Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 05:16 PM EDT

PDB ID	:	8T9D
EMDB ID	:	EMD-41107
Title	:	CryoEM structure of TR-TRAP
Authors	:	Zhao, H.; Asturias, F.
Deposited on	:	2023-06-23
Resolution	:	4.66 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:

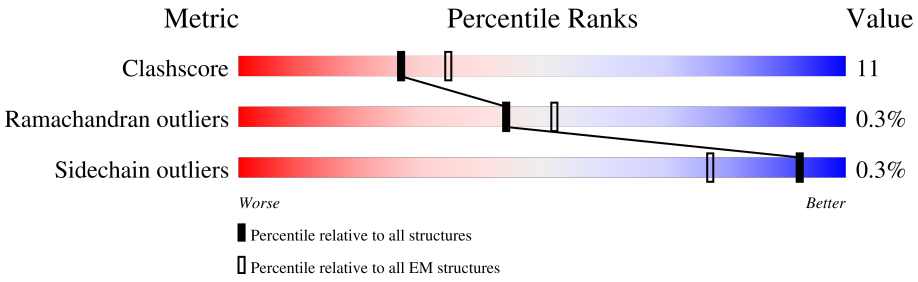
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1581	29% · 70%
2	B	270	57% · 41%
3	C	246	· 49% 21% · 28%
4	D	233	69% 31%
5	E	268	66% · 32%
6	F	146	47% · 50%
7	G	135	23% 90% 10%
8	H	117	78% 9% · · 10%

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Mol	Chain	Length	Quality of chain
9	I	1454	66% 10% 24%
10	J	788	16% 5% 79%
11	K	877	60% 23% 17%
12	L	651	71% 12% 17%
13	M	208	79% 7% 13%
14	O	212	75% 7% 18%
15	P	144	79% 21%
16	Q	200	58% 8% 34%
17	R	1368	70% 24% 5%
18	S	989	78% 13% 9%
19	T	747	23% 74%
20	V	311	77% 10% 13%
21	W	178	58% 8% 34%
22	X	200	48% 13% 38%
23	Y	178	65% 10% 26%
24	Z	131	78% 21%
25	a	20	100%
26	9	2174	99%

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 49136 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 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	467	2354	1405	476	473	0	0

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	158	793	475	158	160	0	0

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	178	931	564	185	182	0	0

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	161	801	479	161	161	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	181	902	537	181	183	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	73	379	228	74	76	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	122	Total	C	N	O	0	0
			608	362	123	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	105	Total	C	N	O	S	0	0
			583	354	116	112	1		

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	1102	Total	C	N	O	S	0	0
			6855	4319	1271	1245	20		

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1176	753	216	203	4		

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	732	Total	C	N	O	S	0	0
			5037	3245	903	866	23		

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	543	Total	C	N	O	S	0	0
			3393	2134	632	622	5		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	180	Total	C	N	O	S	0	0
			1146	729	218	197	2		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	174	Total	C	N	O	S	0	0
			1022	645	180	193	4		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	114	Total	C	N	O	0	0
			568	340	114	114		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	131	Total	C	N	O	0	0
			759	467	145	147		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	1294	Total	C	N	O	S	0	0
			9758	6300	1684	1721	53		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	901	Total	C	N	O	S	0	0
			5888	3751	1061	1049	27		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	192	Total	C	N	O	S	0	0
			1302	837	223	237	5		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	270	Total	C	N	O	S	0	0
			1683	1067	307	306	3		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	118	Total	C	N	O	S	0	0
			781	489	146	144	2		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	123	Total	C	N	O	S	0	0
			842	530	150	159	3		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	132	Total	C	N	O	S	0	0
			839	523	167	146	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	103	Total	C	N	O	0	0
			516	308	103	105		

- Molecule 25 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 13.

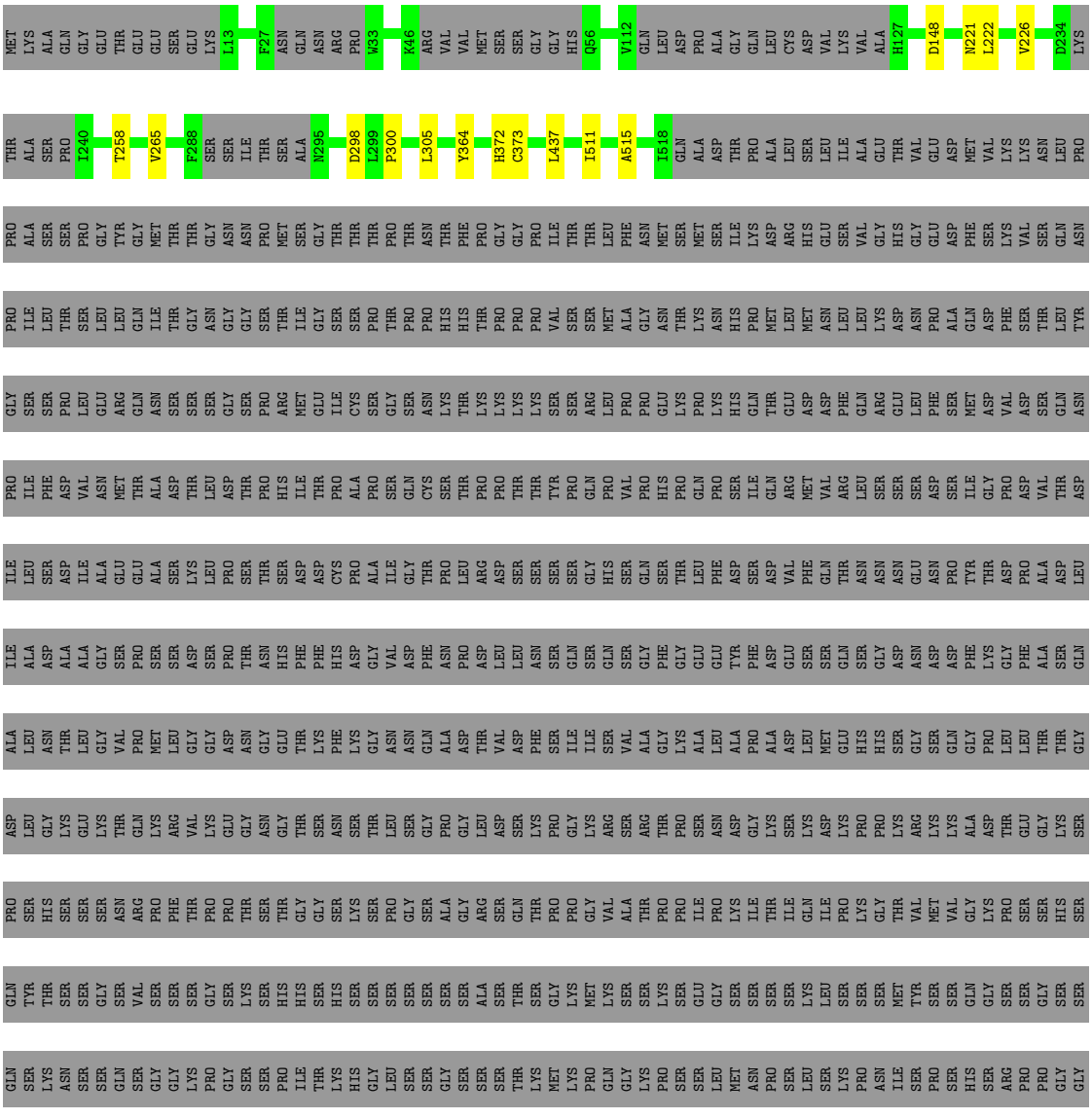
Mol	Chain	Residues	Atoms				AltConf	Trace
26	9	24	Total	C	N	O	0	0
			120	72	24	24		

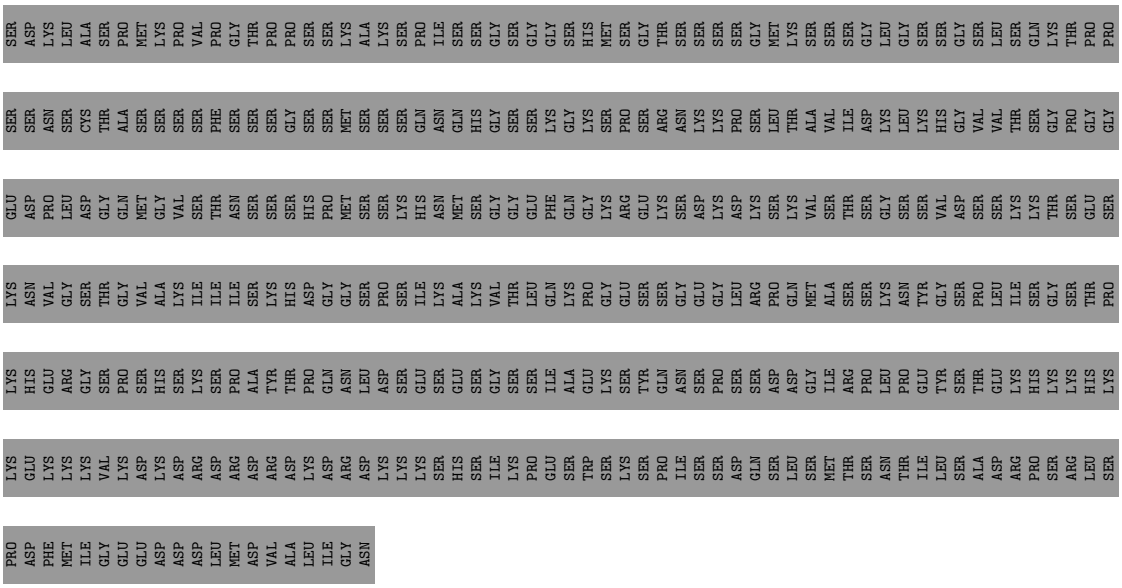
3 Residue-property plots (i)

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 1

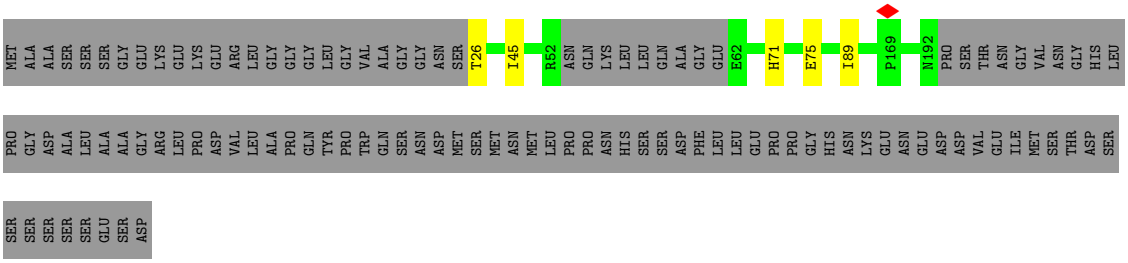
Chain A:





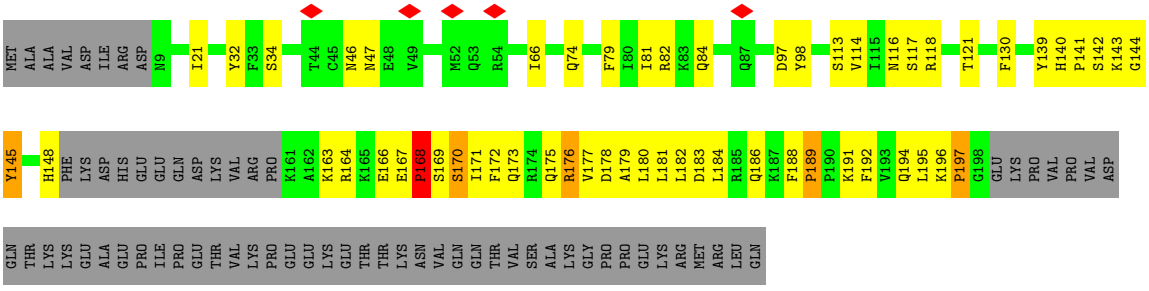
• Molecule 2: Mediator of RNA polymerase II transcription subunit 4

Chain B:



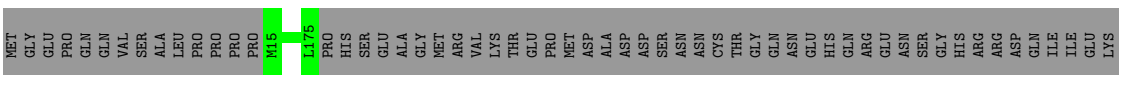
• Molecule 3: Mediator of RNA polymerase II transcription subunit 6

Chain C:



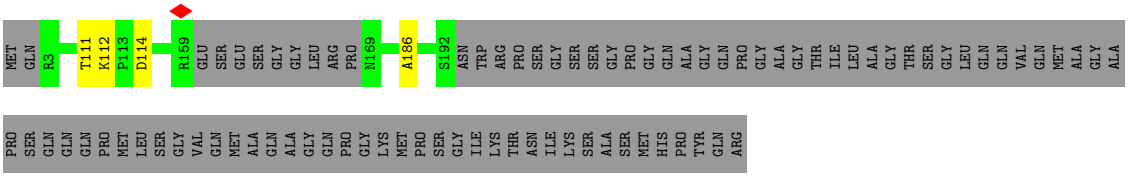
• Molecule 4: Mediator of RNA polymerase II transcription subunit 7

Chain D:



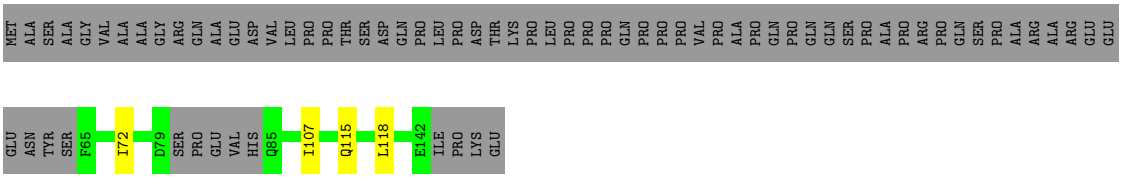
• Molecule 5: Mediator of RNA polymerase II transcription subunit 8

Chain E:



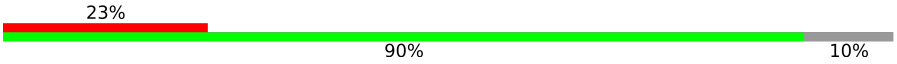
• Molecule 6: Mediator of RNA polymerase II transcription subunit 9

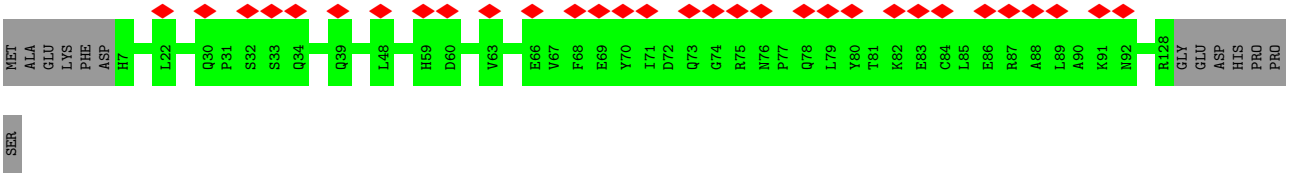
Chain F:



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

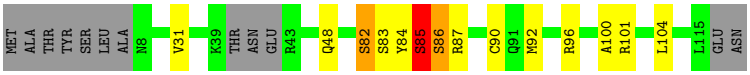
Chain G:





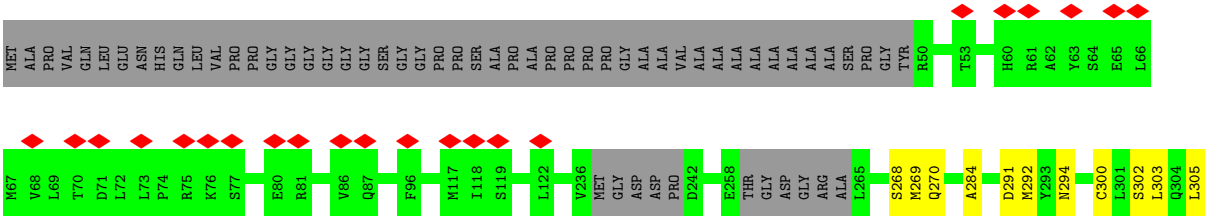
• Molecule 8: Mediator of RNA polymerase II transcription subunit 11

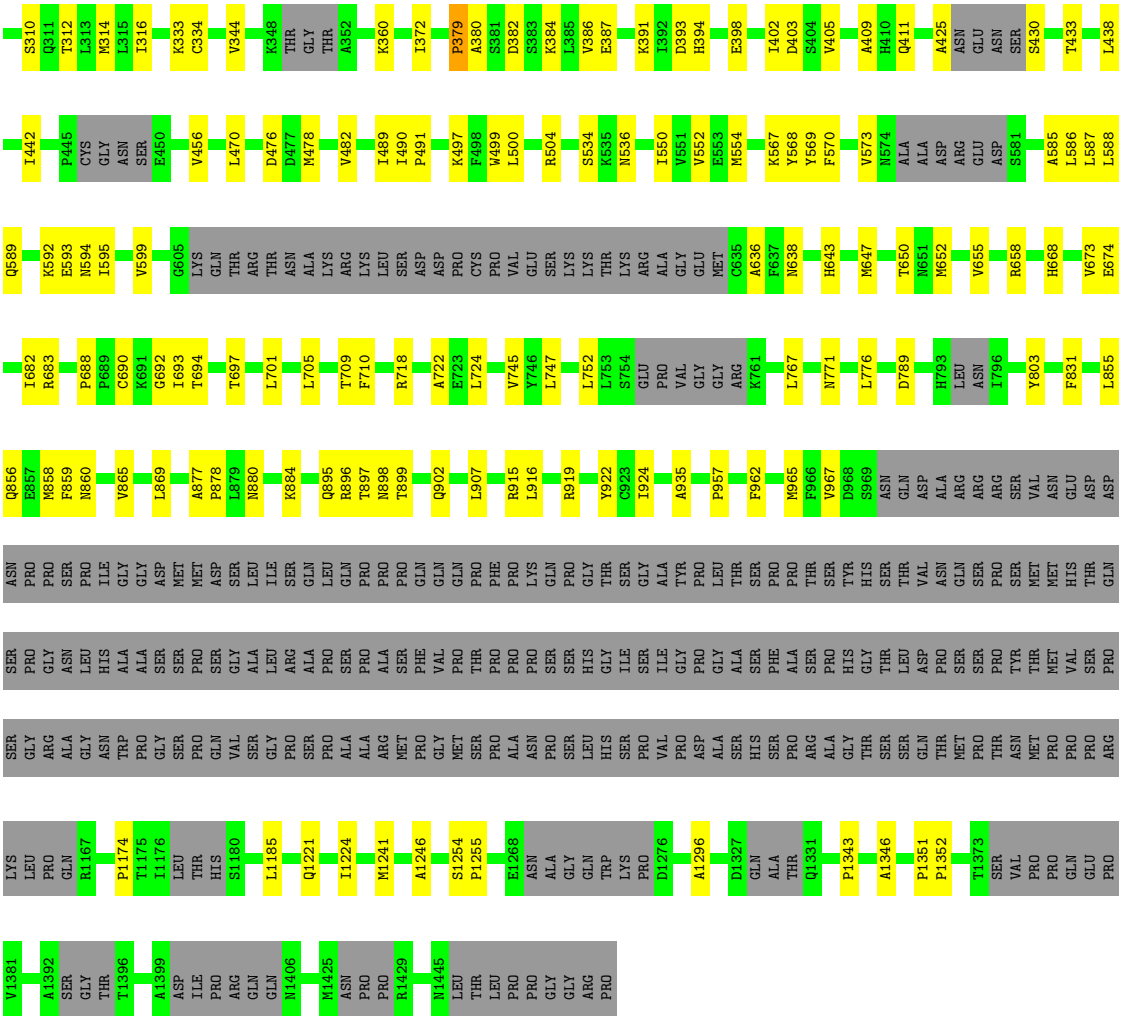
Chain H:



• Molecule 9: Mediator of RNA polymerase II transcription subunit 14

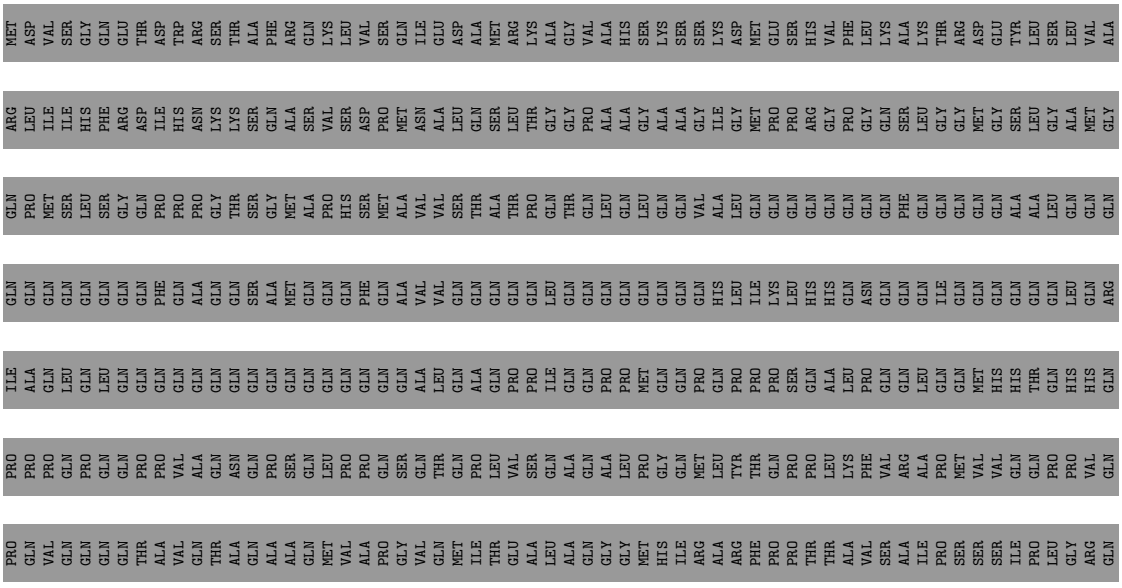
Chain I:

