Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 04:04 PM JST

PDB ID	:	7ENJ
EMDB ID	:	EMD-31211
Title	:	Human Mediator (deletion of MED1-IDR) in a Tail-bent conformation (MED-B)
Authors	:	Yin, X.; Li, J.; Wu, Z.; Liu, W.; Xu, Y.
Deposited on	:	2021-04-17
Resolution	:	4.40 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:

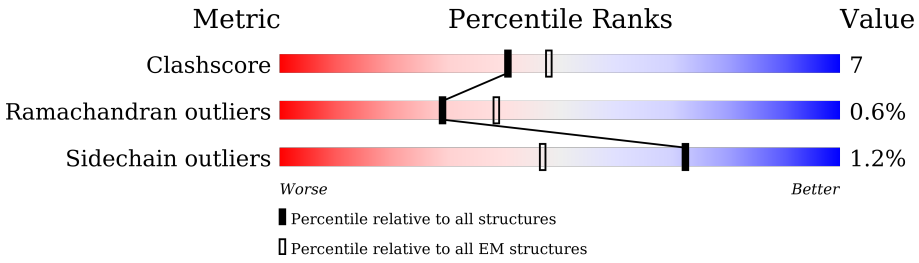
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 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	24% 5% 70%
2	B	20	100%
3	D	270	49% 9% 41%
4	F	246	50% 18% 32%
5	G	233	53% 15% 31%
6	H	268	58% 9% 32%
7	I	146	40% 9% 50%
8	J	135	83% 7% 10%

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Mol	Chain	Length	Quality of chain
9	K	117	78% 18%
10	N	1454	58% 11% 30%
11	O	788	17% 80%
12	P	877	11% 39% 8% 52%
13	Q	651	70% 13% 15%
14	R	208	72% 20% 8%
15	S	244	27% 69%
16	T	212	72% 19% 9%
17	U	144	67% 16% 16%
18	V	200	52% 12% 35%
19	W	1368	10% 82% 15%
20	X	989	77% 13% 9%
21	Z	600	12% 84%
22	0	311	69% 15% 14%
23	1	178	48% 7% 44%
24	2	200	52% 5% 42%
25	3	178	60% 8% 31%
26	4	131	68% 18% 14%

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 57971 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	S		
1	A	467	3578	2278	613	663	24	0	0

- Molecule 2 is a protein called Unknown Chain.

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

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	167	1374	888	238	243	5	0	0

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

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

- Molecule 6 is a protein called Isoform 2 of Mediator of RNA polymerase II transcription subunit 8.

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

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 9.

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

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 10.

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

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 11.

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

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 14.

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

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 15.

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

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	420	Total	C	N	O	S	0	0
			3226	2047	555	602	22		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	551	Total	C	N	O	S	0	0
			4361	2760	780	801	20		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 18.

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

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	75	Total	C	N	O	S	0	0
			476	295	85	94	2		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 20.

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

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 21.

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

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 22.

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

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 23.

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

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 24.

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

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	97	Total	C	N	O	S	0	0
			765	472	136	154	3		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	267	Total	C	N	O	S	0	0
			2159	1373	384	390	12		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	99	Total	C	N	O	S	0	0
			817	511	143	160	3		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	115	Total	C	N	O	S	0	0
			899	563	155	172	9		

- Molecule 25 is a protein called Mediator of RNA polymerase II transcription subunit 30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	122	Total	C	N	O	S	0	0
			1022	639	187	189	7		

- Molecule 26 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	113	Total	C	N	O	S	0	0
			986	642	171	168	5		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

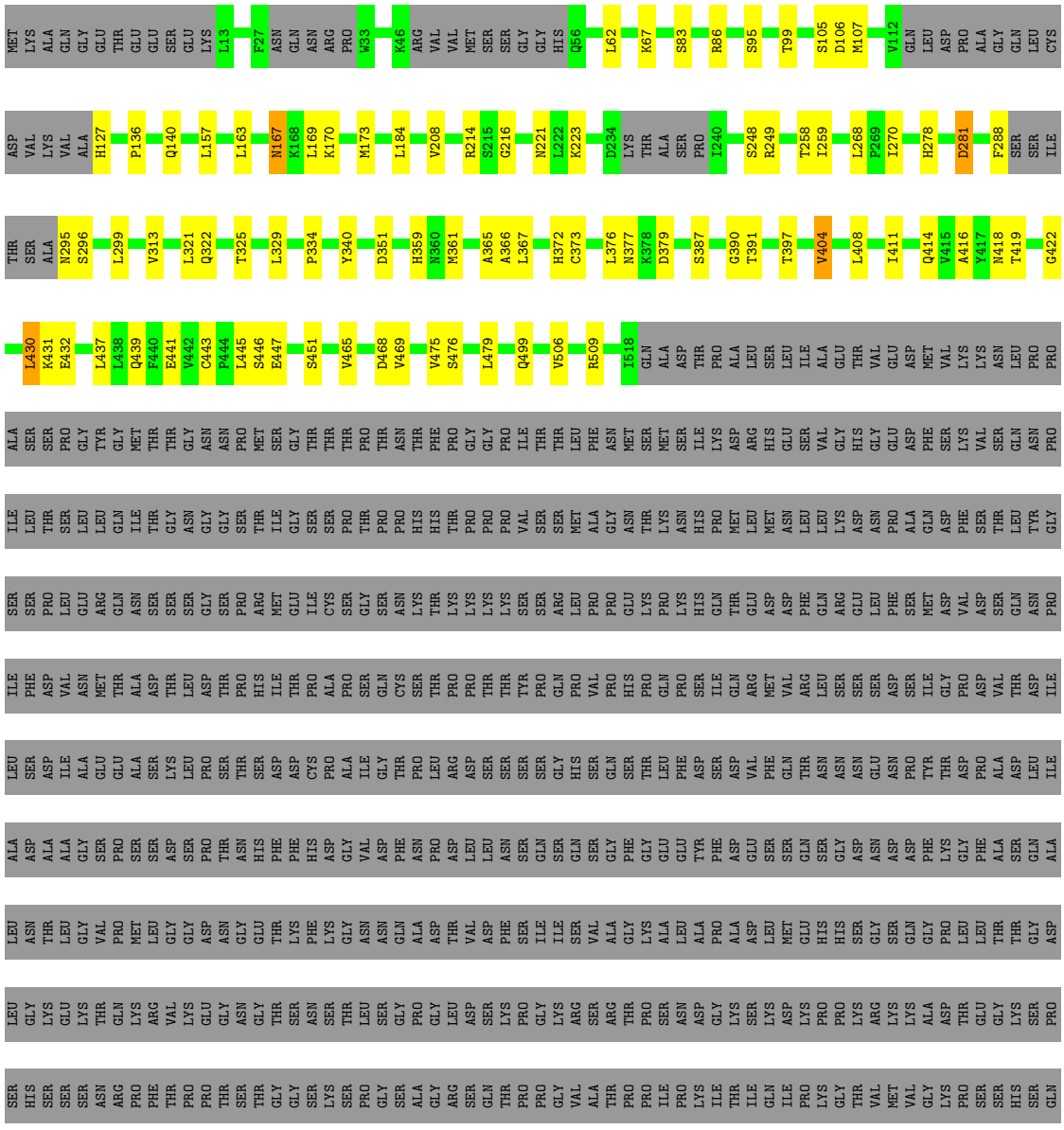
Mol	Chain	Residues	Atoms		AltConf
27	0	1	Total	Zn	0
			1	1	

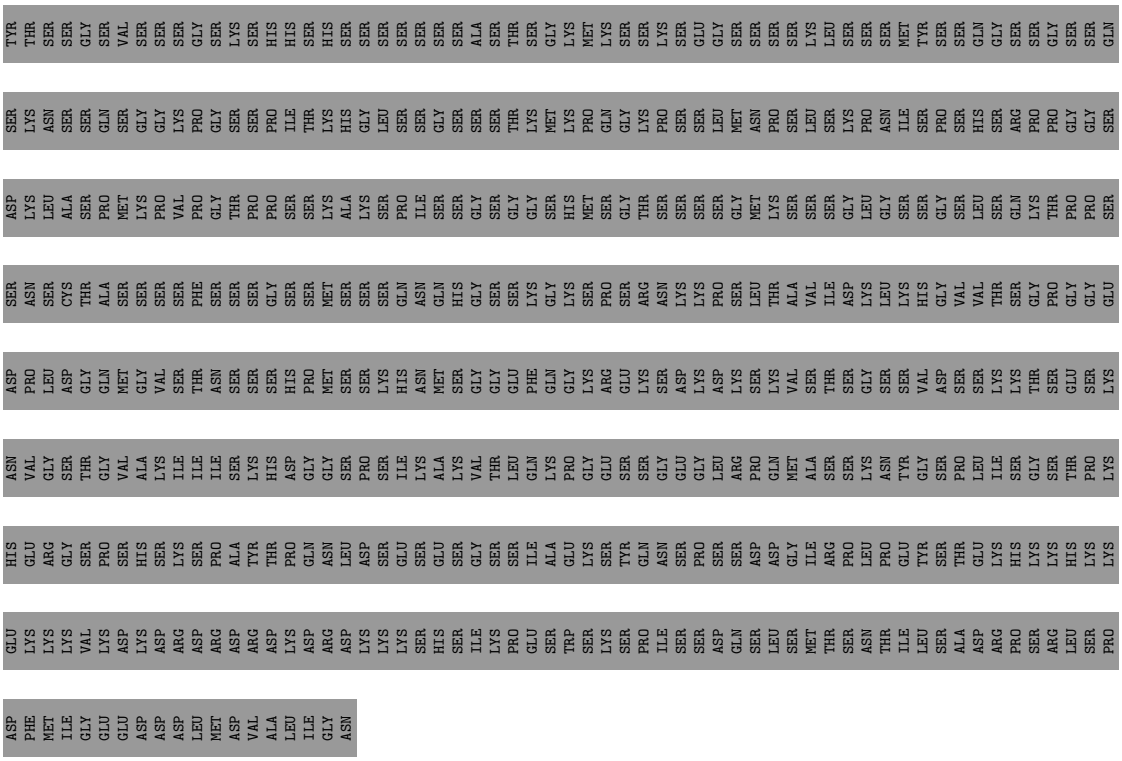
3 Residue-property plots (i)

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 1

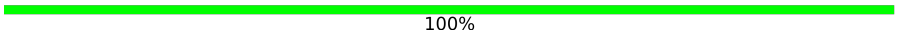
Chain A:





• Molecule 2: Unknown Chain

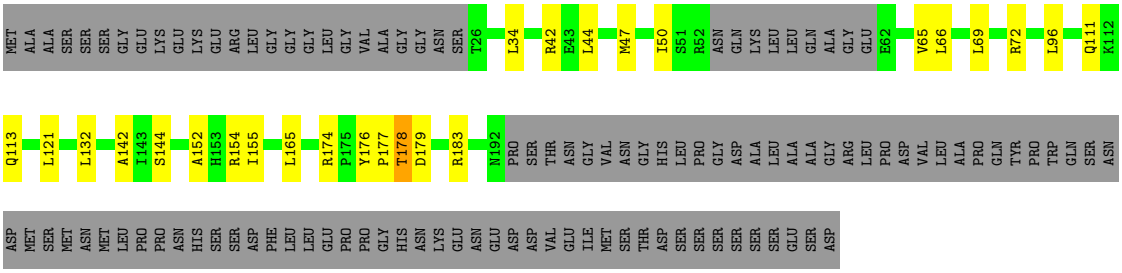
Chain B:



There are no outlier residues recorded for this chain.

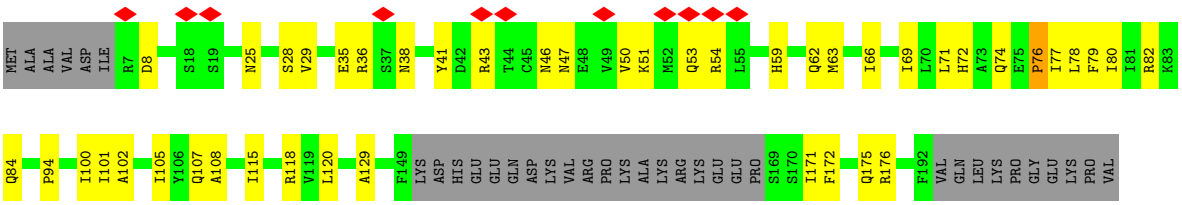
• Molecule 3: Mediator of RNA polymerase II transcription subunit 4

Chain D:



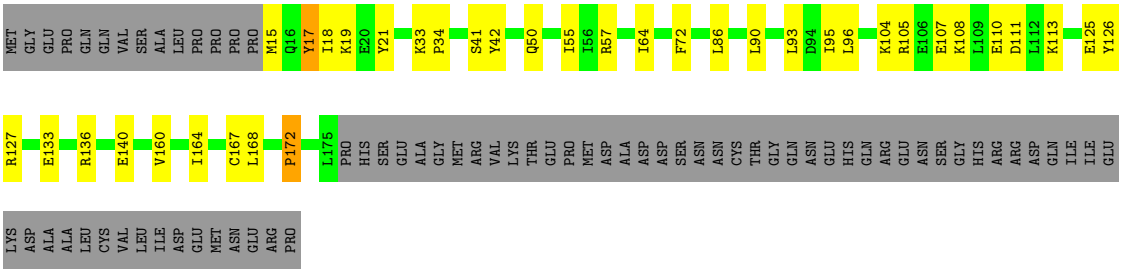
• Molecule 4: Mediator of RNA polymerase II transcription subunit 6

Chain F:



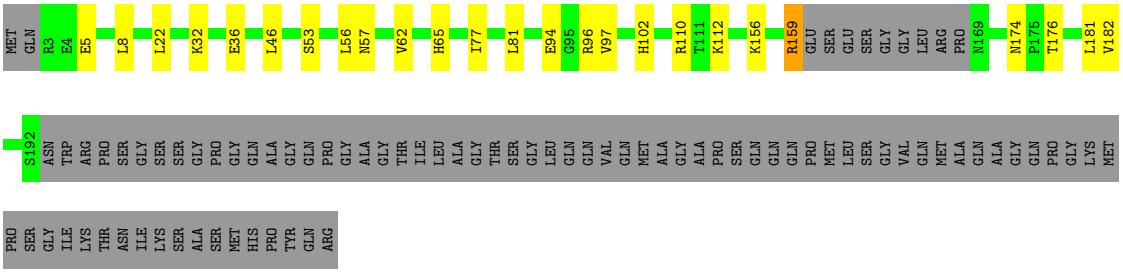
• Molecule 5: Mediator of RNA polymerase II transcription subunit 7

Chain G:



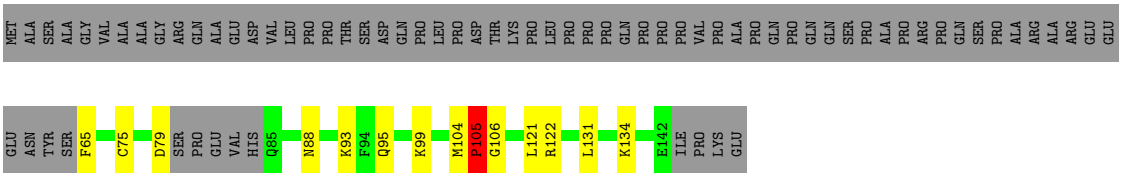
• Molecule 6: Isoform 2 of Mediator of RNA polymerase II transcription subunit 8

Chain H:



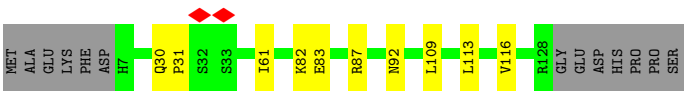
• Molecule 7: Mediator of RNA polymerase II transcription subunit 9

Chain I:



• Molecule 8: Mediator of RNA polymerase II transcription subunit 10

Chain J:

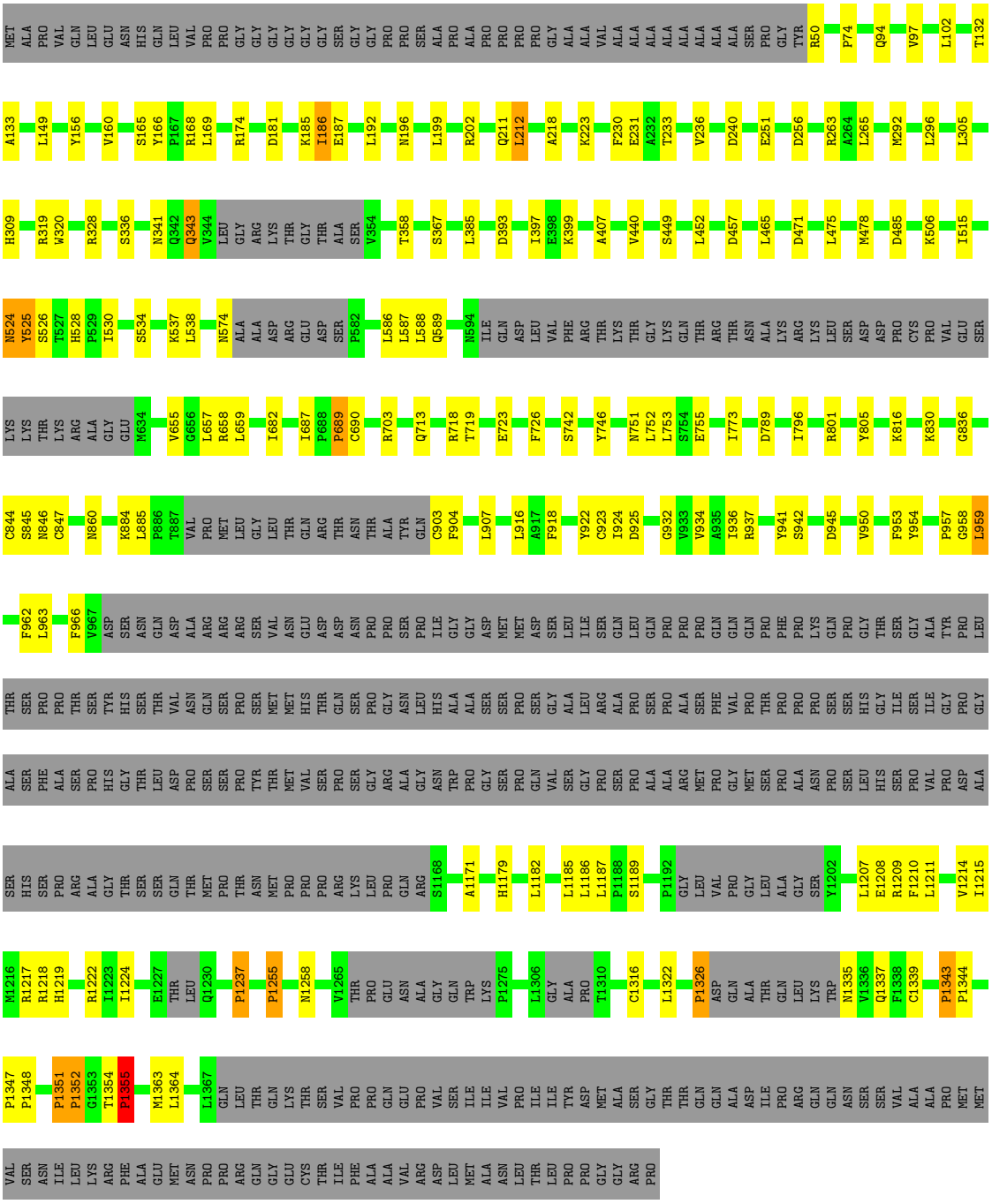


• Molecule 9: Mediator of RNA polymerase II transcription subunit 11

Chain K:

