB2	21:T:82:GLY:H	1.60	0.67
19:R:60:LEU:HB3	19:R:68:PHE:HB3	1.77	0.67
2:1:128:LEU:HD11	23:V:129:GLU:OE1	1.94	0.67
9:F:174:ARG:NH1	15:N:265:LEU:O	2.27	0.67
18:Q:216:PHE:CD2	18:Q:306:GLU:HG2	2.29	0.67
2:1:125:LYS:HA	23:V:133:GLU:OE2	1.94	0.67
25:X:743:TRP:O	25:X:747:ASN:ND2	2.27	0.67
17:P:219:ALA:HB3	17:P:291:SER:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:78:LEU:HD22	15:N:178:ILE:HG13	1.77	0.66
8:D:27:ARG:NH1	12:I:103:THR:HB	2.10	0.66
22:U:127:GLN:HA	22:U:130:LEU:HD23	1.77	0.66
15:N:375:ASP:HB3	15:N:376:PRO:CD	2.10	0.66
6:A:476:SER:OG	6:A:478:LYS:NZ	2.28	0.66
2:1:125:LYS:HE2	23:V:137:SER:HB3	1.78	0.66
1:0:112:LYS:HD3	1:0:115:ASN:HD22	1.61	0.66
15:N:356:LYS:O	15:N:375:ASP:HB2	1.96	0.66
15:N:935:ALA:HB1	15:N:1174:PRO:HB2	1.77	0.66
2:1:101:GLN:HG2	4:3:114:LEU:HD21	1.76	0.66
6:A:265:VAL:HA	6:A:300:PRO:HA	1.78	0.66
6:A:315:ARG:NH2	6:A:389:GLN:OE1	2.28	0.66
10:G:109:LEU:HD22	15:N:135:ARG:CZ	2.25	0.66
12:I:109:LEU:HD23	12:I:114:GLN:CG	2.26	0.66
10:G:64:ILE:HG12	10:G:117:VAL:HG11	1.78	0.65
6:A:305:LEU:HB2	6:A:396:ILE:HB	1.79	0.65
17:P:96:LEU:HB2	17:P:108:TRP:HB2	1.77	0.65
17:P:583:ILE:HD12	17:P:599:LEU:HD22	1.78	0.65
18:Q:496:ASN:HB3	18:Q:503:ARG:HB2	1.79	0.65
9:F:171:ILE:HG13	9:F:173:GLN:H	1.60	0.65
15:N:245:TRP:H	15:N:282:LEU:HD22	1.62	0.65
17:P:231:ALA:HB2	17:P:283:LEU:HD13	1.78	0.65
24:W:1071:LEU:HA	24:W:1074:ARG:HE	1.60	0.65
10:G:101:GLY:CA	15:N:128:LEU:CD2	2.75	0.65
23:V:130:LEU:C	23:V:130:LEU:HD13	2.18	0.65
6:A:310:PRO:HB2	6:A:392:LEU:HB3	1.79	0.64
9:F:129:ALA:HB1	18:Q:98:VAL:HG23	1.78	0.64
17:P:60:ARG:HG2	17:P:80:HIS:HB2	1.78	0.64
17:P:634:ASN:HB3	17:P:640:ARG:HH21	1.62	0.64
25:X:765:VAL:HG21	25:X:808:ALA:HB1	1.80	0.64
17:P:282:HIS:HB2	17:P:297:CYS:HB3	1.79	0.64
15:N:135:ARG:HD2	15:N:135:ARG:O	1.97	0.64
15:N:355:HIS:HB3	15:N:377:PRO:HG3	1.80	0.64
15:N:707:ASP:OD2	16:O:684:ARG:NH1	2.30	0.64
6:A:371:GLN:HB2	6:A:436:GLY:HA3	1.78	0.64
17:P:62:ILE:HB	17:P:76:ILE:HB	1.80	0.64
10:G:101:GLY:HA2	15:N:128:LEU:HD21	1.75	0.64
10:G:87:ILE:HD12	13:J:124:TYR:CD1	2.33	0.64
18:Q:607:SER:H	18:Q:610:LEU:HD12	1.63	0.64
21:T:112:THR:HG22	21:T:129:VAL:HG22	1.79	0.64
6:A:171:THR:O	6:A:175:LEU:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:796:ILE:O	15:N:816:LYS:NZ	2.31	0.63
1:0:39:MET:HB2	1:0:48:ARG:HE	1.64	0.63
2:1:115:VAL:HG22	4:3:142:ILE:CD1	2.18	0.63
10:G:101:GLY:CA	15:N:128:LEU:HD23	2.27	0.63
15:N:372:ILE:O	15:N:372:ILE:HG12	1.98	0.63
8:D:26:THR:N	8:D:86:GLN:HE22	1.94	0.63
15:N:154:ILE:N	15:N:155:PRO:HD2	2.14	0.63
15:N:374:HIS:CE1	15:N:379:PRO:CD	2.81	0.63
10:G:104:LYS:HD2	20:S:72:PRO:HG3	1.79	0.63
17:P:402:MET:SD	17:P:461:MET:CE	2.87	0.63
18:Q:461:GLN:HB2	18:Q:478:LEU:HB2	1.81	0.63
24:W:853:MET:HA	24:W:857:TYR:HB2	1.80	0.63
15:N:421:ARG:NH1	15:N:429:SER:OG	2.26	0.63
8:D:132:LEU:HD22	22:U:108:VAL:HG22	1.80	0.62
10:G:96:LEU:O	15:N:129:PHE:CZ	2.52	0.62
17:P:141:VAL:HA	17:P:161:ARG:HH22	1.63	0.62
15:N:667:PRO:HG2	15:N:686:LYS:HB3	1.81	0.62
15:N:1337:GLN:HA	15:N:1355:PRO:HA	1.80	0.62
17:P:548:HIS:HB3	17:P:732:LEU:HB3	1.80	0.62
25:X:792:LEU:HD21	25:X:907:LEU:HD23	1.80	0.62
6:A:168:LYS:HD3	6:A:169:LEU:HD12	1.81	0.62
13:J:72:ASP:OD1	15:N:98:ARG:NH1	2.33	0.62
24:W:373:MET:HG3	24:W:425:MET:HB2	1.80	0.62
4:3:44:ILE:HD12	4:3:92:LEU:HD13	1.81	0.62
6:A:488:ILE:HG23	6:A:515:ALA:HB2	1.82	0.62
15:N:455:PHE:HB2	15:N:464:GLN:HB2	1.82	0.62
15:N:553:GLU:HB3	15:N:567:LYS:HB2	1.81	0.62
17:P:64:ILE:HB	17:P:74:HIS:HB3	1.82	0.62
9:F:49:VAL:HG23	9:F:50:VAL:HG23	1.81	0.62
23:V:130:LEU:HD13	23:V:130:LEU:O	1.99	0.62
24:W:767:TRP:HD1	24:W:768:LYS:HG3	1.62	0.62
25:X:779:VAL:HA	25:X:782:VAL:HG12	1.81	0.62
2:1:143:LEU:HG	23:V:119:LEU:HD11	1.82	0.61
17:P:488:TRP:NE1	17:P:529:MET:SD	2.73	0.61
8:D:124:ALA:O	8:D:127:GLN:NE2	2.32	0.61
23:V:100:GLN:HG3	23:V:101:ARG:HE	1.64	0.61
18:Q:494:GLN:HB3	18:Q:505:VAL:HB	1.81	0.61
6:A:183:ASP:HA	6:A:186:LYS:HD2	1.83	0.61
24:W:958:ASN:HD21	24:W:961:LEU:HD23	1.65	0.61
6:A:460:ASP:CG	25:X:11:LEU:HD21	2.21	0.61
6:A:163:LEU:HB2	6:A:170:LYS:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:441:PRO:HA	15:N:451:CYS:HA	1.82	0.61
15:N:643:HIS:HB2	18:Q:560:ILE:HG23	1.82	0.61
18:Q:18:GLN:HE21	18:Q:18:GLN:HA	1.65	0.61
25:X:585:ILE:HD12	25:X:624:LEU:HG	1.83	0.61
6:A:64:THR:HA	6:A:67:LYS:HG2	1.83	0.61
10:G:109:LEU:HD13	15:N:135:ARG:HG3	1.82	0.61
17:P:286:LEU:HD11	17:P:396:ARG:HG3	1.81	0.61
20:S:65:PHE:HB3	20:S:68:MET:HE2	1.82	0.61
25:X:274:GLN:HG3	25:X:276:ILE:HG13	1.80	0.61
17:P:220:PHE:H	17:P:289:ASP:HA	1.65	0.61
17:P:640:ARG:HB3	17:P:643:HIS:HB3	1.82	0.61
6:A:186:LYS:O	6:A:190:MET:N	2.29	0.60
15:N:587:LEU:HD12	15:N:589:GLN:HE22	1.64	0.60
17:P:626:LEU:HD11	17:P:724:LEU:HD22	1.82	0.60
18:Q:18:GLN:HA	18:Q:18:GLN:NE2	2.16	0.60
6:A:420:LEU:HD23	6:A:502:MET:O	2.01	0.60
17:P:12:MET:N	17:P:458:SER:OG	2.33	0.60
24:W:585:ILE:HA	24:W:589:LEU:HB2	1.82	0.60
7:B:8:UNK:O	7:B:12:UNK:N	2.34	0.60
15:N:825:ASN:OD1	15:N:832:HIS:ND1	2.28	0.60
24:W:247:THR:O	24:W:249:ARG:NH1	2.34	0.60
2:1:93:CYS:HA	2:1:96:LEU:HB2	1.83	0.60
12:I:109:LEU:HD23	12:I:114:GLN:HG3	1.82	0.60
16:O:735:LEU:HD21	24:W:73:PRO:HB2	1.83	0.60
18:Q:576:GLY:O	18:Q:619:ARG:NH2	2.34	0.60
24:W:698:THR:O	24:W:1223:GLN:NE2	2.35	0.60
5:4:21:GLU:HB3	5:4:58:TRP:HH2	1.66	0.60
8:D:156:SER:HB2	8:D:161:VAL:HG12	1.83	0.60
15:N:247:LEU:HD13	15:N:278:VAL:HG11	1.83	0.60
15:N:1251:VAL:HA	15:N:1263:LEU:HA	1.83	0.60
15:N:197:GLN:OE1	15:N:200:ARG:NH1	2.34	0.60
15:N:387:GLU:O	15:N:391:LYS:NZ	2.35	0.60
1:0:127:LEU:CD2	2:1:74:ARG:HG3	2.31	0.60
1:0:282:GLN:NE2	1:0:304:ALA:O	2.34	0.60
6:A:379:ASP:OD1	6:A:386:ARG:NH1	2.34	0.60
15:N:1218:ARG:HG2	15:N:1219:HIS:CD2	2.37	0.60
6:A:443:CYS:SG	6:A:451:SER:OG	2.60	0.60
12:I:107:ILE:HG22	12:I:107:ILE:O	2.00	0.60
15:N:591:PHE:HD1	24:W:25:MET:HE2	1.65	0.60
8:D:82:LEU:HA	8:D:85:ASN:HB2	1.84	0.60
15:N:458:LEU:HD11	18:Q:325:ILE:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:530:ILE:HD12	15:N:533:LEU:HD12	1.81	0.60
25:X:955:LEU:HD11	25:X:968:LEU:HB2	1.84	0.59
8:D:34:LEU:HD13	12:I:96:GLU:HG2	1.82	0.59
19:R:52:LEU:HB2	19:R:132:LYS:HD3	1.84	0.59
6:A:208:VAL:CG1	6:A:222:LEU:HD13	2.31	0.59
6:A:408:LEU:HA	6:A:411:ILE:HD12	1.85	0.59
2:1:88:ALA:O	2:1:91:THR:OG1	2.20	0.59
15:N:186:ILE:HG23	15:N:186:ILE:O	2.01	0.59
15:N:457:ASP:OD1	15:N:462:MET:N	2.35	0.59
17:P:697:TRP:O	17:P:701:ARG:N	2.34	0.59
21:T:129:VAL:HG11	21:T:200:ILE:HD13	1.84	0.59
24:W:559:LEU:HD11	24:W:563:LEU:HD23	1.85	0.59
15:N:711:ARG:HD2	18:Q:549:LEU:HD23	1.83	0.59
6:A:376:LEU:HA	6:A:442:VAL:HB	1.85	0.59
15:N:690:CYS:SG	15:N:691:LYS:N	2.76	0.59
22:U:118:ILE:O	22:U:122:LEU:N	2.33	0.59
6:A:305:LEU:HD11	6:A:404:VAL:HG23	1.84	0.59
15:N:725:VAL:HA	15:N:744:HIS:HA	1.84	0.59
25:X:134:CYS:SG	25:X:164:ARG:NH2	2.76	0.59
15:N:444:GLU:H	15:N:562:THR:HB	1.68	0.59
15:N:660:GLU:HA	15:N:663:ASN:HB2	1.85	0.59
24:W:727:TRP:HB2	24:W:747:ASN:HD21	1.67	0.59
2:1:119:ARG:NH1	4:3:141:GLU:OE2	2.33	0.59
15:N:540:ILE:HB	15:N:550:ILE:HB	1.84	0.59
2:1:118:LEU:O	2:1:122:LEU:N	2.36	0.59
2:1:123:GLN:O	2:1:127:ALA:N	2.36	0.59
17:P:186:GLY:H	17:P:210:ARG:HG3	1.66	0.59
15:N:506:LYS:O	15:N:510:LYS:NZ	2.29	0.58
17:P:214:ALA:N	17:P:231:ALA:O	2.36	0.58
15:N:707:ASP:CG	16:O:684:ARG:HH11	2.06	0.58
23:V:117:ILE:HG12	23:V:120:ARG:HH21	1.69	0.58
17:P:688:LEU:HB2	17:P:691:ARG:HH21	1.67	0.58
20:S:109:LEU:O	20:S:113:PRO:HD2	2.03	0.58
25:X:979:ARG:HH12	25:X:983:ALA:HB2	1.67	0.58
6:A:304:PHE:HB2	6:A:306:LYS:HZ2	1.69	0.58
25:X:554:VAL:HG11	25:X:583:ALA:HB3	1.84	0.58
9:F:174:ARG:HA	9:F:177:VAL:HB	1.86	0.58
17:P:261:PRO:HD2	17:P:337:LEU:HD12	1.85	0.58
15:N:779:CYS:HA	15:N:782:GLU:HB2	1.85	0.58
18:Q:203:ILE:HG23	18:Q:224:VAL:HB	1.85	0.58
25:X:773:CYS:HA	25:X:776:MET:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:726:PHE:O	15:N:743:ARG:N	2.37	0.58
2:1:128:LEU:HD11	23:V:129:GLU:CD	2.23	0.58
10:G:25:ASN:HD22	10:G:32:PRO:HB3	1.68	0.58
18:Q:381:GLU:HA	18:Q:384:LYS:HG2	1.86	0.58
18:Q:425:GLU:HG2	18:Q:430:LYS:HE3	1.84	0.58
25:X:821:TYR:HH	25:X:942:SER:N	2.02	0.58
15:N:711:ARG:CD	18:Q:549:LEU:HD23	2.34	0.58
15:N:804:ASN:OD1	15:N:807:LYS:N	2.29	0.58
17:P:309:TRP:HB3	17:P:339:TRP:HB3	1.85	0.58
20:S:65:PHE:HB3	20:S:68:MET:CE	2.33	0.58
6:A:288:PHE:HD1	6:A:296:SER:H	1.51	0.58
15:N:657:LEU:HD23	15:N:682:ILE:HD12	1.85	0.58
17:P:743:GLN:HB3	17:P:746:GLN:HB2	1.86	0.58
23:V:118:THR:O	23:V:122:GLU:HG3	2.04	0.58
17:P:212:ARG:NH1	17:P:232:ASP:O	2.37	0.57
18:Q:216:PHE:HE1	18:Q:218:HIS:HB2	1.48	0.57
15:N:340:TRP:HZ2	15:N:405:VAL:HG13	1.68	0.57
15:N:534:SER:O	15:N:537:LYS:NZ	2.33	0.57
15:N:568:TYR:HB2	15:N:591:PHE:HB2	1.85	0.57
15:N:802:VAL:H	15:N:809:ILE:HG22	1.68	0.57
24:W:753:ARG:NH2	24:W:832:TYR:O	2.36	0.57
2:1:101:GLN:HG3	4:3:114:LEU:CD2	2.29	0.57
15:N:359:ILE:HD12	15:N:372:ILE:HG22	1.86	0.57
24:W:339:ILE:HD11	24:W:575:GLU:HB2	1.87	0.57
24:W:1102:ALA:O	24:W:1106:HIS:ND1	2.37	0.57
6:A:318:VAL:HA	6:A:329:LEU:HD13	1.86	0.57
6:A:386:ARG:HH11	6:A:387:SER:H	1.51	0.57
11:H:70:LEU:HD11	11:H:72:ARG:HH21	1.69	0.57
15:N:452:LEU:HD11	15:N:465:LEU:HB3	1.86	0.57
15:N:507:GLN:NE2	15:N:508:SER:OG	2.36	0.57
19:R:17:ASN:ND2	19:R:104:ASN:OD1	2.36	0.57
24:W:57:GLU:O	24:W:60:ILE:HB	2.04	0.57
25:X:796:SER:O	25:X:799:HIS:ND1	2.37	0.57
2:1:113:GLU:OE2	4:3:31:ALA:HB3	2.04	0.57
15:N:530:ILE:HD11	15:N:551:VAL:HG11	1.87	0.57
15:N:683:ARG:HA	15:N:709:THR:HA	1.86	0.57
17:P:377:TYR:H	17:P:459:PRO:HB3	1.68	0.57
24:W:696:HIS:HB2	24:W:736:PRO:HG3	1.85	0.57
6:A:66:GLN:HE22	12:I:73:ILE:CD1	2.16	0.57
13:J:127:ILE:HG13	20:S:65:PHE:HE1	1.69	0.57
15:N:683:ARG:HD2	16:O:684:ARG:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:1154:THR:HG21	24:W:1218:HIS:HB2	1.85	0.57
6:A:84:ILE:HD11	6:A:147:PHE:HB3	1.87	0.57
6:A:502:MET:O	6:A:502:MET:HG2	2.05	0.57
10:G:96:LEU:HB2	13:J:102:MET:CE	2.33	0.57
17:P:737:GLY:O	17:P:741:ARG:NH1	2.38	0.57
14:K:19:ARG:NH2	14:K:55:SER:OG	2.38	0.57
15:N:361:ILE:HD12	15:N:370:LEU:CD2	2.34	0.57
23:V:90:ASP:HB3	23:V:92:PRO:HD3	1.85	0.57
24:W:176:CYS:O	24:W:1330:ARG:NH2	2.37	0.57
24:W:332:GLN:NE2	24:W:575:GLU:OE2	2.37	0.57
15:N:279:GLN:O	15:N:283:PHE:N	2.35	0.57
17:P:402:MET:HE3	17:P:403:ALA:HB2	1.86	0.57
17:P:668:LEU:HD23	17:P:669:LYS:HG2	1.85	0.57
15:N:676:ASP:OD2	18:Q:593:MET:CB	2.53	0.57
24:W:467:LEU:HD12	24:W:474:ILE:HA	1.87	0.57
10:G:126:TYR:HA	10:G:129:HIS:HB3	1.86	0.56
15:N:819:SER:N	15:N:836:GLY:O	2.37	0.56
15:N:927:TYR:HB2	15:N:935:ALA:HB3	1.87	0.56
16:O:673:SER:OG	16:O:674:ILE:N	2.38	0.56
6:A:498:VAL:HA	6:A:502:MET:HA	1.87	0.56
14:K:78:PRO:HA	18:Q:195:LYS:HD3	1.86	0.56
24:W:666:THR:HA	24:W:669:LEU:HB2	1.87	0.56
5:4:77:GLU:HA	5:4:80:GLN:HG2	1.86	0.56
13:J:95:VAL:HG11	15:N:122:LEU:HD22	1.86	0.56
15:N:887:THR:O	15:N:903:CYS:N	2.39	0.56
17:P:821:GLN:HA	17:P:824:ILE:HB	1.87	0.56
1:0:211:ARG:NH1	1:0:212:THR:O	2.39	0.56
19:R:111:SER:OG	19:R:112:GLU:N	2.37	0.56
6:A:364:TYR:HB3	6:A:430:LEU:HD23	1.87	0.56
6:A:459:ASN:ND2	6:A:485:ASP:OD1	2.38	0.56
18:Q:336:PHE:HB2	18:Q:339:LEU:HB3	1.88	0.56
22:U:118:ILE:HA	22:U:121:ALA:HB3	1.87	0.56
24:W:467:LEU:HD11	24:W:491:PRO:HB3	1.88	0.56
24:W:867:LEU:HD12	24:W:966:VAL:HG22	1.88	0.56
25:X:905:PHE:HA	25:X:908:ILE:HD12	1.87	0.56
17:P:579:ARG:HD2	17:P:600:LYS:HE3	1.88	0.56
24:W:384:ILE:HG23	24:W:385:GLN:HG2	1.88	0.56
25:X:294:ILE:HD13	25:X:351:ALA:HA	1.87	0.56
10:G:96:LEU:HD21	15:N:132:THR:HG21	1.88	0.56
13:J:75:ARG:HD2	13:J:79:LEU:HD22	1.87	0.56
21:T:28:LEU:HD12	21:T:31:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:43:ALA:HA	25:X:46:LEU:HD12	1.86	0.56
25:X:284:GLU:HA	25:X:287:LYS:HG2	1.88	0.56
15:N:669:GLN:HG3	15:N:685:LEU:HD21	1.88	0.56
15:N:717:ASN:HD21	18:Q:552:SER:HA	1.71	0.56
17:P:436:LEU:HD13	17:P:443:LEU:HB3	1.86	0.56
5:4:104:HIS:HA	5:4:110:ARG:HH22	1.71	0.56
6:A:489:CYS:HA	6:A:514:LYS:HD3	1.88	0.56
19:R:95:ASP:O	19:R:98:ARG:NH1	2.39	0.56
25:X:505:GLN:HB3	25:X:672:ARG:HE	1.71	0.56
6:A:446:SER:HB3	6:A:449:ARG:HE	1.71	0.55
7:B:11:UNK:O	7:B:15:UNK:N	2.40	0.55
15:N:471:ASP:N	15:N:471:ASP:OD1	2.36	0.55
24:W:308:VAL:HG22	24:W:334:LEU:HD21	1.88	0.55
24:W:985:GLU:HA	24:W:1025:LYS:HG2	1.86	0.55
25:X:506:THR:OG1	25:X:672:ARG:NH2	2.38	0.55
4:3:88:LEU:HA	4:3:91:LYS:HG2	1.89	0.55
17:P:781:HIS:O	17:P:784:ARG:NH2	2.40	0.55
24:W:516:ALA:HA	24:W:558:ALA:HB3	1.88	0.55
6:A:179:SER:OG	6:A:270:ILE:O	2.21	0.55
10:G:84:SER:O	10:G:88:ASN:ND2	2.38	0.55