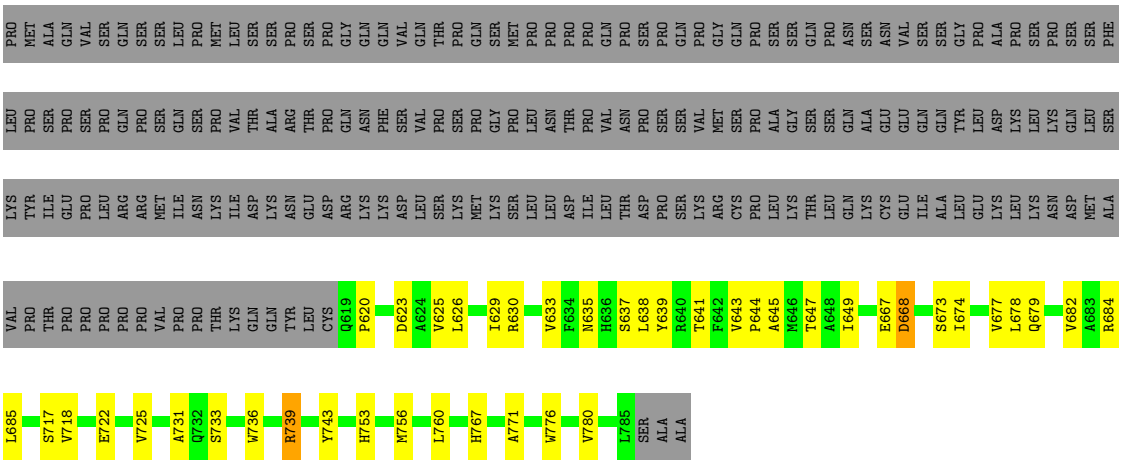




• Molecule 10: Mediator of RNA polymerase II transcription subunit 15

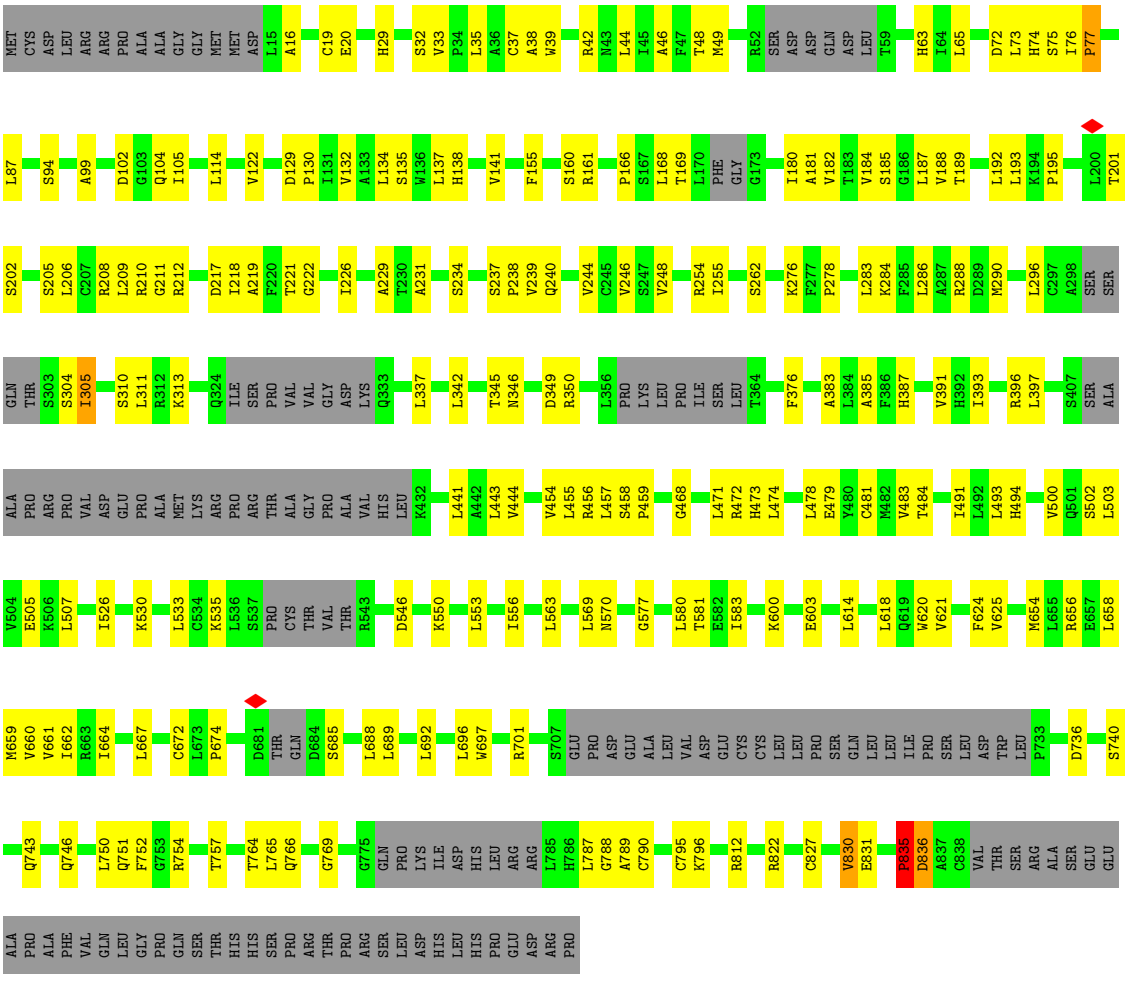
Chain J:





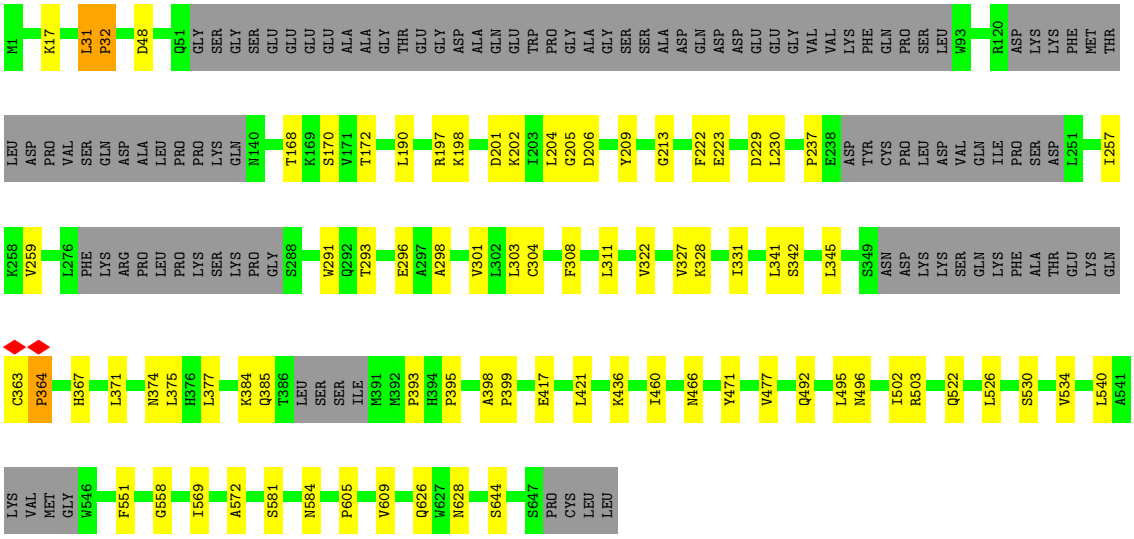
• Molecule 11: Mediator of RNA polymerase II transcription subunit 16

Chain K:



• Molecule 12: Mediator of RNA polymerase II transcription subunit 17

Chain L:

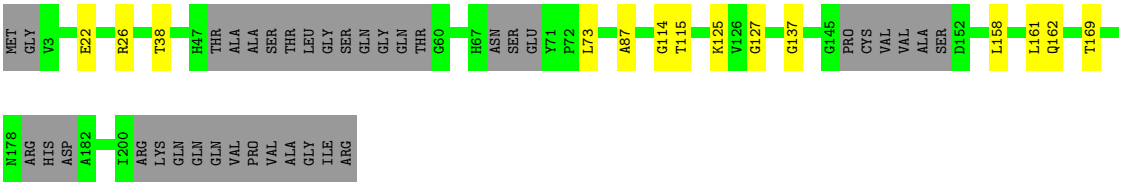


• Molecule 13: Mediator of RNA polymerase II transcription subunit 18

Chain M:

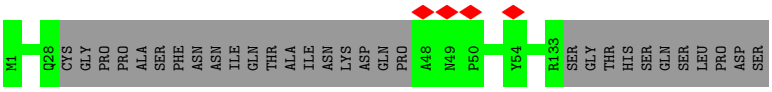
• Molecule 14: Mediator of RNA polymerase II transcription subunit 20

Chain O:



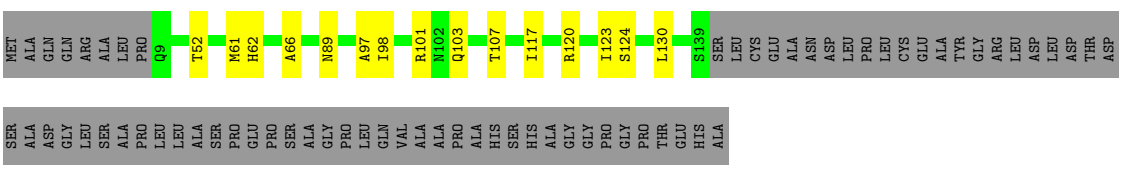
• Molecule 15: Mediator of RNA polymerase II transcription subunit 21

Chain P:



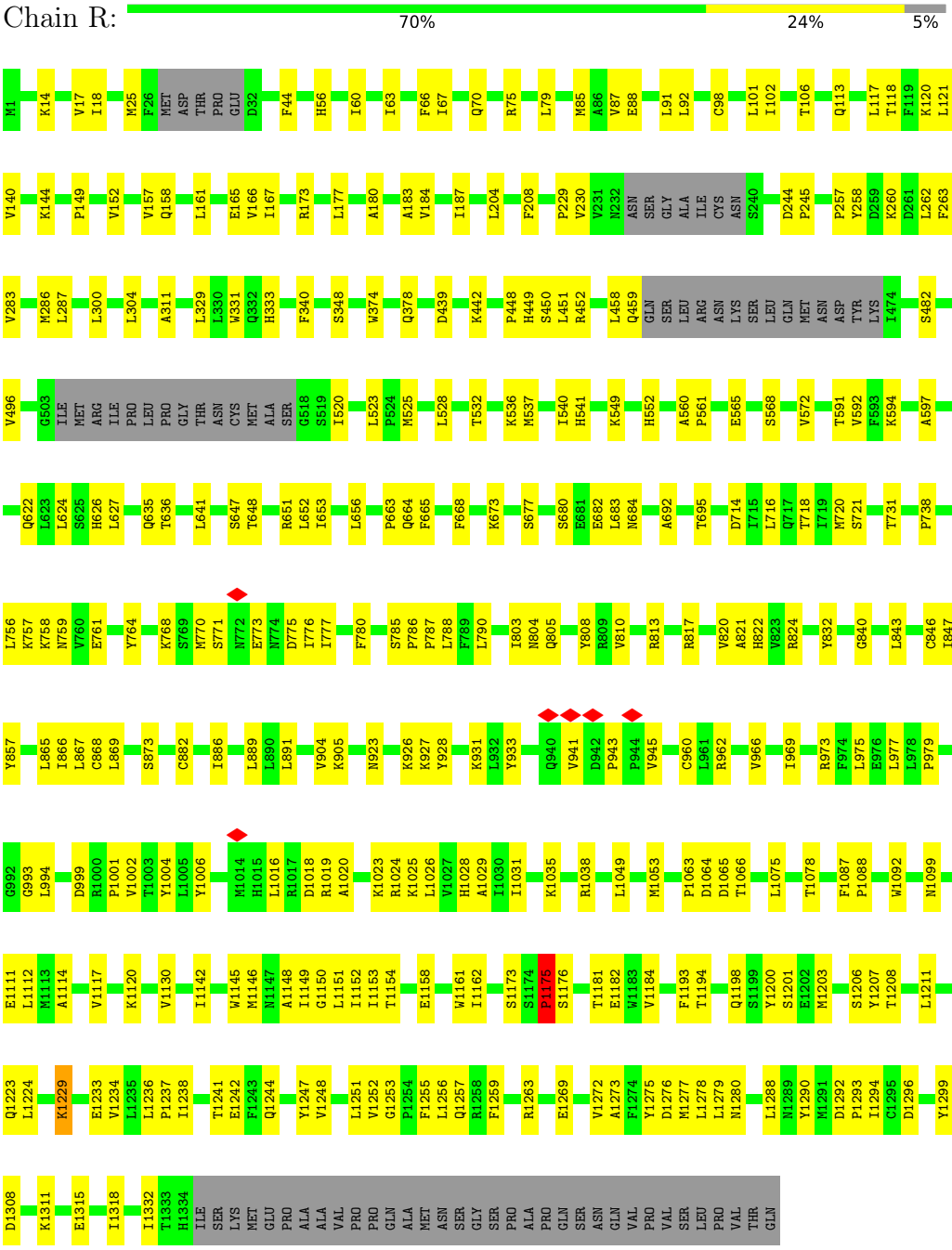
• Molecule 16: Mediator of RNA polymerase II transcription subunit 22

Chain Q:



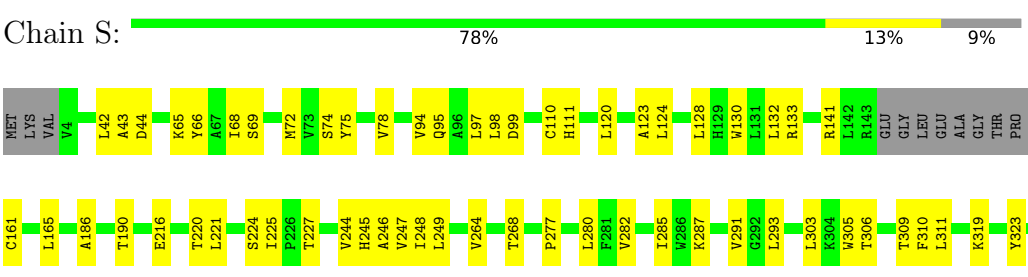
• Molecule 17: Mediator of RNA polymerase II transcription subunit 23

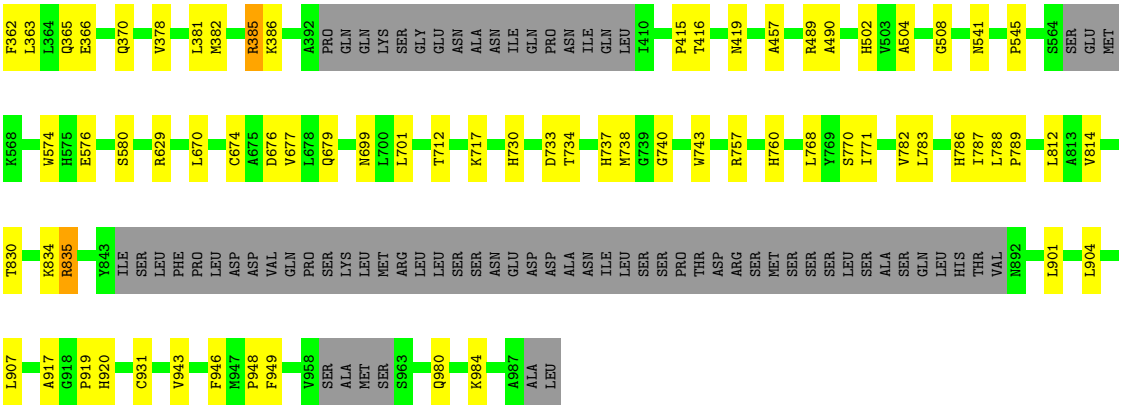
Chain R:



• Molecule 18: Mediator of RNA polymerase II transcription subunit 24

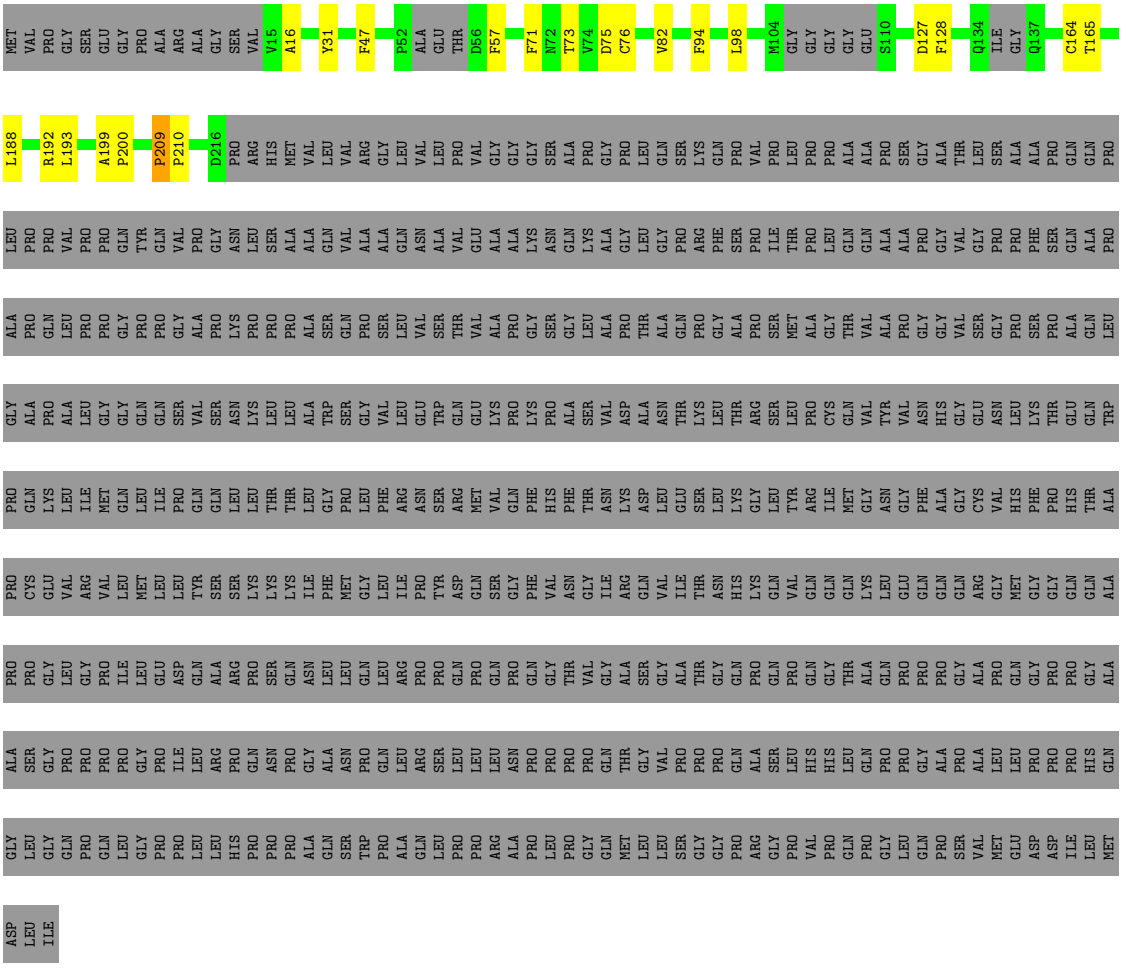
Chain S:





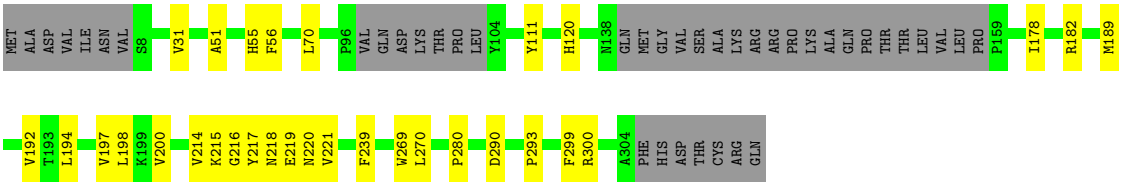
• Molecule 19: Mediator of RNA polymerase II transcription subunit 25

Chain T:



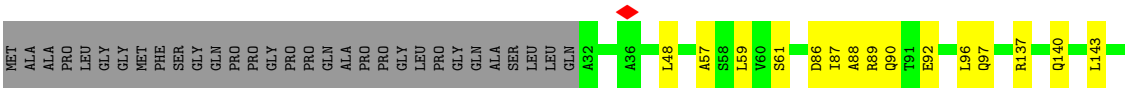
• Molecule 20: Mediator of RNA polymerase II transcription subunit 27

Chain V:



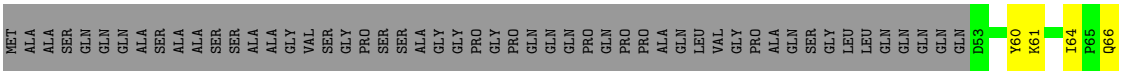
• Molecule 21: Mediator of RNA polymerase II transcription subunit 28

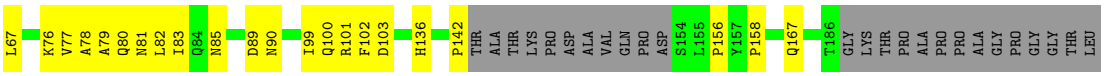
Chain W:



• Molecule 22: Mediator of RNA polymerase II transcription subunit 29

Chain X:



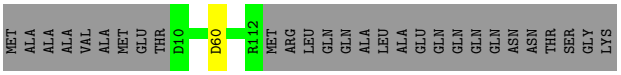


• Molecule 23: Mediator of RNA polymerase II transcription subunit 30

Chain Y:

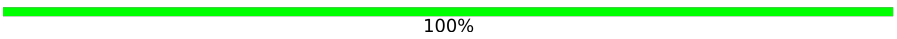
• Molecule 24: Mediator of RNA polymerase II transcription subunit 31

Chain Z:



• Molecule 25: Unknown Peptide

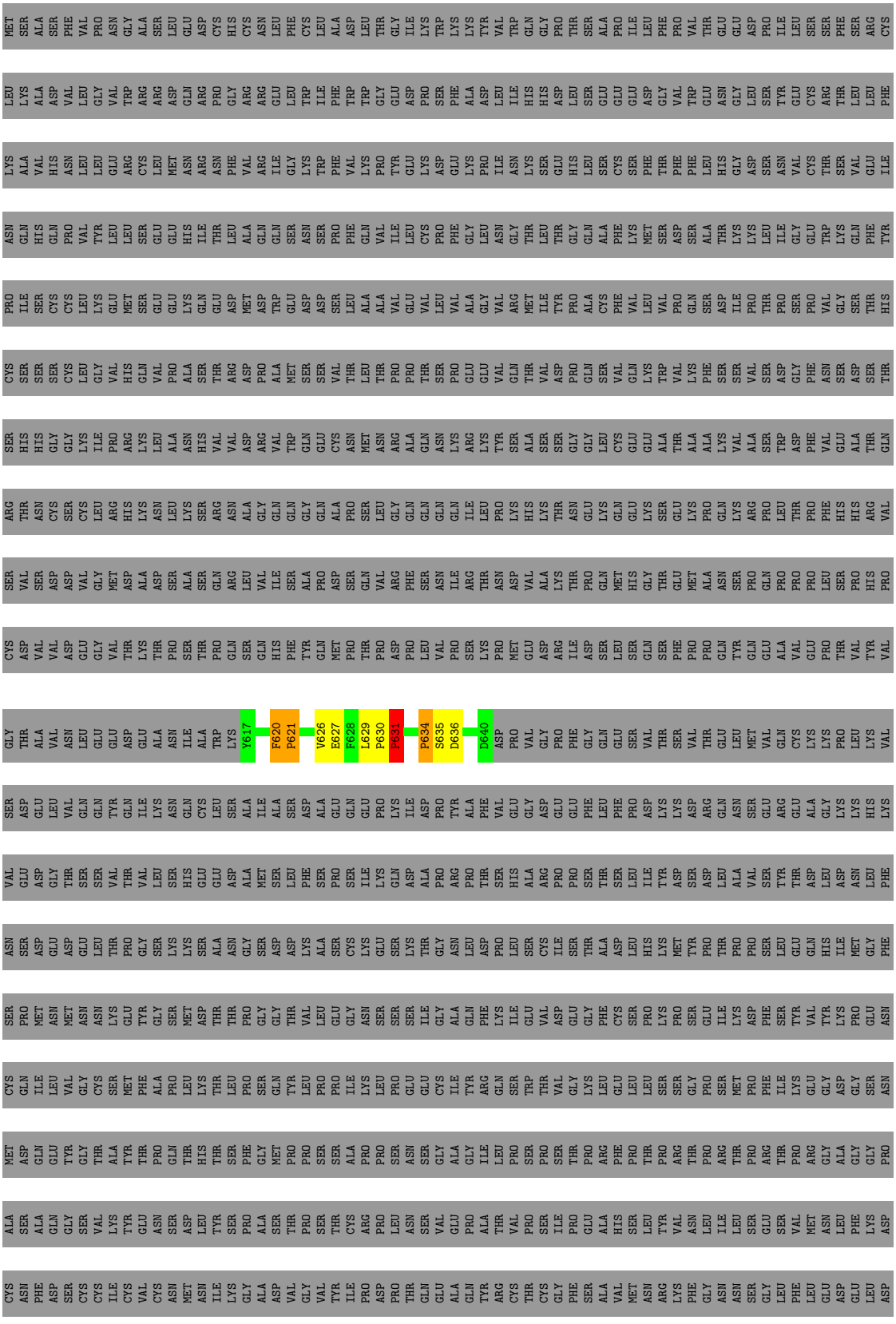
Chain a:



There are no outlier residues recorded for this chain.