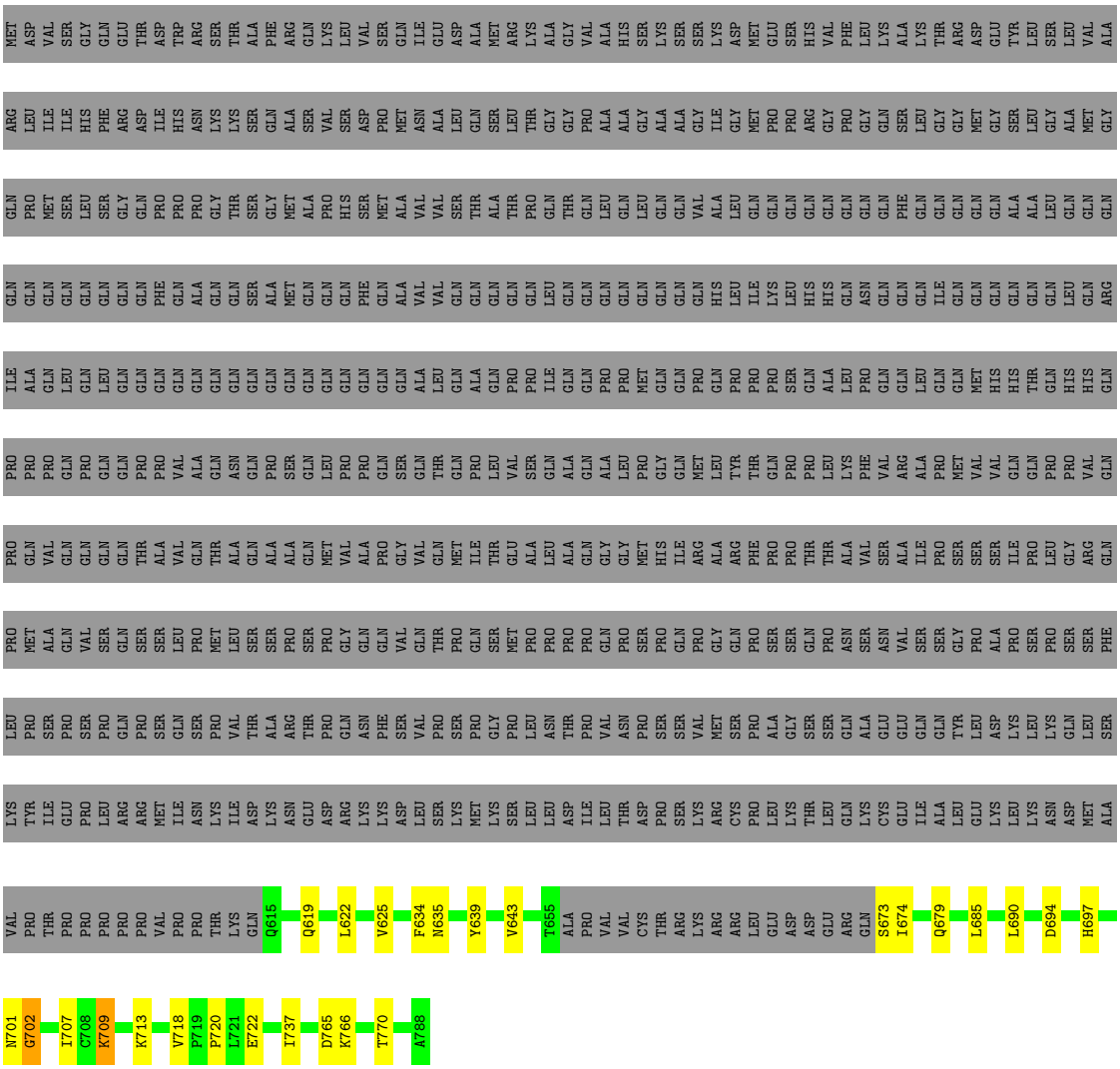
• Molecule 10: Mediator of RNA polymerase II transcription subunit 14

Chain N:



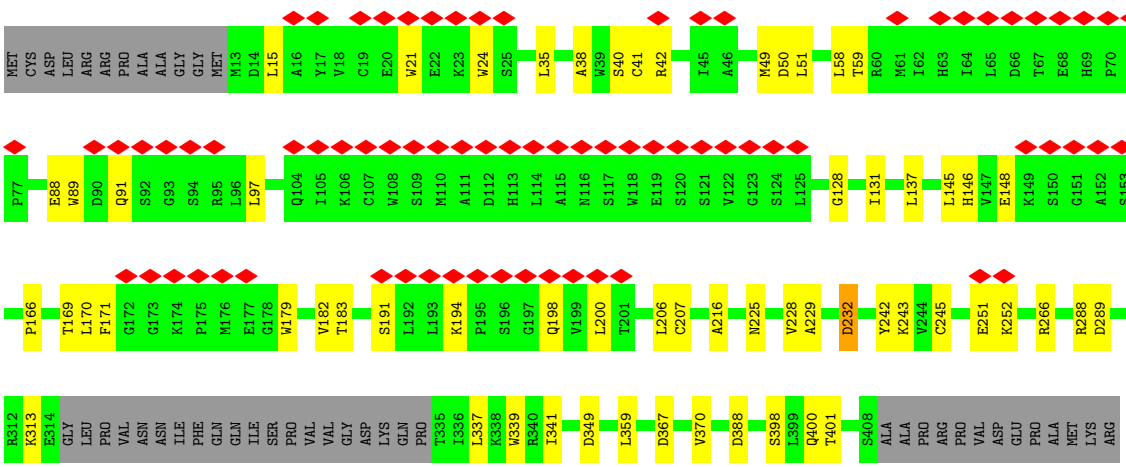
• Molecule 11: Mediator of RNA polymerase II transcription subunit 15

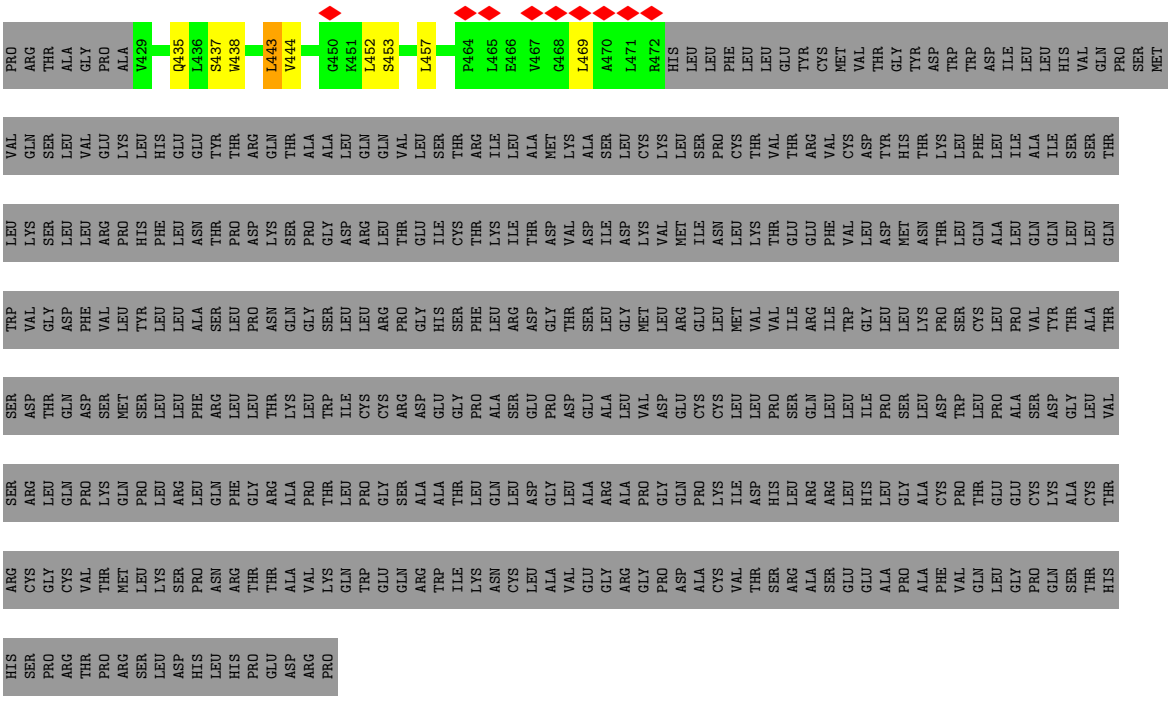
Chain O:



• Molecule 12: Mediator of RNA polymerase II transcription subunit 16

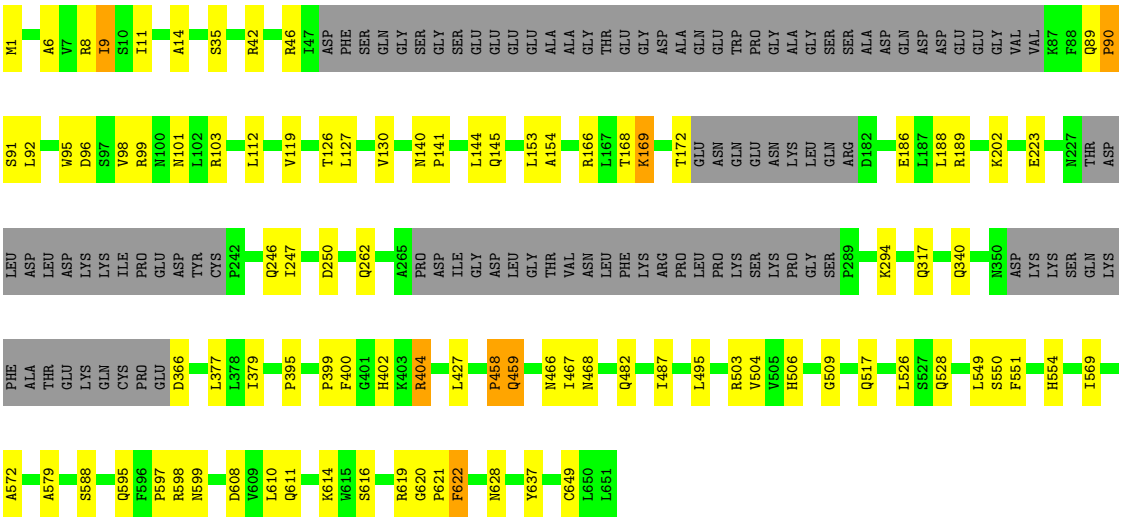
Chain P:





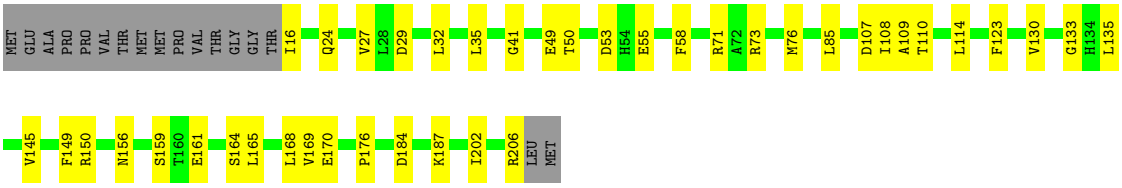
• Molecule 13: Mediator of RNA polymerase II transcription subunit 17

Chain Q:



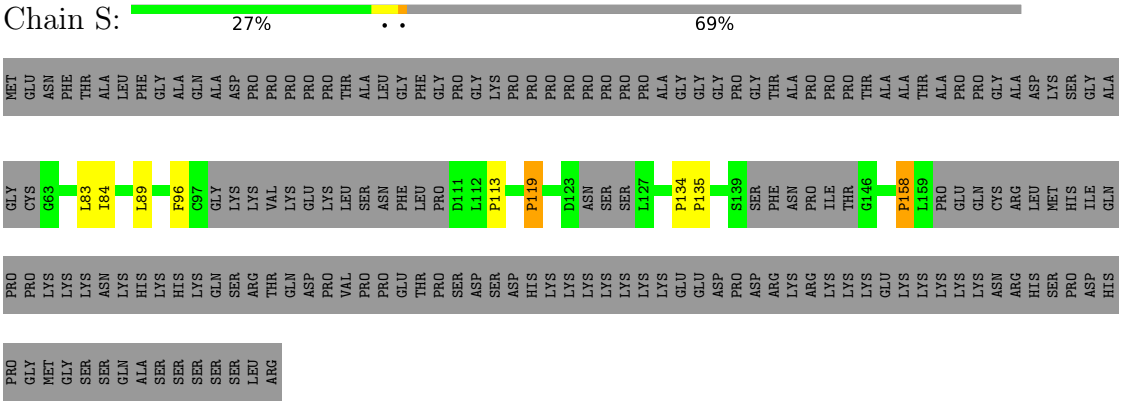
• Molecule 14: Mediator of RNA polymerase II transcription subunit 18

Chain R:



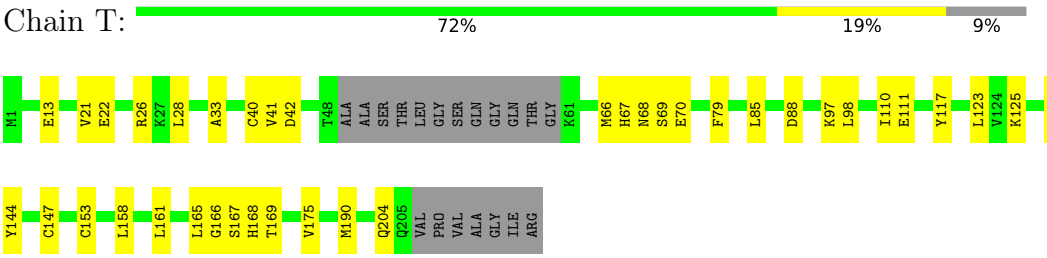
• Molecule 15: Mediator of RNA polymerase II transcription subunit 19

Chain S:



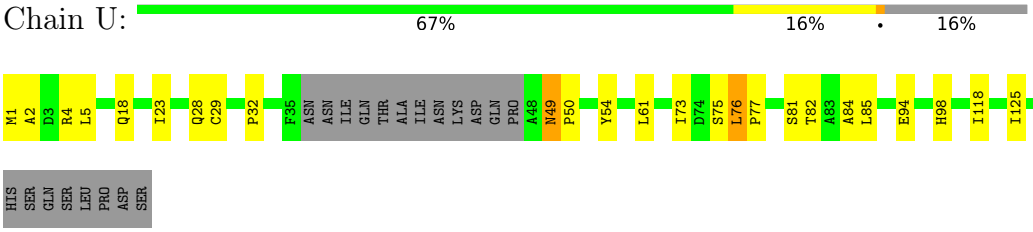
• Molecule 16: Mediator of RNA polymerase II transcription subunit 20

Chain T:



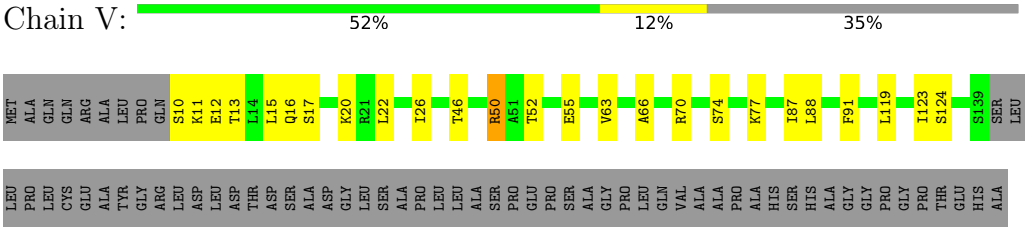
• Molecule 17: Mediator of RNA polymerase II transcription subunit 21

Chain U:



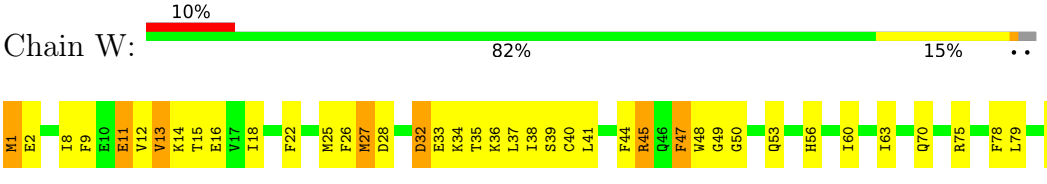
• Molecule 18: Mediator of RNA polymerase II transcription subunit 22

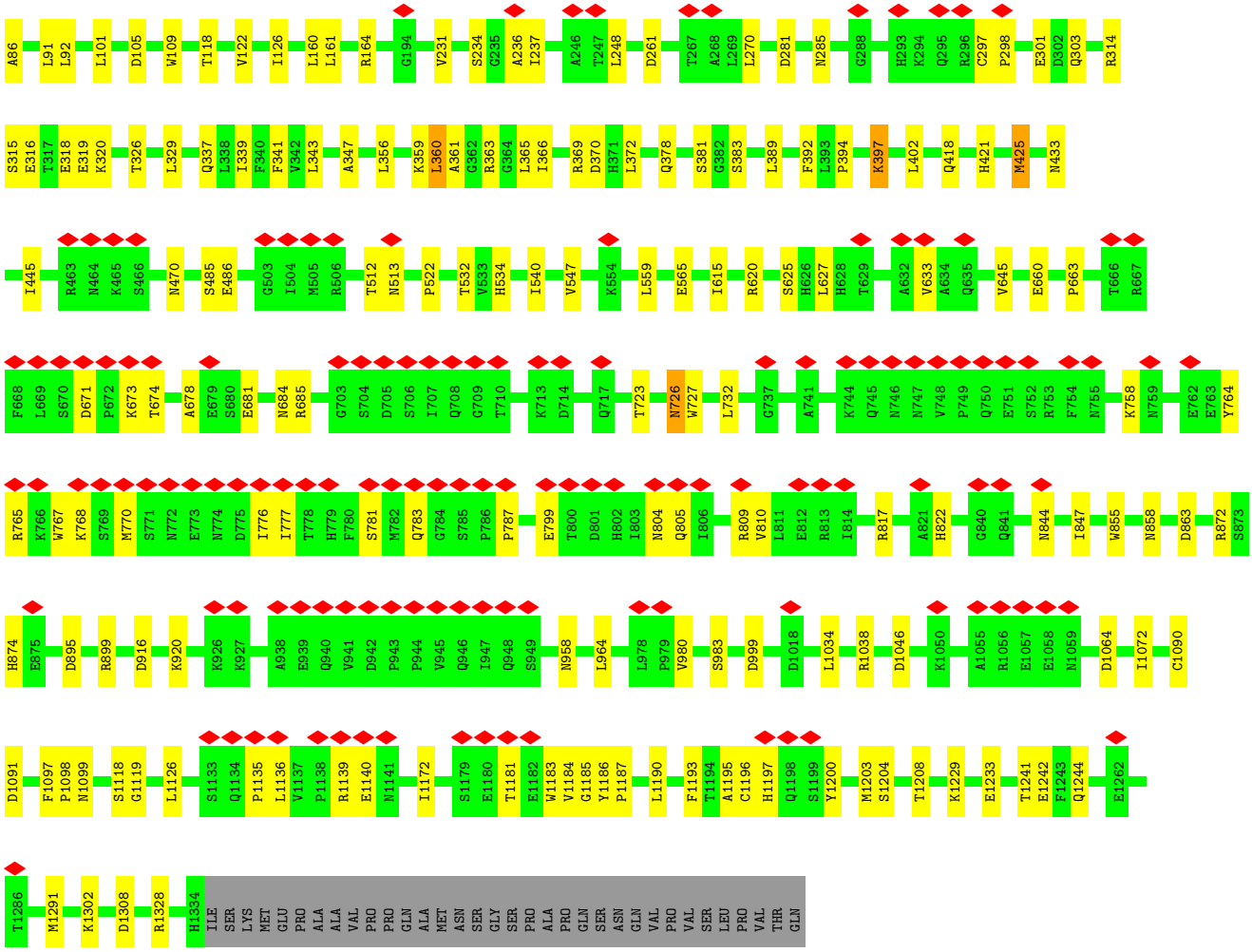
Chain V:



