Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 11:58 pm GMT

PDB ID	:	6TED
EMDB ID	:	EMD-10480
Title	:	Structure of complete, activated transcription complex Pol II-DSIF-PAF-SPT6 uncovers allosteric elongation activation by RTF1
Authors	:	Vos, S.M.; Farnung, L.; Cramer, P.
Deposited on	:	2019-11-11
Resolution	:	3.10 Å(reported)
Based on initial models	:	4L1U, 6GMH, 6AFO

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

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

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

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

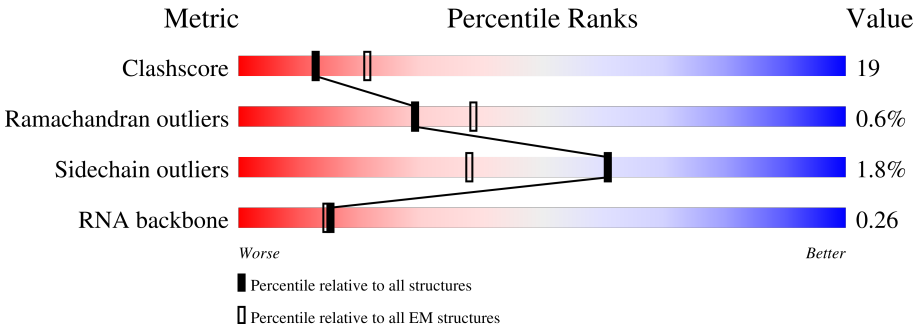
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1984	42% 28% 28%
2	B	1251	57% 28% 5% 10%
3	C	275	66% 23% 5% 6%
4	D	142	61% 43% 45% 11%
5	E	210	63% 34%
6	F	127	49% 11% 39%
7	G	172	52% 55% 44%

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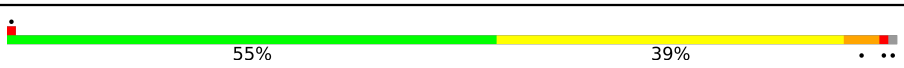
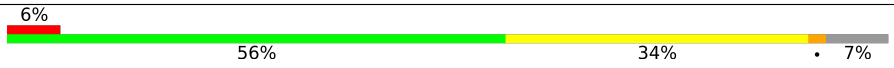
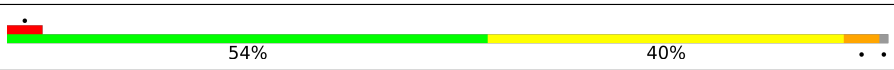
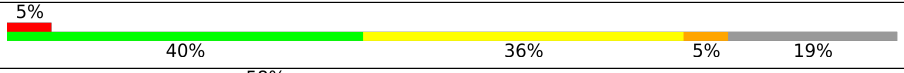
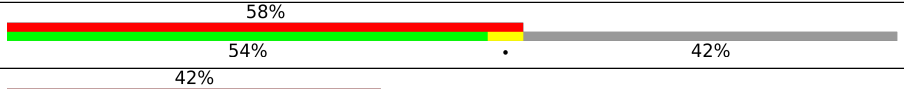
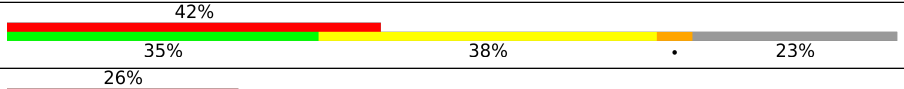
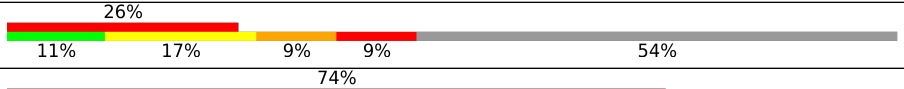
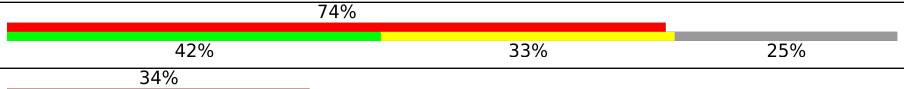
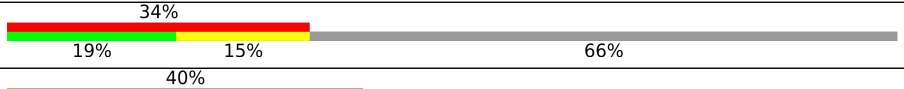
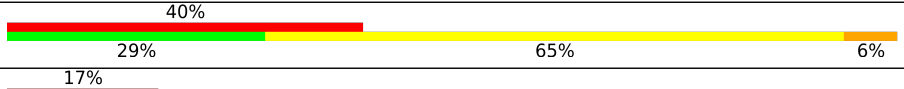
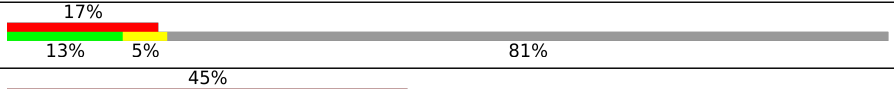
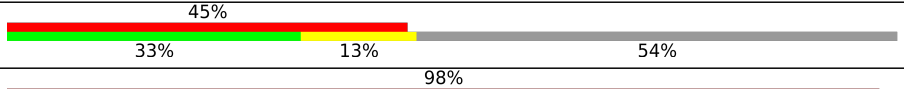
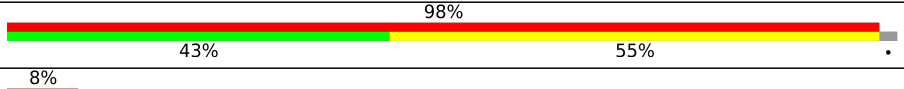
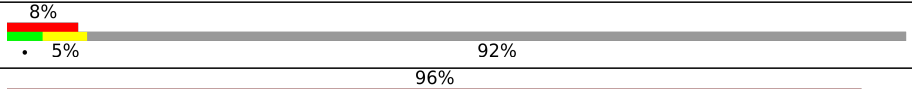
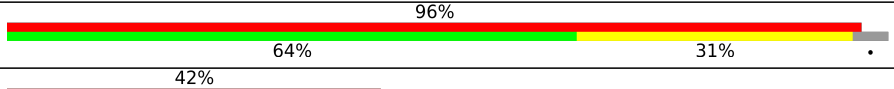
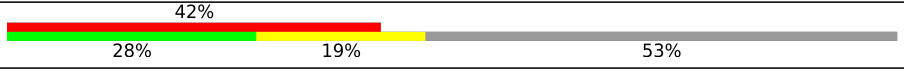
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	48	
15	P	46	
16	Q	1179	
17	R	713	
18	T	48	
19	U	666	
20	V	531	
21	W	305	
22	X	531	
23	Y	121	
24	Z	1087	

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 57142 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1426	11255	7074	2014	2095	2	70	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1122	8980	5684	1576	1656	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	1004	630	170	200	4	0	0

- Molecule 5 is a protein called RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1720	1089	300	323	8	0	0

- Molecule 6 is a protein called RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	78	626	401	106	114	5	0	0

- Molecule 7 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			390	240	77	67	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	N	O	S	0	0
			4737	2583	1071	1076	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	37	Total	C	N	O	P	0	0
			773	361	158	217	37		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 16 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	890	Total	C	N	O	S	0	0
			7226	4579	1264	1352	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 17 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	244	Total	C	N	O	S	0	0
			1832	1148	340	337	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	48	Total	C	N	O	P	0	0
			974	462	168	296	48		

- Molecule 19 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	125	Total	C	N	O	S	0	0
			852	534	151	166	1		

- Molecule 20 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	244	Total	C	N	O	S	0	0
			1703	1061	305	333	4		

- Molecule 21 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 22 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	43	Total	C	N	O	0	0
			353	220	69	64		

- Molecule 23 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 24 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Z	510	Total	C	N	O	P	S	0	0
			4023	2550	709	745	1	18		

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	Y	1	Total	Zn	0
			1	1	

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

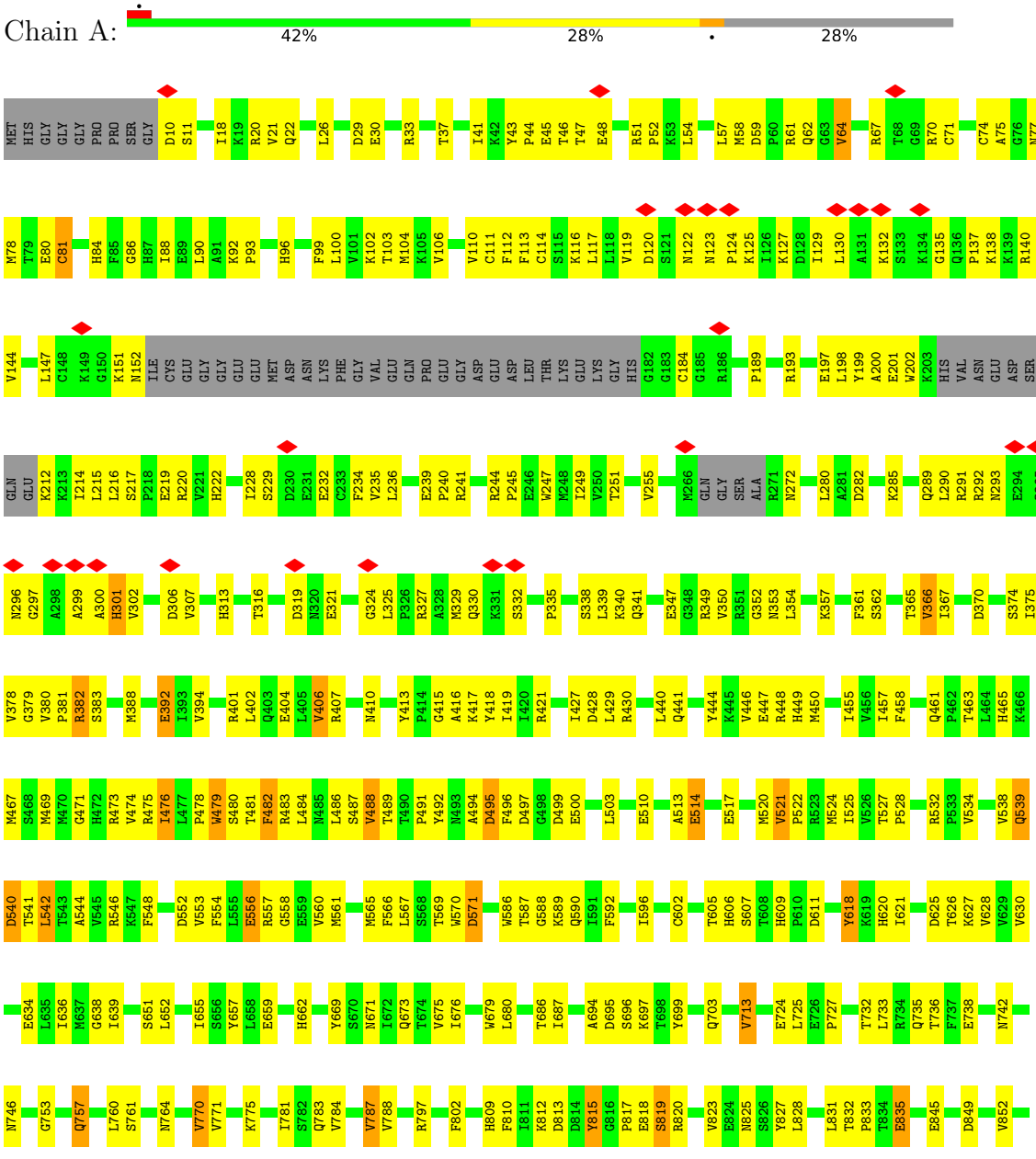
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Mg	0
			1	1	

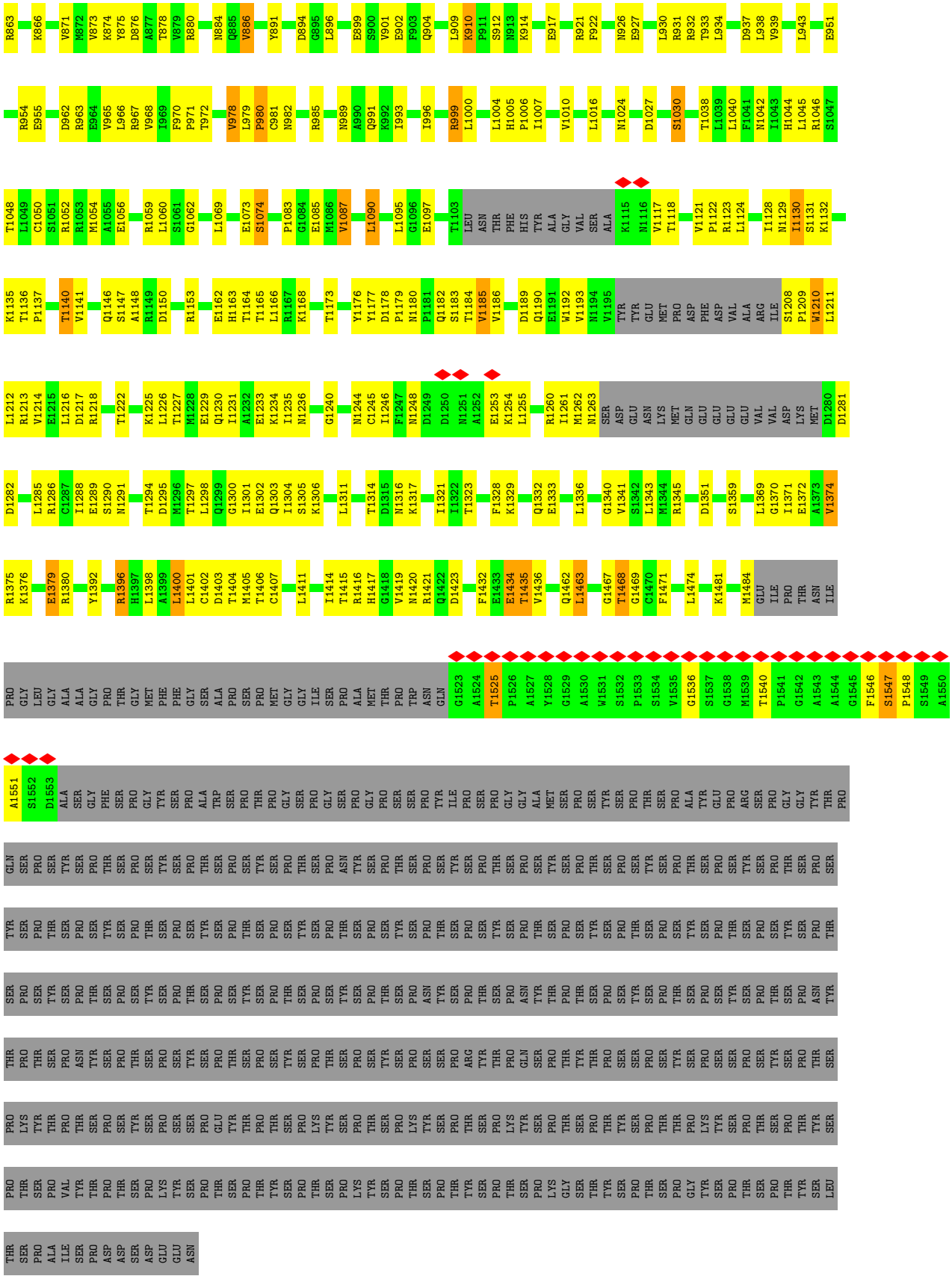
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:



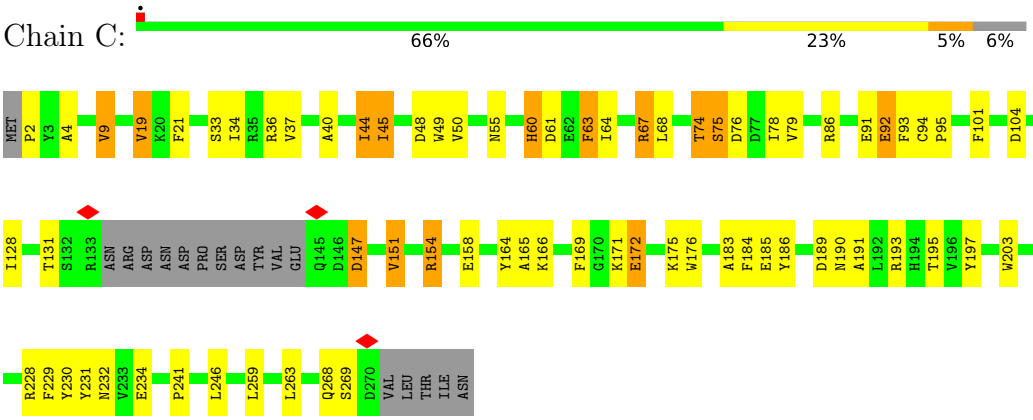


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

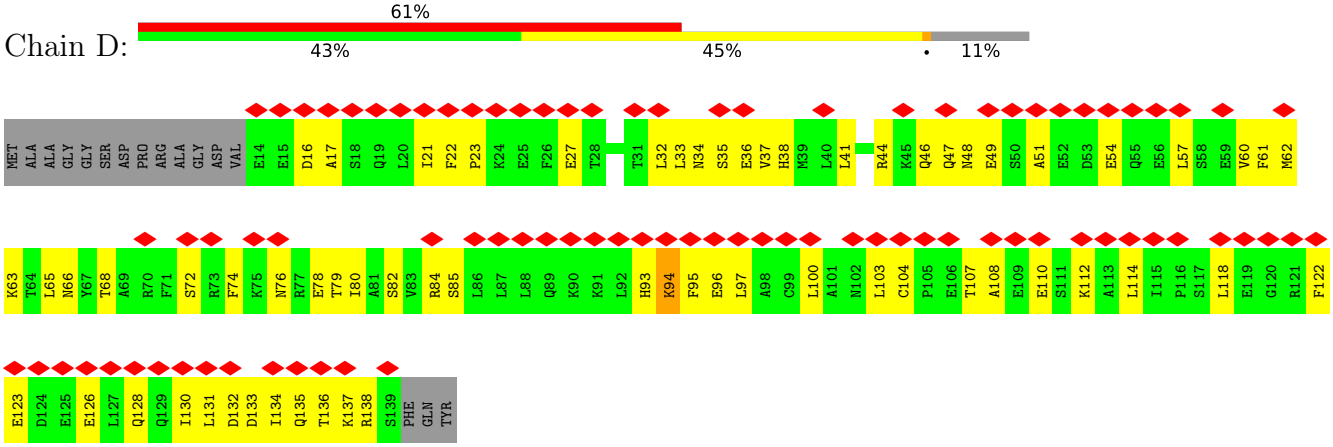
• Molecule 3: RNA polymerase II subunit C

Chain C:



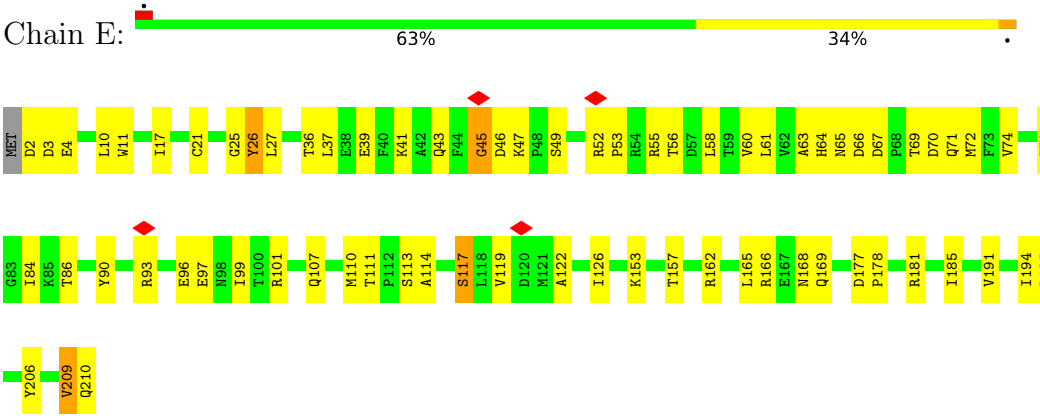
• Molecule 4: RNA polymerase II subunit D

Chain D:



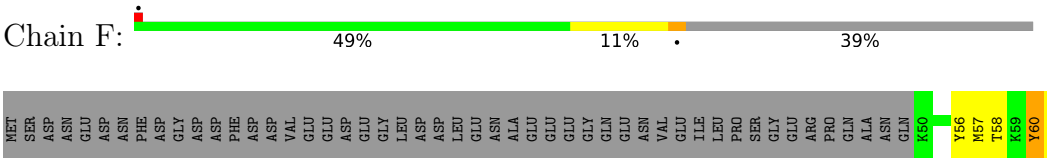
• Molecule 5: RNA polymerase II subunit E

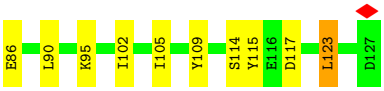
Chain E:



