Full wwPDB EM Validation Report ⓘ

Feb 27, 2024 – 07:45 AM EST

PDB ID	:	6UXW
EMDB ID	:	EMD-20934
Title	:	SWI/SNF nucleosome complex with ADP-BeFx
Authors	:	He, Y.; Han, Y.
Deposited on	:	2019-11-08
Resolution	:	8.96 Å(reported)
Based on initial models	:	4I6M, 5Z3V

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:

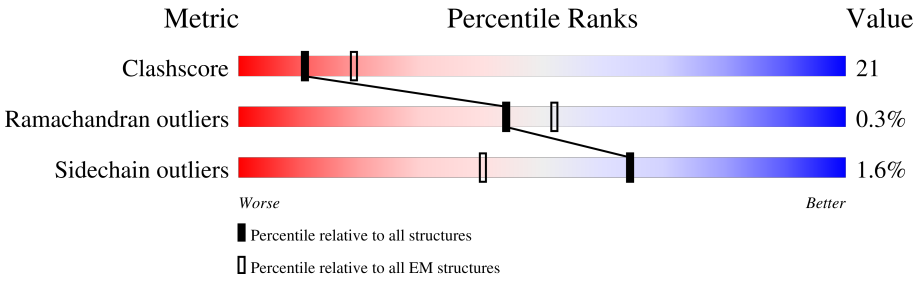
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.96 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	R	135	21% 59% 13% 27%
1	V	135	8% 56% 14% 30%
2	S	102	19% 62% 19% 20%
2	W	102	11% 62% 16% 23%
3	T	129	24% 77% 6% 17%
3	X	129	16% 74% 9% 17%
4	U	122	11% 68% 8% 24%
4	Y	122	9% 66% 10% 24%

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Mol	Chain	Length	Quality of chain
5	a	185	8% 81% 16%
6	b	200	6% 76% 22%
7	P	477	36% 53% 27% 16%
8	Q	467	50% 62% 21% 15%
9	Z	157	18% 21% 12% 66%
10	A	1703	26% 26% 20% 54%
11	B	1314	16% 21% 63%
12	C	905	6% 10% 17% 73%
13	D	825	9% 11% 81%
13	E	825	8% 9% 83%
13	F	825	16% 10% 73%
13	G	825	14% 9% 76%
14	H	566	20% 25% 55%
15	I	179	6% 34% 26% 39%
16	J	67	58% 42%
16	K	67	39% 58%
16	L	67	18% 27% 73%
16	N	67	27% 42% 55%
16	O	67	6% 25% 73%
17	M	83	8% 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	BEF	A	1803	-	-	X	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 41275 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	V	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	102	ALA	GLY	conflict	UNP P84233
V	102	ALA	GLY	conflict	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
2	W	79	Total	C	N	O	S	0	0
			627	395	121	110	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	T	107	Total	C	N	O	0	0
			811	510	158	143		
3	X	107	Total	C	N	O	0	0
			815	513	159	143		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	99	ARG	GLY	conflict	UNP P06897
T	123	SER	ALA	conflict	UNP P06897
X	99	ARG	GLY	conflict	UNP P06897

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Chain	Residue	Modelled	Actual	Comment	Reference
X	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	Y	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	29	THR	SER	conflict	UNP P02281
Y	29	THR	SER	conflict	UNP P02281

- Molecule 5 is a DNA chain called 601 sequence bottom strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	155	Total	C	N	O	P	0	0
			3160	1502	574	929	155		

- Molecule 6 is a DNA chain called 601 sequence top strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	155	Total	C	N	O	P	0	0
			3195	1514	595	931	155		

- Molecule 7 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	399	Total	C	N	O	S	3	0
			3227	2081	528	603	15		

- Molecule 8 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	396	Total	C	N	O	S	1	0
			3198	2053	523	615	7		

- Molecule 9 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 10 is a protein called Transcription regulatory protein SNF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	778	Total	C	N	O	S	1	0
			6385	4041	1139	1185	20		

- Molecule 11 is a protein called SWI/SNF chromatin-remodeling complex subunit SWI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	482	Total	C	N	O	S	0	0
			3890	2519	637	723	11		

- Molecule 12 is a protein called SWI/SNF chromatin-remodeling complex subunit SNF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	245	Total	C	N	O	S	0	0
			2005	1256	346	395	8		

- Molecule 13 is a protein called SWI/SNF complex subunit SWI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	159	Total	C	N	O	S	0	0
			1322	853	225	239	5		
13	E	139	Total	C	N	O	S	0	0
			1152	746	198	205	3		
13	F	221	Total	C	N	O	S	0	0
			1583	987	287	304	5		
13	G	197	Total	C	N	O	S	0	0
			1435	904	258	268	5		

- Molecule 14 is a protein called Transcription regulatory protein SNF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	257	Total	C	N	O	S	0	0
			2085	1323	355	400	7		

- Molecule 15 is a protein called Transcription regulatory protein SNF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	109	Total	C	N	O	S	0	0
			818	504	155	156	3		

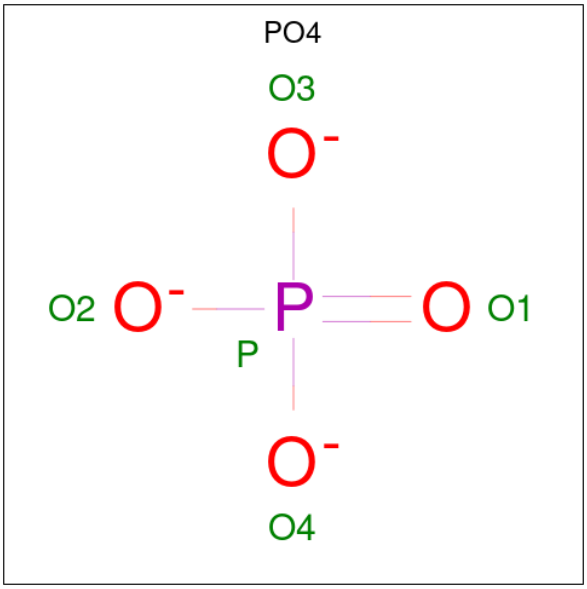
- Molecule 16 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	J	67	Total	C	N	O	0	0
			336	201	67	68		
16	K	28	Total	C	N	O	0	0
			140	84	28	28		
16	L	18	Total	C	N	O	0	0
			90	54	18	18		
16	N	30	Total	C	N	O	0	0
			150	90	30	30		
16	O	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 17 is a protein called SWI/SNF global transcription activator complex subunit SWP82.

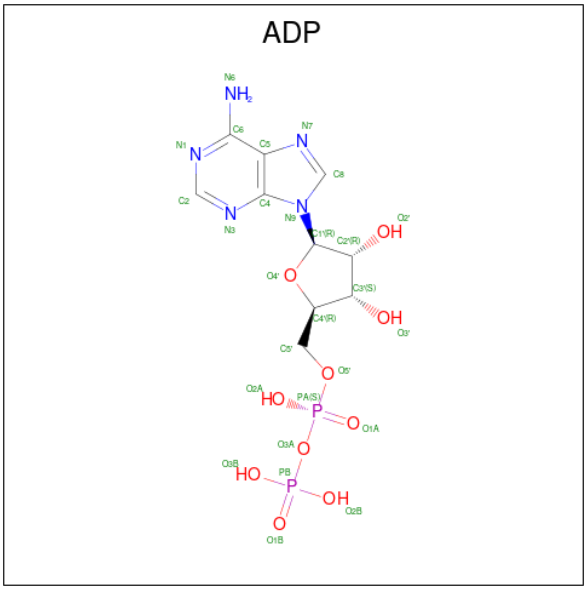
Mol	Chain	Residues	Atoms				AltConf	Trace
17	M	83	Total	C	N	O	0	0
			416	249	83	84		

- Molecule 18 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



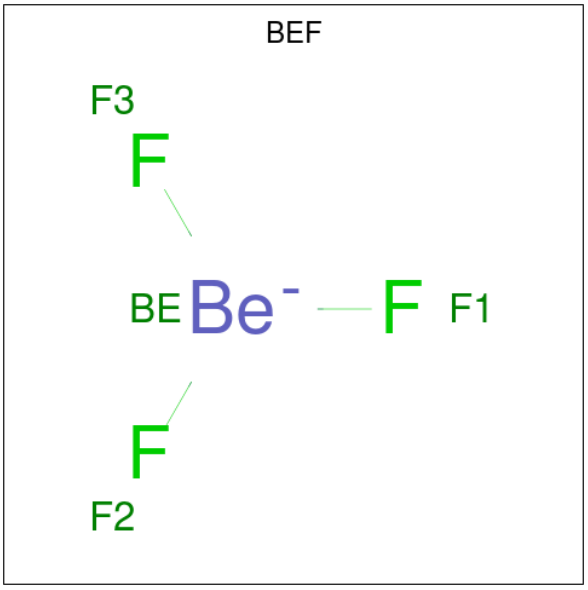
Mol	Chain	Residues	Atoms			AltConf
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	P	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	Q	1	Total	O	P	0
			5	4	1	
18	A	1	Total	O	P	0
			5	4	1	

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	Be	F		0
			4	1	3		

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Mg		0
			1	1		

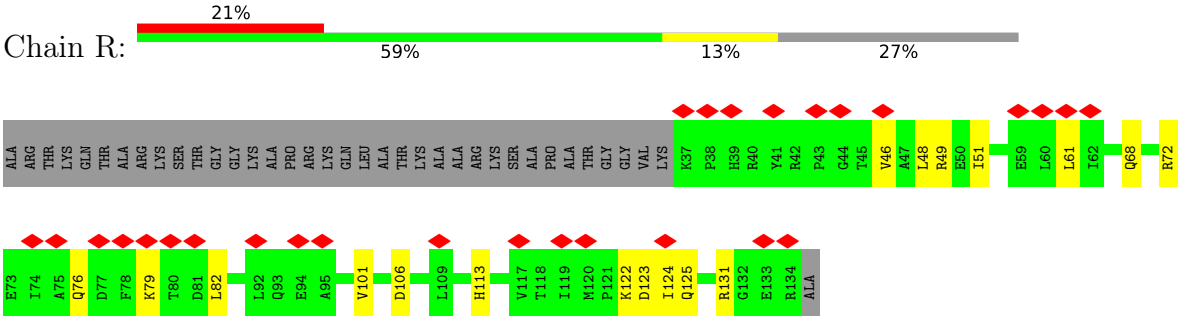
- Molecule 22 is water.

Mol	Chain	Residues	Atoms			AltConf
22	P	33	Total	O		0
			33	33		
22	Q	51	Total	O		0
			51	51		
22	Z	2	Total	O		0
			2	2		

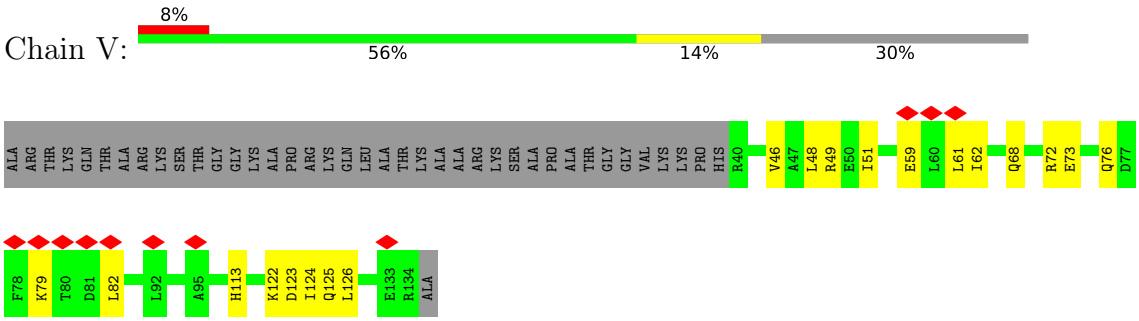
3 Residue-property plots (i)

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.

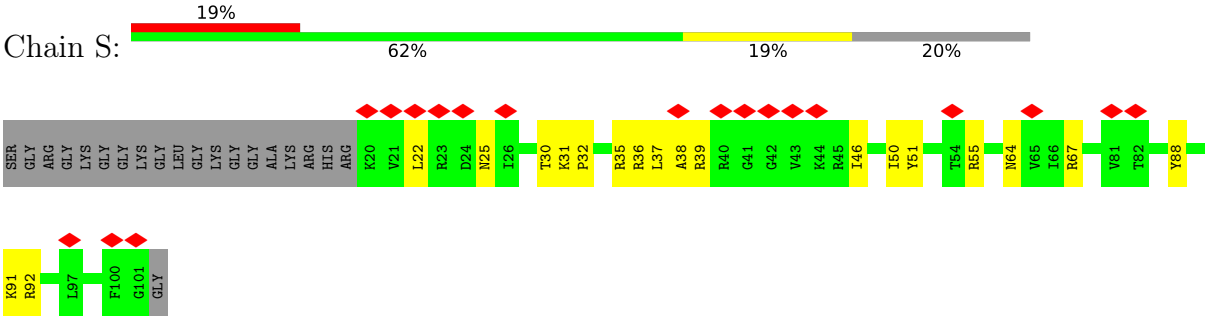
• Molecule 1: Histone H3.2



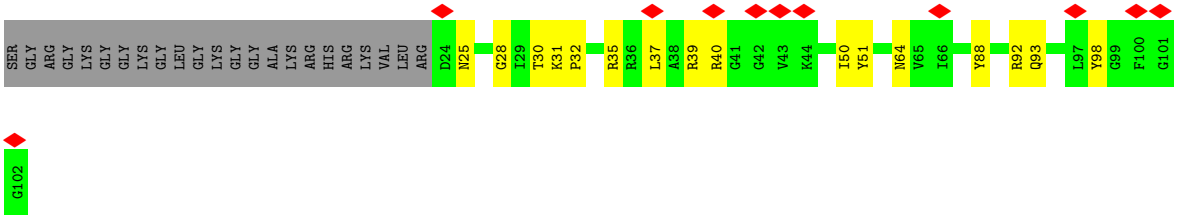
• Molecule 1: Histone H3.2



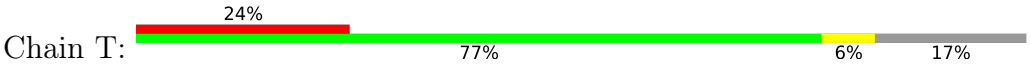
• Molecule 2: Histone H4

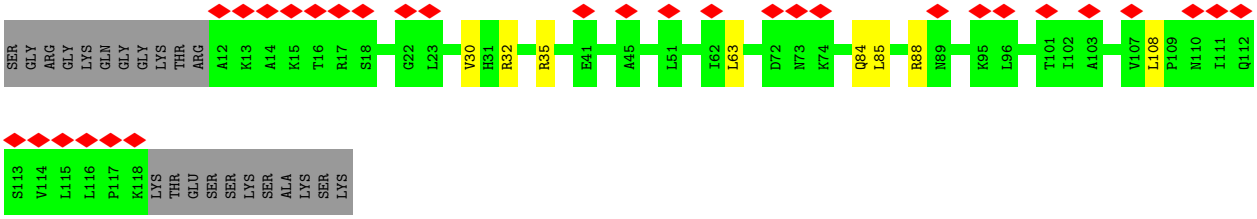


• Molecule 2: Histone H4

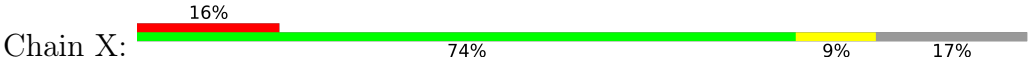


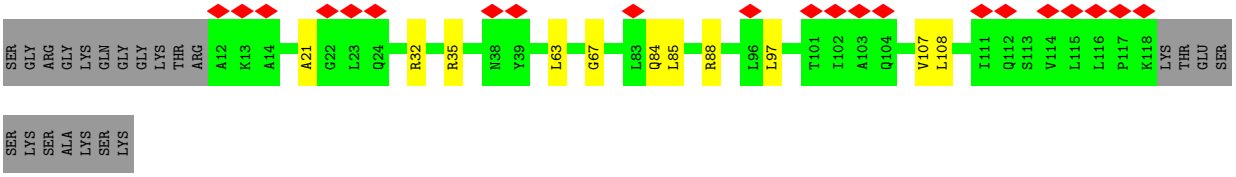
• Molecule 3: Histone H2A type 1



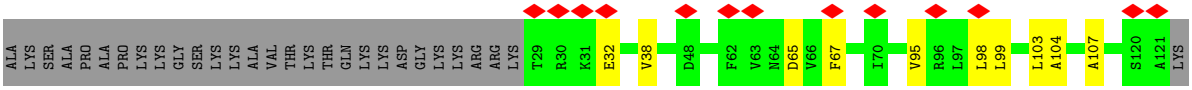


• Molecule 3: Histone H2A type 1

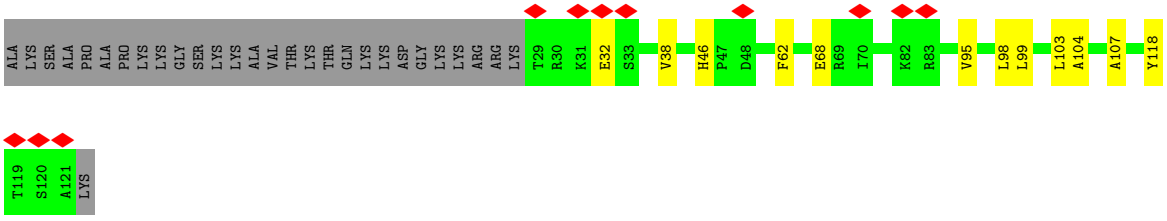




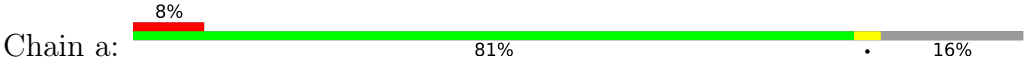
• Molecule 4: Histone H2B 1.1

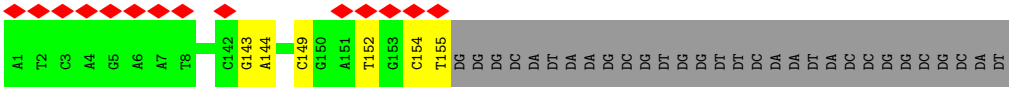


• Molecule 4: Histone H2B 1.1



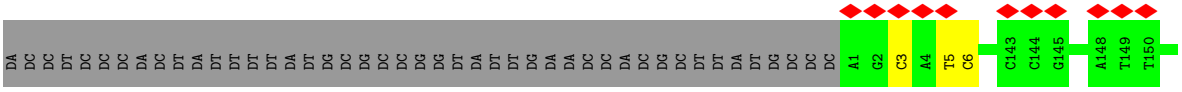
• Molecule 5: 601 sequence bottom strand





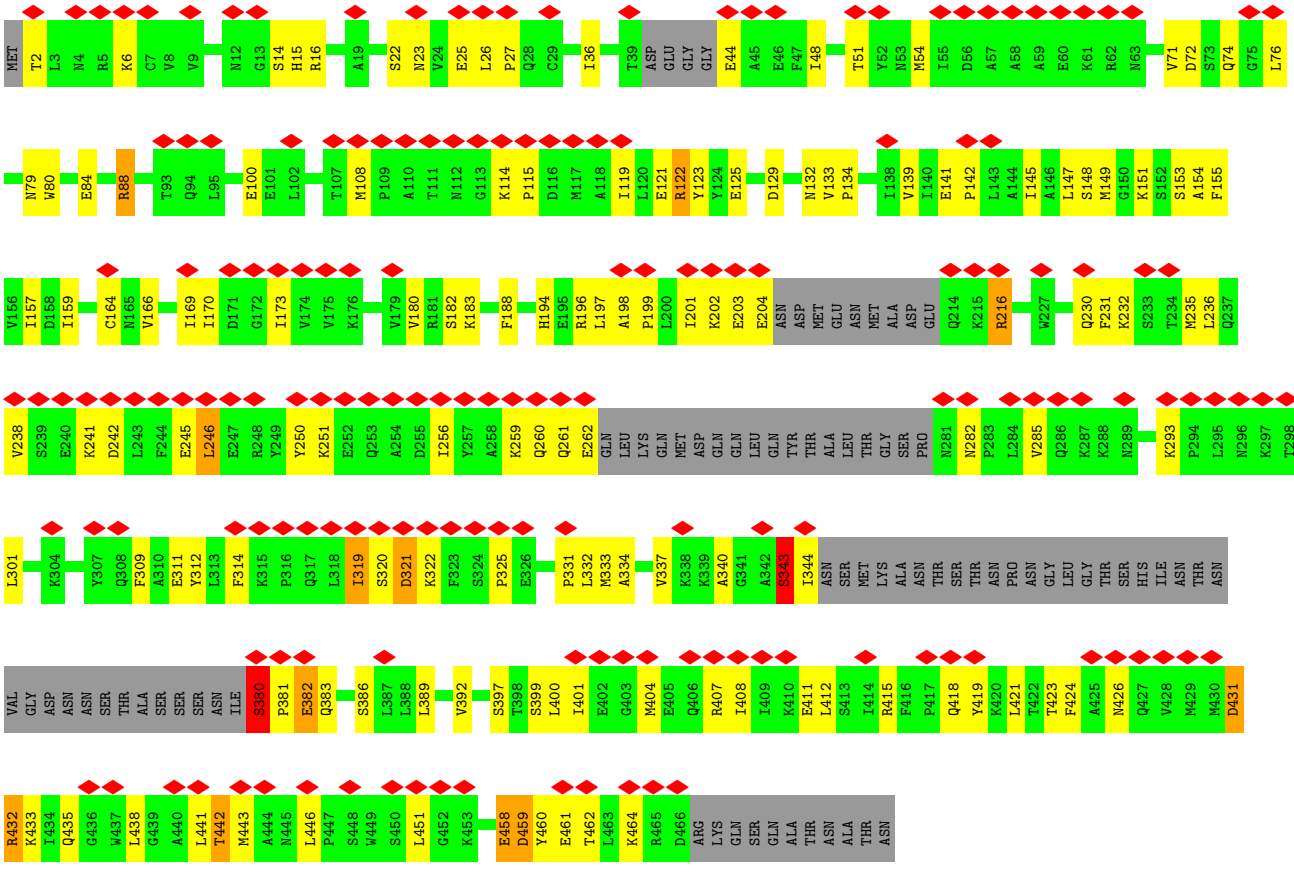
• Molecule 6: 601 sequence top strand

Chain b:



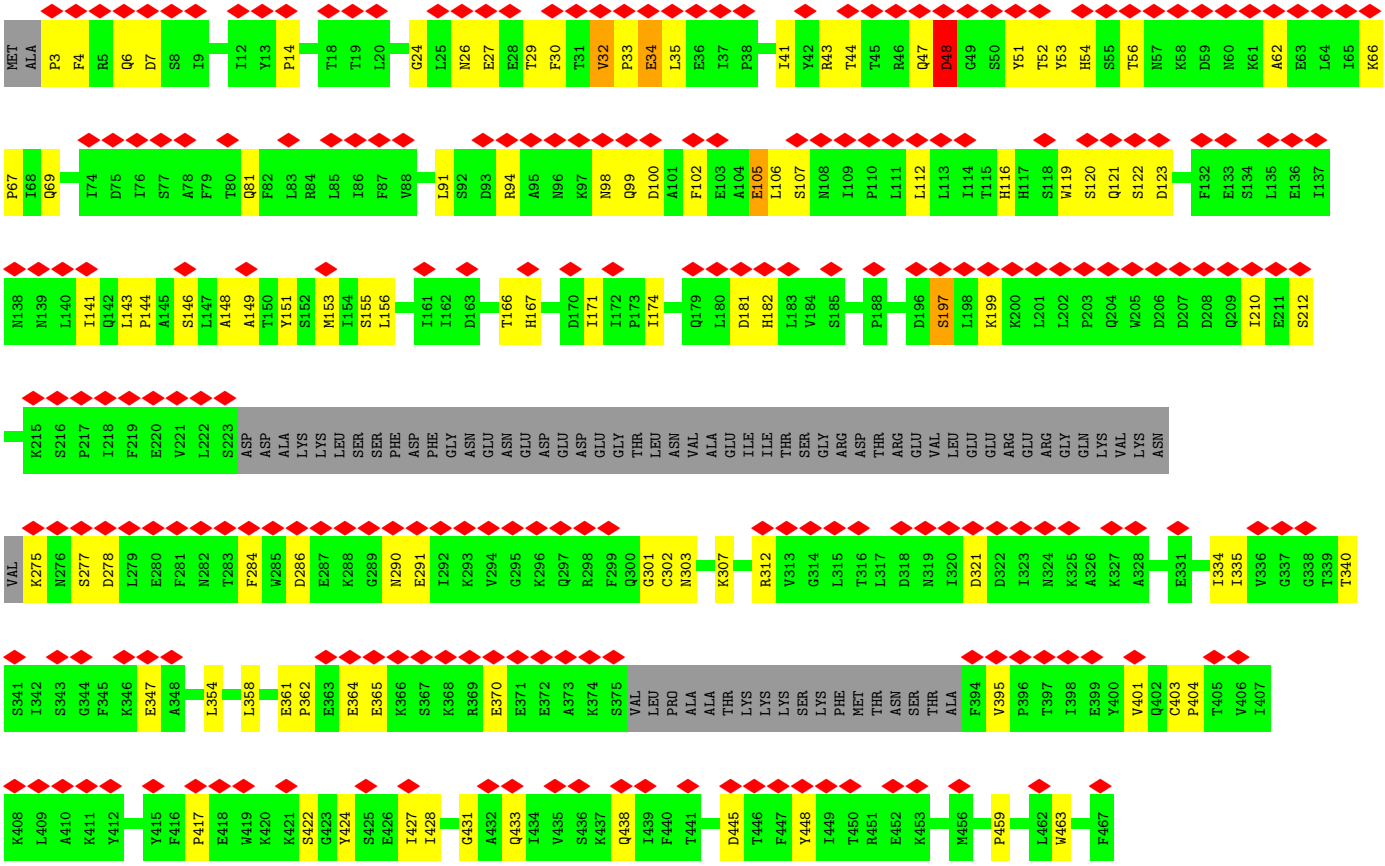
• Molecule 7: Actin-related protein 7

Chain P:



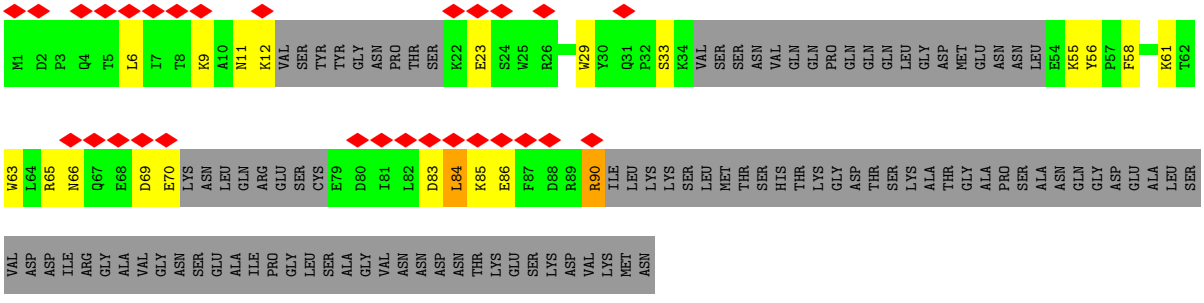
• Molecule 8: Actin-like protein ARP9

Chain Q:



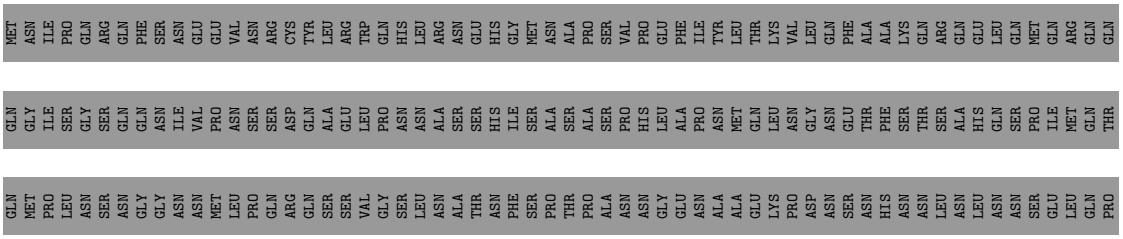
• Molecule 9: Regulator of Ty1 transposition protein 102