• Molecule 19: Mediator of RNA polymerase II transcription subunit 23

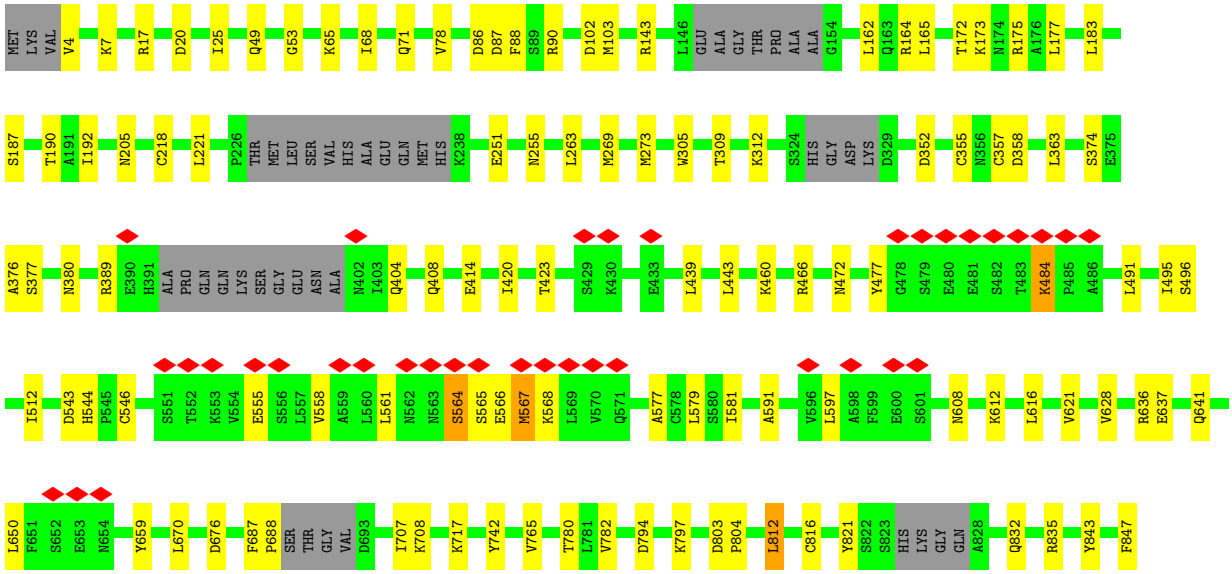
Chain W:

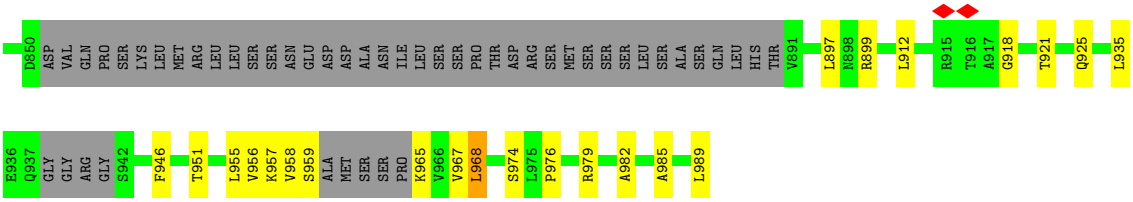




• Molecule 20: Mediator of RNA polymerase II transcription subunit 24

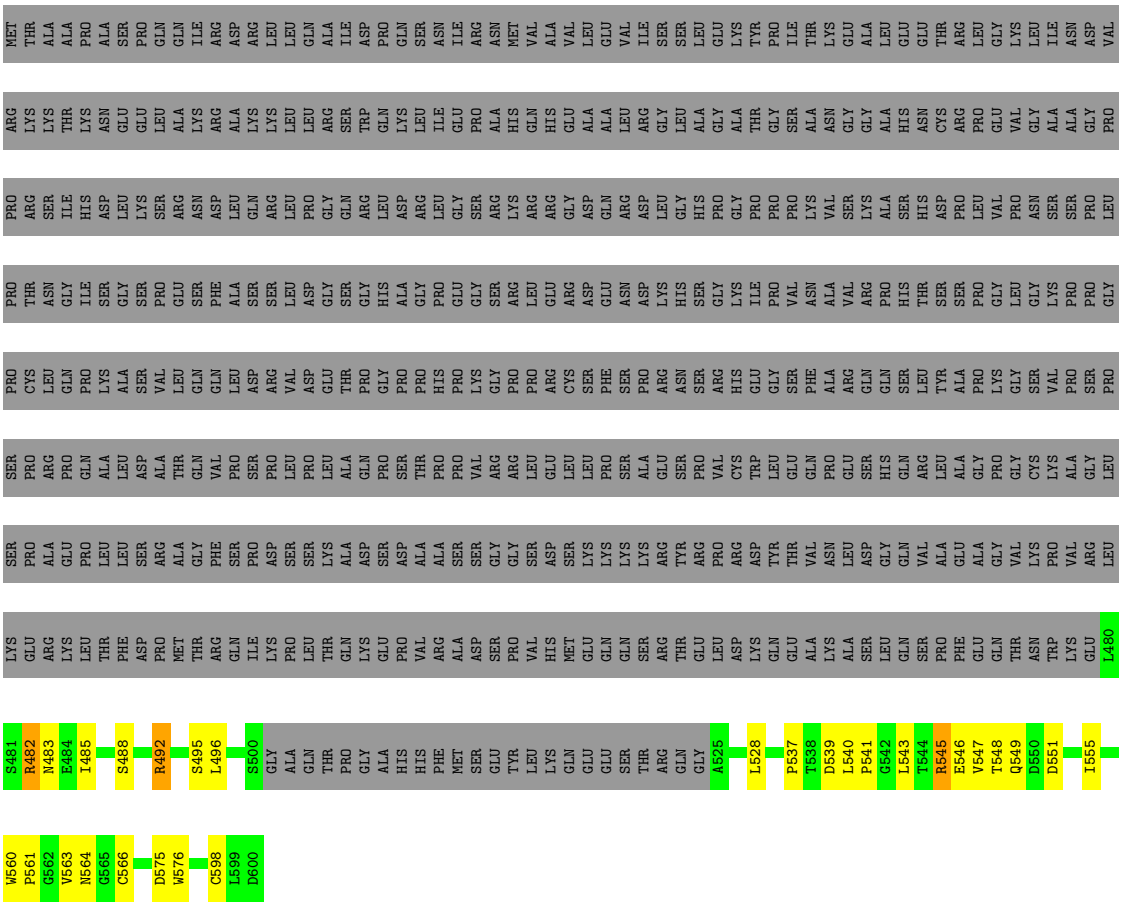
Chain X:





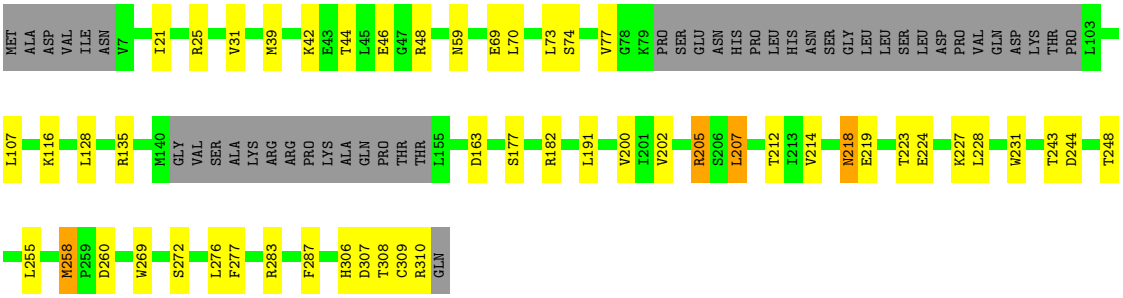
• Molecule 21: Mediator of RNA polymerase II transcription subunit 26

Chain Z:



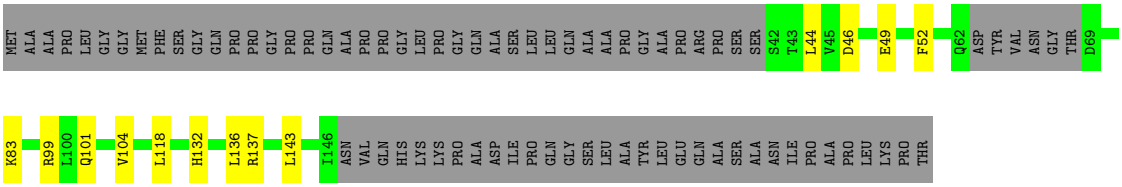
• Molecule 22: Mediator of RNA polymerase II transcription subunit 27

Chain 0:



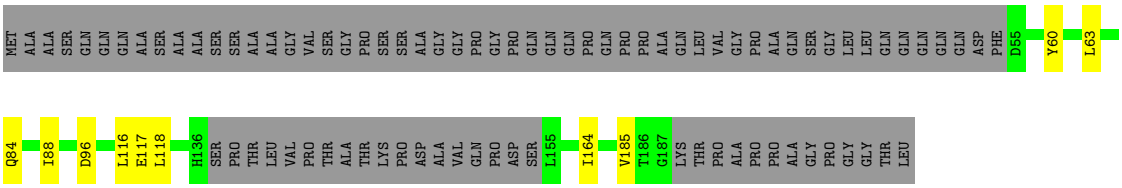
• Molecule 23: Mediator of RNA polymerase II transcription subunit 28

Chain 1:



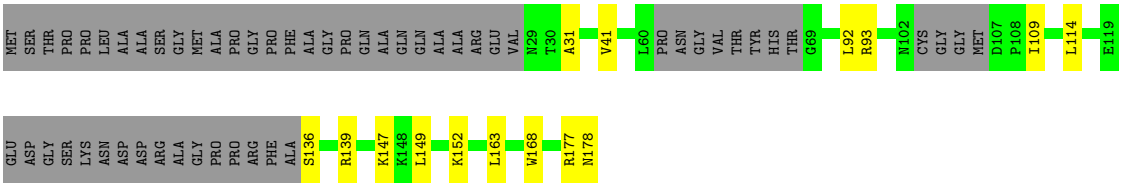
• Molecule 24: Mediator of RNA polymerase II transcription subunit 29

Chain 2:



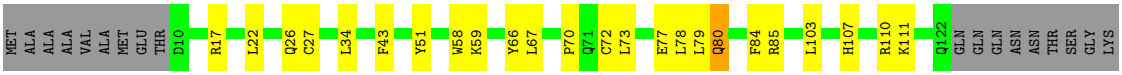
• Molecule 25: Mediator of RNA polymerase II transcription subunit 30

Chain 3:



• Molecule 26: Mediator of RNA polymerase II transcription subunit 31

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.452	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	539.648, 539.648, 539.648	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.108, 2.108, 2.108	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/3653	0.63	0/4961
3	D	0.41	0/1281	0.57	0/1718
4	F	0.37	0/1411	0.64	0/1916
5	G	0.51	0/1374	0.61	0/1847
6	H	0.35	0/1441	0.56	0/1946
7	I	0.37	0/612	0.58	0/815
8	J	0.33	0/849	0.54	1/1150 (0.1%)
9	K	0.43	0/885	0.53	0/1190
10	N	0.51	0/7923	0.65	11/10761 (0.1%)
11	O	0.59	0/1261	0.69	0/1731
12	P	0.70	0/3296	0.70	0/4476
13	Q	0.52	0/4444	0.61	0/6000
14	R	0.50	0/1562	0.60	0/2101
15	S	0.37	0/480	0.74	5/651 (0.8%)
16	T	0.58	0/1530	0.64	0/2066
17	U	0.53	0/927	0.65	0/1257
18	V	0.56	0/1072	0.65	0/1440
19	W	0.58	0/11056	0.62	0/15023
20	X	0.58	0/7191	0.62	0/9728
21	Z	0.51	0/781	0.65	0/1067
22	0	0.57	0/2201	0.61	0/2972
23	1	0.47	0/825	0.54	0/1107
24	2	0.47	0/911	0.56	0/1229
25	3	0.46	0/1029	0.54	0/1378
26	4	0.48	0/1013	0.61	0/1364
All	All	0.54	0/59008	0.62	17/79894 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	N	1351	PRO	N-CA-CB	7.45	112.24	103.30
10	N	1343	PRO	N-CA-CB	7.27	112.03	103.30
10	N	1355	PRO	N-CA-CB	6.91	111.60	103.30
8	J	31	PRO	N-CA-CB	6.54	111.16	103.30
10	N	1352	PRO	N-CA-CB	6.29	110.86	103.30
10	N	1326	PRO	N-CA-CB	6.13	110.66	103.30
15	S	135	PRO	N-CA-CB	6.04	110.55	103.30
10	N	1237	PRO	N-CA-CB	5.88	110.36	103.30
10	N	1255	PRO	N-CA-CB	5.83	110.30	103.30
15	S	119	PRO	N-CA-CB	5.81	110.28	103.30
15	S	134	PRO	N-CA-CB	5.79	110.25	103.30
15	S	113	PRO	N-CA-CB	5.74	110.18	103.30
10	N	1348	PRO	N-CA-CB	5.70	110.14	103.30
10	N	1344	PRO	N-CA-CB	5.67	110.10	103.30
10	N	74	PRO	N-CA-CB	5.63	110.06	103.30
15	S	158	PRO	N-CA-CB	5.62	110.05	103.30
10	N	1347	PRO	N-CA-CB	5.42	109.81	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3578	0	3522	62	0
2	B	100	0	22	0	0
3	D	1268	0	1305	23	0
4	F	1374	0	1357	34	0
5	G	1348	0	1373	31	0
6	H	1422	0	1440	17	0
7	I	605	0	628	9	0
8	J	840	0	718	8	0
9	K	879	0	886	18	0
10	N	7772	0	7557	161	0
11	O	1226	0	1217	20	0
12	P	3226	0	3240	55	0
13	Q	4361	0	4445	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	R	1532	0	1542	23	0
15	S	476	0	347	4	0
16	T	1499	0	1484	27	0
17	U	918	0	905	27	0
18	V	1063	0	1051	24	0
19	W	10774	0	10838	182	0
20	X	7061	0	7223	91	0
21	Z	765	0	728	20	0
22	0	2159	0	2176	44	0
23	1	817	0	818	13	0
24	2	899	0	908	10	0
25	3	1022	0	1054	14	0
26	4	986	0	965	26	0
27	0	1	0	0	0	0
All	All	57971	0	57749	867	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 7.