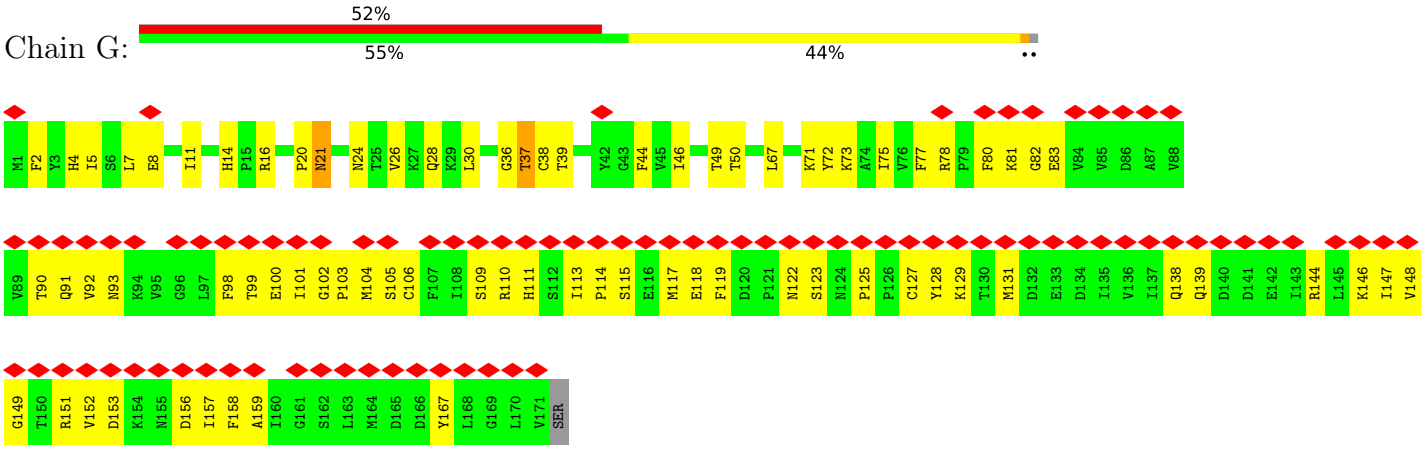
• Molecule 6: RNA polymerase II subunit F

Chain F:

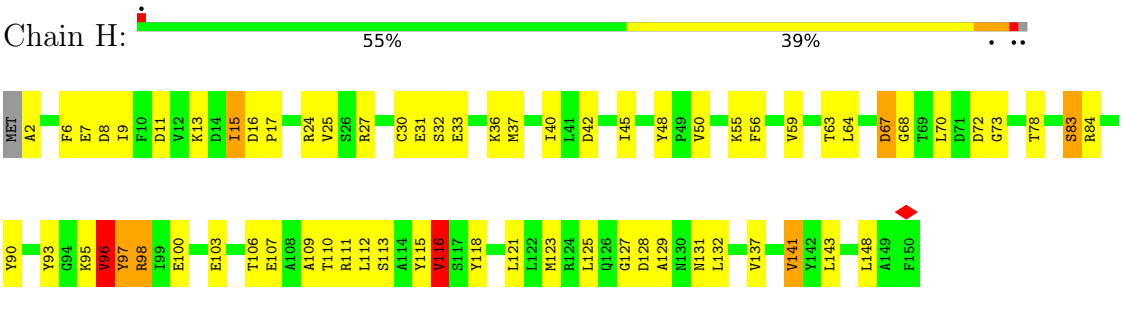




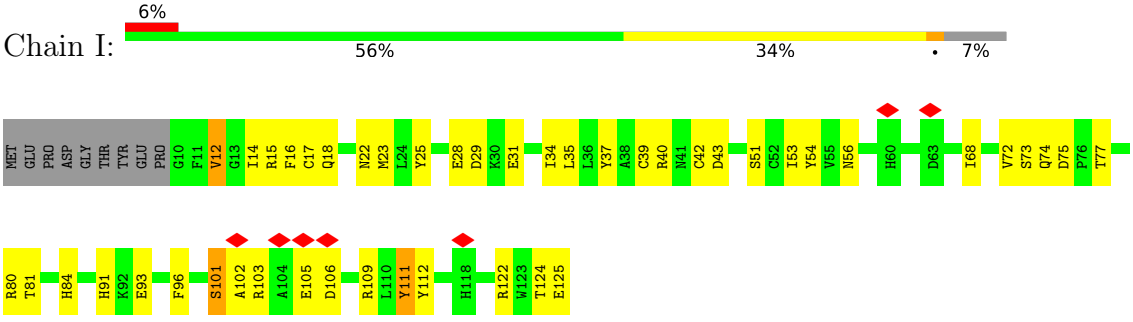
• Molecule 7: RNA polymerase II subunit G



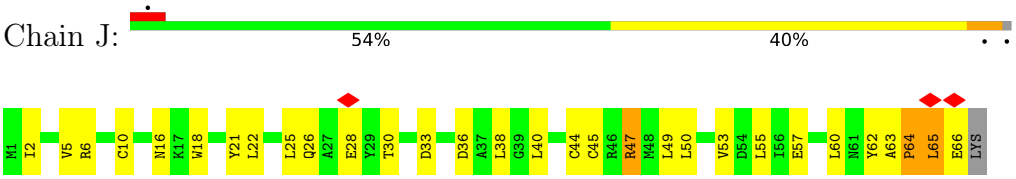
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

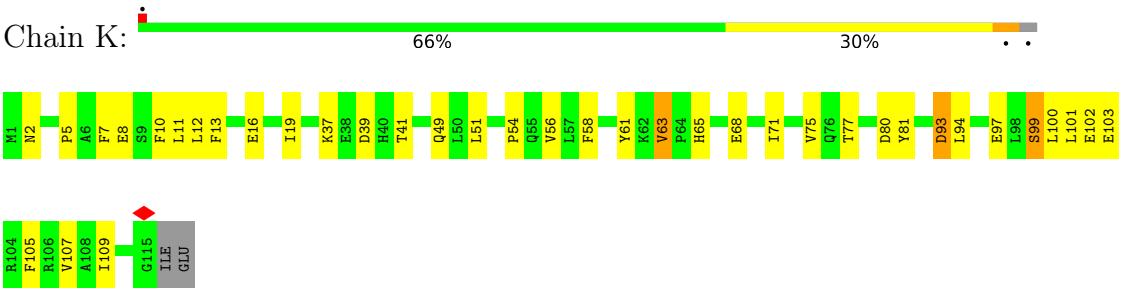


• Molecule 10: Uncharacterized protein



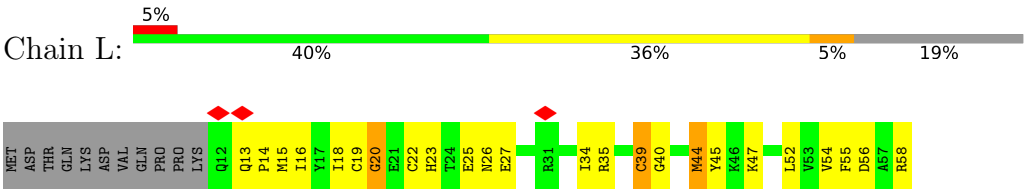
• Molecule 11: Uncharacterized protein

Chain K:



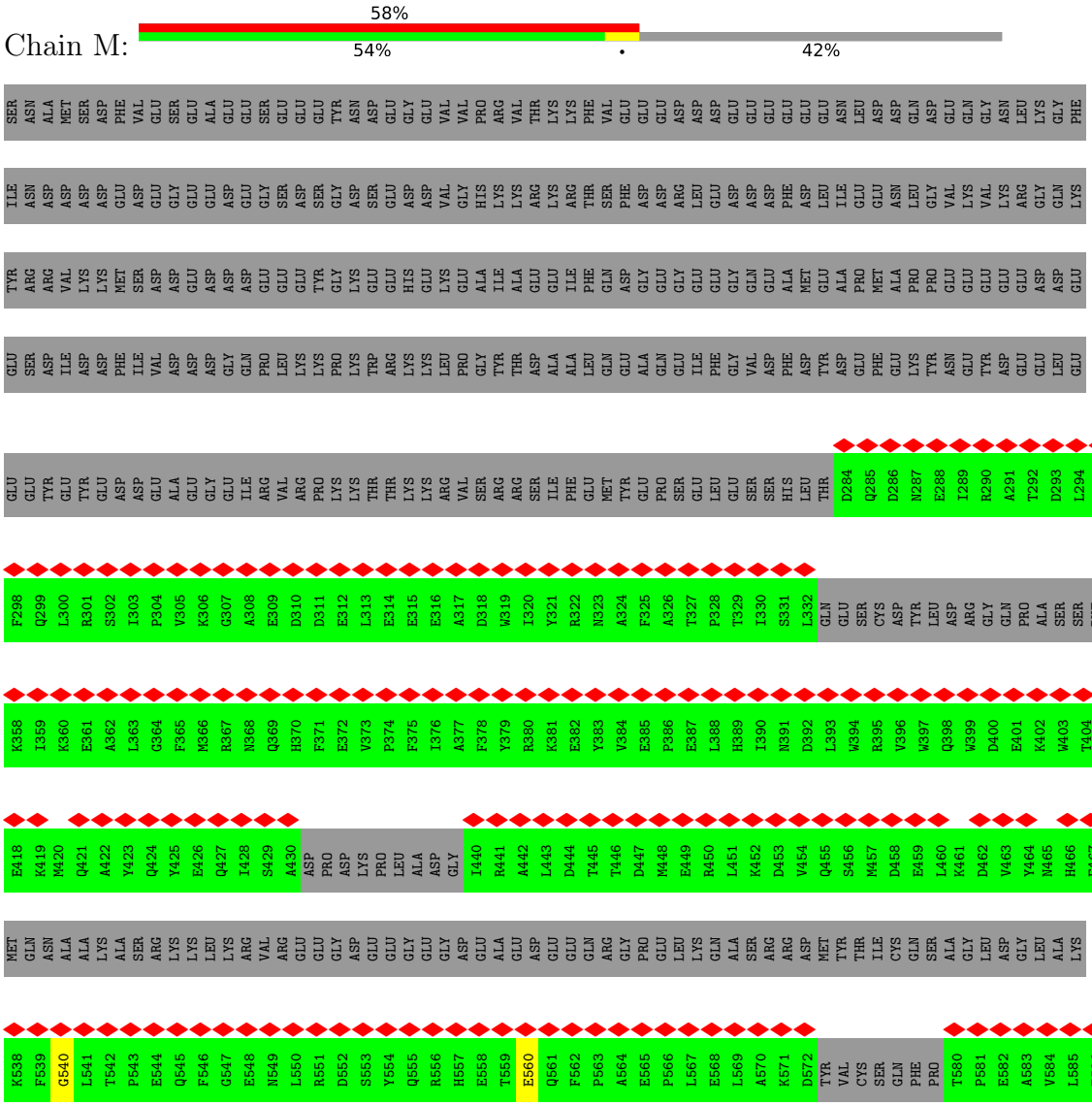
• Molecule 12: Uncharacterized protein

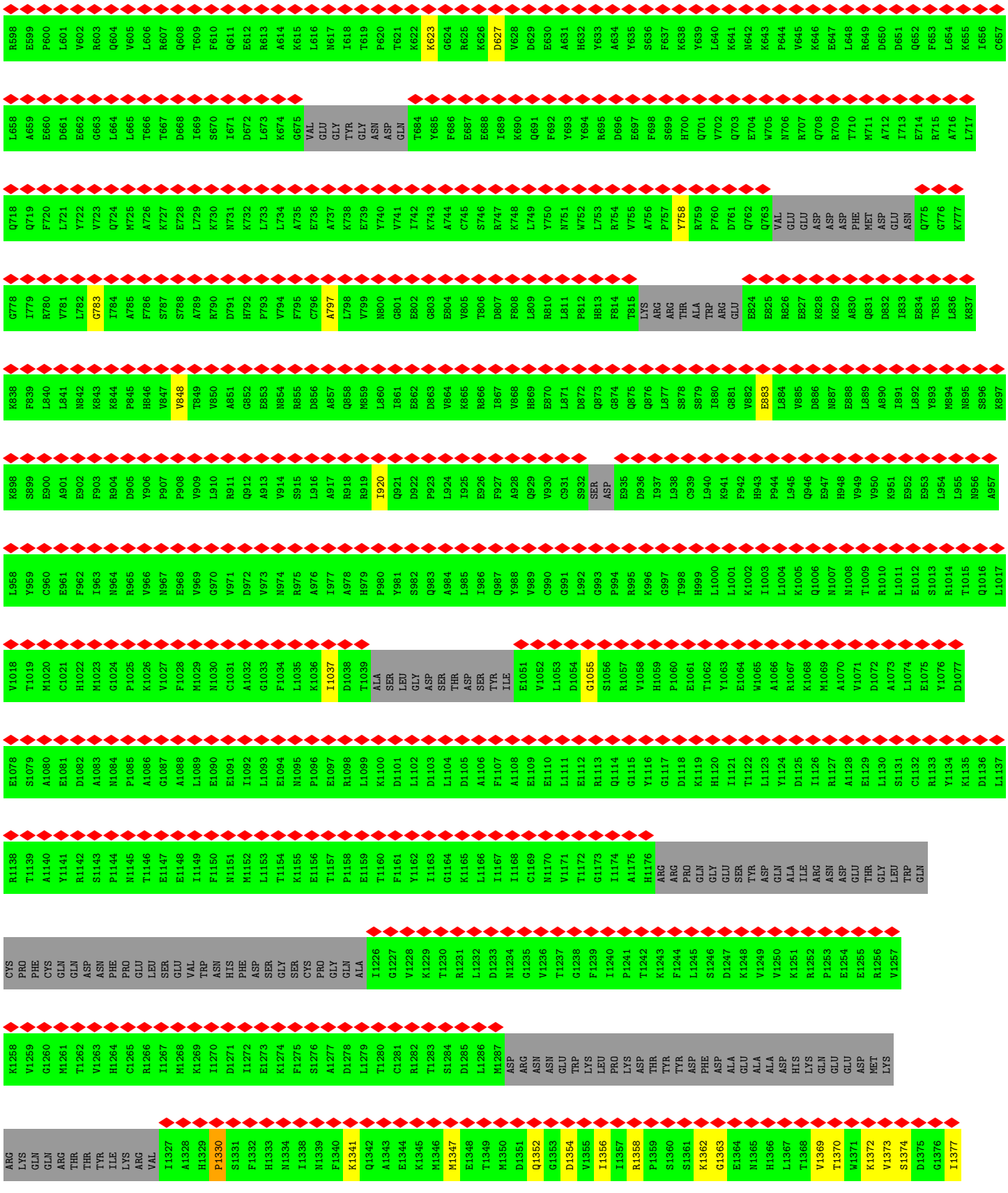
Chain L:



• Molecule 13: Transcription elongation factor SPT6

Chain M:

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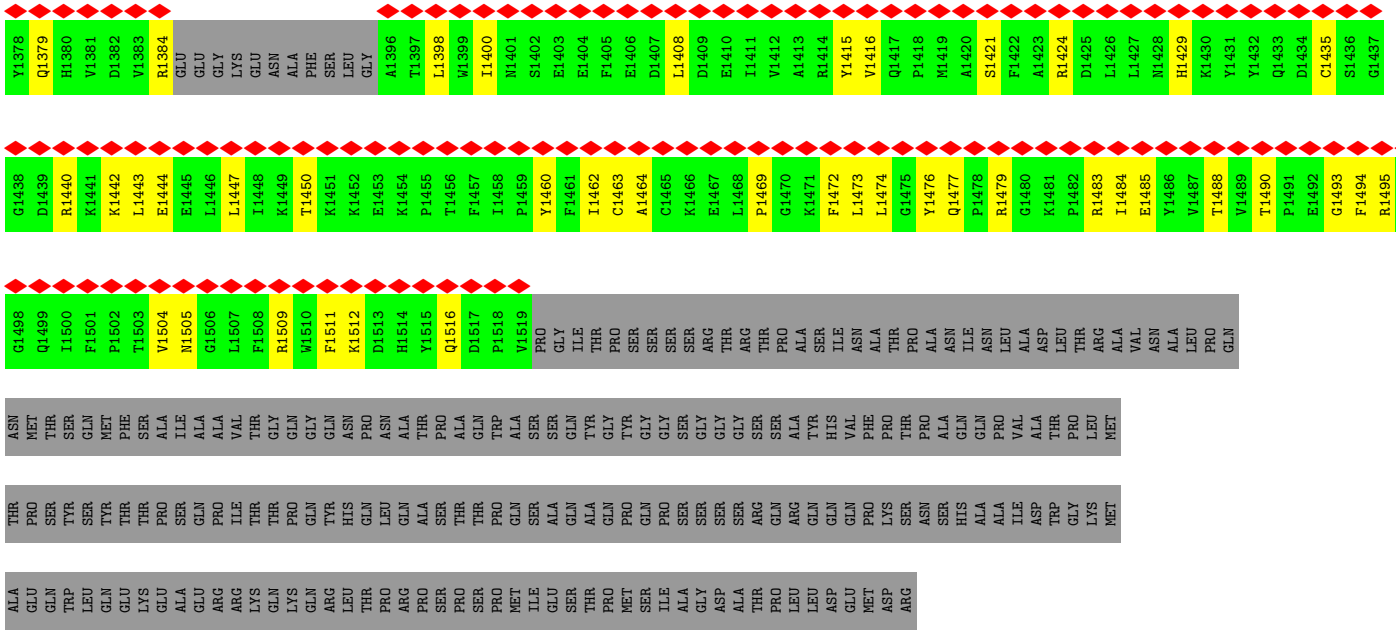
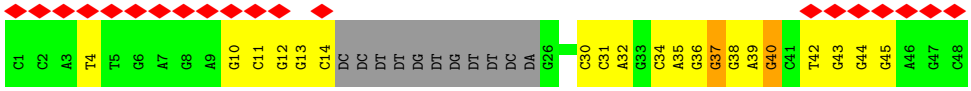
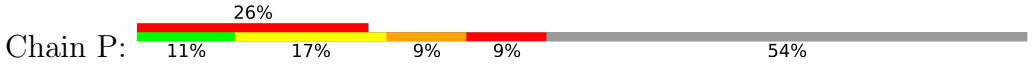
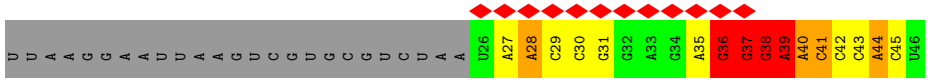


• Molecule 14: DNA (37-MER)

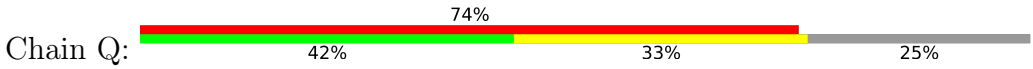


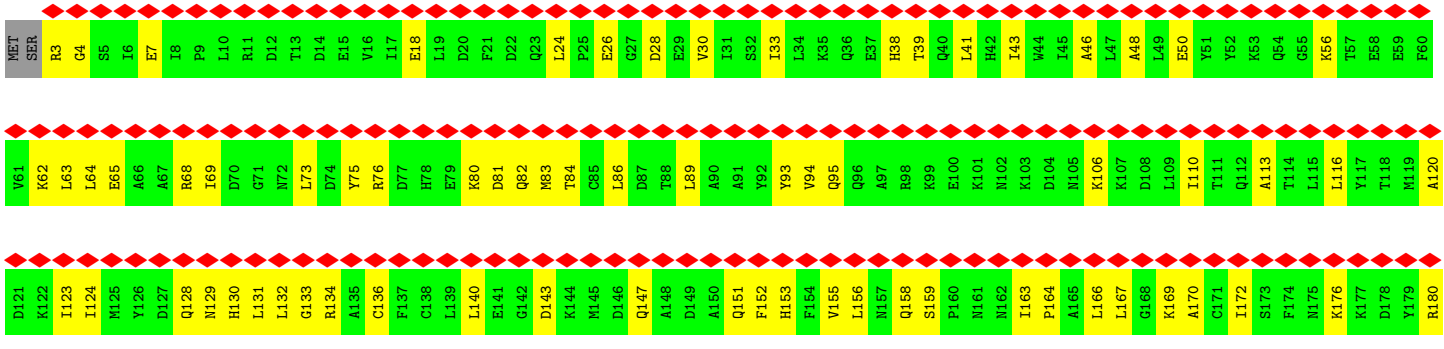
• Molecule 15: RNA (5'-R(P*UP*AP*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')