15:N:804:ASN:HD21	15:N:807:LYS:HB2	1.70	0.55
21:T:119:TYR:O	21:T:122:PHE:HB2	2.07	0.55
24:W:1082:LYS:HG3	24:W:1084:PRO:HD2	1.86	0.55
15:N:312:THR:OG1	15:N:329:TYR:OH	2.24	0.55
25:X:610:LYS:O	25:X:659:TYR:OH	2.24	0.55
15:N:374:HIS:ND1	15:N:379:PRO:CG	2.70	0.55
19:R:34:SER:O	19:R:37:HIS:HB2	2.07	0.55
24:W:294:LYS:NZ	24:W:344:PHE:O	2.39	0.55
24:W:886:ILE:HG21	24:W:970:VAL:HG11	1.87	0.55
25:X:912:LEU:HD22	25:X:954:GLU:HB3	1.88	0.55
8:D:30:LEU:HD22	12:I:99:LYS:HG2	1.89	0.55
10:G:131:ALA:HB1	15:N:154:ILE:CD1	2.34	0.55
2:1:143:LEU:HD21	23:V:119:LEU:CG	2.36	0.55
11:H:8:LEU:HG	11:H:69:PRO:HG3	1.89	0.55
15:N:279:GLN:HA	15:N:282:LEU:HB2	1.87	0.55
17:P:750:LEU:HA	17:P:754:ARG:HH21	1.72	0.55
18:Q:216:PHE:CE2	18:Q:306:GLU:HG3	2.42	0.55
19:R:145:VAL:HG22	19:R:169:VAL:HG13	1.89	0.55
15:N:711:ARG:HD3	18:Q:549:LEU:HB3	1.88	0.55
17:P:312:ARG:O	17:P:340:ARG:NH2	2.40	0.55
20:S:112:LEU:HB3	20:S:113:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:251:GLU:HG3	25:X:263:LEU:HD13	1.89	0.55
25:X:539:ILE:HG12	25:X:629:ARG:HG2	1.87	0.55
10:G:96:LEU:O	15:N:129:PHE:HZ	1.89	0.54
17:P:364:THR:OG1	17:P:367:ASP:HB2	2.07	0.54
18:Q:5:ARG:HG3	18:Q:7:VAL:HG13	1.89	0.54
24:W:213:ARG:NH1	25:X:759:GLU:OE1	2.38	0.54
6:A:288:PHE:HB2	6:A:296:SER:HB2	1.89	0.54
8:D:174:ARG:NH1	8:D:176:TYR:OH	2.40	0.54
10:G:97:ILE:CG1	13:J:102:MET:SD	2.86	0.54
24:W:941:VAL:HG12	24:W:943:PRO:HD2	1.89	0.54
25:X:135:THR:HG22	25:X:161:CYS:HB3	1.88	0.54
25:X:472:ASN:HD22	25:X:525:PHE:HB2	1.72	0.54
1:0:133:LEU:HG	1:0:135:ARG:HH12	1.72	0.54
9:F:61:ASN:OD1	9:F:86:ARG:NH2	2.40	0.54
15:N:217:VAL:HA	15:N:222:VAL:HA	1.89	0.54
15:N:443:LEU:HG	15:N:500:LEU:HD23	1.89	0.54
18:Q:489:LYS:O	18:Q:507:ARG:NH1	2.40	0.54
1:0:260:ASP:OD2	1:0:264:ARG:NH2	2.41	0.54
15:N:250:LEU:HD22	15:N:271:ILE:HG23	1.88	0.54
24:W:1153:ILE:HG12	24:W:1161:TRP:HB3	1.89	0.54
12:I:109:LEU:HD23	12:I:114:GLN:NE2	2.16	0.54
15:N:376:PRO:HB2	15:N:377:PRO:HD3	1.88	0.54
19:R:150:ARG:HB2	19:R:163:LEU:HD12	1.89	0.54
25:X:472:ASN:HA	25:X:475:THR:HG22	1.88	0.54
9:F:80:ILE:O	9:F:82:ARG:NH1	2.40	0.54
15:N:761:LYS:HA	15:N:764:GLU:HB2	1.89	0.54
17:P:131:ILE:HA	17:P:183:THR:HA	1.89	0.54
17:P:359:LEU:HD22	17:P:378:PRO:HG2	1.90	0.54
17:P:656:ARG:HG2	17:P:693:LEU:HD13	1.90	0.54
1:0:241:LYS:NZ	1:0:295:THR:OG1	2.39	0.54
3:2:185:VAL:HG12	3:2:186:THR:HG23	1.89	0.54
6:A:322:GLN:HG2	6:A:329:LEU:H	1.73	0.54
8:D:97:GLU:HA	8:D:100:VAL:HG22	1.90	0.54
15:N:358:THR:CG2	15:N:375:ASP:OD2	2.47	0.54
18:Q:138:LYS:HB3	18:Q:143:THR:HG21	1.89	0.54
24:W:373:MET:O	24:W:377:LEU:N	2.38	0.54
24:W:688:ILE:HD11	24:W:719:ILE:HG21	1.89	0.54
6:A:210:TYR:HB3	6:A:223:LYS:HB2	1.90	0.54
15:N:683:ARG:HD2	16:O:684:ARG:CG	2.38	0.54
17:P:248:VAL:HA	17:P:253:CYS:HA	1.89	0.54
17:P:796:LYS:NZ	17:P:824:ILE:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:113:LYS:HG3	25:X:116:GLU:H	1.71	0.54
25:X:657:GLN:O	25:X:662:ARG:NH2	2.41	0.54
17:P:527:LEU:HD13	17:P:550:LYS:HZ3	1.73	0.54
18:Q:216:PHE:CD2	18:Q:306:GLU:CG	2.90	0.54
9:F:65:GLY:O	9:F:86:ARG:NH1	2.42	0.53
15:N:356:LYS:H	15:N:376:PRO:HD2	1.72	0.53
24:W:581:ILE:HA	24:W:584:PHE:HB2	1.90	0.53
24:W:732:LEU:HG	24:W:740:GLN:HG2	1.89	0.53
24:W:978:LEU:O	24:W:981:SER:OG	2.22	0.53
24:W:1127:LEU:O	24:W:1131:LEU:N	2.31	0.53
15:N:882:ILE:HG23	15:N:916:LEU:HD21	1.90	0.53
15:N:925:ASP:HB3	15:N:927:TYR:HE1	1.73	0.53
18:Q:1:MET:SD	18:Q:1:MET:N	2.76	0.53
25:X:783:LEU:HA	25:X:787:ILE:HD12	1.90	0.53
5:4:28:LEU:HD11	5:4:76:LEU:HD13	1.91	0.53
15:N:1316:CYS:O	15:N:1320:MET:N	2.36	0.53
17:P:595:VAL:HG12	17:P:599:LEU:HD21	1.90	0.53
22:U:3:ASP:O	22:U:6:THR:OG1	2.25	0.53
24:W:148:ILE:O	24:W:198:HIS:NE2	2.41	0.53
24:W:501:GLY:HA3	24:W:517:SER:HB3	1.90	0.53
24:W:1050:LYS:O	24:W:1054:ASN:ND2	2.41	0.53
4:3:92:LEU:HA	4:3:95:VAL:HG22	1.90	0.53
15:N:808:LEU:HB3	15:N:822:ILE:HB	1.90	0.53
21:T:47:HIS:O	21:T:103:GLN:N	2.41	0.53
15:N:376:PRO:HD2	15:N:377:PRO:CD	2.37	0.53
2:1:139:TRP:HD1	23:V:119:LEU:HD13	1.74	0.53
15:N:493:ILE:HA	15:N:496:LEU:HB2	1.91	0.53
2:1:89:ARG:HD3	18:Q:544:MET:CG	2.29	0.53
8:D:104:ASP:OD2	8:D:108:GLN:NE2	2.42	0.53
17:P:359:LEU:HD13	17:P:378:PRO:HB2	1.90	0.53
15:N:737:ARG:NH1	15:N:803:TYR:O	2.42	0.53
21:T:116:ARG:HD2	21:T:125:LYS:HZ3	1.74	0.53
6:A:208:VAL:HG12	6:A:222:LEU:CD1	2.38	0.53
10:G:96:LEU:HB2	13:J:102:MET:HE2	1.90	0.53
15:N:458:LEU:HD21	18:Q:325:ILE:CG2	2.39	0.53
18:Q:404:ARG:HH21	18:Q:421:LEU:HD21	1.74	0.53
24:W:296:ARG:NH2	24:W:348:SER:OG	2.42	0.53
25:X:414:GLU:HG3	25:X:415:PRO:HD3	1.90	0.53
8:D:118:GLU:HG2	22:U:122:LEU:HD12	1.89	0.53
15:N:675:GLY:HA3	18:Q:622:PHE:CE1	2.44	0.53
15:N:700:ALA:O	15:N:704:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:39:VAL:HA	8:D:42:ARG:HD2	1.91	0.52
15:N:376:PRO:N	15:N:377:PRO:CD	2.72	0.52
2:1:69:ASP:N	2:1:71:GLU:OE1	2.42	0.52
6:A:187:MET:HB3	6:A:208:VAL:HG21	1.90	0.52
6:A:206:GLY:O	6:A:412:ARG:NH1	2.42	0.52
15:N:703:ARG:HH22	18:Q:614:LYS:CG	2.20	0.52
17:P:208:ARG:NH2	25:X:680:GLN:O	2.42	0.52
25:X:408:GLN:HA	25:X:411:LEU:HB2	1.91	0.52
1:0:211:ARG:HH11	1:0:212:THR:H	1.58	0.52
15:N:678:PHE:HE1	18:Q:581:SER:HB2	1.75	0.52
15:N:845:SER:OG	15:N:846:ASN:N	2.41	0.52
15:N:1212:GLY:HA2	15:N:1215:ILE:HG22	1.91	0.52
23:V:50:ARG:NH1	23:V:53:GLN:OE1	2.43	0.52
24:W:349:PHE:HD2	24:W:391:ASP:HB3	1.73	0.52
25:X:179:HIS:ND1	25:X:225:ILE:O	2.43	0.52
1:0:40:ARG:HA	17:P:790:CYS:HB3	1.90	0.52
15:N:806:ARG:HH12	15:N:824:TRP:H	1.58	0.52
17:P:393:ILE:HG21	17:P:402:MET:HE3	1.91	0.52
17:P:738:LEU:HB3	17:P:742:LEU:HD23	1.90	0.52
18:Q:152:SER:OG	23:V:61:MET:SD	2.68	0.52
18:Q:589:GLY:O	18:Q:591:LYS:NZ	2.42	0.52
24:W:234:SER:HB2	24:W:660:GLU:HB3	1.91	0.52
6:A:178:GLN:HA	6:A:181:GLU:HB2	1.90	0.52
15:N:334:CYS:HB2	15:N:360:LYS:HG2	1.90	0.52
15:N:465:LEU:HD12	15:N:478:MET:HG3	1.91	0.52
2:1:56:PHE:CE2	3:2:185:VAL:HG21	2.44	0.52
8:D:117:ALA:HB1	10:G:163:MET:SD	2.49	0.52
15:N:541:LYS:HE2	15:N:547:GLN:H	1.74	0.52
24:W:27:MET:N	24:W:27:MET:SD	2.83	0.52
24:W:1216:TRP:O	24:W:1258:ARG:NH1	2.42	0.52
8:D:106:ASP:OD1	8:D:109:GLN:NE2	2.42	0.52
13:J:61:ILE:O	15:N:50:ARG:N	2.42	0.52
15:N:192:LEU:HD23	15:N:195:LEU:HD12	1.92	0.52
15:N:445:PRO:O	15:N:504:ARG:NH2	2.43	0.52
15:N:480:LYS:O	15:N:484:ASP:N	2.41	0.52
21:T:136:ARG:NH1	21:T:205:GLN:O	2.43	0.52
6:A:398:PHE:HB2	6:A:403:ARG:HB2	1.91	0.52
8:D:127:GLN:OE1	10:G:152:ARG:NH2	2.43	0.52
14:K:76:GLY:O	14:K:77:GLN:NE2	2.43	0.52
15:N:308:LEU:CD1	15:N:370:LEU:HD11	2.21	0.52
15:N:370:LEU:O	15:N:392:ILE:HD11	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:639:LYS:CE	18:Q:562:SER:HA	2.39	0.52
24:W:793:LEU:HG	24:W:803:ILE:HG12	1.92	0.52
25:X:352:ASP:OD2	25:X:389:ARG:NH1	2.43	0.52
6:A:258:THR:H	6:A:306:LYS:HZ1	1.57	0.52
6:A:317:PHE:HA	6:A:320:LYS:HD2	1.91	0.52
15:N:457:ASP:OD1	15:N:457:ASP:N	2.42	0.52
15:N:535:LYS:NZ	15:N:536:ASN:OD1	2.39	0.52
18:Q:224:VAL:HG22	18:Q:245:VAL:HG12	1.91	0.52
18:Q:546:TRP:HA	18:Q:574:PRO:HD3	1.90	0.52
24:W:1046:ASP:N	24:W:1046:ASP:OD1	2.43	0.52
25:X:633:LEU:HA	25:X:636:ARG:HD2	1.92	0.52
6:A:357:LEU:HD13	6:A:427:ARG:HH21	1.75	0.52
15:N:751:ASN:ND2	15:N:755:GLU:O	2.43	0.52
17:P:310:SER:OG	17:P:312:ARG:NH1	2.43	0.52
6:A:187:MET:HB3	6:A:208:VAL:CG2	2.40	0.51
17:P:483:VAL:HG13	17:P:484:THR:HG23	1.91	0.51
24:W:735:PHE:O	24:W:740:GLN:NE2	2.43	0.51
25:X:558:VAL:O	25:X:562:ASN:ND2	2.43	0.51
25:X:637:GLU:HA	25:X:640:LEU:HD12	1.92	0.51
15:N:376:PRO:HD2	15:N:377:PRO:HD2	1.91	0.51
15:N:403:ASP:O	15:N:407:ALA:N	2.38	0.51
18:Q:226:LYS:NZ	18:Q:242:PRO:O	2.43	0.51
25:X:162:LEU:HD21	25:X:211:LEU:HD22	1.91	0.51
25:X:530:GLN:HG3	25:X:531:THR:HG23	1.92	0.51
2:1:139:TRP:HE1	23:V:122:GLU:HB2	1.75	0.51
15:N:372:ILE:N	15:N:372:ILE:CD1	2.73	0.51
15:N:680:HIS:CD2	18:Q:557:LEU:HD11	2.45	0.51
15:N:737:ARG:HH22	15:N:805:TYR:HE1	1.58	0.51
15:N:1177:LEU:HD23	15:N:1181:ALA:HB3	1.92	0.51
21:T:36:GLN:OE1	21:T:118:GLN:NE2	2.43	0.51
24:W:188:ARG:NH1	24:W:193:GLU:OE2	2.43	0.51
6:A:379:ASP:HA	6:A:387:SER:HB3	1.92	0.51
10:G:51:CYS:HB3	10:G:54:LEU:HD21	1.92	0.51
15:N:781:LEU:HD12	15:N:782:GLU:HG3	1.91	0.51
16:O:636:HIS:HE1	17:P:616:GLN:HG2	1.76	0.51
1:0:137:ALA:H	18:Q:486:GLN:HG3	1.74	0.51
6:A:343:ILE:HA	6:A:346:PHE:HB3	1.92	0.51
15:N:918:PHE:N	15:N:922:TYR:O	2.44	0.51
17:P:218:ILE:HG12	17:P:228:VAL:HG12	1.92	0.51
17:P:663:ARG:NH2	17:P:684:ASP:OD2	2.44	0.51
6:A:338:PRO:HA	6:A:389:GLN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:806:ARG:NH2	15:N:824:TRP:O	2.34	0.51
10:G:90:LEU:HD21	13:J:109:LEU:CG	2.41	0.51
19:R:82:PRO:HG2	19:R:109:ALA:HB1	1.92	0.51
24:W:271:ARG:HH12	24:W:307:LEU:HA	1.75	0.51
24:W:1018:ASP:OD1	24:W:1018:ASP:N	2.43	0.51
25:X:737:HIS:HB2	25:X:831:ARG:HD3	1.92	0.51
25:X:776:MET:HA	25:X:779:VAL:HG22	1.91	0.51
3:2:123:ALA:HA	3:2:126:CYS:HB2	1.92	0.51
15:N:384:LYS:O	15:N:388:ARG:N	2.39	0.51
17:P:100:ASP:N	17:P:100:ASP:OD1	2.44	0.51
17:P:702:ASP:HB3	17:P:705:PRO:HB3	1.92	0.51
2:1:71:GLU:HG3	2:1:74:ARG:HH21	1.76	0.51
2:1:128:LEU:O	2:1:132:HIS:N	2.30	0.51
11:H:155:SER:O	11:H:159:ARG:NH1	2.43	0.51
15:N:445:PRO:HG2	15:N:635:CYS:HB3	1.93	0.51
15:N:507:GLN:NE2	15:N:636:ALA:O	2.44	0.51
15:N:589:GLN:HA	24:W:26:PHE:HE1	1.75	0.51
24:W:569:ARG:NH2	24:W:912:TRP:O	2.44	0.51
25:X:498:LEU:HD22	25:X:665:ILE:HG23	1.93	0.51
25:X:612:LYS:HD2	25:X:656:LEU:HD21	1.92	0.51
25:X:628:VAL:HG11	25:X:677:VAL:HG13	1.93	0.51
25:X:753:LEU:HD22	25:X:800:SER:HB2	1.92	0.51
15:N:683:ARG:HH11	15:N:685:LEU:HD23	1.76	0.51
15:N:723:GLU:HG2	15:N:744:HIS:HB2	1.92	0.51
18:Q:103:ARG:HE	18:Q:106:LEU:HD22	1.76	0.51
21:T:116:ARG:HA	21:T:124:VAL:O	2.11	0.51
1:0:18:ILE:HD12	1:0:21:ILE:HD11	1.93	0.50
6:A:81:LEU:HD11	6:A:142:LEU:HD11	1.92	0.50
21:T:28:LEU:O	21:T:32:GLY:N	2.41	0.50
24:W:1034:LEU:HD13	24:W:1038:ARG:HH11	1.75	0.50
25:X:282:VAL:HG21	25:X:334:VAL:HG12	1.93	0.50
8:D:79:LEU:O	8:D:83:ALA:N	2.40	0.50
17:P:588:THR:OG1	17:P:701:ARG:NH1	2.43	0.50
24:W:803:ILE:HB	24:W:940:GLN:HE22	1.77	0.50
6:A:258:THR:H	6:A:306:LYS:NZ	2.09	0.50
15:N:121:PHE:HE1	15:N:125:GLN:HE21	1.57	0.50
15:N:154:ILE:N	15:N:155:PRO:CD	2.74	0.50
15:N:225:ARG:HE	15:N:227:GLU:HG3	1.77	0.50
15:N:376:PRO:CD	15:N:377:PRO:CD	2.89	0.50
24:W:1172:ILE:O	24:W:1244:GLN:NE2	2.44	0.50
5:4:29:ALA:HB2	5:4:72:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:506:VAL:HG22	6:A:509:ARG:HH22	1.77	0.50
19:R:129:PHE:HB2	19:R:148:ILE:HG23	1.93	0.50
24:W:238:CYS:HG	24:W:240:SER:HG	1.59	0.50
24:W:891:LEU:O	24:W:897:ARG:NH2	2.43	0.50
24:W:964:LEU:HD13	24:W:994:LEU:HG	1.93	0.50
25:X:423:THR:HG23	25:X:424:MET:HE2	1.93	0.50
2:1:128:LEU:HB3	23:V:133:GLU:HG2	1.93	0.50
10:G:100:PRO:O	15:N:128:LEU:HD23	2.10	0.50
17:P:345:THR:HB	17:P:400:GLN:HA	1.93	0.50
2:1:89:ARG:CD	18:Q:544:MET:HG2	2.30	0.50
6:A:320:LYS:HB3	6:A:410:LEU:HD13	1.94	0.50
15:N:371:GLN:CD	15:N:373:PHE:HE2	2.15	0.50
15:N:545:LEU:HD12	15:N:652:MET:HG3	1.93	0.50
17:P:311:LEU:HD13	17:P:339:TRP:CE2	2.47	0.50
17:P:585:THR:HA	17:P:697:TRP:HH2	1.77	0.50
18:Q:397:SER:HB2	19:R:73:ARG:HH21	1.77	0.50
21:T:184:TYR:OH	21:T:192:GLN:OE1	2.30	0.50
24:W:506:ARG:HH22	24:W:557:VAL:HG13	1.75	0.50
24:W:1047:THR:HA	24:W:1050:LYS:HD2	1.94	0.50
25:X:517:ARG:HG2	25:X:523:PRO:HD3	1.94	0.50
8:D:109:GLN:NE2	10:G:174:ASP:HB3	2.22	0.50
25:X:951:THR:HA	25:X:954:GLU:HG2	1.93	0.50
8:D:104:ASP:HA	8:D:107:ILE:HD12	1.94	0.50
10:G:145:GLN:HA	10:G:148:GLU:HG3	1.94	0.50
15:N:592:LYS:HG2	24:W:25:MET:HE1	1.93	0.50
21:T:38:THR:HG22	21:T:115:THR:HG22	1.94	0.50
24:W:94:PRO:HG2	24:W:128:GLY:HA3	1.94	0.50
25:X:274:GLN:CG	25:X:276:ILE:HD11	2.41	0.50
2:1:143:LEU:CD2	23:V:119:LEU:HG	2.38	0.50
10:G:168:LEU:HD23	10:G:171:LEU:HD13	1.94	0.50
15:N:722:ALA:O	15:N:747:LEU:N	2.43	0.50
24:W:700:PHE:HA	24:W:1222:GLY:HA3	1.94	0.50
25:X:271:LYS:HG3	25:X:276:ILE:HB	1.94	0.50
1:0:201:ILE:HD13	1:0:228:LEU:HD22	1.93	0.49
2:1:125:LYS:CE	23:V:137:SER:HB2	2.34	0.49
5:4:19:GLN:NE2	8:D:190:MET:SD	2.85	0.49
8:D:129:LYS:HD3	8:D:132:LEU:HD12	1.94	0.49
15:N:712:LEU:O	18:Q:550:SER:HA	2.11	0.49
17:P:60:ARG:O	17:P:78:SER:OG	2.30	0.49
17:P:220:PHE:HD1	17:P:289:ASP:HA	1.77	0.49
4:3:136:SER:O	4:3:139:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:40:ARG:NH1	10:G:17:TYR:OH	2.45	0.49
6:A:188:ALA:O	6:A:202:LYS:NZ	2.45	0.49
6:A:343:ILE:O	6:A:347:GLU:N	2.45	0.49
9:F:169:SER:OG	15:N:263:ARG:NH2	2.45	0.49
15:N:221:ARG:HB3	15:N:233:THR:HB	1.93	0.49
15:N:376:PRO:CB	15:N:377:PRO:HD3	2.42	0.49