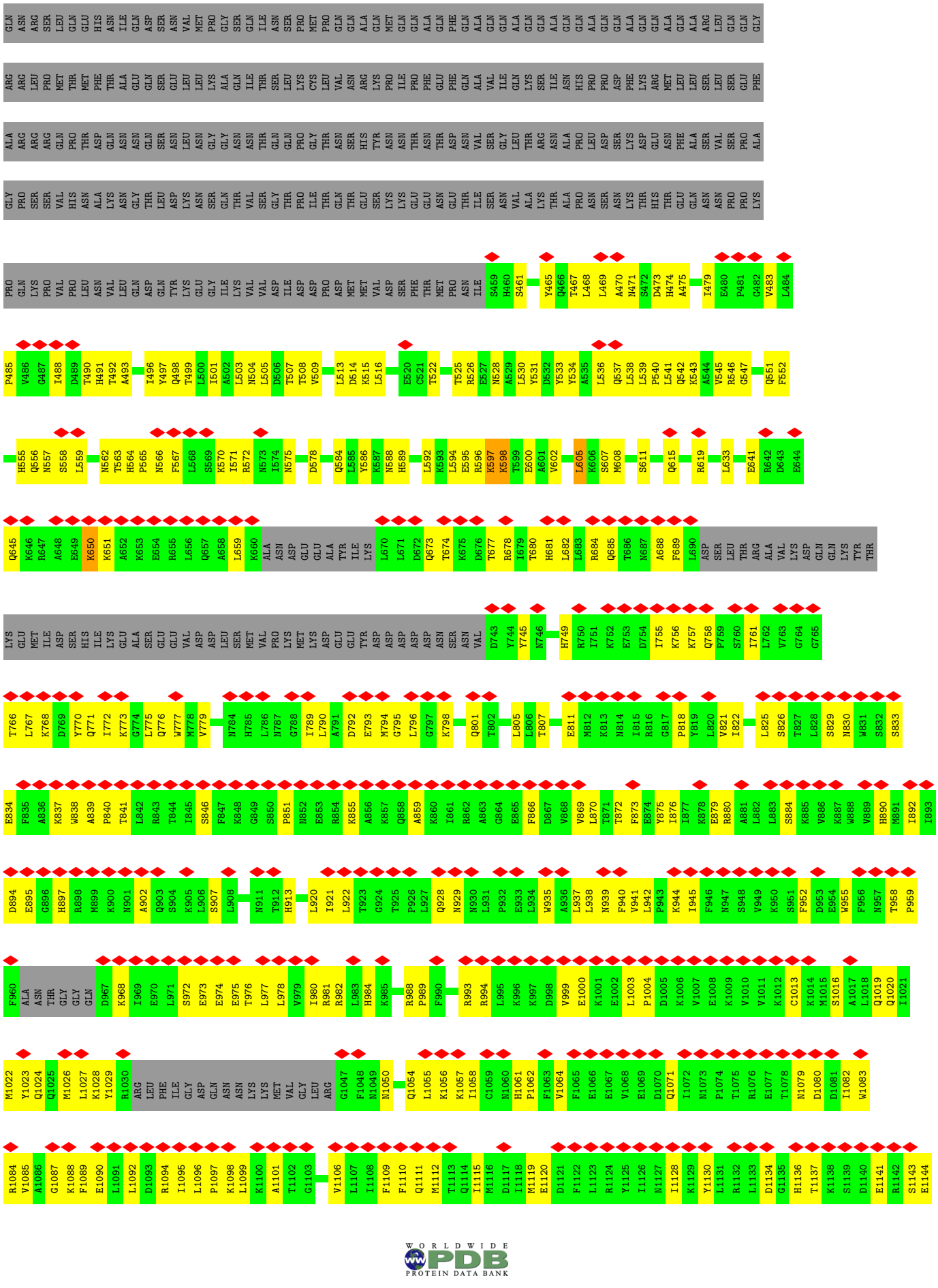
Chain Z:

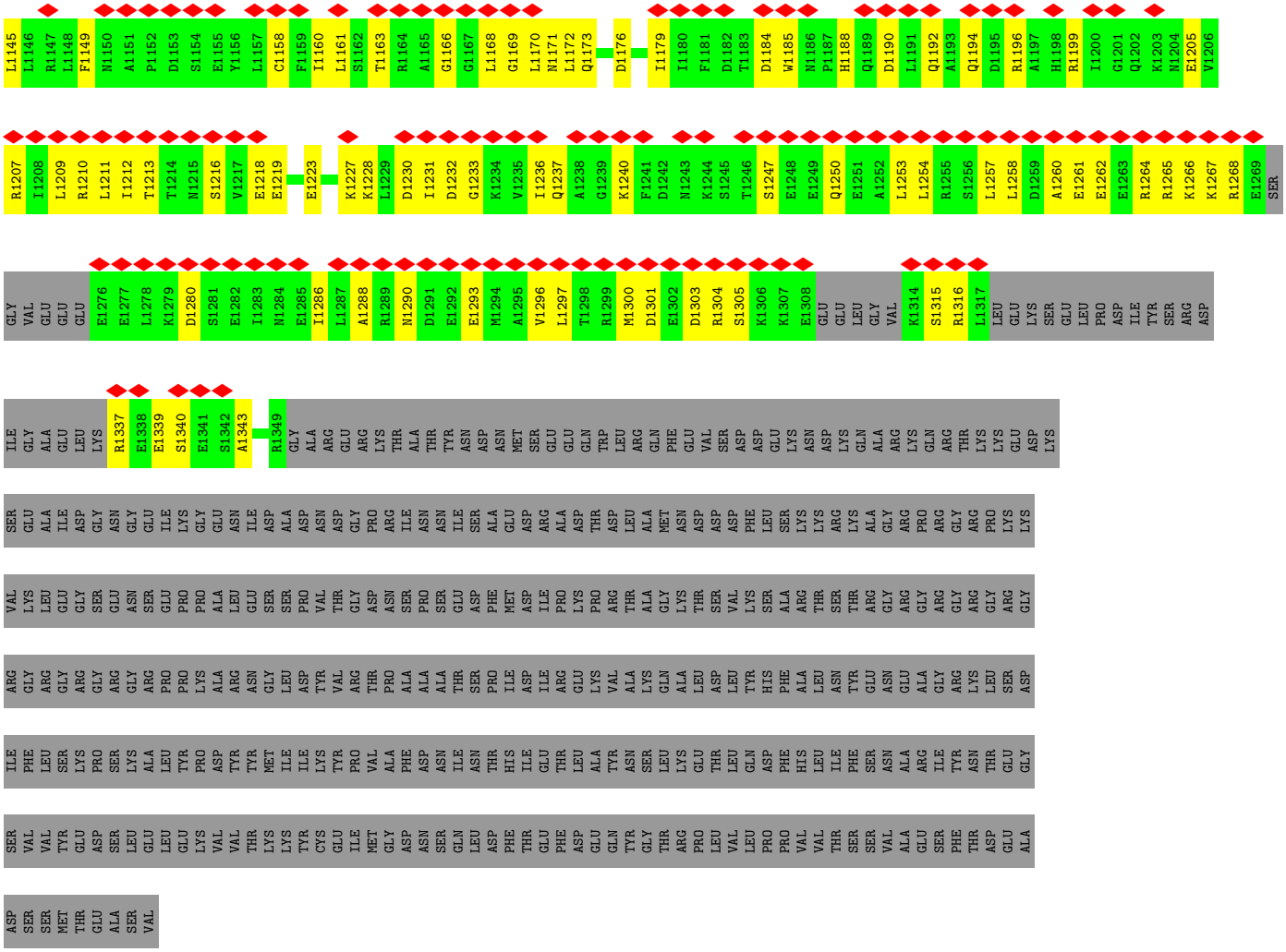


• Molecule 10: Transcription regulatory protein SNF2

Chain A:

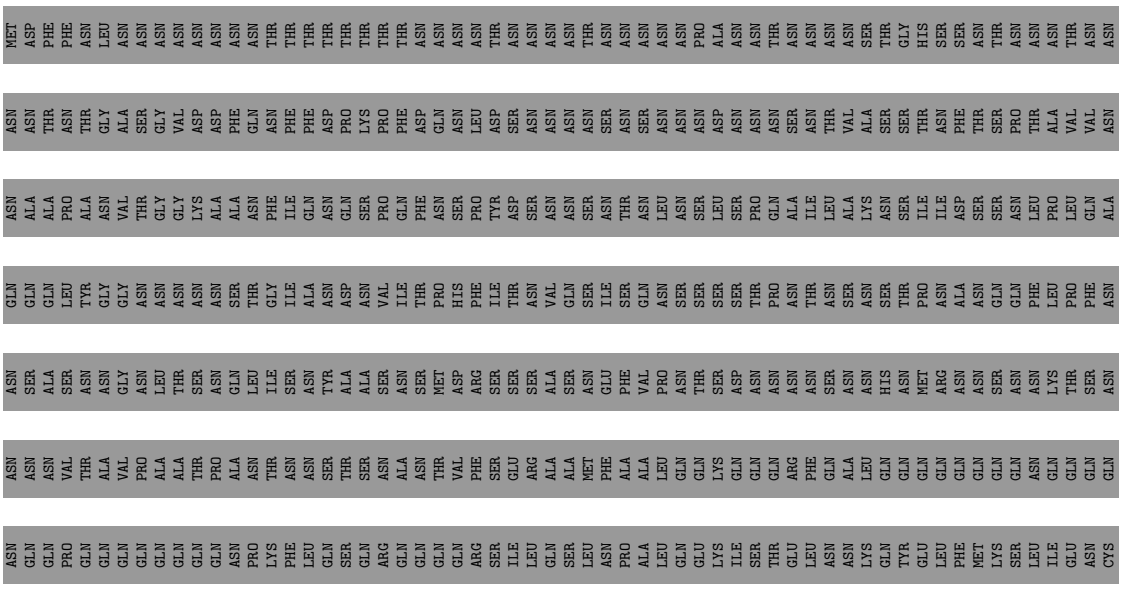


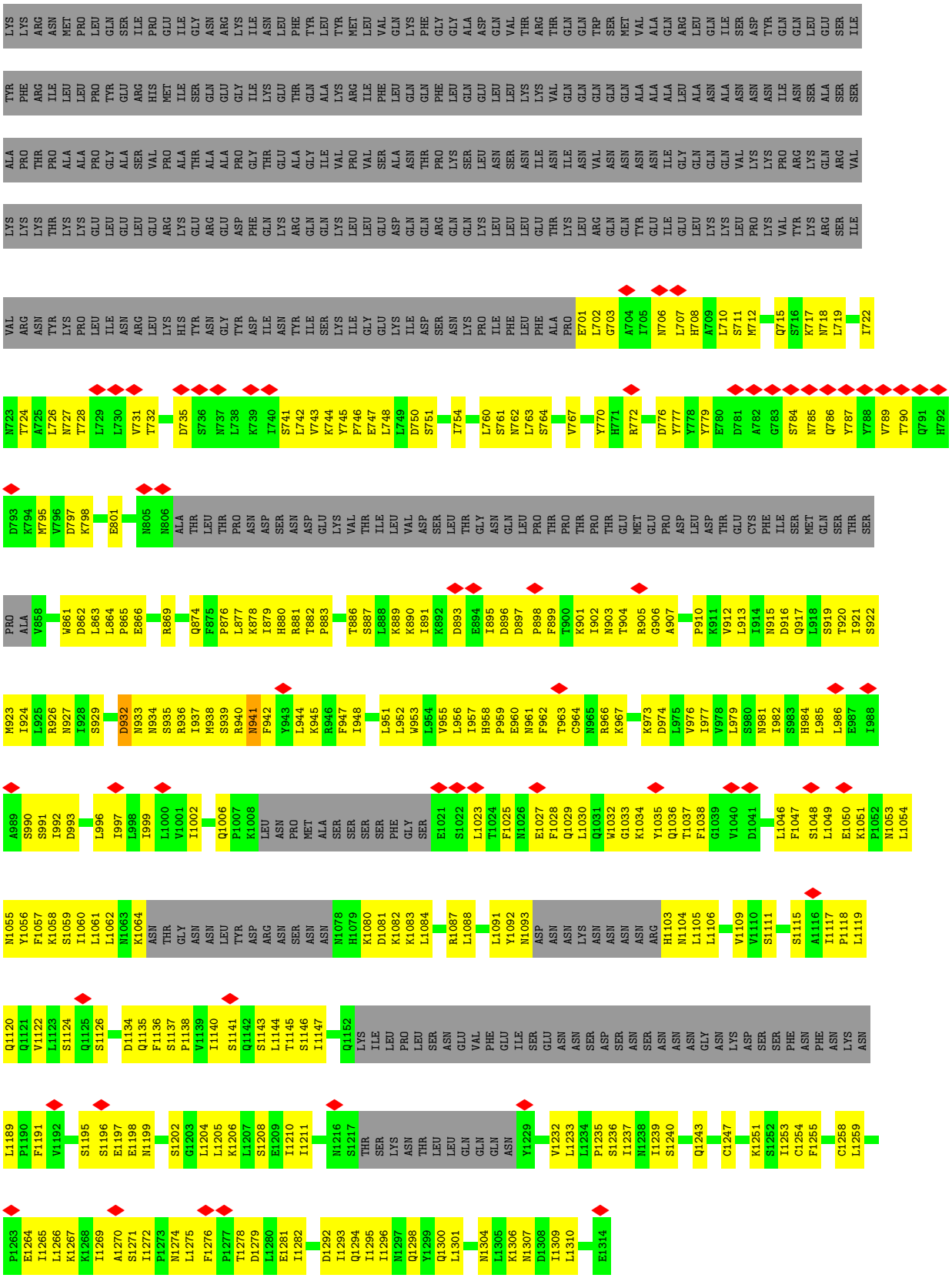




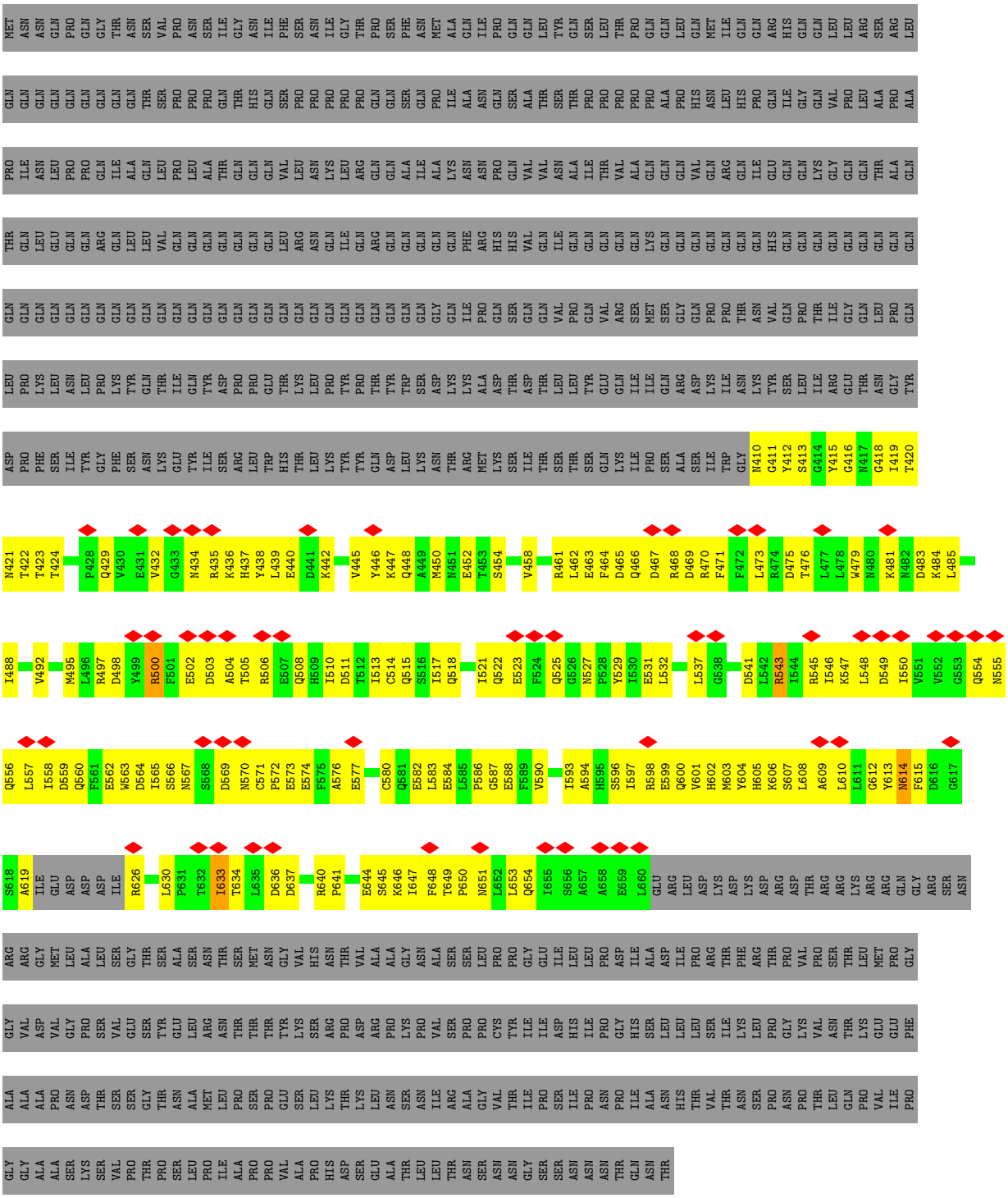
• Molecule 11: SWI/SNF chromatin-remodeling complex subunit SWI1

Chain B: 16% 21% 63%



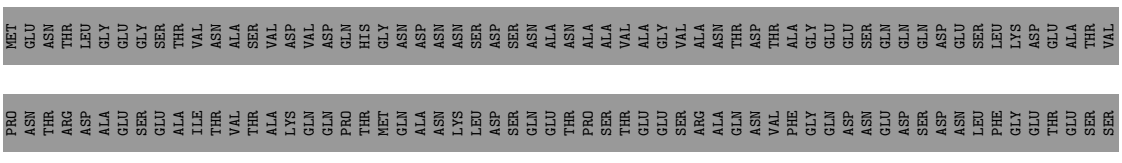


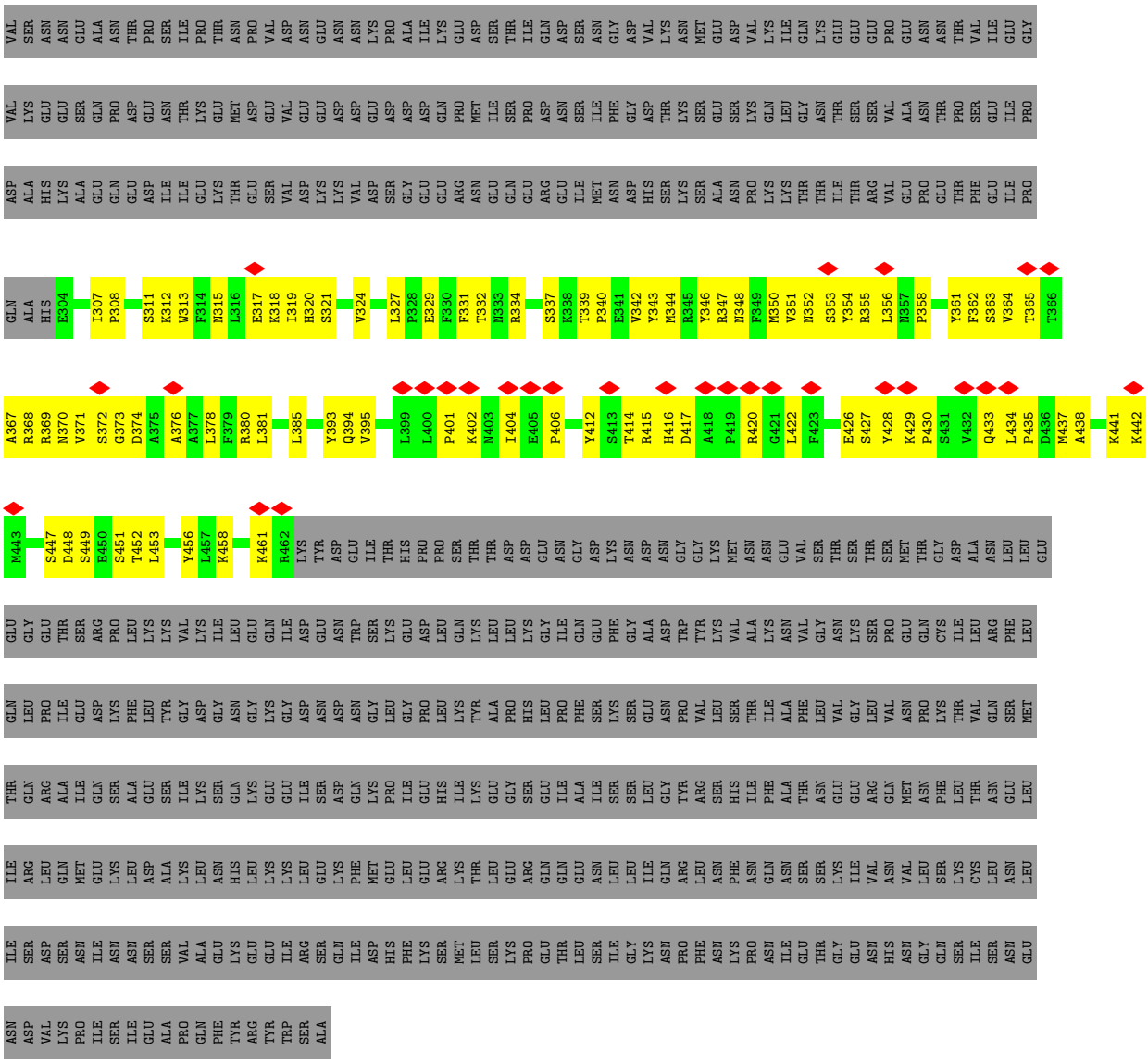
• Molecule 12: SWI/SNF chromatin-remodeling complex subunit SNF5



• Molecule 13: SWI/SNF complex subunit SWI3

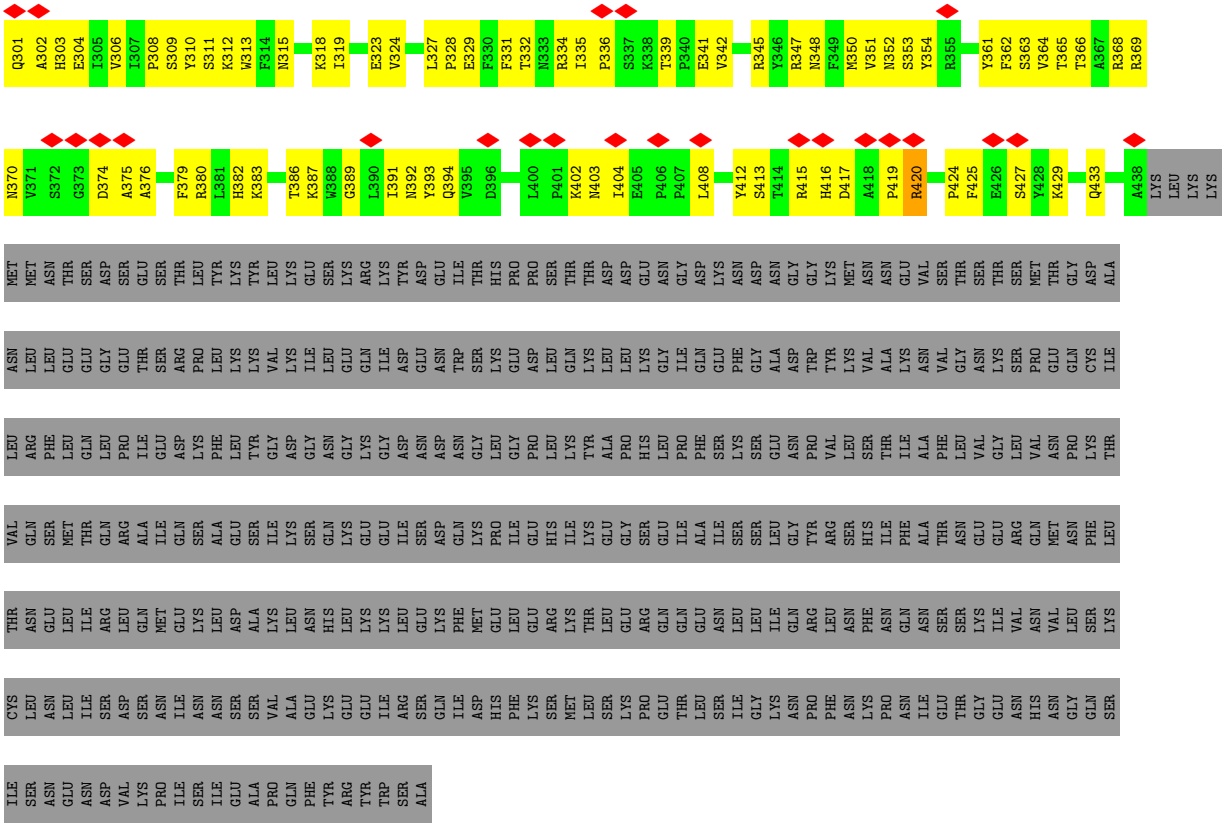
Chain D:



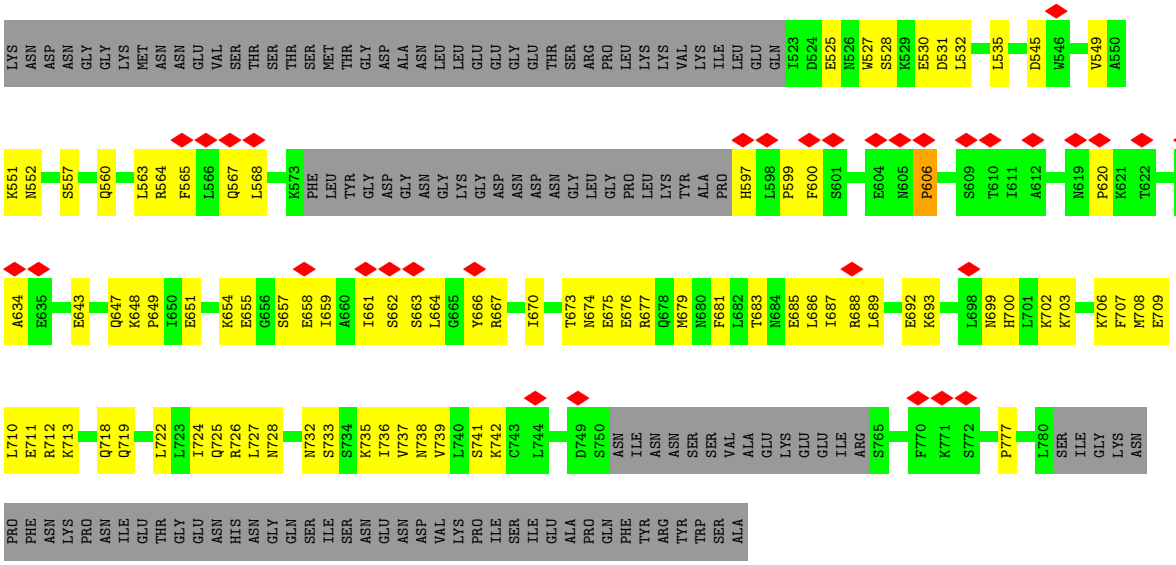


• Molecule 13: SWI/SNF complex subunit SWI3

Chain E:

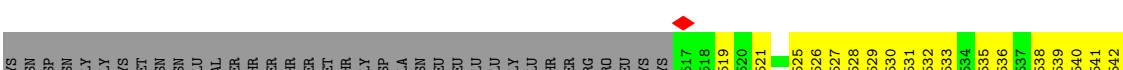

Q301 A302 H303 E304 I305 V306 I307 P308 S309 Y310 S311 K312 W313 F314 N315 K318 I319 E323 V324 L327 P328 E329 F330 F331 T332 N333 R334 I335 P336 S337 K338 T339 P340 E341 V342 R345 Y346 R347 N348 F349 M350 V351 N352 S353 Y354 R355 Y361 F362 S363 V364 T365 T366 A367 R368 R369
N370 V371 S372 G373 D374 A375 A376 F379 R380 L381 H382 K383 T386 K387 W388 G389 L390 I391 N392 Y393 Q394 V395 D396 L400 P401 K402 N403 I404 E405 P406 P407 L408 Y412 S413 T414 R415 H416 D417 A418 P419 R420 P424 F425 E426 S427 Y428 K429 Q433 A438 LYS LEU LYS LYS
MET MET ASN THR SER ASP SER GLU SER THR LEU TYR LYS TYR LEU LYS GLU SER LYS ARG LYS TYR ASP GLU ILE THR HIS PRO PRO SER THR THR ASP ASP GLU ASN GLY ASP LYS ASN ASP ASN GLY GLY LYS MET ASN ASN GLU VAL SER THR SER THR SER ASN LYS THR THR ASP ALA
ASN LEU LEU GLU GLU GLY GLU THR SER ARG PRO LEU LYS LYS VAL LYS ILE LEU GLU GLN ILE ASP GLU ASN TRP SER LYS GLU ASP LEU GLN LYS LEU LEU LYS GLY ILE GLN GLU PHE GLY ALA ASP TRP TYR TYR LYS VAL ALA LYS ASN VAL GLY ASN LYS SER PRO GLU GLN CYS ILE
LEU ARG PHE LEU GLN LEU PRO ILE GLU ASP LYS PHE LEU TYR GLY ASP GLY ASN GLY LYS GLY ASP ASN ASP ASN GLY LEU GLY PRO LEU LYS TYR ALA PRO HIS LEU PRO PHE SER LYS SER GLU ASN PRO VAL LEU SER THR ILE ALA PHE LEU VAL GLY LEU VAL ASN PRO LYS THR
VAL GLN SER MET THR GLN ARG ALA ILE GLN SER ALA GLU SER ILE LYS SER GLN LYS GLU GLU ILE SER ASP GLN LYS PRO ILE GLU GLU HIS ILE LYS GLU GLY SER GLU ILE ALA ILE SER SER LEU GLY TYR ARG SER HIS ILE PHE ALA THR ASN GLU GLU GLU ARG GLN MET ASN PHE LEU
THR ASN GLU LEU ILE ARG LEU GLN MET GLU LYS LEU ASP ALA LYS LEU ASN HIS LEU LYS LYS LEU GLU LYS PHE MET GLU LEU GLU GLU ARG LYS THR LEU GLU GLY GLN GLN GLU ASN LEU LEU ILE GLN ARG LEU ASN PHE ASN GLN ASN SER SER LYS ILE VAL ASN VAL LEU SER LYS
CYS LEU ASN LEU ILE SER ASP SER ASN ILE ASN ASN SER SER VAL ALA GLU LYS GLU GLU ILE ARG SER GLN ILE ASP HIS PHE LYS SER MET LEU SER LYS PRO GLU THR LEU SER ILE GLY LYS ASN PRO PHE ASN LYS PRO ASN ILE GLU THR GLY GLU ASN HIS ASN GLY GLN SER
ILE SER ASN GLU ASN ASP VAL LYS PRO ILE SER ILE GLU ALA ALA PRO GLN PHE TYR ARG TYR TRP SER ALA
• Molecule 13: SWI/SNF complex subunit SWI3
Chain F:

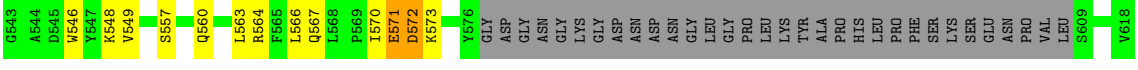

MET GLU ASN THR LEU GLY GLU GLY SER THR VAL ASN ALA SER VAL ASP VAL ASP GLN HIS GLY ASN ASP ASN ASN SER ASP SER ASN ALA ASN ALA ALA VAL ALA GLY VAL ALA ASN THR ASP THR ALA GLY GLU GLU SER GLN GLN GLN ASP GLU SER LEU LYS ASP GLU ALA THR VAL
PRO ASN THR ARG ASP ALA GLU SER GLU ALA ILE THR VAL THR ALA LYS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

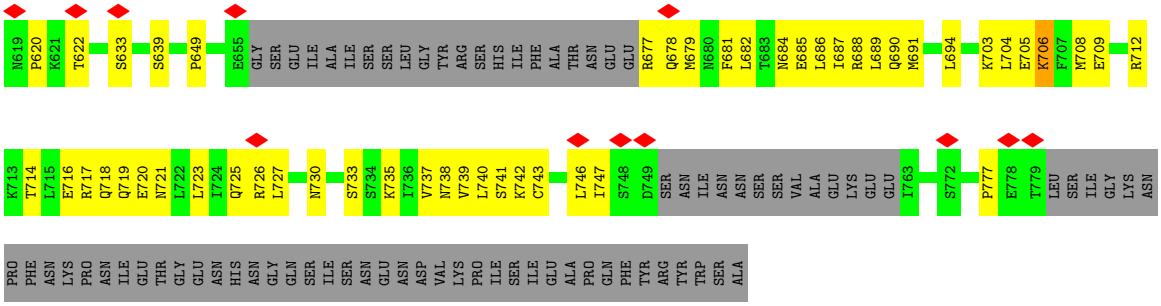


• Molecule 13: SWI/SNF complex subunit SWI3

Chain G:

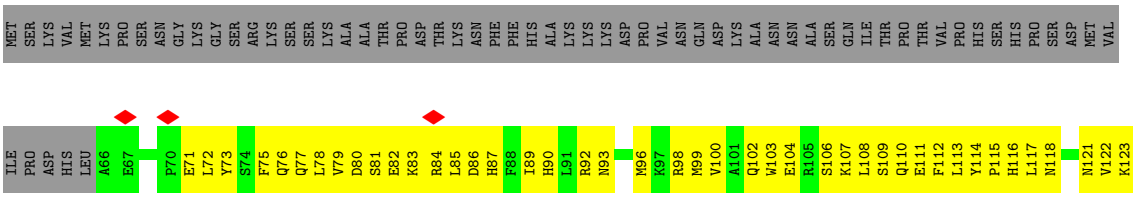


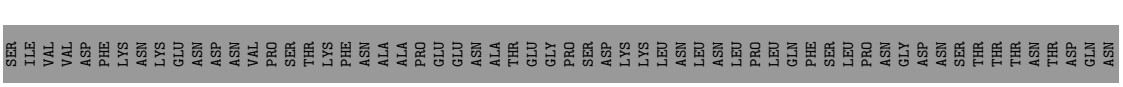


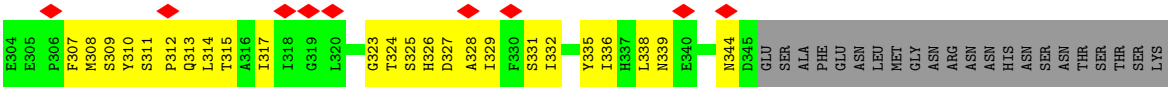


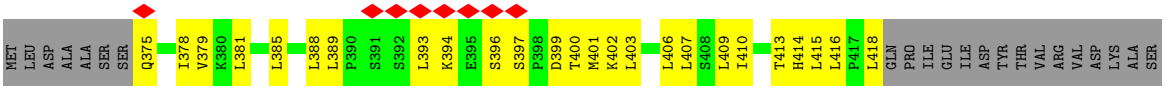
• Molecule 14: Transcription regulatory protein SNF12

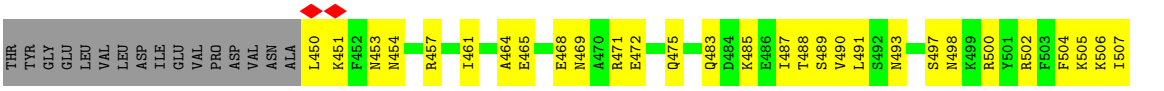
Chain H:

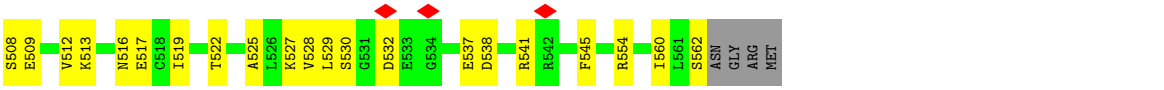






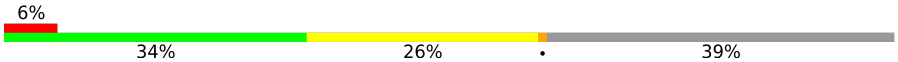


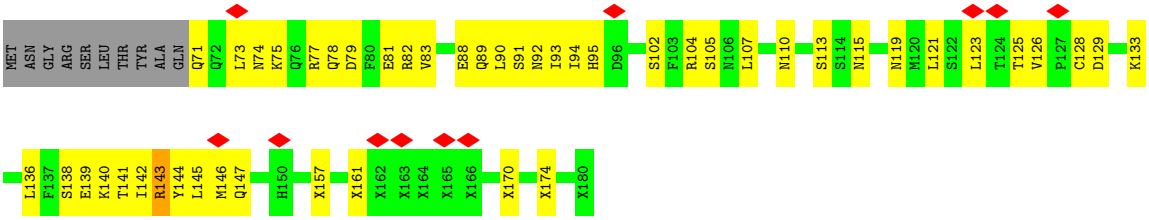




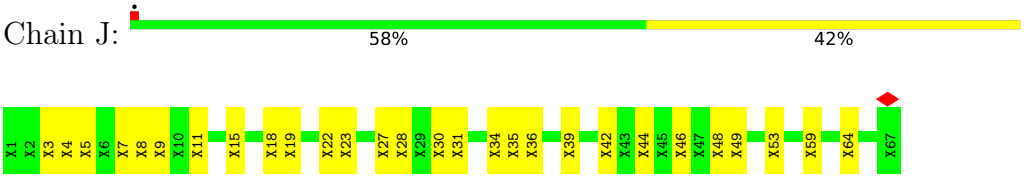
• Molecule 15: Transcription regulatory protein SNF6

Chain I:

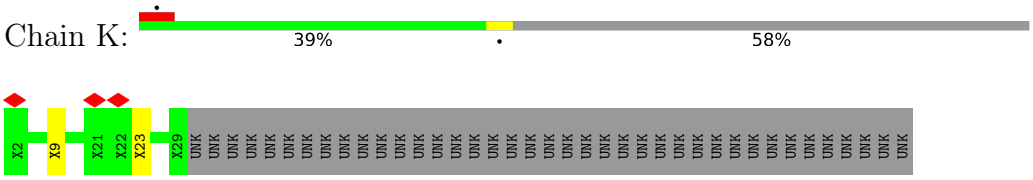




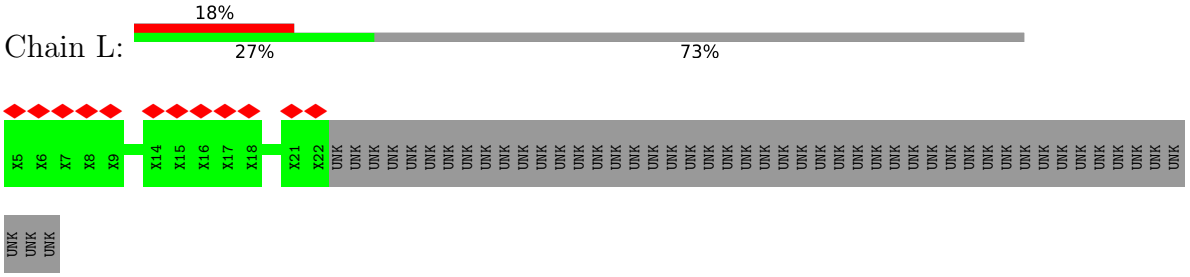
• Molecule 16: Unknown protein



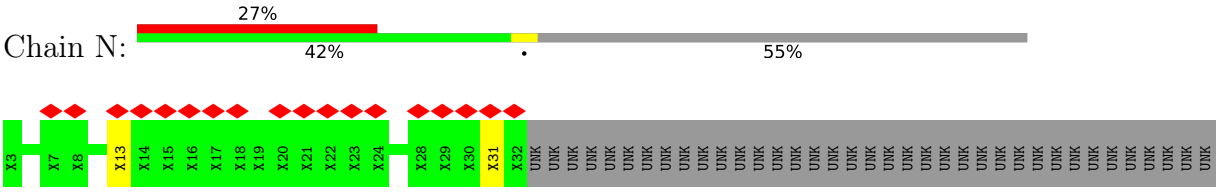
• Molecule 16: Unknown protein



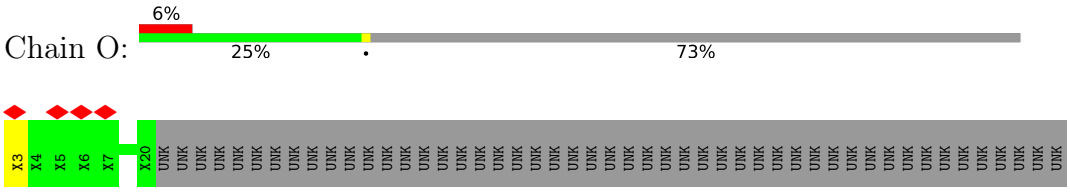
• Molecule 16: Unknown protein



• Molecule 16: Unknown protein

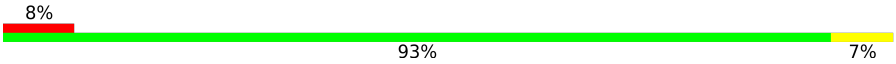


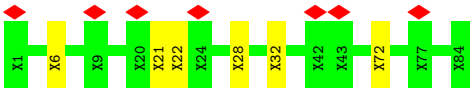
• Molecule 16: Unknown protein



• Molecule 17: SWI/SNF global transcription activator complex subunit SWP82

Chain M:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF amplitude correction was performed following 3D auto refinement in relion.	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	76.5	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	0.171	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.24, 2.24, 2.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ADP, BEF

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	R	0.24	0/813	0.38	0/1093
1	V	0.24	0/789	0.38	0/1059
2	S	0.24	0/660	0.42	0/885
2	W	0.25	0/634	0.41	0/848
3	T	0.24	0/821	0.40	0/1112
3	X	0.24	0/825	0.40	0/1116
4	U	0.24	0/729	0.37	0/985
4	Y	0.24	0/737	0.37	0/993
5	a	0.58	6/3541 (0.2%)	0.94	0/5458
6	b	0.55	4/3587 (0.1%)	0.92	0/5539
7	P	0.43	0/3303	0.61	1/4465 (0.0%)
8	Q	0.45	0/3269	0.59	0/4432
9	Z	0.41	0/501	0.57	0/669
10	A	0.28	0/6488	0.50	1/8732 (0.0%)
11	B	0.38	0/3958	0.52	0/5364
12	C	0.35	0/2040	0.54	0/2756
13	D	0.34	0/1359	0.47	0/1838
13	E	0.40	0/1189	0.51	0/1616
13	F	0.32	0/1596	0.52	5/2154 (0.2%)
13	G	0.33	0/1446	0.51	3/1949 (0.2%)
14	H	0.35	0/2119	0.47	0/2856
15	I	0.32	0/682	0.48	0/913
All	All	0.39	10/41086 (0.0%)	0.61	10/56832 (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.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	B	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	153	DG	C1'-N9	-5.53	1.39	1.47
6	b	5	DT	C1'-N1	5.24	1.56	1.49
5	a	149	DC	C1'-N1	5.22	1.56	1.49
5	a	155	DT	C1'-N1	5.19	1.55	1.49
6	b	6	DC	C1'-N1	5.17	1.55	1.49
5	a	154	DC	C1'-N1	5.16	1.55	1.49
5	a	152	DT	C1'-N1	5.16	1.55	1.49
6	b	3	DC	C1'-N1	5.14	1.55	1.49
5	a	144	DA	C1'-N9	-5.14	1.40	1.47
5	a	143	DG	C1'-N9	-5.03	1.40	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	606	PRO	N-CA-CB	6.96	111.65	103.30
13	G	620	PRO	N-CA-CB	6.12	110.64	103.30
13	F	649	PRO	N-CA-CB	6.05	110.56	103.30
7	P	380	SER	C-N-CD	5.93	140.86	128.40
13	F	599	PRO	N-CA-CB	5.90	110.38	103.30
13	F	777	PRO	N-CA-CB	5.71	110.15	103.30
13	G	777	PRO	N-CA-CB	5.64	110.07	103.30
13	G	649	PRO	N-CA-CB	5.58	110.00	103.30
10	A	959	PRO	N-CA-CB	5.57	109.99	103.30
13	F	620	PRO	N-CA-CB	5.35	109.72	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	B	776	ASP	Peptide
11	B	932	ASP	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	R	801	0	831	15	0
1	V	779	0	815	16	0
2	S	653	0	695	13	0
2	W	627	0	663	14	0
3	T	811	0	849	6	0
3	X	815	0	860	9	0
4	U	718	0	725	8	0
4	Y	726	0	747	10	0
5	a	3160	0	1741	0	0
6	b	3195	0	1742	0	0
7	P	3227	0	3251	170	0
8	Q	3198	0	3187	67	0
9	Z	490	0	467	19	0
10	A	6385	0	6494	327	0
11	B	3890	0	4008	253	0
12	C	2005	0	1939	165	0
13	D	1322	0	1325	95	0
13	E	1152	0	1137	86	0
13	F	1583	0	1397	74	0
13	G	1435	0	1294	59	0
14	H	2085	0	2104	139	0
15	I	818	0	708	67	0
16	J	336	0	70	20	0
16	K	140	0	33	3	0
16	L	90	0	21	0	0
16	N	150	0	41	3	0
16	O	90	0	21	2	0
17	M	416	0	92	4	0
18	A	5	0	0	0	0
18	P	25	0	0	0	0
18	Q	30	0	0	1	0
19	A	27	0	12	6	0
20	A	4	0	0	4	0
21	A	1	0	0	0	0
22	P	33	0	0	4	0
22	Q	51	0	0	4	0
22	Z	2	0	0	0	0
All	All	41275	0	37269	1458	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 21.