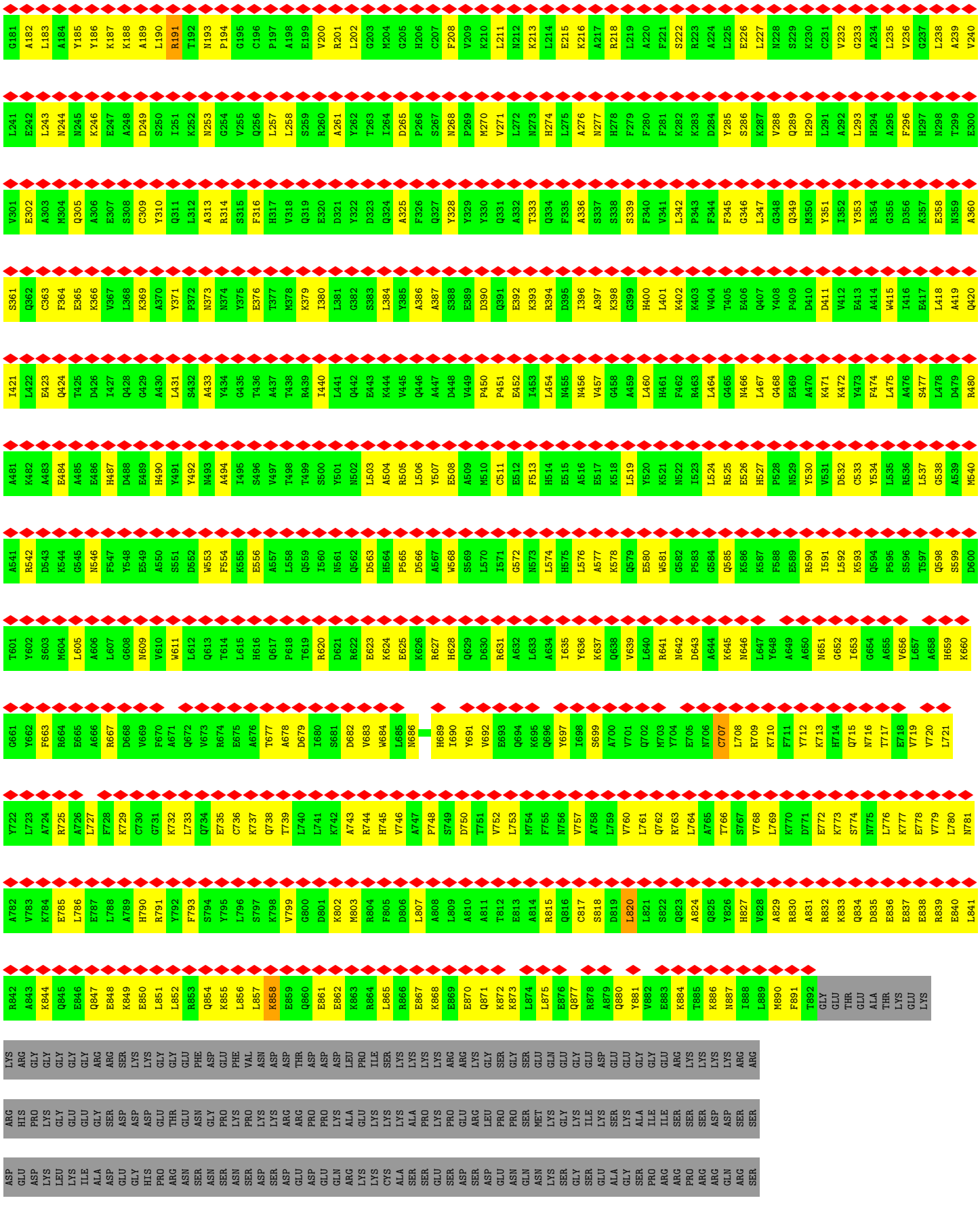




• Molecule 16: RNA polymerase-associated protein CTR9 homolog



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A782 V783 K784 E785 L786 E787 L788 A789 H790 R791 Y792 F793 S794 Y795 L796 S797 K798 V799 G800 D801 K802 M803 R804 F805 D806 L807 A808 L809 A810 A811 T812 E813 A814 R815 Q816 C817 S818 D819 L820 L821 S822 Q823 A824 Q825 Y826 H827 V828 A829 R830 A831 R832 K833 Q834 D835 E836 E837 E838 R839 E840 L841
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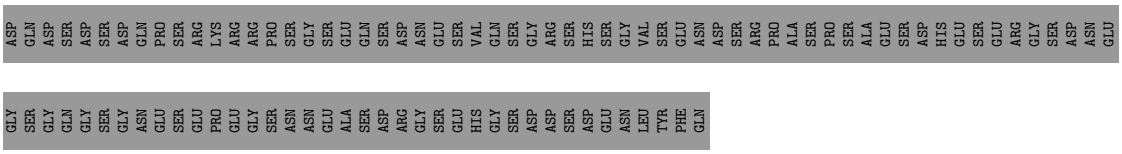
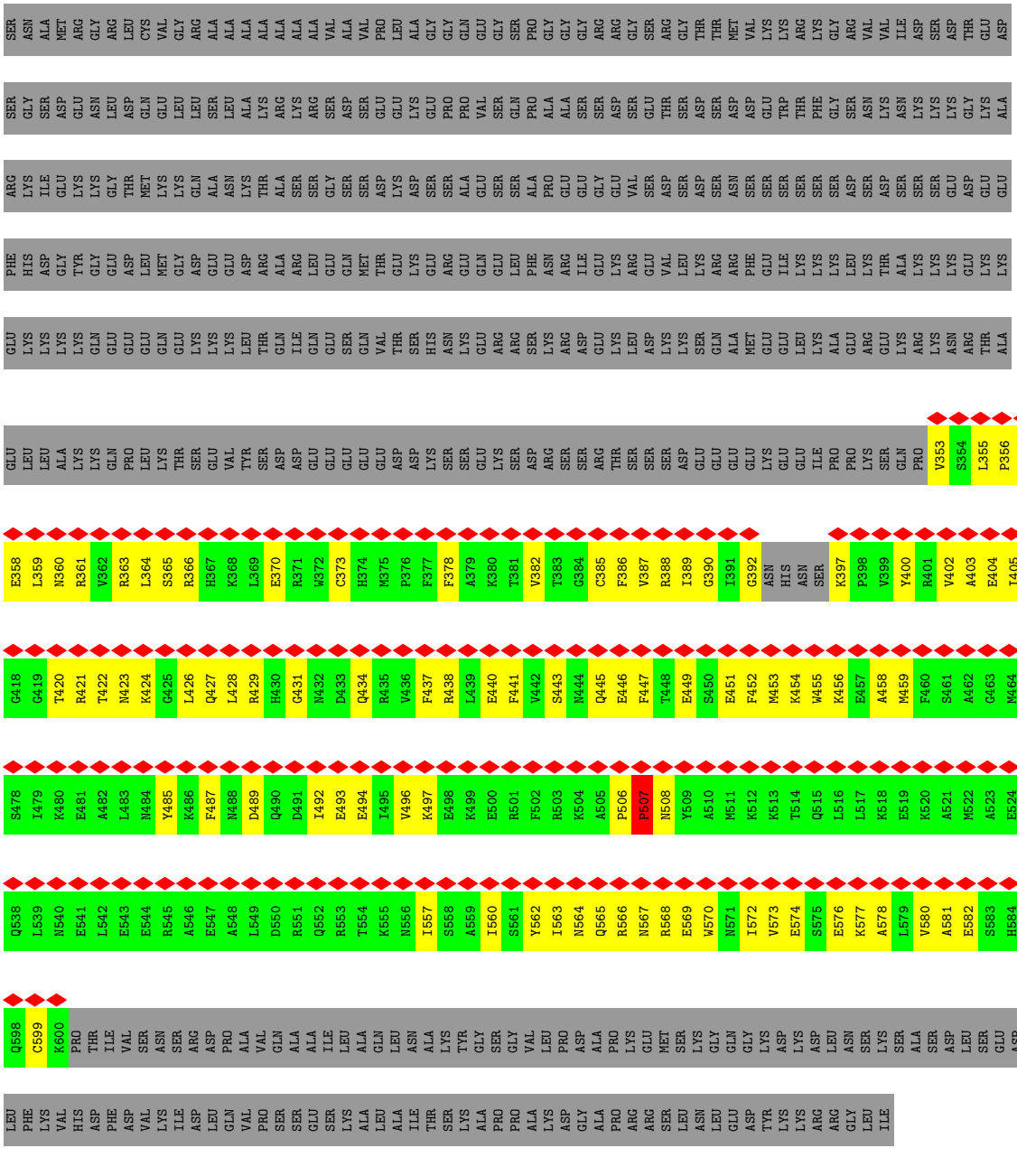
LYS ARG GLY GLY GLY GLY GLY ARG ARG SER LYS LYS GLY GLY GLU PHE ASP GLU PHE VAL ASN ASP ASP THR ASP ASP ASP LEU PRO ILE SER LYS LYS LYS ARG ARG LYS GLY SER GLY SER GLU GLN GLU GLY GLU ASP GLU GLU GLY GLY GLU ARG LYS LYS LYS ARG ARG
ARG HIS PRO LYS GLY GLU GLU GLY SER ASP ASP GLY ASP GLU THR GLU ASN GLY PRO LYS PRO LYS LYS ARG ARG PRO PRO LYS ALA GLU LYS LYS LYS ALA PRO LYS PRO GLU ARG LEU PRO PRO SER MET LYS GLY LYS ILE LYS SER LYS LYS ALA ILE ILE SER SER ASP ASP SER ARG
ASP GLU ASP LYS LEU LYS ILE ALA ASP GLU GLY HIS PRO ARG ASN SER ASN SER ASN SER ASP SER ASP GLU ASN GLN ASN LYS SER GLY SER GLU ALA GLY SER PRO ARG ARG ARG GLN ARG SER
WORLDWIDE PDB PROTEIN DATA BANK



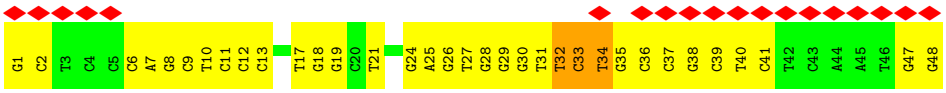
• Molecule 17: RNA polymerase-associated protein RTF1 homolog

Chain R:



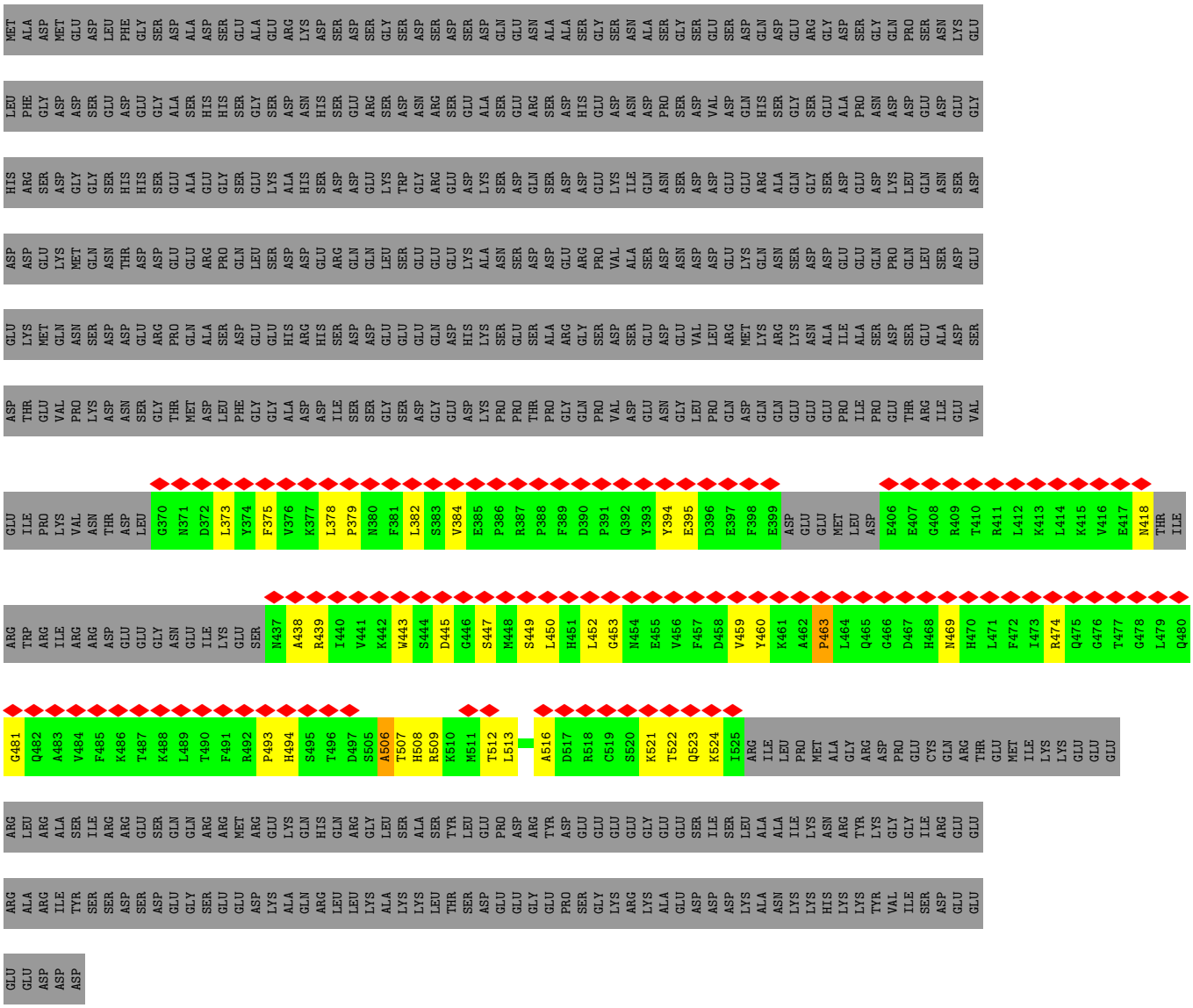
• Molecule 18: Template DNA

Chain T:



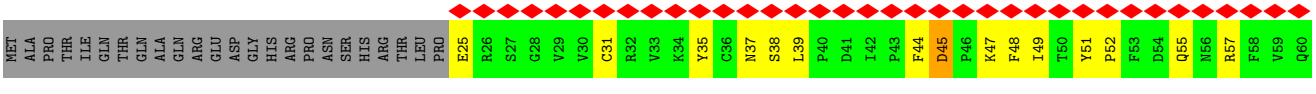
• Molecule 19: RNA polymerase-associated protein LEO1

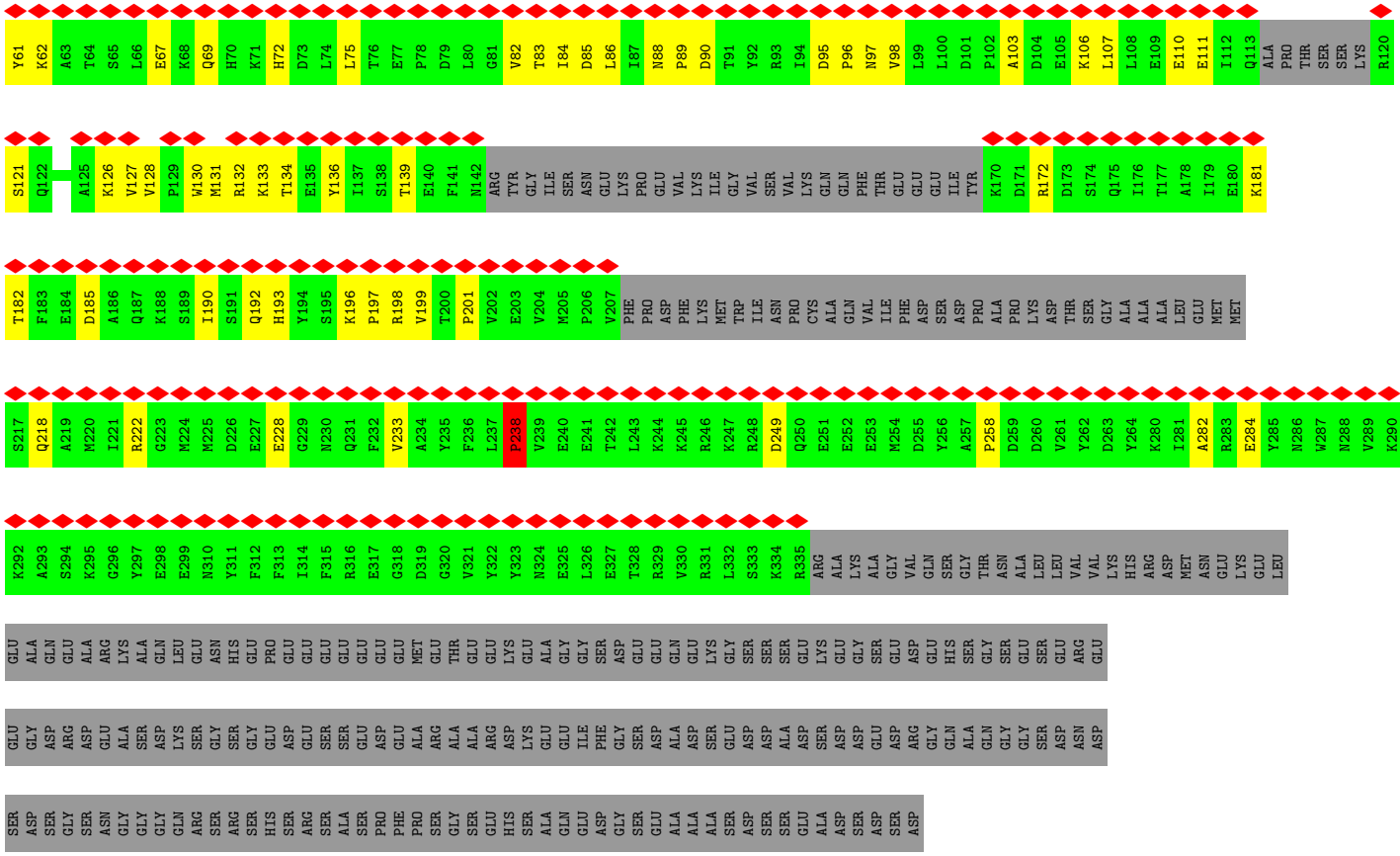
Chain U:



• Molecule 20: RNA polymerase II-associated factor 1 homolog

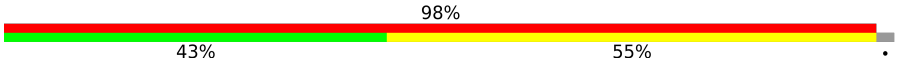
Chain V:





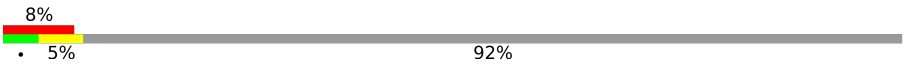
• Molecule 21: WD repeat-containing protein 61

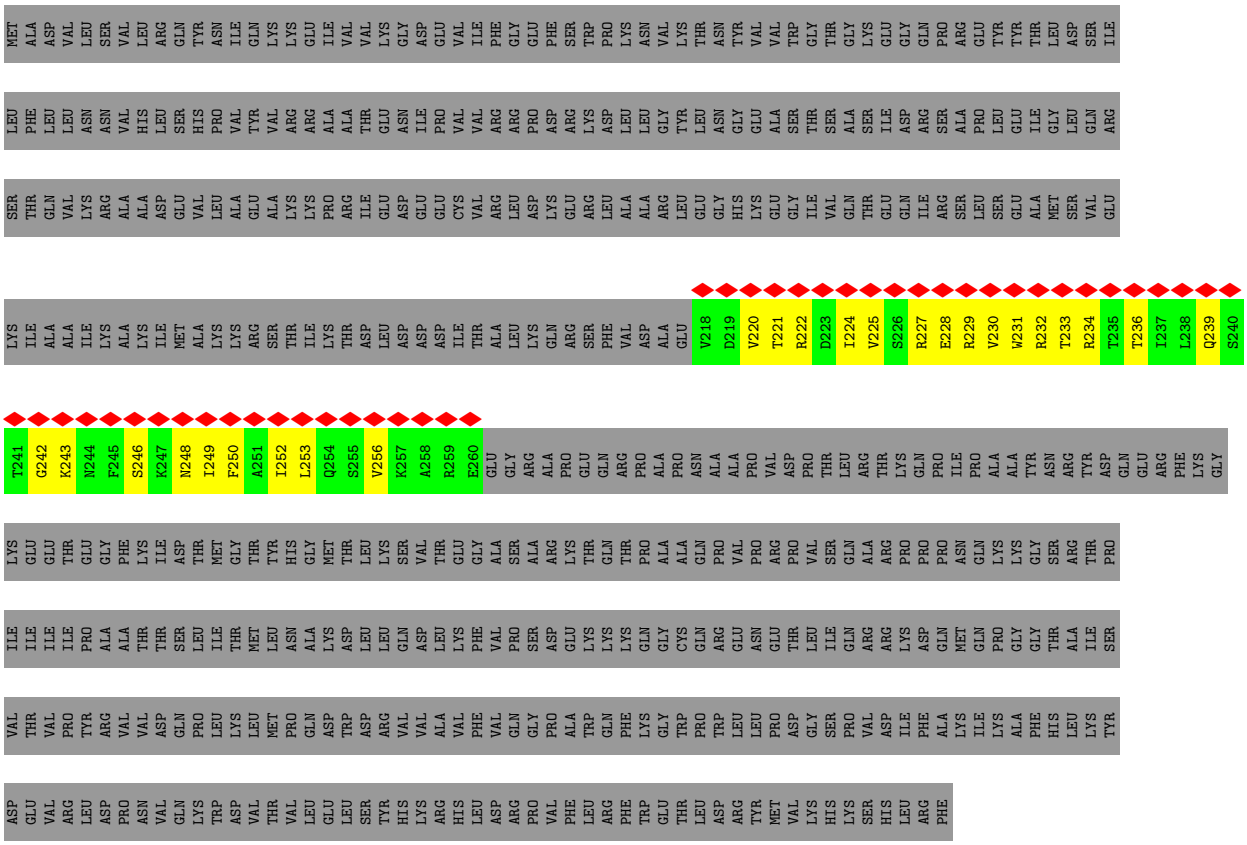
Chain W:



• Molecule 22: Parafibromin

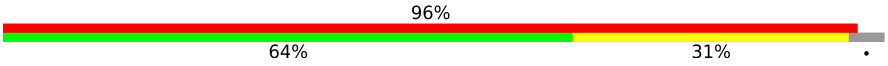
Chain X:





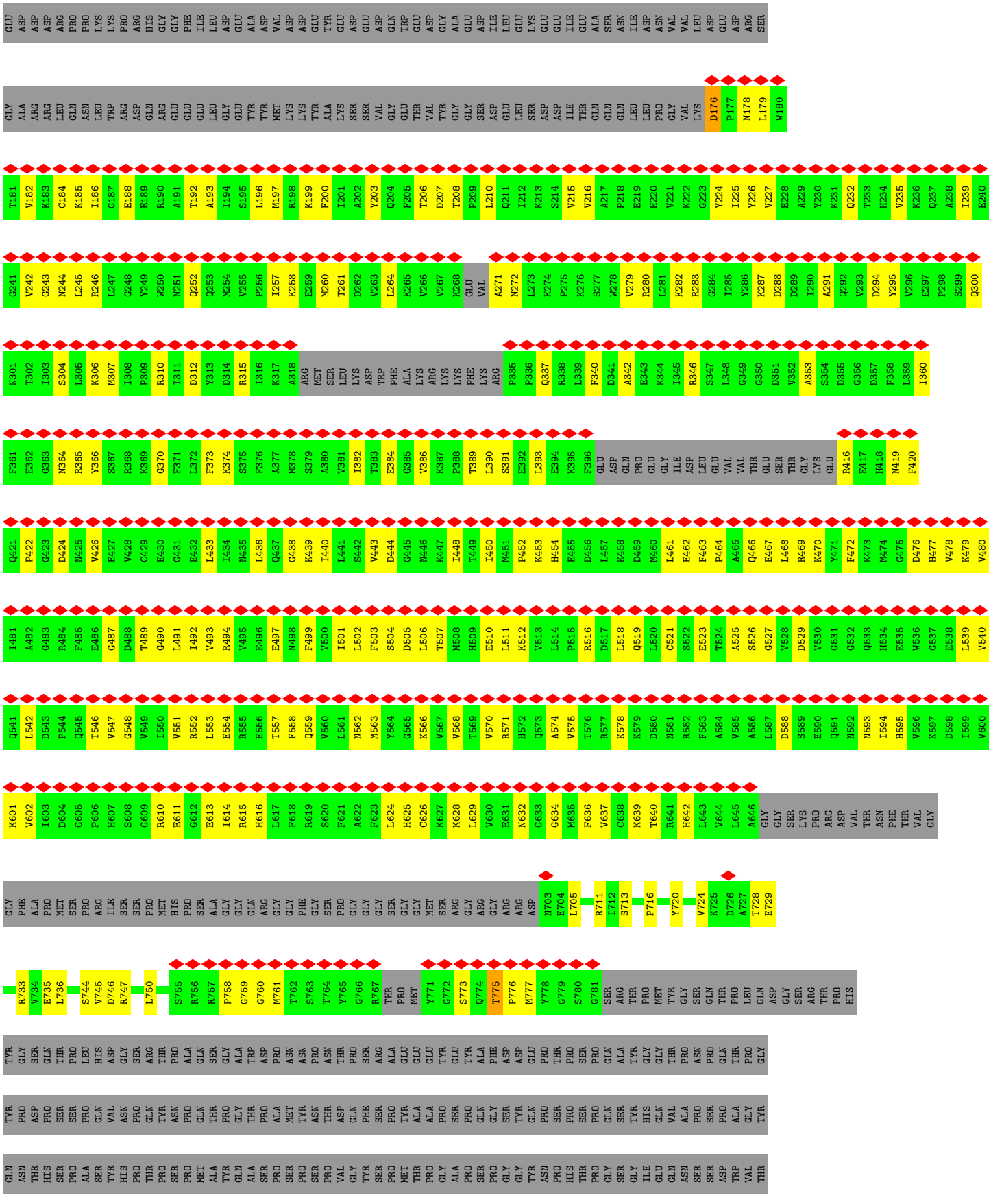
• Molecule 23: Transcription elongation factor SPT4

Chain Y:



• Molecule 24: Transcription elongation factor SPT5

Chain Z: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GLY ALA ARG ARG LEU GLN ASN LEU TRP ARG ASP GLN ARG GLU GLU GLU LEU GLY GLU TYR TYR MET LYS LYS TYR ALA LYS SER SER VAL GLY GLU THR VAL TYR GLY GLY SER ASP GLU LEU SER ASP ASP ILE THR GLN GLN GLN LEU LEU PRO GLY VAL LYS D176 P177 N178 L179 W180
T181 V182 K183 C184 K185 I186 G187 E188 E189 R190 A191 T192 A193 I194 S195 L196 M197 R198 K199 F200 I201 A202 Y203 Q204 F205 T206 D207 T208 P209 L210 Q211 I212 K213 S214 V215 V216 A217 P218 E219 H220 V221 K222 G223 Y224 I225 Y226 V227 E228 A229 Y230 K231 Q232 T233 H234 V235 K236 Q237 A238 I239 E240
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GLY PHE ALA PRO MET SER PRO ARG ILE SER SER PRO MET HIS PRO SER ALA GLY GLY GLN ARG GLY GLY PHE GLY SER PRO GLY GLY GLY SER GLY GLY MET SER ARG GLY ARG GLY ARG ARG ASP N703 E704 L705 R711 I712 S713 P716 Y720 V724 K725 D726 A727 T728 E729
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TYR GLY SER GLN THR PRO LEU HIS ASP GLY SER ARG THR PRO ALA GLN SER GLY ALA TRP ASP PRO ASN ASN PRO ASN THR PRO SER ARG ALA GLU GLU GLU TYR GLU TYR ALA PHE ASP ASP GLU PRO THR PRO SER PRO GLN ALA TYR GLY GLY THR PRO ASN PRO GLN THR PRO GLY
TYR PRO ASP PRO SER SER PRO GLN VAL ASN PRO GLN TYR ASN PRO GLN THR PRO GLY THR PRO ALA MET TYR ASN THR ASP GLN PHE SER PRO TYR ALA ALA PRO SER PRO GLN GLY SER TYR GLN PRO SER PRO SER PRO GLN SER TYR HIS GLN VAL ALA PRO SER PRO ALA GLY TYR
GLN ASN THR HIS SER PRO ALA SER TYR HIS PRO THR PRO SER PRO MET ALA TYR GLN ALA SER PRO SER PRO VAL GLY TYR SER PRO MET THR PRO GLY ALA PRO SER PRO GLY GLY TYR ASN PRO HIS THR PRO GLY SER GLY ILE GLU GLN ASN SER SER ASP TRP VAL THR

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

LYS VAL ILE LEU GLY GLU ASP ARG GLU ALA THR GLY VAL LEU LEU SER ILE ASP GLY GLU ASP GLY ILE VAL ARG MET ASP LEU ASP GLU GLN LEU LYS ILE LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	446195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.40	97/11437 (0.8%)	0.89	18/15433 (0.1%)
2	B	1.63	126/9158 (1.4%)	0.97	28/12360 (0.2%)
3	C	1.77	44/2115 (2.1%)	0.96	7/2873 (0.2%)
4	D	0.42	0/1017	0.51	0/1368
5	E	1.29	10/1751 (0.6%)	0.81	1/2366 (0.0%)
6	F	1.69	9/636 (1.4%)	0.89	0/859
7	G	0.75	0/1364	0.62	0/1853
8	H	1.78	31/1219 (2.5%)	0.92	1/1644 (0.1%)
9	I	1.25	4/964 (0.4%)	0.79	0/1305
10	J	1.82	9/533 (1.7%)	1.03	3/719 (0.4%)
11	K	1.68	8/939 (0.9%)	0.92	2/1271 (0.2%)
12	L	1.57	5/395 (1.3%)	1.00	2/525 (0.4%)
13	M	0.26	0/4763	0.48	1/6084 (0.0%)
14	N	0.98	1/870 (0.1%)	0.87	1/1341 (0.1%)
15	P	1.34	3/506 (0.6%)	1.82	22/787 (2.8%)
16	Q	0.36	0/7365	0.51	0/9927
17	R	0.39	0/1860	0.56	2/2509 (0.1%)
18	T	1.68	11/1087 (1.0%)	1.13	6/1674 (0.4%)
19	U	0.34	0/864	0.58	2/1173 (0.2%)
20	V	0.32	0/1728	0.52	2/2357 (0.1%)
21	W	0.37	0/2392	0.53	0/3257
22	X	0.34	0/356	0.52	0/478
23	Y	0.27	0/927	0.48	0/1250
24	Z	0.45	0/4081	0.55	1/5493 (0.0%)
All	All	1.15	358/58327 (0.6%)	0.79	99/78906 (0.1%)

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
1	A	0	2
2	B	0	3
17	R	0	1
All	All	0	6