• Molecule 26: Mediator of RNA polymerase II transcription subunit 13

Chain 9: 99%


Y617
F620
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E627
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S635
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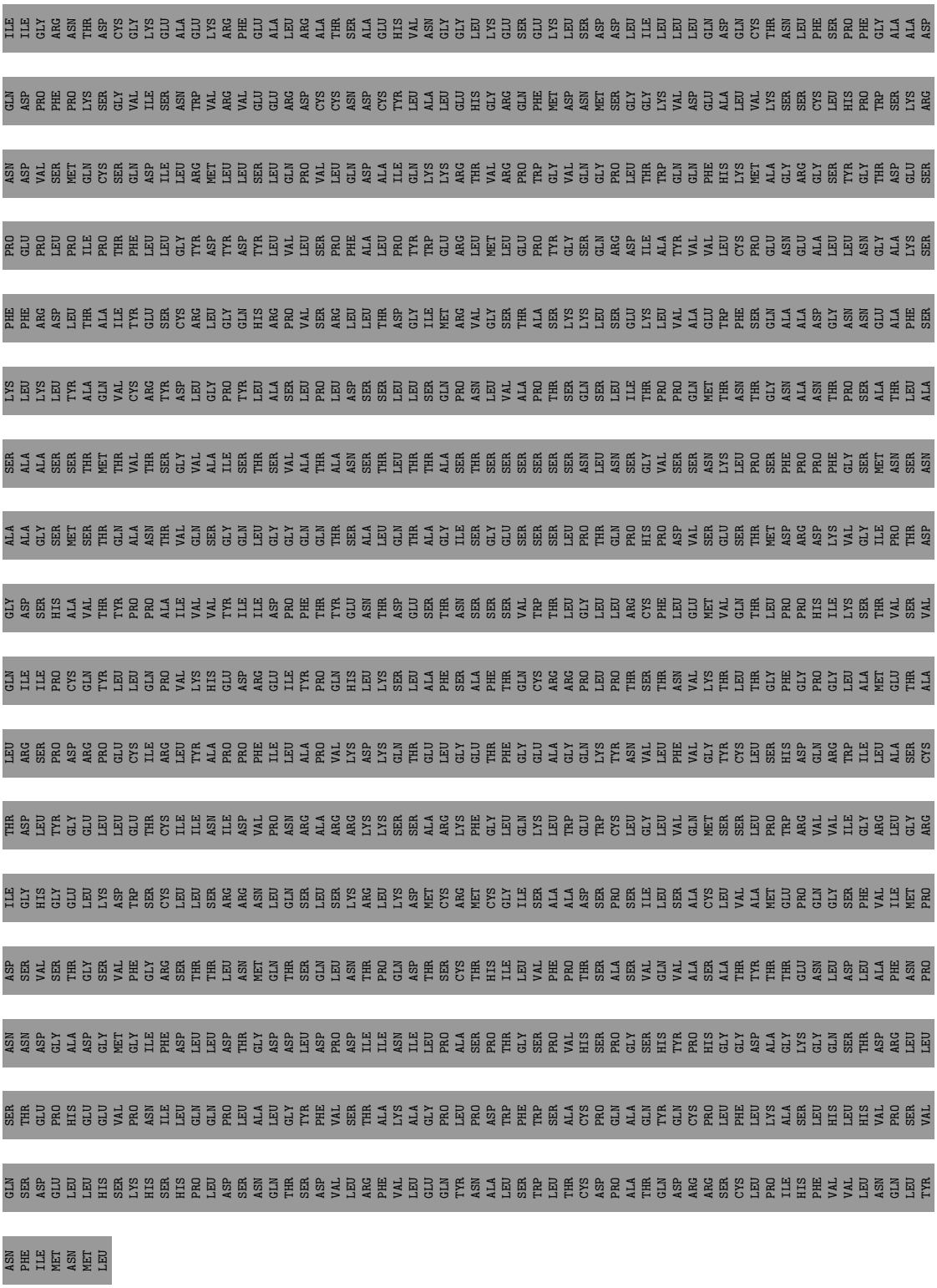
D640