All (1458) 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)
7:P:238:VAL:HG21	7:P:404:MET:SD	1.34	1.68
7:P:36:ILE:HD12	7:P:54:MET:CE	1.34	1.52
13:D:412:TYR:CD1	14:H:560:ILE:HG23	1.62	1.35
7:P:36:ILE:CD1	7:P:54:MET:HE3	1.58	1.33
13:D:412:TYR:CD1	14:H:560:ILE:CG2	2.12	1.33
7:P:155:PHE:CE2	7:P:333:MET:HE3	1.65	1.30
7:P:36:ILE:CD1	7:P:54:MET:CE	2.11	1.29
7:P:238:VAL:CG2	7:P:404:MET:SD	2.19	1.28
10:A:594:LEU:O	10:A:598:LYS:HD3	1.35	1.27
7:P:76:LEU:CD2	7:P:108:MET:CE	2.15	1.25
7:P:157:ILE:CD1	7:P:333:MET:HE2	1.67	1.21
7:P:76:LEU:CD2	7:P:108:MET:HE3	1.67	1.20
7:P:36:ILE:CG1	7:P:54:MET:HE1	1.71	1.19
7:P:36:ILE:CB	7:P:54:MET:HE1	1.75	1.16
7:P:451:LEU:HD13	10:A:608:MET:SD	1.88	1.14
7:P:155:PHE:CE2	7:P:333:MET:CE	2.31	1.12
7:P:76:LEU:HD22	7:P:108:MET:HE1	1.23	1.12
7:P:343:SER:CB	7:P:344:ILE:HA	1.81	1.09
7:P:76:LEU:HD21	7:P:108:MET:HE3	1.33	1.08
10:A:594:LEU:HG	10:A:598:LYS:HE3	1.32	1.08
7:P:157:ILE:HG12	7:P:333:MET:HE1	1.33	1.07
7:P:343:SER:HB3	7:P:344:ILE:HA	1.09	1.05
10:A:594:LEU:CG	10:A:598:LYS:HE3	1.87	1.05
10:A:876:ILE:O	10:A:880:ARG:HB3	1.56	1.05
7:P:216:ARG:HG2	7:P:216:ARG:HH11	1.17	1.04
7:P:157:ILE:HG12	7:P:333:MET:CE	1.87	1.03
7:P:114:LYS:HG3	7:P:115:PRO:HD3	1.37	1.03
13:D:412:TYR:CG	14:H:560:ILE:HG21	1.93	1.03
13:D:412:TYR:CD1	14:H:560:ILE:HG21	1.95	1.01
7:P:122:ARG:HH11	7:P:122:ARG:HG2	1.25	1.00
7:P:25:GLU:O	10:A:619:ARG:NH2	1.96	0.98
10:A:570:LYS:HE2	15:I:90:LEU:H	1.25	0.97
10:A:1190:ASP:O	10:A:1194:GLN:HB2	1.63	0.97
7:P:343:SER:HB3	7:P:344:ILE:CA	1.95	0.97
7:P:76:LEU:HD22	7:P:108:MET:CE	1.86	0.97
13:D:412:TYR:HD1	14:H:560:ILE:HG23	1.16	0.96
10:A:801:GLN:O	10:A:805:LEU:HB2	1.67	0.95
10:A:673:GLN:O	10:A:677:THR:HB	1.66	0.95
7:P:157:ILE:HD11	7:P:333:MET:HE2	1.46	0.94
10:A:1253:LEU:O	10:A:1257:LEU:HB3	1.66	0.94
10:A:807:THR:O	10:A:811:GLU:HB2	1.68	0.93
7:P:36:ILE:CG1	7:P:54:MET:CE	2.41	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:875:TYR:O	10:A:879:GLU:HB2	1.68	0.93
7:P:108:MET:SD	22:P:606:HOH:O	2.27	0.91
11:B:933:ASN:HB2	11:B:936:ARG:HE	1.34	0.91
7:P:157:ILE:CD1	7:P:333:MET:CE	2.48	0.91
13:D:412:TYR:CG	14:H:560:ILE:CG2	2.54	0.90
10:A:972:SER:O	10:A:976:THR:HB	1.71	0.90
7:P:166:VAL:HG21	7:P:333:MET:SD	2.13	0.89
12:C:641:PRO:HG2	13:D:372:SER:OG	1.72	0.89
7:P:84:GLU:OE2	7:P:88:ARG:NH1	2.05	0.89
10:A:594:LEU:CD1	10:A:598:LYS:HE3	2.03	0.88
13:G:519:ILE:HD12	13:G:572:ASP:HB3	1.55	0.88
7:P:157:ILE:HD13	7:P:333:MET:HE2	1.55	0.87
12:C:432:VAL:HG12	12:C:436:LYS:H	1.40	0.86
12:C:644:GLU:HA	12:C:647:ILE:CG1	2.04	0.86
7:P:155:PHE:HE2	7:P:333:MET:HE3	1.15	0.86
7:P:157:ILE:CG1	7:P:333:MET:CE	2.52	0.86
10:A:771:GLN:O	10:A:775:LEU:HB2	1.76	0.86
8:Q:303:ASN:HD21	8:Q:307:LYS:HZ1	1.19	0.85
10:A:794:MET:HE1	10:A:1192:GLN:HA	1.57	0.85
11:B:887:SER:O	11:B:890:LYS:HB3	1.76	0.85
10:A:974:GLU:O	10:A:978:LEU:HB2	1.77	0.85
12:C:439:LEU:HD22	13:E:387:LYS:HG2	1.59	0.85
7:P:76:LEU:CD2	7:P:108:MET:HE1	1.88	0.84
7:P:36:ILE:HD12	7:P:54:MET:HE3	0.84	0.83
10:A:1188:HIS:O	10:A:1192:GLN:HB2	1.78	0.83
13:G:677:ARG:HH11	13:G:678:GLN:H	1.25	0.83
10:A:557:ASN:HB3	11:B:907:ALA:H	1.44	0.83
10:A:570:LYS:NZ	15:I:88:GLU:O	2.13	0.82
12:C:644:GLU:HA	12:C:647:ILE:HG13	1.61	0.81
7:P:157:ILE:CG1	7:P:333:MET:HE1	2.10	0.81
10:A:684:ARG:O	10:A:688:ALA:HB3	1.81	0.81
12:C:505:THR:HA	12:C:508:GLN:HB2	1.63	0.81
7:P:155:PHE:CZ	7:P:333:MET:HE3	2.16	0.81
7:P:166:VAL:CG2	7:P:333:MET:SD	2.68	0.81
7:P:147:LEU:CD2	7:P:443:MET:SD	2.68	0.81
7:P:36:ILE:HD12	7:P:54:MET:SD	2.22	0.80
10:A:597:LYS:HB2	10:A:597:LYS:NZ	1.95	0.80
7:P:36:ILE:CA	7:P:54:MET:HE1	2.13	0.79
10:A:505:LEU:HB2	13:G:573:LYS:HE2	1.64	0.79
13:D:412:TYR:HB2	14:H:560:ILE:HG22	1.65	0.79
12:C:504:ALA:O	12:C:508:GLN:NE2	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:159:ILE:HD11	7:P:408:ILE:HD11	1.65	0.78
8:Q:459:PRO:HG2	9:Z:63:TRP:CD2	2.18	0.78
13:D:414:THR:OG1	13:E:309:SER:N	2.15	0.78
13:D:434:LEU:HD12	13:D:435:PRO:HD2	1.65	0.78
10:A:597:LYS:HA	10:A:600:GLU:HB2	1.66	0.78
7:P:36:ILE:N	7:P:54:MET:CE	2.47	0.77
7:P:36:ILE:N	7:P:54:MET:HE1	1.98	0.77
7:P:114:LYS:HG3	7:P:115:PRO:CD	2.14	0.77
13:E:402:LYS:NZ	13:E:403:ASN:O	2.16	0.77
10:A:793:GLU:O	10:A:794:MET:HG3	1.85	0.76
10:A:768:LYS:H	10:A:771:GLN:HE22	1.32	0.76
10:A:935:TRP:HE1	10:A:952:PHE:HB2	1.49	0.76
14:H:394:LYS:NZ	14:H:401:MET:SD	2.58	0.76
7:P:122:ARG:HH11	7:P:122:ARG:CG	1.99	0.76
12:C:557:LEU:HD11	12:C:651:ASN:HB3	1.68	0.76
10:A:1253:LEU:O	10:A:1257:LEU:CB	2.34	0.75
11:B:1051:LYS:HZ2	11:B:1053:ASN:HB2	1.50	0.75
13:E:341:GLU:OE1	13:E:341:GLU:N	2.20	0.75
7:P:100:GLU:HG2	7:P:132:ASN:HB3	1.68	0.75
8:Q:303:ASN:HD21	8:Q:307:LYS:NZ	1.85	0.75
15:I:110:ASN:OD1	15:I:113:SER:OG	2.04	0.75
7:P:36:ILE:HB	7:P:54:MET:HE1	1.67	0.75
11:B:747:GLU:OE2	12:C:429:GLN:NE2	2.20	0.74
11:B:1103:HIS:O	11:B:1104:ASN:ND2	2.20	0.74
10:A:674:THR:O	10:A:678:ARG:HB2	1.88	0.74
10:A:855:LYS:O	10:A:859:ALA:CB	2.35	0.74
12:C:434:ASN:H	12:C:436:LYS:HG3	1.53	0.74
7:P:216:ARG:HG2	7:P:216:ARG:NH1	1.94	0.74
13:F:700:HIS:HA	13:F:703:LYS:HD2	1.69	0.74
11:B:1084:LEU:O	11:B:1087:ARG:HB3	1.87	0.74
13:F:525:GLU:OE2	13:F:564:ARG:NH1	2.21	0.74
7:P:147:LEU:HD22	7:P:443:MET:SD	2.28	0.73
13:G:540:GLN:HG3	13:G:541:GLU:HG3	1.70	0.73
12:C:562:GLU:HG2	12:C:634:THR:HG21	1.70	0.73
10:A:1254:LEU:O	10:A:1258:LEU:CB	2.35	0.73
12:C:633:ILE:HD12	12:C:633:ILE:H	1.54	0.73
14:H:504:PHE:HA	14:H:507:ILE:HD12	1.69	0.73
7:P:76:LEU:HD23	7:P:108:MET:HE3	1.71	0.73
10:A:798:LYS:HD3	10:A:922:LEU:HB3	1.71	0.73
10:A:572:ARG:NH2	15:I:93:ILE:O	2.21	0.73
10:A:1022:MET:O	10:A:1026:MET:HB3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:414:THR:HG22	13:D:416:HIS:CE1	2.23	0.73
10:A:1004:PRO:HB2	10:A:1205:GLU:HG3	1.71	0.73
11:B:1294:GLN:OE1	11:B:1294:GLN:N	2.18	0.73
10:A:1023:TYR:O	10:A:1027:LEU:HB3	1.89	0.73
18:Q:504:PO4:O2	22:Q:601:HOH:O	2.06	0.72
9:Z:84:LEU:O	9:Z:85:LYS:HB2	1.89	0.72
11:B:715:GLN:HE22	11:B:717:LYS:HB3	1.52	0.72
11:B:732:THR:HG21	11:B:924:ILE:HG13	1.71	0.72
12:C:574:GLU:OE1	12:C:574:GLU:N	2.21	0.72
13:D:412:TYR:HB2	14:H:560:ILE:CG2	2.18	0.72
12:C:605:HIS:O	12:C:609:ALA:N	2.22	0.72
10:A:921:ILE:HD12	10:A:941:VAL:HG22	1.71	0.72
12:C:502:GLU:O	12:C:508:GLN:NE2	2.23	0.71
12:C:630:LEU:O	12:C:633:ILE:HD11	1.89	0.71
14:H:79:VAL:O	14:H:83:LYS:NZ	2.23	0.71
7:P:157:ILE:HD11	7:P:333:MET:CE	2.18	0.71
13:E:318:LYS:O	13:E:347:ARG:NH2	2.22	0.71
10:A:673:GLN:O	10:A:677:THR:CB	2.37	0.71
13:F:739:VAL:HA	13:F:742:LYS:HD2	1.72	0.71
3:T:32:ARG:NH2	4:U:32:GLU:OE2	2.24	0.71
10:A:1254:LEU:O	10:A:1258:LEU:HB2	1.90	0.71
12:C:475:ASP:OD1	13:E:369:ARG:NH1	2.23	0.71
8:Q:14:PRO:O	8:Q:116[B]:HIS:HE1	1.72	0.71
12:C:421:ASN:OD1	13:D:415:ARG:NH2	2.24	0.71
12:C:573:GLU:N	12:C:573:GLU:OE2	2.24	0.71
7:P:157:ILE:CG1	7:P:333:MET:HE2	2.19	0.70
14:H:78:LEU:O	14:H:81:SER:OG	2.08	0.70
14:H:379:VAL:O	14:H:400:THR:HA	1.90	0.70
10:A:533:TYR:CZ	10:A:537:GLN:OE1	2.45	0.70
13:E:312:LYS:HG2	14:H:560:ILE:CD1	2.21	0.70
14:H:393:LEU:HG	14:H:396:SER:HB3	1.74	0.70
7:P:344:ILE:O	7:P:344:ILE:HG23	1.92	0.70
11:B:789:VAL:HG12	11:B:790:THR:H	1.56	0.70
12:C:549:ASP:HA	12:C:557:LEU:O	1.92	0.70
12:C:481:LYS:NZ	12:C:521:ILE:O	2.18	0.70
13:F:597:HIS:N	13:F:600:PHE:O	2.25	0.70
7:P:51:THR:HB	22:P:623:HOH:O	1.91	0.70
12:C:576:ALA:HB1	12:C:590:VAL:HB	1.73	0.70
15:I:157:UNK:O	15:I:161:UNK:N	2.25	0.70
7:P:401:ILE:O	7:P:404:MET:HG2	1.91	0.70
12:C:556:GLN:NE2	12:C:654:GLN:OE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:964:CYS:HB3	11:B:967:LYS:HG2	1.74	0.69
13:G:712:ARG:NH2	14:H:106:SER:OG	2.24	0.69
7:P:183:LYS:O	7:P:183:LYS:HG2	1.91	0.69
10:A:976:THR:O	10:A:980:ILE:HB	1.92	0.69
7:P:14:SER:HA	7:P:71:VAL:HB	1.74	0.69
7:P:36:ILE:CD1	7:P:54:MET:HE1	1.99	0.69
10:A:597:LYS:O	10:A:597:LYS:HE3	1.92	0.69
10:A:594:LEU:O	10:A:598:LYS:CD	2.29	0.69
10:A:789:ILE:HD11	10:A:941:VAL:HG21	1.74	0.69
10:A:855:LYS:O	10:A:859:ALA:HB3	1.92	0.69
12:C:582:GLU:N	12:C:582:GLU:OE1	2.26	0.69
12:C:633:ILE:HD12	12:C:633:ILE:N	2.07	0.69
13:E:308:PRO:O	13:E:311:SER:OG	2.11	0.69
13:G:720:GLU:HA	13:G:723:LEU:HD12	1.75	0.69
10:A:993:ARG:HD3	10:A:1240:LYS:HA	1.75	0.69
7:P:392:VAL:HB	7:P:423:THR:HG22	1.75	0.68
10:A:552:PHE:O	14:H:554:ARG:NH1	2.25	0.68
10:A:807:THR:O	10:A:811:GLU:CB	2.40	0.68
13:E:402:LYS:NZ	16:J:59:UNK:O	2.26	0.68
8:Q:98:ASN:O	8:Q:99:GLN:HG2	1.93	0.68
7:P:155:PHE:CE2	7:P:333:MET:HE1	2.26	0.68
10:A:792:ASP:HB2	10:A:796:LEU:HD22	1.76	0.68
12:C:546:ILE:O	12:C:560:GLN:HA	1.94	0.68
10:A:547:GLY:HA3	13:E:420:ARG:HD2	1.74	0.68
10:A:570:LYS:HE2	15:I:90:LEU:N	2.07	0.68
11:B:797:ASP:O	11:B:801:GLU:N	2.18	0.68
10:A:952:PHE:HA	10:A:955:TRP:HE3	1.58	0.68
13:F:667:ARG:NH2	13:G:639:SER:O	2.27	0.68
15:I:74:ASN:HA	15:I:77:ARG:HE	1.59	0.68
10:A:1184:ASP:HB3	10:A:1190:ASP:HB2	1.75	0.68
14:H:453:ASN:HB2	14:H:457:ARG:HH12	1.59	0.68
10:A:1264:ARG:HA	10:A:1267:LYS:HB2	1.76	0.68
12:C:422:THR:HG22	12:C:423:THR:H	1.59	0.68
10:A:1190:ASP:OD2	10:A:1210:ARG:NH2	2.26	0.67
7:P:311:GLU:OE2	7:P:407:ARG:NH2	2.28	0.67
11:B:1036:GLN:OE1	11:B:1036:GLN:N	2.27	0.67
11:B:1137:SER:HA	11:B:1140:ILE:HD12	1.77	0.67
8:Q:275:LYS:HB3	8:Q:278:ASP:OD2	1.95	0.67
10:A:976:THR:HG23	10:A:980:ILE:HD12	1.74	0.67
10:A:594:LEU:HD11	10:A:598:LYS:HE3	1.77	0.67
13:G:538:GLY:O	13:G:542:PHE:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:19:UNK:O	16:J:23:UNK:N	2.27	0.67
10:A:498:GLN:HA	10:A:501:ILE:HD12	1.76	0.67
10:A:1023:TYR:O	10:A:1027:LEU:CB	2.43	0.67
12:C:559:ASP:OD1	12:C:560:GLN:N	2.28	0.67
10:A:557:ASN:ND2	11:B:907:ALA:O	2.28	0.66
11:B:958:HIS:CE1	11:B:960:GLU:HA	2.30	0.66
8:Q:107:SER:O	9:Z:11:ASN:HA	1.95	0.66
8:Q:303:ASN:ND2	8:Q:307:LYS:NZ	2.43	0.66
10:A:999:VAL:HG23	10:A:1000:GLU:HG3	1.78	0.66
8:Q:303:ASN:ND2	8:Q:307:LYS:HZ1	1.92	0.66
10:A:973:GLU:O	10:A:977:LEU:HB2	1.94	0.66
11:B:891:ILE:O	11:B:895:ILE:N	2.28	0.66
17:M:28:UNK:O	17:M:32:UNK:N	2.28	0.66
7:P:155:PHE:CZ	7:P:333:MET:CE	2.77	0.66
14:H:82:GLU:HA	14:H:85:LEU:HD13	1.78	0.66
7:P:458:GLU:HG2	7:P:459:ASP:N	2.10	0.66
10:A:602:VAL:O	10:A:605:LEU:HD23	1.96	0.66
11:B:929:SER:O	11:B:981:ASN:ND2	2.29	0.66
11:B:1307:ASN:HA	11:B:1310:LEU:HD12	1.76	0.65
15:I:136:LEU:O	15:I:139:GLU:HG2	1.96	0.65
7:P:180:VAL:HG11	7:P:332:LEU:HG	1.78	0.65
10:A:546:ARG:NH2	13:G:566:LEU:O	2.25	0.65
11:B:923:MET:O	11:B:927:ASN:ND2	2.30	0.65
12:C:646:LYS:O	12:C:649:THR:N	2.26	0.65
13:E:365:THR:HB	13:E:368:ARG:HH21	1.62	0.65
15:I:78:GLN:O	15:I:82:ARG:HG2	1.96	0.65
12:C:465:ASP:OD1	12:C:473:LEU:N	2.30	0.64
3:X:32:ARG:NH2	4:Y:32:GLU:OE2	2.30	0.64
7:P:36:ILE:HG13	7:P:54:MET:HE1	1.73	0.64
10:A:592:LEU:O	10:A:596:ARG:HG3	1.98	0.64
12:C:584:GLU:HG3	12:C:586:PRO:HD3	1.79	0.64
13:F:688:ARG:HH11	14:H:86:ASP:HB2	1.62	0.64
13:G:570:ILE:HG13	13:G:570:ILE:O	1.97	0.64
10:A:1168:LEU:HA	10:A:1196:ARG:HH11	1.61	0.64
11:B:974:ASP:HA	11:B:977:ILE:HD12	1.80	0.64
10:A:594:LEU:CD1	10:A:598:LYS:CE	2.75	0.64
10:A:597:LYS:HB2	10:A:597:LYS:HZ1	1.61	0.64
10:A:1050:ASN:O	10:A:1054:GLN:N	2.25	0.64
1:V:59:GLU:O	2:W:40:ARG:NH2	2.28	0.64
10:A:559:LEU:HA	11:B:726:LEU:HD12	1.78	0.64
10:A:594:LEU:O	10:A:597:LYS:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:306:VAL:O	13:E:394:GLN:NE2	2.31	0.64
10:A:826:SER:HB3	10:A:1169:GLY:HA2	1.80	0.64
10:A:1061:HIS:HB2	10:A:1064:VAL:HG13	1.79	0.64
11:B:1196:SER:N	11:B:1197:GLU:OE2	2.27	0.64
12:C:545:ARG:HH12	12:C:649:THR:HG22	1.62	0.64
13:E:404:ILE:HD11	13:E:408:LEU:HD22	1.79	0.64
11:B:933:ASN:O	11:B:936:ARG:HG2	1.99	0.63
11:B:986:LEU:HD11	11:B:1046:LEU:HD13	1.80	0.63
13:F:686:LEU:HD22	15:I:133:LYS:HG2	1.80	0.63
10:A:594:LEU:HG	10:A:598:LYS:CE	2.18	0.63
10:A:1300:MET:HB3	10:A:1304:ARG:HE	1.63	0.63
11:B:1081:ASP:OD1	11:B:1082:LYS:N	2.31	0.63
11:B:990:SER:O	11:B:993:ASP:N	2.31	0.63
11:B:1300:GLN:OE1	11:B:1304:ASN:ND2	2.31	0.63
13:G:525:GLU:O	13:G:564:ARG:NH2	2.25	0.63
16:J:5:UNK:O	16:J:9:UNK:N	2.31	0.63
10:A:790:LEU:HD23	10:A:798:LYS:HG2	1.80	0.63
12:C:511:ASP:N	12:C:511:ASP:OD1	2.31	0.63
12:C:602:HIS:HA	12:C:605:HIS:NE2	2.13	0.63
11:B:719:LEU:HD13	14:H:554:ARG:HH21	1.64	0.63
13:D:426:GLU:HB3	13:E:413:SER:H	1.64	0.63
13:E:354:TYR:OH	13:E:394:GLN:N	2.27	0.63
10:A:555:HIS:HB2	13:D:422:LEU:HD13	1.79	0.63
11:B:1145:THR:HG21	11:B:1239:ILE:HD11	1.80	0.63
13:D:417:ASP:OD2	16:J:64:UNK:N	2.29	0.63
13:E:309:SER:O	13:E:312:LYS:N	2.23	0.63
7:P:148:SER:HB2	7:P:442:THR:HG21	1.79	0.63
10:A:771:GLN:O	10:A:775:LEU:CB	2.47	0.63
13:D:412:TYR:CB	14:H:560:ILE:CG2	2.77	0.63
7:P:121:GLU:O	7:P:125:GLU:HG3	1.98	0.63
12:C:515:GLN:OE1	12:C:518:GLN:NE2	2.31	0.63
13:E:308:PRO:HB2	13:E:310:TYR:CE2	2.34	0.63
11:B:915:ASN:HD21	11:B:962:PHE:HA	1.62	0.62
13:D:354:TYR:OH	13:D:394:GLN:NE2	2.32	0.62
11:B:982:ILE:HB	11:B:1046:LEU:HD11	1.80	0.62
12:C:583:LEU:HD23	12:C:584:GLU:HG2	1.80	0.62
13:F:676:GLU:OE2	13:F:677:ARG:NH2	2.30	0.62
13:D:427:SER:OG	13:D:428:TYR:N	2.32	0.62
14:H:309:SER:OG	14:H:416:LEU:O	2.12	0.62
11:B:706:ASN:OD1	11:B:707:LEU:N	2.33	0.62
10:A:1094:ARG:NH1	10:A:1280:ASP:OD1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1092:TYR:O	11:B:1093:ASN:ND2	2.32	0.62
12:C:454:SER:HB3	13:E:335:ILE:HB	1.80	0.62
13:E:301:GLN:HE21	13:E:303:HIS:H	1.47	0.62
7:P:76:LEU:HD23	7:P:108:MET:CE	2.23	0.62
10:A:584:GLN:O	10:A:588:ASN:ND2	2.33	0.62
10:A:829:SER:HG	10:A:1143:SER:HG	1.45	0.62
13:F:670:ILE:HG21	14:H:508:SER:HB3	1.82	0.62
13:G:528:SER:N	13:G:531:ASP:OD2	2.32	0.62
7:P:153:SER:HA	7:P:169:ILE:O	1.99	0.61
7:P:203:GLU:O	7:P:204:GLU:HB2	2.00	0.61
13:E:374:ASP:OD1	13:E:375:ALA:N	2.33	0.61
13:F:673:THR:O	13:F:677:ARG:HG2	2.00	0.61
7:P:343:SER:CB	7:P:344:ILE:CA	2.66	0.61
8:Q:14:PRO:O	8:Q:116[B]:HIS:CE1	2.53	0.61
10:A:1141:GLU:HA	10:A:1144:GLU:HB3	1.81	0.61
11:B:886:THR:O	11:B:889:LYS:HB2	1.99	0.61
13:D:339:THR:HG23	13:D:342:VAL:H	1.64	0.61
7:P:256:ILE:O	7:P:260:GLN:HB2	2.01	0.61
12:C:471:PHE:HB3	12:C:473:LEU:HG	1.81	0.61
7:P:382:GLU:CD	7:P:382:GLU:H	2.03	0.61
11:B:1195:SER:H	11:B:1251:LYS:HE2	1.65	0.61
16:J:4:UNK:O	16:J:8:UNK:N	2.33	0.61
11:B:979:LEU:HA	11:B:982:ILE:HD12	1.82	0.61
13:D:308:PRO:O	13:D:311:SER:OG	2.17	0.61
10:A:570:LYS:HG3	15:I:90:LEU:C	2.20	0.61
11:B:919:SER:O	11:B:922:SER:OG	2.16	0.61
11:B:1029:GLN:OE1	11:B:1029:GLN:N	2.22	0.61
13:G:557:SER:N	13:G:560:GLN:OE1	2.30	0.61
14:H:457:ARG:HA	14:H:461:ILE:HD11	1.82	0.61
8:Q:47:GLN:O	8:Q:48:ASP:HB3	2.00	0.61
11:B:889:LYS:O	11:B:893:ASP:N	2.29	0.61
11:B:1051:LYS:NZ	11:B:1053:ASN:HD22	1.99	0.61
11:B:1140:ILE:O	11:B:1143:SER:OG	2.17	0.61
10:A:1230:ASP:OD2	10:A:1268:ARG:NH2	2.30	0.61
12:C:465:ASP:O	12:C:470:ARG:NH2	2.34	0.61
13:E:415:ARG:HE	13:E:416:HIS:CE1	2.18	0.61
10:A:792:ASP:HA	10:A:993:ARG:HA	1.81	0.60
11:B:744:LYS:HG3	12:C:437:HIS:CE1	2.36	0.60
11:B:1028:PHE:HZ	11:B:1033:GLY:H	1.48	0.60
10:A:594:LEU:HD11	10:A:598:LYS:CE	2.31	0.60
13:D:332:THR:HG23	13:D:334:ARG:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:104:ARG:HH12	16:K:9:UNK:HA	1.64	0.60
7:P:238:VAL:HG21	7:P:404:MET:CG	2.28	0.60
10:A:533:TYR:OH	10:A:537:GLN:OE1	2.16	0.60
10:A:1199:ARG:NH2	20:A:1803:BEF:F2	2.22	0.60
13:D:318:LYS:O	13:D:347:ARG:NH2	2.34	0.60
7:P:108:MET:CE	7:P:119:ILE:HG21	2.31	0.60
13:F:673:THR:O	13:F:677:ARG:NH1	2.34	0.60
11:B:743:VAL:O	11:B:744:LYS:HD2	2.01	0.60
12:C:410:ASN:HB2	13:D:415:ARG:HD3	1.82	0.60
12:C:564:ASP:OD1	12:C:565:ILE:N	2.33	0.60
13:D:318:LYS:HG2	13:D:319:ILE:H	1.66	0.60
11:B:1206:LYS:O	11:B:1210:ILE:HG12	2.01	0.60
13:G:536:LEU:HA	13:G:539:ILE:HG12	1.82	0.60
13:D:422:LEU:HD23	13:D:422:LEU:H	1.67	0.60
16:J:49:UNK:O	16:J:53:UNK:N	2.34	0.60
7:P:400:LEU:HD12	7:P:433:LYS:HE2	1.84	0.60
12:C:411:GLY:O	12:C:420:THR:OG1	2.19	0.60
12:C:644:GLU:OE1	12:C:644:GLU:N	2.28	0.60
10:A:768:LYS:N	10:A:771:GLN:HE22	2.00	0.59
12:C:564:ASP:OD1	12:C:566:SER:N	2.31	0.59
13:D:371:VAL:HG13	13:D:373:GLY:H	1.67	0.59
13:F:706:LYS:O	13:F:710:LEU:HG	2.01	0.59
10:A:567:PHE:HB2	11:B:926:ARG:CZ	2.32	0.59
10:A:1027:LEU:HA	10:A:1054:GLN:HE22	1.67	0.59
11:B:1233:LEU:O	11:B:1236:SER:OG	2.14	0.59
13:E:302:ALA:O	13:E:303:HIS:ND1	2.35	0.59
11:B:896:ASP:C	15:I:110:ASN:HD22	2.06	0.59
14:H:76:GLN:HG3	14:H:78:LEU:HD23	1.84	0.59
14:H:99:MET:HA	14:H:102:GLN:HE21	1.68	0.59
14:H:109:SER:HA	14:H:112:PHE:CD2	2.37	0.59
10:A:1301:ASP:O	10:A:1305:SER:OG	2.19	0.59
11:B:896:ASP:O	15:I:110:ASN:ND2	2.32	0.59
10:A:1079:ASN:OD1	10:A:1080:ASP:N	2.35	0.59
12:C:543:ARG:HA	12:C:564:ASP:HA	1.84	0.59
12:C:646:LYS:NZ	13:D:370:ASN:O	2.35	0.59
15:I:138:SER:O	15:I:141:THR:OG1	2.18	0.59
9:Z:29:TRP:CD2	9:Z:61:LYS:HD3	2.38	0.59
10:A:1170:LEU:HD13	10:A:1172:LEU:HG	1.85	0.59
11:B:750:ASP:O	11:B:754:ILE:HG12	2.03	0.59
13:D:426:GLU:OE2	13:E:413:SER:N	2.36	0.59
14:H:71:GLU:OE1	14:H:73:TYR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:166:VAL:HG22	7:P:333:MET:SD	2.43	0.59
8:Q:35:LEU:HD11	9:Z:84:LEU:HD13	1.84	0.59
8:Q:53:TYR:CD1	8:Q:81:GLN:HG3	2.37	0.59
11:B:1294:GLN:O	11:B:1298:GLN:HG2	2.02	0.59
12:C:466:GLN:HE21	12:C:468:ARG:HH21	1.50	0.59
13:F:661:ILE:HA	13:F:664:LEU:HD12	1.85	0.59
16:J:11:UNK:O	16:J:15:UNK:N	2.36	0.59
11:B:976:VAL:HA	11:B:979:LEU:HD12	1.84	0.59
8:Q:44:THR:OG1	8:Q:62:ALA:HB2	2.02	0.58
13:G:519:ILE:CD1	13:G:572:ASP:HB3	2.32	0.58
13:G:677:ARG:HH11	13:G:678:GLN:N	1.98	0.58
8:Q:182:HIS:HE1	22:Q:628:HOH:O	1.85	0.58
11:B:1293:ILE:HA	11:B:1296:ILE:HD12	1.86	0.58
12:C:550:ILE:O	12:C:556:GLN:HA	2.03	0.58
7:P:389:LEU:HB3	7:P:421:LEU:HD23	1.84	0.58
10:A:538:LEU:HD13	10:A:541:LEU:HD13	1.85	0.58
11:B:1196:SER:OG	11:B:1251:LYS:NZ	2.37	0.58
13:F:663:SER:HA	13:F:666:TYR:CD2	2.38	0.58
15:I:91:SER:OG	15:I:92:ASN:N	2.36	0.58
10:A:1339:GLU:O	10:A:1343:ALA:HB2	2.03	0.58
13:E:311:SER:O	13:E:313:TRP:N	2.32	0.58
13:F:667:ARG:HA	13:F:670:ILE:HD12	1.85	0.58
4:U:65:ASP:OD2	2:W:98:TYR:OH	2.18	0.58
7:P:380:SER:O	7:P:383:GLN:HB2	2.03	0.58
11:B:869:ARG:HA	11:B:953:TRP:CZ3	2.38	0.58
11:B:1064:LYS:HG3	11:B:1104:ASN:ND2	2.19	0.58
13:G:723:LEU:O	13:G:727:LEU:HG	2.03	0.58
13:G:743:CYS:O	13:G:747:ILE:HG13	2.02	0.58
10:A:542:GLN:OE1	10:A:546:ARG:NH2	2.36	0.58
10:A:1254:LEU:O	10:A:1258:LEU:HB3	2.02	0.58
11:B:926:ARG:O	11:B:929:SER:OG	2.19	0.58
7:P:334:ALA:HB2	7:P:415:ARG:HD3	1.86	0.58
10:A:1171:ASN:ND2	19:A:1802:ADP:O1A	2.37	0.58
11:B:896:ASP:CG	15:I:110:ASN:HB3	2.24	0.58
11:B:944:LEU:O	11:B:948:ILE:HG12	2.04	0.58
12:C:537:LEU:N	13:D:334:ARG:HH22	2.02	0.58
13:E:374:ASP:OD1	13:E:376:ALA:N	2.37	0.58
13:F:692:GLU:HB3	14:H:89:ILE:HG21	1.85	0.58
10:A:595:GLU:HA	10:A:598:LYS:HB2	1.86	0.58
13:F:732:ASN:O	13:F:736:ILE:HG13	2.04	0.58
10:A:1261:GLU:O	10:A:1265:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:461:ARG:NH1	16:N:31:UNK:O	2.36	0.57
7:P:44:GLU:O	7:P:44:GLU:HG2	2.04	0.57
8:Q:199:LYS:HD2	8:Q:210:ILE:HD13	1.85	0.57
10:A:556:GLN:OE1	14:H:554:ARG:NH1	2.37	0.57
14:H:324:THR:HG23	14:H:327:ASP:H	1.69	0.57
7:P:159:ILE:HG23	7:P:164:CYS:SG	2.44	0.57
11:B:866:GLU:OE1	11:B:866:GLU:N	2.30	0.57
12:C:517:ILE:O	12:C:521:ILE:HG23	2.03	0.57
13:G:519:ILE:HD12	13:G:572:ASP:CB	2.32	0.57
10:A:1084:ARG:NH2	10:A:1315:SER:O	2.37	0.57
14:H:111:GLU:HA	14:H:114:TYR:CD2	2.39	0.57
7:P:155:PHE:HE2	7:P:333:MET:CE	1.94	0.57
8:Q:141:ILE:HG12	8:Q:448:TYR:HB3	1.85	0.57
10:A:483:VAL:HG13	10:A:485:PRO:HD3	1.85	0.57
10:A:773:LYS:O	10:A:777:TRP:HB2	2.04	0.57
10:A:798:LYS:HB3	10:A:922:LEU:HD13	1.86	0.57
11:B:874:GLN:HE22	11:B:959:PRO:HD2	1.70	0.57
11:B:880:HIS:CE1	11:B:958:HIS:HB3	2.39	0.57
11:B:1199:ASN:OD1	11:B:1199:ASN:N	2.31	0.57
11:B:1264:GLU:HA	11:B:1267:LYS:HD3	1.85	0.57
12:C:469:ASP:HB2	12:C:471:PHE:HE2	1.68	0.57
10:A:595:GLU:HA	10:A:598:LYS:HG2	1.87	0.57
10:A:796:LEU:HD21	10:A:994:ARG:HB2	1.85	0.57
13:E:354:TYR:CD2	13:E:391:ILE:HA	2.40	0.57
13:E:364:VAL:HB	13:E:382:HIS:CG	2.39	0.57
15:I:139:GLU:O	15:I:143:ARG:HD3	2.04	0.57
7:P:216:ARG:HA	7:P:216:ARG:NE	2.20	0.57
7:P:381:PRO:HG2	7:P:382:GLU:OE2	2.04	0.57
7:P:418:GLN:O	7:P:418:GLN:HG3	2.03	0.57
10:A:559:LEU:HD21	11:B:722:ILE:HG23	1.86	0.57
10:A:1339:GLU:O	10:A:1343:ALA:CB	2.53	0.57
11:B:1058:LYS:HA	11:B:1061:LEU:HD12	1.87	0.57
11:B:1237:ILE:O	11:B:1240:SER:OG	2.18	0.57
13:E:420:ARG:O	13:E:420:ARG:NH1	2.37	0.57
13:G:678:GLN:HB2	13:G:679:MET:HE2	1.87	0.57
1:R:68:GLN:HE21	1:R:72:ARG:HH21	1.52	0.57
10:A:968:LYS:O	10:A:972:SER:OG	2.20	0.57
11:B:864:LEU:HB2	11:B:865:PRO:HD3	1.86	0.57
11:B:1292:ASP:OD1	11:B:1292:ASP:N	2.37	0.57
12:C:464:PHE:HB2	12:C:473:LEU:HB2	1.85	0.57
12:C:488:ILE:O	12:C:492:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:514:CYS:HA	12:C:517:ILE:HD12	1.87	0.57
10:A:1212:ILE:HG23	10:A:1218:GLU:HG3	1.85	0.56
11:B:761:SER:O	11:B:764:SER:OG	2.18	0.56
10:A:855:LYS:O	10:A:859:ALA:HB2	2.05	0.56
11:B:1301:LEU:HA	11:B:1304:ASN:HD22	1.69	0.56
13:E:420:ARG:HD3	13:E:420:ARG:N	2.19	0.56
14:H:519:ILE:O	14:H:522:THR:OG1	2.20	0.56
7:P:241:LYS:NZ	7:P:245:GLU:HB3	2.19	0.56
10:A:555:HIS:O	10:A:558:SER:OG	2.20	0.56
11:B:935:SER:HA	11:B:938:MET:HB2	1.86	0.56
13:D:406:PRO:HA	13:E:352:ASN:HD21	1.70	0.56
13:D:412:TYR:CB	14:H:560:ILE:HG21	2.33	0.56
13:F:657:SER:O	13:F:661:ILE:HG12	2.05	0.56
14:H:490:VAL:HA	14:H:493:ASN:HD22	1.69	0.56
7:P:194:HIS:NE2	7:P:203:GLU:OE1	2.39	0.56
10:A:1199:ARG:NH1	20:A:1803:BEF:F3	2.28	0.56
13:D:324:VAL:HG23	13:D:331:PHE:CD1	2.40	0.56
13:E:308:PRO:HD3	13:E:393:TYR:CE2	2.39	0.56
10:A:589:HIS:ND1	11:B:1050:GLU:HG2	2.20	0.56
12:C:570:ASN:HD21	13:D:380:ARG:NE	2.04	0.56
7:P:72:ASP:OD1	7:P:74:GLN:HB2	2.05	0.56
11:B:785:ASN:HB3	13:E:345:ARG:NH2	2.21	0.56
14:H:498:ASN:O	14:H:502:ARG:HG2	2.05	0.56
3:T:63:LEU:HD11	4:U:38:VAL:HG13	1.87	0.56
10:A:525:THR:HA	10:A:528:ASN:ND2	2.20	0.56
10:A:552:PHE:C	14:H:554:ARG:HH11	2.08	0.56
14:H:117:LEU:O	14:H:118:ASN:ND2	2.39	0.56
15:I:138:SER:O	15:I:142:ILE:HG12	2.06	0.56
10:A:821:VAL:HG12	10:A:892:ILE:HB	1.88	0.56
1:V:68:GLN:HE21	1:V:72:ARG:HH21	1.52	0.56
10:A:546:ARG:CZ	14:H:541:ARG:HE	2.18	0.56
13:D:363:SER:OG	13:D:364:VAL:N	2.39	0.56
13:D:437:MET:O	13:D:441:LYS:N	2.37	0.56
7:P:26:LEU:HB3	7:P:27:PRO:HD2	1.88	0.56
10:A:1134:ASP:OD2	10:A:1136:HIS:NE2	2.39	0.56
15:I:170:UNK:O	15:I:174:UNK:N	2.39	0.56
11:B:880:HIS:HE1	11:B:958:HIS:O	1.89	0.55
13:G:530:GLU:HA	13:G:533:GLN:HB2	1.88	0.55
14:H:532:ASP:OD1	14:H:532:ASP:N	2.37	0.55
7:P:36:ILE:H	7:P:54:MET:CE	2.19	0.55
11:B:999:ILE:O	11:B:1002:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:584:GLU:HB2	13:D:401:PRO:HG3	1.88	0.55
13:F:710:LEU:HD23	13:F:713:LYS:HZ3	1.71	0.55
14:H:512:VAL:O	14:H:516:ASN:ND2	2.39	0.55
1:R:124:ILE:HD11	2:S:50:ILE:HG23	1.88	0.55
7:P:426:ASN:HB3	7:P:432:ARG:HG2	1.88	0.55
10:A:944:LYS:HG2	10:A:945:ILE:HG23	1.88	0.55
10:A:1096:LEU:HD23	10:A:1128:ILE:HD13	1.87	0.55
11:B:745:TYR:N	11:B:745:TYR:CD1	2.74	0.55
12:C:567:ASN:ND2	12:C:570:ASN:OD1	2.40	0.55
13:D:438:ALA:O	13:D:442:LYS:N	2.40	0.55
14:H:307:PHE:HD2	14:H:323:GLY:HA2	1.71	0.55
11:B:941:ASN:O	11:B:944:LEU:N	2.39	0.55
14:H:335:TYR:O	14:H:339:ASN:ND2	2.39	0.55
9:Z:69:ASP:O	9:Z:70:GLU:HG3	2.06	0.55
10:A:1019:GLN:HE22	10:A:1062:PRO:HB3	1.70	0.55
7:P:76:LEU:HD21	7:P:108:MET:CE	2.04	0.55
10:A:822:ILE:HD11	10:A:873:PHE:HA	1.89	0.55
13:G:735:LYS:O	13:G:739:VAL:HG23	2.06	0.55
10:A:1003:LEU:HD12	10:A:1004:PRO:HD2	1.88	0.55
11:B:1243:GLN:NE2	11:B:1247:CYS:SG	2.79	0.55
12:C:649:THR:OG1	13:D:369:ARG:HA	2.06	0.55
14:H:399:ASP:HB2	14:H:401:MET:HG2	1.89	0.55
7:P:48:ILE:HB	7:P:54:MET:SD	2.47	0.55
11:B:1278:THR:OG1	11:B:1281:GLU:HG2	2.07	0.55
13:F:702:LYS:HD3	13:F:706:LYS:HZ1	1.71	0.55
8:Q:43:ARG:HG3	8:Q:53:TYR:CE2	2.42	0.54
10:A:505:LEU:O	10:A:508:THR:OG1	2.17	0.54
13:G:519:ILE:CD1	13:G:572:ASP:CB	2.85	0.54
12:C:599:GLU:HG2	12:C:603:MET:HE3	1.89	0.54
13:E:306:VAL:H	13:E:394:GLN:NE2	2.05	0.54
13:E:424:PRO:HG2	13:E:425:PHE:CE2	2.42	0.54
14:H:311:SER:OG	14:H:314:LEU:HG	2.08	0.54
10:A:1088:LYS:O	10:A:1092:LEU:HB2	2.07	0.54
11:B:947:PHE:HD2	11:B:948:ILE:HD13	1.72	0.54
12:C:475:ASP:OD1	12:C:476:THR:N	2.40	0.54
7:P:147:LEU:HD23	7:P:443:MET:SD	2.47	0.54
11:B:742:LEU:HB2	11:B:745:TYR:CZ	2.42	0.54
11:B:912:VAL:HG12	11:B:963:THR:HG21	1.88	0.54
13:D:426:GLU:HB3	13:E:412:TYR:HA	1.90	0.54
13:G:546:TRP:HA	13:G:549:VAL:HG22	1.90	0.54
8:Q:275:LYS:HE3	8:Q:277:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:685:GLN:HA	10:A:689:PHE:HD2	1.71	0.54
10:A:1109:PHE:HB3	10:A:1163:THR:HG22	1.89	0.54
10:A:1170:LEU:HD12	10:A:1196:ARG:HD2	1.88	0.54
14:H:328:ALA:O	14:H:331:SER:OG	2.20	0.54
15:I:71:GLN:O	15:I:74:ASN:HB2	2.08	0.54
7:P:196:ARG:NH2	7:P:312:TYR:OH	2.39	0.54
10:A:1262:GLU:OE2	10:A:1266:LYS:NZ	2.37	0.54
12:C:415:TYR:CE2	12:C:418:GLY:HA2	2.42	0.54
10:A:1094:ARG:O	10:A:1098:LYS:NZ	2.38	0.54
11:B:745:TYR:CD2	11:B:936:ARG:HD3	2.42	0.54
13:F:719:GLN:HA	13:F:722:LEU:HD12	1.90	0.54
10:A:1173:GLN:NE2	19:A:1802:ADP:O2'	2.41	0.54
11:B:1197:GLU:H	11:B:1199:ASN:CG	2.12	0.54
12:C:609:ALA:HA	12:C:614:ASN:HD21	1.72	0.54
13:F:666:TYR:O	13:F:670:ILE:HG13	2.07	0.54
7:P:16[A]:ARG:NH2	22:P:602:HOH:O	2.40	0.54
10:A:1264:ARG:HG3	10:A:1268:ARG:HH12	1.73	0.54
13:F:710:LEU:HB3	14:H:107:LYS:HD3	1.88	0.54
7:P:381:PRO:C	7:P:383:GLN:H	2.11	0.54
11:B:1037:THR:OG1	11:B:1038:PHE:N	2.41	0.54
13:D:412:TYR:HD1	14:H:560:ILE:CG2	1.83	0.54
13:D:448:ASP:OD1	13:D:448:ASP:N	2.40	0.54
10:A:499:THR:HG21	13:E:427:SER:HB3	1.89	0.53
13:F:708:MET:HG3	13:F:712:ARG:HH21	1.71	0.53
14:H:465:GLU:O	14:H:469:ASN:ND2	2.42	0.53
17:M:21:UNK:HA	17:M:22:UNK:C	2.37	0.53
10:A:504:ASN:O	10:A:507:THR:OG1	2.22	0.53
12:C:464:PHE:HB2	12:C:473:LEU:HD12	1.90	0.53
13:D:449:SER:HA	13:D:452:THR:HB	1.90	0.53
13:F:703:LYS:HA	13:F:707:PHE:CE2	2.43	0.53
7:P:261:GLN:HB2	7:P:262:GLU:OE1	2.09	0.53
10:A:1057:LYS:HB3	10:A:1064:VAL:HG21	1.90	0.53
11:B:952:LEU:HD12	11:B:996:LEU:HD12	1.90	0.53
11:B:710:LEU:HD22	11:B:747:GLU:HG3	1.90	0.53
15:I:115:ASN:OD1	15:I:119:ASN:ND2	2.29	0.53
15:I:133:LYS:HD2	15:I:133:LYS:N	2.24	0.53
8:Q:43:ARG:HD3	8:Q:51:TYR:CD1	2.43	0.53
19:A:1802:ADP:O3B	20:A:1803:BEF:F3	2.16	0.53
11:B:741:SER:O	11:B:936:ARG:NH2	2.36	0.53
11:B:915:ASN:ND2	11:B:963:THR:HG23	2.23	0.53
11:B:1136:PHE:CE2	11:B:1140:ILE:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:27:UNK:O	16:J:31:UNK:N	2.41	0.53
10:A:958:THR:HA	10:A:975:GLU:HB3	1.90	0.53
12:C:641:PRO:HG2	12:C:646:LYS:HD3	1.91	0.53
13:D:447:SER:OG	13:D:451:SER:N	2.36	0.53
10:A:761:ILE:HG22	10:A:839:ALA:HB1	1.91	0.53
11:B:1055:ASN:OD1	11:B:1055:ASN:N	2.38	0.53
11:B:1279:ASP:HA	11:B:1282:ILE:HD12	1.91	0.53
7:P:438:LEU:O	7:P:442:THR:HG23	2.08	0.53
10:A:941:VAL:HG12	10:A:942:LEU:HG	1.91	0.53
11:B:939:SER:OG	11:B:985:LEU:O	2.17	0.53
11:B:953:TRP:CD1	11:B:957:ILE:HD12	2.44	0.53
12:C:577:GLU:O	12:C:580:CYS:HB3	2.09	0.52
7:P:399:SER:OG	7:P:432:ARG:NH1	2.42	0.52
10:A:505:LEU:O	10:A:509:VAL:HG23	2.08	0.52
10:A:1062:PRO:HG3	10:A:1085:VAL:HG21	1.91	0.52
11:B:1143:SER:O	11:B:1146:SER:OG	2.19	0.52
12:C:439:LEU:O	12:C:442:LYS:HG2	2.10	0.52
12:C:518:GLN:HA	12:C:521:ILE:HG12	1.91	0.52
13:F:549:VAL:HA	13:F:552:ASN:HD22	1.75	0.52
13:F:733:SER:O	13:F:737:VAL:HG23	2.09	0.52
13:G:738:ASN:O	13:G:741:SER:OG	2.23	0.52
12:C:469:ASP:HB2	12:C:471:PHE:CE2	2.44	0.52
13:E:417:ASP:HB3	13:E:419:PRO:HD2	1.90	0.52
10:A:575:ASN:N	10:A:578:ASP:OD2	2.43	0.52
11:B:1034:LYS:O	11:B:1037:THR:OG1	2.16	0.52
12:C:495:MET:HE2	13:E:365:THR:HG22	1.89	0.52
14:H:98:ARG:O	14:H:102:GLN:HG3	2.10	0.52
14:H:485:LYS:O	14:H:488:THR:OG1	2.26	0.52
7:P:6:LYS:HE3	8:Q:121:GLN:OE1	2.10	0.52
8:Q:34:GLU:CD	8:Q:34:GLU:H	2.13	0.52
10:A:497:TYR:CE2	10:A:501:ILE:HD11	2.45	0.52
19:A:1802:ADP:O1A	20:A:1803:BEF:F3	2.18	0.52
13:D:344:MET:HG2	13:D:347:ARG:HH12	1.73	0.52
13:D:365:THR:HA	13:D:368:ARG:HG3	1.91	0.52
13:D:449:SER:O	13:D:453:LEU:N	2.28	0.52
13:F:681:PHE:HE1	14:H:497:SER:HB2	1.73	0.52
13:G:564:ARG:HA	13:G:567:GLN:HE21	1.75	0.52
7:P:197:LEU:HD11	7:P:231:PHE:CZ	2.45	0.52
13:G:689:LEU:HB3	15:I:143:ARG:HE	1.73	0.52
14:H:375:GLN:HG2	14:H:402:LYS:HE3	1.91	0.52
14:H:464:ALA:O	14:H:468:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:73:LEU:O	15:I:77:ARG:HG3	2.10	0.52
7:P:80:TRP:NE1	7:P:122:ARG:HD3	2.25	0.52
7:P:426:ASN:O	7:P:432:ARG:NE	2.35	0.52
10:A:1207:ARG:NH1	10:A:1286:ILE:O	2.43	0.52
11:B:1029:GLN:HE21	11:B:1032:TRP:HE1	1.57	0.52
7:P:36:ILE:CB	7:P:54:MET:CE	2.68	0.52
10:A:572:ARG:NH1	15:I:95:HIS:HB2	2.24	0.52
11:B:745:TYR:CD1	11:B:746:PRO:HD3	2.45	0.52
12:C:644:GLU:CA	12:C:647:ILE:HG12	2.38	0.52
13:F:702:LYS:HD3	13:F:706:LYS:HE3	1.91	0.52
16:J:42:UNK:O	16:J:46:UNK:N	2.43	0.52
1:R:61:LEU:HD12	2:S:37:LEU:HD23	1.92	0.51
1:V:61:LEU:HD12	2:W:37:LEU:HD23	1.92	0.51
10:A:641:GLU:O	10:A:645:GLN:HG3	2.10	0.51
11:B:715:GLN:OE1	11:B:717:LYS:N	2.43	0.51
11:B:963:THR:OG1	11:B:964:CYS:N	2.41	0.51
2:W:30:THR:HB	2:W:32:PRO:HD2	1.91	0.51
11:B:932:ASP:HA	11:B:934:ASN:OD1	2.11	0.51
12:C:483:ASP:OD1	12:C:484:LYS:N	2.43	0.51
12:C:497:ARG:HH12	12:C:503:ASP:HA	1.75	0.51
13:D:361:TYR:HB2	13:D:395:VAL:HG11	1.91	0.51
14:H:310:TYR:HB3	14:H:314:LEU:HB2	1.91	0.51
7:P:201:ILE:O	7:P:202:LYS:HB2	2.11	0.51
7:P:446:LEU:HD22	10:A:608:MET:SD	2.50	0.51
11:B:745:TYR:HD2	11:B:936:ARG:HD3	1.76	0.51
13:D:365:THR:OG1	13:D:368:ARG:NH2	2.43	0.51
13:D:426:GLU:CB	13:E:413:SER:H	2.23	0.51
7:P:133:VAL:HG13	7:P:134:PRO:HD2	1.91	0.51
8:Q:32:VAL:HG23	8:Q:33:PRO:HD2	1.92	0.51
10:A:598:LYS:CD	10:A:598:LYS:N	2.73	0.51
11:B:727:ASN:O	11:B:731:VAL:HG23	2.10	0.51
12:C:646:LYS:O	12:C:650:PRO:HD3	2.11	0.51
13:F:735:LYS:O	13:F:739:VAL:HG23	2.11	0.51
14:H:497:SER:HA	14:H:500:ARG:HD3	1.92	0.51
2:S:30:THR:HB	2:S:32:PRO:HD2	1.91	0.51
8:Q:47:GLN:O	8:Q:48:ASP:CB	2.59	0.51
9:Z:85:LYS:O	9:Z:90:ARG:NH1	2.44	0.51
10:A:984:HIS:O	10:A:988:ARG:HG3	2.10	0.51
11:B:1051:LYS:HZ3	11:B:1053:ASN:HD22	1.58	0.51
11:B:1064:LYS:HG3	11:B:1104:ASN:HD22	1.76	0.51
11:B:879:ILE:O	11:B:881:ARG:NE	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:339:THR:HG22	13:E:342:VAL:HG12	1.93	0.51
7:P:320:SER:OG	7:P:322:LYS:N	2.38	0.51
10:A:1016:SER:O	10:A:1020:GLN:N	2.40	0.51
10:A:1057:LYS:O	10:A:1061:HIS:N	2.43	0.51
10:A:1223:GLU:O	10:A:1227:LYS:HG2	2.09	0.51
11:B:1134:ASP:O	11:B:1138:PRO:HD3	2.11	0.51
12:C:547:LYS:O	12:C:548:LEU:HD23	2.10	0.51
7:P:418:GLN:HG2	7:P:419:TYR:CE1	2.46	0.51
10:A:892:ILE:HD12	10:A:920:LEU:HD23	1.92	0.51
10:A:1293:GLU:HA	10:A:1296:VAL:HG22	1.92	0.51
12:C:438:TYR:HB2	13:E:383:LYS:HD2	1.92	0.51
13:F:525:GLU:HB2	13:F:564:ARG:CZ	2.41	0.51
10:A:1024:GLN:O	10:A:1028:LYS:HB2	2.11	0.51
10:A:1098:LYS:HG2	10:A:1297:LEU:HD22	1.93	0.51
12:C:510:ILE:HA	12:C:513:ILE:HD12	1.91	0.51
14:H:506:LYS:HA	14:H:509:GLU:HG2	1.93	0.51
15:I:74:ASN:O	15:I:78:GLN:HG2	2.11	0.51
10:A:866:PHE:CE1	10:A:869:VAL:HG23	2.46	0.51
11:B:1047:PHE:CE1	11:B:1058:LYS:HD2	2.46	0.51
11:B:1054:LEU:HA	11:B:1057:PHE:CD2	2.45	0.51
12:C:450:MET:HG2	12:C:485:LEU:HD11	1.92	0.51
12:C:597:ILE:O	12:C:601:VAL:HG12	2.11	0.51
13:D:364:VAL:O	13:D:367:ALA:N	2.43	0.51
13:E:350:MET:O	13:E:353:SER:OG	2.25	0.51
15:I:78:GLN:HG3	16:O:3:UNK:C	2.40	0.51
11:B:1202:SER:OG	11:B:1204:LEU:HB2	2.11	0.50
12:C:603:MET:O	12:C:607:SER:N	2.26	0.50
13:F:565:PHE:HE1	13:F:634:ALA:H	1.59	0.50
13:G:691:MET:HA	13:G:694:LEU:HD12	1.92	0.50
13:G:705:GLU:O	13:G:709:GLU:HG2	2.11	0.50
14:H:311:SER:HB3	14:H:414:HIS:HB3	1.93	0.50
8:Q:335:ILE:HG22	8:Q:340:THR:HG21	1.93	0.50
10:A:570:LYS:NZ	10:A:571:ILE:HG12	2.26	0.50
12:C:588:GLU:HA	13:E:369:ARG:O	2.11	0.50
12:C:636:ASP:OD1	12:C:637:ASP:N	2.44	0.50
13:D:317:GLU:OE1	13:D:317:GLU:N	2.44	0.50
10:A:563:THR:HG22	10:A:564:HIS:H	1.74	0.50
10:A:795:GLY:HA2	10:A:1199:ARG:HH11	1.76	0.50
11:B:1080:LYS:HA	11:B:1083:LYS:HG2	1.93	0.50
13:F:710:LEU:HA	13:F:713:LYS:HZ3	1.76	0.50
7:P:22:SER:HA	7:P:441:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:141:GLU:HB3	7:P:142:PRO:HD3	1.94	0.50
10:A:551:GLN:HG3	13:E:419:PRO:HG3	1.91	0.50
12:C:458:VAL:N	12:C:479:TRP:O	2.44	0.50
12:C:603:MET:HA	12:C:606:LYS:HB3	1.94	0.50
13:D:344:MET:HG2	13:D:347:ARG:NH1	2.26	0.50
10:A:470:ALA:O	15:I:128:CYS:HB2	2.11	0.50
11:B:715:GLN:NE2	11:B:717:LYS:HB3	2.22	0.50
14:H:75:PHE:HA	14:H:78:LEU:HD21	1.93	0.50
14:H:381:LEU:HD11	14:H:401:MET:SD	2.52	0.50
15:I:74:ASN:HA	15:I:77:ARG:NE	2.26	0.50
8:Q:102:PHE:HZ	9:Z:6:LEU:CD2	2.25	0.50
10:A:467:THR:OG1	10:A:468:LEU:N	2.44	0.50
10:A:1026:MET:HA	10:A:1029:TYR:CD2	2.47	0.50
11:B:1205:LEU:O	11:B:1208:SER:OG	2.25	0.50
12:C:529:TYR:HA	12:C:532:LEU:HB2	1.92	0.50
13:F:674:ASN:OD1	14:H:504:PHE:HB3	2.11	0.50
2:S:92:ARG:NH2	4:U:98:LEU:HD23	2.27	0.50
7:P:407:ARG:O	7:P:411:GLU:HB2	2.12	0.50
10:A:471:ASN:CG	15:I:129:ASP:HB3	2.32	0.50
11:B:1105:LEU:HD23	11:B:1106:LEU:HD23	1.94	0.50
11:B:1258:CYS:SG	11:B:1259:LEU:N	2.84	0.50
10:A:564:HIS:CD2	11:B:966:ARG:HH12	2.30	0.50
13:D:350:MET:O	13:D:353:SER:OG	2.27	0.50
13:G:712:ARG:O	13:G:716:GLU:HG2	2.12	0.50
16:J:44:UNK:O	16:J:48:UNK:N	2.45	0.50
7:P:238:VAL:HG22	7:P:404:MET:SD	2.39	0.50
10:A:565:PRO:HG2	10:A:567:PHE:HE1	1.77	0.50
10:A:968:LYS:O	10:A:972:SER:CB	2.59	0.50
12:C:613:TYR:CE1	12:C:619:ALA:HA	2.46	0.50
13:D:415:ARG:NH1	13:D:416:HIS:O	2.45	0.50
13:E:389:GLY:O	13:E:393:TYR:HB2	2.12	0.50
7:P:418:GLN:HB3	22:P:610:HOH:O	2.10	0.49
11:B:1028:PHE:CE2	11:B:1030:LEU:HA	2.47	0.49
10:A:766:THR:HB	19:A:1802:ADP:HN62	1.77	0.49
10:A:1026:MET:HG2	10:A:1054:GLN:OE1	2.12	0.49
12:C:410:ASN:HB2	13:D:415:ARG:CD	2.42	0.49
13:F:707:PHE:O	13:F:711:GLU:HG2	2.13	0.49
14:H:85:LEU:O	14:H:89:ILE:HG12	2.12	0.49
14:H:336:ILE:HD11	14:H:385:LEU:HD21	1.93	0.49
7:P:183:LYS:O	7:P:183:LYS:CG	2.61	0.49
7:P:460:TYR:CZ	7:P:464:LYS:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:171:ILE:HD13	8:Q:312:ARG:CG	2.42	0.49