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	791	GLU	CA-CB	-15.42	1.20	1.53
2	B	94	SER	C-N	-11.45	1.07	1.34
8	H	116	VAL	CB-CG1	-9.52	1.32	1.52
2	B	690	CYS	CB-SG	-8.84	1.67	1.82
2	B	1047	TYR	CD1-CE1	-8.57	1.26	1.39
2	B	753	TYR	CD2-CE2	-8.37	1.26	1.39
2	B	548	TRP	CB-CG	-8.34	1.35	1.50
1	A	999	ARG	C-N	-8.25	1.15	1.34
8	H	118	TYR	CD1-CE1	-8.14	1.27	1.39
1	A	1050	CYS	CB-SG	-8.09	1.68	1.82
1	A	886	VAL	CB-CG1	-8.08	1.35	1.52
8	H	118	TYR	CD2-CE2	-8.05	1.27	1.39
2	B	29	VAL	CB-CG2	-8.01	1.36	1.52
1	A	827	TYR	CD1-CE1	-7.83	1.27	1.39
3	C	19	VAL	CB-CG2	-7.76	1.36	1.52
2	B	664	TYR	CD1-CE1	-7.73	1.27	1.39
1	A	1374	VAL	CB-CG2	-7.68	1.36	1.52
1	A	492	TYR	CE2-CZ	-7.61	1.28	1.38
10	J	10	CYS	CB-SG	-7.54	1.69	1.82
1	A	492	TYR	CD2-CE2	-7.50	1.28	1.39
18	T	25	DA	C3'-O3'	-7.48	1.34	1.44
2	B	664	TYR	CD2-CE2	-7.39	1.28	1.39
10	J	62	TYR	CD1-CE1	-7.36	1.28	1.39
1	A	514	GLU	CB-CG	-7.34	1.38	1.52
8	H	118	TYR	CE1-CZ	-7.25	1.29	1.38
2	B	1047	TYR	CD2-CE2	-7.21	1.28	1.39
1	A	1396	ARG	CB-CG	-7.17	1.33	1.52
8	H	48	TYR	CD1-CE1	-7.14	1.28	1.39
9	I	72	VAL	CB-CG1	-7.11	1.38	1.52
2	B	108	MET	C-N	-7.10	1.17	1.34
2	B	1047	TYR	CE1-CZ	-7.09	1.29	1.38
1	A	380	VAL	CB-CG2	-7.06	1.38	1.52
2	B	809	VAL	CB-CG1	-7.01	1.38	1.52
2	B	615	TYR	CD1-CE1	-7.01	1.28	1.39
1	A	1379	GLU	CB-CG	-6.96	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	VAL	CB-CG1	-6.96	1.38	1.52
2	B	184	TYR	CD2-CE2	-6.95	1.28	1.39
18	T	28	DG	C3'-O3'	-6.95	1.34	1.44
2	B	753	TYR	CE2-CZ	-6.90	1.29	1.38
2	B	755	GLN	C-N	-6.90	1.18	1.34
3	C	176	TRP	CE3-CZ3	-6.89	1.26	1.38
1	A	560	VAL	CB-CG2	-6.86	1.38	1.52
10	J	45	CYS	CB-SG	-6.86	1.70	1.82
1	A	492	TYR	CD1-CE1	-6.85	1.29	1.39
2	B	662	VAL	CB-CG2	-6.85	1.38	1.52
2	B	693	TYR	CE1-CZ	-6.83	1.29	1.38
2	B	1029	TYR	CD2-CE2	-6.83	1.29	1.39
5	E	191	VAL	CB-CG1	-6.83	1.38	1.52
2	B	615	TYR	CD2-CE2	-6.79	1.29	1.39
3	C	184	PHE	CD1-CE1	-6.79	1.25	1.39
2	B	1029	TYR	CE1-CZ	-6.79	1.29	1.38
2	B	120	TYR	CD2-CE2	-6.77	1.29	1.39
2	B	753	TYR	CE1-CZ	-6.76	1.29	1.38
2	B	1047	TYR	CE2-CZ	-6.75	1.29	1.38
2	B	509	VAL	CB-CG1	-6.74	1.38	1.52
3	C	186	TYR	CD1-CE1	-6.73	1.29	1.39
2	B	753	TYR	CD1-CE1	-6.72	1.29	1.39
2	B	177	CYS	CB-SG	-6.70	1.70	1.82
2	B	504	THR	CB-CG2	-6.69	1.30	1.52
2	B	1105	GLU	CB-CG	-6.66	1.39	1.52
6	F	60	TYR	CD1-CE1	-6.63	1.29	1.39
2	B	1029	TYR	CD1-CE1	-6.61	1.29	1.39
6	F	109	TYR	CD1-CE1	-6.61	1.29	1.39
8	H	115	TYR	CD1-CE1	-6.61	1.29	1.39
3	C	184	PHE	CD2-CE2	-6.60	1.26	1.39
1	A	815	TYR	CD2-CE2	-6.60	1.29	1.39
1	A	815	TYR	CD1-CE1	-6.59	1.29	1.39
8	H	97	TYR	CE1-CZ	-6.58	1.29	1.38
18	T	33	DC	N1-C2	-6.58	1.33	1.40
2	B	801	VAL	CB-CG1	-6.57	1.39	1.52
12	L	55	PHE	CB-CG	-6.56	1.40	1.51
2	B	750	VAL	CB-CG2	-6.55	1.39	1.52
2	B	806	PHE	CD1-CE1	-6.54	1.26	1.39
3	C	229	PHE	CD1-CE1	-6.51	1.26	1.39
18	T	27	DT	C3'-O3'	-6.51	1.35	1.44
2	B	811	TYR	CE1-CZ	-6.48	1.30	1.38
3	C	172	GLU	CB-CG	-6.48	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	CYS	CB-SG	-6.47	1.71	1.82
8	H	115	TYR	CE1-CZ	-6.46	1.30	1.38
3	C	186	TYR	CD2-CE2	-6.46	1.29	1.39
2	B	193	VAL	CB-CG2	-6.45	1.39	1.52
2	B	693	TYR	CD1-CE1	-6.45	1.29	1.39
8	H	90	TYR	CD1-CE1	-6.44	1.29	1.39
1	A	787	VAL	CB-CG2	-6.43	1.39	1.52
3	C	169	PHE	CD1-CE1	-6.43	1.26	1.39
2	B	622	CYS	CB-SG	-6.37	1.71	1.82
1	A	871	VAL	CB-CG1	-6.37	1.39	1.52
3	C	169	PHE	CD2-CE2	-6.35	1.26	1.39
1	A	835	GLU	CB-CG	-6.34	1.40	1.52
1	A	827	TYR	CD2-CE2	-6.34	1.29	1.39
1	A	1140	THR	CA-CB	-6.33	1.36	1.53
1	A	521	VAL	CB-CG2	-6.33	1.39	1.52
2	B	922	ARG	CB-CG	-6.30	1.35	1.52
10	J	5	VAL	CB-CG2	-6.29	1.39	1.52
5	E	191	VAL	CB-CG2	-6.28	1.39	1.52
2	B	919	CYS	CB-SG	-6.28	1.71	1.82
3	C	231	TYR	CD1-CE1	-6.27	1.29	1.39
10	J	62	TYR	CE1-CZ	-6.26	1.30	1.38
6	F	109	TYR	CD2-CE2	-6.26	1.29	1.39
1	A	891	TYR	CD1-CE1	-6.23	1.30	1.39
1	A	630	VAL	CB-CG1	-6.22	1.39	1.52
1	A	590	GLN	CG-CD	-6.22	1.36	1.51
2	B	33	TYR	CE1-CZ	-6.21	1.30	1.38
11	K	56	VAL	CB-CG1	-6.21	1.39	1.52
18	T	33	DC	N1-C6	-6.21	1.33	1.37
2	B	805	PHE	CD2-CE2	-6.21	1.26	1.39
2	B	752	TYR	CE2-CZ	-6.21	1.30	1.38
6	F	60	TYR	CE1-CZ	-6.20	1.30	1.38
2	B	984	CYS	CB-SG	-6.20	1.71	1.82
2	B	809	VAL	CB-CG2	-6.19	1.39	1.52
8	H	90	TYR	CD2-CE2	-6.18	1.30	1.39
2	B	949	TYR	CD1-CE1	-6.18	1.30	1.39
12	L	45	TYR	CE1-CZ	-6.17	1.30	1.38
2	B	1029	TYR	CE2-CZ	-6.17	1.30	1.38
18	T	26	DG	C3'-O3'	-6.17	1.35	1.44
1	A	669	TYR	CD1-CE1	-6.14	1.30	1.39
8	H	115	TYR	CE2-CZ	-6.11	1.30	1.38
8	H	98	ARG	CB-CG	-6.10	1.36	1.52
2	B	236	TRP	CB-CG	-6.10	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	33	DC	C1'-N1	-6.09	1.38	1.47
1	A	474	VAL	CB-CG1	-6.08	1.40	1.52
12	L	45	TYR	CD1-CE1	-6.07	1.30	1.39
2	B	193	VAL	CB-CG1	-6.06	1.40	1.52
2	B	198	GLU	CB-CG	-6.06	1.40	1.52
2	B	924	ARG	CB-CG	-6.06	1.36	1.52
2	B	923	VAL	CB-CG1	-6.05	1.40	1.52
11	K	75	VAL	CB-CG2	-6.05	1.40	1.52
1	A	590	GLN	CB-CG	-6.04	1.36	1.52
3	C	104	ASP	CA-CB	-6.02	1.40	1.53
1	A	873	VAL	CB-CG2	-6.01	1.40	1.52
2	B	707	CYS	CB-SG	-6.01	1.72	1.82
8	H	141	VAL	CB-CG2	-6.00	1.40	1.52
2	B	367	TYR	CD1-CE1	-6.00	1.30	1.39
3	C	186	TYR	CE2-CZ	-5.97	1.30	1.38
1	A	827	TYR	CE1-CZ	-5.97	1.30	1.38
2	B	184	TYR	CE2-CZ	-5.96	1.30	1.38
8	H	115	TYR	CD2-CE2	-5.94	1.30	1.39
18	T	24	DG	C3'-O3'	-5.94	1.36	1.44
18	T	33	DC	N3-C4	-5.93	1.29	1.33
3	C	151	VAL	CB-CG1	-5.90	1.40	1.52
1	A	366	VAL	CB-CG1	-5.89	1.40	1.52
2	B	92	TYR	CD2-CE2	-5.89	1.30	1.39
10	J	6	ARG	CB-CG	-5.89	1.36	1.52
3	C	197	TYR	CE1-CZ	-5.88	1.30	1.38
1	A	458	PHE	CD1-CE1	-5.87	1.27	1.39
3	C	186	TYR	CE1-CZ	-5.87	1.30	1.38
2	B	184	TYR	CD1-CE1	-5.86	1.30	1.39
3	C	197	TYR	CE2-CZ	-5.86	1.30	1.38
2	B	806	PHE	CD2-CE2	-5.85	1.27	1.39
3	C	231	TYR	CD2-CE2	-5.85	1.30	1.39
1	A	377	GLN	CB-CG	-5.84	1.36	1.52
1	A	657	TYR	CD1-CE1	-5.83	1.30	1.39
8	H	96	VAL	CB-CG1	-5.82	1.40	1.52
1	A	669	TYR	CE1-CZ	-5.80	1.31	1.38
8	H	90	TYR	CE2-CZ	-5.80	1.31	1.38
15	P	44	A	N9-C4	-5.80	1.34	1.37
2	B	697	GLU	CG-CD	-5.80	1.43	1.51
2	B	1020	TYR	CD1-CE1	-5.80	1.30	1.39
1	A	669	TYR	CD2-CE2	-5.79	1.30	1.39
1	A	771	VAL	CB-CG2	-5.77	1.40	1.52
2	B	794	VAL	CB-CG2	-5.76	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	907	VAL	CB-CG1	-5.76	1.40	1.52
2	B	184	TYR	CE1-CZ	-5.75	1.31	1.38
2	B	788	TYR	CE2-CZ	-5.74	1.31	1.38
2	B	1093	CYS	CB-SG	-5.74	1.72	1.81
2	B	811	TYR	CD1-CE1	-5.74	1.30	1.39
2	B	1047	TYR	CG-CD1	-5.74	1.31	1.39
12	L	45	TYR	CD2-CE2	-5.72	1.30	1.39
1	A	482	PHE	CD2-CE2	-5.72	1.27	1.39
1	A	784	VAL	CB-CG1	-5.72	1.40	1.52
2	B	1149	VAL	CB-CG2	-5.71	1.40	1.52
2	B	788	TYR	CD1-CE1	-5.71	1.30	1.39
3	C	197	TYR	CD1-CE1	-5.70	1.30	1.39
1	A	556	GLU	CB-CG	-5.69	1.41	1.52
1	A	447	GLU	CB-CG	-5.68	1.41	1.52
8	H	48	TYR	CE1-CZ	-5.68	1.31	1.38
5	E	209	VAL	CB-CG2	-5.67	1.41	1.52
2	B	120	TYR	CD1-CE1	-5.67	1.30	1.39
15	P	40	A	N9-C4	-5.66	1.34	1.37
1	A	556	GLU	CG-CD	-5.66	1.43	1.51
2	B	697	GLU	CB-CG	-5.66	1.41	1.52
1	A	406	VAL	CB-CG1	-5.65	1.41	1.52
1	A	1375	ARG	CG-CD	-5.65	1.37	1.51
11	K	97	GLU	CB-CG	-5.64	1.41	1.52
1	A	901	VAL	CB-CG2	-5.64	1.41	1.52
3	C	169	PHE	CB-CG	-5.63	1.41	1.51
2	B	510	CYS	CB-SG	-5.63	1.72	1.81
2	B	191	GLU	CG-CD	-5.63	1.43	1.51
2	B	785	TYR	CD2-CE2	-5.63	1.30	1.39
5	E	203	TYR	CD2-CE2	-5.63	1.30	1.39
1	A	810	PHE	CD2-CE2	-5.62	1.28	1.39
2	B	788	TYR	CD2-CE2	-5.62	1.30	1.39
2	B	568	PHE	CD1-CE1	-5.61	1.28	1.39
2	B	814	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	815	TYR	CE2-CZ	-5.60	1.31	1.38
11	K	63	VAL	CB-CG1	-5.60	1.41	1.52
2	B	1027	VAL	CB-CG2	-5.60	1.41	1.52
3	C	19	VAL	CB-CG1	-5.59	1.41	1.52
2	B	949	TYR	CD2-CE2	-5.59	1.30	1.39
3	C	185	GLU	CB-CG	-5.59	1.41	1.52
2	B	176	GLU	CB-CG	-5.59	1.41	1.52
11	K	61	TYR	CD1-CE1	-5.57	1.30	1.39
2	B	814	TYR	CE1-CZ	-5.57	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	115	TYR	CG-CD2	-5.57	1.31	1.39
5	E	26	TYR	CD2-CE2	-5.56	1.31	1.39
8	H	50	VAL	CB-CG2	-5.56	1.41	1.52
2	B	671	GLU	CB-CG	-5.56	1.41	1.52
3	C	229	PHE	CD2-CE2	-5.56	1.28	1.39
2	B	367	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	500	GLU	CB-CG	-5.54	1.41	1.52
3	C	230	TYR	CD1-CE1	-5.54	1.31	1.39
3	C	45	ILE	CB-CG2	-5.54	1.35	1.52
2	B	1153	TYR	CE2-CZ	-5.53	1.31	1.38
6	F	102	ILE	C-N	-5.53	1.23	1.34
1	A	479	TRP	CB-CG	-5.53	1.40	1.50
1	A	554	PHE	CD1-CE1	-5.52	1.28	1.39
1	A	810	PHE	CD1-CE1	-5.52	1.28	1.39
1	A	446	VAL	CB-CG2	-5.50	1.41	1.52
9	I	111	TYR	CD1-CE1	-5.50	1.31	1.39
1	A	1471	PHE	CD1-CE1	-5.50	1.28	1.39
3	C	37	VAL	CB-CG1	-5.49	1.41	1.52
1	A	378	VAL	CB-CG1	-5.48	1.41	1.52
2	B	466	VAL	CB-CG2	-5.48	1.41	1.52
2	B	791	GLU	CB-CG	-5.48	1.41	1.52
1	A	618	TYR	CD2-CE2	-5.48	1.31	1.39
15	P	45	C	N1-C6	-5.48	1.33	1.37
3	C	224	GLY	C-N	-5.47	1.21	1.34
3	C	231	TYR	CE1-CZ	-5.46	1.31	1.38
2	B	1018	TYR	CD1-CE1	-5.46	1.31	1.39
2	B	1048	TYR	CB-CG	-5.46	1.43	1.51
1	A	891	TYR	CD2-CE2	-5.46	1.31	1.39
8	H	93	TYR	CD1-CE1	-5.45	1.31	1.39
2	B	752	TYR	CD2-CE2	-5.45	1.31	1.39
1	A	970	PHE	CB-CG	-5.44	1.42	1.51
1	A	548	PHE	CD2-CE2	-5.44	1.28	1.39
6	F	60	TYR	CD2-CE2	-5.44	1.31	1.39
1	A	1085	GLU	CB-CG	-5.43	1.41	1.52
2	B	1088	GLU	CB-CG	-5.43	1.41	1.52
6	F	60	TYR	CE2-CZ	-5.43	1.31	1.38
1	A	64	VAL	CB-CG1	-5.42	1.41	1.52
3	C	231	TYR	CE2-CZ	-5.40	1.31	1.38
11	K	61	TYR	CD2-CE2	-5.40	1.31	1.39
1	A	657	TYR	CD2-CE2	-5.40	1.31	1.39
1	A	891	TYR	CE1-CZ	-5.39	1.31	1.38
1	A	1087	VAL	CB-CG1	-5.39	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	661	VAL	CB-CG1	-5.38	1.41	1.52
11	K	102	GLU	CB-CG	-5.38	1.42	1.52
1	A	566	PHE	CD2-CE2	-5.38	1.28	1.39
8	H	118	TYR	CE2-CZ	-5.38	1.31	1.38
1	A	978	VAL	CB-CG1	-5.37	1.41	1.52
1	A	553	VAL	CB-CG2	-5.36	1.41	1.52
3	C	158	GLU	CB-CG	-5.36	1.42	1.52
8	H	25	VAL	CB-CG1	-5.35	1.41	1.52
2	B	766	TYR	CD2-CE2	-5.35	1.31	1.39
1	A	514	GLU	CG-CD	-5.35	1.44	1.51
8	H	90	TYR	CE1-CZ	-5.34	1.31	1.38
8	H	137	VAL	CB-CG2	-5.34	1.41	1.52
5	E	206	TYR	CD1-CE1	-5.33	1.31	1.39
1	A	886	VAL	CB-CG2	-5.33	1.41	1.52
2	B	615	TYR	CE1-CZ	-5.33	1.31	1.38
1	A	634	GLU	CB-CG	-5.33	1.42	1.52
1	A	382	ARG	CB-CG	-5.31	1.38	1.52
2	B	766	TYR	CD1-CE1	-5.31	1.31	1.39
2	B	664	TYR	CB-CG	-5.30	1.43	1.51
2	B	860	VAL	CB-CG2	-5.30	1.41	1.52
3	C	101	PHE	CD1-CE1	-5.30	1.28	1.39
2	B	568	PHE	CD2-CE2	-5.30	1.28	1.39
1	A	21	VAL	CB-CG2	-5.29	1.41	1.52
10	J	62	TYR	CD2-CE2	-5.29	1.31	1.39
11	K	68	GLU	CB-CG	-5.29	1.42	1.52
2	B	752	TYR	CB-CG	-5.28	1.43	1.51
1	A	26	LEU	C-N	-5.28	1.22	1.34
1	A	787	VAL	CB-CG1	-5.27	1.41	1.52
3	C	197	TYR	CG-CD1	-5.27	1.32	1.39
9	I	111	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	679	TRP	CE3-CZ3	-5.26	1.29	1.38
6	F	56	TYR	CD1-CE1	-5.25	1.31	1.39
5	E	194	ILE	C-N	-5.25	1.22	1.34
2	B	176	GLU	CG-CD	-5.25	1.44	1.51
3	C	197	TYR	CD2-CE2	-5.25	1.31	1.39
1	A	458	PHE	CD2-CE2	-5.25	1.28	1.39
2	B	1006	VAL	CB-CG2	-5.25	1.41	1.52
3	C	184	PHE	CB-CG	-5.25	1.42	1.51
2	B	1153	TYR	CD2-CE2	-5.23	1.31	1.39
3	C	9	VAL	CB-CG2	-5.23	1.41	1.52
2	B	736	TYR	CD2-CE2	-5.23	1.31	1.39
1	A	970	PHE	CD1-CE1	-5.23	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	VAL	CB-CG2	-5.22	1.41	1.52
3	C	176	TRP	CB-CG	-5.22	1.40	1.50
14	N	37	DG	N9-C4	-5.22	1.33	1.38
2	B	743	ARG	CG-CD	-5.22	1.39	1.51
9	I	112	TYR	CD1-CE1	-5.21	1.31	1.39
12	L	54	VAL	CB-CG2	-5.21	1.42	1.52
1	A	713	VAL	CB-CG2	-5.21	1.42	1.52
3	C	234	GLU	CB-CG	-5.21	1.42	1.52
2	B	735	VAL	CB-CG2	-5.21	1.42	1.52
18	T	27	DT	N1-C6	-5.21	1.34	1.38
1	A	770	VAL	CB-CG1	-5.21	1.42	1.52
8	H	115	TYR	CG-CD1	-5.20	1.32	1.39
5	E	206	TYR	CD2-CE2	-5.20	1.31	1.39
5	E	11	TRP	CB-CG	-5.20	1.40	1.50
6	F	65	VAL	CB-CG1	-5.19	1.42	1.52
3	C	50	VAL	CB-CG2	-5.18	1.42	1.52
2	B	1048	TYR	CD1-CE1	-5.18	1.31	1.39
1	A	827	TYR	CG-CD1	-5.17	1.32	1.39
2	B	523	VAL	CB-CG1	-5.17	1.42	1.52
8	H	97	TYR	CD1-CE1	-5.17	1.31	1.39
18	T	32	DT	N1-C2	-5.16	1.33	1.38
2	B	923	VAL	CB-CG2	-5.16	1.42	1.52
2	B	369	VAL	CB-CG2	-5.16	1.42	1.52
1	A	669	TYR	CG-CD2	-5.15	1.32	1.39
2	B	753	TYR	CG-CD2	-5.15	1.32	1.39
1	A	492	TYR	CG-CD2	-5.14	1.32	1.39
2	B	33	TYR	CD1-CE1	-5.14	1.31	1.39
2	B	750	VAL	CB-CG1	-5.14	1.42	1.52
1	A	978	VAL	CB-CG2	-5.13	1.42	1.52
5	E	203	TYR	CD1-CE1	-5.13	1.31	1.39
3	C	101	PHE	CD2-CE2	-5.12	1.29	1.39
3	C	230	TYR	CD2-CE2	-5.12	1.31	1.39
8	H	48	TYR	CD2-CE2	-5.12	1.31	1.39
2	B	918	PHE	CD2-CE2	-5.12	1.29	1.39
3	C	203	TRP	CB-CG	-5.11	1.41	1.50
3	C	21	PHE	CD2-CE2	-5.11	1.29	1.39
10	J	18	TRP	CB-CG	-5.11	1.41	1.50
1	A	1402	CYS	CB-SG	-5.10	1.73	1.81
2	B	666	ASP	CB-CG	-5.10	1.41	1.51
1	A	392	GLU	CB-CG	-5.10	1.42	1.52
1	A	548	PHE	CE1-CZ	-5.09	1.27	1.37
1	A	1392	TYR	CD2-CE2	-5.08	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	TYR	CE2-CZ	-5.07	1.31	1.38
2	B	811	TYR	CG-CD1	-5.07	1.32	1.39
8	H	98	ARG	CG-CD	-5.07	1.39	1.51
2	B	782	ILE	CB-CG2	-5.07	1.37	1.52
10	J	53	VAL	CB-CG2	-5.07	1.42	1.52
1	A	570	TRP	CE3-CZ3	-5.06	1.29	1.38
3	C	49	TRP	CB-CG	-5.06	1.41	1.50
1	A	554	PHE	CD2-CE2	-5.06	1.29	1.39
1	A	618	TYR	CD1-CE1	-5.06	1.31	1.39
1	A	570	TRP	CB-CG	-5.05	1.41	1.50
1	A	521	VAL	CB-CG1	-5.04	1.42	1.52
1	A	675	VAL	CB-CG1	-5.04	1.42	1.52
3	C	164	TYR	CD2-CE2	-5.04	1.31	1.39
2	B	926	VAL	CB-CG1	-5.04	1.42	1.52
1	A	586	TRP	CD2-CE2	-5.04	1.35	1.41
2	B	945	CYS	CB-SG	-5.03	1.73	1.81
8	H	116	VAL	CB-CG2	-5.03	1.42	1.52
2	B	736	TYR	CD1-CE1	-5.03	1.31	1.39
2	B	801	VAL	CB-CG2	-5.03	1.42	1.52
8	H	97	TYR	CE2-CZ	-5.02	1.32	1.38
1	A	81	CYS	CB-SG	-5.02	1.73	1.81
2	B	1018	TYR	CD2-CE2	-5.02	1.31	1.39
2	B	785	TYR	CD1-CE1	-5.01	1.31	1.39
2	B	807	ARG	CG-CD	-5.01	1.39	1.51
8	H	115	TYR	CB-CG	-5.01	1.44	1.51
1	A	479	TRP	CE3-CZ3	-5.01	1.29	1.38
2	B	466	VAL	CB-CG1	-5.01	1.42	1.52
1	A	458	PHE	CB-CG	-5.01	1.42	1.51
1	A	788	VAL	CB-CG1	-5.00	1.42	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	40	A	C8-N9-C4	-13.77	100.29	105.80
15	P	40	A	N7-C8-N9	12.63	120.11	113.80
15	P	41	C	C6-N1-C2	-11.07	115.87	120.30
3	C	224	GLY	C-N-CA	10.22	147.25	121.70
15	P	40	A	C5-N7-C8	-9.32	99.24	103.90
15	P	39	A	C8-N9-C4	-9.26	102.10	105.80
18	T	34	DT	O5'-P-OP1	-9.09	97.52	105.70
1	A	457	ILE	CG1-CB-CG2	-8.95	91.72	111.40
15	P	39	A	N1-C2-N3	8.41	133.51	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	33	DC	OP1-P-O3'	8.23	123.31	105.20
2	B	473	LEU	CB-CG-CD2	-8.05	97.32	111.00
2	B	411	LEU	CB-CG-CD2	-7.96	97.46	111.00
15	P	40	A	N9-C4-C5	7.60	108.84	105.80
2	B	583	LEU	CB-CG-CD1	-7.48	98.28	111.00
14	N	40	DG	O4'-C1'-N9	7.36	113.15	108.00
15	P	39	A	N9-C4-C5	7.34	108.74	105.80
2	B	567	ILE	CG1-CB-CG2	-7.31	95.31	111.40
1	A	484	LEU	CB-CG-CD2	-7.25	98.67	111.00
2	B	545	LEU	CB-CG-CD2	-7.25	98.68	111.00
15	P	42	C	C6-N1-C2	-7.21	117.42	120.30
1	A	524	MET	CG-SD-CE	-7.09	88.86	100.20
3	C	68	LEU	CB-CG-CD1	-6.96	99.16	111.00
2	B	668	LEU	CB-CG-CD2	-6.96	99.17	111.00
17	R	507	PRO	N-CA-CB	6.88	111.56	103.30
15	P	41	C	N3-C2-O2	-6.85	117.11	121.90
1	A	542	LEU	CB-CG-CD2	-6.75	99.52	111.00
15	P	39	A	C6-N1-C2	-6.57	114.66	118.60
1	A	1396	ARG	CG-CD-NE	-6.55	98.03	111.80
15	P	37	G	O4'-C1'-N9	6.53	113.43	108.20
18	T	29	DG	O4'-C4'-C3'	-6.53	101.89	104.50
3	C	67	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	A	1090	LEU	CB-CG-CD2	-6.48	99.98	111.00
15	P	40	A	N3-C4-N9	-6.43	122.25	127.40
2	B	848	LEU	CB-CG-CD1	-6.39	100.13	111.00
18	T	26	DG	O4'-C4'-C3'	-6.36	101.96	104.50
20	V	258	PRO	N-CA-CB	6.33	110.89	103.30
2	B	505	LEU	CA-CB-CG	6.30	129.80	115.30
2	B	501	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	A	486	LEU	CB-CG-CD2	-6.23	100.42	111.00
17	R	506	PRO	N-CA-CB	6.17	110.71	103.30
18	T	27	DT	O4'-C4'-C3'	-6.16	102.04	104.50
1	A	1463	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	A	1095	LEU	CB-CG-CD2	-6.09	100.64	111.00
2	B	163	LEU	CB-CG-CD2	-6.08	100.66	111.00
2	B	411	LEU	CA-CB-CG	6.07	129.27	115.30
11	K	100	LEU	CB-CG-CD2	-6.07	100.69	111.00
15	P	38	G	C6-C5-N7	-5.97	126.82	130.40
5	E	165	LEU	CB-CG-CD2	-5.96	100.86	111.00
13	M	1330	PRO	N-CA-CB	5.95	110.44	103.30
1	A	26	LEU	C-N-CA	-5.94	106.86	121.70
20	V	238	PRO	N-CA-CB	5.92	110.41	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	41	C	O4'-C1'-N1	5.92	112.94	108.20
2	B	395	LEU	CB-CG-CD2	-5.91	100.96	111.00
10	J	55	LEU	CB-CG-CD2	-5.90	100.98	111.00
1	A	1400	LEU	CB-CG-CD2	-5.88	101.00	111.00
15	P	38	G	N7-C8-N9	5.88	116.04	113.10
19	U	463	PRO	N-CA-CB	5.78	110.23	103.30
15	P	38	G	C4-N9-C1'	5.76	133.98	126.50
2	B	556	ILE	C-N-CA	-5.73	107.38	121.70
18	T	32	DT	O4'-C1'-N1	5.71	112.00	108.00
1	A	979	LEU	CB-CG-CD1	-5.68	101.35	111.00
11	K	93	ASP	CB-CG-OD1	-5.63	113.23	118.30
2	B	1014	LEU	CB-CG-CD2	-5.63	101.43	111.00
15	P	41	C	C6-N1-C1'	5.60	127.52	120.80
2	B	866	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	A	1398	LEU	CB-CG-CD2	-5.55	101.56	111.00
15	P	41	C	C5-C6-N1	5.54	123.77	121.00
19	U	493	PRO	N-CA-CB	5.50	109.90	103.30
3	C	228	ARG	NE-CZ-NH1	-5.49	117.56	120.30
2	B	1015	LEU	CB-CG-CD2	-5.48	101.68	111.00
2	B	115	LEU	CB-CG-CD2	-5.44	101.76	111.00
24	Z	758	PRO	N-CA-CB	5.43	109.82	103.30
2	B	542	LEU	CB-CG-CD2	-5.42	101.78	111.00
2	B	576	ILE	CG1-CB-CG2	-5.39	99.54	111.40
2	B	21	LEU	CA-CB-CG	5.39	127.70	115.30
15	P	36	G	P-O3'-C3'	5.37	126.15	119.70
1	A	938	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	B	403	LEU	CB-CG-CD1	-5.32	101.96	111.00
8	H	121	LEU	CB-CG-CD2	-5.30	101.99	111.00
10	J	50	LEU	CB-CG-CD2	-5.25	102.08	111.00
2	B	751	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	A	80	GLU	C-N-CA	-5.23	108.63	121.70
2	B	371	ARG	NE-CZ-NH1	-5.22	117.69	120.30
12	L	44	MET	CG-SD-CE	-5.21	91.86	100.20
2	B	959	GLU	C-N-CA	-5.18	111.42	122.30
2	B	395	LEU	CA-CB-CG	-5.16	103.43	115.30
15	P	39	A	N7-C8-N9	5.16	116.38	113.80
10	J	65	LEU	CA-CB-CG	5.14	127.13	115.30
3	C	67	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	565	MET	CG-SD-CE	-5.12	92.01	100.20
2	B	377	LEU	CB-CG-CD1	-5.10	102.32	111.00
2	B	146	LYS	CA-CB-CG	5.10	124.62	113.40
1	A	567	LEU	CB-CG-CD1	-5.05	102.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	P	38	G	C8-N9-C4	-5.04	104.38	106.40
1	A	484	LEU	CA-CB-CG	5.03	126.86	115.30
2	B	665	ILE	CG1-CB-CG2	-5.02	100.35	111.40
12	L	20	GLY	N-CA-C	-5.02	100.56	113.10
3	C	44	ILE	CG1-CB-CG2	-5.00	100.40	111.40
3	C	154	ARG	CG-CD-NE	-5.00	101.30	111.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1434	GLU	Peptide
1	A	910	LYS	Peptide
2	B	20	ASP	Peptide
2	B	547	GLU	Peptide
2	B	686	GLU	Peptide
17	R	592	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	A	11255	0	11374	435	0
2	B	8980	0	9017	295	0
3	C	2072	0	2019	45	0
4	D	1004	0	980	55	0
5	E	1720	0	1737	73	0
6	F	626	0	657	11	0
7	G	1333	0	1321	80	0
8	H	1197	0	1156	44	0
9	I	942	0	873	38	0
10	J	524	0	541	19	0
11	K	920	0	942	28	0
12	L	390	0	397	13	0
13	M	4737	0	2262	46	0
14	N	773	0	412	38	0
15	P	452	0	229	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	7226	0	7169	355	0
17	R	1832	0	1687	114	0
18	T	974	0	541	39	0
19	U	852	0	668	31	0
20	V	1703	0	1426	85	0
21	W	2333	0	2246	155	0
22	X	353	0	371	28	0
23	Y	911	0	908	27	0
24	Z	4023	0	4035	181	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	Y	1	0	0	0	0
26	A	1	0	0	0	0
All	All	57142	0	52968	2040	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 19.