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	35000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.563	Depositor
Minimum map value	-0.198	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	621.60004, 621.60004, 621.60004	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/2348	0.42	1/3260 (0.0%)
2	B	0.23	0/791	0.34	0/1100
3	C	0.68	2/933 (0.2%)	0.73	3/1289 (0.2%)
4	D	0.23	0/800	0.34	0/1116
5	E	0.23	0/900	0.40	0/1252
6	F	0.22	0/377	0.33	0/521
7	G	0.23	0/607	0.33	0/845
8	H	0.22	0/585	0.43	0/805
9	I	0.24	0/6977	0.43	4/9621 (0.0%)
10	J	0.24	0/1212	0.46	1/1678 (0.1%)
11	K	0.24	0/5145	0.48	4/7058 (0.1%)
12	L	0.25	0/3451	0.44	3/4749 (0.1%)
13	M	0.23	0/1169	0.42	0/1598
14	O	0.25	0/1036	0.40	0/1424
15	P	0.22	0/566	0.31	0/788
16	Q	0.22	0/763	0.38	0/1053
17	R	0.24	0/10006	0.43	5/13665 (0.0%)
18	S	0.24	0/6009	0.42	2/8258 (0.0%)
19	T	0.27	0/1340	0.48	1/1842 (0.1%)
20	V	0.23	0/1721	0.39	0/2377
21	W	0.23	0/793	0.37	0/1086
22	X	0.23	0/855	0.39	0/1172
23	Y	0.22	0/848	0.35	0/1160
24	Z	0.22	0/515	0.46	1/718 (0.1%)
26	9	0.82	0/119	1.02	3/165 (1.8%)
All	All	0.26	2/49866 (0.0%)	0.44	28/68600 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	189	PRO	N-CA	13.28	1.69	1.47
3	C	188	PHE	C-N	6.00	1.45	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	168	PRO	CA-N-CD	-9.16	98.68	111.50
19	T	209	PRO	CA-N-CD	-8.76	99.24	111.50
17	R	1175	PRO	CA-N-CD	-8.64	99.41	111.50
12	L	32	PRO	CA-N-CD	-8.49	99.61	111.50
12	L	364	PRO	CA-N-CD	-8.48	99.62	111.50
11	K	77	PRO	CA-N-CD	-8.43	99.69	111.50
9	I	379	PRO	CA-N-CD	-8.34	99.82	111.50
11	K	835	PRO	CA-N-CD	-8.12	100.13	111.50
3	C	197	PRO	CA-N-CD	-7.60	100.86	111.50
3	C	170	SER	C-N-CA	7.35	140.07	121.70
26	9	634	PRO	N-CA-CB	5.90	110.38	103.30
26	9	631	PRO	N-CA-CB	5.87	110.35	103.30
26	9	621	PRO	N-CA-CB	5.61	110.03	103.30
10	J	668	ASP	CB-CG-OD2	5.26	123.04	118.30
17	R	1064	ASP	CB-CG-OD2	5.24	123.01	118.30
18	S	327	ASP	CB-CG-OD2	5.24	123.01	118.30
9	I	789	ASP	CB-CG-OD2	5.22	123.00	118.30
17	R	1018	ASP	CB-CG-OD2	5.21	122.99	118.30
17	R	775	ASP	CB-CG-OD2	5.21	122.99	118.30
24	Z	60	ASP	CB-CG-OD2	5.20	122.98	118.30
18	S	44	ASP	CB-CG-OD2	5.20	122.98	118.30
12	L	48	ASP	CB-CG-OD2	5.18	122.97	118.30
11	K	72	ASP	CB-CG-OD2	5.18	122.96	118.30
17	R	439	ASP	CB-CG-OD2	5.17	122.96	118.30
9	I	476	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	148	ASP	CB-CG-OD2	5.17	122.95	118.30
11	K	836	ASP	CB-CG-OD2	5.16	122.95	118.30
9	I	382	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	82	SER	Peptide
8	H	85	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2354	0	1078	12	0
2	B	793	0	374	7	0
3	C	931	0	479	94	0
4	D	801	0	327	0	0
5	E	902	0	408	15	0
6	F	379	0	182	6	0
7	G	608	0	260	0	0
8	H	583	0	357	15	0
9	I	6855	0	5052	109	0
10	J	1176	0	1036	36	0
11	K	5037	0	4491	183	0
12	L	3393	0	2495	73	0
13	M	1146	0	845	10	0
14	O	1022	0	684	7	0
15	P	568	0	286	0	0
16	Q	759	0	459	30	0
17	R	9758	0	9145	239	0
18	S	5888	0	4727	105	0
19	T	1302	0	1025	20	0
20	V	1683	0	1190	23	0
21	W	781	0	618	10	0
22	X	842	0	710	31	0
23	Y	839	0	637	17	0
24	Z	516	0	227	0	0
25	a	100	0	23	0	0
26	9	120	0	43	8	0
All	All	49136	0	37158	949	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 (949) 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)
3:C:130:PHE:CE2	16:Q:62:HIS:CB	1.82	1.57
19:T:209:PRO:CD	19:T:210:PRO:HD2	1.19	1.57
3:C:189:PRO:N	3:C:189:PRO:CA	1.69	1.53
19:T:209:PRO:HD2	19:T:210:PRO:CD	1.08	1.53
3:C:118:ARG:HA	5:E:112:LYS:CB	1.03	1.50
3:C:118:ARG:CA	5:E:112:LYS:CB	1.96	1.43
17:R:1233:GLU:OE2	17:R:1234:VAL:HG23	1.26	1.34
16:Q:123:ILE:HG21	23:Y:167:ILE:CB	1.56	1.33
3:C:141:PRO:CB	12:L:170:SER:O	1.77	1.32
3:C:117:SER:CB	5:E:111:THR:CB	2.10	1.29
3:C:130:PHE:CD2	16:Q:62:HIS:CB	2.17	1.25
3:C:140:HIS:CB	12:L:170:SER:CB	2.14	1.24
20:V:215:LYS:CB	20:V:220:ASN:ND2	2.06	1.18
17:R:1233:GLU:CD	17:R:1234:VAL:HG23	1.66	1.15
16:Q:123:ILE:CG2	23:Y:167:ILE:CB	2.24	1.15
3:C:130:PHE:HE2	16:Q:62:HIS:CB	1.31	1.14
8:H:31:VAL:HG11	8:H:48:GLN:CB	1.79	1.13
8:H:31:VAL:CG1	8:H:48:GLN:CB	2.28	1.11
8:H:31:VAL:HG11	8:H:48:GLN:CA	1.79	1.10
3:C:116:ASN:CB	16:Q:52:THR:O	2.01	1.09
9:I:569:TYR:HA	9:I:593:GLU:OE2	1.52	1.08
3:C:130:PHE:CE2	16:Q:62:HIS:CA	2.37	1.06
18:S:363:LEU:HD11	18:S:386:LYS:CE	1.86	1.05
3:C:121:THR:HA	5:E:114:ASP:CB	1.86	1.05
11:K:383:ALA:HA	11:K:393:ILE:HG23	1.37	1.01
2:B:89:ILE:HG23	6:F:118:LEU:CB	1.90	1.00
12:L:168:THR:O	12:L:172:THR:HG21	1.61	1.00
3:C:148:HIS:O	12:L:230:LEU:HD23	1.60	0.99
17:R:1233:GLU:OE2	17:R:1234:VAL:CG2	2.11	0.99
22:X:99:ILE:HG22	22:X:100:GLN:H	1.25	0.99
9:I:270:GLN:CB	26:9:631:PRO:O	2.11	0.98
3:C:175:GLN:O	3:C:178:ASP:N	1.95	0.98
11:K:796:LYS:HA	11:K:812:ARG:NH2	1.79	0.97
3:C:196:LYS:CB	26:9:620:PHE:O	2.11	0.97
17:R:56:HIS:HD1	17:R:60:ILE:HG13	1.27	0.97
18:S:363:LEU:CD1	18:S:386:LYS:HE2	1.94	0.97
9:I:554:MET:CB	9:I:567:LYS:HE3	1.94	0.96
9:I:270:GLN:HB2	26:9:631:PRO:O	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:350:ARG:N	11:K:387:HIS:NE2	2.00	0.96
18:S:363:LEU:HD11	18:S:386:LYS:HE2	0.99	0.95
2:B:89:ILE:CG2	6:F:118:LEU:CB	2.44	0.95
18:S:943:VAL:HG22	18:S:949:PHE:HZ	1.30	0.95
17:R:106:THR:OG1	17:R:144:LYS:HE2	1.64	0.95
20:V:215:LYS:CB	20:V:220:ASN:HD21	1.74	0.94
22:X:99:ILE:HG22	22:X:100:GLN:N	1.81	0.94
9:I:569:TYR:CA	9:I:593:GLU:OE2	2.16	0.93
18:S:247:VAL:HG23	18:S:770:SER:OG	1.67	0.91
18:S:370:GLN:HE22	18:S:382:MET:HG2	1.34	0.91
17:R:1088:PRO:HB2	17:R:1092:TRP:HE1	1.34	0.91
13:M:142:LYS:NZ	13:M:144:MET:SD	2.44	0.91
19:T:209:PRO:CD	19:T:210:PRO:CD	2.01	0.90
3:C:191:LYS:CB	9:I:284:ALA:HB2	2.01	0.90
17:R:56:HIS:ND1	17:R:60:ILE:HG13	1.86	0.90
9:I:379:PRO:HG2	9:I:411:GLN:CB	2.02	0.90
12:L:168:THR:O	12:L:172:THR:CG2	2.20	0.90
17:R:17:VAL:HG12	17:R:18:ILE:N	1.88	0.88
18:S:943:VAL:HG12	18:S:943:VAL:O	1.73	0.88
22:X:99:ILE:CG2	22:X:100:GLN:H	1.86	0.88
3:C:167:GLU:OE2	9:I:268:SER:CA	2.19	0.87
18:S:306:THR:OG1	18:S:310:PHE:HE2	1.57	0.87
3:C:148:HIS:O	12:L:230:LEU:CD2	2.23	0.86
3:C:130:PHE:CZ	16:Q:62:HIS:O	2.28	0.86
17:R:520:ILE:HG22	17:R:520:ILE:O	1.76	0.86
22:X:80:GLN:HB3	22:X:99:ILE:CD1	2.05	0.85
11:K:454:VAL:HG12	11:K:455:LEU:N	1.90	0.85
8:H:31:VAL:HG11	8:H:48:GLN:HA	1.55	0.85
11:K:577:GLY:O	11:K:581:THR:HG23	1.77	0.85
11:K:76:ILE:HG23	11:K:77:PRO:HD3	1.58	0.84
17:R:448:PRO:O	17:R:452:ARG:HG3	1.77	0.84
3:C:140:HIS:CA	12:L:170:SER:CB	2.55	0.83
11:K:39:TRP:HB2	11:K:44:LEU:HA	1.57	0.83
8:H:31:VAL:HG12	8:H:48:GLN:CB	2.08	0.83
12:L:17:LYS:CB	12:L:32:PRO:HG2	2.08	0.83
3:C:130:PHE:HZ	16:Q:62:HIS:O	1.61	0.83
11:K:16:ALA:HB3	11:K:456:ARG:HE	1.44	0.81
10:J:633:VAL:CG2	11:K:812:ARG:HD3	2.10	0.81
11:K:383:ALA:CA	11:K:393:ILE:HG23	2.10	0.80
9:I:270:GLN:HB3	26:9:631:PRO:O	1.80	0.80
19:T:209:PRO:HD2	19:T:210:PRO:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:568:TYR:O	9:I:593:GLU:CD	2.21	0.80
1:A:226:VAL:HG12	1:A:226:VAL:O	1.81	0.79
3:C:116:ASN:CB	16:Q:52:THR:C	2.50	0.79
3:C:46:ASN:N	3:C:66:ILE:O	2.15	0.79
11:K:454:VAL:HG12	11:K:455:LEU:H	1.46	0.79
11:K:76:ILE:CG2	11:K:77:PRO:CD	2.61	0.78
17:R:525:MET:HG2	17:R:565:GLU:HB3	1.65	0.78
22:X:77:VAL:HG23	22:X:99:ILE:HG21	1.65	0.78
1:A:265:VAL:HG22	1:A:300:PRO:HA	1.65	0.78
20:V:221:VAL:HG12	20:V:221:VAL:O	1.83	0.78
17:R:17:VAL:HG12	17:R:18:ILE:H	1.46	0.77
9:I:568:TYR:C	9:I:593:GLU:OE2	2.22	0.77
11:K:234:SER:H	11:K:278:PRO:HD2	1.50	0.77
12:L:395:PRO:HG2	12:L:399:PRO:HD2	1.65	0.77
11:K:796:LYS:HA	11:K:812:ARG:HH22	1.50	0.76
9:I:344:VAL:HG12	9:I:344:VAL:O	1.84	0.76
11:K:471:LEU:HB2	11:K:503:LEU:HD21	1.67	0.76
18:S:306:THR:O	18:S:310:PHE:HD2	1.68	0.76
9:I:333:LYS:O	9:I:334:CYS:SG	2.43	0.76
3:C:171:ILE:HA	26:9:635:SER:CB	2.15	0.76
11:K:42:ARG:HD3	11:K:831:GLU:HG2	1.66	0.76
18:S:224:SER:HA	18:S:227:THR:CG2	2.16	0.75
9:I:907:LEU:HD23	9:I:915:ARG:HB3	1.67	0.75
12:L:363:CYS:HB3	12:L:364:PRO:HD3	1.69	0.75
18:S:943:VAL:HG22	18:S:949:PHE:CZ	2.19	0.75
17:R:840:GLY:HA2	17:R:843:LEU:HD13	1.68	0.74
11:K:454:VAL:CG1	11:K:455:LEU:H	2.00	0.74
20:V:200:VAL:HG22	20:V:214:VAL:HG23	1.69	0.74
9:I:334:CYS:SG	9:I:360:LYS:CB	2.76	0.74
10:J:643:VAL:O	10:J:647:THR:HG23	1.87	0.74
17:R:487:CYS:HB3	17:R:491:PRO:HG2	1.70	0.74
11:K:284:LYS:HE3	11:K:290:MET:HB3	1.70	0.73
18:S:378:VAL:HG12	18:S:378:VAL:O	1.87	0.73
12:L:31:LEU:N	12:L:32:PRO:HD3	2.03	0.73
18:S:370:GLN:HE22	18:S:382:MET:CG	2.01	0.73
22:X:77:VAL:HG23	22:X:99:ILE:CG2	2.18	0.73
17:R:904:VAL:HG13	17:R:905:LYS:HD2	1.70	0.73
3:C:148:HIS:C	12:L:229:ASP:O	2.28	0.72
10:J:633:VAL:HG23	11:K:812:ARG:HD3	1.71	0.72
12:L:257:ILE:HG13	12:L:345:LEU:HB3	1.71	0.72
17:R:17:VAL:CG1	17:R:18:ILE:H	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:449:HIS:HA	17:R:452:ARG:NE	2.05	0.72
3:C:121:THR:CA	5:E:114:ASP:CB	2.67	0.71
12:L:363:CYS:HB3	12:L:364:PRO:CD	2.19	0.71
3:C:195:LEU:O	3:C:197:PRO:HD3	1.90	0.71
11:K:383:ALA:HB1	11:K:393:ILE:HG12	1.72	0.71
9:I:568:TYR:O	9:I:593:GLU:OE2	2.08	0.71
17:R:17:VAL:CG1	17:R:18:ILE:N	2.54	0.71
9:I:379:PRO:HD2	9:I:380:ALA:H	1.55	0.71
11:K:76:ILE:HG23	11:K:77:PRO:CD	2.20	0.71
17:R:1175:PRO:HD2	17:R:1176:SER:N	2.06	0.70
18:S:224:SER:HA	18:S:227:THR:HG23	1.72	0.70
18:S:378:VAL:HG13	18:S:381:LEU:HB3	1.72	0.70
3:C:130:PHE:HE2	16:Q:62:HIS:CA	1.91	0.70
3:C:171:ILE:N	26:9:635:SER:CB	2.55	0.70
17:R:230:VAL:O	17:R:1099:ASN:ND2	2.24	0.70
11:K:454:VAL:CG1	11:K:455:LEU:N	2.54	0.70
20:V:197:VAL:HB	20:V:217:TYR:HA	1.74	0.70
3:C:34:SER:HA	3:C:47:ASN:HA	1.74	0.70
11:K:441:LEU:HB2	11:K:459:PRO:HA	1.75	0.69
23:Y:51:ILE:HD11	23:Y:78:LEU:HD23	1.75	0.69
11:K:19:CYS:SG	11:K:20:GLU:N	2.65	0.69
11:K:76:ILE:HG22	11:K:77:PRO:HD2	1.72	0.69
11:K:751:GLN:NE2	11:K:789:ALA:HB3	2.07	0.69
17:R:1175:PRO:HD2	17:R:1176:SER:H	1.57	0.69
2:B:89:ILE:HG21	6:F:118:LEU:CB	2.21	0.69
9:I:379:PRO:HD2	9:I:380:ALA:N	2.07	0.69
10:J:626:LEU:HD21	22:X:83:ILE:HB	1.74	0.69
11:K:827:CYS:H	11:K:830:VAL:CB	2.06	0.69
17:R:56:HIS:CE1	17:R:60:ILE:HG13	2.27	0.69
3:C:167:GLU:OE2	9:I:269:MET:N	2.25	0.69
8:H:101:ARG:NH2	21:W:143:LEU:O	2.26	0.68
11:K:35:LEU:HD11	11:K:49:MET:SD	2.34	0.68
11:K:444:VAL:HA	11:K:454:VAL:HG13	1.76	0.68
22:X:99:ILE:HG23	22:X:100:GLN:OE1	1.93	0.68
9:I:569:TYR:N	9:I:593:GLU:OE2	2.26	0.68
11:K:248:VAL:HG11	11:K:254:ARG:HB2	1.73	0.68
17:R:770:MET:HA	17:R:773:GLU:HG2	1.74	0.68
18:S:306:THR:OG1	18:S:310:PHE:CE2	2.41	0.68
9:I:393:ASP:O	9:I:394:HIS:ND1	2.27	0.68
17:R:1302:LYS:HA	17:R:1306:THR:HG22	1.76	0.68
3:C:140:HIS:HA	12:L:170:SER:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:827:CYS:SG	11:K:830:VAL:CB	2.82	0.68
11:K:620:TRP:HZ3	11:K:751:GLN:OE1	1.77	0.68
12:L:311:LEU:HD13	12:L:331:ILE:HD13	1.75	0.68
3:C:114:VAL:O	5:E:111:THR:HA	1.94	0.67
3:C:189:PRO:N	3:C:189:PRO:CB	2.55	0.67
11:K:385:ALA:HA	11:K:391:VAL:HG23	1.75	0.67
17:R:458:LEU:HG	17:R:459:GLN:HG2	1.74	0.67
11:K:75:SER:O	11:K:76:ILE:HG13	1.95	0.67
3:C:141:PRO:N	12:L:170:SER:O	2.27	0.67
3:C:176:ARG:O	3:C:179:ALA:N	2.26	0.67
18:S:311:LEU:HD11	18:S:457:ALA:HA	1.77	0.67
9:I:880:ASN:OD1	9:I:884:LYS:NZ	2.28	0.67
11:K:29:HIS:ND1	18:S:907:LEU:CD1	2.58	0.67
17:R:1224:LEU:HD11	17:R:1263:ARG:HG3	1.75	0.67
3:C:140:HIS:H	3:C:143:LYS:HA	1.59	0.67
11:K:796:LYS:CA	11:K:812:ARG:NH2	2.56	0.67
3:C:130:PHE:HD2	16:Q:62:HIS:CB	2.02	0.67
11:K:751:GLN:NE2	11:K:788:GLY:O	2.26	0.67
11:K:743:GLN:O	11:K:746:GLN:NE2	2.27	0.67
19:T:209:PRO:CG	19:T:210:PRO:CD	2.72	0.67
3:C:141:PRO:CA	12:L:170:SER:O	2.43	0.67
3:C:148:HIS:C	12:L:230:LEU:HD23	2.14	0.66
3:C:191:LYS:CB	9:I:284:ALA:CB	2.72	0.66
11:K:48:THR:O	11:K:49:MET:HG2	1.95	0.66
3:C:181:LEU:O	3:C:183:ASP:N	2.27	0.66
9:I:442:ILE:HG12	9:I:500:LEU:HD21	1.78	0.66
11:K:614:LEU:HA	11:K:618:LEU:HB2	1.76	0.66
16:Q:103:GLN:O	16:Q:107:THR:HG23	1.96	0.66
19:T:192:ARG:HG3	19:T:193:LEU:HD12	1.78	0.66
18:S:306:THR:O	18:S:310:PHE:CD2	2.49	0.66
22:X:80:GLN:HB3	22:X:99:ILE:HD12	1.76	0.66
11:K:835:PRO:O	11:K:836:ASP:OD1	2.13	0.65
17:R:1275:TYR:HA	17:R:1278:LEU:HD12	1.78	0.65
20:V:198:LEU:HA	20:V:216:GLY:HA2	1.78	0.65
11:K:304:SER:O	11:K:305:ILE:HG13	1.95	0.65
3:C:171:ILE:CA	26:9:635:SER:CB	2.75	0.65
17:R:283:VAL:HA	17:R:286:MET:HG2	1.78	0.65
20:V:182:ARG:HG2	20:V:189:MET:H	1.62	0.65
17:R:482:SER:HA	17:R:487:CYS:HB2	1.79	0.65
20:V:290:ASP:HB3	20:V:300:ARG:HA	1.77	0.65
10:J:630:ARG:HH12	10:J:637:SER:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:740:GLY:H	18:S:743:TRP:HE1	1.44	0.65
11:K:29:HIS:ND1	18:S:907:LEU:HD11	2.11	0.65
11:K:76:ILE:HG22	11:K:77:PRO:CD	2.25	0.65
16:Q:61:MET:O	16:Q:66:ALA:N	2.30	0.65
19:T:164:CYS:SG	19:T:165:THR:N	2.69	0.65
17:R:549:LYS:HA	17:R:552:HIS:HD2	1.62	0.65
11:K:65:LEU:HD22	11:K:73:LEU:CD2	2.27	0.65
11:K:535:LYS:HE2	11:K:757:THR:HB	1.78	0.65
17:R:1103:HIS:O	17:R:1106:HIS:ND1	2.30	0.65
17:R:1112:LEU:HD13	17:R:1117:VAL:HG21	1.79	0.64
20:V:218:ASN:O	20:V:221:VAL:HG23	1.97	0.64
3:C:118:ARG:N	5:E:112:LYS:CB	2.59	0.64
11:K:94:SER:HB3	11:K:105:ILE:HG13	1.80	0.64
11:K:141:VAL:HG12	11:K:161:ARG:HB3	1.77	0.64
17:R:790:LEU:HD22	17:R:822:HIS:HB3	1.77	0.64
11:K:32:SER:O	11:K:33:VAL:HG23	1.96	0.64
17:R:1001:PRO:HA	17:R:1004:TYR:HB3	1.80	0.64
20:V:215:LYS:CB	20:V:220:ASN:CG	2.65	0.64
18:S:247:VAL:HG23	18:S:770:SER:HG	1.62	0.64
12:L:206:ASP:HA	12:L:222:PHE:HE2	1.62	0.64
9:I:504:ARG:HE	9:I:636:ALA:HB2	1.61	0.64
11:K:65:LEU:HD22	11:K:73:LEU:HD22	1.78	0.64
11:K:795:CYS:O	11:K:812:ARG:NH1	2.30	0.64
22:X:81:ASN:O	22:X:85:ASN:ND2	2.31	0.63
8:H:86:SER:O	8:H:90:CYS:N	2.31	0.63
11:K:77:PRO:HD2	11:K:77:PRO:O	1.99	0.63
17:R:1233:GLU:CD	17:R:1234:VAL:CG2	2.57	0.63
9:I:718:ARG:NH1	9:I:752:LEU:O	2.31	0.63
3:C:116:ASN:CB	16:Q:52:THR:CB	2.77	0.63
12:L:393:PRO:HB2	12:L:395:PRO:HD3	1.79	0.63
17:R:1219:SER:HB2	17:R:1223:GLN:HE21	1.64	0.63
11:K:180:ILE:HD11	11:K:193:LEU:HB2	1.81	0.63
17:R:158:GLN:HA	17:R:161:LEU:HD12	1.81	0.63
17:R:448:PRO:O	17:R:452:ARG:CG	2.46	0.63
17:R:869:LEU:HD11	17:R:886:ILE:HG12	1.82	0.62
17:R:1087:PHE:HB2	17:R:1088:PRO:HD3	1.81	0.62
10:J:739:ARG:O	10:J:743:TYR:HB2	1.98	0.62
11:K:827:CYS:N	11:K:830:VAL:CB	2.62	0.62
3:C:167:GLU:OE2	9:I:268:SER:HA	1.97	0.62
17:R:1238:ILE:O	17:R:1238:ILE:HG22	1.99	0.62
3:C:130:PHE:CE2	16:Q:62:HIS:C	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:376:PHE:H	11:K:473:HIS:HE1	1.48	0.62
11:K:193:LEU:O	11:K:201:THR:OG1	2.17	0.62
19:T:188:LEU:HD12	19:T:192:ARG:HD3	1.81	0.62
10:J:633:VAL:HB	11:K:812:ARG:NH1	2.15	0.61
10:J:677:VAL:HG23	10:J:678:LEU:HD12	1.82	0.61
10:J:736:TRP:HB3	10:J:739:ARG:HB2	1.82	0.61
17:R:609:SER:HB2	17:R:651:ARG:HD2	1.82	0.61
5:E:186:ALA:O	13:M:71:ARG:NH1	2.33	0.61
18:S:415:PRO:O	18:S:419:ASN:ND2	2.34	0.61
12:L:223:GLU:H	12:L:237:PRO:HD2	1.66	0.61
10:J:630:ARG:HH22	10:J:637:SER:H	1.47	0.61
17:R:520:ILE:O	17:R:520:ILE:CG2	2.47	0.61
3:C:142:SER:O	3:C:145:TYR:N	2.34	0.61
11:K:137:LEU:HD23	11:K:138:HIS:HD2	1.65	0.61
10:J:776:TRP:O	10:J:780:VAL:HG23	2.00	0.60
14:O:73:LEU:HA	14:O:87:ALA:HA	1.83	0.60
17:R:270:LEU:HA	17:R:273:VAL:HG12	1.83	0.60
17:R:682:GLU:HG3	17:R:867:LEU:HD23	1.81	0.60
17:R:173:ARG:O	17:R:177:LEU:N	2.31	0.60
18:S:737:HIS:O	18:S:834:LYS:NZ	2.34	0.60
1:A:364:TYR:HA	1:A:373:CYS:HA	1.84	0.60
17:R:1020:ALA:HA	17:R:1023:LYS:HB3	1.84	0.60
9:I:690:CYS:CB	9:I:771:ASN:OD1	2.49	0.60
18:S:72:MET:HB3	18:S:75:TYR:HD2	1.66	0.60
19:T:209:PRO:HD3	19:T:210:PRO:HD2	1.62	0.60
11:K:168:LEU:HD13	11:K:246:VAL:HG23	1.82	0.60
17:R:1016:LEU:O	17:R:1020:ALA:N	2.26	0.60
18:S:712:THR:O	18:S:717:LYS:NZ	2.35	0.60
3:C:140:HIS:N	3:C:144:GLY:H	2.00	0.60
3:C:175:GLN:O	3:C:177:VAL:N	2.35	0.60
18:S:733:ASP:OD1	18:S:830:THR:HG21	2.02	0.59
11:K:664:ILE:HD12	11:K:667:LEU:HD12	1.83	0.59
12:L:198:LYS:HE3	12:L:205:GLY:H	1.67	0.59
18:S:943:VAL:O	18:S:943:VAL:CG1	2.45	0.59
3:C:180:LEU:O	3:C:183:ASP:N	2.34	0.59
16:Q:130:LEU:HD11	23:Y:156:LEU:HD11	1.84	0.59
1:A:265:VAL:HG11	1:A:298:ASP:CB	2.32	0.59
9:I:386:VAL:HG12	9:I:386:VAL:O	2.02	0.59
9:I:916:LEU:O	9:I:924:ILE:N	2.34	0.59
17:R:975:LEU:HD21	17:R:1019:ARG:HG3	1.84	0.59
17:R:977:LEU:HG	17:R:979:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1149:ILE:O	17:R:1153:ILE:HG12	2.02	0.59
17:R:1256:LEU:HA	17:R:1259:PHE:HD2	1.68	0.59
8:H:82:SER:O	8:H:84:TYR:N	2.36	0.59
17:R:647:SER:HB2	17:R:651:ARG:HH21	1.68	0.59
12:L:197:ARG:HH21	16:Q:89:ASN:HA	1.68	0.59
9:I:344:VAL:O	9:I:344:VAL:CG1	2.50	0.59
18:S:782:VAL:O	18:S:786:HIS:ND1	2.33	0.59
3:C:148:HIS:CA	12:L:229:ASP:O	2.51	0.58
18:S:370:GLN:NE2	18:S:378:VAL:HG12	2.18	0.58
10:J:633:VAL:HG21	11:K:812:ARG:HD3	1.82	0.58
11:K:835:PRO:O	11:K:835:PRO:HD2	2.02	0.58
12:L:364:PRO:HD2	12:L:364:PRO:O	2.04	0.58
10:J:673:SER:OG	10:J:674:ILE:N	2.36	0.58
18:S:72:MET:SD	18:S:75:TYR:CE2	2.96	0.58
2:B:26:THR:N	6:F:107:ILE:O	2.37	0.58
12:L:572:ALA:HA	12:L:581:SER:HA	1.86	0.58
23:Y:164:ARG:HH21	23:Y:168:TRP:HE1	1.52	0.58
9:I:831:PHE:H	9:I:860:ASN:HD21	1.51	0.58
9:I:897:THR:HG23	9:I:899:THR:H	1.69	0.58
11:K:48:THR:O	11:K:49:MET:CG	2.51	0.58
11:K:305:ILE:HG12	11:K:346:ASN:HA	1.86	0.58
17:R:161:LEU:O	17:R:165:GLU:N	2.32	0.58
17:R:1276:ASP:O	17:R:1280:ASN:ND2	2.37	0.58
9:I:935:ALA:HA	9:I:1174:PRO:HA	1.86	0.58
17:R:1173:SER:O	17:R:1244:GLN:NE2	2.37	0.58
22:X:80:GLN:HB3	22:X:99:ILE:HD13	1.84	0.58
22:X:80:GLN:CB	22:X:99:ILE:HD13	2.34	0.58
17:R:123:ARG:O	17:R:123:ARG:NH2	2.37	0.57
17:R:770:MET:HG3	17:R:777:ILE:HD12	1.86	0.57
11:K:459:PRO:HB2	11:K:493:LEU:HD13	1.85	0.57
17:R:1233:GLU:OE1	17:R:1234:VAL:HG23	2.03	0.57
17:R:1302:LYS:NZ	17:R:1332:ILE:O	2.34	0.57
3:C:181:LEU:C	3:C:183:ASP:H	2.07	0.57
9:I:1343:PRO:HG2	9:I:1346:ALA:HB2	1.87	0.57
11:K:35:LEU:CD1	11:K:49:MET:SD	2.92	0.57
10:J:725:VAL:HG22	10:J:731:ALA:HB2	1.85	0.57
11:K:600:LYS:NZ	11:K:603:GLU:O	2.26	0.57
17:R:1203:MET:O	17:R:1206:SER:OG	2.22	0.57
10:J:767:HIS:H	10:J:771:ALA:HB3	1.70	0.57
17:R:1288:LEU:HD21	17:R:1294:ILE:HD11	1.87	0.57
18:S:946:PHE:HB3	18:S:948:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:991:LEU:HD23	17:R:994:LEU:HD22	1.87	0.57
11:K:102:ASP:OD1	11:K:102:ASP:N	2.37	0.57
17:R:123:ARG:HB2	17:R:166:VAL:HG12	1.87	0.57
17:R:718:THR:O	17:R:721:SER:OG	2.18	0.57
11:K:288:ARG:NH2	11:K:311:LEU:O	2.35	0.56
3:C:140:HIS:CB	3:C:145:TYR:H	2.18	0.56
17:R:592:VAL:HA	17:R:597:ALA:HB2	1.87	0.56
18:S:378:VAL:O	18:S:378:VAL:CG1	2.52	0.56
23:Y:51:ILE:HD13	23:Y:81:ASN:HD22	1.69	0.56
11:K:32:SER:O	11:K:33:VAL:CG2	2.53	0.56
17:R:1023:LYS:HD3	17:R:1026:LEU:HB2	1.87	0.56
18:S:277:PRO:HG2	18:S:280:LEU:HB2	1.86	0.56
20:V:51:ALA:O	20:V:55:HIS:CD2	2.58	0.56
23:Y:51:ILE:CD1	23:Y:81:ASN:HD22	2.18	0.56
12:L:477:VAL:HG13	12:L:492:GLN:HE21	1.71	0.56
13:M:142:LYS:NZ	13:M:143:ILE:O	2.35	0.56
11:K:212:ARG:HE	18:S:738:MET:HA	1.68	0.56
12:L:322:VAL:HG12	12:L:322:VAL:O	2.05	0.56
11:K:76:ILE:CG2	11:K:77:PRO:HD2	2.30	0.56
17:R:85:MET:HA	17:R:88:GLU:HG2	1.88	0.56
17:R:1075:LEU:O	17:R:1078:THR:OG1	2.22	0.56
17:R:1175:PRO:CD	17:R:1176:SER:N	2.69	0.56
17:R:1181:THR:HG23	17:R:1182:GLU:H	1.69	0.56
18:S:917:ALA:HA	18:S:920:HIS:CE1	2.40	0.56
10:J:682:VAL:HA	10:J:685:LEU:HD23	1.86	0.56
9:I:569:TYR:HA	9:I:593:GLU:CD	2.24	0.56
9:I:470:LEU:H	9:I:499:TRP:HZ2	1.54	0.56
11:K:132:VAL:HB	11:K:181:ALA:HB1	1.88	0.56
12:L:168:THR:O	12:L:172:THR:HG23	2.04	0.56
17:R:442:LYS:HG2	19:T:57:PHE:CZ	2.41	0.56
18:S:504:ALA:O	18:S:508:GLY:N	2.36	0.56
22:X:82:LEU:HA	22:X:85:ASN:HD21	1.70	0.56
2:B:89:ILE:HD13	6:F:115:GLN:HA	1.88	0.56
11:K:16:ALA:HB2	11:K:764:THR:HA	1.87	0.56
11:K:114:LEU:HD22	11:K:835:PRO:CD	2.35	0.56
11:K:789:ALA:O	11:K:790:CYS:SG	2.63	0.56
12:L:605:PRO:O	12:L:609:VAL:N	2.38	0.56
17:R:67:ILE:HD12	17:R:79:LEU:HD13	1.88	0.56
9:I:379:PRO:CD	9:I:380:ALA:H	2.18	0.55
11:K:468:GLY:O	11:K:472:ARG:HG3	2.06	0.55
12:L:31:LEU:N	12:L:32:PRO:CD	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:449:HIS:N	17:R:452:ARG:HE	2.04	0.55
18:S:366:GLU:HB3	18:S:382:MET:SD	2.45	0.55
21:W:137:ARG:HD3	21:W:140:GLN:HE21	1.71	0.55
18:S:224:SER:HA	18:S:227:THR:HG21	1.88	0.55
18:S:378:VAL:HG13	18:S:381:LEU:HD23	1.89	0.55
19:T:75:ASP:OD1	19:T:76:CYS:N	2.39	0.55
22:X:61:LYS:HA	22:X:64:ILE:HD12	1.88	0.55
13:M:58:PHE:HA	13:M:125:MET:HA	1.87	0.55
17:R:865:LEU:HD12	17:R:889:LEU:HD11	1.88	0.55
17:R:1088:PRO:HB2	17:R:1092:TRP:NE1	2.13	0.55
18:S:730:HIS:O	18:S:734:THR:HG23	2.06	0.55
11:K:305:ILE:HG23	11:K:345:THR:O	2.07	0.55
11:K:796:LYS:CB	11:K:812:ARG:CZ	2.85	0.55
12:L:540:LEU:O	21:W:89:ARG:NH2	2.37	0.55
13:M:131:ALA:HB2	13:M:148:ILE:HD13	1.88	0.55
3:C:142:SER:H	3:C:145:TYR:CB	2.20	0.55
12:L:530:SER:O	12:L:534:VAL:HG23	2.07	0.55
18:S:768:LEU:HA	18:S:771:ILE:HG22	1.88	0.55
8:H:92:MET:O	8:H:96:ARG:HG3	2.06	0.55
17:R:44:PHE:HE2	17:R:92:LEU:HD21	1.71	0.55
3:C:130:PHE:CE2	16:Q:62:HIS:HA	2.35	0.55
11:K:443:LEU:HB2	11:K:457:LEU:HD12	1.88	0.55
17:R:113:GLN:O	17:R:117:LEU:HG	2.08	0.54
17:R:1063:PRO:O	17:R:1066:THR:OG1	2.22	0.54
13:M:53:ASP:HA	13:M:75:SER:HA	1.88	0.54
16:Q:123:ILE:HG21	23:Y:167:ILE:CA	2.32	0.54
17:R:624:LEU:HD12	17:R:652:LEU:HD11	1.88	0.54
20:V:216:GLY:O	20:V:219:GLU:HG3	2.08	0.54
23:Y:160:MET:O	23:Y:164:ARG:HG2	2.08	0.54
11:K:383:ALA:CB	11:K:393:ILE:HG23	2.37	0.54
17:R:984:LEU:HD11	17:R:1026:LEU:HD22	1.90	0.54
9:I:692:GLY:O	9:I:694:THR:HG23	2.08	0.54
9:I:722:ALA:HB3	9:I:747:LEU:HB2	1.90	0.54
11:K:16:ALA:HB1	11:K:765:LEU:H	1.71	0.54
17:R:1023:LYS:HA	17:R:1026:LEU:HB2	1.90	0.54
17:R:635:GLN:OE1	17:R:817:ARG:NH2	2.41	0.53
9:I:776:LEU:HD21	9:I:803:TYR:HE1	1.73	0.53
12:L:331:ILE:N	12:L:342:SER:OG	2.37	0.53
17:R:847:ILE:HA	17:R:851:ASN:HD21	1.74	0.53
18:S:293:LEU:HB3	18:S:305:TRP:HB3	1.90	0.53
18:S:757:ARG:HD2	18:S:760:HIS:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:56:HIS:CE1	17:R:60:ILE:CG1	2.92	0.53
17:R:91:LEU:HG	17:R:92:LEU:HD12	1.91	0.53
9:I:895:GLN:HG2	9:I:1296:ALA:H	1.73	0.53
9:I:312:THR:O	9:I:316:ILE:HG12	2.09	0.53
11:K:391:VAL:HG11	11:K:457:LEU:CD1	2.39	0.53
18:S:95:GLN:O	18:S:98:LEU:HG	2.09	0.53
18:S:216:GLU:O	18:S:220:THR:HG23	2.09	0.53
22:X:60:TYR:CZ	22:X:64:ILE:HD11	2.44	0.53
9:I:379:PRO:CD	9:I:380:ALA:N	2.68	0.52
11:K:736:ASP:O	11:K:740:SER:OG	2.22	0.52
11:K:796:LYS:CB	11:K:812:ARG:NH2	2.72	0.52
18:S:310:PHE:HE1	18:S:365:GLN:HB2	1.74	0.52
9:I:592:LYS:O	9:I:595:ILE:N	2.38	0.52
11:K:63:HIS:HA	11:K:75:SER:HA	1.91	0.52
11:K:134:LEU:HB3	11:K:219:ALA:HB2	1.91	0.52
11:K:244:VAL:HB	11:K:255:ILE:HG23	1.92	0.52
17:R:1175:PRO:CD	17:R:1176:SER:H	2.22	0.52
11:K:349:ASP:C	11:K:387:HIS:NE2	2.61	0.52
11:K:659:MET:HA	11:K:662:ILE:HG12	1.92	0.52
9:I:402:ILE:HG21	12:L:327:VAL:HG12	1.92	0.52
11:K:284:LYS:NZ	11:K:286:LEU:O	2.42	0.52
17:R:244:ASP:OD1	17:R:244:ASP:N	2.43	0.52
20:V:269:TRP:HE3	20:V:270:LEU:HD22	1.75	0.52
11:K:19:CYS:SG	11:K:769:GLY:N	2.82	0.52
17:R:449:HIS:HA	17:R:452:ARG:CD	2.39	0.52
21:W:92:GLU:O	21:W:96:LEU:HG	2.10	0.52
3:C:163:LYS:O	3:C:164:ARG:HG3	2.10	0.52
11:K:313:LYS:HG3	11:K:337:LEU:HD13	1.92	0.52
11:K:478:LEU:HD22	11:K:507:LEU:HD11	1.91	0.52
18:S:310:PHE:HE1	18:S:365:GLN:CB	2.23	0.52
9:I:573:VAL:HA	9:I:585:ALA:HB3	1.91	0.52
17:R:14:LYS:HA	17:R:75:ARG:HH22	1.75	0.52
17:R:449:HIS:CA	17:R:452:ARG:NE	2.72	0.52
18:S:370:GLN:NE2	18:S:382:MET:HG2	2.15	0.52
22:X:156:PRO:HB2	22:X:158:PRO:HD2	1.91	0.52
3:C:113:SER:HA	16:Q:52:THR:CB	2.39	0.52
11:K:692:LEU:O	11:K:696:LEU:HG	2.10	0.52
17:R:757:LYS:O	17:R:761:GLU:HG2	2.09	0.52
17:R:824:ARG:HA	17:R:868:CYS:SG	2.49	0.52
9:I:855:LEU:O	9:I:858:MET:HG3	2.10	0.51
11:K:38:ALA:HB3	11:K:87:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:104:GLN:HB2	11:K:122:VAL:HA	1.91	0.51
11:K:114:LEU:HD22	11:K:835:PRO:HD2	1.92	0.51
22:X:101:ARG:HG3	22:X:103:ASP:HB3	1.92	0.51
1:A:511:ILE:HA	1:A:515:ALA:HB3	1.93	0.51
3:C:166:GLU:O	3:C:167:GLU:HG3	2.10	0.51