15:N:937:ARG:HE	15:N:943:LEU:HG	1.76	0.49
15:N:1301:ALA:O	15:N:1305:LEU:N	2.43	0.49
18:Q:209:TYR:C	18:Q:214:SER:OG	2.50	0.49
24:W:16:GLU:OE1	24:W:19:GLU:N	2.44	0.49
24:W:620:ARG:NH2	24:W:652:LEU:O	2.45	0.49
24:W:797:LEU:HA	24:W:801:ASP:H	1.78	0.49
6:A:441:GLU:OE1	6:A:453:SER:OG	2.30	0.49
10:G:90:LEU:CD2	13:J:109:LEU:HD12	2.36	0.49
10:G:90:LEU:HD23	13:J:109:LEU:CD1	2.34	0.49
10:G:109:LEU:HD22	15:N:135:ARG:NE	2.26	0.49
10:G:143:LYS:HA	10:G:146:ARG:HE	1.77	0.49
11:H:140:ILE:HG21	18:Q:146:LEU:HA	1.92	0.49
17:P:106:LYS:HE2	17:P:123:GLY:HA3	1.95	0.49
18:Q:366:ASP:N	18:Q:366:ASP:OD1	2.43	0.49
19:R:40:ARG:HH12	23:V:98:ILE:HD11	1.78	0.49
24:W:1203:MET:HG3	24:W:1205:CYS:H	1.78	0.49
2:1:132:HIS:O	2:1:136:LEU:N	2.40	0.49
15:N:722:ALA:HB3	15:N:747:LEU:HB2	1.93	0.49
17:P:14:ASP:O	17:P:456:ARG:N	2.40	0.49
17:P:182:VAL:HG23	17:P:218:ILE:HD11	1.94	0.49
19:R:21:TYR:HB2	19:R:173:VAL:HB	1.95	0.49
24:W:1295:CYS:HA	24:W:1298:LEU:HD12	1.93	0.49
8:D:87:GLY:O	8:D:91:HIS:ND1	2.38	0.49
15:N:361:ILE:CD1	15:N:370:LEU:HD23	2.40	0.49
17:P:535:LYS:HD3	17:P:541:VAL:HG23	1.93	0.49
19:R:58:PHE:HB3	19:R:123:PHE:HD2	1.77	0.49
24:W:253:LYS:HZ1	24:W:1254:PRO:HA	1.78	0.49
24:W:863:ASP:HB2	24:W:966:VAL:HG21	1.93	0.49
24:W:866:ILE:HG23	24:W:886:ILE:HD12	1.93	0.49
24:W:981:SER:HB3	24:W:1022:LEU:HD22	1.93	0.49
25:X:363:LEU:HD12	25:X:364:LEU:HG	1.95	0.49
18:Q:595:GLN:NE2	18:Q:619:ARG:O	2.46	0.49
10:G:91:ASP:OD2	13:J:124:TYR:OH	2.26	0.49
12:I:86:ASP:OD1	12:I:86:ASP:N	2.45	0.49
13:J:75:ARG:HA	20:S:102:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:197:ARG:HH22	18:Q:221:THR:HG22	1.77	0.49
24:W:144:LYS:O	24:W:147:THR:OG1	2.25	0.49
5:4:23:GLU:O	5:4:27:CYS:N	2.36	0.49
5:4:107:HIS:CE1	15:N:168:ARG:HE	2.31	0.49
6:A:320:LYS:HD3	6:A:410:LEU:HD22	1.95	0.49
15:N:247:LEU:HB3	15:N:275:HIS:CD2	2.48	0.49
15:N:918:PHE:HB3	15:N:922:TYR:HB2	1.95	0.49
24:W:882:CYS:HA	24:W:885:ILE:HD12	1.95	0.49
2:1:80:CYS:SG	2:1:81:ILE:N	2.85	0.49
15:N:280:SER:O	15:N:284:ALA:N	2.45	0.49
15:N:917:ALA:HA	15:N:923:CYS:HA	1.94	0.49
15:N:666:ILE:O	15:N:668:HIS:ND1	2.32	0.49
15:N:699:LYS:O	15:N:703:ARG:N	2.44	0.49
19:R:156:ASN:HD22	19:R:156:ASN:C	2.14	0.49
24:W:561:PRO:HA	24:W:564:VAL:HG22	1.95	0.49
5:4:46:LYS:HA	5:4:49:VAL:HG22	1.94	0.48
17:P:432:LYS:N	17:P:446:ILE:O	2.43	0.48
17:P:582:GLU:HA	17:P:585:THR:HG22	1.94	0.48
21:T:40:CYS:HA	21:T:112:THR:O	2.14	0.48
24:W:794:TRP:HA	24:W:797:LEU:HG	1.95	0.48
24:W:816:ALA:HA	24:W:819:LEU:HB2	1.95	0.48
25:X:629:ARG:O	25:X:636:ARG:NH2	2.46	0.48
3:2:160:TYR:HA	3:2:163:VAL:HG22	1.95	0.48
8:D:112:LYS:HA	8:D:115:LYS:HG2	1.94	0.48
20:S:112:LEU:N	20:S:113:PRO:CD	2.76	0.48
25:X:314:PRO:HB3	25:X:370:GLN:HG3	1.95	0.48
25:X:757:ARG:HE	25:X:760:HIS:CE1	2.32	0.48
5:4:21:GLU:HB3	5:4:58:TRP:CH2	2.48	0.48
6:A:208:VAL:HG12	6:A:222:LEU:HD22	1.95	0.48
6:A:363:PHE:HB2	6:A:374:TYR:HB2	1.94	0.48
6:A:426:LYS:HE3	6:A:505:PRO:HG2	1.94	0.48
15:N:193:HIS:HA	15:N:196:ASN:HB2	1.96	0.48
17:P:71:TRP:HB2	17:P:753:GLY:H	1.78	0.48
17:P:699:CYS:O	17:P:707:SER:OG	2.30	0.48
25:X:303:LEU:HD12	25:X:410:ILE:HD11	1.95	0.48
2:1:135:LYS:HG2	2:1:139:TRP:CZ3	2.34	0.48
7:B:7:UNK:O	7:B:11:UNK:N	2.46	0.48
11:H:105:VAL:HA	11:H:108:HIS:HD1	1.78	0.48
15:N:849:ASN:HA	15:N:852:LEU:HB2	1.95	0.48
17:P:393:ILE:HG21	17:P:402:MET:CE	2.44	0.48
17:P:489:TRP:HH2	17:P:739:VAL:HB	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:726:ASN:HD22	24:W:750:GLN:HG2	1.79	0.48
24:W:966:VAL:HA	24:W:969:ILE:HG22	1.95	0.48
24:W:1252:VAL:HG12	24:W:1256:LEU:HG	1.94	0.48
5:4:22:LEU:HD11	5:4:66:TYR:HB3	1.95	0.48
10:G:72:PHE:HB3	10:G:74:HIS:CE1	2.49	0.48
10:G:162:GLU:O	10:G:166:ASN:ND2	2.47	0.48
15:N:493:ILE:O	15:N:497:LYS:N	2.46	0.48
17:P:14:ASP:HB2	17:P:456:ARG:HB2	1.95	0.48
18:Q:595:GLN:HG2	18:Q:619:ARG:HB2	1.95	0.48
24:W:503:GLY:HA2	24:W:506:ARG:HH21	1.78	0.48
24:W:1210:ALA:O	24:W:1213:HIS:HB2	2.14	0.48
24:W:1241:THR:HG23	24:W:1243:PHE:H	1.78	0.48
25:X:274:GLN:HG3	25:X:276:ILE:CG1	2.42	0.48
1:0:49:GLU:OE2	1:0:50:LYS:NZ	2.41	0.48
4:3:83:ARG:NH1	4:3:84:GLN:OE1	2.44	0.48
6:A:210:TYR:H	6:A:223:LYS:H	1.61	0.48
15:N:555:LEU:O	15:N:565:SER:N	2.45	0.48
15:N:806:ARG:HG3	15:N:807:LYS:HD2	1.96	0.48
2:1:101:GLN:HG2	2:1:105:GLN:HE22	1.78	0.48
10:G:136:ARG:O	10:G:139:MET:HG3	2.14	0.48
15:N:330:HIS:ND1	15:N:334:CYS:SG	2.84	0.48
15:N:592:LYS:HG2	24:W:25:MET:CE	2.42	0.48
15:N:929:ARG:HE	16:O:655:THR:HG21	1.78	0.48
15:N:1224:ILE:O	15:N:1230:GLN:N	2.47	0.48
24:W:523:LEU:O	24:W:569:ARG:NH1	2.44	0.48
25:X:169:LEU:HD13	25:X:221:LEU:HD22	1.95	0.48
15:N:320:TRP:HB3	15:N:322:ASP:H	1.79	0.48
15:N:495:GLN:HA	15:N:498:PHE:CD2	2.48	0.48
17:P:39:TRP:HE1	17:P:43:ASN:HA	1.79	0.48
17:P:825:LYS:NZ	17:P:826:ASN:OD1	2.39	0.48
19:R:32:LEU:HD21	19:R:145:VAL:HG11	1.96	0.48
24:W:507:ILE:HD12	24:W:508:PRO:HD2	1.95	0.48
2:1:143:LEU:HD21	23:V:119:LEU:CD1	2.43	0.48
3:2:81:ASN:ND2	3:2:100:GLN:O	2.42	0.48
6:A:367:LEU:HD13	6:A:509:ARG:HH11	1.78	0.48
11:H:30:ILE:HG23	18:Q:99:ARG:HH12	1.78	0.48
15:N:942:SER:OG	15:N:945:ASP:O	2.25	0.48
17:P:742:LEU:HD13	17:P:748:LEU:HD23	1.96	0.48
5:4:23:GLU:HA	5:4:26:GLN:HB2	1.95	0.48
6:A:208:VAL:CG1	6:A:222:LEU:CD1	2.92	0.48
6:A:462:LEU:HB2	25:X:52:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:301:LEU:HD11	15:N:366:VAL:HG23	1.94	0.48
15:N:807:LYS:HG3	15:N:823:GLN:HB3	1.95	0.48
18:Q:329:ASN:HB3	18:Q:345:LEU:HB3	1.96	0.48
24:W:1005:LEU:HD22	24:W:1026:LEU:HD21	1.96	0.48
24:W:1090:CYS:SG	24:W:1091:ASP:N	2.86	0.48
25:X:193:GLU:HA	25:X:196:LEU:HB3	1.95	0.48
1:0:163:ASP:OD1	1:0:182:ARG:NH2	2.44	0.47
4:3:167:ILE:HA	4:3:170:ILE:HG22	1.95	0.47
10:G:131:ALA:CB	15:N:154:ILE:HD11	2.36	0.47
10:G:134:THR:HA	10:G:137:VAL:HG22	1.96	0.47
17:P:311:LEU:HD11	17:P:337:LEU:HB3	1.96	0.47
17:P:358:LYS:HB3	17:P:438:TRP:HE3	1.78	0.47
24:W:1322:LYS:O	24:W:1326:LYS:N	2.45	0.47
6:A:187:MET:HA	6:A:190:MET:HB3	1.97	0.47
24:W:755:ASN:O	24:W:759:ASN:ND2	2.47	0.47
6:A:222:LEU:HB2	6:A:255:ALA:HB3	1.96	0.47
9:F:42:ASP:N	9:F:42:ASP:OD1	2.46	0.47
17:P:355:ALA:HB3	17:P:383:ALA:HB3	1.96	0.47
22:U:109:TYR:HA	22:U:112:ASP:HB2	1.97	0.47
24:W:534:HIS:HA	24:W:537:MET:HG3	1.96	0.47
24:W:655:ALA:HA	24:W:1000:ARG:HD2	1.96	0.47
24:W:834:PHE:HB2	24:W:885:ILE:HD11	1.97	0.47
6:A:375:PHE:O	6:A:442:VAL:N	2.47	0.47
15:N:202:ARG:NH2	15:N:243:VAL:O	2.47	0.47
17:P:655:LEU:HD23	17:P:658:LEU:HD21	1.96	0.47
19:R:184:ASP:OD1	19:R:185:ASP:N	2.47	0.47
1:0:30:ARG:NH2	1:0:33:ASP:OD2	2.48	0.47
4:3:45:VAL:O	4:3:48:THR:OG1	2.23	0.47
6:A:496:LYS:O	6:A:500:ARG:N	2.47	0.47
6:A:498:VAL:O	6:A:502:MET:N	2.47	0.47
8:D:44:LEU:HA	8:D:47:MET:HG3	1.95	0.47
15:N:794:LEU:HA	15:N:797:PHE:HB3	1.95	0.47
15:N:1214:VAL:HG22	15:N:1217:ARG:HH21	1.79	0.47
24:W:101:LEU:HD13	24:W:118:THR:HG23	1.95	0.47
24:W:374:TRP:O	24:W:377:LEU:HB3	2.15	0.47
24:W:1064:ASP:OD1	24:W:1064:ASP:N	2.42	0.47
24:W:1273:ALA:O	24:W:1277:MET:HG3	2.15	0.47
2:1:128:LEU:HD11	23:V:129:GLU:OE2	2.14	0.47
6:A:278:HIS:ND1	6:A:279:PRO:CD	2.58	0.47
6:A:464:CYS:HB3	6:A:480:TYR:HB2	1.96	0.47
8:D:154:ARG:HE	8:D:155:ILE:HG23	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:152:ARG:HA	10:G:155:LYS:HE3	1.95	0.47
11:H:9:GLU:HA	11:H:12:LEU:HG	1.96	0.47
15:N:234:LEU:HD11	15:N:247:LEU:HD12	1.97	0.47
15:N:440:VAL:O	15:N:452:LEU:N	2.46	0.47
18:Q:454:ARG:NH2	18:Q:522:GLN:OE1	2.46	0.47
21:T:129:VAL:HG11	21:T:200:ILE:HG21	1.97	0.47
24:W:1318:ILE:HD11	24:W:1329:LEU:HD22	1.96	0.47
25:X:273:MET:SD	25:X:934:CYS:SG	3.12	0.47
1:0:295:THR:O	1:0:297:ARG:NH1	2.47	0.47
2:1:92:GLU:O	2:1:96:LEU:N	2.37	0.47
6:A:313:VAL:HG12	6:A:414:GLN:HG2	1.97	0.47
6:A:503:SER:O	6:A:507:THR:HG23	2.15	0.47
13:J:85:LEU:HD13	20:S:93:TYR:HB2	1.97	0.47
15:N:782:GLU:HG2	15:N:785:ARG:HH22	1.80	0.47
17:P:565:ARG:NH1	17:P:566:PRO:O	2.47	0.47
24:W:173:ARG:O	24:W:1328:ARG:NH1	2.46	0.47
25:X:274:GLN:O	25:X:276:ILE:HG13	2.14	0.47
25:X:297:PRO:HG2	25:X:301:GLU:HG3	1.96	0.47
4:3:162:GLN:HB3	14:K:103:LYS:HE3	1.96	0.47
6:A:462:LEU:HD12	25:X:52:ILE:HB	1.97	0.47
6:A:498:VAL:HG13	6:A:502:MET:HA	1.97	0.47
8:D:180:LEU:HD12	8:D:181:GLU:HG2	1.97	0.47
15:N:269:MET:SD	15:N:270:GLN:NE2	2.88	0.47
15:N:402:ILE:O	15:N:406:HIS:N	2.42	0.47
17:P:30:CYS:HB2	17:P:52:ARG:HG2	1.96	0.47
17:P:345:THR:OG1	17:P:346:ASN:N	2.48	0.47
25:X:169:LEU:O	25:X:175:ARG:NH1	2.48	0.47
5:4:30:ASN:HB2	8:D:182:MET:HE1	1.95	0.47
6:A:386:ARG:HD2	6:A:386:ARG:HA	1.60	0.47
15:N:371:GLN:OE1	15:N:373:PHE:CE2	2.61	0.47
15:N:643:HIS:CG	18:Q:560:ILE:HG12	2.48	0.47
2:1:60:VAL:HG11	3:2:182:ALA:HB2	1.98	0.46
6:A:187:MET:CB	6:A:208:VAL:HG21	2.45	0.46
6:A:386:ARG:NH2	6:A:389:GLN:HE21	2.12	0.46
8:D:28:GLU:OE1	12:I:107:ILE:HD12	2.14	0.46
15:N:574:ASN:HB2	15:N:583:ALA:HA	1.97	0.46
15:N:707:ASP:CG	16:O:684:ARG:NH1	2.69	0.46
18:Q:42:ARG:HH21	18:Q:46:ARG:HB3	1.80	0.46
19:R:107:ASP:O	21:T:90:ASN:ND2	2.48	0.46
21:T:154:TRP:HZ2	21:T:171:GLY:HA2	1.80	0.46
24:W:153:SER:HA	25:X:916:THR:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:408:TYR:OH	24:W:452:ARG:NH1	2.40	0.46
24:W:975:LEU:HD22	24:W:1016:LEU:HD21	1.97	0.46
25:X:666:MET:HA	25:X:669:ILE:HD12	1.97	0.46
6:A:59:VAL:HG11	8:D:52:ARG:HD3	1.96	0.46
15:N:224:PHE:HD2	15:N:234:LEU:HD13	1.80	0.46
15:N:499:TRP:HA	15:N:502:GLN:HB2	1.96	0.46
17:P:63:HIS:HB3	17:P:73:LEU:HD21	1.98	0.46
20:S:109:LEU:O	20:S:113:PRO:HD3	2.10	0.46
25:X:543:ASP:HA	25:X:548:ARG:HH12	1.80	0.46
1:0:200:VAL:HG22	1:0:214:VAL:HG23	1.97	0.46
8:D:136:GLU:O	8:D:140:LYS:NZ	2.47	0.46
15:N:149:LEU:HD21	15:N:152:PHE:HZ	1.81	0.46
24:W:188:ARG:NH2	24:W:256:LEU:O	2.48	0.46
24:W:708:GLN:HA	24:W:713:LYS:HD2	1.98	0.46
24:W:891:LEU:HD23	24:W:897:ARG:HD3	1.98	0.46
15:N:521:GLN:NE2	21:T:30:MET:SD	2.88	0.46
15:N:886:PRO:HD2	15:N:904:PHE:HD2	1.80	0.46
23:V:35:GLU:HB3	23:V:64:ARG:HD3	1.98	0.46
24:W:831:VAL:O	24:W:835:SER:OG	2.26	0.46
24:W:1308:ASP:OD1	24:W:1308:ASP:N	2.49	0.46
1:0:73:LEU:HD13	1:0:76:LEU:HD21	1.96	0.46
1:0:121:ALA:HB2	4:3:60:LEU:HD23	1.97	0.46
10:G:154:GLN:HA	10:G:157:LEU:HG	1.97	0.46
11:H:61:LYS:HD2	23:V:53:GLN:HG3	1.98	0.46
15:N:268:SER:HA	15:N:271:ILE:HD12	1.98	0.46
15:N:818:SER:OG	15:N:846:ASN:ND2	2.46	0.46
17:P:102:ASP:H	17:P:130:PRO:HA	1.79	0.46
17:P:180:ILE:HG22	17:P:190:VAL:HG13	1.97	0.46
21:T:191:VAL:O	21:T:194:MET:HG3	2.14	0.46
24:W:623:LEU:HD23	24:W:627:LEU:HD23	1.97	0.46
25:X:975:LEU:HB3	25:X:978:GLY:H	1.80	0.46
2:1:100:LEU:HD12	2:1:103:SER:HB3	1.96	0.46
2:1:128:LEU:HD13	23:V:133:GLU:CG	2.44	0.46
3:2:96:ASP:N	3:2:96:ASP:OD1	2.44	0.46
3:2:120:LEU:O	3:2:124:HIS:N	2.45	0.46
5:4:61:PRO:HA	5:4:64:ALA:HB3	1.96	0.46
11:H:65:HIS:HB2	23:V:48:VAL:HG13	1.98	0.46
15:N:183:ILE:HG13	18:Q:46:ARG:CZ	2.46	0.46
15:N:791:PRO:HB2	15:N:793:HIS:CE1	2.51	0.46
24:W:701:PHE:CG	24:W:736:PRO:HB3	2.50	0.46
24:W:732:LEU:HD12	24:W:735:PHE:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:103:ASP:N	3:2:103:ASP:OD1	2.49	0.46
6:A:177:LEU:HD22	6:A:259:ILE:HG12	1.97	0.46
15:N:683:ARG:HE	16:O:684:ARG:HG2	1.79	0.46
17:P:626:LEU:HD22	17:P:727:PRO:HD3	1.98	0.46
24:W:448:PRO:HG2	24:W:451:LEU:HB3	1.96	0.46
25:X:222:ILE:HD12	25:X:225:ILE:HD12	1.97	0.46
25:X:491:LEU:HD23	25:X:491:LEU:HA	1.77	0.46
25:X:831:ARG:HA	25:X:834:LYS:HD2	1.96	0.46
6:A:190:MET:SD	6:A:191:TYR:N	2.88	0.46
15:N:221:ARG:HB2	15:N:223:LYS:HE2	1.98	0.46
17:P:615:GLN:O	17:P:619:GLN:N	2.47	0.46
1:0:269:TRP:HA	1:0:302:LEU:HD21	1.98	0.46
8:D:73:ASP:OD2	12:I:66:LEU:HD22	2.16	0.46
17:P:735:SER:O	17:P:741:ARG:NH1	2.38	0.46
21:T:76:PHE:CE2	21:T:190:MET:HE1	2.51	0.46
24:W:57:GLU:OE2	24:W:61:GLN:NE2	2.41	0.46
25:X:757:ARG:HB2	25:X:760:HIS:HB2	1.96	0.46
6:A:340:TYR:CD1	6:A:376:LEU:HB3	2.51	0.46
9:F:171:ILE:HG13	9:F:173:GLN:N	2.29	0.46
15:N:480:LYS:HA	15:N:483:ASN:HB2	1.97	0.46
15:N:772:SER:HG	15:N:824:TRP:HD1	1.64	0.46
15:N:783:PHE:O	15:N:787:LEU:N	2.48	0.46
24:W:122:VAL:HA	24:W:125:ILE:HG12	1.98	0.46
24:W:859:ILE:HG13	24:W:934:PHE:HE1	1.81	0.46
25:X:534:PRO:HB3	25:X:539:ILE:HD12	1.97	0.46
8:D:34:LEU:CD1	12:I:96:GLU:HG2	2.47	0.45
15:N:386:VAL:O	15:N:390:MET:HG2	2.16	0.45
16:O:674:ILE:HB	16:O:678:LEU:HD11	1.98	0.45
17:P:383:ALA:HA	17:P:393:ILE:HD12	1.98	0.45
25:X:274:GLN:CD	25:X:276:ILE:HD11	2.35	0.45
1:0:68:ASN:ND2	16:O:615:GLN:OE1	2.46	0.45
1:0:231:TRP:HZ2	18:Q:467:ILE:HG22	1.81	0.45
6:A:321:LEU:HG	6:A:407:ILE:HD12	1.98	0.45
15:N:340:TRP:CZ2	15:N:405:VAL:HG13	2.50	0.45
15:N:468:TYR:OH	18:Q:515:SER:HB2	2.16	0.45