10:A:488:ILE:HD11	13:G:622:THR:HA	1.94	0.49
10:A:566:ASN:HD22	15:I:94:ILE:HG12	1.77	0.49
11:B:956:LEU:HD12	11:B:996:LEU:HD13	1.95	0.49
11:B:1059:SER:O	11:B:1062:LEU:HB2	2.13	0.49
13:D:327:LEU:HB3	13:D:329:GLU:OE2	2.12	0.49
13:E:332:THR:HG23	13:E:334:ARG:H	1.75	0.49
13:E:362:PHE:N	13:E:392:ASN:OD1	2.41	0.49
1:R:113:HIS:NE2	1:V:123:ASP:OD1	2.46	0.49
11:B:869:ARG:HG2	11:B:953:TRP:CD2	2.48	0.49
11:B:1035:TYR:O	11:B:1038:PHE:N	2.45	0.49
11:B:1189:LEU:HB2	11:B:1191:PHE:CE2	2.48	0.49
11:B:1232:VAL:C	11:B:1235:PRO:HD2	2.33	0.49
11:B:1292:ASP:O	11:B:1296:ILE:HG13	2.13	0.49
12:C:518:GLN:O	12:C:522:GLN:HG2	2.13	0.49
13:E:402:LYS:HZ3	16:J:59:UNK:C	2.23	0.49
13:F:675:GLU:O	13:F:679:MET:HG2	2.13	0.49
15:I:139:GLU:HG3	15:I:143:ARG:NH1	2.27	0.49
2:S:91:LYS:NZ	4:Y:68:GLU:OE1	2.46	0.49
11:B:742:LEU:HB2	11:B:745:TYR:CE1	2.47	0.49
13:D:361:TYR:CG	13:D:362:PHE:N	2.80	0.49
13:F:643:GLU:O	13:F:647:GLN:N	2.33	0.49
2:W:92:ARG:NH2	4:Y:98:LEU:HD23	2.28	0.49
10:A:570:LYS:O	15:I:92:ASN:ND2	2.46	0.49
10:A:1261:GLU:HA	10:A:1264:ARG:HG2	1.94	0.49
12:C:527:ASN:HB3	12:C:531:GLU:CD	2.33	0.49
14:H:100:VAL:O	14:H:104:GLU:HG3	2.11	0.49
16:J:18:UNK:O	16:J:22:UNK:N	2.46	0.49
7:P:170:ILE:O	7:P:173:ILE:HG22	2.13	0.49
7:P:389:LEU:O	7:P:421:LEU:HA	2.13	0.49
8:Q:286:ASP:HB2	8:Q:290:ASN:HB2	1.95	0.49
11:B:915:ASN:ND2	11:B:963:THR:H	2.11	0.49
12:C:445:VAL:O	12:C:448:GLN:NE2	2.45	0.49
2:W:31:LYS:HB3	2:W:32:PRO:HD3	1.94	0.49
8:Q:153:MET:HG3	8:Q:334:ILE:HD13	1.95	0.49
10:A:541:LEU:O	10:A:545:VAL:HG22	2.13	0.49
10:A:1090:GLU:O	10:A:1094:ARG:HG2	2.13	0.49
11:B:952:LEU:HB3	11:B:996:LEU:HD12	1.94	0.49
10:A:755:ILE:HG22	10:A:757:LYS:H	1.78	0.49
10:A:977:LEU:HB3	10:A:981:ARG:NH1	2.28	0.49
10:A:1111:GLN:HG3	10:A:1112:MET:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:411:GLY:O	13:D:415:ARG:NH2	2.45	0.49
12:C:412:TYR:HB2	12:C:419:ILE:HA	1.94	0.49
14:H:512:VAL:HG13	14:H:513:LYS:H	1.78	0.49
15:I:143:ARG:HD2	15:I:146:MET:HE1	1.93	0.49
10:A:830:ASN:O	10:A:833:SER:N	2.46	0.48
10:A:890:HIS:NE2	10:A:892:ILE:HD11	2.28	0.48
11:B:1056:TYR:O	11:B:1060:ILE:HG13	2.13	0.48
13:E:402:LYS:HA	16:J:59:UNK:CB	2.43	0.48
13:F:659:ILE:HD13	13:G:633:SER:H	1.77	0.48
13:F:724:ILE:O	13:F:727:LEU:HG	2.12	0.48
13:F:738:ASN:O	13:F:741:SER:OG	2.26	0.48
3:X:21:ALA:HB2	4:Y:118:TYR:HB2	1.95	0.48
10:A:937:LEU:O	10:A:941:VAL:HG23	2.13	0.48
11:B:745:TYR:HE2	11:B:936:ARG:HB2	1.78	0.48
12:C:518:GLN:O	12:C:521:ILE:HG12	2.13	0.48
13:G:721:ASN:O	13:G:725:GLN:HG2	2.13	0.48
13:G:730:ASN:O	13:G:733:SER:OG	2.27	0.48
10:A:921:ILE:HD11	10:A:940:PHE:HD2	1.77	0.48
10:A:1232:ASP:O	10:A:1236:ILE:N	2.46	0.48
12:C:645:SER:O	12:C:648:PHE:HD2	1.96	0.48
14:H:92:ARG:O	14:H:96:MET:HG2	2.13	0.48
14:H:326:HIS:O	14:H:329:ILE:HG12	2.13	0.48
14:H:329:ILE:HA	14:H:332:ILE:HG12	1.96	0.48
10:A:542:GLN:HG3	10:A:543:LYS:N	2.28	0.48
10:A:837:LYS:HG3	10:A:838:TRP:CD1	2.48	0.48
10:A:939:ASN:ND2	10:A:945:ILE:HG13	2.28	0.48
13:F:563:LEU:O	13:F:567:GLN:N	2.47	0.48
15:I:81:GLU:HB2	15:I:82:ARG:NH1	2.28	0.48
11:B:1278:THR:HG21	14:H:113:LEU:HD21	1.96	0.48
7:P:241:LYS:O	7:P:242:ASP:C	2.52	0.48
10:A:776:GLN:HA	10:A:779:VAL:HB	1.96	0.48
10:A:846:SER:HA	10:A:870:LEU:O	2.13	0.48
11:B:1006:GLN:NE2	11:B:1029:GLN:HE22	2.12	0.48
12:C:461:ARG:C	12:C:462:LEU:HD22	2.34	0.48
13:G:703:LYS:O	13:G:706:LYS:HG3	2.13	0.48
14:H:90:HIS:HA	14:H:93:ASN:OD1	2.14	0.48
15:I:88:GLU:OE2	15:I:89:GLN:NE2	2.37	0.48
8:Q:148:ALA:O	8:Q:431:GLY:HA3	2.14	0.48
10:A:1096:LEU:HD12	10:A:1099:LEU:HD12	1.96	0.48
11:B:902:ILE:O	11:B:904:THR:N	2.46	0.48
13:F:725:GLN:HE22	13:F:728:ASN:HD22	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:286:ASP:HB3	8:Q:290:ASN:H	1.79	0.48
10:A:650:LYS:HE2	10:A:650:LYS:HA	1.95	0.48
11:B:1124:SER:OG	11:B:1126:SER:O	2.31	0.48
13:D:340:PRO:O	13:D:344:MET:HG3	2.14	0.48
13:E:335:ILE:HD12	13:E:336:PRO:HD2	1.96	0.48
13:F:662:SER:OG	13:F:663:SER:N	2.46	0.48
15:I:125:THR:OG1	15:I:126:VAL:N	2.47	0.48
1:V:46:VAL:HG22	1:V:49:ARG:HH22	1.78	0.48
2:W:88:TYR:O	2:W:92:ARG:HB2	2.14	0.48
10:A:1106:VAL:HB	10:A:1158:CYS:SG	2.53	0.48
11:B:786:GLN:HG2	11:B:787:TYR:H	1.77	0.48
11:B:942:PHE:HA	11:B:945:LYS:HE3	1.95	0.48
11:B:993:ASP:O	11:B:997:ILE:HG12	2.14	0.48
11:B:1275:LEU:HG	11:B:1276:PHE:CG	2.48	0.48
13:G:532:LEU:O	13:G:536:LEU:HG	2.14	0.48
14:H:76:GLN:HG3	14:H:78:LEU:H	1.79	0.48
14:H:76:GLN:HE21	14:H:78:LEU:HA	1.79	0.48
14:H:410:ILE:HD13	14:H:414:HIS:HB2	1.95	0.48
15:I:139:GLU:HG3	15:I:143:ARG:HH12	1.79	0.48
10:A:492:THR:OG1	10:A:493:ALA:N	2.47	0.48
10:A:801:GLN:O	10:A:805:LEU:CB	2.52	0.48
10:A:895:GLU:HG3	10:A:1168:LEU:HD13	1.96	0.48
12:C:593:ILE:O	12:C:596:SER:OG	2.22	0.48
8:Q:30:PHE:HB3	8:Q:433:GLN:OE1	2.14	0.47
11:B:761:SER:OG	11:B:762:ASN:N	2.47	0.47
11:B:1106:LEU:HA	11:B:1109:VAL:HG23	1.96	0.47
13:E:364:VAL:HB	13:E:382:HIS:ND1	2.29	0.47
13:F:727:LEU:HD21	14:H:122:VAL:HG21	1.96	0.47
14:H:529:LEU:HD21	15:I:107:LEU:HB3	1.96	0.47
3:X:32:ARG:HA	3:X:35:ARG:HE	1.79	0.47
7:P:458:GLU:O	7:P:461:GLU:N	2.47	0.47
10:A:570:LYS:O	10:A:572:ARG:N	2.47	0.47
10:A:602:VAL:HA	10:A:605:LEU:HD22	1.96	0.47
10:A:938:LEU:HD23	10:A:944:LYS:NZ	2.29	0.47
12:C:416:GLY:N	13:E:393:TYR:CZ	2.82	0.47
13:F:651:GLU:O	13:F:655:GLU:HG2	2.14	0.47
13:G:685:GLU:HA	13:G:688:ARG:HH12	1.79	0.47
7:P:216:ARG:NH1	7:P:216:ARG:CG	2.69	0.47
8:Q:151:TYR:CD1	10:A:633:LEU:HD12	2.50	0.47
10:A:473:ASP:CG	10:A:475:ALA:H	2.16	0.47
10:A:586:TYR:CZ	11:B:1048:SER:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1110:PHE:CE2	10:A:1160:ILE:HG12	2.50	0.47
10:A:1257:LEU:HD12	10:A:1260:ALA:HB3	1.96	0.47
11:B:866:GLU:H	11:B:866:GLU:CD	2.16	0.47
11:B:939:SER:O	11:B:945:LYS:NZ	2.46	0.47
11:B:973:LYS:O	11:B:977:ILE:HG13	2.13	0.47
11:B:1088:LEU:HA	11:B:1091:LEU:HB2	1.95	0.47
11:B:1144:LEU:O	11:B:1147:ILE:HG22	2.14	0.47
12:C:440:GLU:OE1	12:C:440:GLU:N	2.29	0.47
14:H:123:LYS:HD2	14:H:454:ASN:ND2	2.29	0.47
1:R:46:VAL:HG22	1:R:49:ARG:HH22	1.78	0.47
7:P:188:PHE:HZ	7:P:319:ILE:HD13	1.80	0.47
8:Q:120:SER:HB2	8:Q:123:ASP:H	1.78	0.47
10:A:921:ILE:HD11	10:A:940:PHE:CD2	2.49	0.47
11:B:898:PRO:HB2	11:B:899:PHE:CE2	2.48	0.47
13:D:358:PRO:HB2	13:D:394:GLN:NE2	2.28	0.47
14:H:75:PHE:CZ	14:H:77:GLN:HA	2.50	0.47
4:Y:95:VAL:HG13	4:Y:99:LEU:HD12	1.96	0.47
7:P:15:HIS:ND1	7:P:16[B]:ARG:HG2	2.29	0.47
10:A:1161:LEU:HD21	10:A:1166:GLY:C	2.35	0.47
11:B:718:ASN:HB2	11:B:770:TYR:CD2	2.49	0.47
13:F:563:LEU:O	13:F:568:LEU:N	2.44	0.47
8:Q:26:ASN:O	8:Q:27:GLU:HB2	2.15	0.47
8:Q:417:PRO:HD2	22:Q:622:HOH:O	2.15	0.47
11:B:703:GLY:O	12:C:424:THR:HG23	2.14	0.47
11:B:762:ASN:HB2	11:B:767:VAL:HG13	1.97	0.47
11:B:1062:LEU:HD23	11:B:1106:LEU:HD12	1.97	0.47
11:B:1306:LYS:O	11:B:1310:LEU:HG	2.14	0.47
12:C:498:ASP:O	12:C:500:ARG:NH1	2.48	0.47
13:D:318:LYS:NZ	13:D:319:ILE:O	2.48	0.47
13:E:348:ASN:HA	13:E:351:VAL:HG12	1.97	0.47
3:T:32:ARG:HA	3:T:35:ARG:HE	1.80	0.47
7:P:337:VAL:O	7:P:340:ALA:HB3	2.15	0.47
8:Q:364:GLU:HG2	8:Q:365:GLU:N	2.29	0.47
9:Z:9:LYS:HD2	9:Z:12:LYS:HE2	1.97	0.47
10:A:562:ASN:OD1	10:A:563:THR:N	2.48	0.47
10:A:681:HIS:HD2	10:A:684:ARG:HB2	1.80	0.47
10:A:755:ILE:O	10:A:776:GLN:NE2	2.47	0.47
10:A:1219:GLU:O	10:A:1223:GLU:HG2	2.14	0.47
11:B:901:LYS:HA	11:B:901:LYS:HD3	1.63	0.47
13:D:433:GLN:N	13:D:433:GLN:OE1	2.48	0.47
14:H:99:MET:O	14:H:102:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:453:ASN:O	14:H:457:ARG:NH1	2.47	0.47
2:W:25:ASN:O	2:W:28:GLY:N	2.37	0.47
3:X:63:LEU:HD11	4:Y:38:VAL:HG13	1.96	0.47
8:Q:403:CYS:HB2	8:Q:404:PRO:HA	1.97	0.47
10:A:674:THR:O	10:A:678:ARG:CB	2.62	0.47
10:A:1056:LYS:HD3	10:A:1185:TRP:HZ2	1.79	0.47
11:B:789:VAL:HG12	11:B:790:THR:N	2.28	0.47
12:C:446:TYR:CE1	12:C:485:LEU:HB3	2.50	0.47
12:C:446:TYR:HE1	12:C:485:LEU:HB3	1.79	0.47
12:C:562:GLU:CG	12:C:634:THR:HG21	2.43	0.47
12:C:594:ALA:O	12:C:597:ILE:HB	2.13	0.47
12:C:602:HIS:HA	12:C:605:HIS:CE1	2.49	0.47
12:C:630:LEU:O	12:C:633:ILE:CD1	2.59	0.47
12:C:640:ARG:HA	12:C:641:PRO:HD3	1.45	0.47
13:D:429:LYS:HE3	13:E:420:ARG:HH22	1.79	0.47
13:D:458:LYS:HA	13:D:461:LYS:HE2	1.97	0.47
13:F:683:THR:HA	15:I:133:LYS:HE3	1.97	0.47
13:G:525:GLU:C	13:G:527:TRP:H	2.18	0.47
1:V:73:GLU:OE1	2:W:25:ASN:HB2	2.14	0.47
2:W:64:ASN:HB3	2:W:93:GLN:HE22	1.80	0.47
10:A:490:THR:OG1	10:A:491:HIS:N	2.48	0.47
10:A:894:ASP:OD1	10:A:895:GLU:N	2.48	0.47
11:B:863:LEU:H	11:B:863:LEU:HD23	1.80	0.47
11:B:1028:PHE:HE1	11:B:1032:TRP:HD1	1.63	0.47
13:F:689:LEU:O	13:F:693:LYS:HG2	2.15	0.47
4:U:95:VAL:HG13	4:U:99:LEU:HD12	1.96	0.47
14:H:308:MET:SD	14:H:415:LEU:HG	2.55	0.47
1:V:124:ILE:HD11	2:W:50:ILE:HG23	1.97	0.46
7:P:259:LYS:HD2	7:P:259:LYS:O	2.14	0.46
10:A:825:LEU:HD23	10:A:872:THR:HG21	1.96	0.46
11:B:1051:LYS:O	11:B:1053:ASN:N	2.45	0.46
11:B:1195:SER:H	11:B:1251:LYS:CE	2.28	0.46
12:C:447:LYS:HD2	13:E:328:PRO:HG3	1.97	0.46
13:D:374:ASP:O	13:D:378:LEU:HG	2.15	0.46
13:E:306:VAL:H	13:E:394:GLN:HE22	1.60	0.46
14:H:489:SER:O	14:H:493:ASN:ND2	2.49	0.46
8:Q:370:GLU:HG3	8:Q:395:VAL:HG21	1.97	0.46
12:C:605:HIS:HA	12:C:608:LEU:HB3	1.96	0.46
12:C:653:LEU:HB2	16:N:13:UNK:HA	1.97	0.46
13:D:307:ILE:HD11	13:D:312:LYS:HA	1.96	0.46
13:G:714:THR:O	13:G:718:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:742:LYS:O	13:G:746:LEU:HG	2.14	0.46
15:I:104:ARG:NH1	16:K:9:UNK:HA	2.30	0.46
3:X:67:GLY:HA3	4:Y:46:HIS:CD2	2.51	0.46
14:H:78:LEU:HD13	14:H:84:ARG:NH1	2.31	0.46
1:V:62:ILE:HD11	2:W:37:LEU:HD11	1.97	0.46
7:P:6:LYS:HD2	7:P:23:ASN:ND2	2.30	0.46
7:P:36:ILE:HG13	7:P:54:MET:CE	2.32	0.46
8:Q:302:CYS:HB2	22:Q:635:HOH:O	2.16	0.46
10:A:678:ARG:HA	10:A:681:HIS:HB3	1.97	0.46
11:B:920:THR:O	11:B:924:ILE:HG22	2.15	0.46
12:C:646:LYS:HG2	13:D:372:SER:HB3	1.97	0.46
13:D:426:GLU:HB3	13:E:413:SER:N	2.28	0.46
7:P:325:PRO:O	7:P:331:PRO:HG2	2.15	0.46
10:A:556:GLN:HB3	11:B:718:ASN:HD21	1.81	0.46
10:A:1061:HIS:CE1	10:A:1089:PHE:HZ	2.34	0.46
12:C:466:GLN:O	12:C:470:ARG:NH2	2.45	0.46
10:A:471:ASN:HB3	15:I:129:ASP:HB3	1.97	0.46
10:A:756:LYS:HG2	10:A:772:ILE:HG21	1.97	0.46
10:A:1237:GLN:HA	10:A:1240:LYS:HE3	1.97	0.46
13:E:361:TYR:CG	13:E:362:PHE:N	2.83	0.46
9:Z:23:GLU:OE2	9:Z:65:ARG:HD3	2.16	0.46
10:A:1170:LEU:HD22	10:A:1172:LEU:HD11	1.98	0.46
12:C:523:GLU:O	12:C:606:LYS:HE3	2.15	0.46
13:F:655:GLU:HA	13:F:658:GLU:OE1	2.15	0.46
13:F:708:MET:HG3	13:F:712:ARG:NH2	2.30	0.46
13:G:563:LEU:HG	13:G:567:GLN:NE2	2.30	0.46
7:P:164:CYS:HB2	7:P:182:SER:HB3	1.98	0.46
11:B:724:THR:O	11:B:728:THR:HG22	2.15	0.46
12:C:563:TRP:HZ3	13:D:376:ALA:HB2	1.81	0.46
1:R:113:HIS:CG	1:V:126:LEU:HD22	2.51	0.46
9:Z:83:ASP:C	9:Z:84:LEU:O	2.52	0.46
10:A:540:PRO:HB2	13:D:430:PRO:O	2.16	0.46
11:B:735:ASP:OD1	11:B:735:ASP:N	2.49	0.46
11:B:899:PHE:HE1	14:H:517:GLU:HB2	1.81	0.46
13:F:549:VAL:HA	13:F:552:ASN:ND2	2.29	0.46
14:H:314:LEU:HA	14:H:317:ILE:HD12	1.97	0.46
15:I:133:LYS:HD2	15:I:133:LYS:H	1.81	0.46
8:Q:143:LEU:HD12	8:Q:144:PRO:HD2	1.98	0.46
8:Q:424:TYR:CD1	8:Q:427:ILE:HD12	2.51	0.46
9:Z:33:SER:HB3	9:Z:55:LYS:HD3	1.98	0.46
11:B:1197:GLU:N	11:B:1199:ASN:OD1	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1198:GLU:O	14:H:98:ARG:NH1	2.42	0.46
13:F:528:SER:H	13:F:531:ASP:HB2	1.80	0.46
13:G:677:ARG:HD2	13:G:677:ARG:HA	1.68	0.46
7:P:236:LEU:HD22	7:P:309:PHE:CD2	2.51	0.45
10:A:1083:TRP:HB2	10:A:1089:PHE:HB3	1.98	0.45
11:B:1255:PHE:HA	11:B:1258:CYS:SG	2.56	0.45
12:C:644:GLU:CA	12:C:647:ILE:CG1	2.85	0.45
7:P:334:ALA:CB	7:P:415:ARG:HD3	2.46	0.45
8:Q:121:GLN:HG2	8:Q:463:TRP:CH2	2.52	0.45
8:Q:286:ASP:CB	8:Q:290:ASN:H	2.29	0.45
9:Z:56:TYR:HB3	9:Z:58:PHE:CE2	2.50	0.45
10:A:570:LYS:HG3	15:I:90:LEU:O	2.16	0.45
10:A:974:GLU:HG2	10:A:978:LEU:HD12	1.98	0.45
10:A:1141:GLU:O	10:A:1145:LEU:HB2	2.17	0.45
10:A:1188:HIS:O	10:A:1192:GLN:CB	2.57	0.45
11:B:718:ASN:O	11:B:722:ILE:HG12	2.16	0.45
12:C:640:ARG:NH2	17:M:72:UNK:O	2.49	0.45
13:D:321:SER:HA	13:D:324:VAL:HG12	1.97	0.45
13:F:685:GLU:O	13:F:689:LEU:HG	2.15	0.45
1:R:72:ARG:O	1:R:76:GLN:HG3	2.17	0.45
7:P:320:SER:OG	7:P:321:ASP:N	2.49	0.45
8:Q:30:PHE:N	8:Q:30:PHE:CD1	2.85	0.45
8:Q:212:SER:HB3	8:Q:284:PHE:HE2	1.81	0.45
11:B:708:HIS:CE1	11:B:710:LEU:HD11	2.51	0.45
12:C:463:GLU:HA	12:C:473:LEU:O	2.16	0.45
13:F:528:SER:N	13:F:531:ASP:OD2	2.50	0.45
7:P:419:TYR:N	7:P:419:TYR:CD1	2.84	0.45
10:A:766:THR:O	19:A:1802:ADP:N6	2.49	0.45
10:A:973:GLU:HA	10:A:977:LEU:HD12	1.98	0.45
10:A:1264:ARG:O	10:A:1268:ARG:HG3	2.16	0.45
13:D:344:MET:HB2	13:D:344:MET:HE2	1.80	0.45
13:F:683:THR:O	13:F:687:ILE:HG12	2.15	0.45
14:H:121:ASN:OD1	14:H:122:VAL:HG23	2.17	0.45
1:R:113:HIS:HE1	1:V:122:LYS:HG3	1.81	0.45
8:Q:354:LEU:HD22	8:Q:358:LEU:HD22	1.99	0.45
10:A:1061:HIS:CD2	10:A:1115:ILE:HA	2.52	0.45
10:A:1288:ALA:C	10:A:1290:ASN:H	2.20	0.45
11:B:907:ALA:CB	11:B:913:LEU:HB2	2.46	0.45
12:C:529:TYR:CD1	12:C:532:LEU:HB2	2.51	0.45
12:C:613:TYR:C	12:C:615:PHE:H	2.19	0.45
12:C:613:TYR:OH	12:C:626:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:429:LYS:NZ	13:E:433:GLN:HE21	2.14	0.45
13:F:527:TRP:HE3	13:F:531:ASP:HB3	1.81	0.45
13:G:687:ILE:HA	13:G:690:GLN:OE1	2.16	0.45
14:H:378:ILE:HB	14:H:400:THR:HG22	1.98	0.45
14:H:525:ALA:HA	14:H:528:VAL:HG12	1.97	0.45
14:H:537:GLU:HG3	14:H:538:ASP:H	1.82	0.45
3:X:84:GLN:HE21	3:X:88:ARG:HG3	1.81	0.45
11:B:917:GLN:O	11:B:921:ILE:HG12	2.16	0.45
14:H:71:GLU:O	14:H:72:LEU:HD23	2.15	0.45
15:I:88:GLU:HB3	15:I:89:GLN:HE22	1.82	0.45
2:S:51:TYR:HB3	2:S:55:ARG:HH12	1.82	0.45
3:T:84:GLN:HE21	3:T:88:ARG:HG3	1.81	0.45
1:V:72:ARG:O	1:V:76:GLN:HG3	2.16	0.45
11:B:1196:SER:N	11:B:1251:LYS:HZ3	2.15	0.45
7:P:282:ASN:O	7:P:285:VAL:HG22	2.16	0.45
10:A:595:GLU:HA	10:A:598:LYS:CG	2.45	0.45
10:A:1079:ASN:H	10:A:1082:ILE:HD12	1.81	0.45
10:A:1176:ASP:OD1	10:A:1176:ASP:N	2.50	0.45
12:C:527:ASN:OD1	12:C:531:GLU:N	2.50	0.45
14:H:77:GLN:OE1	14:H:79:VAL:HB	2.17	0.45
14:H:99:MET:CE	14:H:103:TRP:HE1	2.30	0.45
4:Y:99:LEU:O	4:Y:104:ALA:HB2	2.17	0.45
8:Q:146:SER:HB2	8:Q:174:ILE:HD11	1.99	0.45
11:B:1266:LEU:O	11:B:1270:ALA:N	2.45	0.45
15:I:75:LYS:HA	16:O:3:UNK:N	2.32	0.45
7:P:36:ILE:N	7:P:54:MET:HE2	2.31	0.45
7:P:145:ILE:O	7:P:149:MET:HG2	2.17	0.45
9:Z:33:SER:HB3	9:Z:55:LYS:CD	2.46	0.45
11:B:710:LEU:HD12	11:B:711:SER:N	2.32	0.45
11:B:934:ASN:O	11:B:938:MET:N	2.49	0.45
13:G:737:VAL:O	13:G:740:LEU:HG	2.17	0.45
10:A:473:ASP:OD1	10:A:474:HIS:N	2.50	0.44
10:A:1013:CYS:HB2	10:A:1213:THR:HG22	1.99	0.44
10:A:1209:LEU:HD21	10:A:1286:ILE:HG21	1.99	0.44
11:B:785:ASN:HD22	13:E:341:GLU:HB3	1.82	0.44
11:B:1265:ILE:HG13	11:B:1266:LEU:H	1.82	0.44
12:C:466:GLN:O	12:C:468:ARG:N	2.47	0.44
13:E:324:VAL:HG12	13:E:331:PHE:CZ	2.52	0.44
14:H:86:ASP:OD1	14:H:87:HIS:N	2.50	0.44
10:A:546:ARG:NH1	14:H:541:ARG:HE	2.15	0.44
10:A:575:ASN:O	11:B:1135:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:589:HIS:CE1	11:B:1050:GLU:HG2	2.53	0.44
10:A:1061:HIS:HD2	10:A:1115:ILE:HG13	1.82	0.44
11:B:748:LEU:O	11:B:751:SER:OG	2.33	0.44
12:C:587:GLY:O	12:C:590:VAL:HG22	2.16	0.44
13:E:312:LYS:HG2	14:H:560:ILE:HD11	1.97	0.44
13:F:654:LYS:O	13:F:657:SER:OG	2.28	0.44
14:H:325:SER:HB3	14:H:415:LEU:HD22	2.00	0.44
7:P:232:LYS:HA	7:P:236:LEU:HG	1.99	0.44
10:A:770:TYR:HB3	10:A:999:VAL:HG12	2.00	0.44
10:A:1173:GLN:HA	10:A:1199:ARG:HB3	1.99	0.44
11:B:795:MET:O	11:B:798:LYS:HB2	2.17	0.44
12:C:651:ASN:HD21	13:D:368:ARG:HH22	1.66	0.44
13:D:381:LEU:O	13:D:385:LEU:HG	2.17	0.44
13:G:726:ARG:HG2	13:G:730:ASN:HD21	1.82	0.44
14:H:111:GLU:O	14:H:114:TYR:N	2.46	0.44
4:U:99:LEU:O	4:U:104:ALA:HB2	2.17	0.44
3:X:97:LEU:HD21	4:Y:62:PHE:HE1	1.82	0.44
8:Q:102:PHE:HZ	9:Z:6:LEU:HD23	1.82	0.44
10:A:558:SER:O	10:A:559:LEU:HD23	2.18	0.44
10:A:680:THR:O	10:A:684:ARG:HG2	2.18	0.44
11:B:718:ASN:HD22	11:B:719:LEU:HD23	1.83	0.44
11:B:1119:LEU:H	11:B:1122:VAL:HG22	1.82	0.44
12:C:571:CYS:HB2	12:C:574:GLU:OE2	2.18	0.44
13:E:323:GLU:O	13:E:327:LEU:N	2.51	0.44
14:H:81:SER:HA	14:H:83:LYS:HE2	1.98	0.44
14:H:389:LEU:HB2	14:H:409:LEU:HD21	1.98	0.44
9:Z:66:ASN:HB3	9:Z:70:GLU:HB2	1.98	0.44
10:A:597:LYS:CD	10:A:597:LYS:C	2.86	0.44
10:A:1055:LEU:HA	10:A:1058:ILE:HG12	1.98	0.44
11:B:1034:LYS:HA	11:B:1034:LYS:HD3	1.74	0.44
12:C:475:ASP:OD2	13:E:368:ARG:NH1	2.48	0.44
13:D:343:TYR:HA	13:D:346:TYR:CD2	2.53	0.44
13:F:685:GLU:OE2	14:H:83:LYS:HD3	2.17	0.44
14:H:418:LEU:HD23	14:H:418:LEU:HA	1.82	0.44
10:A:876:ILE:O	10:A:880:ARG:CB	2.46	0.44
10:A:902:ALA:O	10:A:907:SER:OG	2.32	0.44
11:B:903:ASN:ND2	11:B:906:GLY:O	2.51	0.44
11:B:1027:GLU:HG3	11:B:1118:PRO:HD2	1.99	0.44
14:H:338:LEU:HD12	14:H:339:ASN:N	2.32	0.44
15:I:115:ASN:O	15:I:119:ASN:ND2	2.51	0.44
1:R:106:ASP:OD2	1:R:131:ARG:NH2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:566:ASN:OD1	10:A:566:ASN:N	2.51	0.44
10:A:1087:GLY:HA2	10:A:1316:ARG:HH12	1.83	0.44
11:B:784:SER:O	11:B:784:SER:OG	2.33	0.44
11:B:878:LYS:HG2	11:B:881:ARG:HD3	1.99	0.44
11:B:919:SER:O	11:B:923:MET:HG3	2.18	0.44
13:G:743:CYS:HA	13:G:746:LEU:HD12	1.98	0.44
10:A:1216:SER:OG	10:A:1219:GLU:OE1	2.28	0.44
11:B:862:ASP:OD1	11:B:862:ASP:N	2.49	0.44
11:B:1030:LEU:N	11:B:1120:GLN:OE1	2.51	0.44
13:D:308:PRO:HD3	13:D:393:TYR:CD2	2.53	0.44
13:F:545:ASP:OD1	13:F:545:ASP:N	2.51	0.44
10:A:597:LYS:HD3	10:A:598:LYS:HD2	1.99	0.44
10:A:1055:LEU:HD23	10:A:1058:ILE:HD11	2.00	0.44
11:B:1023:LEU:HD22	11:B:1111:SER:HB3	1.99	0.44
13:D:369:ARG:NH2	13:D:370:ASN:HD21	2.16	0.44
13:F:530:GLU:OE2	13:F:530:GLU:N	2.28	0.44
13:F:655:GLU:HA	13:F:658:GLU:CD	2.38	0.44
13:G:535:LEU:O	13:G:539:ILE:HG23	2.17	0.44
13:G:682:LEU:HA	13:G:685:GLU:CD	2.38	0.44
1:V:79:LYS:HD3	1:V:82:LEU:HD21	2.00	0.43
7:P:129:ASP:OD2	7:P:460:TYR:HE2	2.01	0.43
7:P:458:GLU:O	7:P:459:ASP:C	2.56	0.43
8:Q:286:ASP:HB2	8:Q:290:ASN:O	2.18	0.43
9:Z:83:ASP:O	9:Z:86:GLU:HG3	2.18	0.43
11:B:711:SER:OG	11:B:712:MET:N	2.51	0.43
11:B:745:TYR:HD1	11:B:745:TYR:H	1.64	0.43
11:B:1091:LEU:HD23	11:B:1091:LEU:HA	1.85	0.43
12:C:452:GLU:HA	13:E:334:ARG:NH1	2.32	0.43
12:C:572:PRO:HD2	12:C:598:ARG:HH22	1.83	0.43
13:D:402:LYS:O	13:D:404:ILE:HG23	2.17	0.43
13:G:521:GLU:N	13:G:521:GLU:OE1	2.51	0.43
14:H:483:GLN:O	14:H:487:ILE:HG12	2.18	0.43
15:I:138:SER:OG	15:I:139:GLU:N	2.51	0.43
1:R:122:LYS:HA	1:R:125:GLN:HG2	2.00	0.43
10:A:496:ILE:HG13	10:A:497:TYR:N	2.32	0.43
10:A:1184:ASP:HB3	10:A:1190:ASP:CB	2.46	0.43
11:B:1117:ILE:HB	11:B:1118:PRO:HD3	2.00	0.43
13:D:347:ARG:HG3	13:D:348:ASN:N	2.32	0.43
14:H:491:LEU:HD23	14:H:491:LEU:HA	1.70	0.43
14:H:513:LYS:HA	14:H:516:ASN:HD22	1.83	0.43
1:V:122:LYS:HA	1:V:125:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:381:PRO:HG2	7:P:382:GLU:CD	2.39	0.43
10:A:1261:GLU:HG3	10:A:1264:ARG:HH21	1.82	0.43
11:B:777:TYR:CD1	11:B:777:TYR:N	2.86	0.43
11:B:984:HIS:O	11:B:986:LEU:HD12	2.18	0.43
13:D:352:ASN:O	13:D:356:LEU:HG	2.18	0.43
13:E:379:PHE:CZ	13:E:383:LYS:HD3	2.53	0.43
15:I:142:ILE:HA	15:I:145:LEU:HG	1.99	0.43
2:S:31:LYS:HB3	2:S:32:PRO:HD3	2.01	0.43
2:S:88:TYR:O	2:S:92:ARG:HB2	2.17	0.43
7:P:151:LYS:HE3	7:P:424:PHE:CE1	2.53	0.43
11:B:1049:LEU:HD23	11:B:1049:LEU:HA	1.77	0.43
12:C:547:LYS:HB2	12:C:560:GLN:NE2	2.33	0.43
12:C:548:LEU:HD21	12:C:600:GLN:HG3	1.99	0.43
13:E:416:HIS:CE1	16:J:36:UNK:HA	2.53	0.43
14:H:344:ASN:N	14:H:344:ASN:OD1	2.52	0.43
14:H:403:LEU:O	14:H:407:LEU:HG	2.17	0.43
2:S:38:ALA:HB3	2:S:46:ILE:HD11	2.00	0.43
10:A:1233:GLY:O	10:A:1237:GLN:HB2	2.18	0.43
11:B:910:PRO:O	11:B:913:LEU:HB3	2.17	0.43
12:C:435:ARG:NH1	12:C:438:TYR:OH	2.51	0.43
12:C:511:ASP:O	12:C:515:GLN:HG2	2.19	0.43
12:C:525:GLN:N	12:C:525:GLN:OE1	2.51	0.43
12:C:549:ASP:HB2	12:C:558:ILE:HD13	2.01	0.43
12:C:554:GLN:NE2	12:C:555:ASN:HB2	2.33	0.43
16:J:30:UNK:O	16:J:34:UNK:N	2.51	0.43
8:Q:197:SER:HB3	8:Q:301:GLY:HA2	1.99	0.43
10:A:503:LEU:O	10:A:507:THR:HG23	2.19	0.43
10:A:522:THR:O	10:A:526:ARG:HG3	2.18	0.43
10:A:770:TYR:HB2	10:A:994:ARG:NE	2.33	0.43
11:B:890:LYS:HB3	11:B:890:LYS:HE3	1.88	0.43
12:C:446:TYR:CD1	12:C:485:LEU:HD22	2.53	0.43
13:D:339:THR:HG22	13:D:342:VAL:HG22	2.00	0.43
13:F:709:GLU:C	13:F:713:LYS:HZ2	2.21	0.43
1:R:79:LYS:HD3	1:R:82:LEU:HD21	2.00	0.43
8:Q:66:LYS:HA	8:Q:67:PRO:HD3	1.78	0.43
10:A:461:SER:HG	10:A:465:TYR:HH	1.66	0.43
10:A:514:ASP:OD1	10:A:515:LYS:N	2.52	0.43
10:A:745:TYR:HA	10:A:749:HIS:HD2	1.82	0.43
10:A:913:HIS:O	10:A:913:HIS:ND1	2.51	0.43
11:B:879:ILE:HG22	11:B:880:HIS:N	2.34	0.43
12:C:641:PRO:HB2	12:C:646:LYS:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:529:LYS:O	13:G:533:GLN:HG3	2.19	0.43
14:H:413:THR:HB	14:H:414:HIS:CE1	2.53	0.43
1:R:48:LEU:HD23	1:R:51:ILE:HD12	2.00	0.43
7:P:122:ARG:HG2	7:P:122:ARG:NH1	2.06	0.43
7:P:180:VAL:CG1	7:P:332:LEU:HG	2.48	0.43
7:P:314:PHE:CZ	7:P:407:ARG:HG3	2.54	0.43
7:P:381:PRO:C	7:P:383:GLN:N	2.72	0.43
10:A:1054:GLN:HG3	10:A:1055:LEU:HG	2.01	0.43
11:B:1202:SER:H	11:B:1274:ASN:CB	2.31	0.43
12:C:607:SER:HA	12:C:610:LEU:HG	2.00	0.43
13:D:308:PRO:HG3	13:D:393:TYR:CE1	2.54	0.43
13:D:311:SER:O	13:D:313:TRP:N	2.49	0.43
14:H:80:ASP:O	14:H:82:GLU:N	2.45	0.43
1:V:48:LEU:HD23	1:V:51:ILE:HD12	2.00	0.43
10:A:929:ASN:ND2	10:A:1228:LYS:HB3	2.33	0.43
11:B:779:TYR:O	13:E:319:ILE:HG12	2.18	0.43
12:C:467:ASP:HA	12:C:470:ARG:NH2	2.34	0.43
12:C:469:ASP:N	12:C:469:ASP:OD1	2.50	0.43
11:B:763:LEU:HD11	11:B:961:ASN:HB2	2.00	0.43
11:B:1064:LYS:NZ	11:B:1103:HIS:O	2.44	0.43
11:B:1211:ILE:HG21	11:B:1237:ILE:HB	2.00	0.43
13:E:327:LEU:HD23	13:E:327:LEU:HA	1.81	0.43
14:H:312:PRO:HA	14:H:315:THR:HG22	2.01	0.43
14:H:512:VAL:HG13	14:H:513:LYS:N	2.34	0.43
15:I:136:LEU:O	15:I:140:LYS:HG2	2.19	0.43
10:A:1247:SER:O	10:A:1250:GLN:HG2	2.18	0.42
11:B:992:ILE:O	11:B:996:LEU:HD23	2.18	0.42
13:E:386:THR:OG1	13:E:391:ILE:HD11	2.18	0.42
14:H:313:GLN:H	14:H:313:GLN:CD	2.22	0.42
14:H:388:LEU:HG	14:H:414:HIS:CE1	2.54	0.42
15:I:79:ASP:O	15:I:83:VAL:HG12	2.18	0.42
2:S:22:LEU:HB3	2:S:25:ASN:ND2	2.34	0.42
10:A:1097:PRO:O	10:A:1101:ALA:HB2	2.19	0.42
11:B:760:LEU:HD11	11:B:951:LEU:HA	2.01	0.42
11:B:990:SER:OG	11:B:991:SER:N	2.52	0.42
13:E:339:THR:HG23	13:E:342:VAL:H	1.84	0.42
14:H:335:TYR:O	14:H:338:LEU:HG	2.19	0.42
14:H:468:GLU:HA	14:H:471:ARG:NH1	2.33	0.42
7:P:198:ALA:N	7:P:199:PRO:HD2	2.34	0.42
8:Q:6:GLN:O	8:Q:24:GLY:HA2	2.19	0.42
10:A:539:LEU:HD13	13:G:570:ILE:HG21	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:559:LEU:HD21	11:B:722:ILE:HD12	2.02	0.42
10:A:851:PRO:O	10:A:855:LYS:HG3	2.19	0.42
10:A:1179:ILE:HG23	10:A:1211:LEU:HD13	2.01	0.42
11:B:787:TYR:CE1	13:E:345:ARG:HB3	2.55	0.42
11:B:938:MET:HE3	11:B:940:ARG:HE	1.84	0.42
11:B:1253:ILE:HG13	11:B:1254:CYS:N	2.33	0.42
13:D:420:ARG:O	13:D:420:ARG:HG3	2.19	0.42
14:H:397:SER:HB2	14:H:399:ASP:OD1	2.19	0.42
7:P:80:TRP:CE2	7:P:122:ARG:HD3	2.53	0.42
10:A:559:LEU:HD12	11:B:916:ASP:OD1	2.18	0.42
10:A:678:ARG:O	10:A:682:LEU:HG	2.20	0.42
10:A:1095:ILE:O	10:A:1099:LEU:HG	2.19	0.42
10:A:1110:PHE:CZ	10:A:1119:MET:HG2	2.55	0.42
11:B:899:PHE:CE2	14:H:506:LYS:HD2	2.54	0.42
11:B:1267:LYS:HB3	13:G:717:ARG:CZ	2.50	0.42
12:C:541:ASP:OD1	12:C:541:ASP:N	2.52	0.42
13:E:415:ARG:NH2	16:J:39:UNK:C	2.82	0.42
15:I:102:SER:O	15:I:105:SER:N	2.51	0.42
3:T:30:VAL:HG13	4:U:67:PHE:HE1	1.85	0.42
9:Z:9:LYS:HD2	9:Z:12:LYS:NZ	2.34	0.42
10:A:513:LEU:O	10:A:516:LEU:HG	2.18	0.42
10:A:536:LEU:HD13	10:A:536:LEU:HA	1.78	0.42
11:B:882:THR:HA	11:B:883:PRO:HD3	1.87	0.42
12:C:412:TYR:HB2	12:C:420:THR:H	1.83	0.42
13:E:362:PHE:CE1	13:E:366:THR:HB	2.55	0.42
13:G:681:PHE:HA	13:G:684:ASN:ND2	2.34	0.42
14:H:84:ARG:O	14:H:87:HIS:HB2	2.19	0.42
14:H:115:PRO:HG2	14:H:116:HIS:CD2	2.54	0.42
7:P:431:ASP:O	7:P:435:GLN:HB2	2.19	0.42
11:B:1035:TYR:N	11:B:1036:GLN:OE1	2.52	0.42
11:B:1053:ASN:HB3	11:B:1057:PHE:CZ	2.54	0.42
13:D:347:ARG:O	13:D:351:VAL:HG12	2.19	0.42
13:D:402:LYS:HE2	13:D:402:LYS:HB2	1.71	0.42
8:Q:91:LEU:CD2	8:Q:106:LEU:HD22	2.50	0.42
8:Q:445:ASP:HA	8:Q:448:TYR:CE1	2.55	0.42
11:B:1295:ILE:H	11:B:1295:ILE:HD12	1.84	0.42
12:C:415:TYR:OH	12:C:419:ILE:N	2.52	0.42
12:C:613:TYR:CZ	12:C:619:ALA:HA	2.55	0.42
13:F:670:ILE:CG2	14:H:508:SER:HB3	2.47	0.42
14:H:541:ARG:HG2	14:H:545:PHE:HE2	1.84	0.42
15:I:144:TYR:HA	15:I:147:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1337:ARG:O	10:A:1340:SER:N	2.52	0.42
11:B:1265:ILE:O	11:B:1269:ILE:N	2.30	0.42
12:C:555:ASN:OD1	12:C:654:GLN:N	2.48	0.42
13:F:726:ARG:CZ	15:I:161:UNK:HA	2.49	0.42
10:A:531:TYR:HA	10:A:534:TYR:CD2	2.55	0.42
13:F:532:LEU:HA	13:F:535:LEU:HB3	2.02	0.42
13:G:682:LEU:O	13:G:686:LEU:HG	2.20	0.42
15:I:110:ASN:HA	15:I:113:SER:OG	2.20	0.42
1:R:101:VAL:HG11	3:X:107:VAL:HG21	2.02	0.42
10:A:469:LEU:HA	15:I:128:CYS:SG	2.60	0.42
10:A:595:GLU:HA	10:A:598:LYS:CB	2.49	0.42
10:A:978:LEU:O	10:A:982:ARG:HG2	2.20	0.42
11:B:952:LEU:HA	11:B:955:VAL:HG12	2.01	0.42
12:C:567:ASN:OD1	12:C:569:ASP:N	2.46	0.42
13:F:718:GLN:HE22	13:G:719:GLN:HB2	1.85	0.42
14:H:505:LYS:O	14:H:508:SER:OG	2.16	0.42
15:I:102:SER:O	15:I:105:SER:OG	2.20	0.42
3:X:85:LEU:HD23	3:X:108:LEU:HD23	2.02	0.41
7:P:197:LEU:HD11	7:P:231:PHE:CE1	2.55	0.41
8:Q:361:GLU:HA	8:Q:362:PRO:HD3	1.94	0.41
10:A:546:ARG:NH1	10:A:546:ARG:HB2	2.35	0.41
10:A:570:LYS:HZ2	10:A:571:ILE:HG12	1.85	0.41
10:A:586:TYR:OH	11:B:1048:SER:HA	2.20	0.41
10:A:884:SER:HB2	10:A:913:HIS:HA	2.02	0.41
10:A:988:ARG:HB2	10:A:989:PRO:HD3	2.00	0.41
10:A:1019:GLN:OE1	10:A:1058:ILE:HB	2.20	0.41
12:C:505:THR:OG1	12:C:506:ARG:NH1	2.52	0.41
13:F:551:LYS:HA	13:F:551:LYS:HD3	1.62	0.41
13:F:557:SER:H	13:F:560:GLN:CD	2.24	0.41
13:G:526:ASN:O	13:G:527:TRP:HD1	2.02	0.41
14:H:86:ASP:HA	14:H:89:ILE:HG12	2.02	0.41
15:I:71:GLN:O	15:I:75:LYS:HG3	2.20	0.41
15:I:74:ASN:HA	15:I:77:ARG:HH21	1.85	0.41
1:R:123:ASP:OD1	1:V:113:HIS:NE2	2.52	0.41
10:A:564:HIS:HB3	11:B:966:ARG:HH22	1.85	0.41
10:A:818:PRO:HB3	10:A:866:PHE:CZ	2.55	0.41
10:A:1137:THR:OG1	10:A:1141:GLU:OE2	2.36	0.41
10:A:1149:PHE:CZ	10:A:1172:LEU:HD13	2.55	0.41
10:A:1228:LYS:HA	10:A:1231:ILE:HD12	2.02	0.41
11:B:1202:SER:H	11:B:1274:ASN:ND2	2.17	0.41
12:C:413:SER:H	12:C:420:THR:HG23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:588:GLU:HG3	13:E:370:ASN:HD22	1.85	0.41
12:C:636:ASP:HA	13:D:337:SER:OG	2.20	0.41
13:D:329:GLU:OE1	13:D:329:GLU:N	2.42	0.41
13:E:323:GLU:H	13:E:323:GLU:HG2	1.72	0.41
2:S:35:ARG:O	2:S:39:ARG:HG2	2.19	0.41
7:P:418:GLN:HG2	7:P:419:TYR:CD1	2.56	0.41
10:A:530:LEU:HG	10:A:534:TYR:CE2	2.55	0.41
10:A:758:GLN:HB3	10:A:767:LEU:HD21	2.02	0.41
10:A:895:GLU:N	10:A:922:LEU:O	2.53	0.41
13:D:453:LEU:HD12	13:D:456:TYR:HB2	2.01	0.41
13:F:699:ASN:HB2	13:F:703:LYS:HZ2	1.85	0.41
13:F:726:ARG:HD3	13:F:726:ARG:HA	1.94	0.41
14:H:106:SER:O	14:H:110:GLN:HG2	2.19	0.41
4:Y:103:LEU:O	4:Y:107:ALA:CB	2.69	0.41
7:P:235:MET:SD	8:Q:401:VAL:HG21	2.60	0.41
10:A:1120:GLU:HG2	10:A:1130:TYR:CE2	2.55	0.41
10:A:1303:ASP:OD1	10:A:1304:ARG:N	2.49	0.41
12:C:541:ASP:HA	12:C:543:ARG:HH11	1.85	0.41
12:C:613:TYR:C	12:C:615:PHE:N	2.74	0.41
13:D:420:ARG:NH2	17:M:6:UNK:H	2.18	0.41
13:E:424:PRO:HG2	13:E:425:PHE:CD2	2.56	0.41
13:F:702:LYS:HD3	13:F:706:LYS:NZ	2.35	0.41
14:H:527:LYS:HD2	14:H:527:LYS:HA	1.74	0.41
15:I:81:GLU:HB2	15:I:82:ARG:HH12	1.83	0.41
16:J:34:UNK:O	16:J:35:UNK:C	2.67	0.41
16:J:35:UNK:O	16:J:36:UNK:C	2.69	0.41
10:A:681:HIS:HE1	10:A:944:LYS:HA	1.86	0.41
10:A:1237:GLN:O	10:A:1240:LYS:HG2	2.21	0.41
11:B:876:PRO:O	11:B:877:LEU:HD22	2.20	0.41
11:B:897:ASP:N	11:B:897:ASP:OD1	2.53	0.41
11:B:1027:GLU:HG2	11:B:1115:SER:HA	2.03	0.41
11:B:1292:ASP:HB2	11:B:1295:ILE:HB	2.02	0.41
13:D:355:ARG:O	13:D:358:PRO:HD3	2.20	0.41
13:G:542:PHE:CD2	13:G:548:LYS:HD3	2.56	0.41
16:J:27:UNK:O	16:J:28:UNK:C	2.68	0.41
1:R:122:LYS:HG3	1:V:113:HIS:HE1	1.84	0.41
7:P:108:MET:SD	7:P:123:TYR:HE2	2.43	0.41
10:A:834:GLU:O	10:A:838:TRP:HB2	2.20	0.41
11:B:1271:SER:O	11:B:1272:ILE:HD13	2.20	0.41
12:C:498:ASP:OD2	13:E:363:SER:HB2	2.21	0.41
14:H:99:MET:HG3	14:H:103:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:121:LEU:HD23	15:I:121:LEU:HA	1.74	0.41
2:S:64:ASN:O	2:S:67:ARG:HG2	2.21	0.41
7:P:412:LEU:HD12	7:P:412:LEU:HA	1.76	0.41
8:Q:3:PRO:HA	8:Q:4:PHE:HA	1.67	0.41
10:A:1061:HIS:NE2	10:A:1115:ILE:HG23	2.36	0.41
10:A:1071:GLN:HE22	10:A:1343:ALA:HA	1.86	0.41
13:E:312:LYS:HD2	13:E:312:LYS:HA	1.83	0.41
13:G:704:LEU:O	13:G:708:MET:HG2	2.21	0.41
16:J:3:UNK:O	16:J:7:UNK:N	2.54	0.41
8:Q:112:LEU:HD12	8:Q:141:ILE:HD12	2.02	0.41
8:Q:166:THR:HG22	8:Q:167:HIS:CE1	2.56	0.41
10:A:479:ILE:HG12	16:K:23:UNK:O	2.20	0.41
12:C:447:LYS:CD	13:E:328:PRO:HG3	2.51	0.41
13:D:320:HIS:HD2	13:D:321:SER:N	2.19	0.41
13:E:329:GLU:OE2	13:E:380:ARG:NE	2.48	0.41
7:P:203:GLU:O	7:P:204:GLU:CB	2.66	0.41
7:P:458:GLU:O	7:P:460:TYR:N	2.53	0.41
8:Q:26:ASN:HB3	8:Q:29:THR:O	2.21	0.41
9:Z:84:LEU:O	9:Z:85:LYS:CB	2.61	0.41
10:A:611:SER:O	10:A:615:GLN:HG3	2.21	0.41
10:A:840:PRO:O	10:A:841:THR:OG1	2.34	0.41
10:A:895:GLU:OE1	10:A:897:HIS:NE2	2.51	0.41
10:A:928:GLN:NE2	10:A:929:ASN:HD22	2.19	0.41
10:A:1149:PHE:CE2	10:A:1172:LEU:HD13	2.56	0.41
11:B:861:TRP:HD1	12:C:447:LYS:HE2	1.86	0.41
11:B:879:ILE:HG22	11:B:880:HIS:CD2	2.55	0.41
11:B:883:PRO:O	11:B:886:THR:HG23	2.21	0.41
11:B:905:ARG:HA	11:B:905:ARG:NE	2.36	0.41
11:B:933:ASN:O	11:B:937:ILE:HG13	2.21	0.41
11:B:1309:ILE:HD13	11:B:1309:ILE:HA	1.82	0.41
12:C:466:GLN:H	12:C:466:GLN:CD	2.24	0.41
12:C:584:GLU:HG3	12:C:586:PRO:CD	2.50	0.41
12:C:606:LYS:O	12:C:609:ALA:HB3	2.21	0.41
12:C:653:LEU:HD12	16:N:13:UNK:HA	2.03	0.41
13:E:315:ASN:HB2	13:E:318:LYS:HG2	2.03	0.41
13:F:702:LYS:HD3	13:F:706:LYS:CE	2.50	0.41
14:H:109:SER:HA	14:H:112:PHE:CE2	2.56	0.41
14:H:309:SER:O	14:H:415:LEU:HD12	2.21	0.41
14:H:406:LEU:O	14:H:410:ILE:N	2.45	0.41
14:H:450:LEU:HG	14:H:451:LYS:H	1.85	0.41
15:I:123:LEU:HD23	15:I:123:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:142:ILE:HG22	15:I:146:MET:SD	2.60	0.41
2:W:31:LYS:HG3	2:W:51:TYR:CE2	2.56	0.41
2:W:35:ARG:O	2:W:39:ARG:HG2	2.21	0.41
7:P:381:PRO:O	7:P:383:GLN:N	2.53	0.41
7:P:446:LEU:CD2	10:A:608:MET:SD	3.09	0.41
7:P:451:LEU:CD1	10:A:608:MET:SD	2.82	0.41
10:A:493:ALA:HA	10:A:496:ILE:HG12	2.02	0.41
10:A:598:LYS:N	10:A:598:LYS:HD2	2.34	0.41
11:B:958:HIS:HE1	11:B:960:GLU:OE1	2.04	0.41
11:B:1233:LEU:H	11:B:1233:LEU:HG	1.65	0.41
13:D:315:ASN:C	13:D:317:GLU:H	2.25	0.41
14:H:108:LEU:HD23	14:H:108:LEU:HA	1.90	0.41
3:T:85:LEU:HD23	3:T:108:LEU:HD23	2.02	0.40
7:P:154:ALA:N	7:P:169:ILE:O	2.53	0.40
8:Q:105:GLU:H	8:Q:105:GLU:HG3	1.62	0.40
8:Q:146:SER:O	8:Q:149:ALA:HB3	2.21	0.40
8:Q:156:LEU:HA	8:Q:156:LEU:HD23	1.76	0.40
10:A:546:ARG:NH1	14:H:541:ARG:HH11	2.19	0.40
10:A:556:GLN:HG3	11:B:719:LEU:HD22	2.03	0.40
10:A:1019:GLN:NE2	10:A:1062:PRO:HB3	2.35	0.40
11:B:741:SER:OG	11:B:742:LEU:N	2.53	0.40
11:B:878:LYS:HG2	11:B:881:ARG:CZ	2.51	0.40
12:C:411:GLY:O	13:D:415:ARG:NE	2.50	0.40
13:E:376:ALA:HB1	13:E:380:ARG:HH12	1.86	0.40
4:U:103:LEU:O	4:U:107:ALA:CB	2.69	0.40
7:P:36:ILE:HB	7:P:54:MET:CE	2.42	0.40
7:P:108:MET:HE1	7:P:119:ILE:HG21	2.03	0.40
7:P:389:LEU:HD22	7:P:421:LEU:CD2	2.52	0.40
8:Q:119:TRP:N	8:Q:119:TRP:CD1	2.89	0.40
10:A:938:LEU:HD23	10:A:944:LYS:HZ3	1.86	0.40
11:B:1046:LEU:HA	11:B:1046:LEU:HD23	1.75	0.40
12:C:438:TYR:HB3	13:E:383:LYS:HZ1	1.86	0.40
12:C:604:TYR:O	12:C:607:SER:OG	2.26	0.40
14:H:311:SER:CB	14:H:414:HIS:HB3	2.51	0.40
14:H:472:GLU:O	14:H:475:GLN:HB3	2.21	0.40
7:P:139:VAL:HG11	7:P:443:MET:HG3	2.03	0.40
7:P:246:LEU:HD13	7:P:250:TYR:HE2	1.87	0.40
8:Q:148:ALA:HB1	8:Q:428:ILE:O	2.22	0.40
10:A:572:ARG:HH22	15:I:95:HIS:N	2.19	0.40
10:A:1250:GLN:O	10:A:1254:LEU:HG	2.21	0.40
11:B:785:ASN:HB3	13:E:345:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1057:PHE:O	11:B:1061:LEU:HG	2.20	0.40
11:B:1275:LEU:HD12	11:B:1276:PHE:H	1.85	0.40
13:F:681:PHE:CZ	14:H:498:ASN:HA	2.56	0.40
13:G:571:GLU:OE1	13:G:571:GLU:HA	2.20	0.40
2:S:32:PRO:O	2:S:36:ARG:HG3	2.22	0.40
8:Q:354:LEU:HD23	8:Q:354:LEU:HA	1.89	0.40
10:A:572:ARG:HH22	15:I:95:HIS:H	1.67	0.40
11:B:701:GLU:O	11:B:702:LEU:HD23	2.20	0.40
11:B:1025:PHE:HD1	11:B:1025:PHE:HA	1.67	0.40
12:C:550:ILE:HD12	12:C:550:ILE:HA	1.96	0.40
13:E:304:GLU:OE1	13:E:304:GLU:N	2.54	0.40
13:F:567:GLN:O	13:F:568:LEU:HD23	2.21	0.40
14:H:78:LEU:HB3	14:H:84:ARG:HH12	1.87	0.40
7:P:188:PHE:CZ	7:P:319:ILE:HD13	2.57	0.40
7:P:381:PRO:HG2	7:P:382:GLU:H	1.86	0.40
10:A:567:PHE:O	11:B:926:ARG:NE	2.54	0.40
11:B:896:ASP:OD2	15:I:110:ASN:HB3	2.21	0.40
11:B:964:CYS:SG	11:B:966:ARG:HB3	2.61	0.40
11:B:1141:SER:O	11:B:1145:THR:HG22	2.20	0.40
12:C:630:LEU:O	12:C:633:ILE:CG1	2.69	0.40
14:H:121:ASN:OD1	14:H:122:VAL:N	2.53	0.40
14:H:528:VAL:C	14:H:530:SER:H	2.25	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	R	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	V	93/135 (69%)	89 (96%)	4 (4%)	0	100	100
2	S	80/102 (78%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	77/102 (76%)	73 (95%)	4 (5%)	0	100	100
3	T	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	X	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	U	91/122 (75%)	88 (97%)	3 (3%)	0	100	100
4	Y	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
7	P	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	12	48
8	Q	391/467 (84%)	367 (94%)	22 (6%)	2 (0%)	29	69
9	Z	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	6	35
10	A	763/1703 (45%)	667 (87%)	96 (13%)	0	100	100
11	B	468/1314 (36%)	364 (78%)	104 (22%)	0	100	100
12	C	241/905 (27%)	176 (73%)	63 (26%)	2 (1%)	19	60
13	D	157/825 (19%)	130 (83%)	27 (17%)	0	100	100
13	E	137/825 (17%)	113 (82%)	24 (18%)	0	100	100
13	F	215/825 (26%)	186 (86%)	27 (13%)	2 (1%)	17	57
13	G	189/825 (23%)	164 (87%)	24 (13%)	1 (0%)	29	69
14	H	249/566 (44%)	217 (87%)	32 (13%)	0	100	100
15	I	78/179 (44%)	66 (85%)	12 (15%)	0	100	100
All	All	4064/10044 (40%)	3573 (88%)	478 (12%)	13 (0%)	44	77