All (867) 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)
12:P:171:PHE:CZ	19:W:394:PRO:HA	1.29	1.58
5:G:18:ILE:HD11	26:4:51:TYR:OH	1.35	1.22
12:P:171:PHE:CE1	19:W:394:PRO:HA	1.74	1.20
12:P:171:PHE:CZ	19:W:394:PRO:CA	2.25	1.20
10:N:922:TYR:CE2	10:N:1215:ILE:HD13	1.76	1.18
10:N:659:LEU:HD11	19:W:18:ILE:HG21	1.26	1.16
10:N:885:LEU:HD21	10:N:1186:LEU:HD22	1.31	1.07
10:N:962:PHE:HB2	10:N:1210:PHE:CE2	1.88	1.06
10:N:932:GLY:HA2	10:N:1179:HIS:CE1	1.90	1.06
10:N:922:TYR:HE2	10:N:1215:ILE:HD13	0.83	1.00
10:N:885:LEU:HD21	10:N:1186:LEU:CD2	1.93	0.98
10:N:922:TYR:HE2	10:N:1215:ILE:CD1	1.76	0.98
10:N:934:VAL:HG11	10:N:1182:LEU:HD22	1.44	0.97
19:W:1:MET:SD	19:W:1:MET:N	2.35	0.97
19:W:38:ILE:HA	19:W:85:MET:HE1	1.47	0.96
12:P:171:PHE:CE1	19:W:394:PRO:CA	2.48	0.96
10:N:962:PHE:CG	10:N:1210:PHE:CD2	2.56	0.93
19:W:27:MET:SD	19:W:27:MET:N	2.34	0.92
10:N:918:PHE:CE1	10:N:1208:GLU:HG3	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:957:PRO:HB2	10:N:1217:ARG:NH2	1.90	0.87
5:G:18:ILE:CD1	26:4:51:TYR:OH	2.22	0.84
19:W:13:VAL:HG12	19:W:79:LEU:HD21	1.62	0.82
10:N:962:PHE:CB	10:N:1210:PHE:CE2	2.63	0.82
10:N:962:PHE:CD1	10:N:1210:PHE:CD2	2.67	0.82
18:V:10:SER:N	18:V:13:THR:HG1	1.76	0.82
10:N:587:LEU:HA	19:W:39:SER:HB2	1.63	0.80
12:P:171:PHE:HZ	19:W:394:PRO:CA	1.81	0.79
3:D:176:TYR:HB2	3:D:177:PRO:HD2	1.65	0.77
5:G:18:ILE:HD11	26:4:51:TYR:HH	1.49	0.77
6:H:22:LEU:HA	6:H:56:LEU:HD13	1.66	0.77
11:O:720:PRO:HD3	20:X:71:GLN:HG3	1.66	0.77
19:W:45:ARG:C	19:W:45:ARG:HD2	2.06	0.76
20:X:566:GLU:C	20:X:568:LYS:H	1.89	0.76
10:N:659:LEU:CD1	19:W:18:ILE:HG21	2.13	0.75
17:U:28:GLN:HE22	21:Z:482:ARG:HA	1.50	0.75
12:P:171:PHE:HZ	19:W:394:PRO:HA	0.98	0.75
10:N:918:PHE:CE1	10:N:1208:GLU:CG	2.70	0.74
1:A:221:ASN:ND2	1:A:249:ARG:HH21	1.86	0.74
10:N:962:PHE:CD1	10:N:1210:PHE:HD2	2.04	0.73
14:R:55:GLU:HG2	14:R:73:ARG:HG2	1.69	0.73
10:N:957:PRO:HB2	10:N:1217:ARG:HH22	1.54	0.72
10:N:957:PRO:HD2	10:N:1214:VAL:HG11	1.72	0.72
22:0:214:VAL:H	22:0:243:THR:HG22	1.53	0.72
13:Q:119:VAL:HG13	13:Q:127:LEU:HD21	1.72	0.72
19:W:14:LYS:O	19:W:18:ILE:HG23	1.90	0.72
14:R:55:GLU:OE1	14:R:71:ARG:HB3	1.88	0.71
3:D:177:PRO:HG3	26:4:27:CYS:HA	1.71	0.71
10:N:962:PHE:CG	10:N:1210:PHE:CE2	2.78	0.71
10:N:659:LEU:HD21	19:W:18:ILE:HG22	1.71	0.70
6:H:32:LYS:O	6:H:36:GLU:HB2	1.90	0.70
5:G:18:ILE:HD11	26:4:51:TYR:CZ	2.27	0.70
4:F:77:ILE:HB	4:F:102:ALA:H	1.57	0.69
9:K:112:GLU:O	9:K:116:GLU:HB2	1.92	0.69
5:G:126:TYR:CE2	17:U:76:LEU:HG	2.28	0.69
1:A:270:ILE:HG22	1:A:270:ILE:O	1.94	0.68
4:F:53:GLN:O	4:F:54:ARG:HG3	1.93	0.68
19:W:1291:MET:SD	19:W:1328:ARG:NH2	2.67	0.68
19:W:38:ILE:HG12	19:W:85:MET:HE3	1.76	0.67
1:A:62:LEU:HD22	3:D:66:LEU:HD22	1.76	0.67
10:N:918:PHE:HE1	10:N:1208:GLU:HG3	1.55	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:318:GLU:HG2	19:W:320:LYS:H	1.59	0.67
5:G:127:ARG:NH1	10:N:149:LEU:O	2.27	0.67
13:Q:595:GLN:NE2	13:Q:619:ARG:O	2.27	0.67
10:N:230:PHE:CZ	10:N:296:LEU:HD13	2.29	0.66
17:U:49:ASN:H	17:U:49:ASN:ND2	1.93	0.66
4:F:25:ASN:H	4:F:28:SER:HB3	1.58	0.66
9:K:35:LEU:HD22	13:Q:154:ALA:HA	1.76	0.66
17:U:82:THR:HG21	21:Z:540:LEU:H	1.61	0.66
10:N:587:LEU:HA	19:W:39:SER:CB	2.26	0.66
21:Z:555:ILE:HA	21:Z:564:ASN:HD21	1.61	0.66
1:A:313:VAL:HG12	1:A:414:GLN:HG2	1.77	0.66
3:D:34:LEU:HD22	7:I:99:LYS:HD3	1.78	0.66
5:G:95:ILE:HG21	5:G:105:ARG:HB3	1.79	0.65
4:F:74:GLN:HB3	4:F:78:LEU:HB3	1.78	0.65
19:W:45:ARG:HH11	19:W:45:ARG:HB3	1.60	0.65
20:X:912:LEU:HD22	20:X:958:VAL:HG21	1.77	0.65
10:N:957:PRO:HD2	10:N:1214:VAL:CG1	2.26	0.65
12:P:50:ASP:HA	12:P:59:THR:HG22	1.79	0.65
20:X:566:GLU:O	20:X:568:LYS:N	2.28	0.65
10:N:885:LEU:CD2	10:N:1186:LEU:HD22	2.19	0.65
6:H:181:LEU:HB3	14:R:168:LEU:HD12	1.79	0.64
19:W:1183:TRP:CZ2	19:W:1185:GLY:HA3	2.32	0.64
26:4:107:HIS:HA	26:4:110:ARG:HH21	1.62	0.64
20:X:143:ARG:HH22	20:X:205:ASN:HB2	1.62	0.64
20:X:968:LEU:HD22	20:X:985:ALA:HB3	1.79	0.64
19:W:1184:VAL:HG22	19:W:1184:VAL:O	1.98	0.64
18:V:22:LEU:HD12	18:V:26:ILE:HD13	1.79	0.63
22:0:74:SER:HA	24:2:60:TYR:HE2	1.62	0.63
10:N:589:GLN:HB3	19:W:27:MET:HA	1.81	0.63
13:Q:247:ILE:HD11	13:Q:294:LYS:HB3	1.78	0.63
19:W:281:ASP:OD1	19:W:281:ASP:N	2.31	0.63
10:N:932:GLY:HA2	10:N:1179:HIS:NE2	2.12	0.63
20:X:780:THR:HG22	20:X:816:CYS:HB3	1.80	0.63
10:N:957:PRO:CB	10:N:1217:ARG:NH2	2.61	0.63
20:X:567:MET:H	20:X:612:LYS:NZ	1.96	0.63
10:N:918:PHE:HE1	10:N:1208:GLU:CG	2.12	0.62
19:W:425:MET:SD	19:W:425:MET:N	2.72	0.62
10:N:936:ILE:HD11	10:N:963:LEU:HD22	1.81	0.62
10:N:1189:SER:O	10:N:1209:ARG:NH1	2.33	0.62
1:A:136:PRO:O	1:A:140:GLN:HB2	2.00	0.62
1:A:506:VAL:HG22	1:A:509:ARG:HH22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:844:CYS:O	22:0:116:LYS:NZ	2.32	0.62
19:W:1181:THR:O	19:W:1184:VAL:HB	2.00	0.62
20:X:637:GLU:O	20:X:641:GLN:NE2	2.31	0.62
3:D:113:GLN:NE2	5:G:167:CYS:SG	2.69	0.62
17:U:4:ARG:NH1	21:Z:566:CYS:SG	2.71	0.62
18:V:50:ARG:O	18:V:50:ARG:NH1	2.33	0.62
20:X:251:GLU:HG3	20:X:263:LEU:HD13	1.82	0.62
9:K:76:GLY:HA2	18:V:11:LYS:CE	2.28	0.61
19:W:41:LEU:HD12	19:W:41:LEU:O	1.99	0.61
4:F:171:ILE:HG22	10:N:263:ARG:HH11	1.65	0.61
10:N:923:CYS:HB2	10:N:953:PHE:CD1	2.34	0.61
1:A:359:HIS:HD2	1:A:361:MET:H	1.48	0.61
12:P:148:GLU:HB3	12:P:370:VAL:HG21	1.82	0.61
20:X:650:LEU:HB2	20:X:659:TYR:HE2	1.64	0.61
10:N:903:CYS:SG	10:N:904:PHE:N	2.74	0.61
20:X:484:LYS:HA	20:X:484:LYS:NZ	2.16	0.61
12:P:225:ASN:ND2	12:P:245:CYS:SG	2.74	0.61
12:P:443:LEU:HD23	12:P:457:LEU:HD21	1.82	0.60
19:W:48:TRP:C	19:W:50:GLY:H	2.05	0.60
4:F:82:ARG:HH21	4:F:94:PRO:HB3	1.66	0.60
12:P:171:PHE:CE1	19:W:394:PRO:HG3	2.37	0.60
13:Q:223:GLU:HB2	13:Q:246:GLN:HB2	1.84	0.60
13:Q:598:ARG:HG3	13:Q:620:GLY:H	1.65	0.60
20:X:414:GLU:OE2	20:X:460:LYS:NZ	2.34	0.60
10:N:659:LEU:HD21	19:W:18:ILE:CG2	2.31	0.60
10:N:801:ARG:HH21	23:1:83:LYS:HE3	1.66	0.60
4:F:129:ALA:HB1	13:Q:98:VAL:HG23	1.82	0.60
10:N:1316:CYS:HA	10:N:1339:CYS:H	1.65	0.60
12:P:166:PRO:HG2	12:P:169:THR:HG22	1.84	0.60
13:Q:141:PRO:O	13:Q:145:GLN:HB2	2.02	0.60
23:1:99:ARG:NH1	25:3:31:ALA:O	2.34	0.60
12:P:97:LEU:HD11	12:P:179:TRP:HB3	1.83	0.60
4:F:100:ILE:HG22	4:F:105:ILE:HG22	1.83	0.59
16:T:33:ALA:HB1	16:T:117:TYR:HB3	1.84	0.59
19:W:765:ARG:HA	19:W:768:LYS:HE2	1.84	0.59
10:N:954:TYR:HD2	10:N:1218:ARG:HH22	1.47	0.59
14:R:85:LEU:HG	14:R:114:LEU:HD11	1.84	0.59
17:U:81:SER:HA	17:U:85:LEU:HD23	1.85	0.59
19:W:28:ASP:O	19:W:32:ASP:HB2	2.02	0.59
19:W:32:ASP:O	19:W:36:LYS:HG3	2.01	0.59
18:V:16:GLN:O	18:V:20:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:524:ASN:HA	19:W:45:ARG:HH22	1.67	0.59
3:D:96:LEU:HD22	7:I:121:LEU:HB3	1.84	0.59
11:O:690:LEU:HB2	11:O:709:LYS:HB2	1.84	0.59
19:W:359:LYS:O	19:W:361:ALA:N	2.33	0.59
1:A:107:MET:HG3	1:A:157:LEU:HB3	1.85	0.58
5:G:15:MET:SD	5:G:15:MET:N	2.76	0.58
19:W:53:GLN:O	19:W:56:HIS:HB2	2.03	0.58
23:1:104:VAL:HG11	25:3:114:LEU:HD22	1.84	0.58
6:H:156:LYS:HA	6:H:159:ARG:HH21	1.67	0.58
20:X:404:GLN:NE2	20:X:408:GLN:OE1	2.37	0.58
19:W:726:ASN:ND2	19:W:726:ASN:H	2.02	0.58
19:W:48:TRP:O	19:W:50:GLY:N	2.37	0.58
19:W:764:TYR:OH	19:W:799:GLU:OE2	2.22	0.58
4:F:120:LEU:HB2	18:V:52:THR:HG22	1.86	0.58
26:4:59:LYS:NZ	26:4:77:GLU:HG2	2.18	0.58
8:J:92:ASN:HD21	15:S:83:LEU:H	1.52	0.58
10:N:687:ILE:HD12	10:N:687:ILE:N	2.18	0.58
16:T:110:ILE:HD11	16:T:129:VAL:HG12	1.86	0.58
20:X:687:PHE:HB2	20:X:688:PRO:HD3	1.86	0.58
10:N:941:TYR:HE2	10:N:1171:ALA:HB3	1.69	0.57
13:Q:599:ASN:ND2	13:Q:616:SER:O	2.37	0.57
17:U:61:LEU:HD22	21:Z:496:LEU:HD21	1.85	0.57
10:N:718:ARG:NH2	10:N:752:LEU:O	2.37	0.57
19:W:369:ARG:NH1	19:W:402:LEU:O	2.37	0.57
20:X:439:LEU:HB3	20:X:495:ILE:HG21	1.86	0.57
20:X:566:GLU:C	20:X:568:LYS:N	2.57	0.57
20:X:968:LEU:CD2	20:X:985:ALA:HB3	2.34	0.57
22:0:307:ASP:O	22:0:310:ARG:NH1	2.37	0.57
9:K:75:THR:HG23	9:K:77:GLN:H	1.69	0.57
20:X:581:ILE:HD11	20:X:616:LEU:HD22	1.87	0.57
13:Q:186:GLU:HG2	13:Q:189:ARG:HH21	1.69	0.57
16:T:68:ASN:ND2	16:T:190:MET:SD	2.78	0.57
1:A:167:ASN:O	1:A:170:LYS:HB2	2.05	0.57
1:A:367:LEU:HD13	1:A:509:ARG:HH11	1.70	0.57
5:G:96:LEU:HD21	10:N:132:THR:HG21	1.87	0.57
19:W:855:TRP:O	19:W:858:ASN:ND2	2.37	0.57
26:4:43:PHE:HA	26:4:85:ARG:HH21	1.70	0.57
5:G:55:ILE:HG23	13:Q:1:MET:HG2	1.87	0.57
19:W:35:THR:HA	19:W:38:ILE:HG13	1.87	0.57
19:W:45:ARG:HD2	19:W:45:ARG:O	2.04	0.57
4:F:47:ASN:HB3	4:F:51:LYS:HZ1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:379:ILE:HD13	13:Q:427:LEU:HD11	1.87	0.56
11:O:625:VAL:HG23	11:O:634:PHE:HZ	1.70	0.56
6:H:53:SER:O	6:H:57:ASN:HB2	2.06	0.56
12:P:243:LYS:NZ	12:P:245:CYS:SG	2.79	0.56
16:T:153:CYS:O	16:T:153:CYS:SG	2.62	0.56
19:W:1034:LEU:HD22	19:W:1038:ARG:HD2	1.86	0.56
20:X:955:LEU:HB3	20:X:967:VAL:HG21	1.87	0.56
23:1:46:ASP:OD1	25:3:93:ARG:NH1	2.39	0.56
10:N:341:ASN:HB2	10:N:343:GLN:HE21	1.69	0.56
22:0:283:ARG:HD3	22:0:309:CYS:HB3	1.87	0.56
12:P:232:ASP:OD1	12:P:232:ASP:N	2.31	0.56
10:N:657:LEU:HD23	10:N:682:ILE:HD12	1.88	0.56
10:N:655:VAL:HG22	10:N:658:ARG:HH21	1.71	0.56
12:P:251:GLU:O	12:P:251:GLU:CD	2.44	0.56
4:F:41:TYR:OH	4:F:51:LYS:NZ	2.38	0.56
20:X:172:THR:HB	20:X:965:LYS:HE2	1.88	0.56
19:W:261:ASP:N	19:W:261:ASP:OD1	2.38	0.56
16:T:147:CYS:SG	16:T:153:CYS:HB3	2.46	0.55
18:V:10:SER:O	18:V:13:THR:OG1	2.25	0.55
19:W:895:ASP:O	19:W:899:ARG:NH1	2.35	0.55
1:A:105:SER:OG	1:A:167:ASN:ND2	2.38	0.55
10:N:962:PHE:CD1	10:N:1210:PHE:CE2	2.94	0.55
14:R:27:VAL:HG21	14:R:35:LEU:HD22	1.88	0.55
19:W:231:VAL:O	19:W:1099:ASN:ND2	2.39	0.55
20:X:376:ALA:O	20:X:380:ASN:ND2	2.38	0.55
10:N:168:ARG:NH2	13:Q:14:ALA:O	2.39	0.55
17:U:81:SER:HB3	21:Z:563:VAL:HG22	1.87	0.55
11:O:765:ASP:OD2	11:O:766:LYS:NZ	2.40	0.55
10:N:166:TYR:HE1	26:4:73:LEU:HB2	1.71	0.55
19:W:1072:ILE:HD11	19:W:1126:LEU:HD22	1.89	0.55
19:W:433:ASN:ND2	19:W:445:ILE:O	2.35	0.55
10:N:922:TYR:CE2	10:N:1215:ILE:CD1	2.66	0.54
19:W:958:ASN:OD1	19:W:958:ASN:N	2.40	0.54
19:W:625:SER:HB2	19:W:674:THR:HG22	1.89	0.54
22:0:207:LEU:O	22:0:207:LEU:HD22	2.08	0.54
10:N:524:ASN:O	10:N:526:SER:N	2.41	0.54
10:N:916:LEU:HB2	10:N:924:ILE:HG23	1.88	0.54
19:W:781:SER:O	19:W:783:GLN:NE2	2.41	0.54
19:W:109:TRP:HB2	19:W:160:LEU:HD21	1.90	0.54
1:A:163:LEU:HD13	1:A:173:MET:HE2	1.89	0.54
5:G:90:LEU:HD21	8:J:109:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:962:PHE:HB2	10:N:1210:PHE:HE2	1.64	0.54
19:W:627:LEU:HD22	19:W:645:VAL:HG23	1.89	0.54
20:X:358:ASP:OD1	20:X:389:ARG:NE	2.41	0.54
9:K:19:ARG:HG3	9:K:58:HIS:HE1	1.73	0.53
17:U:29:CYS:SG	17:U:29:CYS:O	2.66	0.53
19:W:522:PRO:HG3	19:W:565:GLU:HG2	1.90	0.53
4:F:176:ARG:HH22	10:N:309:HIS:HD2	1.56	0.53
10:N:959:LEU:O	10:N:963:LEU:HG	2.08	0.53
11:O:674:ILE:H	13:Q:611:GLN:HE22	1.56	0.53
19:W:11:GLU:C	19:W:11:GLU:CD	2.67	0.53
20:X:472:ASN:ND2	20:X:496:SER:OG	2.42	0.53
1:A:431:LYS:HG3	1:A:432:GLU:HG2	1.89	0.53
10:N:165:SER:OG	10:N:166:TYR:N	2.40	0.53
22:0:218:ASN:H	22:0:218:ASN:ND2	2.06	0.53
6:H:81:LEU:HD11	6:H:102:HIS:HA	1.90	0.53
13:Q:404:ARG:HH22	22:0:224:GLU:HG3	1.73	0.53
19:W:1302:LYS:NZ	19:W:1308:ASP:OD1	2.41	0.53
10:N:202:ARG:HD3	10:N:236:VAL:HG11	1.90	0.53
10:N:966:PHE:CE2	10:N:1185:LEU:HD13	2.44	0.53
19:W:339:ILE:O	19:W:343:LEU:HB2	2.08	0.53
19:W:681:GLU:OE2	19:W:685:ARG:NH1	2.41	0.53
4:F:53:GLN:O	4:F:54:ARG:CG	2.56	0.53
5:G:136:ARG:NH1	5:G:140:GLU:OE2	2.42	0.53
11:O:673:SER:OG	11:O:674:ILE:N	2.42	0.53
20:X:628:VAL:HG13	20:X:636:ARG:HG2	1.91	0.53
22:0:107:LEU:HD13	24:2:164:ILE:HG23	1.91	0.53
4:F:8:ASP:OD1	4:F:8:ASP:N	2.40	0.53
10:N:789:ASP:OD1	10:N:789:ASP:N	2.42	0.53
19:W:101:LEU:HD22	19:W:118:THR:HG23	1.90	0.53
20:X:175:ARG:HH21	20:X:221:LEU:HD22	1.73	0.53
20:X:976:PRO:HA	20:X:979:ARG:HE	1.73	0.53
22:0:200:VAL:HG22	22:0:214:VAL:HG22	1.91	0.53
1:A:184:LEU:HD21	1:A:404:VAL:HG11	1.90	0.52
10:N:385:LEU:HD23	10:N:407:ALA:HA	1.92	0.52
11:O:722:GLU:HG2	11:O:737:ILE:HD12	1.91	0.52
18:V:10:SER:OG	18:V:13:THR:HG23	2.09	0.52
13:Q:262:GLN:HE21	13:Q:340:GLN:HE21	1.56	0.52
1:A:173:MET:HG2	1:A:299:LEU:HD13	1.90	0.52
3:D:154:ARG:NH1	5:G:50:GLN:OE1	2.43	0.52
9:K:76:GLY:HA2	18:V:11:LYS:HE2	1.90	0.52
22:0:69:GLU:HA	22:0:69:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:161:LEU:HD22	19:W:164:ARG:HD2	1.91	0.52
1:A:258:THR:OG1	1:A:259:ILE:N	2.42	0.52
7:I:104:MET:N	7:I:105:PRO:HD2	2.25	0.52
19:W:418:GLN:HA	19:W:421:HIS:HD2	1.75	0.52
26:4:80:GLN:HE21	26:4:80:GLN:HA	1.74	0.52
10:N:726:PHE:O	10:N:742:SER:HA	2.10	0.52
13:Q:9:ILE:HD12	13:Q:11:ILE:HD11	1.91	0.52
23:1:49:GLU:OE2	25:3:93:ARG:NH2	2.43	0.52
8:J:61:ILE:O	10:N:50:ARG:N	2.43	0.52
12:P:304:SER:OG	12:P:349:ASP:O	2.28	0.52
10:N:528:HIS:HB3	10:N:530:ILE:HG22	1.91	0.52
10:N:958:GLY:O	10:N:1210:PHE:HZ	1.93	0.52
11:O:697:HIS:HA	20:X:957:LYS:HZ2	1.75	0.52
14:R:16:ILE:HD11	14:R:176:PRO:HB3	1.92	0.52
13:Q:467:ILE:HG22	22:0:231:TRP:HZ2	1.75	0.52
18:V:74:SER:HA	18:V:77:LYS:HD2	1.92	0.52
19:W:633:VAL:O	19:W:817:ARG:NH2	2.43	0.52
19:W:767:TRP:HE1	19:W:804:ASN:HD21	1.58	0.51
20:X:86:ASP:O	20:X:88:PHE:N	2.43	0.51
10:N:932:GLY:C	10:N:1179:HIS:NE2	2.63	0.51
12:P:91:GLN:NE2	12:P:137:LEU:O	2.43	0.51
19:W:378:GLN:HE22	19:W:532:THR:HA	1.75	0.51
1:A:365:ALA:HB3	1:A:372:HIS:HB2	1.92	0.51
10:N:1219:HIS:HD2	10:N:1222:ARG:HH11	1.58	0.51
10:N:202:ARG:NH1	10:N:240:ASP:O	2.43	0.51
22:0:163:ASP:OD1	22:0:182:ARG:NH2	2.39	0.51
3:D:44:LEU:HD21	3:D:65:VAL:HG23	1.91	0.51
19:W:16:GLU:HG2	19:W:78:PHE:CE1	2.46	0.51
1:A:270:ILE:O	1:A:270:ILE:CG2	2.59	0.51
1:A:446:SER:OG	1:A:447:GLU:N	2.43	0.51
5:G:41:SER:OG	5:G:42:TYR:N	2.44	0.51
12:P:437:SER:OG	12:P:438:TRP:N	2.43	0.51