24:W:796:MET:O	24:W:800:THR:OG1	2.26	0.45
25:X:562:ASN:O	25:X:604:LYS:NZ	2.50	0.45
25:X:968:LEU:HD11	25:X:985:ALA:HB1	1.97	0.45
2:1:139:TRP:CD1	23:V:119:LEU:HD13	2.51	0.45
6:A:190:MET:O	6:A:194:ALA:N	2.47	0.45
10:G:127:ARG:HH22	22:U:1:MET:H1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:528:HIS:HE1	15:N:588:LEU:HG	1.81	0.45
16:O:700:ASN:O	25:X:915:ARG:NH2	2.42	0.45
17:P:471:LEU:HD12	17:P:506:LYS:HG3	1.98	0.45
17:P:827:CYS:SG	17:P:828:LEU:N	2.89	0.45
24:W:701:PHE:HB2	24:W:738:PRO:HD2	1.98	0.45
25:X:697:TYR:HE1	25:X:727:ARG:HA	1.82	0.45
1:0:79:LYS:HG2	3:2:60:TYR:HB3	1.98	0.45
15:N:821:SER:OG	15:N:834:SER:N	2.50	0.45
15:N:875:THR:HB	15:N:879:LEU:HD12	1.98	0.45
18:Q:597:PRO:HA	18:Q:619:ARG:HA	1.97	0.45
2:1:121:GLU:HA	2:1:124:ARG:HG2	1.98	0.45
6:A:362:ARG:NH1	6:A:375:PHE:HB2	2.32	0.45
11:H:117:VAL:HA	11:H:120:GLN:HG3	1.98	0.45
15:N:300:CYS:O	15:N:304:GLN:N	2.47	0.45
15:N:770:TRP:O	15:N:774:ALA:N	2.46	0.45
5:4:109:SER:HB3	8:D:163:ALA:HB3	1.99	0.45
8:D:105:SER:HA	8:D:108:GLN:HB2	1.99	0.45
15:N:648:CYS:O	15:N:652:MET:HG2	2.16	0.45
16:O:723:LEU:HD13	16:O:725:VAL:HG23	1.98	0.45
18:Q:93:TRP:CG	18:Q:94:PRO:HD3	2.50	0.45
24:W:154:SER:HB2	25:X:917:ALA:H	1.82	0.45
25:X:172:THR:HG22	25:X:175:ARG:HH21	1.81	0.45
1:0:134:LYS:NZ	18:Q:486:GLN:O	2.50	0.45
1:0:166:ILE:HG12	1:0:190:LEU:HD21	1.99	0.45
4:3:177:ARG:NH1	23:V:113:ASP:OD2	2.50	0.45
6:A:445:LEU:HD11	6:A:451:SER:HB3	1.99	0.45
9:F:178:ASP:HA	9:F:181:LEU:HB2	1.99	0.45
15:N:697:THR:HG22	15:N:781:LEU:HD21	1.99	0.45
15:N:846:ASN:CG	15:N:848:HIS:HD1	2.19	0.45
24:W:214:PRO:HG3	24:W:1186:TYR:HE1	1.81	0.45
6:A:344:THR:HA	6:A:425:VAL:HG11	1.98	0.45
15:N:929:ARG:HB3	15:N:933:VAL:HB	1.99	0.45
17:P:439:THR:OG1	17:P:490:ASP:OD2	2.34	0.45
18:Q:311:LEU:HD21	18:Q:343:ILE:HG21	1.99	0.45
24:W:311:ALA:HA	24:W:314:ARG:HG2	1.99	0.45
24:W:418:GLN:O	24:W:421:HIS:HB2	2.17	0.45
25:X:672:ARG:NH1	25:X:694:THR:O	2.50	0.45
3:2:76:LYS:HD2	3:2:76:LYS:HA	1.67	0.45
6:A:178:GLN:O	6:A:182:GLN:N	2.39	0.45
6:A:339:LEU:HD23	6:A:342:LEU:HD12	1.98	0.45
6:A:365:ALA:HB3	6:A:372:HIS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:33:LEU:HD21	18:Q:95:TRP:HB3	1.97	0.45
15:N:376:PRO:CD	15:N:377:PRO:HD2	2.47	0.45
15:N:903:CYS:SG	15:N:904:PHE:N	2.90	0.45
15:N:1282:GLU:O	15:N:1286:GLU:N	2.42	0.45
24:W:201:LEU:HD23	24:W:205:VAL:HG11	1.98	0.45
6:A:174:TYR:HA	6:A:177:LEU:HB3	1.98	0.45
19:R:70:LEU:HD12	19:R:85:LEU:HB2	1.99	0.45
24:W:67:ILE:HG12	24:W:79:LEU:HD13	1.97	0.45
15:N:376:PRO:N	15:N:377:PRO:HD2	2.32	0.44
17:P:652:LEU:HA	17:P:655:LEU:HD12	1.99	0.44
18:Q:138:LYS:HE3	18:Q:143:THR:HG21	1.98	0.44
24:W:370:ASP:OD1	24:W:370:ASP:N	2.50	0.44
24:W:1014:MET:HA	24:W:1017:ARG:HH21	1.82	0.44
5:4:72:CYS:SG	5:4:73:LEU:N	2.90	0.44
8:D:125:VAL:HG11	22:U:115:LEU:HD11	1.99	0.44
11:H:65:HIS:HD2	23:V:48:VAL:HG22	1.82	0.44
15:N:637:PHE:CZ	18:Q:563:ILE:O	2.71	0.44
18:Q:259:VAL:HG12	18:Q:343:ILE:HG13	2.00	0.44
24:W:427:CYS:HA	24:W:430:ILE:HG22	1.99	0.44
24:W:469:MET:HE1	24:W:527:LEU:HB2	1.99	0.44
25:X:128:LEU:HD13	25:X:131:LEU:HD12	1.99	0.44
25:X:905:PHE:HE2	25:X:946:PHE:HB2	1.82	0.44
2:1:100:LEU:HD11	18:Q:631:GLU:OE1	2.17	0.44
15:N:361:ILE:CB	15:N:370:LEU:HD23	2.42	0.44
21:T:45:THR:HG22	21:T:108:SER:HB2	2.00	0.44
23:V:130:LEU:C	23:V:130:LEU:CD1	2.86	0.44
25:X:301:GLU:HA	25:X:304:LYS:HE3	1.98	0.44
6:A:65:LEU:HD13	8:D:63:ASN:HD21	1.82	0.44
6:A:317:PHE:HA	6:A:320:LYS:HB2	1.98	0.44
8:D:104:ASP:O	8:D:108:GLN:N	2.47	0.44
8:D:186:LEU:HB3	8:D:190:MET:HE3	2.00	0.44
15:N:528:HIS:CE1	15:N:588:LEU:HG	2.52	0.44
15:N:941:TYR:HD2	15:N:1172:SER:HB3	1.83	0.44
17:P:109:SER:OG	17:P:119:GLU:OE2	2.36	0.44
17:P:583:ILE:HG22	17:P:586:LYS:HE3	1.99	0.44
17:P:669:LYS:HD3	17:P:669:LYS:HA	1.75	0.44
21:T:118:GLN:HA	21:T:122:PHE:O	2.17	0.44
24:W:852:ASP:O	24:W:857:TYR:N	2.49	0.44
25:X:20:ASP:OD1	25:X:21:TYR:N	2.50	0.44
25:X:420:ILE:HA	25:X:423:THR:HG22	1.99	0.44
15:N:374:HIS:CB	15:N:379:PRO:HD3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:534:SER:HB3	15:N:553:GLU:HG3	1.99	0.44
19:R:23:LEU:HD12	19:R:199:LEU:HB3	1.98	0.44
25:X:320:LEU:O	25:X:324:SER:OG	2.33	0.44
14:K:55:SER:HA	14:K:58:HIS:ND1	2.33	0.44
16:O:758:SER:HB2	24:W:30:PRO:HD2	1.99	0.44
17:P:495:VAL:HB	17:P:536:LEU:HD23	1.99	0.44
19:R:23:LEU:HB3	19:R:199:LEU:HD22	1.99	0.44
24:W:205:VAL:HA	24:W:208:PHE:HB3	1.98	0.44
25:X:319:LYS:HA	25:X:322:LYS:HE2	2.00	0.44
25:X:633:LEU:HB2	25:X:680:GLN:HE22	1.83	0.44
1:0:248:THR:HG21	18:Q:509:GLY:HA2	2.00	0.44
6:A:348:LEU:HD23	6:A:348:LEU:HA	1.84	0.44
10:G:67:LEU:HB2	20:S:66:TYR:CG	2.52	0.44
15:N:960:LYS:O	15:N:964:ASN:N	2.47	0.44
18:Q:223:GLU:HG2	18:Q:246:GLN:HB2	2.00	0.44
18:Q:514:LEU:HD22	18:Q:520:GLU:HB3	2.00	0.44
24:W:182:PHE:O	24:W:185:THR:OG1	2.35	0.44
24:W:382:GLY:HA2	24:W:534:HIS:HB2	2.00	0.44
24:W:546:ARG:HA	24:W:549:LYS:HE2	1.99	0.44
25:X:285:ILE:HG23	25:X:313:ILE:HD11	2.00	0.44
2:1:146:ILE:HD11	23:V:115:LYS:CD	2.41	0.44
6:A:509:ARG:O	6:A:513:ARG:N	2.45	0.44
9:F:9:ASN:HD21	9:F:11:LEU:HD12	1.83	0.44
10:G:109:LEU:HD22	15:N:135:ARG:NH2	2.33	0.44
11:H:16:LEU:HB2	18:Q:113:TYR:HD1	1.82	0.44
15:N:362:ASP:OD1	15:N:363:GLU:N	2.51	0.44
17:P:796:LYS:O	17:P:805:THR:OG1	2.34	0.44
18:Q:608:ASP:N	18:Q:608:ASP:OD1	2.51	0.44
24:W:108:GLU:HG2	24:W:110:GLU:H	1.83	0.44
24:W:763:GLU:HA	24:W:766:LYS:HB2	2.00	0.44
4:3:90:ARG:HA	4:3:90:ARG:HD3	1.83	0.44
9:F:185:ARG:HH22	15:N:299:PHE:HE1	1.66	0.44
12:I:109:LEU:HD21	12:I:114:GLN:NE2	2.15	0.44
15:N:642:ALA:HB1	18:Q:565:ASN:HD22	1.83	0.44
19:R:141:MET:HB2	19:R:171:LEU:HD11	1.99	0.44
21:T:161:LEU:HB3	21:T:169:THR:HG23	1.99	0.44
24:W:318:GLU:HG2	24:W:320:LYS:H	1.83	0.44
24:W:459:GLN:HB3	24:W:463:ARG:NH1	2.33	0.44
24:W:1005:LEU:HD11	24:W:1030:ILE:HG21	2.00	0.44
9:F:50:VAL:HG12	9:F:51:LYS:HG3	2.00	0.43
9:F:68:TYR:HD1	9:F:83:LYS:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:110:SER:O	12:I:114:GLN:N	2.48	0.43
15:N:499:TRP:O	15:N:503:GLN:N	2.34	0.43
24:W:653:ILE:HG21	24:W:686:ALA:HB1	2.00	0.43
25:X:274:GLN:HG3	25:X:274:GLN:O	2.17	0.43
1:0:179:HIS:ND1	1:0:191:LEU:O	2.43	0.43
4:3:107:ASP:HA	4:3:108:PRO:HD3	1.90	0.43
8:D:30:LEU:HD13	12:I:99:LYS:CG	2.48	0.43
10:G:73:ASP:N	10:G:73:ASP:OD1	2.45	0.43
11:H:34:GLU:OE2	18:Q:99:ARG:NH1	2.51	0.43
11:H:122:LYS:O	11:H:126:THR:OG1	2.30	0.43
21:T:38:THR:HA	21:T:115:THR:HA	1.99	0.43
6:A:15:LYS:O	6:A:19:LEU:N	2.43	0.43
6:A:273:LEU:HD12	6:A:273:LEU:HA	1.78	0.43
6:A:339:LEU:HD12	6:A:388:LEU:HB3	2.00	0.43
11:H:59:LEU:HA	11:H:62:VAL:HG12	1.99	0.43
15:N:305:LEU:HD21	15:N:361:ILE:HG21	2.00	0.43
15:N:688:PRO:HA	15:N:689:PRO:HD3	1.88	0.43
15:N:1202:TYR:CD2	15:N:1292:PRO:HB2	2.53	0.43
16:O:768:SER:OG	16:O:769:VAL:N	2.50	0.43
17:P:479:GLU:OE2	17:P:513:ARG:NH2	2.50	0.43
18:Q:191:ARG:HA	18:Q:196:LEU:HD22	2.00	0.43
18:Q:207:LEU:O	18:Q:299:GLN:NE2	2.39	0.43
25:X:789:PRO:O	25:X:793:THR:OG1	2.36	0.43
6:A:375:PHE:HB3	6:A:441:GLU:HA	2.00	0.43
6:A:375:PHE:HD2	6:A:441:GLU:HG2	1.83	0.43
8:D:30:LEU:O	8:D:34:LEU:N	2.48	0.43
13:J:70:TYR:HB3	13:J:75:ARG:HB3	2.00	0.43
15:N:330:HIS:HB2	15:N:334:CYS:H	1.83	0.43
15:N:385:LEU:HD21	15:N:406:HIS:ND1	2.34	0.43
24:W:857:TYR:O	24:W:937:LEU:N	2.51	0.43
24:W:1013:GLU:O	24:W:1017:ARG:NE	2.46	0.43
25:X:329:ASP:N	25:X:329:ASP:OD1	2.51	0.43
2:1:121:GLU:OE2	23:V:138:SER:HB3	2.19	0.43
6:A:345:GLN:HE22	6:A:392:LEU:HD11	1.82	0.43
6:A:374:TYR:CE2	6:A:505:PRO:HG3	2.53	0.43
15:N:186:ILE:HD12	15:N:186:ILE:HA	1.90	0.43
15:N:637:PHE:HD2	15:N:639:LYS:HE3	1.84	0.43
15:N:885:LEU:HD21	15:N:1186:LEU:HD22	2.00	0.43
15:N:1292:PRO:HA	15:N:1294:PHE:CE2	2.53	0.43
17:P:286:LEU:O	17:P:356:LEU:HD13	2.18	0.43
18:Q:262:GLN:O	18:Q:340:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:572:ALA:HA	18:Q:579:ALA:HA	1.99	0.43
24:W:750:GLN:HE22	24:W:874:HIS:HA	1.82	0.43
2:1:139:TRP:HA	2:1:142:VAL:HB	2.00	0.43
13:J:89:LEU:HG	20:S:84:ILE:HD12	1.99	0.43
17:P:375:GLN:HB2	17:P:465:LEU:HD11	1.99	0.43
17:P:690:PHE:HA	17:P:693:LEU:HG	2.00	0.43
18:Q:149:LYS:HD3	18:Q:149:LYS:HA	1.80	0.43
19:R:84:HIS:HD1	19:R:109:ALA:HB2	1.83	0.43
20:S:84:ILE:HG23	20:S:89:LEU:HB3	2.00	0.43
24:W:119:PHE:HA	24:W:122:VAL:HG22	2.01	0.43
24:W:327:SER:O	24:W:331:TRP:N	2.44	0.43
24:W:442:LYS:HE2	24:W:442:LYS:HB2	1.90	0.43
24:W:665:PHE:HE2	24:W:691:LEU:HD21	1.84	0.43
8:D:125:VAL:HA	8:D:128:ALA:HB3	1.99	0.43
13:J:77:PRO:HB3	15:N:105:TRP:CD1	2.53	0.43
15:N:420:LEU:HD13	15:N:427:GLU:HG2	2.01	0.43
17:P:40:SER:OG	17:P:41:CYS:N	2.51	0.43
17:P:560:LEU:HD13	17:P:563:LEU:HD13	2.00	0.43
3:2:122:LEU:O	3:2:126:CYS:N	2.48	0.43
5:4:37:LEU:HD12	5:4:42:TYR:HB2	2.00	0.43
6:A:88:ASN:HD21	6:A:151:SER:HA	1.83	0.43
6:A:148:ASP:OD1	6:A:148:ASP:N	2.51	0.43
9:F:171:ILE:HG12	9:F:174:ARG:HG2	1.99	0.43
12:I:95:GLN:HB3	12:I:99:LYS:HZ2	1.82	0.43
15:N:372:ILE:HG13	15:N:390:MET:HA	2.00	0.43
15:N:807:LYS:HE3	15:N:823:GLN:HB2	2.01	0.43
15:N:903:CYS:HA	15:N:919:ARG:HG2	2.00	0.43
17:P:103:GLY:HA3	17:P:126:VAL:H	1.83	0.43
18:Q:414:ASP:OD1	21:T:71:TYR:OH	2.27	0.43
24:W:13:VAL:HB	24:W:75:ARG:HD2	2.01	0.43
24:W:576:ILE:O	24:W:580:GLY:N	2.51	0.43
25:X:135:THR:HG21	25:X:165:LEU:HD11	1.99	0.43
25:X:415:PRO:O	25:X:419:ASN:ND2	2.51	0.43
2:1:119:ARG:HA	2:1:122:LEU:HB2	2.00	0.43
5:4:60:ASP:N	5:4:60:ASP:OD1	2.52	0.43
11:H:61:LYS:O	11:H:65:HIS:ND1	2.45	0.43
15:N:278:VAL:O	15:N:282:LEU:N	2.45	0.43
15:N:553:GLU:O	15:N:567:LYS:N	2.50	0.43
17:P:496:GLN:HB2	17:P:499:MET:HG2	2.01	0.43
18:Q:384:LYS:O	18:Q:388:SER:N	2.45	0.43
21:T:76:PHE:CE2	21:T:190:MET:CE	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:986:THR:O	24:W:990:HIS:ND1	2.49	0.43
24:W:1065:ASP:HA	24:W:1068:TYR:HD2	1.84	0.43
25:X:746:ASN:O	25:X:750:LYS:NZ	2.39	0.43
6:A:321:LEU:HD22	6:A:329:LEU:HD12	2.01	0.43
8:D:118:GLU:O	8:D:122:ALA:N	2.43	0.43
15:N:455:PHE:N	15:N:464:GLN:O	2.39	0.43
15:N:725:VAL:HG23	15:N:744:HIS:HB3	2.00	0.43
18:Q:156:ALA:HB2	23:V:61:MET:HG2	2.00	0.43
24:W:366:ILE:HG22	24:W:369:ARG:HD3	2.01	0.43
24:W:1198:GLN:HA	25:X:723:TRP:CD1	2.54	0.43
25:X:258:GLY:O	25:X:312:LYS:NZ	2.50	0.43
6:A:177:LEU:O	6:A:181:GLU:N	2.45	0.42
8:D:173:ARG:HD2	8:D:173:ARG:HA	1.88	0.42
10:G:51:CYS:SG	10:G:52:ASP:N	2.92	0.42
15:N:372:ILE:HG13	15:N:389:ALA:O	2.19	0.42
18:Q:96:ASP:OD1	18:Q:97:SER:N	2.52	0.42
24:W:36:LYS:HD2	24:W:36:LYS:HA	1.81	0.42
24:W:73:PRO:HA	24:W:76:ILE:HB	2.00	0.42
25:X:894:ARG:HA	25:X:899:ARG:HH21	1.84	0.42
1:0:274:ILE:HG13	1:0:275:LYS:HD3	2.01	0.42
6:A:219:LEU:HD13	6:A:258:THR:HB	2.00	0.42
15:N:309:HIS:CE1	15:N:331:ALA:HA	2.54	0.42
17:P:376:PHE:HD1	17:P:473:HIS:HD2	1.65	0.42
19:R:58:PHE:HB3	19:R:123:PHE:HB3	2.01	0.42
24:W:366:ILE:HD12	24:W:402:LEU:HD12	2.00	0.42
25:X:606:THR:HG21	25:X:645:GLN:HB3	2.00	0.42
6:A:173:MET:O	6:A:177:LEU:N	2.45	0.42
6:A:314:SER:HB2	6:A:447:GLU:OE1	2.19	0.42
10:G:67:LEU:HD13	20:S:66:TYR:CZ	2.55	0.42
10:G:90:LEU:CD2	13:J:109:LEU:CB	2.92	0.42
15:N:941:TYR:OH	15:N:1168:SER:O	2.30	0.42
17:P:402:MET:SD	17:P:402:MET:C	2.97	0.42
17:P:534:CYS:O	17:P:540:THR:OG1	2.28	0.42
17:P:544:VAL:HB	17:P:548:HIS:CE1	2.54	0.42
2:1:84:PHE:HA	2:1:87:ILE:HG22	2.00	0.42
9:F:69:ILE:HG22	9:F:82:ARG:HH21	1.83	0.42
15:N:102:LEU:HD23	15:N:102:LEU:HA	1.91	0.42
15:N:925:ASP:HB3	15:N:927:TYR:CE1	2.53	0.42
18:Q:202:LYS:HA	18:Q:202:LYS:HD3	1.81	0.42
24:W:506:ARG:HD3	24:W:506:ARG:HA	1.80	0.42
24:W:559:LEU:HD12	24:W:559:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:1075:LEU:HD12	24:W:1075:LEU:HA	1.87	0.42
5:4:17:ARG:CZ	5:4:21:GLU:HG3	2.50	0.42
10:G:91:ASP:OD1	13:J:124:TYR:OH	2.38	0.42
15:N:376:PRO:HD2	15:N:377:PRO:HD3	2.00	0.42
15:N:639:LYS:HE2	18:Q:562:SER:HA	2.00	0.42
15:N:820:ILE:HG22	15:N:835:LEU:HD23	2.01	0.42
18:Q:384:LYS:HA	18:Q:384:LYS:HD3	1.73	0.42
24:W:452:ARG:HA	24:W:455:HIS:HB3	2.00	0.42
2:1:86:ASP:O	2:1:90:GLN:NE2	2.42	0.42
6:A:191:TYR:CD2	6:A:202:LYS:HG2	2.54	0.42
10:G:78:LEU:HD23	10:G:119:VAL:HG23	2.01	0.42
10:G:100:PRO:HG2	15:N:125:GLN:OE1	2.20	0.42
13:J:80:TYR:HD2	15:N:105:TRP:HE1	1.68	0.42
15:N:370:LEU:HB2	15:N:392:ILE:HD11	2.01	0.42
15:N:703:ARG:HA	15:N:703:ARG:HD2	1.85	0.42
15:N:730:PRO:HG2	15:N:780:VAL:HG11	2.02	0.42
15:N:751:ASN:ND2	15:N:756:PRO:O	2.41	0.42
17:P:186:GLY:HA3	17:P:210:ARG:HA	2.02	0.42
17:P:201:THR:O	17:P:252:LYS:NZ	2.44	0.42
18:Q:431:ILE:HD13	18:Q:431:ILE:HA	1.89	0.42
21:T:112:THR:HG23	21:T:197:PHE:HE1	1.84	0.42
24:W:126:ILE:HG21	24:W:169:TYR:HE2	1.83	0.42
1:0:36:LYS:HD2	16:O:643:VAL:HA	2.02	0.42