11:K:218:ILE:HD12	11:K:283:LEU:HB3	1.91	0.51
12:L:168:THR:C	12:L:172:THR:HG23	2.31	0.51
17:R:1049:LEU:HG	17:R:1053:MET:HE3	1.91	0.51
11:K:48:THR:O	11:K:49:MET:SD	2.69	0.51
17:R:1215:VAL:O	17:R:1219:SER:OG	2.17	0.51
17:R:1236:LEU:HB2	17:R:1237:PRO:HD3	1.91	0.51
11:K:229:ALA:HB1	11:K:239:VAL:HB	1.93	0.51
17:R:565:GLU:O	17:R:568:SER:OG	2.27	0.51
1:A:265:VAL:CG1	1:A:298:ASP:CB	2.89	0.51
11:K:656:ARG:O	11:K:660:VAL:HG13	2.11	0.51
9:I:1241:MET:HA	9:I:1246:ALA:HB3	1.92	0.51
18:S:247:VAL:CG2	18:S:770:SER:OG	2.50	0.51
18:S:370:GLN:NE2	18:S:382:MET:CG	2.72	0.51
22:X:99:ILE:CG2	22:X:100:GLN:OE1	2.59	0.51
10:J:635:ASN:HD21	10:J:638:LEU:HD12	1.76	0.51
11:K:396:ARG:HG3	11:K:397:LEU:HG	1.92	0.51
17:R:591:THR:HA	17:R:594:LYS:HB3	1.92	0.51
3:C:82:ARG:O	3:C:84:GLN:N	2.44	0.50
11:K:455:LEU:HD12	11:K:456:ARG:H	1.75	0.50
11:K:570:ASN:HD21	11:K:577:GLY:HA3	1.75	0.50
11:K:697:TRP:CE2	11:K:701:ARG:HD2	2.46	0.50
23:Y:75:LEU:HA	23:Y:78:LEU:HD12	1.92	0.50
9:I:724:LEU:O	9:I:745:VAL:N	2.43	0.50
17:R:999:ASP:N	17:R:999:ASP:OD1	2.45	0.50
22:X:64:ILE:O	22:X:67:LEU:HG	2.12	0.50
11:K:76:ILE:CG2	11:K:77:PRO:HD3	2.27	0.50
11:K:132:VAL:HG21	11:K:182:VAL:HB	1.93	0.50
11:K:248:VAL:HG21	11:K:254:ARG:HG2	1.94	0.50
3:C:81:ILE:CB	3:C:98:TYR:H	2.24	0.50
3:C:130:PHE:HE2	16:Q:62:HIS:C	2.11	0.50
9:I:402:ILE:HD13	12:L:327:VAL:HG11	1.93	0.50
9:I:589:GLN:CB	9:I:593:GLU:OE1	2.59	0.50
11:K:553:LEU:HD13	11:K:624:PHE:CE1	2.47	0.50
17:R:118:THR:O	17:R:121:LEU:HG	2.11	0.50
11:K:507:LEU:HD21	11:K:526:ILE:HD11	1.93	0.50
17:R:374:TRP:O	17:R:378:GLN:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1247:TYR:O	17:R:1251:LEU:HG	2.12	0.50
11:K:16:ALA:HA	11:K:766:GLN:HG2	1.93	0.50
16:Q:62:HIS:HA	16:Q:66:ALA:HB3	1.94	0.50
1:A:226:VAL:O	1:A:226:VAL:CG1	2.55	0.50
9:I:592:LYS:HA	17:R:25:MET:H	1.77	0.50
9:I:433:THR:HA	9:I:438:LEU:HA	1.93	0.49
17:R:1024:ARG:HG3	17:R:1114:ALA:HB1	1.93	0.49
3:C:175:GLN:C	3:C:177:VAL:N	2.64	0.49
20:V:178:ILE:HG22	20:V:192:VAL:HG23	1.93	0.49
22:X:89:ASP:OD1	22:X:90:ASN:N	2.44	0.49
1:A:221:ASN:O	1:A:222:LEU:HG	2.13	0.49
11:K:383:ALA:HB1	11:K:393:ILE:CG1	2.42	0.49
17:R:1198:GLN:HG3	17:R:1200:TYR:H	1.77	0.49
18:S:385:ARG:NH1	18:S:385:ARG:O	2.45	0.49
22:X:80:GLN:CB	22:X:99:ILE:CD1	2.84	0.49
8:H:85:SER:O	8:H:87:ARG:N	2.44	0.49
12:L:259:VAL:HB	12:L:367:HIS:CD2	2.47	0.49
17:R:988:LEU:HD21	17:R:1029:ALA:HB1	1.94	0.49
18:S:783:LEU:O	18:S:787:ILE:HG12	2.12	0.49
18:S:814:VAL:HG21	18:S:931:CYS:HA	1.94	0.49
3:C:181:LEU:C	3:C:183:ASP:N	2.66	0.49
9:I:387:GLU:HB2	9:I:391:LYS:HA	1.94	0.49
14:O:127:GLY:N	14:O:137:GLY:O	2.45	0.49
17:R:808:TYR:OH	17:R:933:TYR:O	2.30	0.49
18:S:490:ALA:HB1	18:S:574:TRP:HE1	1.77	0.49
3:C:197:PRO:HD2	3:C:197:PRO:O	2.12	0.49
9:I:291:ASP:HA	9:I:294:ASN:ND2	2.27	0.49
9:I:372:ILE:HD12	9:I:387:GLU:OE2	2.13	0.49
9:I:831:PHE:O	9:I:856:GLN:NE2	2.45	0.49
17:R:731:THR:HB	17:R:973:ARG:HH22	1.77	0.49
18:S:74:SER:HA	18:S:120:LEU:HD12	1.95	0.49
1:A:265:VAL:HG12	1:A:265:VAL:O	2.13	0.49
9:I:310:SER:O	9:I:314:MET:HG2	2.13	0.49
17:R:622:GLN:O	17:R:626:HIS:ND1	2.31	0.49
17:R:755:ASN:HA	17:R:758:LYS:HD3	1.94	0.49
20:V:70:LEU:O	22:X:61:LYS:NZ	2.33	0.49
3:C:175:GLN:O	3:C:176:ARG:C	2.50	0.48
10:J:637:SER:O	10:J:641:THR:HG23	2.13	0.48
17:R:1028:HIS:HA	17:R:1031:ILE:HG12	1.94	0.48
18:S:78:VAL:HG12	18:S:123:ALA:HB2	1.95	0.48
3:C:139:TYR:HA	3:C:144:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:LEU:C	3:C:197:PRO:HD3	2.33	0.48
9:I:478:MET:O	9:I:482:VAL:HG23	2.13	0.48
11:K:750:LEU:HB3	11:K:752:PHE:CE2	2.48	0.48
12:L:569:ILE:O	12:L:584:ASN:N	2.44	0.48
18:S:264:VAL:O	18:S:268:THR:HG23	2.13	0.48
19:T:127:ASP:OD1	19:T:128:PHE:N	2.47	0.48
10:J:717:SER:OG	10:J:718:VAL:N	2.46	0.48
12:L:374:ASN:HA	12:L:377:LEU:HD12	1.94	0.48
17:R:496:VAL:HG23	17:R:523:LEU:HD21	1.94	0.48
18:S:65:LYS:HA	18:S:68:ILE:HG12	1.94	0.48
18:S:699:ASN:ND2	18:S:701:LEU:H	2.10	0.48
10:J:674:ILE:HD11	10:J:679:GLN:HB3	1.95	0.48
10:J:625:VAL:O	10:J:629:ILE:HG12	2.14	0.48
11:K:685:SER:O	11:K:689:LEU:HG	2.14	0.48
17:R:149:PRO:HG2	17:R:152:VAL:HB	1.94	0.48
17:R:653:ILE:HD12	17:R:656:LEU:HD21	1.96	0.48
10:J:645:ALA:O	10:J:649:ILE:HG22	2.13	0.48
10:J:722:GLU:HA	10:J:733:SER:HB3	1.94	0.48
11:K:129:ASP:N	11:K:185:SER:OG	2.46	0.48
11:K:160:SER:OG	11:K:161:ARG:N	2.47	0.48
17:R:1130:VAL:HG12	17:R:1207:TYR:HB3	1.96	0.48
17:R:1238:ILE:O	17:R:1238:ILE:CG2	2.61	0.48
17:R:1248:VAL:O	17:R:1252:VAL:HG22	2.13	0.48
9:I:534:SER:OG	9:I:552:VAL:HB	2.13	0.48
17:R:117:LEU:HA	17:R:120:LYS:HD2	1.95	0.48
17:R:636:THR:H	17:R:817:ARG:HH22	1.60	0.48
11:K:288:ARG:HA	11:K:311:LEU:HD12	1.96	0.48
11:K:310:SER:HB3	11:K:342:LEU:HD11	1.94	0.48
12:L:201:ASP:OD1	12:L:202:LYS:N	2.42	0.48
12:L:308:PHE:HA	12:L:311:LEU:HG	1.95	0.48
17:R:180:ALA:O	17:R:184:VAL:HG23	2.13	0.48
11:K:219:ALA:HA	11:K:226:ILE:HG23	1.96	0.48
17:R:641:LEU:HD23	17:R:641:LEU:H	1.79	0.48
9:I:570:PHE:O	9:I:587:LEU:HB2	2.13	0.47
9:I:701:LEU:O	9:I:705:LEU:N	2.47	0.47
9:I:859:PHE:HE1	9:I:865:VAL:HG12	1.79	0.47
14:O:158:LEU:O	14:O:162:GLN:HG2	2.13	0.47
16:Q:97:ALA:O	16:Q:101:ARG:NE	2.46	0.47
18:S:757:ARG:HD2	18:S:760:HIS:CD2	2.49	0.47
1:A:372:HIS:HA	1:A:437:LEU:H	1.78	0.47
11:K:210:ARG:CZ	11:K:211:GLY:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:LEU:H	12:L:32:PRO:HD3	1.78	0.47
17:R:340:PHE:CZ	17:R:572:VAL:HB	2.50	0.47
11:K:237:SER:N	11:K:238:PRO:HD3	2.28	0.47
12:L:327:VAL:HG23	12:L:328:LYS:H	1.78	0.47
17:R:764:TYR:O	17:R:768:LYS:HG2	2.14	0.47
18:S:161:CYS:O	18:S:165:LEU:HG	2.15	0.47
3:C:21:ILE:HA	3:C:32:TYR:CB	2.44	0.47
9:I:442:ILE:HD11	9:I:497:LYS:HD3	1.97	0.47
11:K:206:LEU:HD12	11:K:208:ARG:H	1.80	0.47
13:M:53:ASP:OD1	13:M:53:ASP:N	2.43	0.47
17:R:1145:TRP:O	17:R:1149:ILE:HG13	2.14	0.47
23:Y:168:TRP:O	23:Y:170:ILE:N	2.48	0.47
9:I:409:ALA:HB1	9:I:456:VAL:HG11	1.97	0.47
12:L:371:LEU:HA	12:L:374:ASN:HD21	1.80	0.47
12:L:384:LYS:HG3	12:L:385:GLN:HG2	1.95	0.47
17:R:616:GLN:HE22	17:R:618:HIS:HB3	1.79	0.47
17:R:969:ILE:O	17:R:973:ARG:HB3	2.15	0.47
20:V:280:PRO:HG2	20:V:299:PHE:HA	1.97	0.47
17:R:63:ILE:O	17:R:67:ILE:HG12	2.15	0.47
17:R:184:VAL:HG22	17:R:208:PHE:HE2	1.79	0.47
17:R:1035:LYS:O	17:R:1038:ARG:NH2	2.47	0.47
3:C:130:PHE:CE2	16:Q:62:HIS:O	2.64	0.47
3:C:184:LEU:C	3:C:186:GLN:N	2.66	0.47
8:H:31:VAL:CG1	8:H:48:GLN:CA	2.69	0.47
11:K:75:SER:C	11:K:76:ILE:HG13	2.34	0.47
17:R:136:ASP:O	17:R:140:VAL:HG23	2.15	0.47
17:R:184:VAL:HG22	17:R:208:PHE:CE2	2.49	0.47
17:R:618:HIS:O	17:R:622:GLN:HG2	2.14	0.47
17:R:1229:LYS:O	17:R:1233:GLU:HG3	2.15	0.47
9:I:831:PHE:N	9:I:860:ASN:HD21	2.13	0.47
17:R:311:ALA:HB1	17:R:331:TRP:CD1	2.50	0.47
17:R:1224:LEU:HD13	17:R:1259:PHE:CE1	2.49	0.47
3:C:121:THR:CB	5:E:114:ASP:CB	2.93	0.47
11:K:155:PHE:HE1	11:K:479:GLU:HB3	1.79	0.47
11:K:304:SER:C	11:K:305:ILE:HG13	2.35	0.47
18:S:42:LEU:HD12	18:S:43:ALA:N	2.30	0.47
17:R:329:LEU:O	17:R:333:HIS:ND1	2.32	0.47
17:R:804:ASN:O	17:R:805:GLN:HG3	2.15	0.47
18:S:835:ARG:HD3	18:S:835:ARG:O	2.15	0.47
1:A:258:THR:H	1:A:305:LEU:HA	1.80	0.46
9:I:655:VAL:HG23	9:I:658:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:661:VAL:O	11:K:664:ILE:HG22	2.15	0.46
17:R:1024:ARG:HD3	17:R:1025:LYS:HE2	1.98	0.46
23:Y:70:THR:O	23:Y:74:ARG:HG2	2.15	0.46
11:K:787:LEU:HD23	11:K:787:LEU:H	1.79	0.46
17:R:528:LEU:HA	17:R:532:THR:HB	1.98	0.46
18:S:541:ASN:O	18:S:545:PRO:HD2	2.15	0.46
3:C:139:TYR:HA	3:C:144:GLY:H	1.81	0.46
17:R:1158:GLU:O	17:R:1162:ILE:HG12	2.16	0.46
23:Y:45:VAL:O	23:Y:48:THR:OG1	2.29	0.46
10:J:743:TYR:CE1	10:J:753:HIS:HB2	2.51	0.46
11:K:206:LEU:HB2	11:K:209:LEU:HD23	1.97	0.46
17:R:56:HIS:ND1	17:R:60:ILE:CG1	2.70	0.46
17:R:300:LEU:HD23	17:R:304:LEU:HD23	1.97	0.46
17:R:1016:LEU:HD11	17:R:1019:ARG:CZ	2.45	0.46
18:S:282:VAL:HA	18:S:285:ILE:HG22	1.97	0.46
18:S:287:LYS:O	18:S:291:VAL:HG13	2.15	0.46
3:C:118:ARG:N	5:E:111:THR:O	2.30	0.46
11:K:685:SER:O	11:K:688:LEU:HG	2.16	0.46
17:R:923:ASN:O	17:R:927:LYS:HG2	2.16	0.46
17:R:1130:VAL:HG11	17:R:1211:LEU:HD23	1.97	0.46
17:R:1273:ALA:O	17:R:1277:MET:HG2	2.16	0.46
19:T:94:PHE:O	19:T:98:LEU:HG	2.16	0.46
9:I:595:ILE:O	9:I:599:VAL:HG23	2.16	0.46
11:K:563:LEU:HD22	11:K:822:ARG:HD2	1.96	0.46
18:S:141:ARG:HA	18:S:141:ARG:HD3	1.65	0.46
9:I:425:ALA:HA	9:I:430:SER:HA	1.68	0.46
18:S:980:GLN:O	18:S:984:LYS:HG2	2.15	0.46
3:C:168:PRO:HD2	3:C:169:SER:N	2.31	0.46
9:I:490:ILE:N	9:I:491:PRO:HD2	2.31	0.46
16:Q:123:ILE:HD13	23:Y:167:ILE:HA	1.97	0.46
17:R:1002:VAL:O	17:R:1006:TYR:HB2	2.16	0.46
18:S:95:GLN:NE2	18:S:99:ASP:OD2	2.48	0.46
11:K:391:VAL:CG1	11:K:457:LEU:HD13	2.46	0.46
16:Q:117:ILE:HD12	16:Q:120:ARG:HH21	1.80	0.46
17:R:1308:ASP:HB2	17:R:1311:LYS:HD2	1.96	0.46
22:X:142:PRO:HG3	22:X:156:PRO:HA	1.98	0.46
11:K:99:ALA:HA	11:K:129:ASP:HA	1.97	0.46
11:K:211:GLY:HA2	11:K:240:GLN:HE22	1.81	0.46
12:L:436:LYS:HE3	12:L:471:TYR:O	2.16	0.46
16:Q:98:ILE:HA	16:Q:101:ARG:HH11	1.80	0.46
17:R:1107:VAL:O	17:R:1111:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1208:THR:O	17:R:1211:LEU:HG	2.16	0.46
19:T:71:PHE:CZ	19:T:82:VAL:HG23	2.51	0.46
3:C:180:LEU:O	3:C:181:LEU:C	2.52	0.45
12:L:190:LEU:HD12	12:L:291:TRP:HD1	1.80	0.45
12:L:301:VAL:HA	12:L:304:CYS:SG	2.55	0.45
17:R:677:SER:HA	17:R:684:ASN:HD21	1.81	0.45
17:R:1296:ASP:HA	17:R:1299:TYR:HB2	1.98	0.45
12:L:398:ALA:N	12:L:399:PRO:HD3	2.31	0.45
17:R:810:VAL:HA	17:R:813:ARG:HH21	1.81	0.45
17:R:1193:PHE:O	17:R:1194:THR:OG1	2.31	0.45
3:C:194:GLN:O	3:C:195:LEU:HG	2.16	0.45
8:H:84:TYR:CZ	13:M:45:ASN:HA	2.52	0.45
9:I:379:PRO:CG	9:I:411:GLN:CB	2.83	0.45
17:R:229:PRO:HG3	17:R:1218:HIS:NE2	2.32	0.45
18:S:186:ALA:O	18:S:190:THR:HG23	2.15	0.45
3:C:81:ILE:O	3:C:97:ASP:HA	2.16	0.45
10:J:667:GLU:O	10:J:668:ASP:OD1	2.35	0.45
10:J:756:MET:O	10:J:760:LEU:HG	2.16	0.45
12:L:466:ASN:HD22	16:Q:124:SER:HB2	1.81	0.45
12:L:551:PHE:HE1	12:L:572:ALA:HB3	1.80	0.45
17:R:98:CYS:O	17:R:102:ILE:HB	2.17	0.45
18:S:74:SER:O	18:S:78:VAL:HG13	2.16	0.45
9:I:647:MET:HA	9:I:650:THR:HG22	1.98	0.45
11:K:29:HIS:ND1	18:S:907:LEU:HD13	2.29	0.45
11:K:580:LEU:O	11:K:583:ILE:HG12	2.16	0.45
12:L:259:VAL:O	12:L:367:HIS:NE2	2.50	0.45
16:Q:123:ILE:HG22	23:Y:167:ILE:CB	2.37	0.45
17:R:904:VAL:HG23	17:R:993:GLY:HA3	1.98	0.45
18:S:110:CYS:SG	18:S:111:HIS:N	2.90	0.45
23:Y:68:THR:HA	23:Y:71:TYR:HE1	1.82	0.45
9:I:291:ASP:OD1	9:I:292:MET:N	2.49	0.45
9:I:402:ILE:HA	9:I:405:VAL:HG22	1.98	0.45
11:K:491:ILE:HA	11:K:494:HIS:CD2	2.52	0.45
17:R:716:LEU:O	17:R:720:MET:HG2	2.17	0.45
18:S:130:TRP:HA	18:S:133:ARG:HE	1.82	0.45
20:V:31:VAL:HG22	20:V:55:HIS:HB3	1.99	0.45
2:B:71:HIS:O	2:B:75:GLU:HG3	2.17	0.45
9:I:683:ARG:HH12	10:J:684:ARG:NH1	2.15	0.45
14:O:114:GLY:O	14:O:125:LYS:NZ	2.38	0.45
18:S:984:LYS:HA	18:S:984:LYS:HD3	1.84	0.45
19:T:209:PRO:CG	19:T:210:PRO:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:865:VAL:O	9:I:869:LEU:HG	2.17	0.45
9:I:922:TYR:HB3	9:I:957:PRO:HG3	1.98	0.45
11:K:835:PRO:O	11:K:835:PRO:CD	2.65	0.45
17:R:663:PRO:HB2	17:R:664:GLN:HE21	1.81	0.45
17:R:985:GLU:O	17:R:988:LEU:HG	2.17	0.45
17:R:1198:GLN:NE2	17:R:1201:SER:OG	2.35	0.45
1:A:265:VAL:HG13	1:A:298:ASP:C	2.38	0.45
3:C:141:PRO:N	12:L:170:SER:CB	2.80	0.45
9:I:291:ASP:HA	9:I:294:ASN:HD21	1.81	0.45
11:K:795:CYS:O	11:K:812:ARG:NH2	2.49	0.45
18:S:246:ALA:O	18:S:249:LEU:HG	2.16	0.45
3:C:184:LEU:C	3:C:186:GLN:H	2.20	0.45
9:I:693:ILE:O	9:I:697:THR:OG1	2.35	0.45
10:J:620:PRO:HG2	20:V:56:PHE:HE1	1.81	0.45
11:K:65:LEU:CD2	11:K:73:LEU:HD22	2.44	0.44
11:K:383:ALA:CB	11:K:393:ILE:CG2	2.96	0.44
17:R:560:ALA:N	17:R:561:PRO:HD2	2.32	0.44
17:R:962:ARG:O	17:R:966:VAL:HG23	2.17	0.44
17:R:1031:ILE:O	17:R:1035:LYS:HG3	2.17	0.44
12:L:209:TYR:O	12:L:213:GLY:N	2.51	0.44
18:S:245:HIS:NE2	18:S:291:VAL:HG21	2.32	0.44
22:X:78:ALA:HB2	22:X:102:PHE:CE1	2.52	0.44
9:I:504:ARG:HG2	9:I:638:ASN:HD21	1.83	0.44
11:K:276:LYS:O	11:K:296:LEU:N	2.31	0.44
19:T:16:ALA:HB1	19:T:47:PHE:HE1	1.82	0.44
9:I:490:ILE:HG13	9:I:491:PRO:HD3	2.00	0.44
11:K:246:VAL:HG12	11:K:255:ILE:HG13	1.99	0.44
17:R:183:ALA:O	17:R:187:ILE:HG12	2.18	0.44
17:R:258:TYR:CE1	17:R:262:LEU:HD22	2.52	0.44
17:R:1149:ILE:HA	17:R:1152:ILE:HD12	1.99	0.44
3:C:114:VAL:HA	5:E:111:THR:HA	2.00	0.44
11:K:77:PRO:CD	11:K:77:PRO:O	2.64	0.44
12:L:32:PRO:HD2	12:L:32:PRO:O	2.18	0.44
12:L:496:ASN:HA	12:L:502:ILE:HG12	1.99	0.44
17:R:846:CYS:HA	17:R:850:LEU:HB2	1.99	0.44
18:S:674:CYS:O	18:S:679:GLN:NE2	2.50	0.44
18:S:901:LEU:O	18:S:904:LEU:HG	2.17	0.44
8:H:31:VAL:HG11	8:H:48:GLN:N	2.28	0.44
8:H:100:ALA:O	8:H:104:LEU:HG	2.18	0.44
9:I:1254:SER:N	9:I:1255:PRO:HD2	2.33	0.44
11:K:188:VAL:HG23	11:K:189:THR:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:648:THR:O	17:R:651:ARG:HG2	2.17	0.44
17:R:773:GLU:HB2	17:R:776:ILE:HB	2.00	0.44
17:R:1241:THR:OG1	17:R:1242:GLU:N	2.50	0.44
22:X:99:ILE:CG2	22:X:100:GLN:N	2.48	0.44
3:C:170:SER:C	26:9:635:SER:CB	2.86	0.44
11:K:672:CYS:O	11:K:674:PRO:HD3	2.18	0.44
17:R:540:ILE:HG13	17:R:541:HIS:H	1.83	0.44
9:I:643:HIS:CE1	12:L:558:GLY:HA2	2.53	0.44
11:K:37:CYS:HB2	11:K:46:ALA:HB3	1.99	0.44
17:R:785:SER:HB2	17:R:788:LEU:HB3	1.99	0.44
17:R:856:LYS:HA	17:R:857:TYR:HA	1.60	0.44
17:R:941:VAL:HG22	17:R:943:PRO:HD3	2.00	0.44
17:R:1234:VAL:O	17:R:1238:ILE:HD12	2.18	0.44
17:R:1276:ASP:O	17:R:1279:LEU:HG	2.18	0.44
18:S:788:LEU:HB2	18:S:789:PRO:HD3	2.00	0.44
3:C:176:ARG:O	3:C:179:ALA:HB3	2.18	0.44
9:I:402:ILE:HG13	9:I:403:ASP:N	2.33	0.44
9:I:652:MET:HA	9:I:655:VAL:HG12	2.00	0.44
9:I:877:ALA:HB3	9:I:878:PRO:HD3	2.00	0.44
10:J:623:ASP:OD1	10:J:623:ASP:N	2.50	0.44
11:K:193:LEU:HG	11:K:195:PRO:HD3	2.00	0.44
17:R:257:PRO:HD2	17:R:263:PHE:HZ	1.83	0.44
18:S:221:LEU:O	18:S:225:ILE:HG12	2.18	0.44
18:S:305:TRP:O	18:S:309:THR:HG23	2.18	0.44
11:K:391:VAL:HG22	11:K:393:ILE:HG13	2.00	0.43
17:R:102:ILE:HG13	17:R:140:VAL:HG11	2.00	0.43
17:R:738:PRO:HB2	17:R:741:ALA:HB2	1.98	0.43
17:R:745:GLN:CD	17:R:745:GLN:H	2.21	0.43
17:R:803:ILE:HG13	17:R:804:ASN:H	1.82	0.43
18:S:416:THR:HA	18:S:419:ASN:HD21	1.83	0.43
14:O:38:THR:HA	14:O:115:THR:HA	2.00	0.43
17:R:118:THR:O	17:R:122:VAL:HG23	2.18	0.43
9:I:302:SER:O	9:I:305:LEU:HG	2.18	0.43
9:I:683:ARG:HA	9:I:709:THR:HA	2.00	0.43
9:I:1351:PRO:HA	9:I:1352:PRO:HD3	1.89	0.43
10:J:626:LEU:HD23	22:X:79:ALA:HB1	1.99	0.43
11:K:187:LEU:HD12	11:K:188:VAL:HG13	2.00	0.43
17:R:66:PHE:O	17:R:70:GLN:NE2	2.46	0.43
18:S:362:PHE:O	18:S:365:GLN:HG3	2.17	0.43
9:I:489:ILE:HG13	9:I:490:ILE:N	2.34	0.43
9:I:668:HIS:H	9:I:668:HIS:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:673:VAL:O	9:I:674:GLU:HG2	2.18	0.43
10:J:643:VAL:HG22	10:J:644:PRO:HD3	2.01	0.43
11:K:32:SER:C	11:K:33:VAL:HG23	2.37	0.43
11:K:231:ALA:HB3	11:K:238:PRO:HG2	2.00	0.43
18:S:768:LEU:HD22	18:S:812:LEU:HD11	1.99	0.43
20:V:111:TYR:CE2	22:X:136:HIS:HB2	2.52	0.43
3:C:74:GLN:CB	3:C:79:PHE:HA	2.49	0.43
9:I:682:ILE:O	9:I:710:PHE:N	2.46	0.43
11:K:765:LEU:HD12	11:K:765:LEU:HA	1.89	0.43
17:R:490:LEU:HB3	17:R:491:PRO:HD3	2.00	0.43
17:R:1233:GLU:OE1	17:R:1234:VAL:CG2	2.63	0.43
20:V:111:TYR:HE2	22:X:136:HIS:HB2	1.83	0.43
11:K:192:LEU:HD13	11:K:202:SER:HA	1.99	0.43
11:K:569:LEU:HD11	19:T:31:TYR:HE2	1.84	0.43
17:R:866:ILE:HG12	17:R:966:VAL:HG22	2.00	0.43
11:K:74:HIS:CD2	11:K:114:LEU:HD23	2.53	0.43
11:K:530:LYS:O	11:K:533:LEU:HG	2.19	0.43
11:K:550:LYS:O	11:K:553:LEU:HG	2.19	0.43
17:R:540:ILE:HG13	17:R:541:HIS:N	2.34	0.43
20:V:120:HIS:CE1	21:W:59:LEU:HD11	2.53	0.43
21:W:57:ALA:O	21:W:61:SER:OG	2.35	0.43
2:B:45:ILE:CB	6:F:72:ILE:CG2	2.97	0.43
8:H:84:TYR:HB3	8:H:85:SER:H	1.51	0.43
12:L:341:LEU:HD23	12:L:341:LEU:HA	1.90	0.43
17:R:260:LYS:HA	17:R:263:PHE:HD2	1.82	0.43
17:R:348:SER:O	17:R:348:SER:OG	2.37	0.43
17:R:1184:VAL:HG13	18:S:340:PHE:HB3	2.00	0.43
17:R:1255:PHE:HA	17:R:1257:GLN:HE22	1.83	0.43
18:S:734:THR:HA	18:S:737:HIS:ND1	2.33	0.43
20:V:194:LEU:HD23	20:V:194:LEU:HA	1.93	0.43
3:C:121:THR:CB	5:E:112:LYS:O	2.67	0.43
12:L:417:GLU:O	12:L:421:LEU:HG	2.19	0.43
14:O:161:LEU:CB	14:O:169:THR:HG21	2.49	0.43
17:R:1150:GLY:O	17:R:1154:THR:HG23	2.19	0.43
18:S:576:GLU:O	18:S:580:SER:N	2.51	0.43
21:W:86:ASP:O	21:W:90:GLN:HG2	2.18	0.43
11:K:468:GLY:O	11:K:471:LEU:HG	2.18	0.43
12:L:168:THR:C	12:L:172:THR:CG2	2.85	0.43
12:L:364:PRO:CD	12:L:364:PRO:O	2.67	0.43
17:R:1292:ASP:HB3	17:R:1293:PRO:HD3	2.00	0.43
11:K:48:THR:C	11:K:49:MET:HG2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:189:THR:HG21	11:K:205:SER:HB2	2.01	0.42
19:T:209:PRO:HG2	19:T:210:PRO:HD3	2.00	0.42
11:K:391:VAL:HG11	11:K:457:LEU:HD13	2.01	0.42
11:K:481:CYS:HA	11:K:484:THR:HG22	2.00	0.42
17:R:245:PRO:HG2	17:R:287:LEU:HD11	2.00	0.42
17:R:927:LYS:HG3	17:R:928:TYR:N	2.33	0.42
17:R:1142:ILE:O	17:R:1146:MET:HG2	2.19	0.42
18:S:247:VAL:HG22	18:S:770:SER:HA	2.02	0.42
11:K:262:SER:N	18:S:629:ARG:O	2.50	0.42
17:R:1106:HIS:CE1	17:R:1107:VAL:HG12	2.54	0.42
18:S:128:LEU:O	18:S:132:LEU:HG	2.18	0.42
9:I:593:GLU:HA	9:I:594:ASN:HA	1.52	0.42
17:R:260:LYS:HA	17:R:263:PHE:HB2	2.02	0.42
17:R:873:SER:HA	17:R:882:CYS:SG	2.60	0.42
18:S:319:LYS:O	18:S:323:TYR:N	2.42	0.42
9:I:398:GLU:O	9:I:402:ILE:HG23	2.19	0.42
10:J:630:ARG:NH2	10:J:637:SER:H	2.14	0.42
12:L:626:GLN:O	12:L:628:ASN:N	2.51	0.42
13:M:194:LYS:N	13:M:195:PRO:HD2	2.34	0.42
20:V:214:VAL:HG13	20:V:239:PHE:HB3	2.02	0.42
21:W:88:ALA:O	21:W:92:GLU:HG2	2.19	0.42
12:L:198:LYS:HB3	12:L:204:LEU:HA	2.00	0.42
17:R:756:LEU:HA	17:R:759:ASN:ND2	2.35	0.42
17:R:960:CYS:HB2	17:R:994:LEU:HG	2.02	0.42
17:R:1158:GLU:HA	17:R:1161:TRP:NE1	2.35	0.42
9:I:962:PHE:O	9:I:965:MET:HG2	2.19	0.42
11:K:618:LEU:HD23	11:K:618:LEU:HA	1.88	0.42
13:M:52:LEU:HA	13:M:132:LYS:HB2	2.02	0.42
17:R:768:LYS:O	17:R:771:SER:OG	2.30	0.42
19:T:199:ALA:HB3	19:T:200:PRO:HD3	2.00	0.42
9:I:384:LYS:O	9:I:386:VAL:HG23	2.19	0.42
9:I:897:THR:OG1	9:I:898:ASN:N	2.52	0.42
18:S:66:TYR:O	18:S:69:SER:OG	2.38	0.42
18:S:141:ARG:HG3	18:S:155:GLU:N	2.35	0.42
18:S:244:VAL:O	18:S:248:ILE:HG12	2.20	0.42
3:C:140:HIS:O	3:C:141:PRO:C	2.58	0.42
17:R:1065:ASP:OD1	17:R:1066:THR:N	2.53	0.42
17:R:1120:LYS:HE2	17:R:1120:LYS:HB2	1.95	0.42
9:I:831:PHE:HD2	9:I:859:PHE:HE2	1.68	0.41
11:K:42:ARG:CD	11:K:831:GLU:HG2	2.43	0.41
11:K:458:SER:HA	11:K:459:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:553:LEU:HA	11:K:556:ILE:HG22	2.01	0.41
17:R:977:LEU:HD12	17:R:977:LEU:HA	1.81	0.41
18:S:378:VAL:CG1	18:S:381:LEU:HD23	2.49	0.41
3:C:114:VAL:HA	5:E:111:THR:CB	2.50	0.41
11:K:393:ILE:CD1	11:K:443:LEU:HD21	2.50	0.41
12:L:644:SER:HA	21:W:97:GLN:HE21	1.84	0.41
17:R:673:LYS:HD2	17:R:673:LYS:HA	1.76	0.41
17:R:1253:GLY:O	17:R:1256:LEU:HD13	2.20	0.41
17:R:1315:GLU:HA	17:R:1318:ILE:HG22	2.01	0.41
18:S:282:VAL:O	18:S:285:ILE:HG22	2.20	0.41
3:C:178:ASP:O	3:C:179:ALA:C	2.57	0.41
9:I:300:CYS:O	9:I:303:LEU:HG	2.20	0.41
9:I:688:PRO:HG2	9:I:767:LEU:HD11	2.01	0.41
11:K:500:VAL:HA	11:K:503:LEU:HD12	2.02	0.41
11:K:502:SER:O	11:K:505:GLU:HG2	2.20	0.41
12:L:293:THR:O	12:L:296:GLU:HG3	2.20	0.41
11:K:130:PRO:HA	11:K:184:VAL:H	1.86	0.41
12:L:460:ILE:HD13	12:L:460:ILE:HA	1.96	0.41
17:R:624:LEU:O	17:R:627:LEU:HG	2.19	0.41
17:R:891:LEU:HD23	17:R:891:LEU:HA	1.91	0.41
18:S:676:ASP:OD1	18:S:677:VAL:N	2.53	0.41
3:C:140:HIS:H	3:C:144:GLY:H	1.66	0.41
11:K:134:LEU:HD12	11:K:217:ASP:HB3	2.00	0.41
12:L:522:GLN:O	12:L:526:LEU:HG	2.20	0.41
17:R:167:ILE:HG23	17:R:204:LEU:HD11	2.02	0.41
9:I:1221:GLN:HA	9:I:1224:ILE:HG22	2.03	0.41
11:K:134:LEU:HB3	11:K:135:SER:H	1.72	0.41
17:R:101:LEU:HD23	17:R:121:LEU:HD11	2.01	0.41
17:R:680:SER:HB2	17:R:683:LEU:HD13	2.03	0.41
22:X:66:GLN:OE1	22:X:66:GLN:N	2.52	0.41
12:L:298:ALA:HA	12:L:301:VAL:HG12	2.03	0.41
17:R:665:PHE:HA	17:R:668:PHE:CE1	2.56	0.41
17:R:756:LEU:HD21	17:R:832:TYR:CZ	2.55	0.41
18:S:378:VAL:CG1	18:S:381:LEU:HB3	2.45	0.41
3:C:117:SER:O	5:E:112:LYS:O	2.39	0.41
3:C:180:LEU:C	3:C:182:LEU:N	2.72	0.41
11:K:474:LEU:HD21	11:K:493:LEU:HG	2.02	0.41
12:L:495:LEU:HD21	12:L:503:ARG:HD3	2.02	0.41
17:R:692:ALA:O	17:R:695:THR:OG1	2.39	0.41
17:R:926:LYS:HA	17:R:926:LYS:HD2	1.81	0.41
17:R:1142:ILE:H	17:R:1142:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:94:VAL:HA	18:S:97:LEU:HD12	2.02	0.41
19:T:73:THR:HG23	19:T:75:ASP:OD1	2.20	0.41
9:I:668:HIS:HB3	10:J:767:HIS:HD2	1.85	0.41
17:R:450:SER:OG	17:R:451:LEU:N	2.54	0.41
17:R:537:MET:SD	17:R:537:MET:N	2.92	0.41
17:R:680:SER:HB2	17:R:683:LEU:HB2	2.03	0.41
17:R:714:ASP:N	17:R:714:ASP:OD1	2.53	0.41
17:R:786:PRO:HB2	17:R:787:PRO:HD3	2.01	0.41
17:R:847:ILE:HD13	17:R:851:ASN:HD21	1.86	0.41
17:R:1269:GLU:HA	17:R:1272:VAL:HG22	2.03	0.41
17:R:1290:TYR:O	17:R:1293:PRO:HD2	2.21	0.41
17:R:1308:ASP:OD1	17:R:1308:ASP:N	2.53	0.41
10:J:639:TYR:O	10:J:643:VAL:HG22	2.20	0.41
11:K:621:VAL:O	11:K:625:VAL:HG13	2.21	0.41
11:K:654:MET:O	11:K:658:LEU:HG	2.21	0.41
17:R:229:PRO:HG3	17:R:1218:HIS:HE2	1.86	0.41
18:S:225:ILE:HD13	18:S:225:ILE:HA	1.92	0.41
9:I:536:ASN:HA	9:I:550:ILE:HA	2.03	0.40
9:I:586:LEU:HG	9:I:588:LEU:HG	2.03	0.40
9:I:902:GLN:O	9:I:919:ARG:HA	2.21	0.40
17:R:777:ILE:HA	17:R:780:PHE:HB3	2.02	0.40
17:R:927:LYS:HG3	17:R:928:TYR:H	1.86	0.40
17:R:931:LYS:HD2	17:R:931:LYS:HA	1.76	0.40
18:S:120:LEU:HD23	18:S:124:LEU:HD23	2.02	0.40
21:W:48:LEU:HD22	21:W:87:ILE:HD12	2.02	0.40
11:K:221:THR:OG1	11:K:222:GLY:N	2.53	0.40
14:O:22:GLU:O	14:O:26:ARG:HG3	2.20	0.40
17:R:820:VAL:HG13	17:R:821:ALA:H	1.86	0.40
17:R:1148:ALA:HA	17:R:1151:LEU:HD12	2.02	0.40
3:C:167:GLU:OE2	9:I:268:SER:C	2.59	0.40
9:I:967:VAL:HG21	9:I:1185:LEU:HD13	2.04	0.40
11:K:166:PRO:HG2	11:K:169:THR:HB	2.03	0.40
11:K:479:GLU:O	11:K:483:VAL:HG13	2.21	0.40
17:R:87:VAL:HA	17:R:91:LEU:O	2.22	0.40
17:R:157:VAL:O	17:R:161:LEU:HG	2.21	0.40
3:C:118:ARG:N	5:E:111:THR:C	2.74	0.40
3:C:176:ARG:C	3:C:179:ALA:H	2.25	0.40
11:K:750:LEU:HD22	11:K:752:PHE:CE1	2.56	0.40
12:L:303:LEU:HD21	12:L:375:LEU:HD21	2.03	0.40
12:L:477:VAL:HG13	12:L:492:GLN:NE2	2.35	0.40
17:R:448:PRO:C	17:R:452:ARG:HG3	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:1162:ILE:HD13	17:R:1162:ILE:HA	1.90	0.40
18:S:502:HIS:HA	18:S:670:LEU:HD21	2.02	0.40
22:X:167:GLN:HG3	23:Y:61:PRO:HD2	2.02	0.40
10:J:639:TYR:CE1	10:J:643:VAL:HG21	2.56	0.40
10:J:736:TRP:HD1	10:J:743:TYR:HE2	1.69	0.40
11:K:383:ALA:HB2	11:K:393:ILE:CG2	2.52	0.40
11:K:546:ASP:N	11:K:546:ASP:OD1	2.54	0.40
18:S:303:LEU:H	18:S:303:LEU:HD12	1.87	0.40
22:X:76:LYS:O	22:X:80:GLN:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	455/1581 (29%)	430 (94%)	25 (6%)	0	100 100
2	B	154/270 (57%)	151 (98%)	3 (2%)	0	100 100
3	C	174/246 (71%)	118 (68%)	51 (29%)	5 (3%)	4 32
4	D	159/233 (68%)	153 (96%)	6 (4%)	0	100 100
5	E	177/268 (66%)	161 (91%)	16 (9%)	0	100 100
6	F	69/146 (47%)	67 (97%)	2 (3%)	0	100 100
7	G	120/135 (89%)	119 (99%)	1 (1%)	0	100 100
8	H	101/117 (86%)	92 (91%)	6 (6%)	3 (3%)	4 31
9	I	1068/1454 (74%)	958 (90%)	110 (10%)	0	100 100
10	J	165/788 (21%)	144 (87%)	21 (13%)	0	100 100
11	K	710/877 (81%)	598 (84%)	109 (15%)	3 (0%)	34 72
12	L	527/651 (81%)	460 (87%)	66 (12%)	1 (0%)	47 81
13	M	176/208 (85%)	162 (92%)	14 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	O	164/212 (77%)	145 (88%)	19 (12%)	0	100 100
15	P	110/144 (76%)	108 (98%)	2 (2%)	0	100 100
16	Q	129/200 (64%)	123 (95%)	6 (5%)	0	100 100
17	R	1284/1368 (94%)	1127 (88%)	155 (12%)	2 (0%)	47 81
18	S	889/989 (90%)	802 (90%)	86 (10%)	1 (0%)	51 85
19	T	184/747 (25%)	171 (93%)	13 (7%)	0	100 100
20	V	264/311 (85%)	226 (86%)	37 (14%)	1 (0%)	34 72
21	W	116/178 (65%)	113 (97%)	3 (3%)	0	100 100
22	X	119/200 (60%)	115 (97%)	4 (3%)	0	100 100
23	Y	128/178 (72%)	120 (94%)	8 (6%)	0	100 100
24	Z	101/131 (77%)	100 (99%)	1 (1%)	0	100 100
26	9	22/2174 (1%)	6 (27%)	7 (32%)	9 (41%)	0 0
All	All	7565/13806 (55%)	6769 (90%)	771 (10%)	25 (0%)	44 76