12:P:443:LEU:HD12	12:P:443:LEU:C	2.30	0.51
18:V:119:LEU:HD22	23:1:143:LEU:HD11	1.91	0.51
22:0:74:SER:HA	24:2:60:TYR:CE2	2.45	0.51
3:D:47:MET:HA	3:D:50:ILE:HG22	1.91	0.51
7:I:65:PHE:HA	7:I:95:GLN:HE22	1.75	0.51
12:P:398:SER:OG	12:P:400:GLN:NE2	2.43	0.51
17:U:49:ASN:N	17:U:50:PRO:HD2	2.26	0.51
19:W:86:ALA:HB1	19:W:92:LEU:HD13	1.92	0.51
19:W:1118:SER:OG	19:W:1119:GLY:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:115:ILE:HA	13:Q:112:LEU:HD21	1.92	0.51
10:N:174:ARG:HG3	26:4:78:LEU:HD21	1.92	0.51
19:W:1200:TYR:CD2	19:W:1200:TYR:O	2.64	0.51
13:Q:551:PHE:HD1	13:Q:569:ILE:HG22	1.75	0.51
22:0:25:ARG:NH2	24:2:117:GLU:OE1	2.38	0.51
13:Q:509:GLY:HA2	22:0:248:THR:HG21	1.93	0.51
15:S:84:ILE:HG23	15:S:89:LEU:HB3	1.92	0.51
19:W:1185:GLY:O	19:W:1186:TYR:C	2.50	0.51
3:D:121:LEU:HD22	5:G:160:VAL:HG11	1.93	0.50
1:A:430:LEU:H	1:A:430:LEU:HD23	1.77	0.50
10:N:957:PRO:CB	10:N:1217:ARG:HH22	2.21	0.50
19:W:1241:THR:OG1	19:W:1242:GLU:N	2.44	0.50
13:Q:597:PRO:HA	13:Q:619:ARG:HA	1.94	0.50
11:O:713:LYS:O	20:X:25:ILE:HG23	2.11	0.50
14:R:184:ASP:HA	14:R:187:LYS:HE3	1.93	0.50
19:W:726:ASN:ND2	19:W:726:ASN:N	2.60	0.50
22:0:218:ASN:ND2	22:0:218:ASN:N	2.58	0.50
10:N:796:ILE:O	10:N:816:LYS:NZ	2.41	0.50
18:V:12:GLU:HG3	18:V:16:GLN:NE2	2.26	0.50
20:X:20:ASP:N	20:X:20:ASP:OD1	2.44	0.50
26:4:73:LEU:O	26:4:77:GLU:HG3	2.12	0.50
1:A:465:VAL:HG22	1:A:479:LEU:HD12	1.93	0.50
4:F:38:ASN:O	4:F:43:ARG:NH1	2.44	0.50
19:W:25:MET:HA	19:W:25:MET:CE	2.41	0.50
19:W:872:ARG:HB3	19:W:874:HIS:HD2	1.76	0.50
10:N:485:ASP:OD1	10:N:485:ASP:N	2.44	0.50
10:N:589:GLN:HE21	19:W:36:LYS:HG2	1.77	0.50
12:P:171:PHE:CE1	19:W:394:PRO:CG	2.95	0.50
19:W:1172:ILE:O	19:W:1244:GLN:NE2	2.41	0.50
13:Q:495:LEU:HD22	13:Q:504:VAL:HG22	1.94	0.49
19:W:337:GLN:HE21	19:W:341:PHE:HE2	1.59	0.49
20:X:555:GLU:HA	20:X:558:VAL:HG12	1.94	0.49
9:K:109:ARG:HG2	9:K:113:GLN:HE21	1.77	0.49
10:N:713:GLN:HB3	13:Q:550:SER:HA	1.93	0.49
10:N:885:LEU:HD21	10:N:1186:LEU:HD23	1.89	0.49
19:W:70:GLN:HG3	19:W:75:ARG:HG2	1.94	0.49
19:W:366:ILE:HG23	19:W:369:ARG:HD3	1.94	0.49
20:X:374:SER:O	20:X:377:SER:OG	2.30	0.49
23:1:118:LEU:HD22	25:3:149:LEU:HD21	1.93	0.49
3:D:154:ARG:NH2	26:4:66:TYR:O	2.44	0.49
14:R:145:VAL:HG22	14:R:169:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:33:GLU:HA	19:W:36:LYS:HD2	1.94	0.49
19:W:999:ASP:OD1	19:W:999:ASP:N	2.41	0.49
26:4:58:TRP:HB3	26:4:67:LEU:HD11	1.94	0.49
14:R:29:ASP:OD1	14:R:29:ASP:N	2.45	0.49
19:W:9:PHE:O	19:W:13:VAL:HG13	2.11	0.49
19:W:726:ASN:N	19:W:726:ASN:HD22	2.11	0.49
9:K:71:THR:HA	18:V:15:LEU:HD13	1.94	0.49
10:N:393:ASP:OD1	10:N:393:ASP:N	2.43	0.49
19:W:38:ILE:HG12	19:W:85:MET:CE	2.41	0.49
10:N:845:SER:OG	10:N:846:ASN:N	2.45	0.49
3:D:111:GLN:HE21	17:U:125:ILE:HG22	1.77	0.49
5:G:17:TYR:HD2	5:G:19:LYS:HG2	1.76	0.49
4:F:53:GLN:C	4:F:54:ARG:HG3	2.32	0.49
14:R:50:THR:HA	14:R:133:GLY:O	2.13	0.49
19:W:13:VAL:HA	19:W:78:PHE:HE2	1.77	0.49
19:W:980:VAL:O	19:W:983:SER:OG	2.31	0.49
21:Z:539:ASP:HA	21:Z:545:ARG:HD3	1.95	0.49
10:N:534:SER:O	10:N:537:LYS:NZ	2.40	0.49
21:Z:563:VAL:O	21:Z:576:TRP:NE1	2.42	0.49
1:A:278:HIS:HD2	1:A:281:ASP:HB2	1.78	0.49
7:I:88:ASN:N	7:I:88:ASN:OD1	2.46	0.49
12:P:38:ALA:HA	12:P:435:GLN:HE21	1.78	0.49
12:P:51:LEU:HB2	12:P:58:LEU:HB3	1.95	0.49
13:Q:35:SER:OG	13:Q:42:ARG:NH2	2.46	0.49
13:Q:89:GLN:O	13:Q:91:SER:N	2.43	0.49
19:W:1187:PRO:HA	19:W:1190:LEU:HB3	1.94	0.49
20:X:968:LEU:HD21	20:X:982:ALA:HA	1.95	0.49
3:D:165:LEU:HD13	17:U:1:MET:HG2	1.95	0.48
4:F:107:GLN:NE2	4:F:108:ALA:O	2.46	0.48
9:K:76:GLY:HA2	18:V:11:LYS:HE3	1.94	0.48
4:F:50:VAL:HG22	4:F:59:HIS:HB3	1.94	0.48
4:F:84:GLN:HG3	4:F:94:PRO:HA	1.95	0.48
10:N:932:GLY:CA	10:N:1179:HIS:NE2	2.77	0.48
11:O:635:ASN:N	11:O:635:ASN:OD1	2.42	0.48
17:U:94:GLU:O	17:U:98:HIS:ND1	2.35	0.48
22:0:21:ILE:HD13	24:2:116:LEU:HB3	1.95	0.48
1:A:366:ALA:HB2	1:A:430:LEU:HD22	1.96	0.48
5:G:57:ARG:NH2	5:G:125:GLU:O	2.47	0.48
9:K:112:GLU:OE2	23:1:137:ARG:NH2	2.42	0.48
14:R:107:ASP:OD1	14:R:107:ASP:N	2.46	0.48
23:1:101:GLN:NE2	25:3:109:ILE:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:658:ARG:HH22	19:W:22:PHE:HB2	1.79	0.48
10:N:703:ARG:O	13:Q:614:LYS:NZ	2.37	0.48
4:F:62:GLN:HG3	4:F:63:MET:HG2	1.96	0.48
19:W:48:TRP:C	19:W:50:GLY:N	2.67	0.48
1:A:377:ASN:ND2	1:A:441:GLU:OE2	2.44	0.48
8:J:82:LYS:HG2	15:S:96:PHE:HB3	1.95	0.48
10:N:166:TYR:CE2	26:4:70:PRO:HB2	2.48	0.48
10:N:185:LYS:O	10:N:187:GLU:N	2.45	0.48
17:U:76:LEU:HB2	17:U:77:PRO:HD2	1.96	0.48
1:A:443:CYS:SG	1:A:451:SER:OG	2.64	0.48
13:Q:89:GLN:HG2	13:Q:90:PRO:HD2	1.96	0.48
13:Q:459:GLN:NE2	13:Q:482:GLN:OE1	2.46	0.48
13:Q:487:ILE:HD11	22:0:135:ARG:HG2	1.96	0.48
4:F:72:HIS:HB3	4:F:80:ILE:HD13	1.94	0.48
17:U:61:LEU:HD11	21:Z:492:ARG:HG3	1.94	0.48
19:W:105:ASP:OD1	19:W:105:ASP:N	2.46	0.48
20:X:355:CYS:SG	20:X:357:CYS:O	2.72	0.48
20:X:621:VAL:HG11	20:X:670:LEU:HD22	1.96	0.48
10:N:687:ILE:HD12	10:N:687:ILE:H	1.77	0.48
13:Q:95:TRP:HE3	13:Q:98:VAL:HG11	1.79	0.48
19:W:777:ILE:HA	19:W:810:VAL:HG22	1.95	0.48
20:X:544:HIS:HD2	20:X:546:CYS:H	1.62	0.48
5:G:110:GLU:O	5:G:113:LYS:HB3	2.14	0.47
19:W:122:VAL:O	19:W:126:ILE:HB	2.13	0.47
6:H:182:VAL:HG11	14:R:202:ILE:HD13	1.96	0.47
9:K:104:LEU:HD21	18:V:123:ILE:HD11	1.96	0.47
10:N:525:TYR:CG	10:N:525:TYR:O	2.67	0.47
20:X:968:LEU:CD2	20:X:982:ALA:HA	2.44	0.47
10:N:440:VAL:HG13	10:N:452:LEU:HB3	1.95	0.47
12:P:367:ASP:HA	12:P:370:VAL:HG22	1.96	0.47
1:A:223:LYS:NZ	1:A:248:SER:O	2.44	0.47
1:A:379:ASP:HA	1:A:387:SER:HB3	1.96	0.47
4:F:176:ARG:HH22	10:N:309:HIS:CD2	2.32	0.47
10:N:589:GLN:NE2	19:W:36:LYS:HG2	2.29	0.47
12:P:88:GLU:OE2	12:P:288:ARG:NH1	2.47	0.47
13:Q:637:TYR:OH	23:1:99:ARG:NE	2.48	0.47
21:Z:488:SER:OG	21:Z:492:ARG:NH1	2.47	0.47
5:G:21:TYR:HB3	5:G:33:LYS:HE3	1.96	0.47
18:V:12:GLU:HG3	18:V:16:GLN:HE21	1.80	0.47
19:W:234:SER:HB2	19:W:660:GLU:HG3	1.97	0.47
22:0:73:LEU:O	22:0:77:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HB3	1:A:509:ARG:HD3	1.97	0.47
4:F:77:ILE:HD12	4:F:101:ILE:HG23	1.96	0.47
5:G:107:GLU:O	5:G:111:ASP:N	2.47	0.47
12:P:24:TRP:HD1	12:P:51:LEU:HD12	1.79	0.47
12:P:191:SER:HA	12:P:200:LEU:O	2.15	0.47
16:T:166:GLY:O	16:T:169:THR:OG1	2.32	0.47
1:A:468:ASP:OD1	1:A:476:SER:OG	2.28	0.47
3:D:174:ARG:HB2	3:D:178:THR:HG22	1.96	0.47
9:K:104:LEU:HD22	23:1:136:LEU:HD22	1.97	0.47
14:R:156:ASN:OD1	14:R:159:SER:N	2.43	0.47
19:W:360:LEU:HD13	19:W:402:LEU:HD21	1.95	0.47
19:W:1229:LYS:O	19:W:1233:GLU:HB2	2.14	0.47
20:X:352:ASP:HA	20:X:355:CYS:SG	2.55	0.47
10:N:166:TYR:CE1	26:4:73:LEU:HB2	2.49	0.47
10:N:907:LEU:HD11	24:2:118:LEU:HD13	1.96	0.47
10:N:925:ASP:OD2	10:N:937:ARG:NH1	2.48	0.47
14:R:130:VAL:HB	14:R:149:PHE:HB2	1.97	0.47
19:W:1090:CYS:SG	19:W:1091:ASP:N	2.88	0.47
20:X:255:ASN:OD1	20:X:255:ASN:N	2.47	0.47
22:0:205:ARG:O	22:0:205:ARG:HD3	2.15	0.47
13:Q:595:GLN:HB2	13:Q:622:PHE:CE1	2.50	0.47
19:W:270:LEU:HD23	19:W:303:GLN:HG3	1.96	0.47
19:W:787:PRO:HB3	19:W:822:HIS:CD2	2.49	0.47
20:X:566:GLU:OE1	20:X:566:GLU:N	2.48	0.47
20:X:843:TYR:HD1	20:X:847:PHE:HE2	1.62	0.47
1:A:214:ARG:NH2	1:A:216:GLY:O	2.48	0.47
13:Q:595:GLN:HG3	13:Q:621:PRO:O	2.15	0.47
14:R:109:ALA:N	16:T:88:ASP:OD1	2.47	0.47
16:T:144:TYR:HE2	16:T:147:CYS:HG	1.61	0.47
16:T:167:SER:OG	16:T:168:HIS:N	2.48	0.47
19:W:863:ASP:OD1	19:W:863:ASP:N	2.45	0.47
22:0:269:TRP:O	22:0:272:SER:OG	2.31	0.47
1:A:278:HIS:CD2	1:A:281:ASP:HB2	2.50	0.46
12:P:40:SER:OG	12:P:42:ARG:O	2.24	0.46
20:X:543:ASP:OD1	20:X:543:ASP:N	2.48	0.46
1:A:67:LYS:HE3	1:A:83:SER:HB3	1.97	0.46
10:N:751:ASN:ND2	10:N:755:GLU:O	2.49	0.46
11:O:679:GLN:HG2	13:Q:610:LEU:HA	1.98	0.46
11:O:720:PRO:CD	20:X:71:GLN:HG3	2.41	0.46
22:0:218:ASN:N	22:0:218:ASN:HD22	2.14	0.46
12:P:171:PHE:HE2	19:W:397:LYS:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:207:CYS:HB3	12:P:242:TYR:HE2	1.80	0.46
12:P:266:ARG:HH11	12:P:341:ILE:HD13	1.80	0.46
20:X:847:PHE:HB2	20:X:899:ARG:HG2	1.97	0.46
21:Z:560:TRP:HD1	21:Z:561:PRO:HD2	1.80	0.46
26:4:34:LEU:HD11	26:4:79:LEU:HD11	1.98	0.46
19:W:615:ILE:O	19:W:620:ARG:NH2	2.48	0.46
1:A:359:HIS:CD2	1:A:361:MET:H	2.32	0.46
1:A:408:LEU:HD23	1:A:411:ILE:HD12	1.98	0.46
4:F:172:PHE:O	4:F:175:GLN:NE2	2.46	0.46
17:U:49:ASN:H	17:U:49:ASN:HD22	1.63	0.46
10:N:336:SER:HB2	10:N:358:THR:HG22	1.97	0.46
10:N:515:ILE:HD11	22:0:308:THR:HB	1.98	0.46
19:W:485:SER:OG	19:W:486:GLU:N	2.49	0.46
22:0:73:LEU:HA	22:0:73:LEU:HD13	1.82	0.46
3:D:69:LEU:HA	3:D:72:ARG:HD2	1.98	0.46
6:H:77:ILE:O	13:Q:126:THR:N	2.42	0.46
14:R:24:GLN:HG2	14:R:170:GLU:HG2	1.98	0.46
19:W:13:VAL:HG21	19:W:75:ARG:HD3	1.96	0.46
19:W:1195:ALA:C	19:W:1197:HIS:N	2.69	0.46
22:0:258:MET:SD	22:0:258:MET:N	2.74	0.46
8:J:113:LEU:HA	8:J:116:VAL:HG12	1.98	0.46
19:W:370:ASP:N	19:W:370:ASP:OD1	2.49	0.46
22:0:31:VAL:HG22	22:0:59:ASN:HB3	1.98	0.46
1:A:313:VAL:O	1:A:390:GLY:HA3	2.16	0.46
5:G:164:ILE:HD11	17:U:118:ILE:HD12	1.97	0.46
13:Q:99:ARG:HG2	13:Q:103:ARG:HE	1.81	0.46
19:W:397:LYS:HZ3	19:W:397:LYS:HB2	1.81	0.46
3:D:179:ASP:HB2	3:D:183:ARG:HH21	1.79	0.45
12:P:128:GLY:HA3	20:X:708:LYS:HB2	1.97	0.45
20:X:567:MET:H	20:X:612:LYS:HZ1	1.63	0.45
12:P:171:PHE:CE1	19:W:394:PRO:CB	2.99	0.45
19:W:13:VAL:HA	19:W:78:PHE:CE2	2.51	0.45
19:W:671:ASP:OD1	19:W:671:ASP:N	2.44	0.45
22:0:218:ASN:HD22	22:0:219:GLU:H	1.65	0.45
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.74	0.45
19:W:1064:ASP:OD1	19:W:1064:ASP:N	2.37	0.45
21:Z:482:ARG:HD3	21:Z:483:ASN:N	2.31	0.45
1:A:288:PHE:O	1:A:295:ASN:ND2	2.49	0.45
1:A:445:LEU:HD11	1:A:451:SER:HB3	1.98	0.45
4:F:129:ALA:HB2	13:Q:101:ASN:HB2	1.98	0.45
19:W:316:GLU:OE2	19:W:366:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:512:THR:OG1	19:W:513:ASN:ND2	2.50	0.45
19:W:1135:PRO:O	19:W:1136:LEU:HB2	2.17	0.45
19:W:1183:TRP:CH2	19:W:1185:GLY:HA3	2.52	0.45
19:W:1193:PHE:C	19:W:1195:ALA:H	2.19	0.45
10:N:589:GLN:HG2	19:W:27:MET:HB3	1.98	0.45
13:Q:377:LEU:HD13	25:3:177:ARG:HA	1.99	0.45
19:W:315:SER:OG	19:W:319:GLU:OE1	2.31	0.45
22:0:46:GLU:OE1	22:0:46:GLU:N	2.27	0.45
5:G:86:LEU:HD22	8:J:113:LEU:HD11	1.97	0.45
13:Q:466:ASN:OD1	18:V:124:SER:OG	2.29	0.45
19:W:673:LYS:HE2	19:W:678:ALA:HB2	1.99	0.45
13:Q:366:ASP:OD1	13:Q:366:ASP:N	2.50	0.45
19:W:1193:PHE:C	19:W:1195:ALA:N	2.70	0.45
10:N:343:GLN:H	10:N:343:GLN:HG3	1.56	0.45
12:P:41:CYS:SG	12:P:42:ARG:N	2.90	0.45
16:T:41:VAL:O	16:T:111:GLU:HA	2.16	0.45
17:U:84:ALA:HB2	21:Z:540:LEU:HD22	1.97	0.45
5:G:127:ARG:HA	5:G:127:ARG:HD3	1.77	0.45
6:H:96:ARG:HD3	6:H:96:ARG:HA	1.83	0.45
14:R:150:ARG:NH1	14:R:161:GLU:OE2	2.50	0.45
19:W:33:GLU:O	19:W:37:LEU:HG	2.17	0.45
19:W:726:ASN:H	19:W:726:ASN:HD22	1.64	0.45
4:F:118:ARG:HH22	6:H:110:ARG:HB2	1.80	0.45
9:K:32:ILE:HD13	9:K:35:LEU:HD21	1.99	0.45
10:N:587:LEU:HD12	10:N:589:GLN:HE22	1.82	0.45
10:N:962:PHE:CD2	10:N:1210:PHE:CD2	3.05	0.45
20:X:187:SER:O	20:X:190:THR:OG1	2.35	0.45
3:D:144:SER:HB3	13:Q:6:ALA:HB1	1.99	0.44
12:P:21:TRP:HE1	12:P:49:MET:HE3	1.81	0.44
12:P:40:SER:HB3	12:P:89:TRP:CD2	2.52	0.44
18:V:50:ARG:HH11	18:V:50:ARG:HA	1.81	0.44
12:P:15:LEU:HD11	12:P:453:SER:HB2	1.98	0.44
12:P:131:ILE:HD13	12:P:183:THR:HG22	1.99	0.44
20:X:832:GLN:NE2	20:X:835:ARG:HH21	2.15	0.44
10:N:320:TRP:O	13:Q:317:GLN:NE2	2.47	0.44
10:N:589:GLN:HB3	19:W:26:PHE:O	2.16	0.44
11:O:694:ASP:OD1	11:O:707:ILE:HG12	2.18	0.44
19:W:15:THR:O	19:W:18:ILE:HG12	2.17	0.44
19:W:1139:ARG:O	19:W:1140:GLU:HG3	2.17	0.44
22:0:128:LEU:HD23	22:0:128:LEU:HA	1.82	0.44
22:0:202:VAL:HG22	22:0:212:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:0:287:PHE:O	22:0:306:HIS:HE1	2.00	0.44
25:3:41:VAL:HG22	25:3:92:LEU:HD11	1.99	0.44
26:4:78:LEU:HD23	26:4:78:LEU:HA	1.80	0.44
10:N:192:LEU:O	10:N:196:ASN:ND2	2.38	0.44
10:N:449:SER:OG	13:Q:517:GLN:NE2	2.50	0.44
10:N:1185:LEU:HD12	10:N:1185:LEU:O	2.16	0.44
13:Q:140:ASN:O	13:Q:144:LEU:HB2	2.16	0.44
19:W:770:MET:HB3	19:W:776:ILE:HD11	1.99	0.44
1:A:321:LEU:HD22	1:A:329:LEU:HD12	2.00	0.44
1:A:468:ASP:OD1	1:A:468:ASP:N	2.48	0.44
4:F:74:GLN:HG2	4:F:76:PRO:HD2	1.99	0.44
13:Q:503:ARG:NH2	22:0:244:ASP:OD2	2.44	0.44
14:R:49:GLU:HB2	14:R:135:LEU:HB3	1.99	0.44
19:W:236:ALA:HB2	19:W:663:PRO:HG3	2.00	0.44
20:X:177:LEU:HD23	20:X:177:LEU:HA	1.86	0.44
22:0:42:LYS:HB2	22:0:48:ARG:HB3	2.00	0.44
22:0:260:ASP:OD1	22:0:260:ASP:N	2.49	0.44
26:4:103:LEU:O	26:4:110:ARG:NH2	2.51	0.44
12:P:398:SER:O	12:P:400:GLN:N	2.51	0.44
17:U:73:ILE:HA	17:U:76:LEU:HD13	2.00	0.44
19:W:34:LYS:O	19:W:38:ILE:HG13	2.18	0.44
19:W:297:CYS:HA	19:W:298:PRO:HD3	1.88	0.44
19:W:339:ILE:HD11	19:W:378:GLN:HB3	1.99	0.44
19:W:547:VAL:HG13	19:W:559:LEU:HD11	2.00	0.44
20:X:577:ALA:O	20:X:581:ILE:HG13	2.18	0.44
22:0:223:THR:OG1	22:0:224:GLU:N	2.49	0.44
22:0:227:LYS:NZ	25:3:178:ASN:OD1	2.49	0.44
10:N:319:ARG:HG3	10:N:320:TRP:HD1	1.82	0.44
10:N:959:LEU:HD13	10:N:963:LEU:HD11	1.99	0.44
10:N:962:PHE:HD1	10:N:1258:ASN:CB	2.30	0.44
10:N:1219:HIS:CD2	10:N:1222:ARG:HH11	2.35	0.44
19:W:1195:ALA:O	19:W:1197:HIS:N	2.50	0.44
1:A:430:LEU:HD23	1:A:430:LEU:N	2.32	0.44
10:N:230:PHE:HZ	10:N:296:LEU:HD13	1.82	0.44
12:P:469:LEU:HD23	12:P:469:LEU:HA	1.83	0.44
1:A:106:ASP:O	1:A:127:HIS:N	2.50	0.44
1:A:325:THR:HG21	1:A:397:THR:O	2.18	0.44
1:A:441:GLU:HG3	20:X:17:ARG:HH22	1.82	0.44
19:W:1195:ALA:C	19:W:1197:HIS:H	2.21	0.44
20:X:959:SER:O	20:X:965:LYS:N	2.51	0.44
23:1:52:PHE:HE2	24:2:185:VAL:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:H	1:A:499:GLN:HE21	1.66	0.43
4:F:71:LEU:HD11	4:F:82:ARG:HD2	1.99	0.43
6:H:97:VAL:O	6:H:97:VAL:HG12	2.16	0.43
19:W:44:PHE:CE1	19:W:92:LEU:HD11	2.53	0.43