4:3:111:VAL:HG22	18:Q:651:LEU:HG	2.00	0.42
4:3:170:ILE:HD12	4:3:173:MET:HG3	2.01	0.42
6:A:172:LYS:HB3	6:A:299:LEU:HD21	2.02	0.42
10:G:56:ILE:HG23	10:G:57:ARG:HG2	2.01	0.42
15:N:223:LYS:HD3	15:N:233:THR:HG22	2.00	0.42
15:N:467:LEU:HB2	15:N:470:LEU:HD12	2.02	0.42
17:P:34:PRO:HA	17:P:432:LYS:HE3	2.01	0.42
24:W:236:ALA:HB2	24:W:663:PRO:HB3	2.01	0.42
25:X:196:LEU:HD11	25:X:223:ARG:HH11	1.85	0.42
25:X:452:LEU:HD13	25:X:507:TYR:HE2	1.85	0.42
1:0:133:LEU:HD12	1:0:133:LEU:HA	1.91	0.42
2:1:119:ARG:HD3	2:1:122:LEU:HD12	2.01	0.42
14:K:32:ILE:HD13	14:K:35:LEU:HD21	2.02	0.42
15:N:195:LEU:HD23	15:N:198:ILE:HD11	2.02	0.42
15:N:683:ARG:CD	16:O:684:ARG:HG3	2.48	0.42
17:P:434:MET:N	17:P:434:MET:SD	2.93	0.42
17:P:524:THR:HG22	17:P:554:ILE:HD12	2.01	0.42
17:P:732:LEU:O	17:P:734:ALA:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:116:ASP:OD1	19:R:116:ASP:N	2.53	0.42
22:U:102:THR:HA	22:U:105:GLU:HG2	2.01	0.42
24:W:238:CYS:HB3	24:W:241:TRP:HD1	1.85	0.42
24:W:732:LEU:O	24:W:740:GLN:NE2	2.52	0.42
25:X:406:ASN:HA	25:X:409:LEU:HD12	2.02	0.42
6:A:462:LEU:O	6:A:482:GLY:N	2.52	0.42
10:G:100:PRO:C	15:N:128:LEU:HD23	2.41	0.42
10:G:152:ARG:HA	10:G:155:LYS:HG2	2.00	0.42
15:N:202:ARG:NH1	15:N:241:PRO:O	2.50	0.42
15:N:313:LEU:HD23	15:N:313:LEU:HA	1.93	0.42
15:N:376:PRO:CD	15:N:377:PRO:HD3	2.50	0.42
15:N:1186:LEU:HD23	15:N:1207:LEU:HD13	2.01	0.42
17:P:143:LEU:HA	17:P:161:ARG:HA	2.02	0.42
25:X:274:GLN:HG3	25:X:276:ILE:CD1	2.50	0.42
1:0:68:ASN:HB3	1:0:72:ARG:HH12	1.84	0.42
9:F:67:GLU:OE1	9:F:86:ARG:NH1	2.53	0.42
15:N:1224:ILE:HD13	15:N:1224:ILE:HA	1.93	0.42
24:W:416:LYS:HB3	24:W:418:GLN:HG2	2.02	0.42
24:W:617:PRO:HA	24:W:620:ARG:HB2	2.02	0.42
25:X:517:ARG:HH21	25:X:523:PRO:HG3	1.85	0.42
2:1:135:LYS:HE2	2:1:139:TRP:CH2	2.55	0.41
6:A:354:PRO:HG2	6:A:355:ILE:HD12	2.02	0.41
8:D:86:GLN:CD	12:I:106:GLY:CA	2.65	0.41
11:H:19:VAL:O	11:H:23:LYS:HG2	2.20	0.41
15:N:236:VAL:HB	15:N:243:VAL:HG11	2.02	0.41
15:N:449:SER:HB3	18:Q:516:TYR:OH	2.20	0.41
17:P:531:ALA:HB1	17:P:548:HIS:CE1	2.55	0.41
17:P:540:THR:O	17:P:544:VAL:HG13	2.20	0.41
18:Q:598:ARG:NH2	18:Q:605:PRO:O	2.41	0.41
19:R:152:LEU:O	19:R:159:SER:OG	2.37	0.41
24:W:339:ILE:HA	24:W:342:VAL:HG12	2.01	0.41
24:W:982:LYS:O	24:W:985:GLU:HB2	2.20	0.41
2:1:135:LYS:CG	2:1:139:TRP:HZ3	2.23	0.41
5:4:103:LEU:O	5:4:110:ARG:NH1	2.36	0.41
9:F:84:GLN:HA	9:F:94:PRO:HA	2.02	0.41
15:N:343:GLN:H	15:N:343:GLN:HG3	1.68	0.41
15:N:812:TYR:HE1	15:N:820:ILE:HG23	1.85	0.41
17:P:310:SER:HB3	17:P:342:LEU:HD21	2.01	0.41
17:P:784:ARG:HA	17:P:784:ARG:HD3	1.77	0.41
18:Q:391:MET:SD	18:Q:391:MET:N	2.77	0.41
24:W:101:LEU:HD11	24:W:121:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:373:MET:O	24:W:376:LEU:HB3	2.19	0.41
24:W:552:HIS:CE1	24:W:591:THR:HB	2.55	0.41
24:W:714:ASP:OD1	24:W:714:ASP:N	2.51	0.41
6:A:80:ARG:HH21	6:A:147:PHE:HB2	1.84	0.41
6:A:194:ALA:CB	6:A:280:VAL:HG23	2.50	0.41
6:A:366:ALA:HB3	6:A:428:THR:HB	2.02	0.41
6:A:503:SER:OG	6:A:506:VAL:HB	2.19	0.41
9:F:184:LEU:HD23	15:N:299:PHE:CE1	2.56	0.41
12:I:73:ILE:HA	12:I:76:MET:HG3	2.02	0.41
15:N:233:THR:HG23	15:N:249:LYS:HE3	2.01	0.41
15:N:806:ARG:HH12	15:N:824:TRP:N	2.16	0.41
17:P:503:LEU:HD23	17:P:533:LEU:HD11	2.01	0.41
18:Q:139:GLN:HB3	18:Q:142:GLN:HB2	2.01	0.41
19:R:108:ILE:HG12	21:T:90:ASN:HB3	2.01	0.41
24:W:378:GLN:HE22	24:W:532:THR:HG22	1.86	0.41
24:W:431:HIS:NE2	24:W:479:ASN:O	2.43	0.41
24:W:883:TYR:HB3	24:W:974:PHE:CE1	2.55	0.41
24:W:1176:SER:HA	24:W:1180:GLU:HB3	2.02	0.41
25:X:50:ALA:HB2	25:X:60:ILE:HG21	2.03	0.41
9:F:178:ASP:O	9:F:182:LEU:N	2.50	0.41
10:G:83:MET:HG3	13:J:120:ASP:HB2	2.02	0.41
15:N:1192:PRO:HD3	15:N:1209:ARG:CZ	2.51	0.41
17:P:402:MET:SD	17:P:402:MET:O	2.79	0.41
25:X:801:LEU:HD23	25:X:801:LEU:HA	1.95	0.41
6:A:493:PHE:CD2	6:A:514:LYS:HD2	2.56	0.41
10:G:21:TYR:CE1	10:G:33:LYS:HD3	2.55	0.41
13:J:106:LYS:HA	13:J:109:LEU:HD12	2.03	0.41
15:N:328:ARG:NH1	15:N:336:SER:HB3	2.35	0.41
15:N:419:ILE:HD12	15:N:487:LYS:HD3	2.01	0.41
15:N:567:LYS:HB3	15:N:569:TYR:HE1	1.85	0.41
15:N:784:ALA:O	15:N:788:PRO:HD3	2.21	0.41
17:P:431:LEU:HA	17:P:447:ASP:HA	2.02	0.41
17:P:511:TYR:HB2	17:P:526:ILE:HD13	2.01	0.41
18:Q:226:LYS:HA	18:Q:243:LEU:HG	2.02	0.41
23:V:29:ILE:HD11	23:V:75:LEU:HD11	2.03	0.41
24:W:180:ALA:HB1	24:W:208:PHE:HE1	1.85	0.41
24:W:1238:ILE:O	24:W:1244:GLN:NE2	2.52	0.41
1:0:103:LEU:HD12	1:0:107:LEU:HD23	2.03	0.41
2:1:125:LYS:CE	23:V:137:SER:CB	2.89	0.41
2:1:128:LEU:HD22	23:V:133:GLU:HG2	2.02	0.41
5:4:90:ASN:HB3	5:4:92:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:367:LEU:HD21	6:A:426:LYS:NZ	2.36	0.41
15:N:463:PHE:H	15:N:483:ASN:HD21	1.68	0.41
24:W:224:ARG:NH2	24:W:240:SER:O	2.53	0.41
24:W:1142:ILE:HD12	24:W:1145:TRP:HB2	2.02	0.41
25:X:101:MET:O	25:X:167:LYS:NZ	2.50	0.41
25:X:561:LEU:HD11	25:X:588:ILE:HD11	2.02	0.41
25:X:784:LEU:HG	25:X:904:LEU:HD22	2.01	0.41
2:1:71:GLU:HG3	2:1:74:ARG:NH2	2.35	0.41
2:1:128:LEU:HD23	2:1:132:HIS:HB2	2.02	0.41
10:G:112:LEU:HA	10:G:115:LEU:HD12	2.03	0.41
11:H:89:LEU:HD21	11:H:97:VAL:HB	2.02	0.41
13:J:79:LEU:O	13:J:82:LYS:HB2	2.19	0.41
15:N:159:ASP:O	15:N:163:THR:OG1	2.31	0.41
15:N:515:ILE:HD12	15:N:541:LYS:HB3	2.03	0.41
15:N:945:ASP:HB3	15:N:948:LYS:H	1.84	0.41
21:T:79:PHE:CD2	21:T:83:PRO:HD2	2.56	0.41
24:W:764:TYR:HD1	24:W:792:LEU:HD13	1.86	0.41
6:A:156:GLY:O	6:A:160:LEU:N	2.52	0.41
6:A:177:LEU:HD13	6:A:259:ILE:HG23	2.03	0.41
6:A:269:PRO:HB2	6:A:271:ALA:O	2.21	0.41
17:P:227:VAL:HB	17:P:291:SER:OG	2.21	0.41
17:P:286:LEU:O	17:P:356:LEU:HD22	2.20	0.41
17:P:301:GLN:O	17:P:350:ARG:NH1	2.54	0.41
17:P:627:TYR:HB2	17:P:726:ILE:HG23	2.02	0.41
19:R:191:GLU:HA	19:R:194:LYS:HG2	2.03	0.41
24:W:1313:GLN:HA	24:W:1316:LYS:HE2	2.02	0.41
2:1:137:ARG:HG3	2:1:140:GLN:NE2	2.36	0.41
4:3:170:ILE:HD12	4:3:170:ILE:HA	1.95	0.41
6:A:67:LYS:HD3	6:A:67:LYS:HA	1.79	0.41
6:A:280:VAL:O	6:A:280:VAL:HG22	2.21	0.41
6:A:370:GLN:HB2	6:A:509:ARG:HG2	2.02	0.41
6:A:491:ASP:HA	6:A:494:ILE:HG12	2.02	0.41
11:H:37:TYR:CZ	18:Q:94:PRO:HG2	2.55	0.41
11:H:93:THR:O	11:H:96:ARG:NE	2.54	0.41
15:N:385:LEU:HD23	15:N:385:LEU:HA	1.92	0.41
15:N:572:SER:HB3	15:N:586:LEU:HD12	2.03	0.41
15:N:824:TRP:CH2	15:N:829:GLN:HA	2.56	0.41
15:N:1291:GLY:HA2	15:N:1292:PRO:HD3	1.91	0.41
16:O:636:HIS:CD2	17:P:786:HIS:H	2.38	0.41
16:O:764:PRO:O	16:O:767:HIS:ND1	2.42	0.41
17:P:66:ASP:HB2	17:P:799:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:457:LEU:O	17:P:494:HIS:NE2	2.54	0.41
17:P:527:LEU:HD12	17:P:554:ILE:HD13	2.02	0.41
18:Q:591:LYS:HD3	18:Q:591:LYS:HA	1.87	0.41
20:S:103:GLU:O	20:S:107:ASN:HB2	2.21	0.41
23:V:104:GLN:O	23:V:107:THR:OG1	2.38	0.41
24:W:261:ASP:N	24:W:261:ASP:OD1	2.54	0.41
24:W:782:MET:SD	24:W:785:SER:HB3	2.60	0.41
25:X:180:ILE:O	25:X:979:ARG:NE	2.53	0.41
25:X:533:MET:SD	25:X:533:MET:N	2.94	0.41
6:A:339:LEU:HA	6:A:342:LEU:HD12	2.03	0.41
8:D:86:GLN:CG	12:I:106:GLY:HA2	2.48	0.41
8:D:88:LYS:HD2	8:D:89:ILE:HG13	2.03	0.41
8:D:131:LYS:HZ3	10:G:149:THR:HG21	1.86	0.41
15:N:154:ILE:O	15:N:157:ALA:HB3	2.21	0.41
18:Q:331:ILE:HB	18:Q:343:ILE:HB	2.02	0.41
21:T:98:LEU:HB3	21:T:101:PHE:HD2	1.86	0.41
24:W:71:HIS:H	24:W:75:ARG:HH21	1.67	0.41
24:W:111:ARG:HB3	24:W:114:LEU:HB3	2.02	0.41
25:X:630:MET:SD	25:X:630:MET:N	2.91	0.41
1:0:253:TYR:HB2	1:0:262:VAL:HG13	2.03	0.40
5:4:114:ARG:NH2	18:Q:28:GLU:OE2	2.53	0.40
6:A:192:TRP:HE3	6:A:202:LYS:HE3	1.86	0.40
6:A:221:ASN:HA	6:A:256:SER:HA	2.03	0.40
12:I:108:HIS:ND1	12:I:108:HIS:N	2.68	0.40
15:N:1281:LEU:HD21	15:N:1306:LEU:HD11	2.02	0.40
17:P:290:MET:SD	17:P:290:MET:O	2.79	0.40
17:P:780:ASP:O	17:P:784:ARG:NH1	2.54	0.40
17:P:783:ARG:HE	17:P:785:LEU:HD22	1.86	0.40
24:W:1013:GLU:HG3	24:W:1157:PRO:HG2	2.03	0.40
24:W:1062:VAL:HA	24:W:1063:PRO:HD3	1.91	0.40
25:X:97:LEU:HD23	25:X:100:ILE:HD12	2.03	0.40
14:K:94:LEU:HD23	14:K:94:LEU:HA	1.95	0.40
15:N:667:PRO:HB2	15:N:685:LEU:HB2	2.03	0.40
17:P:402:MET:CE	17:P:461:MET:HE1	2.52	0.40
17:P:469:LEU:HD23	17:P:469:LEU:HA	1.85	0.40
18:Q:188:LEU:O	18:Q:191:ARG:NE	2.55	0.40
18:Q:247:ILE:HD11	18:Q:295:LEU:HD23	2.04	0.40
21:T:116:ARG:HB3	21:T:125:LYS:HD3	2.02	0.40
4:3:78:LEU:HD23	4:3:78:LEU:HA	1.92	0.40
4:3:95:VAL:HA	4:3:98:LYS:HB2	2.03	0.40
4:3:168:TRP:HA	4:3:171:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:225:TYR:OH	6:A:502:MET:SD	2.76	0.40
6:A:262:THR:OG1	6:A:264:ALA:O	2.39	0.40
6:A:315:ARG:NH1	6:A:389:GLN:HB2	2.36	0.40
15:N:922:TYR:HE2	15:N:1215:ILE:HD13	1.86	0.40
17:P:439:THR:HB	17:P:477:LEU:HD23	2.03	0.40
21:T:43:CYS:HA	21:T:66:MET:HG2	2.03	0.40
25:X:25:ILE:HG22	25:X:29:LYS:HZ2	1.86	0.40
25:X:25:ILE:HG22	25:X:29:LYS:NZ	2.36	0.40
7:B:9:UNK:O	7:B:13:UNK:N	2.54	0.40
11:H:62:VAL:HA	11:H:65:HIS:HD1	1.86	0.40
15:N:918:PHE:HD2	15:N:922:TYR:HD2	1.68	0.40
15:N:923:CYS:SG	15:N:924:ILE:N	2.94	0.40
17:P:823:TRP:HZ2	17:P:828:LEU:HB2	1.86	0.40
18:Q:215:LEU:HG	18:Q:215:LEU:O	2.20	0.40
25:X:561:LEU:HD13	25:X:605:ILE:HG21	2.03	0.40
1:0:197:VAL:HG12	1:0:198:LEU:HG	2.04	0.40
5:4:17:ARG:NE	5:4:21:GLU:HG3	2.37	0.40
8:D:47:MET:HA	8:D:50:ILE:HG12	2.04	0.40
12:I:109:LEU:CD2	12:I:109:LEU:O	2.70	0.40
15:N:77:SER:O	15:N:81:ARG:N	2.52	0.40
15:N:929:ARG:N	15:N:933:VAL:O	2.55	0.40
15:N:1211:LEU:O	15:N:1215:ILE:N	2.44	0.40
16:O:719:PRO:HA	16:O:720:PRO:HD3	1.92	0.40
17:P:88:GLU:HG2	17:P:288:ARG:HH22	1.86	0.40
24:W:781:SER:HB3	24:W:810:VAL:HG13	2.04	0.40
25:X:406:ASN:HA	25:X:409:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	261/311 (84%)	250 (96%)	11 (4%)	0	100	100
2	1	95/178 (53%)	92 (97%)	3 (3%)	0	100	100
3	2	111/200 (56%)	107 (96%)	4 (4%)	0	100	100
4	3	114/178 (64%)	112 (98%)	2 (2%)	0	100	100
5	4	111/131 (85%)	106 (96%)	5 (4%)	0	100	100
6	A	455/1581 (29%)	427 (94%)	27 (6%)	1 (0%)	44	78
8	D	154/270 (57%)	148 (96%)	6 (4%)	0	100	100
9	F	162/246 (66%)	148 (91%)	14 (9%)	0	100	100
10	G	159/233 (68%)	152 (96%)	7 (4%)	0	100	100
11	H	177/268 (66%)	169 (96%)	7 (4%)	1 (1%)	22	60
12	I	69/146 (47%)	66 (96%)	3 (4%)	0	100	100
13	J	120/135 (89%)	119 (99%)	1 (1%)	0	100	100
14	K	110/117 (94%)	108 (98%)	2 (2%)	0	100	100
15	N	995/1454 (68%)	902 (91%)	89 (9%)	4 (0%)	30	68
16	O	153/788 (19%)	143 (94%)	10 (6%)	0	100	100
17	P	743/877 (85%)	689 (93%)	53 (7%)	1 (0%)	48	83
18	Q	534/651 (82%)	497 (93%)	36 (7%)	1 (0%)	44	78
19	R	189/208 (91%)	177 (94%)	12 (6%)	0	100	100
20	S	67/244 (28%)	65 (97%)	1 (2%)	1 (2%)	8	40
21	T	189/212 (89%)	166 (88%)	23 (12%)	0	100	100
22	U	117/144 (81%)	114 (97%)	3 (3%)	0	100	100
23	V	128/200 (64%)	122 (95%)	6 (5%)	0	100	100
24	W	1332/1368 (97%)	1278 (96%)	54 (4%)	0	100	100
25	X	877/989 (89%)	828 (94%)	49 (6%)	0	100	100
26	a	301/464 (65%)	292 (97%)	8 (3%)	1 (0%)	37	73
27	b	261/283 (92%)	258 (99%)	3 (1%)	0	100	100
28	c	1422/2177 (65%)	1359 (96%)	63 (4%)	0	100	100
29	d	923/2174 (42%)	874 (95%)	49 (5%)	0	100	100
All	All	10329/16227 (64%)	9768 (95%)	551 (5%)	10 (0%)	50	83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	375	ASP
20	S	67	LEU
26	a	338	ASP
11	H	99	VAL
17	P	362	SER
6	A	208	VAL
15	N	153	ALA
18	Q	458	PRO
15	N	524	ASN
15	N	186	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	241/280 (86%)	238 (99%)	3 (1%)	67 78
2	1	94/152 (62%)	93 (99%)	1 (1%)	70 80
3	2	102/163 (63%)	101 (99%)	1 (1%)	73 82
4	3	116/155 (75%)	116 (100%)	0	100 100
5	4	102/115 (89%)	102 (100%)	0	100 100
6	A	394/1391 (28%)	393 (100%)	1 (0%)	91 92
8	D	139/230 (60%)	134 (96%)	5 (4%)	30 50
9	F	150/223 (67%)	149 (99%)	1 (1%)	81 87
10	G	153/216 (71%)	153 (100%)	0	100 100
11	H	161/225 (72%)	160 (99%)	1 (1%)	84 88
12	I	71/133 (53%)	68 (96%)	3 (4%)	25 46
13	J	66/124 (53%)	62 (94%)	4 (6%)	15 37
14	K	94/98 (96%)	93 (99%)	1 (1%)	70 80
15	N	810/1271 (64%)	808 (100%)	2 (0%)	92 94
16	O	141/697 (20%)	140 (99%)	1 (1%)	81 87
17	P	670/766 (88%)	667 (100%)	3 (0%)	89 91
18	Q	488/577 (85%)	485 (99%)	3 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	R	169/183 (92%)	166 (98%)	3 (2%)	54 71
20	S	43/208 (21%)	43 (100%)	0	100 100
21	T	166/178 (93%)	164 (99%)	2 (1%)	67 78
22	U	98/119 (82%)	97 (99%)	1 (1%)	73 82
23	V	122/173 (70%)	122 (100%)	0	100 100
24	W	1203/1232 (98%)	1200 (100%)	3 (0%)	92 94
25	X	789/864 (91%)	786 (100%)	3 (0%)	89 91
26	a	277/412 (67%)	277 (100%)	0	100 100
27	b	241/258 (93%)	240 (100%)	1 (0%)	89 91
28	c	1282/1916 (67%)	1271 (99%)	11 (1%)	75 83
29	d	869/1918 (45%)	862 (99%)	7 (1%)	79 85
All	All	9251/14277 (65%)	9190 (99%)	61 (1%)	80 87