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Q	48	ASP
13	F	606	PRO
7	P	343	SER
12	C	614	ASN
7	P	382	GLU
7	P	459	ASP
9	Z	84	LEU
13	G	572	ASP
7	P	431	ASP
7	P	458	GLU
8	Q	155	SER
13	F	648	LYS
12	C	612	GLY

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	R	84/110 (76%)	84 (100%)	0	100	100
1	V	82/110 (74%)	82 (100%)	0	100	100
2	S	67/78 (86%)	67 (100%)	0	100	100
2	W	64/78 (82%)	64 (100%)	0	100	100
3	T	81/101 (80%)	81 (100%)	0	100	100
3	X	82/101 (81%)	82 (100%)	0	100	100
4	U	77/102 (76%)	77 (100%)	0	100	100
4	Y	79/102 (78%)	79 (100%)	0	100	100
7	P	357/420 (85%)	338 (95%)	19 (5%)	22	47
8	Q	363/423 (86%)	343 (94%)	20 (6%)	21	47
9	Z	53/140 (38%)	52 (98%)	1 (2%)	57	75
10	A	705/1520 (46%)	698 (99%)	7 (1%)	76	86
11	B	460/1218 (38%)	458 (100%)	2 (0%)	91	94
12	C	222/823 (27%)	219 (99%)	3 (1%)	67	80
13	D	150/751 (20%)	150 (100%)	0	100	100
13	E	129/751 (17%)	128 (99%)	1 (1%)	81	89
13	F	138/751 (18%)	138 (100%)	0	100	100
13	G	127/751 (17%)	125 (98%)	2 (2%)	62	79
14	H	239/517 (46%)	238 (100%)	1 (0%)	91	94
15	I	79/133 (59%)	78 (99%)	1 (1%)	69	81
All	All	3638/8980 (40%)	3581 (98%)	57 (2%)	64	79