13:Q:468:ASN:HD21	25:3:168:TRP:HD1	1.67	0.43
16:T:42:ASP:O	16:T:66:MET:HA	2.18	0.43
20:X:676:ASP:OD1	20:X:676:ASP:N	2.50	0.43
1:A:295:ASN:HB3	1:A:296:SER:H	1.68	0.43
1:A:367:LEU:HD12	1:A:372:HIS:CD2	2.53	0.43
3:D:42:ARG:HH21	7:I:93:LYS:HG2	1.82	0.43
13:Q:202:LYS:HD2	13:Q:202:LYS:HA	1.79	0.43
13:Q:579:ALA:HB3	13:Q:595:GLN:HB3	1.99	0.43
19:W:248:LEU:HD23	19:W:248:LEU:HA	1.83	0.43
20:X:564:SER:HB3	20:X:565:SER:H	1.64	0.43
4:F:69:ILE:N	4:F:82:ARG:O	2.47	0.43
6:H:5:GLU:HA	6:H:8:LEU:HD12	1.99	0.43
10:N:962:PHE:CE1	10:N:1210:PHE:HD2	2.35	0.43
12:P:171:PHE:HZ	19:W:394:PRO:C	2.21	0.43
12:P:194:LYS:HG3	12:P:198:GLN:HB3	2.00	0.43
13:Q:402:HIS:HE1	13:Q:404:ARG:HH21	1.65	0.43
13:Q:549:LEU:HD11	13:Q:572:ALA:HB2	1.99	0.43
16:T:147:CYS:SG	16:T:153:CYS:CB	3.07	0.43
18:V:17:SER:HA	18:V:20:LYS:HD2	1.98	0.43
20:X:420:ILE:HA	20:X:423:THR:HG22	1.99	0.43
22:0:70:LEU:HD12	22:0:70:LEU:HA	1.87	0.43
16:T:70:GLU:OE2	16:T:125:LYS:NZ	2.51	0.43
19:W:383:SER:O	19:W:383:SER:OG	2.32	0.43
4:F:94:PRO:HB2	13:Q:130:VAL:HG13	2.00	0.43
9:K:82:SER:OG	9:K:83:SER:N	2.52	0.43
10:N:1322:LEU:O	10:N:1326:PRO:N	2.52	0.43
12:P:216:ALA:HA	12:P:229:ALA:O	2.19	0.43
20:X:707:ILE:HD12	20:X:707:ILE:HA	1.88	0.43
10:N:169:LEU:HD23	10:N:169:LEU:HA	1.87	0.43
10:N:884:LYS:HD2	10:N:1187:LEU:HD21	2.00	0.43
10:N:1185:LEU:HD11	10:N:1207:LEU:HB2	2.01	0.43
11:O:701:ASN:O	11:O:702:GLY:C	2.57	0.43
19:W:326:THR:HA	19:W:329:LEU:HD13	1.99	0.43
1:A:268:LEU:HD12	1:A:299:LEU:HD12	1.99	0.43
1:A:416:ALA:O	1:A:419:THR:OG1	2.33	0.43
5:G:168:LEU:O	5:G:172:PRO:HD2	2.19	0.43
10:N:465:LEU:HD13	10:N:478:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:554:HIS:O	13:Q:554:HIS:ND1	2.51	0.43
16:T:98:LEU:HD23	16:T:98:LEU:HA	1.88	0.43
19:W:389:LEU:HA	19:W:392:PHE:HD2	1.84	0.43
20:X:591:ALA:HB1	20:X:597:LEU:HD23	2.00	0.43
20:X:742:TYR:HA	20:X:782:VAL:HG11	1.99	0.43
1:A:62:LEU:HD13	3:D:66:LEU:HD13	2.00	0.43
1:A:334:PRO:HG2	1:A:391:THR:HG21	1.99	0.43
8:J:83:GLU:HB3	8:J:87:ARG:HH12	1.84	0.43
10:N:475:LEU:HD23	10:N:475:LEU:HA	1.86	0.43
10:N:1187:LEU:HD23	10:N:1187:LEU:HA	1.88	0.43
12:P:35:LEU:HD22	12:P:49:MET:HA	2.01	0.43
12:P:145:LEU:HD22	12:P:359:LEU:HD21	2.00	0.43
13:Q:458:PRO:HB2	13:Q:459:GLN:H	1.55	0.43
13:Q:526:LEU:HD23	13:Q:526:LEU:HA	1.90	0.43
16:T:123:LEU:HD23	16:T:123:LEU:HA	1.83	0.43
19:W:45:ARG:HB3	19:W:45:ARG:NH1	2.31	0.43
19:W:47:PHE:CD1	19:W:47:PHE:C	2.92	0.43
19:W:83:LEU:HD12	19:W:83:LEU:HA	1.90	0.43
19:W:1204:SER:O	19:W:1208:THR:OG1	2.26	0.43
20:X:765:VAL:HG13	20:X:812:LEU:HB2	1.99	0.43
1:A:351:ASP:OD1	1:A:351:ASP:N	2.41	0.43
10:N:292:MET:HG2	10:N:296:LEU:HD12	2.01	0.43
16:T:40:CYS:H	16:T:69:SER:HB3	1.84	0.43
19:W:60:ILE:HA	19:W:63:ILE:HD12	2.01	0.43
5:G:57:ARG:H	5:G:57:ARG:HG2	1.74	0.42
6:H:94:GLU:OE1	6:H:94:GLU:HA	2.19	0.42
10:N:932:GLY:C	10:N:1179:HIS:CD2	2.92	0.42
13:Q:608:ASP:N	13:Q:608:ASP:OD1	2.46	0.42
18:V:50:ARG:NH1	18:V:50:ARG:HA	2.34	0.42
19:W:33:GLU:HA	19:W:36:LYS:CD	2.48	0.42
19:W:41:LEU:HD22	19:W:85:MET:HB3	2.00	0.42
19:W:758:LYS:HA	19:W:758:LYS:HD3	1.81	0.42
9:K:10:ARG:HD2	13:Q:188:LEU:HD11	2.00	0.42
10:N:457:ASP:OD1	10:N:457:ASP:N	2.52	0.42
13:Q:395:PRO:HA	14:R:53:ASP:OD2	2.19	0.42
13:Q:588:SER:O	13:Q:588:SER:OG	2.37	0.42
19:W:9:PHE:O	19:W:12:VAL:HG22	2.20	0.42
19:W:11:GLU:C	19:W:11:GLU:OE2	2.57	0.42
19:W:540:ILE:HD13	19:W:540:ILE:HA	1.92	0.42
19:W:727:TRP:HB2	19:W:732:LEU:HD13	2.02	0.42
20:X:803:ASP:HB2	20:X:804:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Z:575:ASP:OD1	21:Z:575:ASP:N	2.51	0.42
6:H:62:VAL:HA	6:H:65:HIS:CE1	2.54	0.42
12:P:182:VAL:HG21	12:P:228:VAL:HG21	2.01	0.42
16:T:85:LEU:HD23	16:T:85:LEU:HA	1.90	0.42
18:V:87:ILE:HD12	18:V:87:ILE:HA	1.87	0.42
19:W:48:TRP:HB3	19:W:91:LEU:HD21	2.00	0.42
20:X:53:GLY:O	20:X:90:ARG:NH1	2.51	0.42
20:X:821:TYR:HE2	20:X:946:PHE:HE2	1.67	0.42
20:X:955:LEU:HD13	20:X:967:VAL:HG21	2.01	0.42
1:A:95:SER:OG	1:A:99:THR:OG1	2.29	0.42
4:F:29:VAL:HG21	4:F:79:PHE:CG	2.54	0.42
5:G:34:PRO:O	26:4:17:ARG:NH2	2.53	0.42
9:K:23:ALA:O	9:K:27:ASN:ND2	2.45	0.42
10:N:753:LEU:HD23	10:N:753:LEU:HA	1.90	0.42
11:O:685:LEU:HD23	11:O:685:LEU:HA	1.81	0.42
11:O:720:PRO:HD3	20:X:71:GLN:CG	2.43	0.42
19:W:40:CYS:SG	19:W:82:CYS:HB2	2.59	0.42
19:W:356:LEU:HD21	19:W:372:LEU:HD11	2.01	0.42
20:X:173:LYS:HD2	20:X:989:LEU:HD21	2.02	0.42
20:X:363:LEU:HD23	20:X:363:LEU:HA	1.81	0.42
20:X:717:LYS:HB2	20:X:717:LYS:HE3	1.87	0.42
21:Z:537:PRO:HB3	21:Z:543:LEU:HD22	2.01	0.42
10:N:199:LEU:HD23	10:N:199:LEU:HA	1.90	0.42
16:T:147:CYS:SG	22:0:277:PHE:CD1	3.12	0.42
20:X:269:MET:O	20:X:273:MET:HG2	2.19	0.42
9:K:37:LYS:HB3	9:K:37:LYS:HE3	1.84	0.42
10:N:133:ALA:HB2	17:U:23:ILE:HG22	2.02	0.42
10:N:223:LYS:HD3	10:N:233:THR:HG22	2.01	0.42
10:N:836:GLY:O	10:N:846:ASN:ND2	2.52	0.42
19:W:270:LEU:HD12	19:W:270:LEU:HA	1.89	0.42
19:W:381:SER:O	19:W:534:HIS:ND1	2.48	0.42
26:4:79:LEU:HD23	26:4:84:PHE:HD2	1.84	0.42
3:D:142:ALA:O	13:Q:8:ARG:NH2	2.44	0.42
6:H:174:ASN:ND2	6:H:176:THR:OG1	2.52	0.42
7:I:131:LEU:HA	7:I:134:LYS:HD2	2.00	0.42
10:N:586:LEU:HD13	19:W:11:GLU:OE2	2.20	0.42
10:N:936:ILE:HD11	10:N:963:LEU:HD13	2.00	0.42
11:O:685:LEU:HD21	11:O:770:THR:HG22	2.02	0.42
13:Q:598:ARG:HG2	13:Q:621:PRO:HD3	2.01	0.42
13:Q:628:ASN:OD1	13:Q:628:ASN:N	2.52	0.42
20:X:951:THR:HG22	20:X:955:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:4:59:LYS:HZ1	26:4:77:GLU:HG2	1.83	0.42
5:G:127:ARG:HH21	17:U:5:LEU:HB3	1.85	0.42
10:N:962:PHE:HB2	10:N:1210:PHE:CZ	2.46	0.42
16:T:21:VAL:HG21	16:T:128:THR:HG22	2.02	0.42
19:W:1183:TRP:HE1	19:W:1190:LEU:HD13	1.85	0.42
19:W:1291:MET:H	19:W:1291:MET:HG2	1.64	0.42
25:3:147:LYS:HA	25:3:147:LYS:HD3	1.77	0.42
1:A:469:VAL:HA	1:A:475:VAL:HG22	2.01	0.42
12:P:146:HIS:NE2	12:P:160:SER:OG	2.49	0.42
13:Q:96:ASP:OD1	13:Q:96:ASP:N	2.43	0.42
19:W:916:ASP:OD1	19:W:916:ASP:N	2.53	0.42
20:X:65:LYS:HA	20:X:103:MET:HE1	2.02	0.42
22:0:191:LEU:HD12	22:0:228:LEU:HD21	2.02	0.42
10:N:942:SER:OG	10:N:945:ASP:O	2.33	0.42
10:N:959:LEU:HD23	10:N:1210:PHE:CE1	2.55	0.42
10:N:1355:PRO:O	10:N:1363:MET:HA	2.20	0.42
12:P:252:LYS:HD3	12:P:252:LYS:HA	1.76	0.42
17:U:1:MET:HB3	17:U:2:ALA:H	1.70	0.42
19:W:964:LEU:HD12	19:W:964:LEU:HA	1.89	0.42
20:X:7:LYS:HB3	20:X:49:GLN:HE22	1.85	0.42
25:3:149:LEU:HA	25:3:152:LYS:HB2	2.02	0.42
10:N:102:LEU:HD23	10:N:102:LEU:HA	1.89	0.41
16:T:147:CYS:SG	22:0:277:PHE:CG	3.13	0.41
19:W:45:ARG:HA	19:W:91:LEU:CD2	2.50	0.41
19:W:1046:ASP:OD1	19:W:1046:ASP:N	2.52	0.41
20:X:561:LEU:O	20:X:608:ASN:ND2	2.51	0.41
20:X:794:ASP:HB3	20:X:797:LYS:HB2	2.02	0.41
10:N:231:GLU:HB3	10:N:251:GLU:HB3	2.01	0.41
11:O:639:TYR:CZ	11:O:643:VAL:HG11	2.55	0.41
11:O:697:HIS:CA	20:X:957:LYS:NZ	2.83	0.41
19:W:301:GLU:HG3	19:W:347:ALA:HB1	2.03	0.41
19:W:805:GLN:HE22	19:W:809:ARG:HE	1.69	0.41
19:W:1097:PHE:HA	19:W:1098:PRO:HD3	1.90	0.41
20:X:68:ILE:HD11	20:X:78:VAL:HG11	2.01	0.41
22:0:276:LEU:HD23	22:0:276:LEU:HA	1.92	0.41
8:J:92:ASN:ND2	15:S:83:LEU:H	2.18	0.41
10:N:256:ASP:H	10:N:265:LEU:HD21	1.85	0.41
10:N:506:LYS:HE3	10:N:538:LEU:HD11	2.02	0.41
12:P:388:ASP:OD1	12:P:388:ASP:N	2.53	0.41
16:T:22:GLU:O	16:T:26:ARG:HB2	2.20	0.41
19:W:38:ILE:HA	19:W:85:MET:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:397:LYS:HA	19:W:397:LYS:NZ	2.36	0.41
20:X:466:ARG:NH2	20:X:512:ILE:O	2.53	0.41
1:A:288:PHE:HA	1:A:295:ASN:HA	2.03	0.41
1:A:322:GLN:HE21	1:A:329:LEU:H	1.68	0.41
10:N:471:ASP:OD1	10:N:471:ASP:N	2.51	0.41
10:N:773:ILE:HG23	10:N:805:TYR:HB3	2.02	0.41
10:N:1354:THR:HA	10:N:1364:LEU:O	2.20	0.41
13:Q:379:ILE:HD12	13:Q:379:ILE:HA	1.87	0.41
14:R:108:ILE:HG22	14:R:110:THR:HG23	2.01	0.41
18:V:55:GLU:H	18:V:55:GLU:HG2	1.78	0.41
19:W:470:ASN:OD1	19:W:470:ASN:N	2.52	0.41
19:W:684:ASN:HD22	19:W:723:THR:HG21	1.85	0.41
19:W:916:ASP:O	19:W:920:LYS:NZ	2.50	0.41
20:X:183:LEU:HD21	20:X:974:SER:HB3	2.03	0.41
1:A:418:ASN:O	1:A:422:GLY:N	2.54	0.41
4:F:46:ASN:ND2	4:F:66:ILE:O	2.44	0.41
17:U:18:GLN:HE21	21:Z:495:SER:HB3	1.84	0.41
1:A:373:CYS:SG	1:A:439:GLN:NE2	2.90	0.41
5:G:104:LYS:O	5:G:108:LYS:N	2.47	0.41
7:I:75:CYS:O	7:I:79:ASP:N	2.41	0.41
14:R:164:SER:OG	14:R:165:LEU:N	2.53	0.41
3:D:96:LEU:HD11	7:I:122:ARG:HD2	2.03	0.41
4:F:36:ARG:CZ	4:F:43:ARG:HG3	2.50	0.41
6:H:112:LYS:HB2	6:H:112:LYS:HE2	1.86	0.41
10:N:713:GLN:O	10:N:719:THR:HB	2.21	0.41
10:N:884:LYS:CD	10:N:1187:LEU:HD21	2.50	0.41
12:P:444:VAL:HG22	12:P:452:LEU:HD11	2.02	0.41
13:Q:506:HIS:HE1	13:Q:528:GLN:HE21	1.68	0.41
14:R:41:GLY:HA3	18:V:91:PHE:CD2	2.55	0.41
16:T:161:LEU:O	16:T:165:LEU:HB2	2.21	0.41
19:W:237:ILE:HG21	19:W:285:ASN:HB3	2.01	0.41
19:W:314:ARG:NH1	19:W:326:THR:OG1	2.48	0.41
19:W:844:ASN:HA	19:W:847:ILE:HG22	2.02	0.41
21:Z:598:CYS:SG	26:4:111:LYS:NZ	2.77	0.41
26:4:22:LEU:O	26:4:26:GLN:HG3	2.20	0.41
1:A:83:SER:HA	1:A:86:ARG:HD2	2.02	0.41
1:A:373:CYS:HB2	1:A:437:LEU:HD12	2.03	0.41
9:K:41:ASN:HB2	9:K:44:LEU:HB3	2.03	0.41
10:N:94:GLN:HA	10:N:97:VAL:HG12	2.02	0.41
10:N:397:ILE:HD12	10:N:397:ILE:HA	1.91	0.41
10:N:399:LYS:HB3	10:N:399:LYS:HE2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:211:GLN:HG2	10:N:367:SER:HA	2.02	0.41
10:N:574:ASN:OD1	19:W:11:GLU:HG3	2.21	0.41
10:N:723:GLU:HG3	10:N:746:TYR:CE1	2.56	0.41
10:N:830:LYS:HB3	10:N:860:ASN:HD21	1.86	0.41
13:Q:153:LEU:HD12	13:Q:153:LEU:HA	1.92	0.41
16:T:42:ASP:HB2	16:T:67:HIS:HD2	1.86	0.41
19:W:18:ILE:HG23	19:W:18:ILE:H	1.54	0.41
20:X:162:LEU:HD23	20:X:165:LEU:HD12	2.03	0.41
20:X:579:LEU:HD23	20:X:579:LEU:HA	1.92	0.41
20:X:925:GLN:NE2	20:X:958:VAL:O	2.51	0.41
22:0:255:LEU:HD13	22:0:255:LEU:HA	1.96	0.41
24:2:84:GLN:HE21	24:2:88:ILE:HD11	1.84	0.41
24:2:96:ASP:OD1	24:2:96:ASP:N	2.50	0.41
1:A:169:LEU:O	1:A:173:MET:N	2.44	0.41
10:N:212:LEU:HD13	10:N:212:LEU:HA	1.81	0.41
10:N:528:HIS:HE1	10:N:588:LEU:HG	1.86	0.41
16:T:158:LEU:HD12	16:T:158:LEU:HA	1.86	0.41
17:U:54:TYR:OH	21:Z:485:ILE:HA	2.21	0.41
20:X:192:ILE:HD13	20:X:192:ILE:HA	1.92	0.41
23:1:132:HIS:CE1	25:3:163:LEU:HD11	2.56	0.41
13:Q:166:ARG:HG3	13:Q:169:LYS:HE3	2.01	0.40
14:R:58:PHE:HB3	14:R:123:PHE:HB3	2.03	0.40
16:T:28:LEU:HD23	16:T:28:LEU:HA	1.88	0.40
16:T:97:LYS:HD3	16:T:97:LYS:HA	1.93	0.40
19:W:44:PHE:O	19:W:44:PHE:CD1	2.73	0.40
20:X:305:TRP:O	20:X:309:THR:HG23	2.21	0.40
20:X:420:ILE:HA	20:X:420:ILE:HD13	1.91	0.40
20:X:484:LYS:HA	20:X:484:LYS:HZ2	1.84	0.40
21:Z:528:LEU:HD23	21:Z:528:LEU:HA	1.91	0.40
5:G:133:GLU:OE1	5:G:136:ARG:NH2	2.55	0.40
10:N:181:ASP:O	13:Q:46:ARG:NH2	2.54	0.40
10:N:1210:PHE:HD1	10:N:1211:LEU:HD23	1.85	0.40
10:N:1335:ASN:C	10:N:1337:GLN:H	2.25	0.40
12:P:311:LEU:HD13	12:P:339:TRP:CE2	2.57	0.40
12:P:313:LYS:HB3	12:P:337:LEU:HD23	2.04	0.40
17:U:4:ARG:NH1	17:U:75:SER:OG	2.55	0.40
17:U:49:ASN:ND2	17:U:49:ASN:N	2.66	0.40
17:U:76:LEU:C	17:U:76:LEU:CD2	2.89	0.40
20:X:443:LEU:HD11	20:X:495:ILE:HD12	2.01	0.40
20:X:935:LEU:HD23	20:X:935:LEU:HA	1.93	0.40
21:Z:546:GLU:O	21:Z:547:VAL:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:HD2	1:A:376:LEU:HB3	1.86	0.40
3:D:132:LEU:HD23	3:D:132:LEU:HA	1.92	0.40
3:D:152:ALA:HA	3:D:155:ILE:HG22	2.03	0.40
5:G:93:LEU:HD23	5:G:93:LEU:HA	1.90	0.40
10:N:156:TYR:O	10:N:160:VAL:HG23	2.22	0.40
16:T:175:VAL:H	16:T:175:VAL:HG22	1.67	0.40
19:W:37:LEU:C	19:W:85:MET:SD	3.00	0.40
26:4:80:GLN:NE2	26:4:80:GLN:CA	2.85	0.40
10:N:659:LEU:HD11	19:W:18:ILE:CG2	2.19	0.40
10:N:904:PHE:HE2	10:N:1208:GLU:HB2	1.87	0.40
10:N:1224:ILE:HD13	10:N:1224:ILE:HA	1.90	0.40
11:O:619:GLN:HE22	11:O:622:LEU:HD23	1.87	0.40
12:P:206:LEU:HD23	12:P:206:LEU:HA	1.99	0.40
12:P:398:SER:OG	12:P:398:SER:O	2.37	0.40
13:Q:168:THR:O	13:Q:172:THR:OG1	2.36	0.40
20:X:491:LEU:O	20:X:495:ILE:HG12	2.22	0.40
20:X:956:VAL:HG21	20:X:985:ALA:HB1	2.03	0.40
24:2:63:LEU:HD23	24:2:63:LEU:HA	1.94	0.40
25:3:136:SER:OG	25:3:139:ARG:NH1	2.55	0.40
26:4:79:LEU:HD23	26:4:79:LEU:HA	1.79	0.40
6:H:46:LEU:HD11	18:V:66:ALA:HB1	2.03	0.40
10:N:185:LYS:O	10:N:186:ILE:C	2.60	0.40
10:N:305:LEU:HD23	10:N:305:LEU:HA	1.91	0.40
10:N:753:LEU:HB3	22:0:283:ARG:HD2	2.03	0.40
13:Q:112:LEU:HD23	13:Q:112:LEU:HA	1.92	0.40
19:W:363:ARG:HE	19:W:365:LEU:HD11	1.87	0.40
20:X:102:ASP:HB2	20:X:164:ARG:HE	1.87	0.40
20:X:918:GLY:O	20:X:921:THR:OG1	2.40	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%)	429 (94%)	23 (5%)	3 (1%)	22 62
3	D	154/270 (57%)	150 (97%)	3 (2%)	1 (1%)	25 65
4	F	163/246 (66%)	153 (94%)	8 (5%)	2 (1%)	13 50
5	G	159/233 (68%)	151 (95%)	8 (5%)	0	100 100
6	H	177/268 (66%)	165 (93%)	12 (7%)	0	100 100
7	I	69/146 (47%)	66 (96%)	1 (1%)	2 (3%)	4 32
8	J	120/135 (89%)	117 (98%)	2 (2%)	1 (1%)	19 60
9	K	110/117 (94%)	105 (96%)	5 (4%)	0	100 100
10	N	995/1454 (68%)	890 (89%)	94 (9%)	11 (1%)	14 52
11	O	153/788 (19%)	138 (90%)	13 (8%)	2 (1%)	12 48
12	P	414/877 (47%)	382 (92%)	32 (8%)	0	100 100
13	Q	539/651 (83%)	504 (94%)	31 (6%)	4 (1%)	22 62
14	R	189/208 (91%)	180 (95%)	9 (5%)	0	100 100
15	S	67/244 (28%)	60 (90%)	5 (8%)	2 (3%)	4 31
16	T	189/212 (89%)	175 (93%)	13 (7%)	1 (0%)	29 68
17	U	117/144 (81%)	114 (97%)	2 (2%)	1 (1%)	17 56
18	V	128/200 (64%)	125 (98%)	2 (2%)	1 (1%)	19 60
19	W	1332/1368 (97%)	1264 (95%)	64 (5%)	4 (0%)	41 76
20	X	877/989 (89%)	828 (94%)	47 (5%)	2 (0%)	47 81
21	Z	93/600 (16%)	83 (89%)	8 (9%)	2 (2%)	6 38
22	0	261/311 (84%)	245 (94%)	16 (6%)	0	100 100
23	1	95/178 (53%)	91 (96%)	3 (3%)	1 (1%)	14 52
24	2	111/200 (56%)	106 (96%)	5 (4%)	0	100 100
25	3	114/178 (64%)	111 (97%)	3 (3%)	0	100 100
26	4	111/131 (85%)	107 (96%)	3 (3%)	1 (1%)	17 56
All	All	7192/11729 (61%)	6739 (94%)	412 (6%)	41 (1%)	29 65