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	48	ARG
1	0	134	LYS
1	0	205	ARG
2	1	137	ARG
3	2	165	LYS
6	A	502	MET
8	D	88	LYS
8	D	112	LYS
8	D	131	LYS
8	D	137	LYS
8	D	139	ARG
9	F	36	ARG
11	H	138	LYS
12	I	108	HIS
12	I	109	LEU
12	I	110	SER
13	J	92	ASN
13	J	104	LYS
13	J	106	LYS
13	J	115	LYS
14	K	95	LYS
15	N	372	ILE

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Mol	Chain	Res	Type
15	N	691	LYS
16	O	630	ARG
17	P	254	ARG
17	P	289	ASP
17	P	434	MET
18	Q	169	LYS
18	Q	215	LEU
18	Q	403	LYS
19	R	98	ARG
19	R	156	ASN
19	R	206	ARG
21	T	136	ARG
21	T	179	ARG
22	U	92	LYS
24	W	296	ARG
24	W	813	ARG
24	W	1056	ARG
25	X	167	LYS
25	X	173	LYS
25	X	412	ARG
27	b	79	LYS
28	c	65	ASN
28	c	92	ARG
28	c	131	LYS
28	c	516	ARG
28	c	531	LYS
28	c	784	ARG
28	c	988	LYS
28	c	1170	ARG
28	c	1298	LYS
28	c	1453	LYS
28	c	1610	LYS
29	d	231	LYS
29	d	275	ARG
29	d	338	ASP
29	d	1129	VAL
29	d	1198	ASN
29	d	1359	MET
29	d	2153	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	115	ASN
1	0	118	GLN
2	1	70	GLN
2	1	132	HIS
2	1	140	GLN
4	3	57	ASN
10	G	25	ASN
10	G	166	ASN
12	I	95	GLN
12	I	114	GLN
15	N	374	HIS
15	N	507	GLN
15	N	909	GLN
15	N	1219	HIS
16	O	636	HIS
18	Q	18	GLN
18	Q	340	GLN
21	T	118	GLN
24	W	53	GLN
24	W	233	ASN
25	X	26	ASN
26	a	331	GLN
28	c	65	ASN
28	c	101	ASN
28	c	800	ASN
28	c	1369	GLN
28	c	1615	ASN
28	c	1621	GLN
28	c	1729	HIS
29	d	1131	ASN
29	d	1137	ASN
29	d	2108	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