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	P	2	THR
7	P	79	ASN
7	P	88	ARG

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Mol	Chain	Res	Type
7	P	122	ARG
7	P	216	ARG
7	P	230	GLN
7	P	246	LEU
7	P	251	LYS
7	P	293	LYS
7	P	301	LEU
7	P	319	ILE
7	P	321	ASP
7	P	343	SER
7	P	380	SER
7	P	386	SER
7	P	397	SER
7	P	432	ARG
7	P	442	THR
7	P	462	THR
8	Q	7	ASP
8	Q	32	VAL
8	Q	34	GLU
8	Q	41	ILE
8	Q	48	ASP
8	Q	52	THR
8	Q	54	HIS
8	Q	56	THR
8	Q	69	GLN
8	Q	94	ARG
8	Q	100	ASP
8	Q	105	GLU
8	Q	122	SER
8	Q	181	ASP
8	Q	197	SER
8	Q	291	GLU
8	Q	321	ASP
8	Q	347	GLU
8	Q	422	SER
8	Q	438	GLN
9	Z	90	ARG
10	A	597	LYS
10	A	598	LYS
10	A	605	LEU
10	A	607	SER
10	A	650	LYS

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Mol	Chain	Res	Type
10	A	651	LYS
10	A	659	LEU
11	B	772	ARG
11	B	941	ASN
12	C	500	ARG
12	C	543	ARG
12	C	633	ILE
13	E	420	ARG
13	G	571	GLU
13	G	706	LYS
14	H	562	SER
15	I	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	68	GLN
2	S	25	ASN
4	U	46	HIS
1	V	68	GLN
2	W	93	GLN
4	Y	46	HIS
8	Q	303	ASN
8	Q	304	ASN
10	A	460	HIS
10	A	510	ASN
10	A	528	ASN
10	A	564	HIS
10	A	588	ASN
10	A	681	HIS
10	A	749	HIS
10	A	929	ASN
10	A	939	ASN
10	A	1054	GLN
10	A	1071	GLN
10	A	1104	HIS
10	A	1173	GLN
10	A	1202	GLN
11	B	718	ASN
11	B	791	GLN
11	B	874	GLN
11	B	880	HIS

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Mol	Chain	Res	Type
11	B	915	ASN
11	B	984	HIS
11	B	1006	GLN
11	B	1026	ASN
11	B	1053	ASN
11	B	1093	ASN
11	B	1104	ASN
11	B	1215	ASN
11	B	1243	GLN
11	B	1274	ASN
11	B	1298	GLN
11	B	1300	GLN
11	B	1304	ASN
12	C	437	HIS
12	C	448	GLN
12	C	466	GLN
12	C	508	GLN
12	C	595	HIS
12	C	614	ASN
13	D	348	ASN
13	D	394	GLN
13	D	416	HIS
13	E	352	ASN
13	E	357	ASN
13	E	394	GLN
13	E	411	GLN
13	E	433	GLN
13	F	552	ASN
13	F	718	GLN
13	F	728	ASN
13	F	738	ASN
13	G	526	ASN
13	G	533	GLN
13	G	555	ASN
13	G	567	GLN
13	G	699	ASN
13	G	725	GLN
13	G	730	ASN
13	G	745	ASN
14	H	76	GLN
14	H	102	GLN
14	H	118	ASN

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Mol	Chain	Res	Type
14	H	313	GLN
14	H	326	HIS
14	H	469	ASN
14	H	493	ASN
14	H	516	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

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ADP	A	1802	21	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
18	PO4	Q	503	-	4,4,4	0.84	0	6,6,6	0.56	0
18	PO4	Q	506	-	4,4,4	0.82	0	6,6,6	0.58	0
18	PO4	Q	505	-	4,4,4	0.87	0	6,6,6	0.42	0
18	PO4	P	502	-	4,4,4	0.80	0	6,6,6	0.54	0
18	PO4	P	503	-	4,4,4	0.96	0	6,6,6	0.48	0
18	PO4	P	505	-	4,4,4	0.88	0	6,6,6	0.43	0
18	PO4	A	1801	-	4,4,4	0.79	0	6,6,6	0.80	0
18	PO4	P	501	-	4,4,4	0.90	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	PO4	Q	502	-	4,4,4	0.83	0	6,6,6	0.46	0
20	BEF	A	1803	-	0,3,3	-	-	-		
18	PO4	Q	504	-	4,4,4	0.88	0	6,6,6	0.41	0
18	PO4	P	504	-	4,4,4	0.85	0	6,6,6	0.60	0
18	PO4	Q	501	-	4,4,4	0.98	0	6,6,6	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	A	1802	21	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	1802	ADP	C5-C4	2.46	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	1802	ADP	C3'-C2'-C1'	3.33	105.99	100.98
19	A	1802	ADP	PA-O3A-PB	-3.33	121.41	132.83
19	A	1802	ADP	N3-C2-N1	-3.14	123.77	128.68
19	A	1802	ADP	C4-C5-N7	-2.60	106.69	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1802	ADP	C5'-O5'-PA-O1A

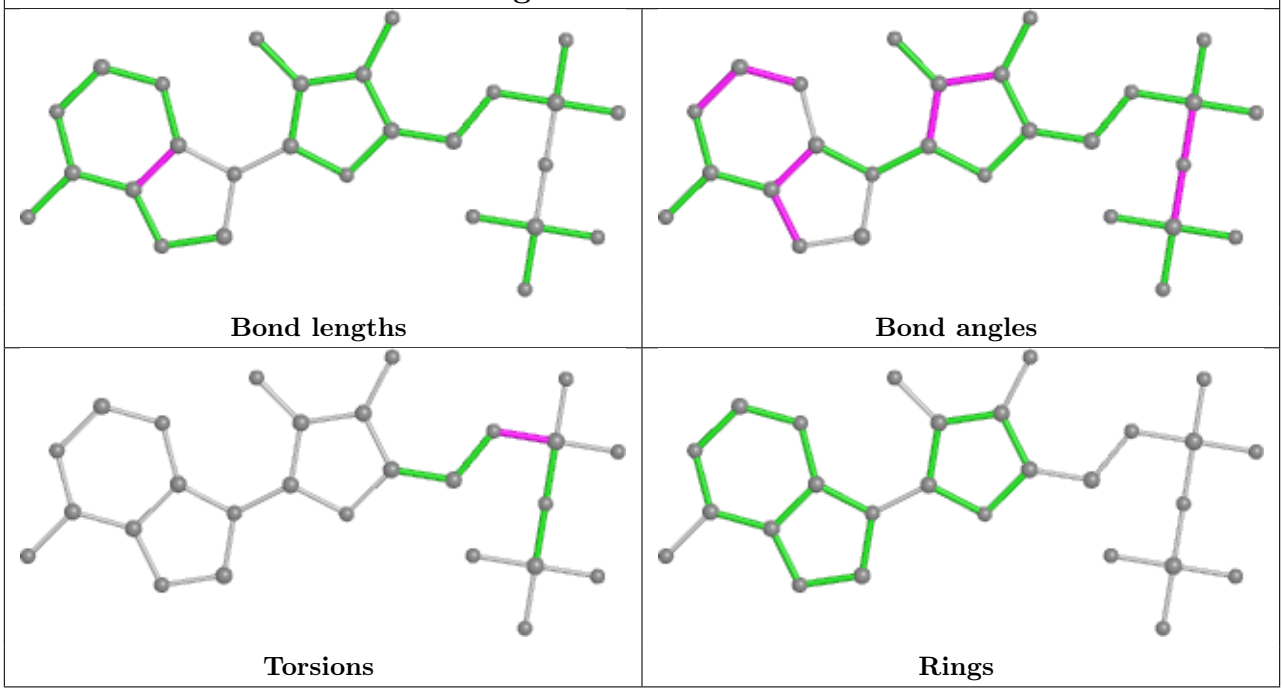
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1802	ADP	6	0
20	A	1803	BEF	4	0
18	Q	504	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	I	1
17	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	150:HIS	C	152:UNK	N	20.17
1	M	22:UNK	C	24:UNK	N	7.86

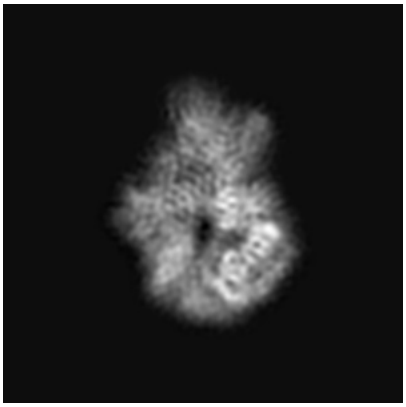
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20934. These allow visual inspection of the internal detail of the map and identification of artifacts.