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	105	PRO
10	N	186	ILE
10	N	525	TYR
10	N	689	PRO

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Mol	Chain	Res	Type
10	N	1351	PRO
10	N	1355	PRO
11	O	709	LYS
13	Q	458	PRO
18	V	50	ARG
20	X	564	SER
1	A	208	VAL
10	N	218	ALA
10	N	1343	PRO
11	O	702	GLY
13	Q	399	PRO
16	T	204	GLN
17	U	32	PRO
19	W	49	GLY
19	W	1196	CYS
20	X	567	MET
10	N	524	ASN
10	N	1237	PRO
13	Q	90	PRO
15	S	158	PRO
19	W	360	LEU
19	W	1203	MET
21	Z	549	GLN
1	A	167	ASN
3	D	178	THR
4	F	35	GLU
10	N	1255	PRO
13	Q	459	GLN
15	S	119	PRO
26	4	72	CYS
1	A	281	ASP
7	I	106	GLY
8	J	30	GLN
10	N	1352	PRO
23	1	44	LEU
4	F	76	PRO
21	Z	541	PRO

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	394/1391 (28%)	392 (100%)	2 (0%)	88 93
3	D	139/230 (60%)	139 (100%)	0	100 100
4	F	151/223 (68%)	151 (100%)	0	100 100
5	G	153/216 (71%)	149 (97%)	4 (3%)	46 67
6	H	161/225 (72%)	160 (99%)	1 (1%)	86 92
7	I	71/133 (53%)	70 (99%)	1 (1%)	67 81
8	J	66/124 (53%)	66 (100%)	0	100 100
9	K	94/98 (96%)	94 (100%)	0	100 100
10	N	810/1271 (64%)	802 (99%)	8 (1%)	76 86
11	O	141/697 (20%)	140 (99%)	1 (1%)	84 90
12	P	364/766 (48%)	357 (98%)	7 (2%)	57 75
13	Q	493/577 (85%)	485 (98%)	8 (2%)	62 79
14	R	169/183 (92%)	166 (98%)	3 (2%)	59 77
15	S	31/208 (15%)	31 (100%)	0	100 100
16	T	166/178 (93%)	163 (98%)	3 (2%)	59 77
17	U	98/119 (82%)	96 (98%)	2 (2%)	55 73
18	V	122/173 (70%)	118 (97%)	4 (3%)	38 61
19	W	1203/1232 (98%)	1191 (99%)	12 (1%)	76 86
20	X	789/864 (91%)	780 (99%)	9 (1%)	73 85
21	Z	89/512 (17%)	84 (94%)	5 (6%)	21 48
22	0	241/280 (86%)	234 (97%)	7 (3%)	42 64
23	1	94/152 (62%)	94 (100%)	0	100 100
24	2	102/163 (63%)	102 (100%)	0	100 100
25	3	116/155 (75%)	116 (100%)	0	100 100
26	4	102/115 (89%)	101 (99%)	1 (1%)	76 86
All	All	6359/10285 (62%)	6281 (99%)	78 (1%)	72 84

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	VAL
1	A	430	LEU
5	G	17	TYR
5	G	64	ILE
5	G	72	PHE
5	G	172	PRO
6	H	159	ARG
7	I	105	PRO
10	N	212	LEU
10	N	328	ARG
10	N	343	GLN
10	N	689	PRO
10	N	690	CYS
10	N	847	CYS
10	N	950	VAL
10	N	959	LEU
11	O	718	VAL
12	P	162	VAL
12	P	170	LEU
12	P	232	ASP
12	P	289	ASP
12	P	295	LEU
12	P	401	THR
12	P	443	LEU
13	Q	9	ILE
13	Q	92	LEU
13	Q	169	LYS
13	Q	250	ASP
13	Q	400	PHE
13	Q	404	ARG
13	Q	622	PHE
13	Q	649	CYS
14	R	32	LEU
14	R	76	MET
14	R	206	ARG
16	T	13	GLU
16	T	79	PHE
16	T	130	THR
17	U	49	ASN
17	U	76	LEU
18	V	46	THR
18	V	63	VAL
18	V	70	ARG

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Mol	Chain	Res	Type
18	V	88	LEU
19	W	1	MET
19	W	2	GLU
19	W	8	ILE
19	W	11	GLU
19	W	13	VAL
19	W	27	MET
19	W	32	ASP
19	W	45	ARG
19	W	47	PHE
19	W	397	LYS
19	W	425	MET
19	W	726	ASN
20	X	4	VAL
20	X	87	ASP
20	X	218	CYS
20	X	312	LYS
20	X	477	TYR
20	X	484	LYS
20	X	812	LEU
20	X	897	LEU
20	X	968	LEU
21	Z	482	ARG
21	Z	492	ARG
21	Z	545	ARG
21	Z	548	THR
21	Z	551	ASP
22	0	39	MET
22	0	44	THR
22	0	177	SER
22	0	205	ARG
22	0	207	LEU
22	0	218	ASN
22	0	258	MET
26	4	80	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	221	ASN
1	A	278	HIS

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	322	GLN
1	A	359	HIS
1	A	439	GLN
1	A	459	ASN
3	D	77	GLN
3	D	113	GLN
3	D	191	ASN
4	F	59	HIS
4	F	62	GLN
4	F	74	GLN
5	G	47	ASN
5	G	129	HIS
6	H	7	GLN
6	H	18	GLN
9	K	58	HIS
9	K	66	GLN
9	K	77	GLN
9	K	113	GLN
10	N	267	HIS
10	N	294	ASN
10	N	309	HIS
10	N	330	HIS
10	N	411	GLN
10	N	589	GLN
10	N	590	GLN
10	N	638	ASN
10	N	669	GLN
10	N	846	ASN
10	N	848	HIS
10	N	849	ASN
10	N	856	GLN
10	N	964	ASN
11	O	619	GLN
11	O	679	GLN
11	O	740	GLN
11	O	746	ASN
11	O	753	HIS
12	P	63	HIS
12	P	69	HIS
12	P	80	HIS
12	P	225	ASN

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Mol	Chain	Res	Type
12	P	272	ASN
12	P	282	HIS
12	P	387	HIS
12	P	400	GLN
12	P	435	GLN
13	Q	100	ASN
13	Q	139	GLN
13	Q	193	HIS
13	Q	310	GLN
13	Q	340	GLN
13	Q	402	HIS
13	Q	411	GLN
13	Q	459	GLN
13	Q	468	ASN
13	Q	492	GLN
13	Q	506	HIS
13	Q	517	GLN
13	Q	599	ASN
17	U	28	GLN
17	U	49	ASN
17	U	56	GLN
17	U	97	ASN
17	U	119	GLN
18	V	16	GLN
19	W	46	GLN
19	W	378	GLN
19	W	421	HIS
19	W	513	ASN
19	W	726	ASN
19	W	783	GLN
19	W	822	HIS
19	W	851	ASN
19	W	874	HIS
19	W	921	HIS
19	W	923	ASN
19	W	925	HIS
19	W	972	HIS
19	W	1059	ASN
19	W	1134	GLN
19	W	1300	HIS
19	W	1320	ASN
20	X	8	GLN

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Mol	Chain	Res	Type
20	X	179	HIS
20	X	217	GLN
20	X	266	GLN
20	X	361	ASN
20	X	380	ASN
20	X	402	ASN
20	X	404	GLN
20	X	472	ASN
20	X	502	HIS
20	X	544	HIS
21	Z	564	ASN
22	0	75	ASN
22	0	218	ASN
22	0	306	HIS
24	2	84	GLN
25	3	42	GLN
26	4	80	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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.

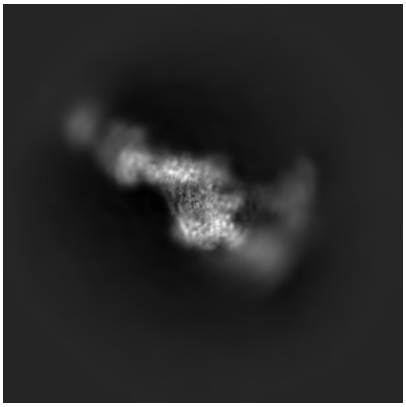
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31211. These allow visual inspection of the internal detail of the map and identification of artifacts.

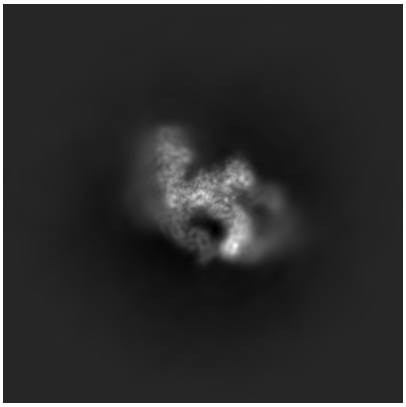
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

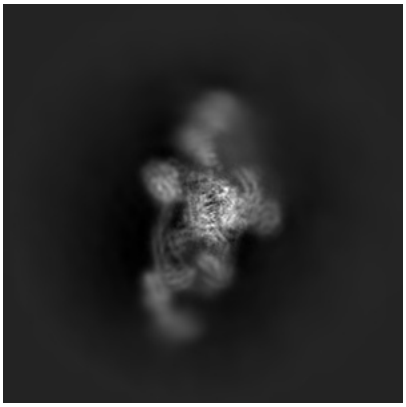
6.1.1 Primary map



X



Y



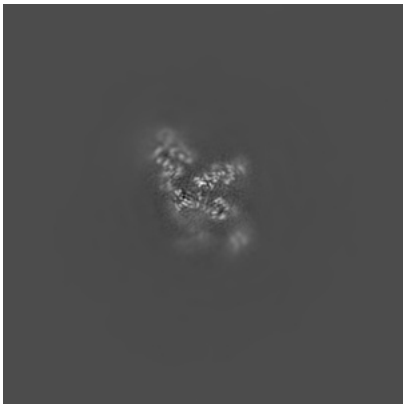
Z

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

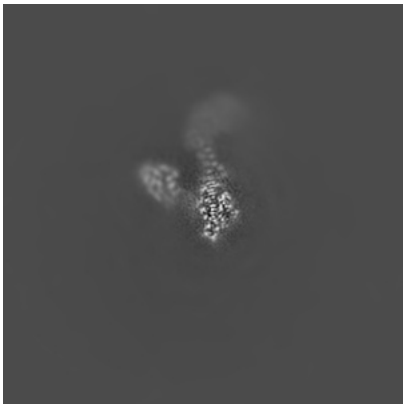
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