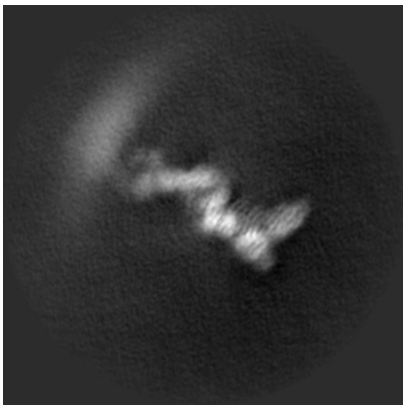
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41565. These allow visual inspection of the internal detail of the map and identification of artifacts.

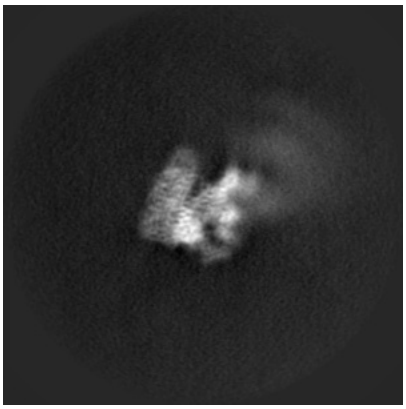
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

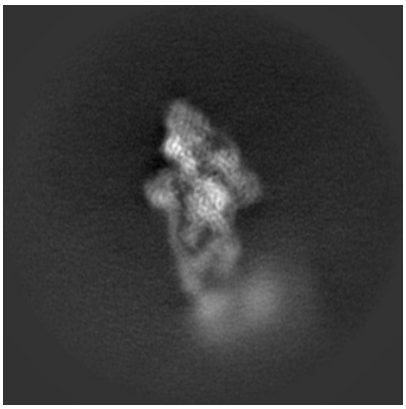
6.1.1 Primary map



X

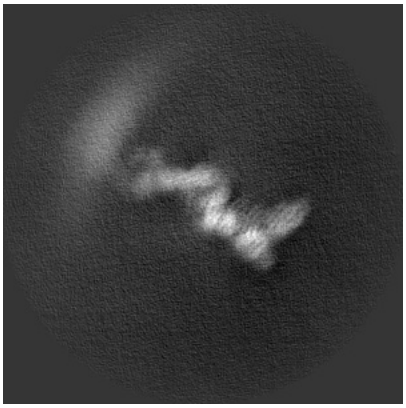


Y

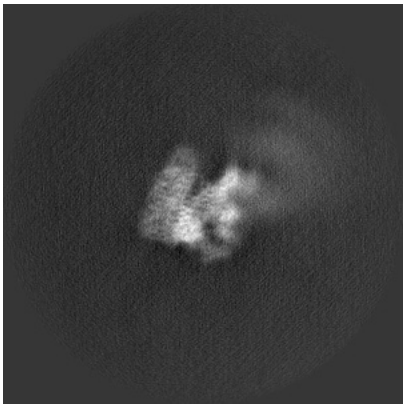


Z

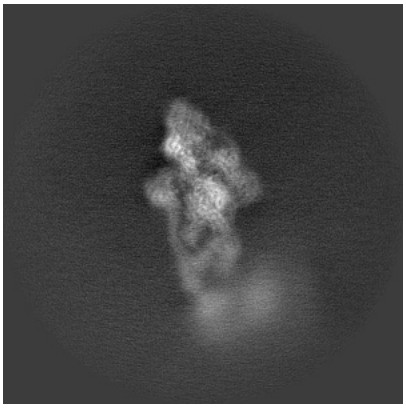
6.1.2 Raw map



X



Y

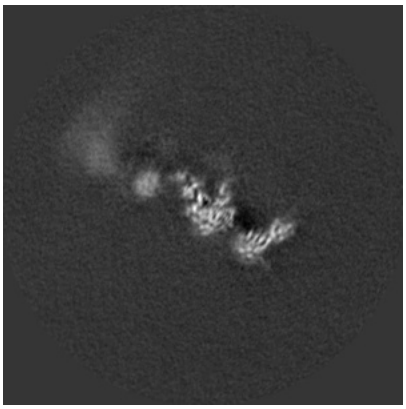


Z

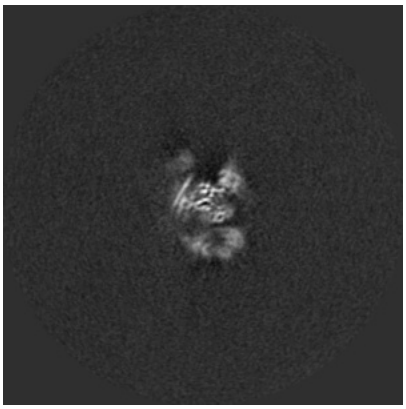
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

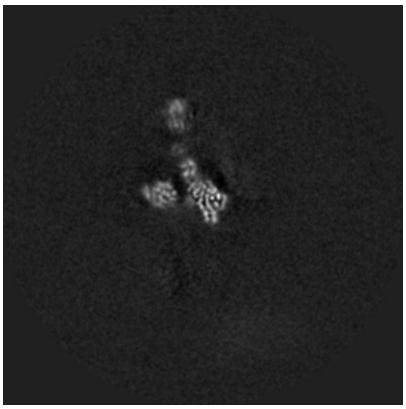
6.2.1 Primary map



X Index: 160

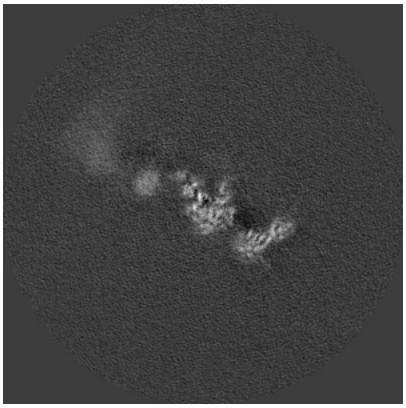


Y Index: 160

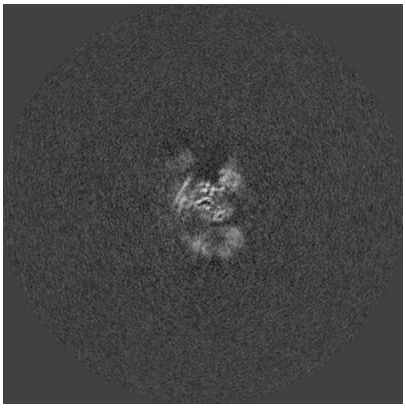


Z Index: 160

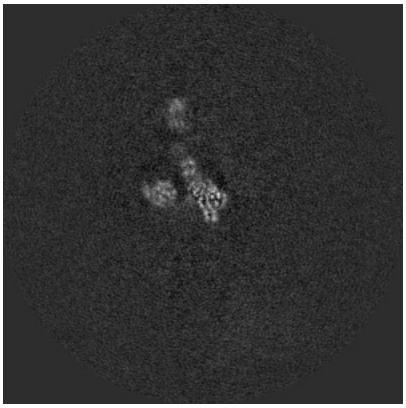
6.2.2 Raw map



X Index: 160



Y Index: 160

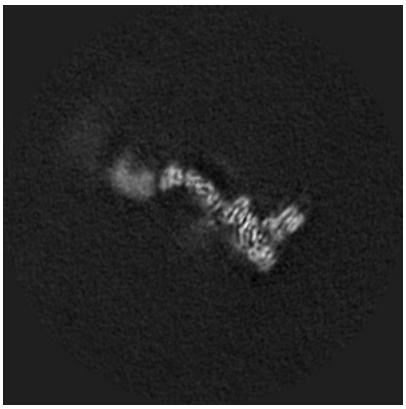


Z Index: 160

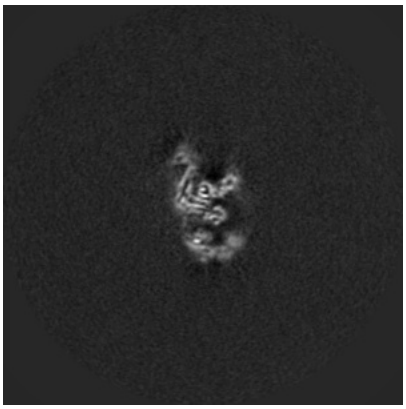
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

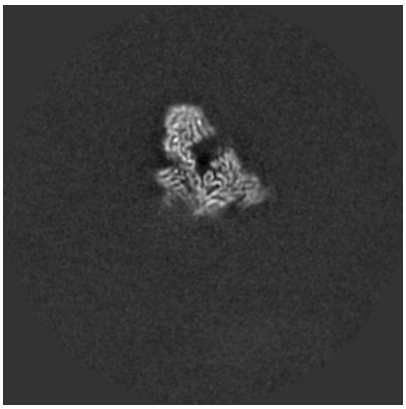
6.3.1 Primary map



X Index: 149

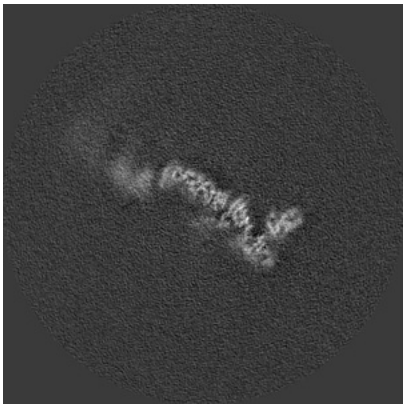


Y Index: 165



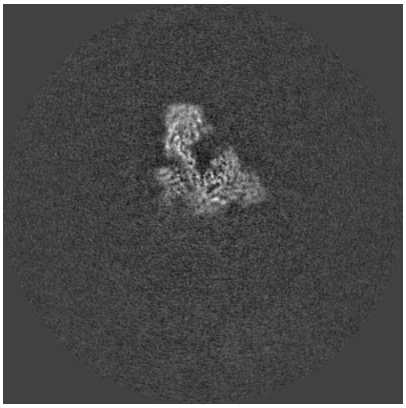
Z Index: 145

6.3.2 Raw map



X Index: 152

Y Index: 166

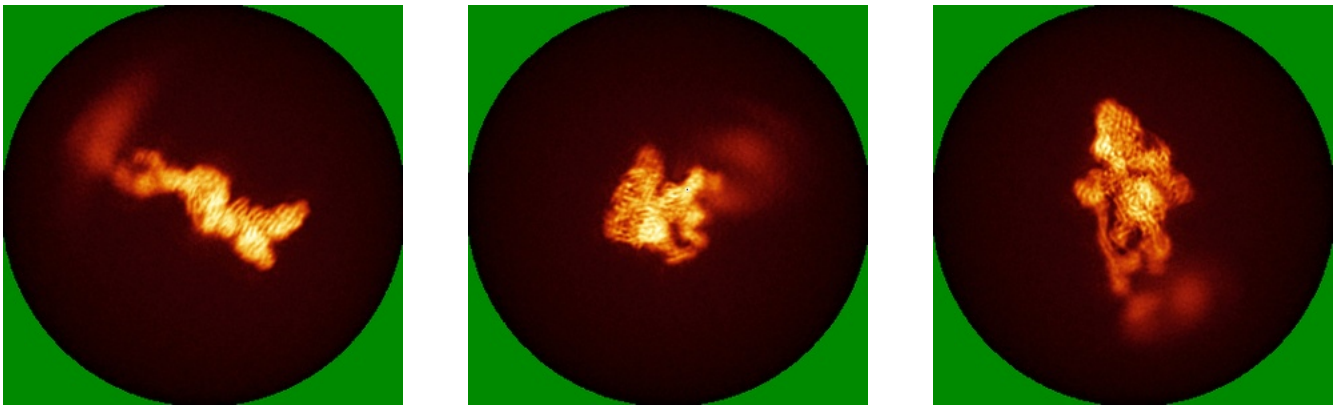


Z Index: 146

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

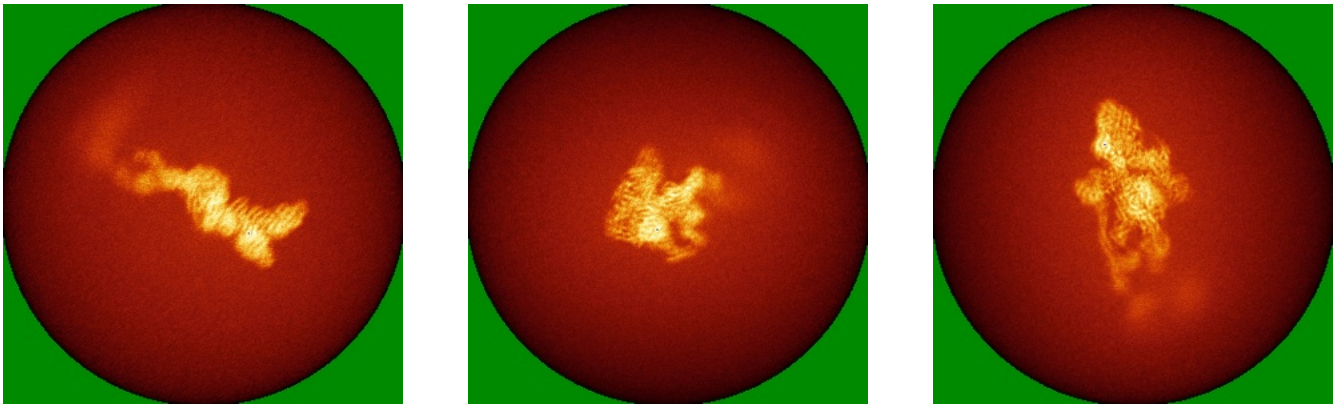
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

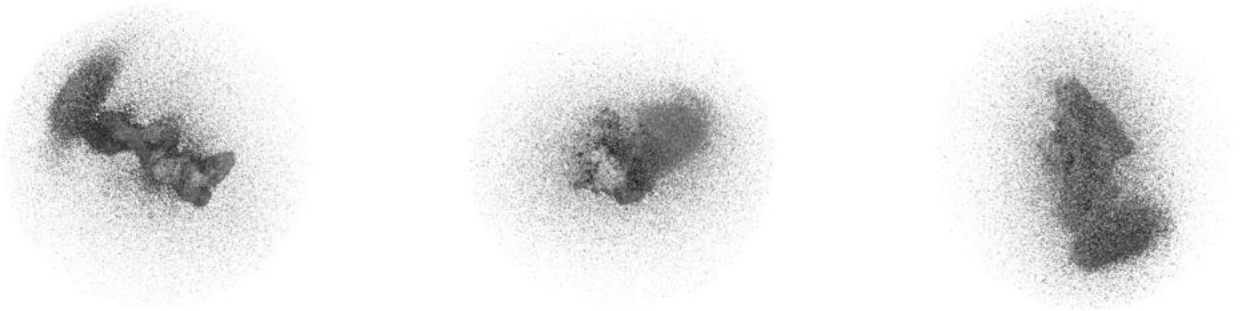
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

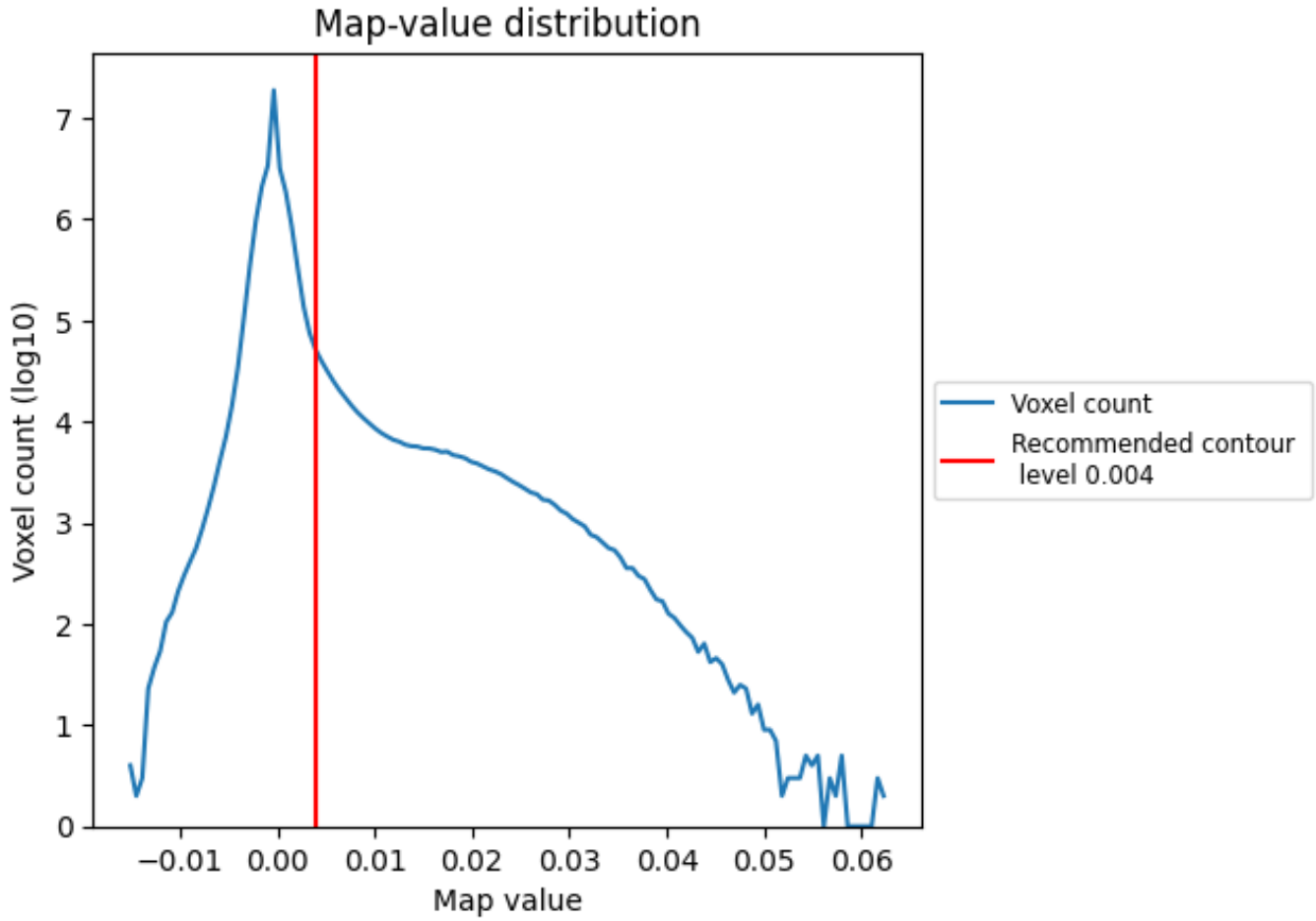
6.6 Mask visualisation (i)