All (2040) 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)
8:H:37:MET:HE2	8:H:127:GLY:HA3	1.42	0.99
2:B:953:ASP:OD1	3:C:36:ARG:NH2	1.96	0.98
1:A:609:HIS:HD1	1:A:626:THR:HG1	1.04	0.94
16:Q:505:ARG:HH21	20:V:44:PHE:HB2	1.32	0.93
1:A:904:GLN:NE2	1:A:981:CYS:O	2.01	0.91
2:B:105:PRO:HG2	19:U:512:THR:HA	1.51	0.91
16:Q:830:ARG:HA	16:Q:833:LYS:HE2	1.54	0.90
21:W:278:TRP:HB2	21:W:293:GLY:HA2	1.51	0.90
1:A:1227:THR:H	1:A:1230:GLN:HE21	1.19	0.90
14:N:30:DC:H42	18:T:19:DG:H1	1.18	0.89
23:Y:7:PRO:HG3	23:Y:23:LYS:HA	1.53	0.89
2:B:332:LYS:NZ	2:B:333:GLU:OE1	2.07	0.88
21:W:40:LEU:HD12	21:W:66:GLY:HA3	1.53	0.88
16:Q:727:LEU:HB3	16:Q:732:LYS:HB3	1.57	0.87
17:R:388:ARG:NH1	17:R:446:GLU:O	2.08	0.87
16:Q:768:VAL:HG21	16:Q:778:GLU:HG3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:103:ARG:NH2	9:I:105:GLU:OE2	2.08	0.86
17:R:387:VAL:HG13	17:R:405:ILE:HD11	1.58	0.86
24:Z:478:VAL:HB	24:Z:518:LEU:HD11	1.58	0.85
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.10	0.85
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.40	0.85
18:T:41:DC:H4'	24:Z:283:ARG:HE	1.41	0.85
3:C:193:ARG:NH2	3:C:218:ALA:O	2.09	0.85
21:W:35:VAL:HB	21:W:47:TRP:HB2	1.59	0.85
8:H:98:ARG:NH2	8:H:100:GLU:OE1	2.09	0.85
2:B:85:LEU:HB2	2:B:131:THR:HB	1.59	0.85
23:Y:75:GLN:O	23:Y:111:ARG:NH1	2.09	0.85
16:Q:682:ASP:O	16:Q:686:ASN:ND2	2.09	0.84
1:A:197:GLU:HB2	1:A:215:LEU:HD11	1.60	0.84
17:R:570:TRP:HB3	20:V:133:LYS:HE2	1.61	0.83
1:A:404:GLU:OE2	1:A:407:ARG:NH1	2.12	0.82
9:I:54:TYR:OH	9:I:56:ASN:ND2	2.12	0.82
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.12	0.82
4:D:107:THR:HG23	4:D:110:GLU:H	1.43	0.82
14:N:37:DG:N1	18:T:12:DC:N3	2.27	0.82
1:A:392:GLU:OE2	1:A:401:ARG:NH2	2.11	0.81
5:E:166:ARG:HH22	5:E:168:ASN:HD22	1.26	0.81
16:Q:387:ALA:N	16:Q:390:ASP:OD2	2.13	0.81
21:W:14:ALA:N	21:W:296:GLN:O	2.13	0.81
21:W:172:ILE:HB	21:W:186:LEU:HB2	1.61	0.81
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.62	0.81
16:Q:643:ASP:OD2	22:X:239:GLN:NE2	2.11	0.81
4:D:76:ASN:HD22	4:D:79:THR:HG23	1.45	0.81
10:J:25:LEU:HB3	17:R:563:ILE:HD11	1.61	0.81
21:W:237:ASN:HD22	21:W:279:GLY:HA2	1.45	0.81
23:Y:3:LEU:O	23:Y:8:LYS:NZ	2.12	0.81
21:W:95:ASN:O	21:W:97:LYS:NZ	2.12	0.81
16:Q:276:ALA:HB1	16:Q:288:VAL:HG23	1.61	0.81
16:Q:737:LYS:HZ2	16:Q:764:LEU:HD13	1.46	0.80
1:A:1182:GLN:O	1:A:1192:TRP:NE1	2.14	0.80
21:W:35:VAL:N	21:W:47:TRP:O	2.12	0.80
2:B:756:LYS:NZ	20:V:134:THR:OG1	2.15	0.80
1:A:1525:TPO:O3P	13:M:1358:ARG:NH2	2.15	0.80
15:P:39:A:H3'	15:P:40:A:H8	1.47	0.80
16:Q:268:ASN:HD22	16:Q:271:VAL:H	1.29	0.79
1:A:1536:GLY:O	13:M:1483:ARG:NH2	2.16	0.79
7:G:111:HIS:HB3	24:Z:494:ARG:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:237:ASN:HB3	21:W:280:VAL:HG22	1.65	0.79
16:Q:41:LEU:HD23	16:Q:81:ASP:HB3	1.65	0.79
16:Q:534:TYR:HH	16:Q:553:TRP:HD1	1.31	0.79
1:A:1180:ASN:O	1:A:1183:SER:OG	2.00	0.79
20:V:47:LYS:HB3	22:X:228:GLU:HB2	1.63	0.79
1:A:539:GLN:O	1:A:541:THR:N	2.16	0.78
2:B:297:MET:HG2	2:B:377:LEU:HD11	1.65	0.78
3:C:154:ARG:NH1	10:J:63:ALA:HB2	1.98	0.78
1:A:349:ARG:HE	2:B:1157:LEU:HD22	1.46	0.78
15:P:38:G:H2'	15:P:39:A:H8	1.49	0.78
15:P:40:A:H2'	15:P:41:C:C6	2.19	0.78
1:A:1189:ASP:HA	1:A:1192:TRP:HE3	1.49	0.78
14:N:14:DC:N4	18:T:35:DG:O6	2.16	0.78
16:Q:268:ASN:HD21	16:Q:270:MET:HB3	1.49	0.78
1:A:413:TYR:O	1:A:415:GLY:N	2.17	0.78
16:Q:568:TRP:HE1	16:Q:591:ILE:HD12	1.49	0.78
24:Z:216:VAL:HB	24:Z:226:TYR:HB2	1.65	0.77
9:I:101:SER:OG	9:I:102:ALA:O	2.03	0.77
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.66	0.77
19:U:394:TYR:O	20:V:172:ARG:NH2	2.17	0.77
24:Z:728:THR:O	24:Z:747:ARG:NH1	2.18	0.77
16:Q:624:LYS:HG3	16:Q:627:ARG:HH21	1.47	0.76
1:A:272:ASN:ND2	18:T:34:DT:O2	2.19	0.76
1:A:1189:ASP:HA	1:A:1192:TRP:CE3	2.20	0.76
2:B:622:CYS:HB3	2:B:666:ASP:HB3	1.68	0.76
1:A:571:ASP:OD1	1:A:571:ASP:N	2.13	0.76
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.66	0.76
11:K:77:THR:OG1	11:K:81:TYR:O	2.04	0.76
17:R:562:TYR:O	17:R:566:ARG:NE	2.18	0.76
20:V:47:LYS:HE3	22:X:230:VAL:HG22	1.67	0.76
16:Q:353:TYR:OH	20:V:57:ARG:O	2.04	0.76
1:A:659:GLU:OE1	1:A:985:ARG:NH1	2.19	0.75
1:A:1434:GLU:O	1:A:1436:VAL:N	2.19	0.75
16:Q:314:ARG:HH12	16:Q:349:GLN:HE22	1.33	0.75
2:B:834:ARG:NH2	2:B:841:ARG:O	2.20	0.75
1:A:819:SER:O	1:A:819:SER:OG	2.05	0.74
2:B:1142:ASN:HD21	2:B:1145:GLN:HB2	1.52	0.74
1:A:713:VAL:HG21	1:A:817:PRO:HD3	1.67	0.74
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.68	0.74
14:N:37:DG:O6	18:T:12:DC:N4	2.20	0.74
1:A:296:ASN:OD1	1:A:297:GLY:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ALA:HB3	1:A:302:VAL:HG12	1.69	0.74
1:A:1467:GLY:O	1:A:1469:GLY:N	2.20	0.74
2:B:677:MET:H	2:B:682:LEU:HD22	1.52	0.74
20:V:193:HIS:HB2	20:V:199:VAL:HG12	1.70	0.74
1:A:239:GLU:OE2	1:A:241:ARG:NH1	2.21	0.74
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.21	0.74
24:Z:438:GLY:HA3	24:Z:452:PRO:HB2	1.68	0.74
2:B:388:TYR:H	2:B:504:THR:HG21	1.51	0.73
24:Z:492:ILE:HG22	24:Z:502:LEU:HB3	1.70	0.73
24:Z:554:GLU:OE2	24:Z:559:GLN:NE2	2.21	0.73
15:P:39:A:C3'	15:P:40:A:H8	2.01	0.73
21:W:214:ILE:N	21:W:228:LEU:O	2.21	0.73
24:Z:353:ALA:HB3	24:Z:360:ILE:HB	1.69	0.73
16:Q:424:GLN:HB2	22:X:231:TRP:CE3	2.24	0.73
24:Z:188:GLU:O	24:Z:192:THR:OG1	2.05	0.73
24:Z:295:TYR:N	24:Z:304:SER:OG	2.17	0.73
1:A:1184:THR:O	1:A:1186:VAL:N	2.22	0.73
21:W:169:ASP:N	21:W:169:ASP:OD1	2.22	0.73
2:B:898:THR:O	2:B:899:SER:OG	2.05	0.72
8:H:32:SER:HB3	8:H:37:MET:H	1.52	0.72
2:B:84:TYR:HB3	2:B:132:VAL:HG23	1.70	0.72
2:B:309:PHE:O	9:I:40:ARG:NH2	2.22	0.72
2:B:650:ASN:N	19:U:460:TYR:OH	2.17	0.72
4:D:131:LEU:HA	4:D:134:ILE:HD12	1.71	0.72
5:E:81:LYS:NZ	14:N:39:DA:OP1	2.19	0.72
1:A:539:GLN:O	1:A:542:LEU:N	2.21	0.72
21:W:272:ASP:O	21:W:274:GLN:NE2	2.22	0.72
8:H:103:GLU:HG3	8:H:109:ALA:HB2	1.71	0.72
19:U:438:ALA:O	19:U:439:ARG:NH1	2.20	0.72
20:V:110:GLU:HG3	20:V:111:GLU:H	1.53	0.72
1:A:289:GLN:O	1:A:293:ASN:HB2	1.89	0.72
12:L:19:CYS:SG	12:L:20:GLY:N	2.62	0.72
21:W:251:SER:OG	21:W:253:ASP:OD1	2.05	0.72
2:B:348:LEU:O	2:B:361:LYS:NZ	2.22	0.72
7:G:11:ILE:HD11	7:G:26:VAL:HG13	1.70	0.72
23:Y:93:LEU:HD22	23:Y:97:ILE:HD11	1.70	0.72
2:B:595:ASP:OD1	2:B:596:ILE:N	2.20	0.71
16:Q:163:ILE:HB	16:Q:194:PRO:HG3	1.72	0.71
21:W:81:SER:HB3	21:W:91:TRP:HE1	1.55	0.71
16:Q:302:GLU:HG3	16:Q:305:GLN:HE21	1.55	0.71
8:H:128:ASP:OD1	8:H:131:ASN:ND2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:401:LEU:HD22	16:Q:418:LEU:HG	1.72	0.71
17:R:405:ILE:HG23	17:R:426:LEU:HD11	1.72	0.71
5:E:80:PRO:HA	5:E:107:GLN:HB3	1.72	0.71
10:J:64:PRO:O	12:L:23:HIS:NE2	2.23	0.71
18:T:8:DG:H1'	18:T:9:DC:H5'	1.73	0.71
21:W:256:VAL:HB	21:W:270:PHE:HB2	1.72	0.71
24:Z:504:SER:OG	24:Z:507:THR:O	2.08	0.71
16:Q:384:LEU:HD13	16:Q:397:ALA:HB2	1.73	0.71
19:U:507:THR:O	19:U:509:ARG:N	2.24	0.71
24:Z:470:LYS:HB2	24:Z:516:ARG:HA	1.72	0.71
5:E:36:THR:N	5:E:39:GLU:OE2	2.16	0.70
9:I:109:ARG:HD3	9:I:124:THR:HG21	1.72	0.70
16:Q:799:VAL:O	16:Q:802:LYS:NZ	2.23	0.70
17:R:405:ILE:HG12	17:R:426:LEU:HD21	1.72	0.70
7:G:151:ARG:O	7:G:158:PHE:N	2.22	0.70
10:J:44:CYS:O	10:J:47:ARG:NH1	2.25	0.70
1:A:77:ASN:OD1	1:A:78:MET:N	2.25	0.70
16:Q:729:LYS:HE2	16:Q:732:LYS:HD2	1.72	0.70
1:A:244:ARG:HE	1:A:245:PRO:HD2	1.57	0.70
3:C:74:THR:OG1	3:C:74:THR:O	2.09	0.70
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.25	0.70
7:G:110:ARG:HH21	7:G:118:GLU:HA	1.56	0.70
9:I:42:CYS:SG	9:I:43:ASP:N	2.65	0.70
24:Z:563:MET:HA	24:Z:637:VAL:HG11	1.73	0.70
24:Z:759:GLY:O	24:Z:761:MET:N	2.24	0.70
2:B:85:LEU:N	2:B:131:THR:O	2.25	0.70
1:A:100:LEU:HD23	1:A:193:ARG:HE	1.57	0.69
19:U:450:LEU:HD21	19:U:452:LEU:HD23	1.73	0.69
4:D:37:VAL:HG21	7:G:2:PHE:CD2	2.27	0.69
1:A:357:LYS:NZ	2:B:1112:ASP:OD1	2.26	0.69
1:A:686:THR:OG1	1:A:687:ILE:N	2.25	0.69
16:Q:624:LYS:HG3	16:Q:627:ARG:NH2	2.07	0.69
5:E:97:GLU:HB2	5:E:99:ILE:HG12	1.74	0.69
13:M:1379:GLN:HG2	13:M:1469:PRO:HB2	1.73	0.69
17:R:428:LEU:HB2	17:R:437:PHE:CD2	2.27	0.69
21:W:231:HIS:HD1	21:W:235:VAL:HG22	1.57	0.69
24:Z:502:LEU:HG	24:Z:511:LEU:HB3	1.75	0.69
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.25	0.69
7:G:91:GLN:HG2	7:G:93:ASN:HD21	1.58	0.69
24:Z:525:ALA:HB1	24:Z:552:ARG:HH22	1.58	0.69
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1462:ILE:HD11	13:M:1472:PHE:HB3	1.74	0.69
21:W:113:ALA:HB3	21:W:122:ALA:HB3	1.74	0.69
1:A:999:ARG:NH2	8:H:103:GLU:OE2	2.24	0.69
4:D:34:ASN:O	4:D:68:THR:OG1	2.09	0.69
17:R:564:ASN:HD21	20:V:136:TYR:C	1.96	0.69
1:A:1212:LEU:HD21	1:A:1289:GLU:HB3	1.75	0.69
16:Q:752:VAL:HG22	16:Q:803:MET:HE2	1.75	0.69
24:Z:450:ILE:HG23	24:Z:452:PRO:HD3	1.74	0.69
5:E:2:ASP:OD2	5:E:4:GLU:N	2.25	0.69
7:G:152:VAL:HG22	7:G:157:ILE:HG22	1.74	0.69
17:R:410:GLU:OE1	17:R:423:ASN:ND2	2.25	0.69
8:H:36:LYS:HG3	16:Q:709:ARG:HH22	1.57	0.68
17:R:366:ARG:NH1	24:Z:775:TPO:OG1	2.26	0.68
4:D:23:PRO:HG2	7:G:78:ARG:HH12	1.58	0.68
13:M:1488:THR:HB	13:M:1495:ARG:HB3	1.75	0.68
17:R:570:TRP:HD1	20:V:133:LYS:HD2	1.57	0.68
20:V:192:GLN:HB2	20:V:197:PRO:HB3	1.74	0.68
13:M:1512:LYS:O	13:M:1516:GLN:NE2	2.24	0.68
16:Q:886:LYS:O	16:Q:890:MET:HG2	1.94	0.68
15:P:39:A:H3'	15:P:40:A:C8	2.29	0.68
1:A:487:SER:OG	1:A:673:GLN:NE2	2.26	0.68
24:Z:433:LEU:HB3	24:Z:436:LEU:HD12	1.75	0.68
24:Z:478:VAL:HG21	24:Z:502:LEU:HD22	1.74	0.68
21:W:289:ILE:HB	21:W:301:TYR:HB2	1.74	0.68
16:Q:86:LEU:HD11	16:Q:116:LEU:HB3	1.76	0.68
7:G:123:SER:OG	7:G:125:PRO:O	2.11	0.68
16:Q:590:ARG:HA	16:Q:593:LYS:HG3	1.76	0.67
2:B:633:LEU:HD11	2:B:679:PRO:HB2	1.76	0.67
2:B:649:ASN:HB2	19:U:460:TYR:OH	1.93	0.67
6:F:86:GLU:OE2	6:F:95:LYS:NZ	2.17	0.67
1:A:1212:LEU:HD12	1:A:1285:LEU:HD13	1.77	0.67
16:Q:394:ARG:HB3	16:Q:398:LYS:HE3	1.76	0.67
24:Z:419:ASN:OD1	24:Z:516:ARG:NH1	2.27	0.67
1:A:140:ARG:HH22	1:A:234:PHE:HD1	1.41	0.67
1:A:611:ASP:N	1:A:611:ASP:OD1	2.25	0.67
1:A:1024:ASN:O	5:E:162:ARG:NH2	2.28	0.67
5:E:82:VAL:HG22	5:E:86:THR:OG1	1.93	0.67
21:W:13:GLN:NE2	21:W:15:HIS:O	2.27	0.67
17:R:406:THR:OG1	17:R:427:GLN:O	2.11	0.67
1:A:112:PHE:O	1:A:113:PHE:HB2	1.93	0.67
1:A:116:LYS:NZ	1:A:184:CYS:SG	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:TRP:CE2	2:B:679:PRO:HG3	2.30	0.67
2:B:565:THR:HG21	2:B:580:PRO:HB3	1.77	0.67
2:B:1136:GLU:HB2	2:B:1143:LYS:HG2	1.77	0.67
16:Q:484:GLU:HB3	16:Q:487:HIS:HB2	1.76	0.66
24:Z:295:TYR:H	24:Z:304:SER:HG	1.42	0.66
2:B:1157:LEU:O	2:B:1161:GLU:HG3	1.95	0.66
4:D:128:GLN:NE2	4:D:132:ASP:OD1	2.27	0.66
24:Z:184:CYS:SG	24:Z:185:LYS:N	2.68	0.66
7:G:21:ASN:OD1	7:G:21:ASN:N	2.23	0.66
7:G:109:SER:HB3	24:Z:493:VAL:HG21	1.77	0.66
19:U:474:ARG:H	20:V:218:GLN:HA	1.60	0.66
21:W:236:LEU:N	21:W:250:SER:O	2.27	0.66
21:W:292:VAL:HG12	21:W:298:ILE:HG12	1.76	0.66
1:A:200:ALA:HB3	1:A:214:ILE:HG12	1.78	0.66
14:N:37:DG:N2	18:T:12:DC:O2	2.26	0.66
1:A:413:TYR:O	1:A:449:HIS:HD2	1.77	0.66
1:A:1118:THR:O	1:A:1123:ARG:HB2	1.96	0.66
2:B:1003:ASN:O	2:B:1005:ALA:N	2.27	0.66
16:Q:534:TYR:OH	16:Q:556:GLU:OE1	2.12	0.66
3:C:212:ASP:OD1	3:C:212:ASP:N	2.28	0.66
13:M:1373:VAL:HG21	13:M:1379:GLN:HG3	1.76	0.66
21:W:66:GLY:O	21:W:83:SER:OG	2.11	0.66
1:A:539:GLN:NE2	2:B:790:GLN:O	2.28	0.66
14:N:34:DC:H2"	14:N:35:DA:C8	2.30	0.66
16:Q:268:ASN:ND2	16:Q:271:VAL:H	1.93	0.66
16:Q:420:GLN:O	22:X:229:ARG:NH1	2.28	0.66
24:Z:613:GLU:O	24:Z:625:HIS:N	2.28	0.66
14:N:10:DG:H2"	14:N:11:DC:C5	2.30	0.66
21:W:46:VAL:HB	21:W:58:TRP:HB2	1.77	0.66
2:B:354:SER:OG	2:B:355:ASP:N	2.26	0.65
3:C:154:ARG:HH11	10:J:63:ALA:HB2	1.61	0.65
21:W:130:VAL:HB	21:W:144:LEU:HD12	1.78	0.65
6:F:105:ILE:HD12	6:F:117:ASP:HB3	1.78	0.65
11:K:13:PHE:HB2	11:K:16:GLU:HG3	1.77	0.65
16:Q:494:ALA:HB1	22:X:224:ILE:HG12	1.78	0.65
17:R:494:GLU:HA	17:R:497:LYS:HD2	1.79	0.65
23:Y:4:GLU:O	23:Y:27:GLN:NE2	2.29	0.65
5:E:27:LEU:O	16:Q:877:GLN:NE2	2.29	0.65
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.19	0.65