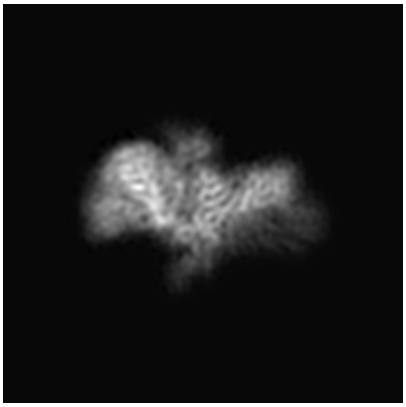
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

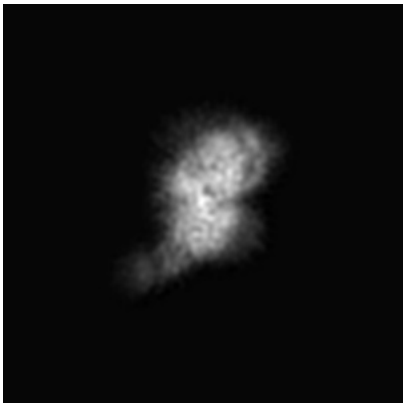
6.1.1 Primary map



X



Y

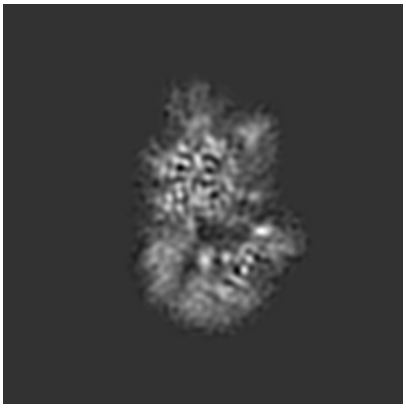


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 96

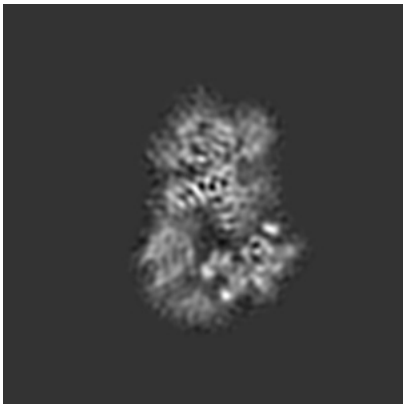
Y Index: 96

Z Index: 96

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: 102

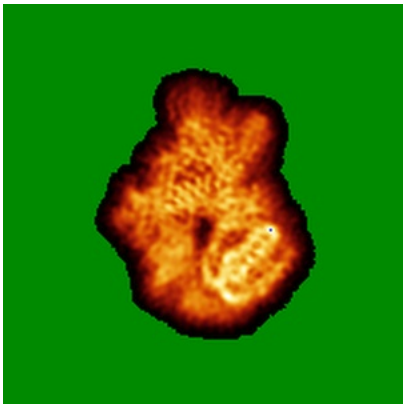
Y Index: 107

Z Index: 97

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

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

6.4.1 Primary map



X

Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

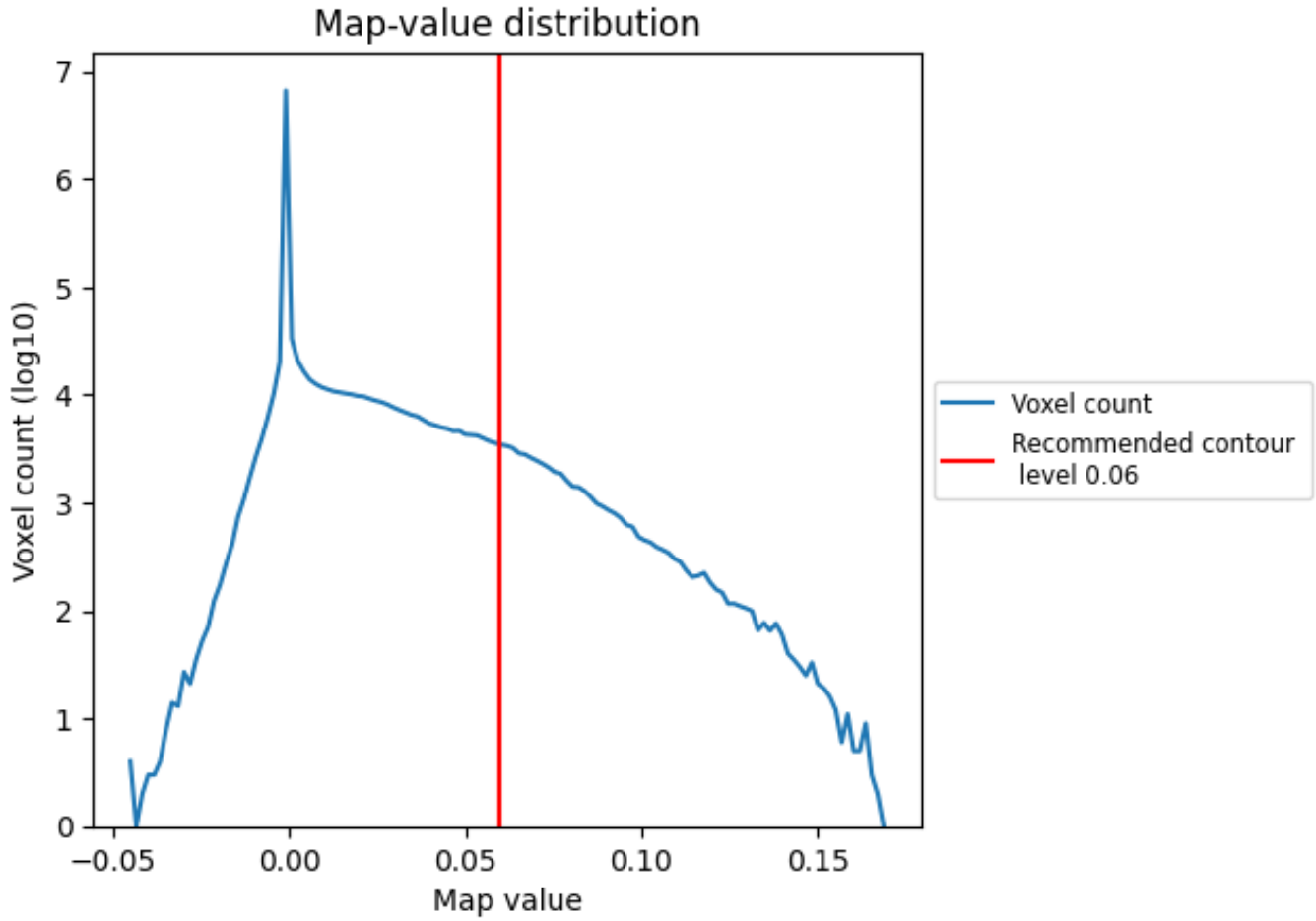
6.6 Mask visualisation (i)

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

7 Map analysis

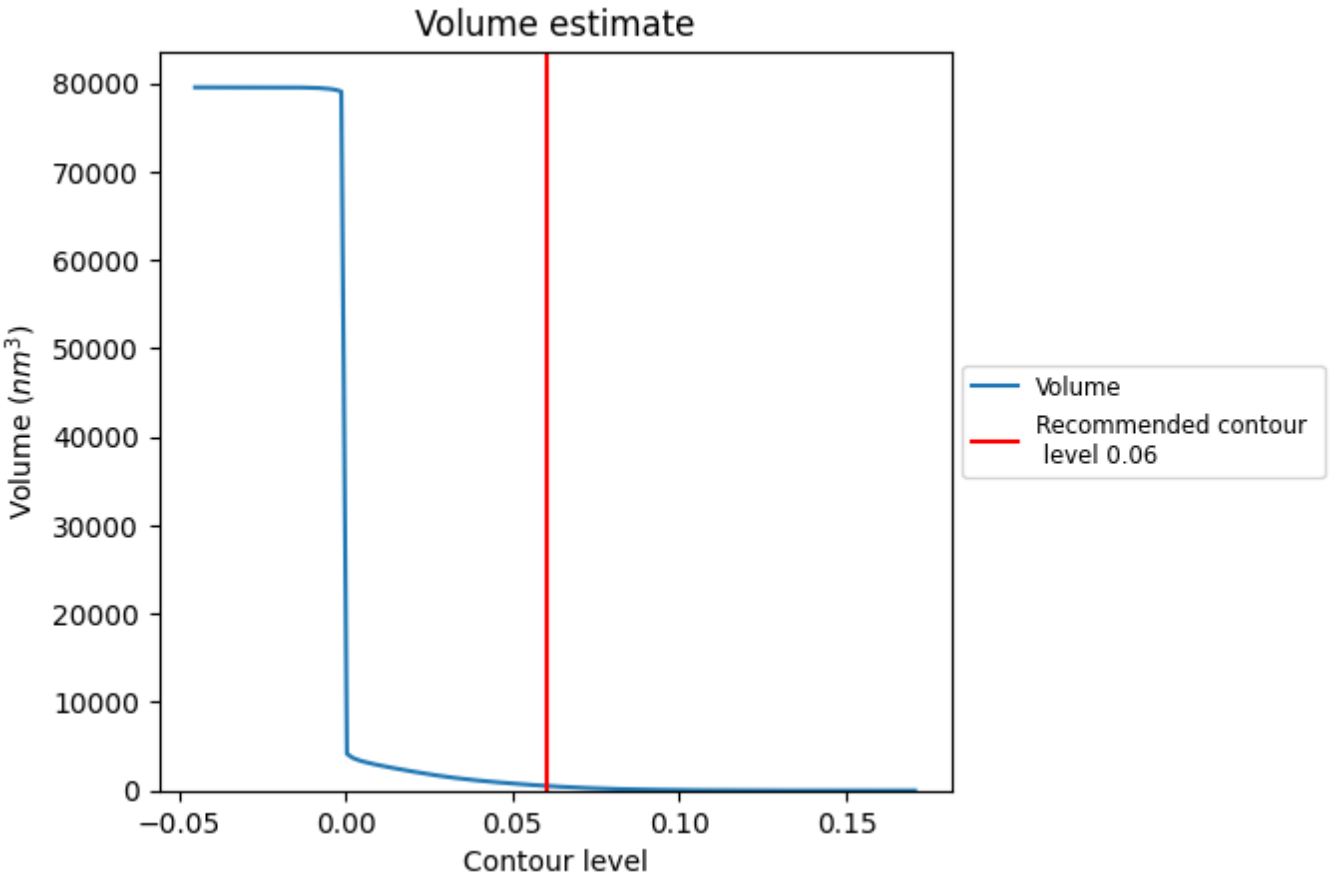
This section contains the results of statistical analysis of the map.

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.

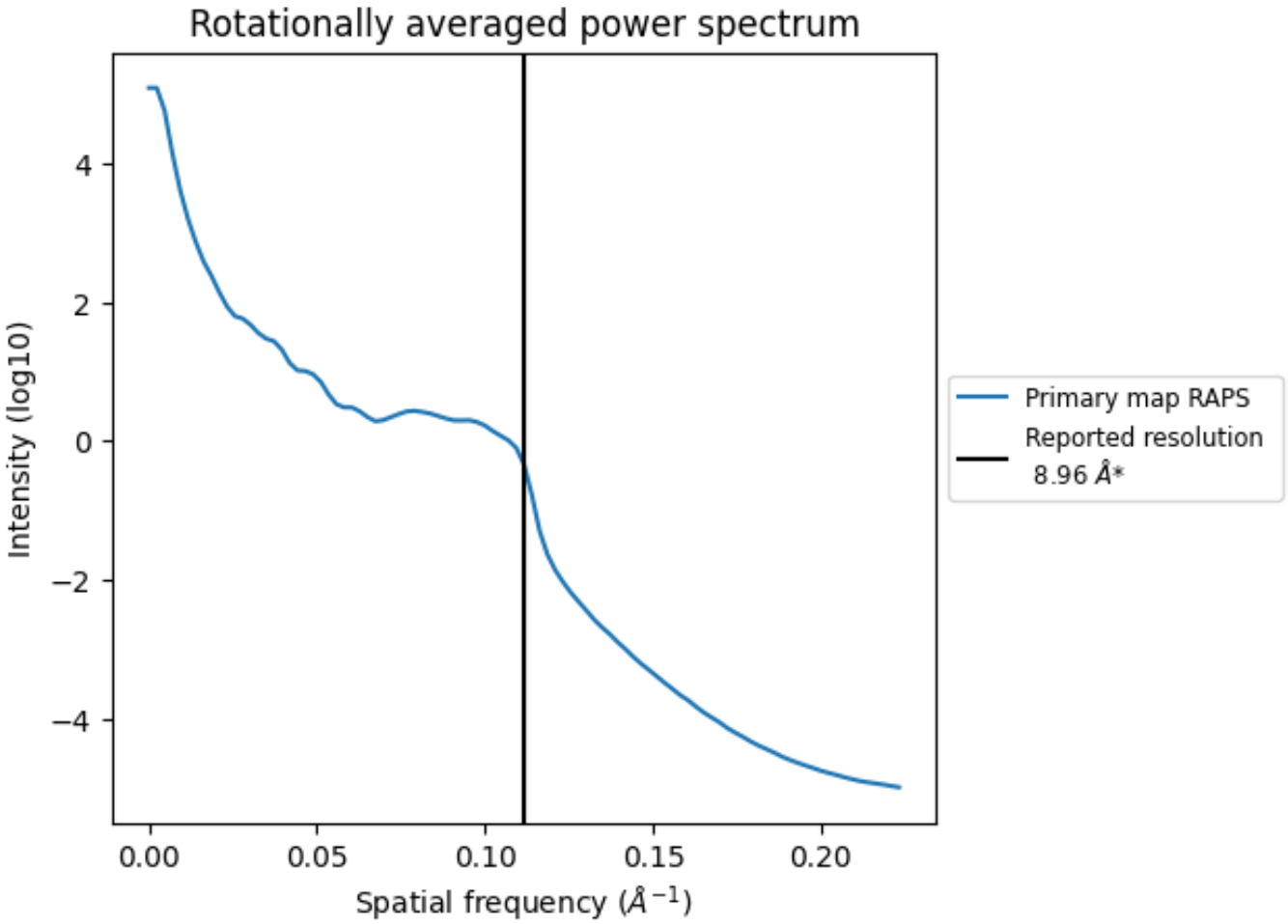
7.2 Volume estimate



The volume at the recommended contour level is 531 nm^3; this corresponds to an approximate mass of 480 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)

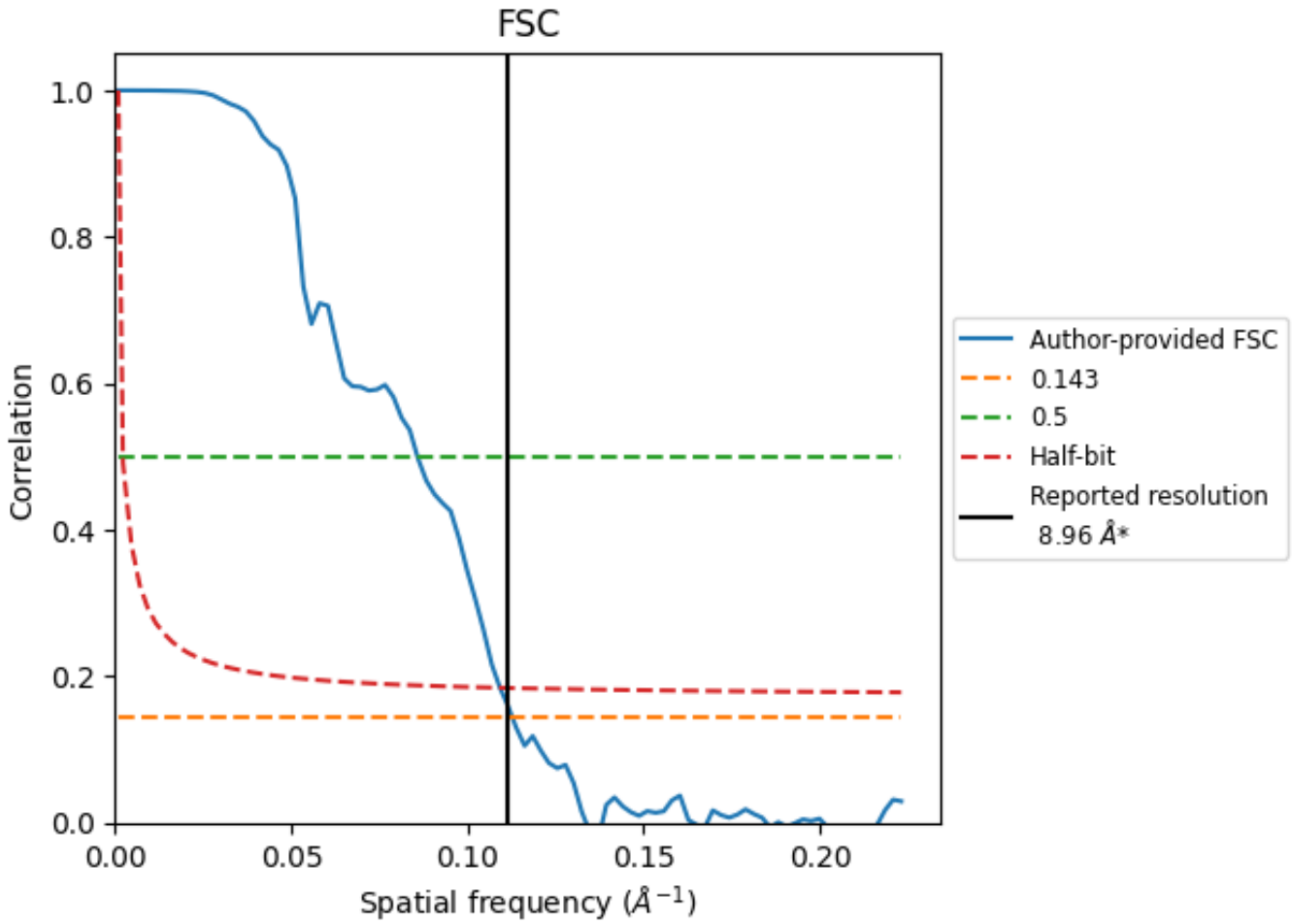


*Reported resolution corresponds to spatial frequency of 0.112 Å^{-1}

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 0.112 Å^{-1}

8.2 Resolution estimates (i)

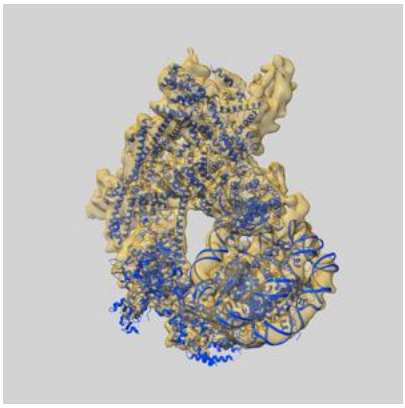
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.96	-	-
Author-provided FSC curve	8.86	11.64	9.15
Unmasked-calculated*	-	-	-

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

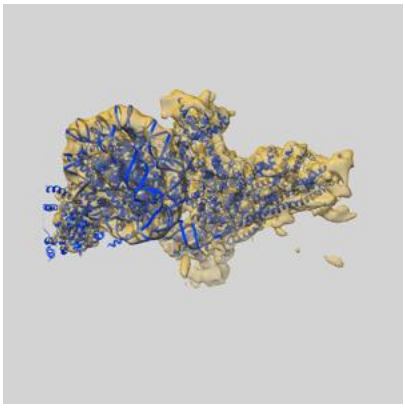
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20934 and PDB model 6UXW. Per-residue inclusion information can be found in section 3 on page 10.

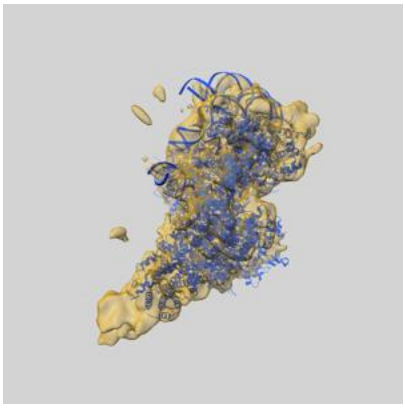
9.1 Map-model overlay



X



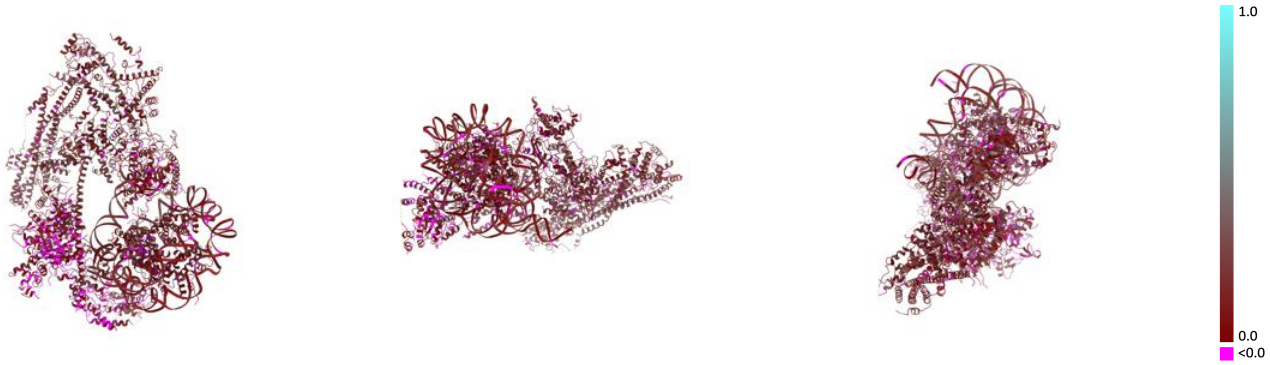
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

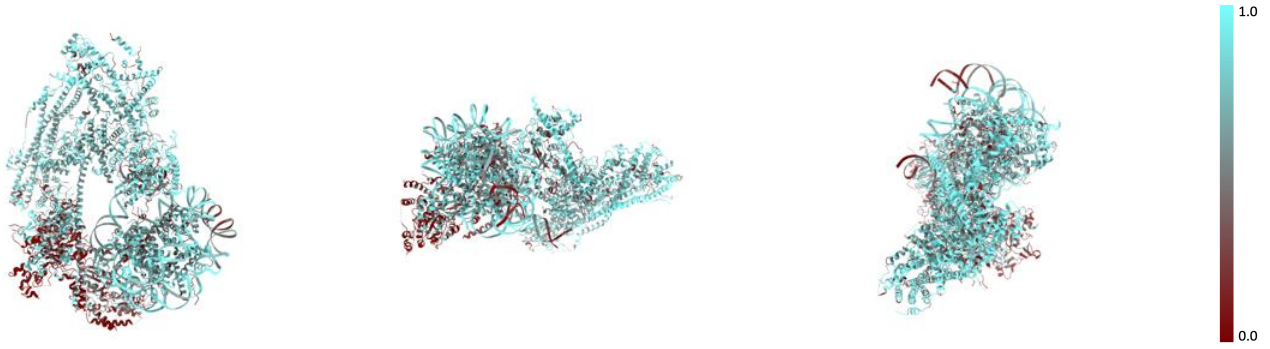
9.2 Q-score mapped to coordinate model



X Y Z

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

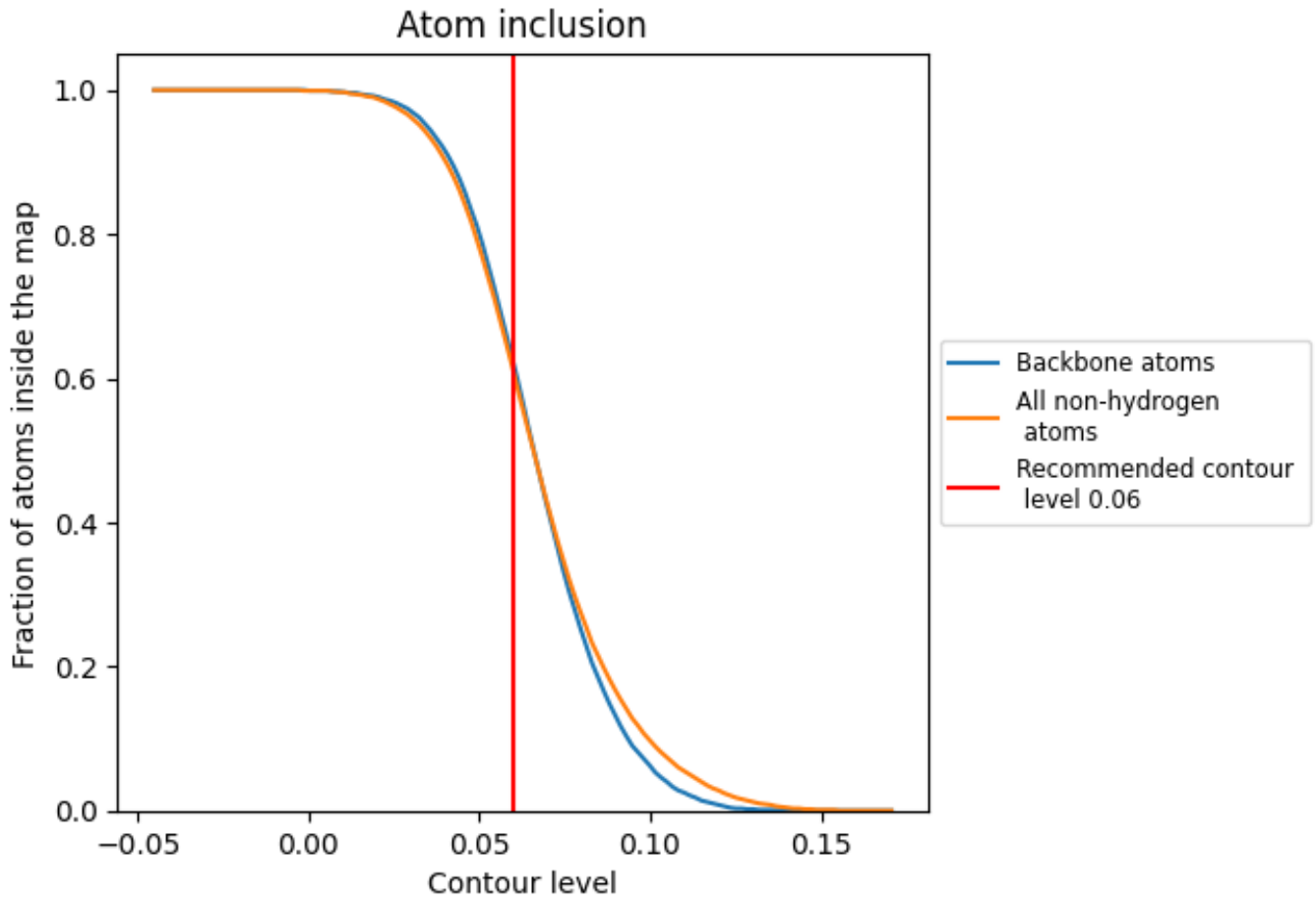
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6090	0.1220
A	0.3700	0.0820
B	0.6980	0.1540
C	0.6370	0.1420
D	0.7220	0.1270
E	0.7080	0.1410
F	0.7600	0.1580
G	0.7540	0.1690
H	0.7300	0.1660
I	0.7700	0.1710
J	0.9670	0.2740
K	0.8860	0.2370
L	0.3000	0.1970
M	0.8890	0.2170
N	0.4270	0.0640
O	0.7440	0.1650
P	0.5240	0.0750
Q	0.3550	0.0520
R	0.5820	0.1120
S	0.6010	0.1060
T	0.5800	0.1100
U	0.6930	0.1590
V	0.6590	0.1260
W	0.6770	0.1050
X	0.6730	0.1180
Y	0.7000	0.1370
Z	0.4380	0.0930
a	0.7290	0.1300
b	0.7540	0.1380