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	168	PRO
3	C	176	ARG
8	H	86	SER
11	K	835	PRO
26	9	621	PRO
26	9	626	VAL
26	9	629	LEU
26	9	630	PRO
26	9	631	PRO
26	9	634	PRO
3	C	145	TYR
26	9	636	ASP
3	C	173	GLN
8	H	83	SER
8	H	85	SER
26	9	627	GLU
3	C	172	PHE
12	L	31	LEU
11	K	830	VAL
17	R	1175	PRO
26	9	620	PHE

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Mol	Chain	Res	Type
20	V	293	PRO
17	R	945	VAL
18	S	919	PRO
11	K	305	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	A	13/1391 (1%)	13 (100%)	0	100 100
2	B	3/230 (1%)	3 (100%)	0	100 100
3	C	12/223 (5%)	11 (92%)	1 (8%)	11 36
5	E	3/225 (1%)	3 (100%)	0	100 100
6	F	6/133 (4%)	6 (100%)	0	100 100
7	G	1/124 (1%)	1 (100%)	0	100 100
8	H	14/98 (14%)	14 (100%)	0	100 100
9	I	401/1271 (32%)	400 (100%)	1 (0%)	93 96
10	J	104/697 (15%)	103 (99%)	1 (1%)	76 86
11	K	418/766 (55%)	417 (100%)	1 (0%)	93 96
12	L	199/577 (34%)	199 (100%)	0	100 100
13	M	62/183 (34%)	62 (100%)	0	100 100
14	O	47/178 (26%)	47 (100%)	0	100 100
16	Q	25/173 (14%)	25 (100%)	0	100 100
17	R	956/1232 (78%)	954 (100%)	2 (0%)	93 96
18	S	402/864 (46%)	399 (99%)	3 (1%)	84 90
19	T	96/601 (16%)	96 (100%)	0	100 100
20	V	95/280 (34%)	95 (100%)	0	100 100
21	W	55/152 (36%)	55 (100%)	0	100 100
22	X	67/163 (41%)	67 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	Y	47/155 (30%)	47 (100%)	0	100 100
24	Z	1/115 (1%)	1 (100%)	0	100 100
All	All	3027/9831 (31%)	3018 (100%)	9 (0%)	92 95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	192	PHE
9	I	896	ARG
10	J	739	ARG
11	K	754	ARG
17	R	536	LYS
17	R	1229	LYS
18	S	385	ARG
18	S	489	ARG
18	S	835	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	638	ASN
9	I	663	ASN
9	I	860	ASN
10	J	628	ASN
10	J	635	ASN
11	K	473	HIS
11	K	598	ASN
12	L	367	HIS
12	L	466	ASN
13	M	134	HIS
16	Q	102	ASN
17	R	103	ASN
17	R	276	GLN
17	R	552	HIS
17	R	664	GLN
17	R	684	ASN
17	R	696	HIS
17	R	726	ASN
17	R	874	HIS
17	R	918	HIS