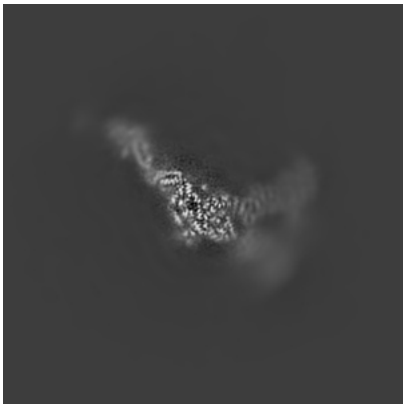


Z Index: 128

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: 131

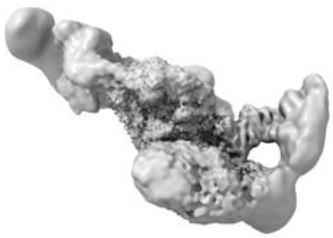
Y Index: 133

Z Index: 148

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

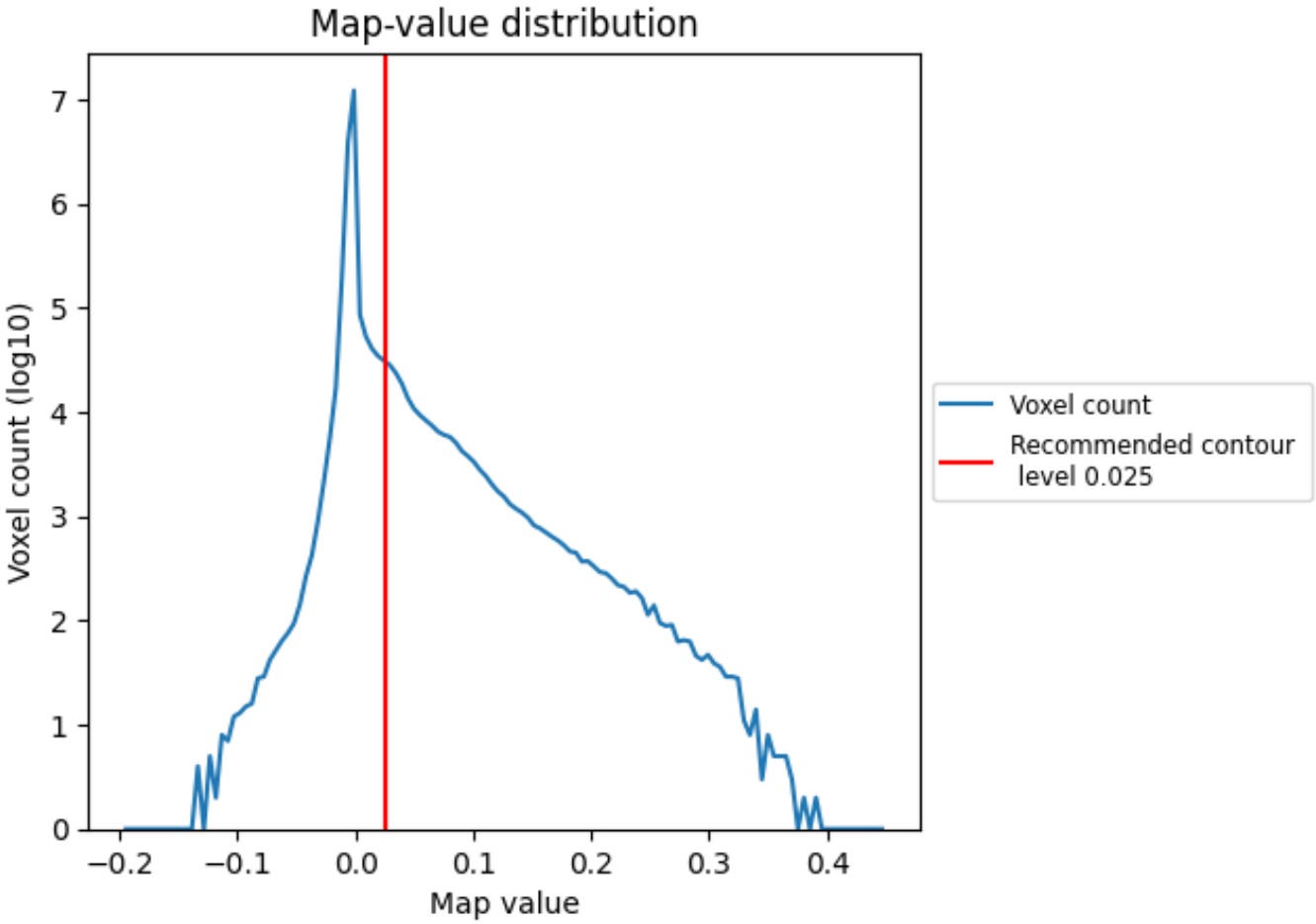
6.5 Mask visualisation (i)

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

7 Map analysis

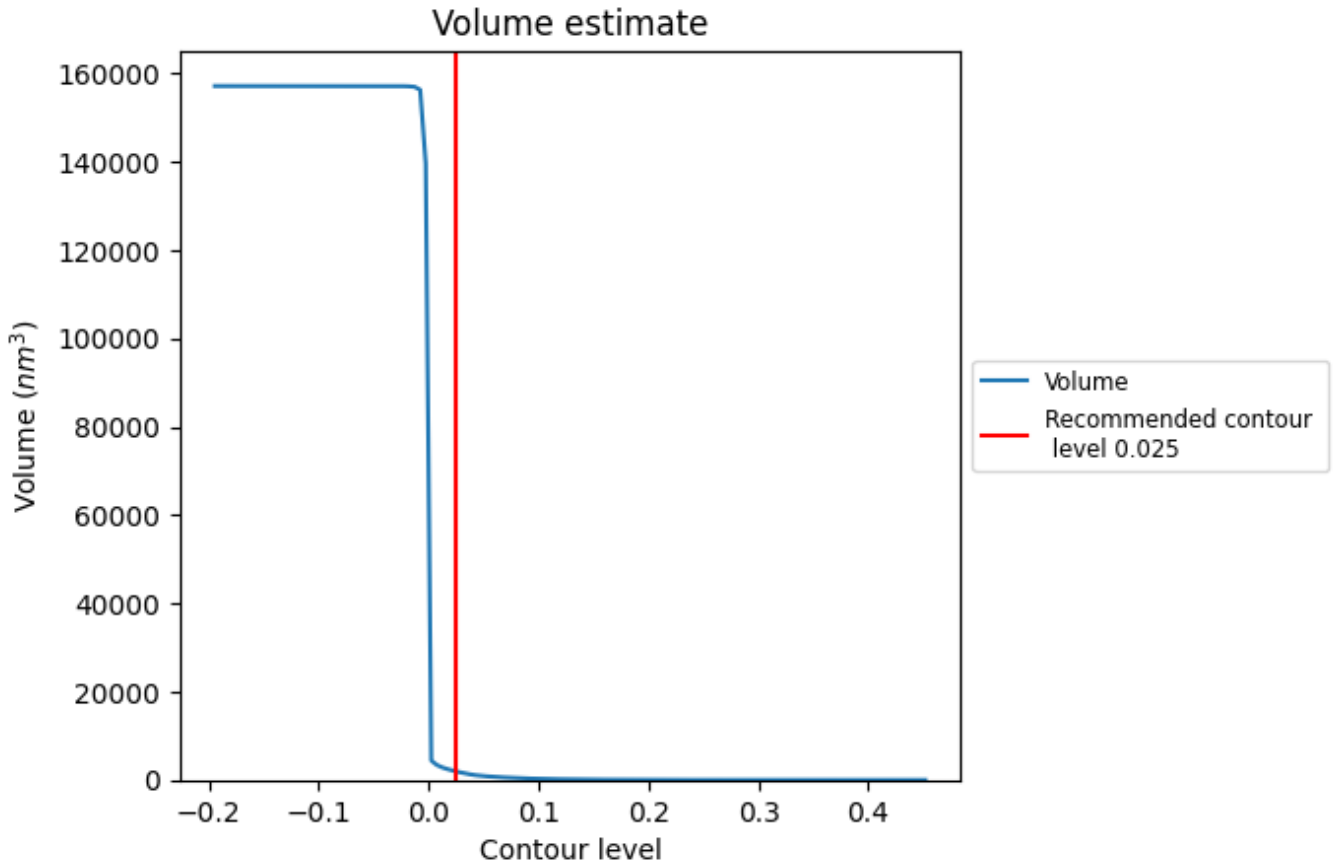
This section contains the results of statistical analysis of the map.

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.

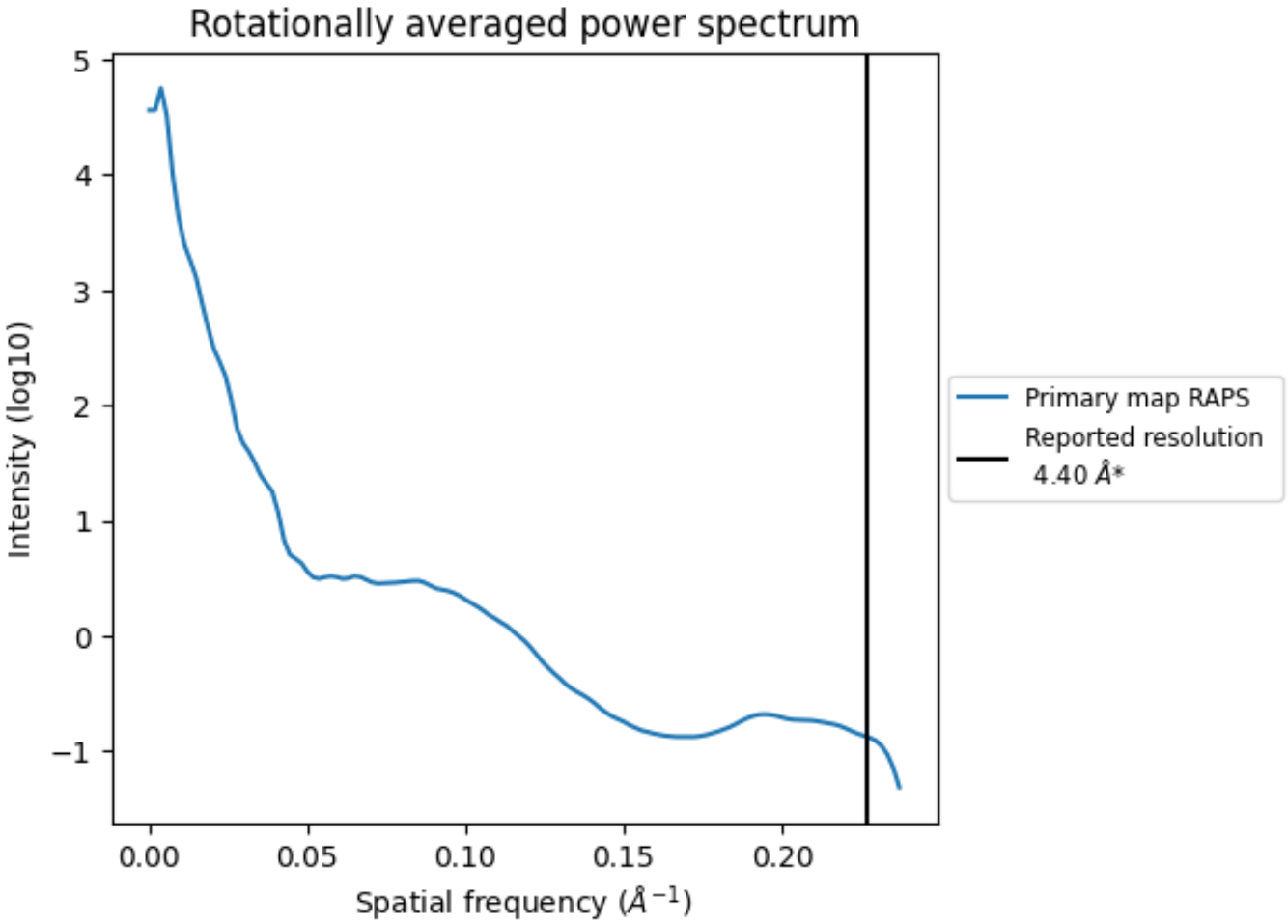
7.2 Volume estimate



The volume at the recommended contour level is 1941 nm^3; this corresponds to an approximate mass of 1753 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 0.227 Å^{-1}

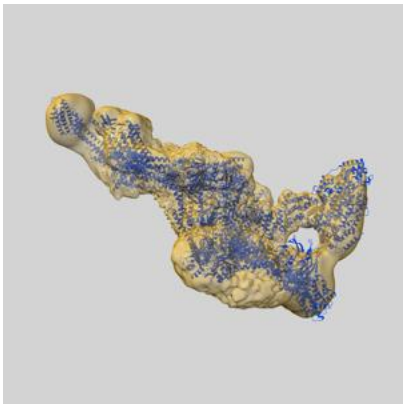
8 Fourier-Shell correlation

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

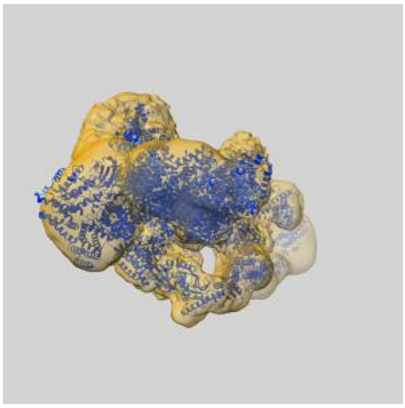
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31211 and PDB model 7ENJ. Per-residue inclusion information can be found in section 3 on page 8.

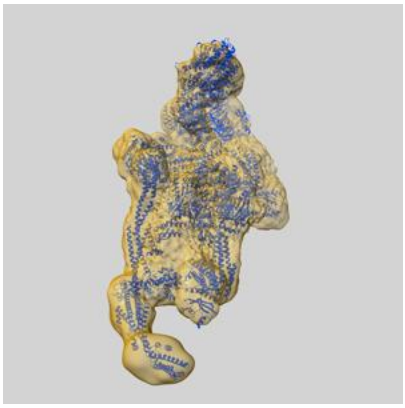
9.1 Map-model overlay



X



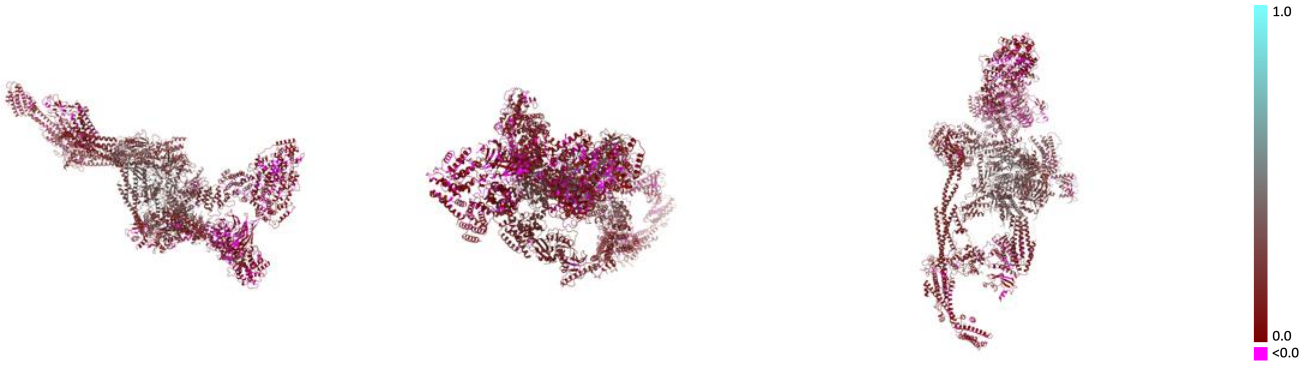
Y



Z

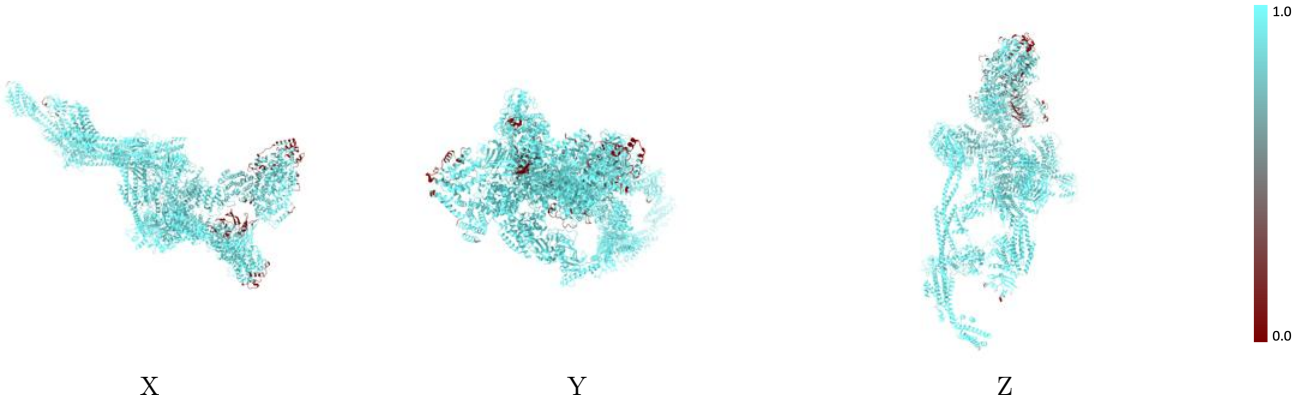
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



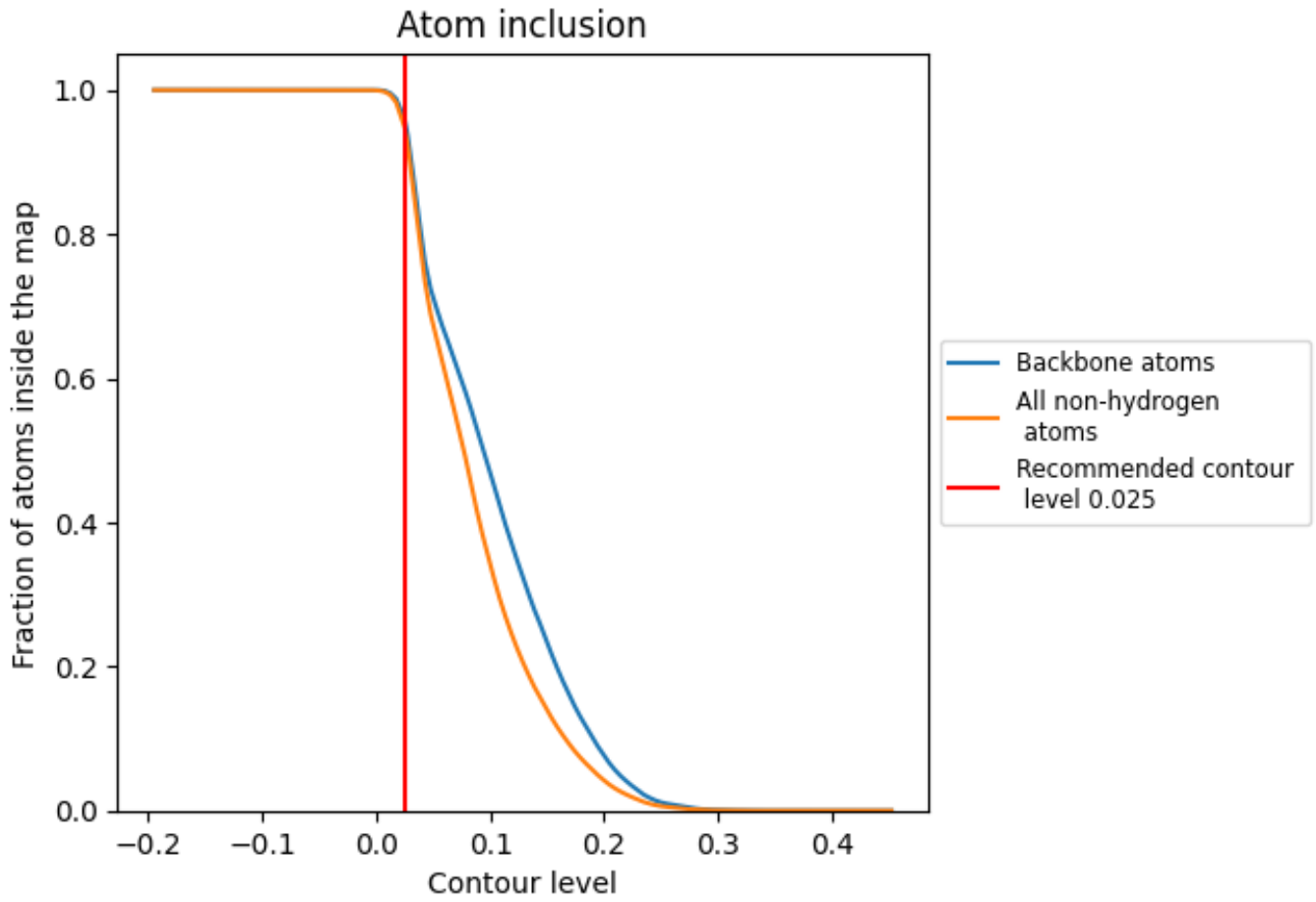
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9484	0.1700
0	0.9901	0.3050
1	0.9888	0.2680
2	0.9798	0.1760
3	0.9960	0.2600
4	1.0000	0.1390
A	0.9989	0.1700
B	1.0000	0.2470
D	1.0000	0.1460
F	0.9268	0.1040
G	0.9977	0.1410
H	0.9914	0.1280
I	1.0000	0.1760
J	0.9867	0.0890
K	0.9965	0.2260
N	0.9922	0.2530
O	0.9901	0.2660
P	0.7448	0.0330
Q	0.9939	0.3020
R	0.9947	0.2920
S	0.9979	0.0740
T	0.9973	0.3000
U	1.0000	0.1220
V	0.9962	0.2190
W	0.8597	0.0900
X	0.9498	0.0960
Z	1.0000	0.0960