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

7 Map analysis

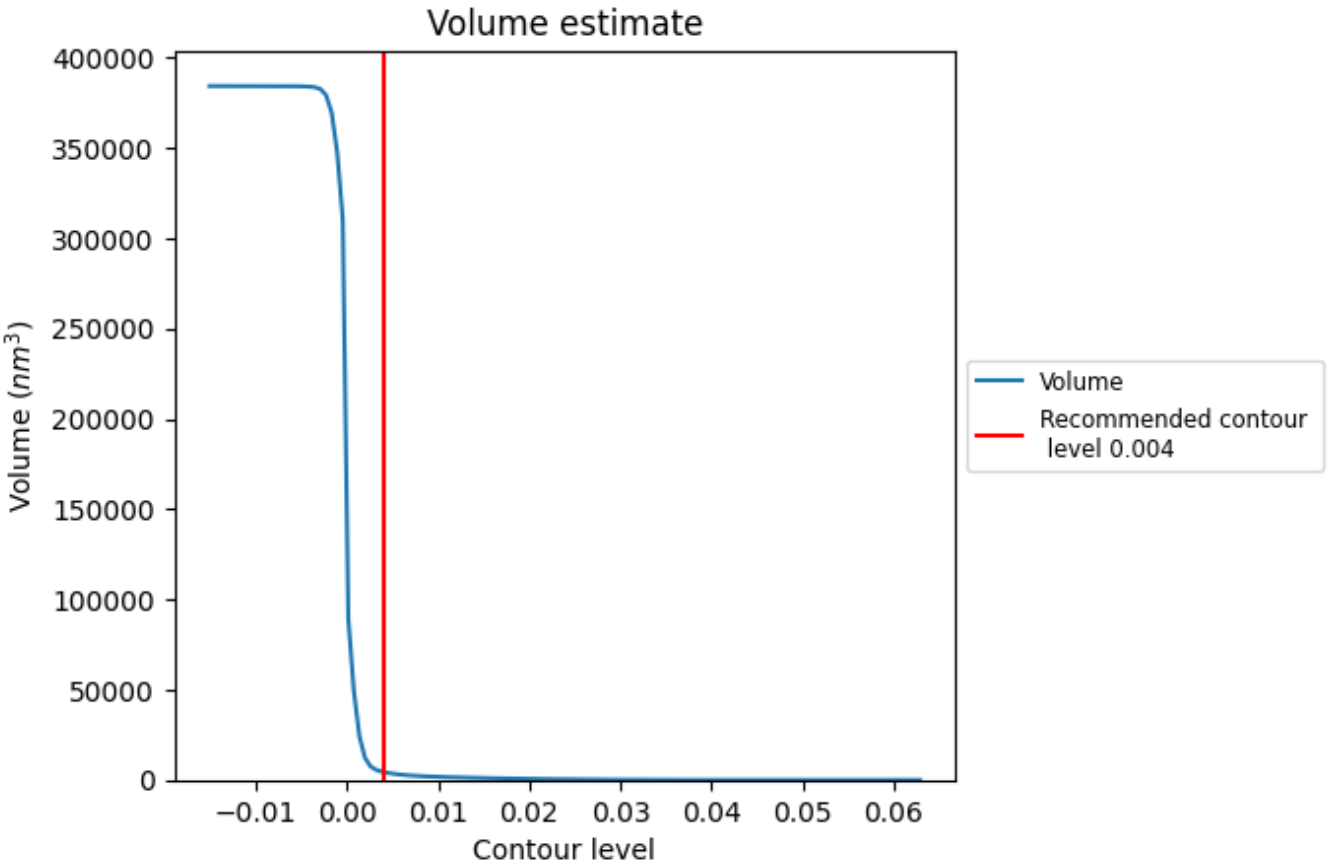
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

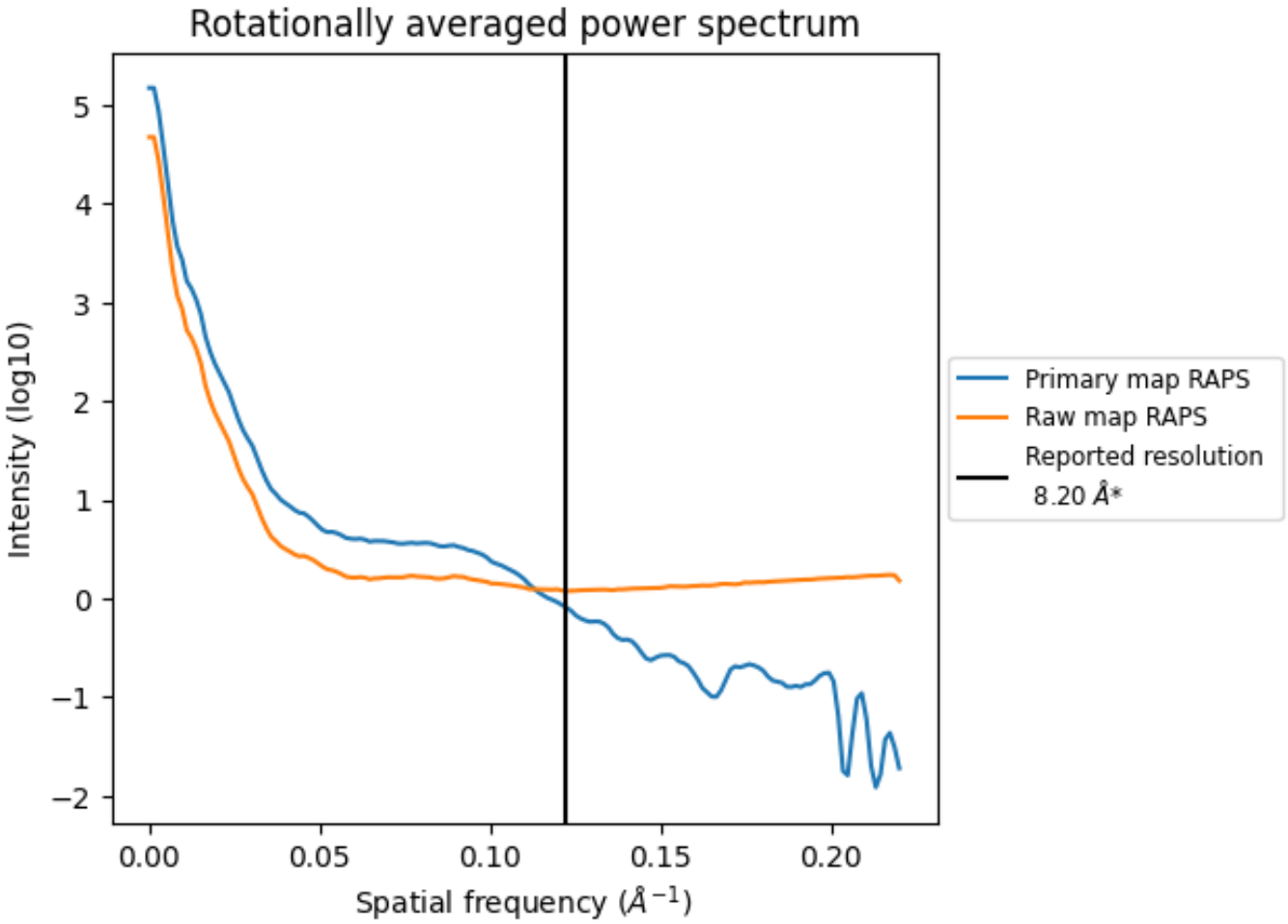
7.2 Volume estimate



The volume at the recommended contour level is 4396 nm^3; this corresponds to an approximate mass of 3971 kDa.

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

7.3 Rotationally averaged power spectrum (i)

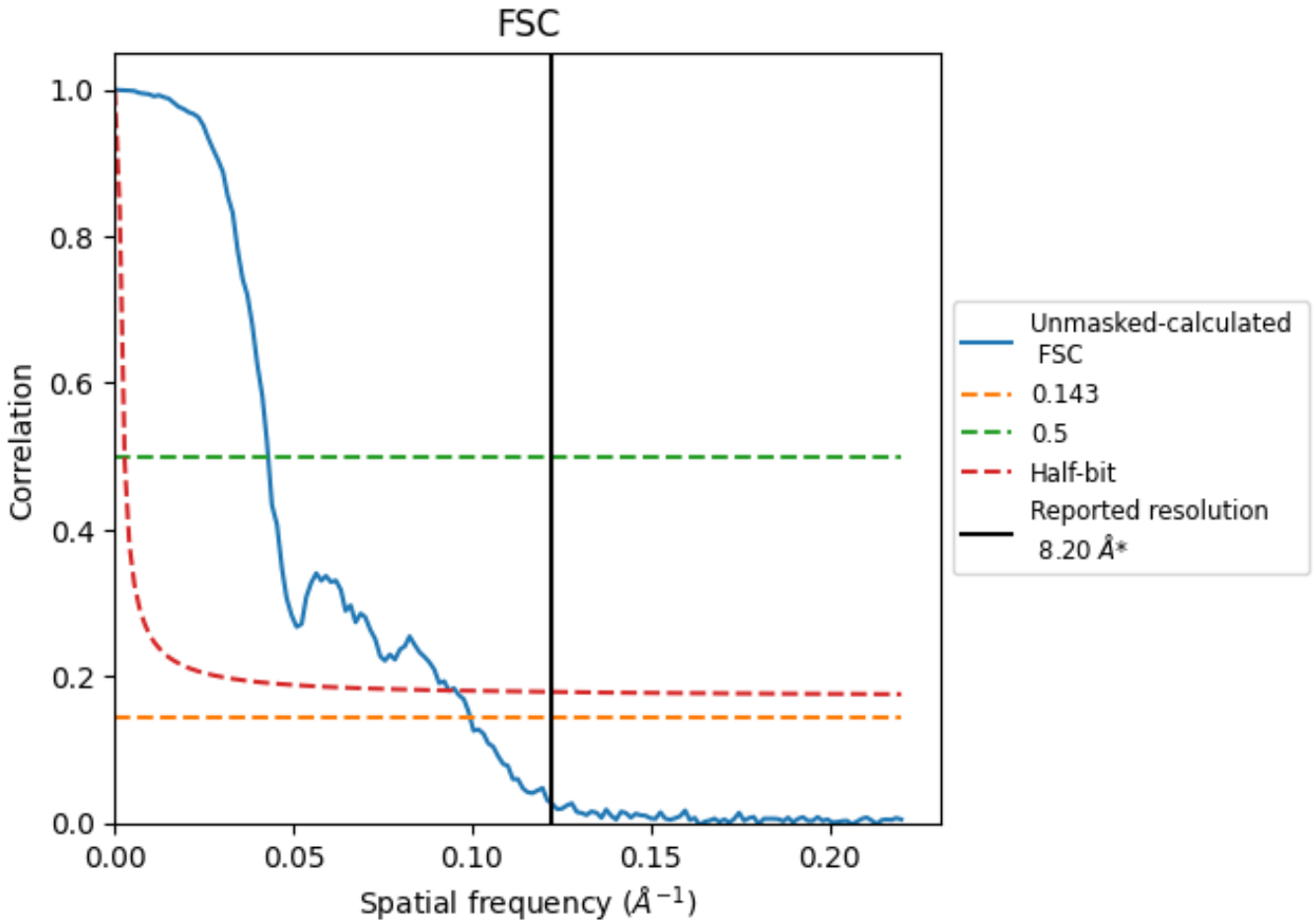


*Reported resolution corresponds to spatial frequency of 0.122 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.122 Å^{-1}

8.2 Resolution estimates (i)

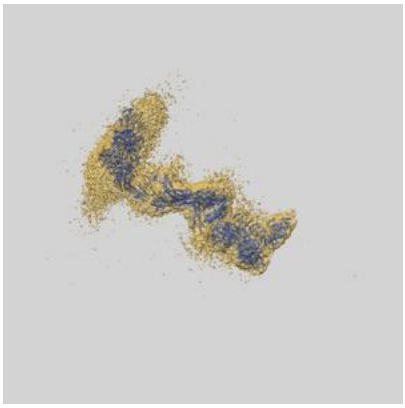
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.05	23.31	10.70

*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 10.05 differs from the reported value 8.2 by more than 10 %

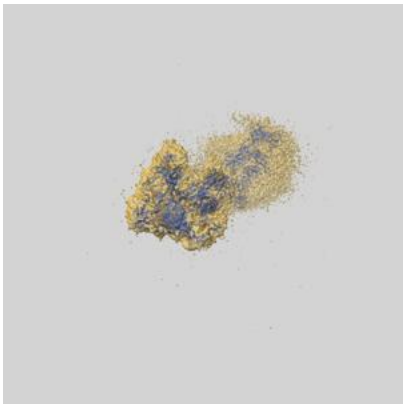
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41565 and PDB model 8TQW. Per-residue inclusion information can be found in section 3 on page 9.

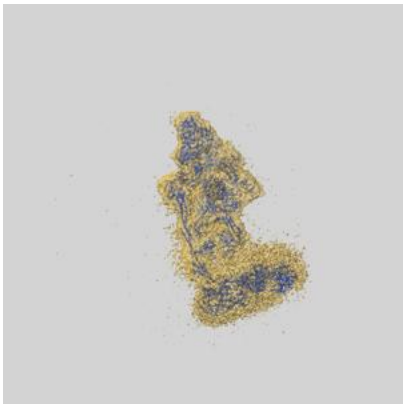
9.1 Map-model overlay



X



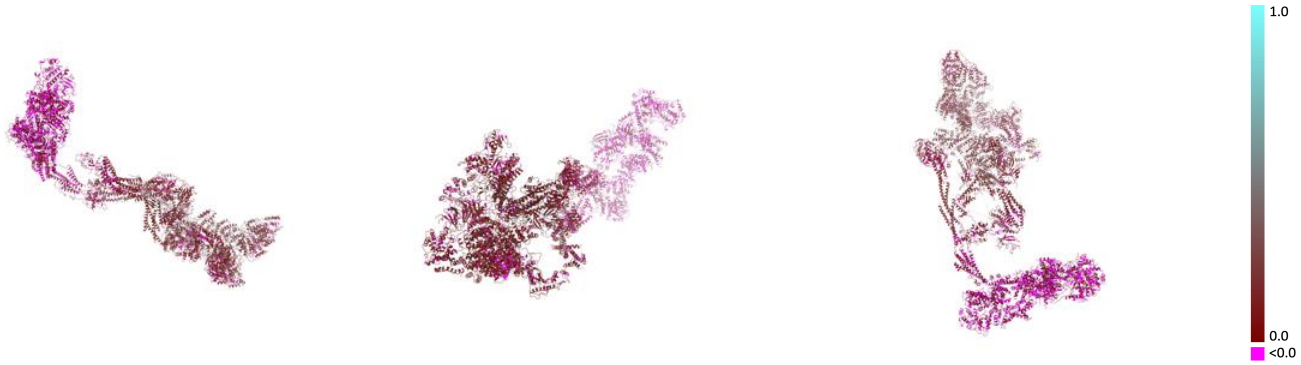
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

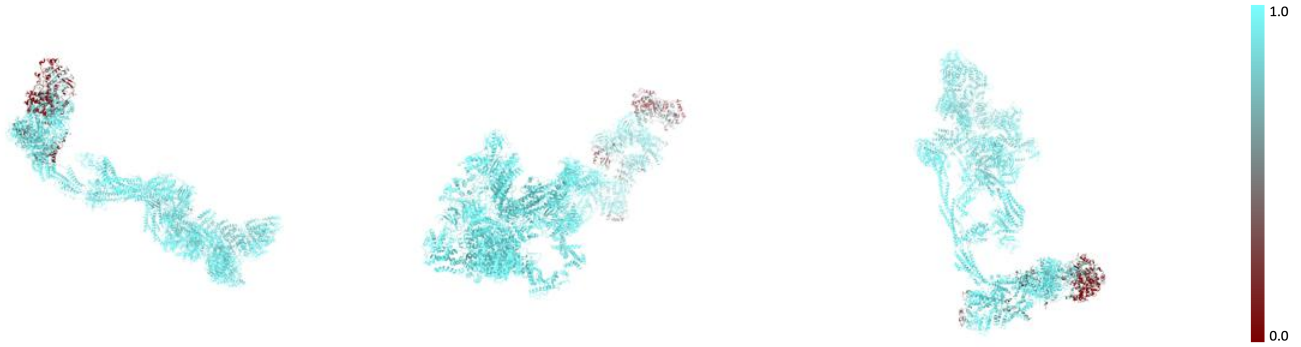
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

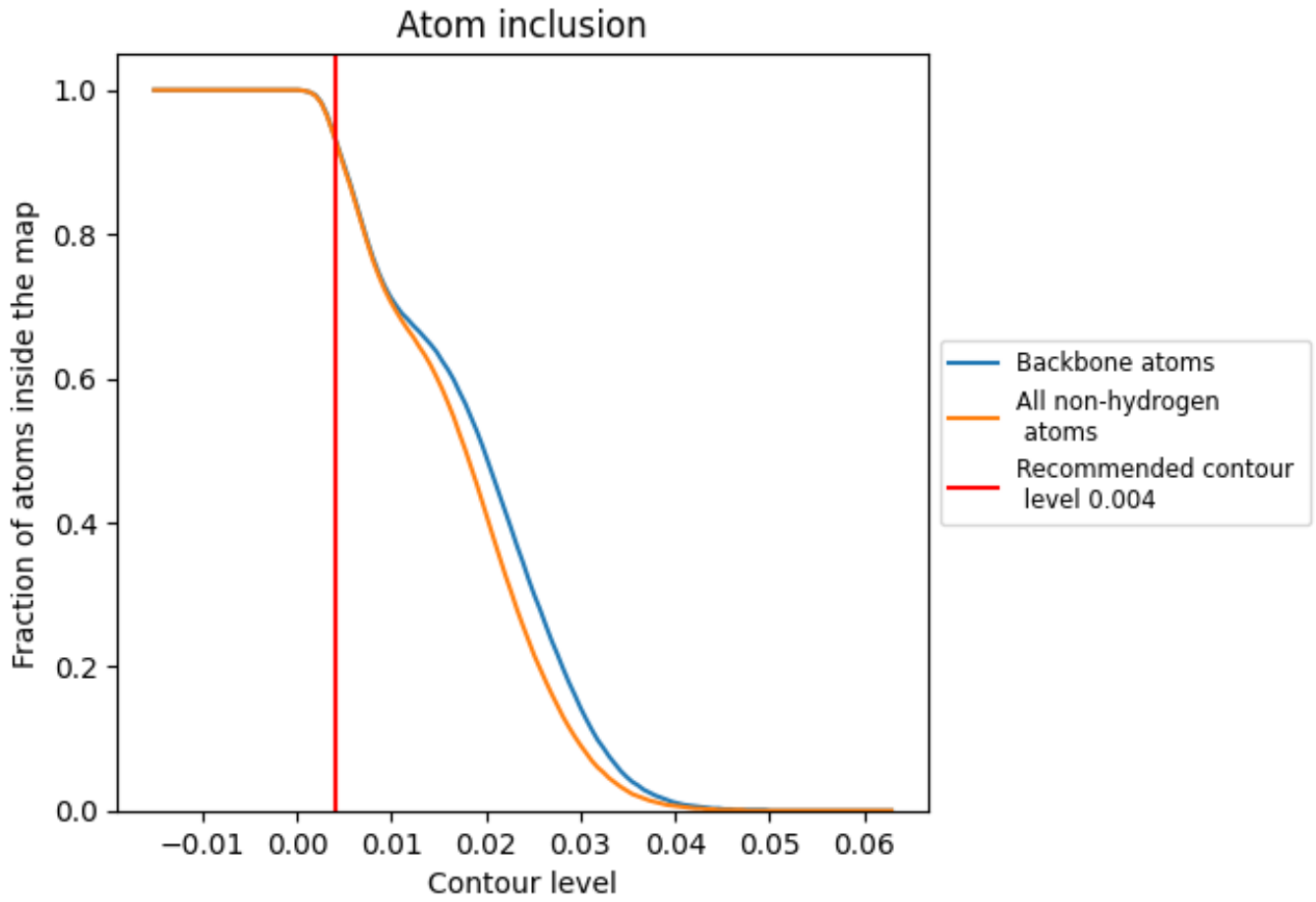
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.1110
0	0.9980	0.1790
1	1.0000	0.1670
2	1.0000	0.1470
3	1.0000	0.1610
4	1.0000	0.0940
A	1.0000	0.1290
B	1.0000	0.2460
D	1.0000	0.1340
F	1.0000	0.0940
G	0.9990	0.0980
H	0.9950	0.1220
I	1.0000	0.1670
J	0.9960	0.0370
K	1.0000	0.1270
N	1.0000	0.1720
O	1.0000	0.2010
P	0.9990	0.1450
Q	1.0000	0.1780
R	1.0000	0.1390
S	1.0000	0.0690
T	1.0000	0.1490
U	0.9960	0.0850
V	1.0000	0.1440
W	1.0000	0.1550
X	0.9990	0.1660
a	0.3260	0.0050
b	0.2570	0.0040
c	0.8820	0.0110
d	0.8920	0.0170