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Mol	Chain	Res	Type
17	R	1028	HIS
17	R	1054	ASN
17	R	1165	HIS
17	R	1223	GLN
17	R	1300	HIS
18	S	370	GLN
18	S	419	ASN
18	S	699	ASN
18	S	747	ASN
18	S	760	HIS
18	S	836	HIS
18	S	920	HIS
20	V	55	HIS
20	V	106	GLN
20	V	220	ASN
20	V	252	HIS
21	W	97	GLN
21	W	140	GLN
22	X	84	GLN
22	X	85	ASN
23	Y	81	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

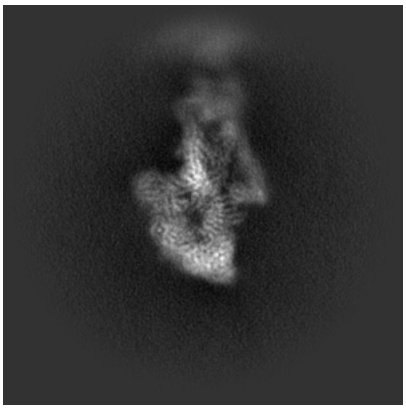
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41107. These allow visual inspection of the internal detail of the map and identification of artifacts.

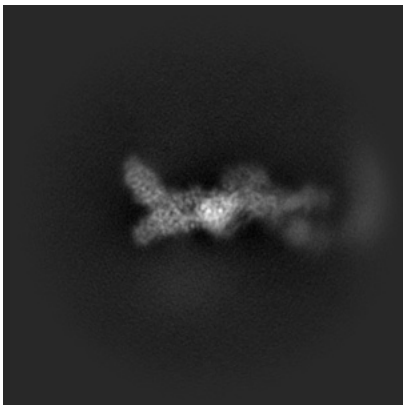
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

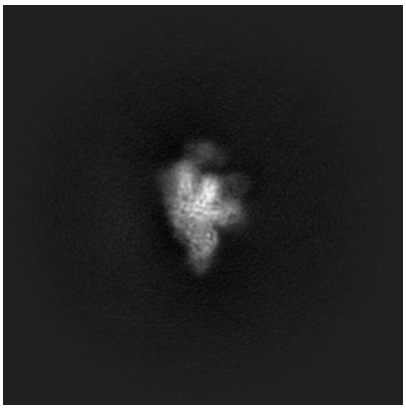
6.1.1 Primary map



X

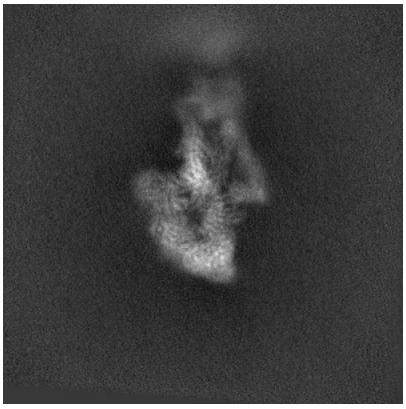


Y

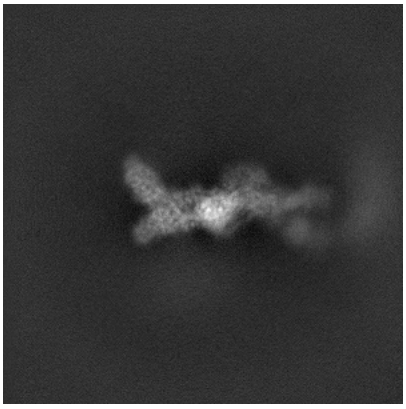


Z

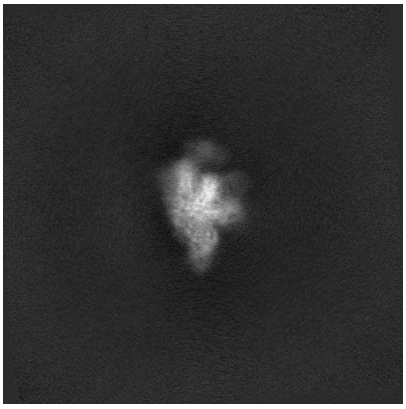
6.1.2 Raw map



X



Y

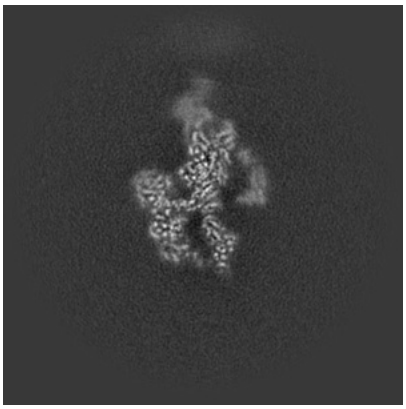


Z

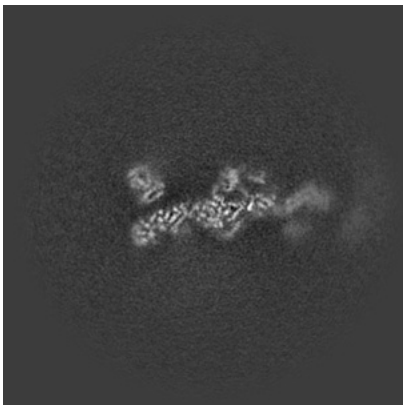
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

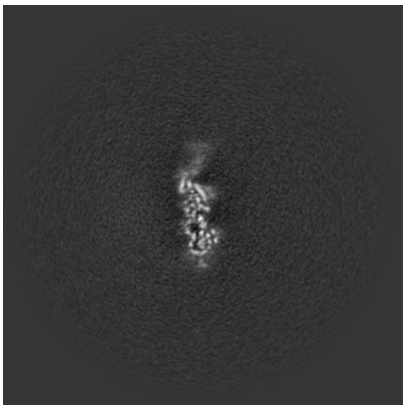
6.2.1 Primary map



X Index: 280

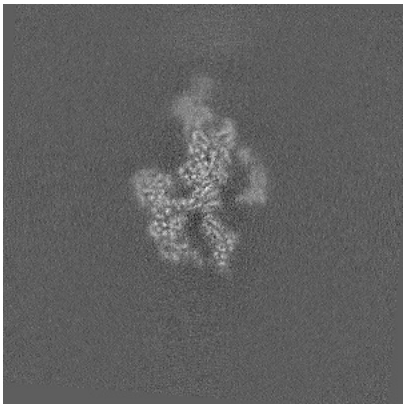


Y Index: 280

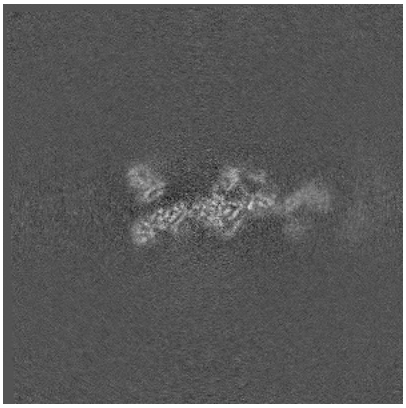


Z Index: 280

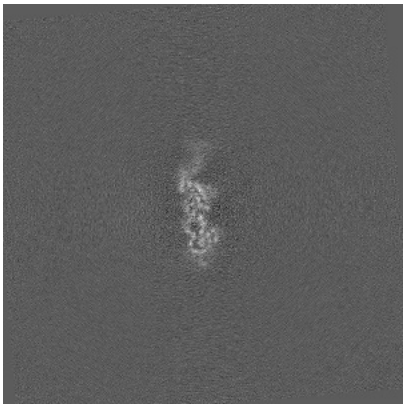
6.2.2 Raw map



X Index: 280



Y Index: 280

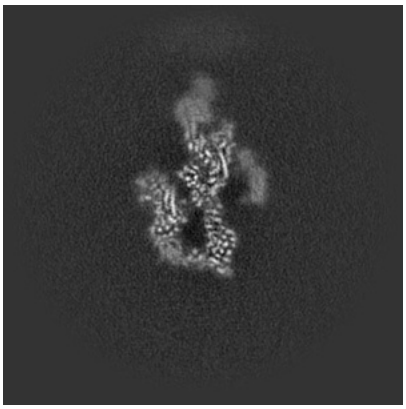


Z Index: 280

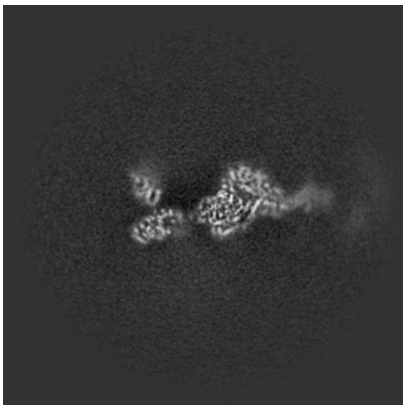
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



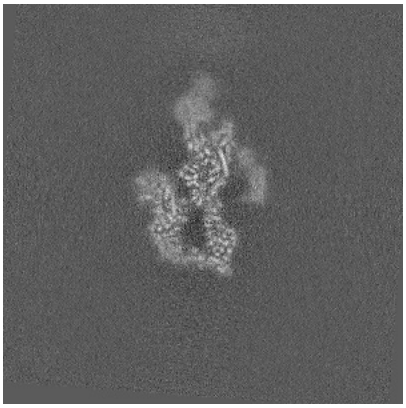
X Index: 286



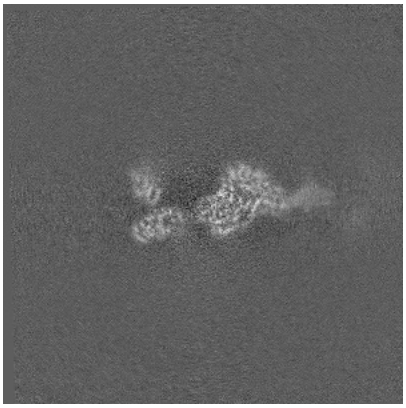
Y Index: 270

Z Index: 297

6.3.2 Raw map



X Index: 285



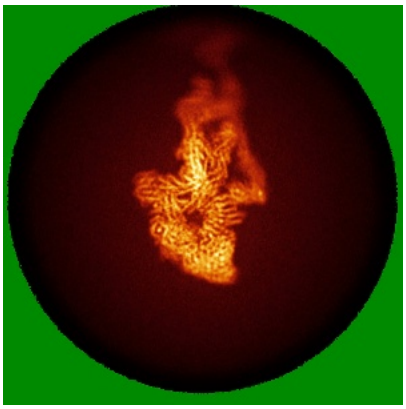
Y Index: 270

Z Index: 297

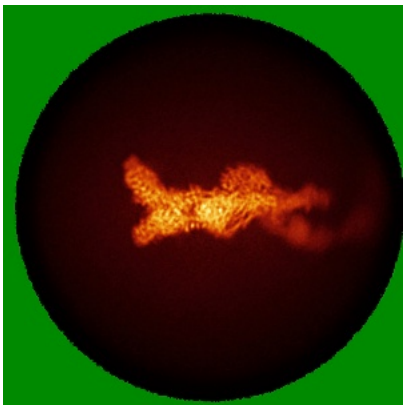
The images above show the largest variance slices of the map in three orthogonal directions.

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

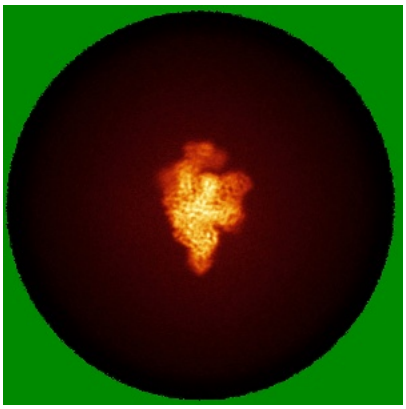
6.4.1 Primary map



X

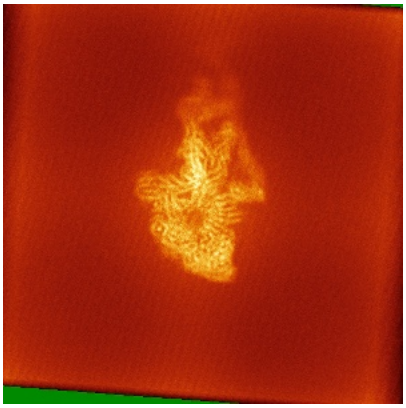


Y

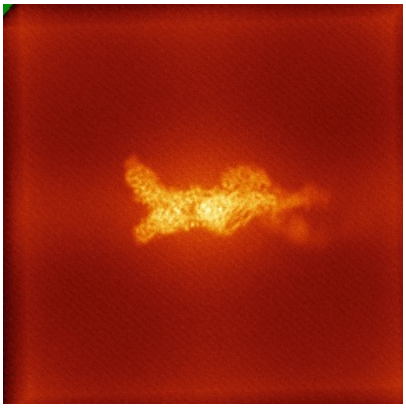


Z

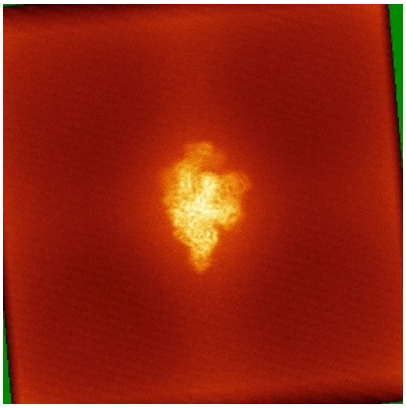
6.4.2 Raw map



X



Y

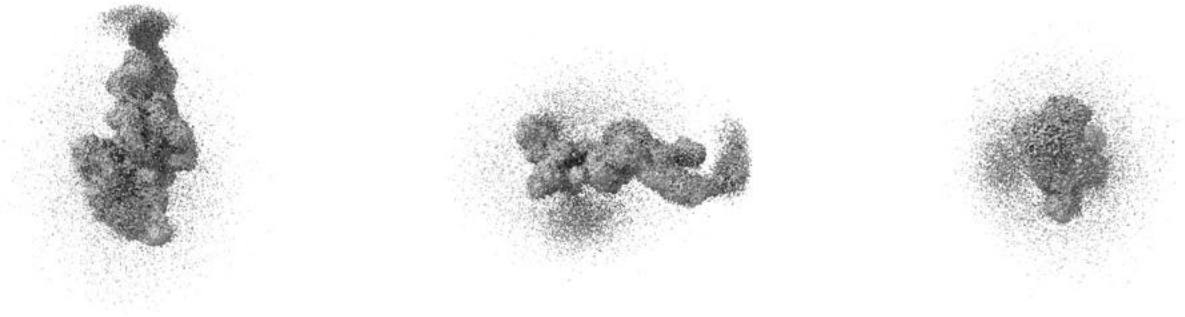


Z

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)

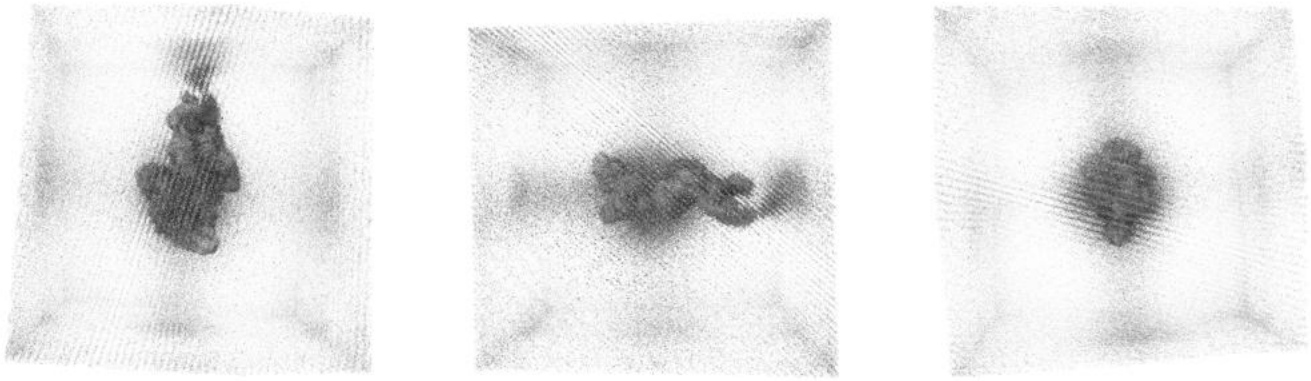
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

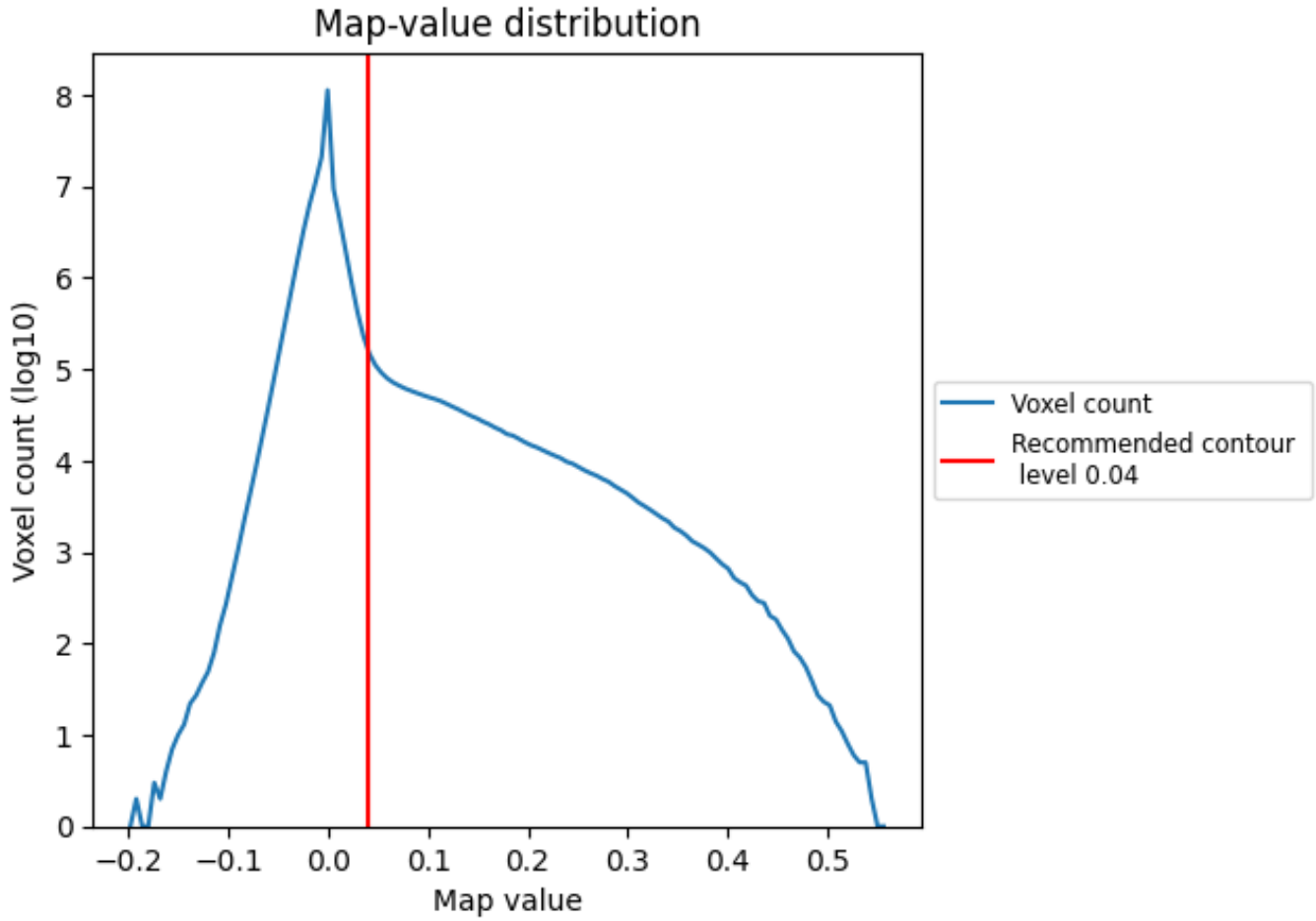
6.6 Mask visualisation (i)