5:E:93:ARG:HA	5:E:96:GLU:OE1	1.97	0.65
14:N:30:DC:N3	18:T:19:DG:N2	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:342:LEU:HD11	20:V:67:GLU:HG2	1.78	0.65
16:Q:86:LEU:HG	16:Q:120:ALA:HB2	1.76	0.65
2:B:1071:ASN:O	2:B:1073:GLN:N	2.29	0.65
14:N:30:DC:N4	18:T:19:DG:H1	1.93	0.65
16:Q:211:LEU:HD12	16:Q:213:LYS:HZ1	1.62	0.65
1:A:1184:THR:C	1:A:1186:VAL:H	2.00	0.65
8:H:72:ASP:OD1	8:H:73:GLY:N	2.29	0.65
21:W:218:ASP:N	21:W:223:ASN:O	2.29	0.65
23:Y:14:ARG:HH21	23:Y:54:SER:HA	1.61	0.65
24:Z:539:LEU:HD22	24:Z:616:HIS:HB3	1.79	0.65
21:W:195:SER:OG	21:W:236:LEU:O	2.15	0.65
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.79	0.65
16:Q:856:LEU:HD23	16:Q:857:LEU:HD22	1.78	0.65
24:Z:558:PHE:N	24:Z:570:VAL:O	2.30	0.65
2:B:223:SER:OG	2:B:350:HIS:ND1	2.26	0.64
16:Q:605:LEU:O	16:Q:609:ASN:ND2	2.30	0.64
5:E:71:GLN:HB2	5:E:99:ILE:HG22	1.78	0.64
16:Q:568:TRP:CZ3	16:Q:592:LEU:HB2	2.32	0.64
20:V:45:ASP:N	20:V:45:ASP:OD1	2.30	0.64
24:Z:470:LYS:NZ	24:Z:518:LEU:O	2.31	0.64
4:D:76:ASN:HD21	4:D:78:GLU:HB2	1.61	0.64
5:E:113:SER:OG	14:N:40:DG:OP1	2.15	0.64
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.13	0.64
21:W:214:ILE:HB	21:W:228:LEU:HB3	1.78	0.64
24:Z:282:LYS:O	24:Z:287:LYS:NZ	2.28	0.64
17:R:569:GLU:O	17:R:573:VAL:HG23	1.97	0.64
20:V:48:PHE:HB2	22:X:229:ARG:HB2	1.78	0.64
1:A:329:MET:HA	1:A:335:PRO:HA	1.80	0.64
1:A:1140:THR:OG1	1:A:1140:THR:O	2.12	0.64
2:B:100:GLU:OE1	2:B:100:GLU:N	2.24	0.64
7:G:153:ASP:N	7:G:156:ASP:O	2.23	0.64
21:W:26:THR:HG23	21:W:284:GLY:HA2	1.80	0.64
16:Q:710:LYS:HB2	16:Q:712:TYR:CD1	2.32	0.64
2:B:497:LYS:HG3	2:B:498:PRO:HD3	1.80	0.64
14:N:31:DC:H2"	14:N:32:DA:C8	2.32	0.64
2:B:577:HIS:NE2	2:B:583:LEU:HD11	2.13	0.64
24:Z:519:GLN:NE2	24:Z:521:CYS:SG	2.71	0.64
1:A:376:ASP:CG	1:A:473:ARG:HH21	2.01	0.63
17:R:355:LEU:HG	17:R:357:GLU:H	1.62	0.63
2:B:787:GLY:O	2:B:790:GLN:HG3	1.98	0.63
21:W:92:ASP:HB3	21:W:95:ASN:OD1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:HG23	2:B:408:PHE:CZ	2.33	0.63
2:B:184:TYR:CE2	2:B:191:GLU:HG2	2.33	0.63
3:C:2:PRO:HB3	11:K:54:PRO:HD2	1.79	0.63
14:N:38:DG:H2"	14:N:39:DA:C8	2.34	0.63
1:A:1540:THR:HG23	13:M:1479:ARG:HE	1.62	0.63
2:B:93:LEU:O	19:U:507:THR:HA	1.99	0.63
8:H:2:ALA:C	8:H:84:ARG:HH22	2.02	0.63
16:Q:123:ILE:HG13	16:Q:124:ILE:HG12	1.80	0.63
16:Q:398:LYS:O	16:Q:402:LYS:HD3	1.99	0.63
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.81	0.63
18:T:38:DG:H2"	18:T:39:DC:C5	2.33	0.63
21:W:48:LYS:N	21:W:55:ASP:O	2.27	0.63
5:E:166:ARG:NH2	5:E:168:ASN:HD22	1.95	0.63
7:G:36:GLY:O	24:Z:628:LYS:NZ	2.23	0.63
8:H:8:ASP:OD1	8:H:32:SER:OG	2.05	0.63
17:R:355:LEU:HD12	17:R:356:PRO:HD2	1.81	0.63
17:R:404:GLU:OE1	17:R:455:TRP:NE1	2.32	0.63
24:Z:733:ARG:NH1	24:Z:744:SER:OG	2.31	0.63
8:H:30:CYS:HG	8:H:56:PHE:HZ	1.47	0.63
16:Q:286:SER:O	16:Q:290:HIS:ND1	2.32	0.63
16:Q:611:TRP:HE1	16:Q:628:HIS:HA	1.63	0.63
2:B:67:LEU:H	2:B:83:ARG:HB2	1.64	0.63
16:Q:239:ALA:HB2	16:Q:257:LEU:HB3	1.81	0.63
1:A:694:ALA:HB3	1:A:699:TYR:CE1	2.34	0.62
16:Q:576:LEU:HD21	16:Q:585:GLN:HE22	1.64	0.62
16:Q:128:GLN:HE22	20:V:86:LEU:HD13	1.64	0.62
16:Q:835:ASP:OD1	16:Q:839:ARG:NE	2.32	0.62
21:W:206:VAL:HG11	21:W:238:VAL:HG21	1.81	0.62
5:E:64:HIS:N	5:E:70:ASP:O	2.31	0.62
1:A:481:THR:O	1:A:483:ARG:NH1	2.32	0.62
4:D:114:LEU:HD21	7:G:167:TYR:HB2	1.80	0.62
4:D:135:GLN:OE1	4:D:138:ARG:NH1	2.32	0.62
1:A:381:PRO:HB3	1:A:480:SER:HA	1.81	0.62
1:A:922:PHE:H	1:A:1052:ARG:HH11	1.48	0.62
8:H:110:THR:O	8:H:129:ALA:N	2.32	0.62
11:K:5:PRO:HG2	11:K:8:GLU:HG3	1.81	0.62
1:A:556:GLU:OE1	1:A:556:GLU:N	2.33	0.62
2:B:100:GLU:HA	2:B:105:PRO:HG3	1.82	0.62
5:E:55:ARG:HB2	5:E:78:GLU:HG3	1.82	0.62
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.11	0.62
9:I:35:LEU:HD21	9:I:53:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HG	2:B:84:TYR:OH	2.00	0.62
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.82	0.62
16:Q:394:ARG:HD2	16:Q:421:ILE:HG23	1.82	0.62
16:Q:849:LYS:O	16:Q:852:LEU:HG	2.00	0.62
24:Z:506:LEU:HD11	24:Z:552:ARG:HH21	1.63	0.62
8:H:83:SER:OG	8:H:84:ARG:N	2.33	0.62
9:I:12:VAL:HG21	9:I:53:ILE:O	2.00	0.62
21:W:206:VAL:HG22	21:W:216:ILE:HG12	1.81	0.62
8:H:32:SER:OG	8:H:33:GLU:N	2.33	0.61
12:L:56:ASP:O	12:L:58:ARG:N	2.33	0.61
17:R:564:ASN:OD1	20:V:136:TYR:N	2.29	0.61
1:A:797:ARG:NH2	1:A:815:TYR:O	2.32	0.61
1:A:876:ASP:HB3	1:A:878:THR:HG22	1.82	0.61
5:E:39:GLU:OE1	5:E:39:GLU:N	2.24	0.61
8:H:2:ALA:O	8:H:84:ARG:NH2	2.30	0.61
16:Q:86:LEU:HD12	16:Q:89:LEU:HB2	1.80	0.61
1:A:30:GLU:HA	1:A:33:ARG:HE	1.63	0.61
1:A:200:ALA:HB2	1:A:216:LEU:HD21	1.81	0.61
1:A:1468:THR:H	6:F:60:TYR:HB3	1.66	0.61
2:B:19:PRO:O	2:B:21:LEU:N	2.32	0.61
16:Q:249:ASP:O	16:Q:253:ASN:ND2	2.33	0.61
17:R:364:LEU:HB2	17:R:387:VAL:HG12	1.81	0.61
24:Z:366:TYR:O	24:Z:373:PHE:N	2.28	0.61
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.34	0.61
16:Q:715:GLN:HB2	16:Q:746:VAL:HG11	1.83	0.61
20:V:110:GLU:HG3	20:V:111:GLU:N	2.14	0.61
1:A:88:ILE:O	1:A:90:LEU:N	2.33	0.61
16:Q:38:HIS:HE1	16:Q:73:LEU:HD13	1.66	0.61
16:Q:68:ARG:HE	16:Q:89:LEU:HD12	1.65	0.61
24:Z:390:LEU:HD12	24:Z:393:LEU:HD12	1.82	0.61
1:A:1303:GLN:O	1:A:1340:GLY:HA3	2.01	0.61
3:C:190:ASN:ND2	3:C:195:THR:O	2.20	0.61
16:Q:862:GLU:HA	16:Q:865:LEU:HG	1.82	0.61
2:B:228:SER:O	2:B:405:ARG:NH1	2.34	0.61
3:C:91:GLU:OE1	24:Z:713:SER:HB2	2.01	0.61
5:E:45:GLY:HA3	5:E:53:PRO:HD3	1.82	0.61
16:Q:729:LYS:HB2	16:Q:732:LYS:HD2	1.82	0.61
1:A:47:THR:HA	1:A:52:PRO:HA	1.81	0.61
1:A:1244:ASN:HB2	1:A:1262:MET:HE1	1.81	0.61
1:A:1481:LYS:O	13:M:1384:ARG:NH1	2.34	0.61
2:B:144:HIS:CD2	2:B:431:LEU:HD21	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:158:GLN:HG3	16:Q:159:SER:H	1.66	0.61
1:A:1301:ILE:HG22	1:A:1345:ARG:HH21	1.65	0.60
16:Q:379:LYS:HZ1	20:V:61:TYR:HE2	1.47	0.60
21:W:26:THR:HA	21:W:284:GLY:HA2	1.83	0.60
1:A:222:HIS:HB2	1:A:249:ILE:HD11	1.82	0.60
16:Q:646:ASN:HA	22:X:239:GLN:HA	1.82	0.60
20:V:196:LYS:O	20:V:198:ARG:HG3	2.01	0.60
21:W:53:ARG:NH1	21:W:54:LEU:O	2.34	0.60
23:Y:66:PRO:HB2	23:Y:78:SER:HA	1.82	0.60
24:Z:554:GLU:OE1	24:Z:557:THR:OG1	2.18	0.60
7:G:151:ARG:HB3	7:G:158:PHE:O	2.01	0.60
4:D:48:ASN:HD22	4:D:57:LEU:HG	1.66	0.60
16:Q:65:GLU:OE1	16:Q:93:TYR:OH	2.15	0.60
1:A:123:ASN:O	1:A:127:LYS:HG2	2.02	0.60
16:Q:80:LYS:O	16:Q:83:MET:HG3	2.01	0.60
16:Q:222:SER:O	16:Q:226:GLU:HG2	2.01	0.60
21:W:27:ASN:O	21:W:32:SER:OG	2.19	0.60
6:F:114:SER:OG	6:F:115:TYR:N	2.33	0.60
16:Q:163:ILE:HG21	16:Q:189:ALA:HA	1.83	0.60
16:Q:313:ALA:HB2	16:Q:328:TYR:HB2	1.83	0.60
23:Y:19:CYS:SG	23:Y:21:LEU:HB2	2.42	0.60
3:C:55:ASN:ND2	3:C:60:HIS:O	2.34	0.60
16:Q:48:ALA:HB2	16:Q:63:LEU:HD11	1.84	0.60
16:Q:65:GLU:HA	16:Q:89:LEU:HD11	1.82	0.60
21:W:176:ASP:HB2	21:W:183:LEU:HD11	1.83	0.60
1:A:760:LEU:HD22	1:A:764:ASN:ND2	2.16	0.60
20:V:233:VAL:O	20:V:238:PRO:N	2.35	0.60
2:B:784:SER:O	2:B:784:SER:OG	2.14	0.60
10:J:36:ASP:OD1	10:J:36:ASP:N	2.28	0.60
21:W:125:THR:OG1	21:W:131:ASN:ND2	2.34	0.60
1:A:217:SER:OG	1:A:220:ARG:N	2.35	0.60
5:E:45:GLY:CA	5:E:53:PRO:HD3	2.32	0.60
16:Q:581:TRP:O	16:Q:585:GLN:HB2	2.02	0.60
16:Q:620:ARG:HG3	16:Q:625:GLU:HB2	1.84	0.60
24:Z:629:LEU:HB2	24:Z:634:GLY:HA2	1.83	0.60
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.35	0.59
1:A:1222:THR:O	1:A:1225:LYS:N	2.34	0.59
3:C:189:ASP:O	3:C:191:ALA:N	2.34	0.59
1:A:1210:TRP:CZ2	1:A:1281:ASP:HB3	2.37	0.59
4:D:60:VAL:HA	4:D:63:LYS:HG2	1.82	0.59
7:G:109:SER:HB2	24:Z:503:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:CYS:O	2:B:691:SER:OG	2.21	0.59
2:B:743:ARG:NH1	2:B:745:ASP:OD1	2.35	0.59
16:Q:351:TYR:HB2	16:Q:360:ALA:HB2	1.83	0.59
16:Q:708:LEU:HD21	16:Q:719:VAL:HG21	1.83	0.59
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.84	0.59
11:K:49:GLN:NE2	11:K:93:ASP:OD2	2.34	0.59
1:A:64:VAL:HG11	1:A:78:MET:HA	1.84	0.59
24:Z:365:ARG:HD3	24:Z:374:LYS:HD2	1.84	0.59
24:Z:499:PHE:HD1	24:Z:512:LYS:HB3	1.67	0.59
16:Q:776:LEU:O	16:Q:779:VAL:HG22	2.03	0.59
1:A:379:GLY:HA2	1:A:475:ARG:O	2.02	0.59
1:A:1231:ILE:O	1:A:1235:ILE:HB	2.03	0.59
2:B:650:ASN:N	2:B:650:ASN:OD1	2.36	0.59
3:C:60:HIS:HB2	3:C:63:PHE:HB2	1.83	0.59
16:Q:371:TYR:HE2	16:Q:373:ASN:HD21	1.51	0.59
16:Q:505:ARG:NH2	20:V:44:PHE:HB2	2.12	0.59
16:Q:419:ALA:HB2	16:Q:433:ALA:HB3	1.83	0.59
1:A:620:HIS:O	8:H:97:TYR:OH	2.15	0.59
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.85	0.59
16:Q:201:ARG:HH12	16:Q:227:LEU:HD13	1.68	0.59
1:A:1005:HIS:HD2	1:A:1007:ILE:H	1.49	0.59
2:B:177:CYS:SG	2:B:180:ASP:N	2.74	0.59
4:D:103:LEU:O	7:G:144:ARG:NH2	2.36	0.59
16:Q:24:LEU:HD11	16:Q:56:LYS:HZ3	1.68	0.59
16:Q:624:LYS:HA	16:Q:627:ARG:HH21	1.67	0.59
15:P:39:A:C2	15:P:40:A:C5	2.91	0.58
21:W:8:LEU:N	21:W:300:ILE:O	2.30	0.58
1:A:476:ILE:O	1:A:476:ILE:HG13	2.00	0.58
2:B:912:ASN:OD1	2:B:912:ASN:N	2.26	0.58
9:I:17:CYS:N	9:I:22:ASN:O	2.27	0.58
14:N:11:DC:H2"	14:N:12:DG:C8	2.38	0.58
16:Q:884:LYS:O	16:Q:887:ASN:N	2.34	0.58
16:Q:774:SER:H	16:Q:830:ARG:NH1	1.99	0.58
17:R:574:GLU:HA	17:R:577:LYS:HG2	1.84	0.58
2:B:565:THR:HA	2:B:610:ARG:HB3	1.86	0.58
5:E:93:ARG:HB2	16:Q:891:PHE:CE1	2.38	0.58
8:H:63:THR:HG21	8:H:68:GLY:HA2	1.85	0.58
8:H:78:THR:O	8:H:78:THR:OG1	2.21	0.58
17:R:353:VAL:HG12	17:R:469:LEU:HD13	1.86	0.58
19:U:445:ASP:OD2	19:U:447:SER:OG	2.19	0.58
1:A:202:TRP:CE3	1:A:212:LYS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:ARG:NE	1:A:1056:GLU:OE2	2.36	0.58
15:P:37:G:HO2'	15:P:38:G:H8	1.52	0.58
20:V:88:ASN:OD1	20:V:89:PRO:HD3	2.04	0.58
24:Z:562:ASN:HD21	24:Z:566:LYS:HG3	1.67	0.58
1:A:367:ILE:HA	1:A:482:PHE:O	2.04	0.58
1:A:394:VAL:HG23	1:A:444:TYR:O	2.04	0.58
2:B:743:ARG:HB3	2:B:743:ARG:HH11	1.69	0.58
5:E:66:ASP:OD1	5:E:67:ASP:N	2.36	0.58
17:R:363:ARG:NH2	17:R:365:SER:OG	2.36	0.58
1:A:11:SER:O	2:B:1135:TYR:OH	2.14	0.58
1:A:370:ASP:OD2	11:K:65:HIS:NE2	2.36	0.58
2:B:577:HIS:CD2	2:B:583:LEU:HD11	2.38	0.58
2:B:646:ARG:C	2:B:648:TYR:H	2.07	0.58
1:A:552:ASP:OD1	8:H:24:ARG:NH1	2.37	0.58
2:B:83:ARG:O	2:B:83:ARG:NH2	2.37	0.58
1:A:1190:GLN:O	1:A:1193:VAL:HG12	2.04	0.58
1:A:1244:ASN:HB2	1:A:1262:MET:CE	2.34	0.58
4:D:46:GLN:HA	4:D:49:GLU:CD	2.24	0.58
13:M:1356:ILE:HG22	13:M:1370:THR:HB	1.85	0.58
15:P:37:G:O2'	15:P:38:G:H8	1.86	0.58
15:P:38:G:H2'	15:P:39:A:C8	2.35	0.58
16:Q:95:GLN:NE2	20:V:84:ILE:O	2.37	0.58
17:R:493:GLU:OE1	17:R:493:GLU:N	2.22	0.58
2:B:715:ASP:OD1	2:B:715:ASP:N	2.19	0.58
24:Z:416:ARG:HE	24:Z:466:GLN:HE21	1.52	0.57
2:B:1115:GLN:HG2	2:B:1150:ARG:HG2	1.86	0.57
16:Q:156:LEU:HD11	16:Q:169:LYS:HE2	1.87	0.57
16:Q:504:ALA:HB2	16:Q:519:LEU:HB3	1.86	0.57
17:R:407:GLY:H	17:R:427:GLN:HB3	1.69	0.57
24:Z:424:ASP:HB2	24:Z:440:ILE:HD12	1.84	0.57
1:A:1177:TYR:OH	1:A:1282:ASP:HA	2.04	0.57
2:B:721:ARG:NH1	2:B:940:GLY:O	2.36	0.57
5:E:90:TYR:HA	16:Q:891:PHE:HZ	1.69	0.57
1:A:392:GLU:HG2	1:A:402:LEU:HD11	1.86	0.57
1:A:699:TYR:O	1:A:703:GLN:HG2	2.05	0.57
2:B:235:ILE:HG13	2:B:348:LEU:HD13	1.85	0.57
7:G:37:THR:HA	24:Z:628:LYS:NZ	2.20	0.57
11:K:63:VAL:HG22	11:K:71:ILE:HG22	1.86	0.57
7:G:122:ASN:OD1	7:G:123:SER:N	2.38	0.57
16:Q:384:LEU:HG	16:Q:386:ALA:H	1.69	0.57
24:Z:280:ARG:HH21	24:Z:288:ASP:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.86	0.57
21:W:27:ASN:HB2	21:W:31:ASN:HD21	1.70	0.57
24:Z:192:THR:HG23	24:Z:245:LEU:HD21	1.85	0.57
1:A:96:HIS:HD2	1:A:99:PHE:CD2	2.23	0.57
1:A:546:ARG:HG2	1:A:546:ARG:O	2.04	0.57
1:A:1146:GLN:NE2	1:A:1150:ASP:OD2	2.36	0.57
1:A:1484:MET:HB2	13:M:1362:LYS:HE3	1.87	0.57
11:K:39:ASP:OD1	11:K:39:ASP:N	2.35	0.57
16:Q:474:PHE:HB2	16:Q:503:LEU:HD13	1.85	0.57
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.87	0.57
1:A:962:ASP:CG	1:A:1046:ARG:HH21	2.08	0.57
16:Q:208:PHE:HD1	16:Q:213:LYS:HD2	1.70	0.57
21:W:48:LYS:HB2	21:W:57:GLN:HB2	1.85	0.57
1:A:282:ASP:HB3	1:A:313:HIS:CE1	2.39	0.57
1:A:1146:GLN:OE1	1:A:1153:ARG:HD3	2.05	0.57