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

7 Map analysis

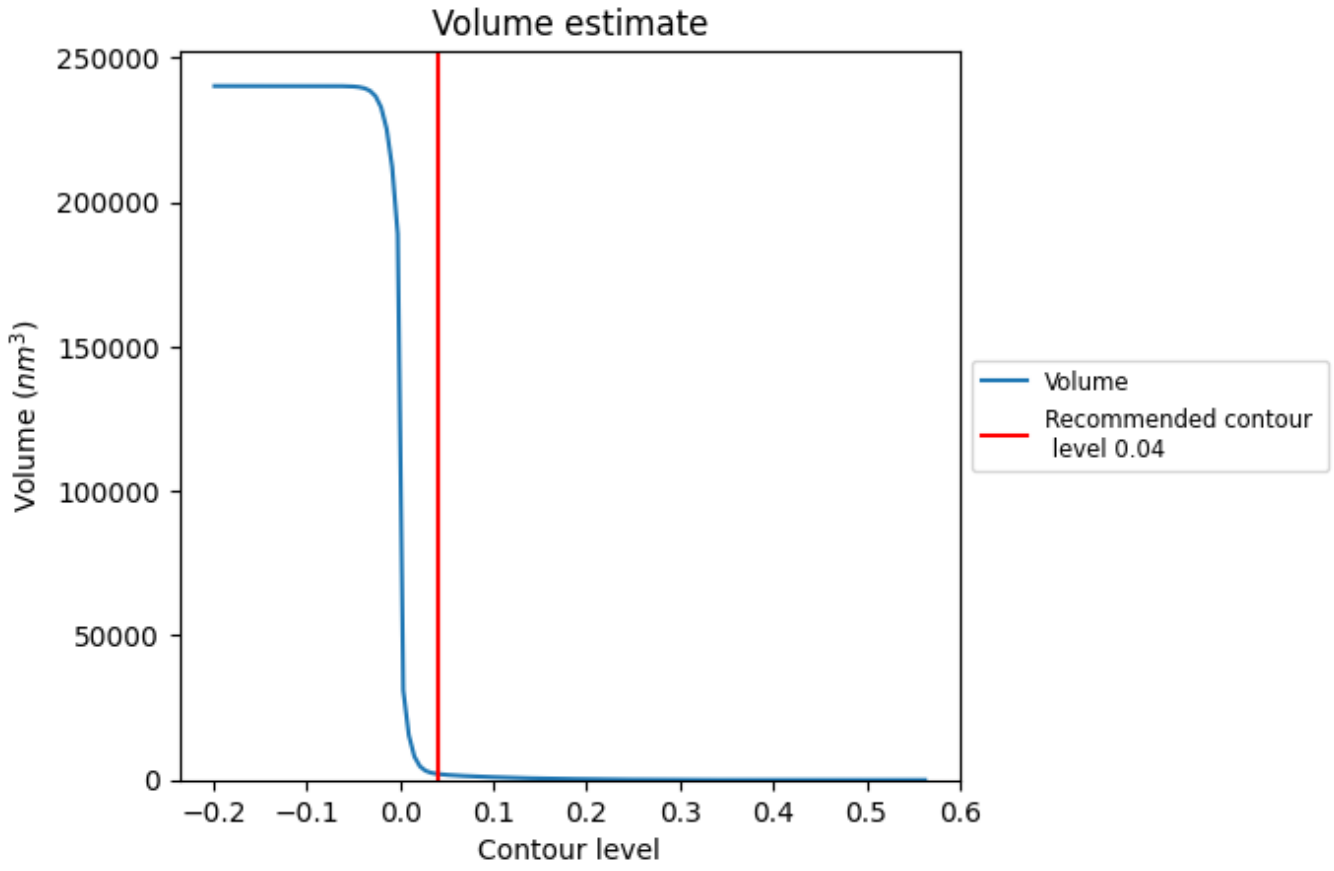
This section contains the results of statistical analysis of the map.

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.

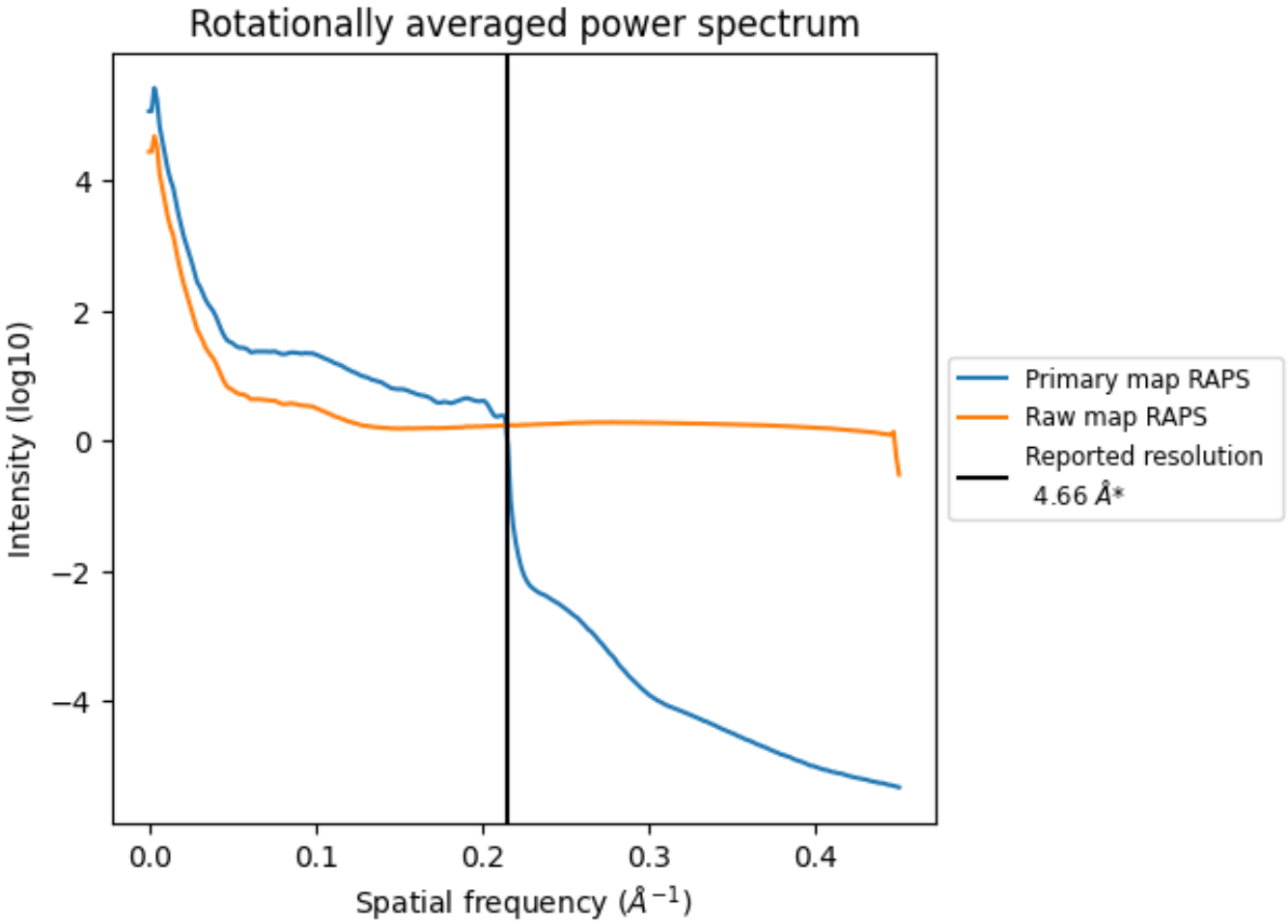
7.2 Volume estimate



The volume at the recommended contour level is 2101 nm^3; this corresponds to an approximate mass of 1898 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)

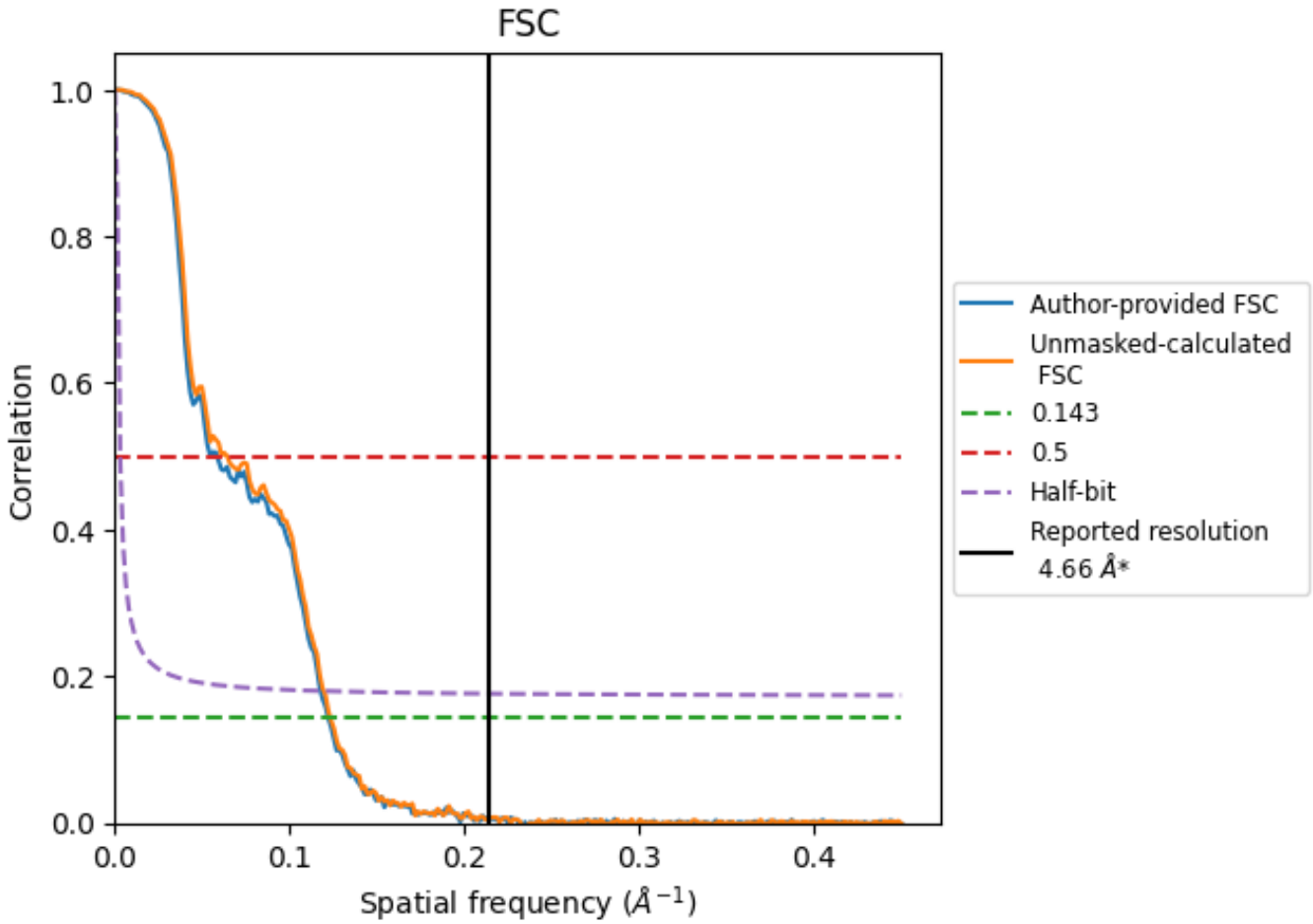


*Reported resolution corresponds to spatial frequency of 0.215 $Å^{-1}$

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 0.215 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.66	-	-
Author-provided FSC curve	8.18	17.06	8.47
Unmasked-calculated*	8.10	15.55	8.35

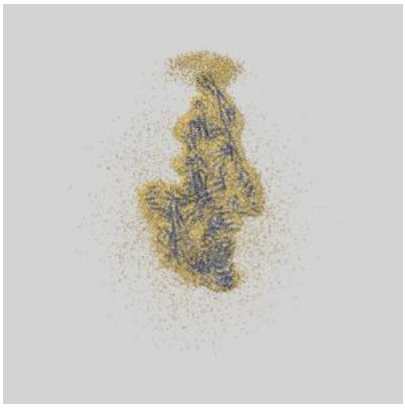
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.18 differs from the reported value 4.66 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.10 differs from the reported value 4.66 by more than 10 %

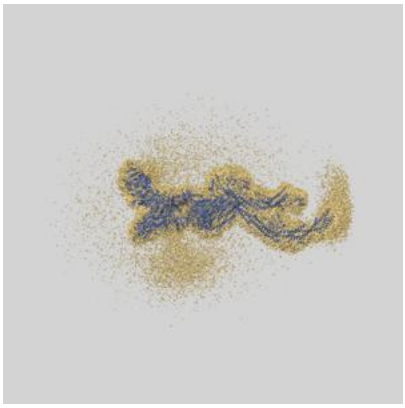
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41107 and PDB model 8T9D. Per-residue inclusion information can be found in section 3 on page 8.

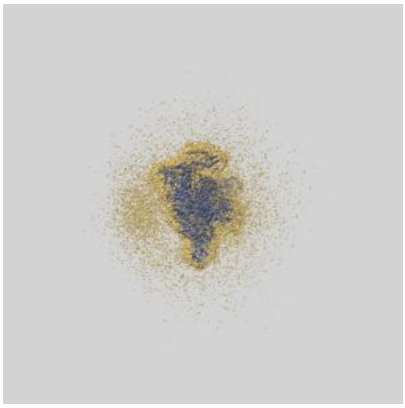
9.1 Map-model overlay



X



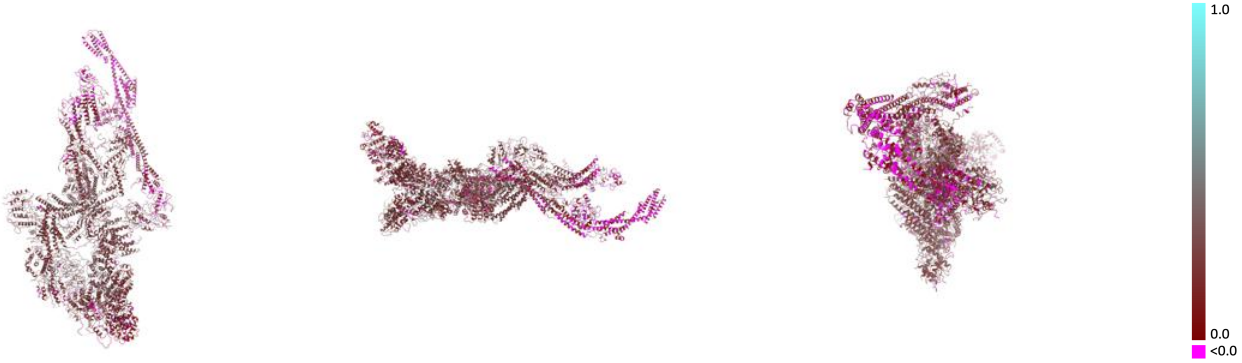
Y



Z

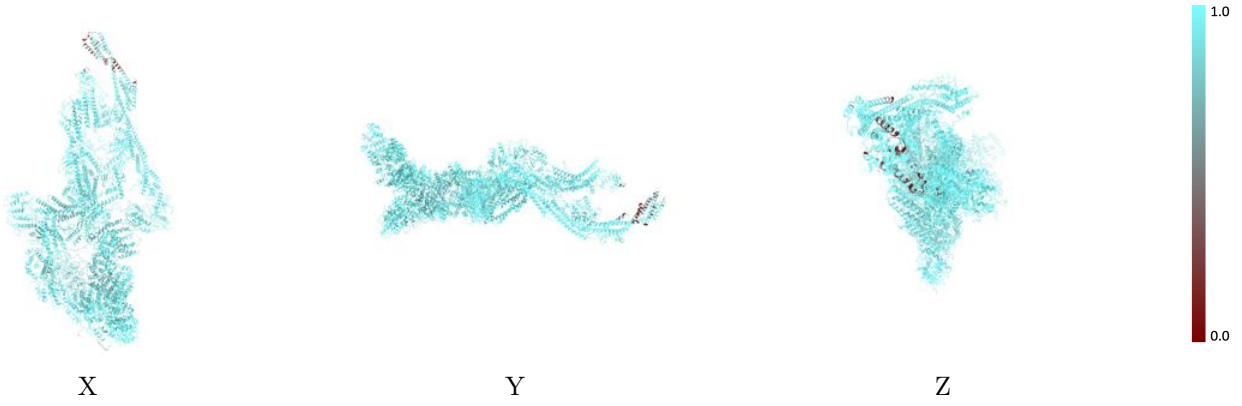
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



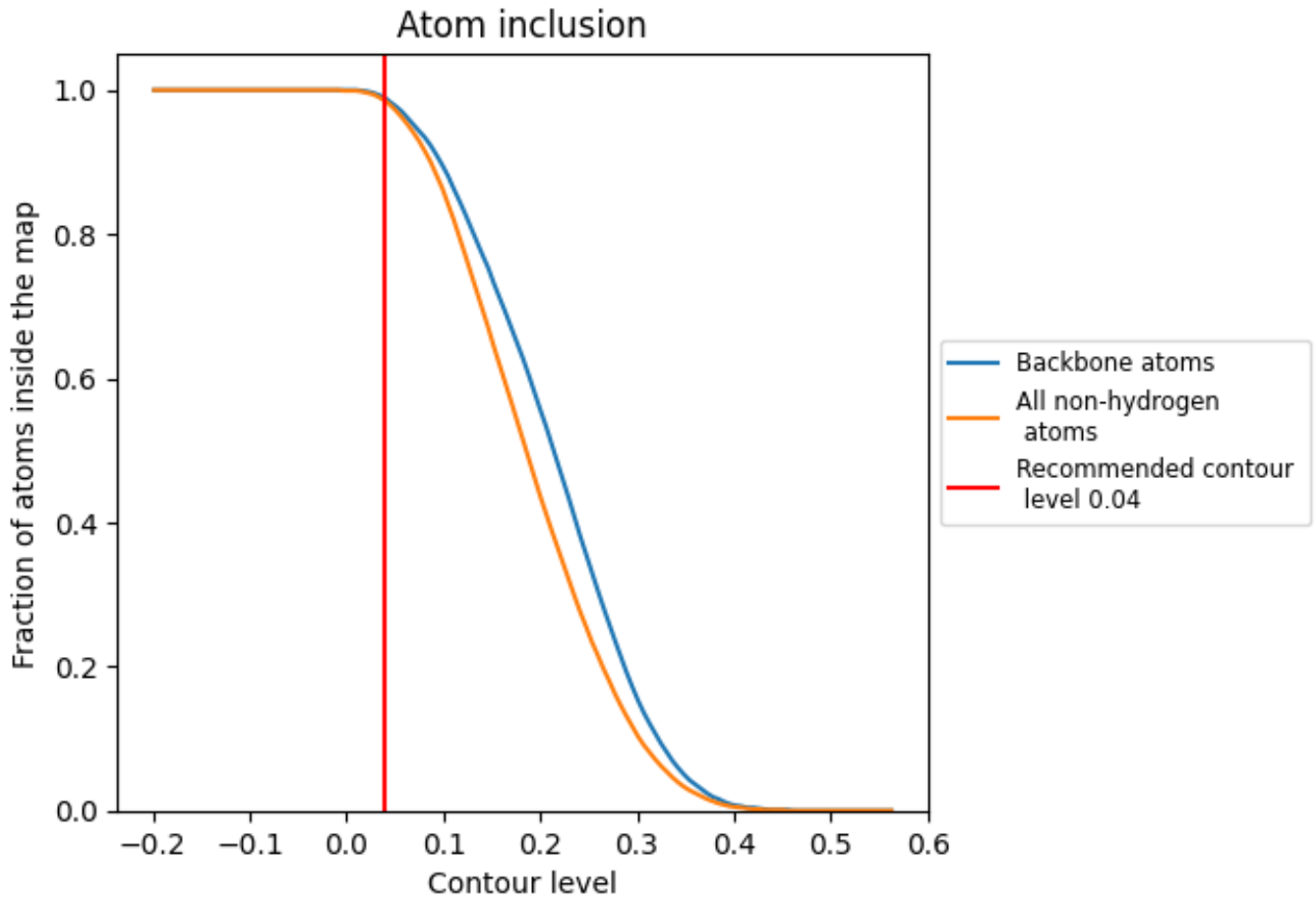
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9850	0.2150
9	1.0000	0.2220
A	0.9970	0.1740
B	0.9950	0.1190
C	0.9630	0.1290
D	0.9950	0.0790
E	0.9950	0.1370
F	1.0000	0.1670
G	0.7220	0.0500
H	0.9970	0.1930
I	0.9800	0.2420
J	0.9910	0.2480
K	0.9890	0.2450
L	0.9880	0.2410
M	0.9990	0.2300
O	1.0000	0.2760
P	0.9600	0.0750
Q	0.9930	0.1920
R	0.9840	0.1950
S	0.9920	0.2380
T	0.9950	0.2050
V	0.9960	0.3020
W	0.9910	0.2380
X	1.0000	0.2500
Y	0.9990	0.2570
Z	0.9940	0.0880
a	1.0000	0.2080