20:V:55:GLN:OE1	20:V:57:ARG:NE	2.35	0.57
24:Z:450:ILE:HG21	24:Z:468:LEU:HD11	1.86	0.57
1:A:92:LYS:HD2	1:A:307:VAL:HG11	1.87	0.56
1:A:117:LEU:HG	1:A:232:GLU:OE2	2.05	0.56
21:W:152:LEU:HD12	21:W:168:ILE:HA	1.85	0.56
1:A:1005:HIS:CD2	1:A:1007:ILE:H	2.23	0.56
3:C:4:ALA:HB2	11:K:93:ASP:HB2	1.86	0.56
16:Q:188:LYS:HB3	16:Q:191:ARG:HH11	1.70	0.56
16:Q:678:ALA:O	16:Q:684:TRP:NE1	2.38	0.56
17:R:560:ILE:HA	17:R:563:ILE:HG22	1.87	0.56
24:Z:501:ILE:HD11	24:Z:510:GLU:HB3	1.87	0.56
1:A:140:ARG:NH2	1:A:234:PHE:HD1	2.03	0.56
1:A:299:ALA:O	1:A:301:HIS:N	2.39	0.56
1:A:538:VAL:O	1:A:538:VAL:HG12	2.06	0.56
1:A:809:HIS:HE1	2:B:506:TRP:CZ2	2.23	0.56
2:B:177:CYS:HB2	2:B:738:THR:OG1	2.06	0.56
2:B:995:GLU:OE1	20:V:131:MET:HB3	2.05	0.56
5:E:55:ARG:O	5:E:56:THR:OG1	2.23	0.56
13:M:1505:ASN:O	13:M:1509:ARG:HG2	2.05	0.56
2:B:285:LEU:HD23	9:I:16:PHE:HZ	1.70	0.56
7:G:110:ARG:HH12	7:G:115:SER:HA	1.69	0.56
14:N:12:DG:H2"	14:N:13:DG:H8	1.70	0.56
21:W:68:VAL:HG13	21:W:83:SER:HA	1.87	0.56
9:I:25:TYR:O	9:I:37:TYR:HA	2.04	0.56
18:T:33:DC:H2"	18:T:34:DT:OP1	2.04	0.56
20:V:61:TYR:N	20:V:62:LYS:HA	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:384:VAL:HA	19:U:418:ASN:HB3	1.86	0.56
1:A:353:ASN:OD1	2:B:1071:ASN:ND2	2.39	0.56
2:B:897:ARG:HB2	2:B:900:GLU:HG3	1.88	0.56
16:Q:802:LYS:HE2	16:Q:807:LEU:HB2	1.87	0.56
23:Y:14:ARG:NH1	23:Y:55:SER:OG	2.39	0.56
1:A:886:VAL:HG12	5:E:169:GLN:O	2.06	0.56
1:A:1370:GLY:O	1:A:1374:VAL:HG23	2.06	0.56
15:P:39:A:C3'	15:P:40:A:C8	2.87	0.56
16:Q:777:LYS:HE3	16:Q:781:ASN:HD21	1.71	0.56
19:U:395:GLU:HA	20:V:172:ARG:HH21	1.71	0.56
24:Z:478:VAL:HG11	24:Z:492:ILE:HG23	1.87	0.56
1:A:1211:LEU:HD12	1:A:1213:ARG:N	2.21	0.56
1:A:1234:LYS:HE2	1:A:1298:LEU:HA	1.87	0.56
2:B:639:HIS:O	2:B:643:LEU:HB2	2.06	0.56
4:D:104:CYS:HB3	4:D:135:GLN:HE22	1.70	0.56
17:R:415:TYR:CZ	17:R:438:ARG:HB3	2.41	0.56
24:Z:420:PHE:HB3	24:Z:440:ILE:HD13	1.88	0.56
2:B:218:THR:HG23	2:B:238:SER:HB3	1.88	0.56
2:B:1129:ASN:HB3	2:B:1134:THR:HG22	1.87	0.56
18:T:12:DC:H2"	18:T:13:DC:H5'	1.88	0.56
20:V:127:VAL:HG23	20:V:128:VAL:H	1.71	0.56
21:W:163:LEU:O	21:W:175:PHE:N	2.34	0.56
1:A:469:MET:HG3	2:B:1093:CYS:SG	2.46	0.55
3:C:60:HIS:HB2	3:C:63:PHE:H	1.71	0.55
14:N:39:DA:H2"	14:N:40:DG:O4'	2.07	0.55
20:V:95:ASP:OD1	20:V:95:ASP:N	2.39	0.55
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.38	0.55
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.87	0.55
21:W:81:SER:HB3	21:W:91:TRP:NE1	2.20	0.55
21:W:112:LEU:HD22	21:W:121:LEU:HD21	1.87	0.55
24:Z:472:PHE:HB3	24:Z:476:ASP:OD2	2.06	0.55
2:B:588:ARG:O	2:B:592:ARG:HD3	2.07	0.55
17:R:492:ILE:O	17:R:496:VAL:HG13	2.07	0.55
21:W:9:PHE:HB3	21:W:300:ILE:CG1	2.35	0.55
24:Z:364:ASN:O	24:Z:374:LYS:NZ	2.39	0.55
1:A:760:LEU:HD13	1:A:764:ASN:HD22	1.71	0.55
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.88	0.55
16:Q:302:GLU:HG3	16:Q:305:GLN:NE2	2.20	0.55
17:R:592:ASP:O	17:R:594:PHE:N	2.37	0.55
1:A:365:THR:HG22	1:A:366:VAL:H	1.70	0.55
7:G:118:GLU:O	7:G:128:TYR:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:108:ASP:HA	21:W:126:HIS:CE1	2.41	0.55
2:B:279:VAL:HG23	2:B:312:GLN:O	2.06	0.55
4:D:74:PHE:HE2	4:D:80:ILE:HG12	1.72	0.55
16:Q:451:PRO:HD3	16:Q:480:ARG:HG3	1.88	0.55
16:Q:772:GLU:HA	16:Q:773:LYS:HB2	1.88	0.55
24:Z:542:LEU:HD22	24:Z:570:VAL:HG11	1.87	0.55
1:A:528:PRO:HB3	1:A:899:GLU:HG3	1.87	0.55
17:R:363:ARG:NE	17:R:446:GLU:HA	2.21	0.55
18:T:31:DT:H2"	18:T:32:DT:H5'	1.89	0.55
22:X:250:PHE:CE1	22:X:253:LEU:HD22	2.42	0.55
1:A:1208:SER:O	1:A:1260:ARG:HD3	2.07	0.55
2:B:756:LYS:NZ	20:V:134:THR:HG1	2.02	0.55
7:G:46:ILE:HB	7:G:75:ILE:HG13	1.89	0.55
16:Q:772:GLU:HB3	16:Q:774:SER:CB	2.37	0.55
24:Z:416:ARG:NE	24:Z:466:GLN:HE21	2.04	0.55
1:A:874:LYS:HG3	1:A:880:ARG:HG3	1.89	0.55
2:B:649:ASN:ND2	19:U:460:TYR:OH	2.40	0.55
13:M:1369:VAL:HG11	13:M:1416:VAL:HG21	1.88	0.55
17:R:569:GLU:O	17:R:572:ILE:HG22	2.07	0.55
1:A:229:SER:OG	1:A:232:GLU:HB2	2.07	0.55
14:N:43:DG:H2"	14:N:44:DG:C8	2.42	0.55
16:Q:94:VAL:HG23	16:Q:140:LEU:HD11	1.89	0.55
16:Q:313:ALA:HB2	16:Q:328:TYR:CB	2.37	0.55
16:Q:761:LEU:HD22	16:Q:785:GLU:HB3	1.89	0.55
17:R:449:GLU:O	17:R:453:MET:HG2	2.07	0.55
7:G:7:LEU:N	7:G:72:TYR:O	2.40	0.54
9:I:17:CYS:HB3	9:I:22:ASN:H	1.72	0.54
13:M:1476:TYR:OH	13:M:1483:ARG:NH1	2.40	0.54
16:Q:568:TRP:CD2	16:Q:592:LEU:HD13	2.42	0.54
17:R:360:ASN:HA	17:R:363:ARG:HB2	1.89	0.54
21:W:31:ASN:HB2	21:W:72:ILE:HG21	1.90	0.54
21:W:41:ASP:OD1	21:W:41:ASP:N	2.40	0.54
1:A:350:VAL:HA	1:A:354:LEU:HB2	1.89	0.54
8:H:27:ARG:HD3	8:H:42:ASP:OD2	2.06	0.54
2:B:714:PRO:HD2	2:B:1001:PRO:HG3	1.88	0.54
2:B:859:ARG:HH12	2:B:901:THR:HG22	1.72	0.54
10:J:57:GLU:OE1	17:R:557:ILE:HG12	2.06	0.54
17:R:471:GLU:HG2	17:R:474:LYS:HE3	1.88	0.54
1:A:62:GLN:HE22	1:A:255:VAL:HG13	1.71	0.54
1:A:117:LEU:C	1:A:119:VAL:H	2.11	0.54
2:B:342:VAL:HG23	2:B:346:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:309:CYS:HB3	16:Q:328:TYR:HD1	1.73	0.54
16:Q:546:ASN:HD22	16:Q:577:ALA:HB2	1.73	0.54
24:Z:610:ARG:HD2	24:Z:629:LEU:HD21	1.89	0.54
1:A:340:LYS:HG3	1:A:1436:VAL:HG11	1.90	0.54
1:A:522:PRO:O	1:A:662:HIS:HB2	2.07	0.54
2:B:309:PHE:HD2	9:I:40:ARG:NE	2.04	0.54
5:E:166:ARG:HH22	5:E:168:ASN:ND2	1.99	0.54
16:Q:316:PHE:HB2	16:Q:325:ALA:HB2	1.90	0.54
16:Q:525:ARG:HG3	16:Q:526:GLU:HG3	1.88	0.54
16:Q:776:LEU:HD22	16:Q:831:ALA:HA	1.88	0.54
21:W:76:LEU:HD12	21:W:77:PRO:HD2	1.89	0.54
24:Z:235:VAL:O	24:Z:239:ILE:HG12	2.07	0.54
1:A:48:GLU:OE1	1:A:51:ARG:HB2	2.08	0.54
1:A:606:HIS:HB3	1:A:626:THR:HB	1.89	0.54
5:E:111:THR:HG23	5:E:114:ALA:H	1.73	0.54
15:P:39:A:C2	18:T:33:DC:O2	2.61	0.54
17:R:385:CYS:O	17:R:405:ILE:HD12	2.08	0.54
21:W:236:LEU:HD13	21:W:278:TRP:CE3	2.42	0.54
1:A:1130:ILE:HD11	1:A:1405:MET:CE	2.38	0.54
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.54
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.40	0.54
16:Q:46:ALA:O	16:Q:50:GLU:HG2	2.08	0.54
19:U:450:LEU:CD2	19:U:452:LEU:HD23	2.37	0.54
21:W:19:ILE:HG12	21:W:39:SER:OG	2.06	0.54
1:A:255:VAL:HG23	1:A:280:LEU:HD13	1.89	0.54
16:Q:274:HIS:HA	16:Q:277:ASN:ND2	2.23	0.54
16:Q:505:ARG:HE	20:V:44:PHE:HB3	1.73	0.54
2:B:169:ARG:NH2	20:V:139:THR:OG1	2.40	0.54
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.38	0.54
4:D:133:ASP:O	4:D:136:THR:OG1	2.22	0.54
9:I:39:CYS:SG	9:I:40:ARG:N	2.81	0.54
16:Q:364:PHE:HB3	16:Q:380:ILE:HD11	1.90	0.54
21:W:29:LYS:O	21:W:77:PRO:HB3	2.08	0.54
2:B:159:THR:HA	2:B:164:ASN:ND2	2.22	0.54
17:R:452:PHE:CZ	17:R:456:LYS:HE2	2.43	0.54
19:U:379:PRO:HD2	19:U:382:LEU:HD12	1.89	0.54
21:W:233:SER:HG	21:W:251:SER:HB2	1.71	0.54
13:M:1463:CYS:O	13:M:1473:LEU:N	2.30	0.53
16:Q:147:GLN:O	16:Q:151:GLN:HG2	2.08	0.53
16:Q:392:GLU:HG2	16:Q:393:LYS:HG2	1.90	0.53
16:Q:553:TRP:HD1	16:Q:556:GLU:OE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.90	0.53
2:B:22:TRP:CH2	2:B:679:PRO:HD3	2.43	0.53
2:B:141:GLN:O	2:B:143:GLN:N	2.42	0.53
2:B:959:GLU:OE1	2:B:959:GLU:N	2.41	0.53
17:R:356:PRO:HB3	17:R:452:PHE:HB2	1.90	0.53
17:R:560:ILE:O	17:R:563:ILE:HG22	2.08	0.53
1:A:606:HIS:CG	1:A:607:SER:H	2.26	0.53
1:A:727:PRO:HA	1:A:736:THR:HG21	1.89	0.53
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.40	0.53
7:G:100:GLU:OE1	7:G:105:SER:HB3	2.08	0.53
7:G:117:MET:HB3	7:G:128:TYR:HB3	1.89	0.53
9:I:29:ASP:HB3	9:I:34:ILE:HG13	1.89	0.53
16:Q:772:GLU:HB3	16:Q:774:SER:HB3	1.89	0.53
21:W:228:LEU:HD13	21:W:264:ARG:HB3	1.90	0.53
21:W:256:VAL:O	21:W:269:THR:HA	2.07	0.53
1:A:64:VAL:HG12	1:A:81:CYS:SG	2.48	0.53
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.43	0.53
16:Q:190:LEU:O	16:Q:193:ASN:ND2	2.41	0.53
16:Q:454:LEU:HA	16:Q:457:VAL:HG12	1.91	0.53
16:Q:867:GLU:O	16:Q:871:GLN:HG3	2.08	0.53
20:V:45:ASP:HB3	22:X:232:ARG:HE	1.73	0.53
21:W:33:GLU:O	21:W:49:TRP:N	2.41	0.53
23:Y:40:LEU:HD22	23:Y:42:MET:HB3	1.89	0.53
24:Z:244:ASN:HB3	24:Z:245:LEU:HD22	1.90	0.53
1:A:141:LEU:HA	1:A:144:VAL:HG22	1.89	0.53
5:E:45:GLY:HA3	5:E:52:ARG:HB2	1.91	0.53
8:H:9:ILE:HD12	8:H:148:LEU:HD11	1.90	0.53
12:L:35:ARG:HH21	12:L:40:GLY:CA	2.20	0.53
13:M:1440:ARG:O	13:M:1444:GLU:HG2	2.08	0.53
16:Q:631:ARG:O	16:Q:635:ILE:HG12	2.09	0.53
1:A:589:LYS:NZ	1:A:625:ASP:OD2	2.36	0.53
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.74	0.53
1:A:1227:THR:N	1:A:1230:GLN:HE21	1.98	0.53
7:G:117:MET:N	7:G:117:MET:SD	2.80	0.53
22:X:233:THR:O	22:X:236:THR:OG1	2.22	0.53
24:Z:279:VAL:HA	24:Z:386:VAL:HG21	1.90	0.53
1:A:241:ARG:HB2	1:A:241:ARG:CZ	2.39	0.53
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.89	0.53
2:B:957:THR:HG22	2:B:1028:LEU:HD22	1.90	0.53
5:E:119:VAL:HA	5:E:122:ALA:HB2	1.90	0.53
2:B:395:LEU:HD11	2:B:532:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:623:GLU:O	16:Q:627:ARG:NE	2.42	0.53
16:Q:776:LEU:O	16:Q:780:LEU:HD12	2.08	0.53
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.42	0.53
2:B:741:HIS:CD2	2:B:742:VAL:HG23	2.43	0.53
2:B:789:ASN:O	2:B:968:ASN:HB2	2.09	0.53
2:B:833:THR:C	2:B:835:GLU:H	2.11	0.53
7:G:109:SER:HB3	24:Z:493:VAL:HG11	1.91	0.53
13:M:1352:GLN:HE22	13:M:1373:VAL:C	2.11	0.53
16:Q:769:LEU:HD13	16:Q:824:ALA:HB2	1.91	0.53
16:Q:777:LYS:HA	16:Q:780:LEU:HD13	1.91	0.53
21:W:9:PHE:H	21:W:300:ILE:HB	1.73	0.53
24:Z:479:LYS:NZ	24:Z:521:CYS:O	2.28	0.53
4:D:130:ILE:HA	4:D:133:ASP:OD2	2.09	0.53
9:I:68:ILE:HB	9:I:122:ARG:HD3	1.91	0.53
11:K:93:ASP:OD1	11:K:93:ASP:N	2.41	0.53
16:Q:26:GLU:HG3	16:Q:28:ASP:H	1.74	0.53
21:W:108:ASP:HA	21:W:126:HIS:ND1	2.23	0.53
21:W:248:VAL:HG12	21:W:258:VAL:HG22	1.90	0.53
1:A:1180:ASN:ND2	1:A:1182:GLN:HE21	2.07	0.52
7:G:8:GLU:HA	7:G:71:LYS:HA	1.91	0.52
7:G:37:THR:OG1	7:G:38:CYS:N	2.42	0.52
10:J:65:LEU:HD12	10:J:66:GLU:OE1	2.09	0.52
16:Q:244:ASN:ND2	20:V:69:GLN:HA	2.24	0.52
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.91	0.52
4:D:61:PHE:CE2	4:D:65:LEU:HD21	2.44	0.52
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.91	0.52
17:R:355:LEU:HD11	17:R:357:GLU:HG2	1.90	0.52
17:R:403:ALA:HB1	17:R:428:LEU:HB3	1.91	0.52
18:T:17:DT:H2"	18:T:18:DG:C8	2.44	0.52
18:T:35:DG:C2	18:T:36:DC:C2	2.97	0.52
16:Q:384:LEU:HD21	16:Q:386:ALA:HB3	1.91	0.52
16:Q:763:ARG:HG2	20:V:25:GLU:HG3	1.91	0.52
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.90	0.52
2:B:609:GLU:O	2:B:609:GLU:HG2	2.09	0.52
13:M:1447:LEU:HB3	13:M:1477:GLN:HG3	1.91	0.52
17:R:577:LYS:O	17:R:580:VAL:HG22	2.09	0.52
24:Z:422:PRO:HG3	24:Z:443:VAL:HG21	1.91	0.52
1:A:129:ILE:HD13	1:A:132:LYS:NZ	2.24	0.52
16:Q:420:GLN:HA	22:X:229:ARG:HH22	1.75	0.52
21:W:172:ILE:N	21:W:186:LEU:O	2.42	0.52
21:W:289:ILE:N	21:W:301:TYR:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:193:ALA:O	24:Z:197:MET:HG3	2.10	0.52
2:B:1136:GLU:HA	2:B:1143:LYS:HA	1.90	0.52
4:D:51:ALA:O	4:D:54:GLU:HB2	2.10	0.52
4:D:82:SER:O	4:D:85:SER:OG	2.25	0.52
5:E:209:VAL:O	5:E:210:GLN:HB2	2.10	0.52
7:G:93:ASN:O	7:G:128:TYR:OH	2.27	0.52
16:Q:239:ALA:HA	16:Q:257:LEU:HD13	1.92	0.52
16:Q:774:SER:O	16:Q:830:ARG:NH2	2.41	0.52
18:T:9:DC:C6	18:T:10:DT:H72	2.45	0.52
2:B:1010:LYS:HE3	20:V:130:TRP:CZ3	2.43	0.52
4:D:63:LYS:HA	4:D:66:ASN:HD21	1.75	0.52
4:D:63:LYS:HE2	7:G:102:GLY:O	2.10	0.52
16:Q:380:ILE:HD12	16:Q:400:HIS:HE1	1.75	0.52
17:R:473:ASN:HA	17:R:476:GLU:CD	2.30	0.52
21:W:39:SER:HB2	21:W:41:ASP:OD1	2.10	0.52
21:W:217:TYR:HA	21:W:224:LEU:HA	1.91	0.52
1:A:525:ILE:O	1:A:534:VAL:HG22	2.09	0.52
1:A:1229:GLU:O	1:A:1233:GLU:HG3	2.10	0.52
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.92	0.52
7:G:7:LEU:O	7:G:72:TYR:N	2.27	0.52
16:Q:511:CYS:O	21:W:229:SER:OG	2.24	0.52
16:Q:790:HIS:HA	16:Q:793:PHE:CD2	2.45	0.52
17:R:452:PHE:HB3	17:R:453:MET:HE2	1.92	0.52
21:W:176:ASP:HB2	21:W:183:LEU:HD21	1.92	0.52
24:Z:588:ASP:HA	24:Z:640:THR:O	2.10	0.52
1:A:1546:PHE:HD2	13:M:1516:GLN:HG3	1.75	0.51
2:B:388:TYR:OH	2:B:524:LYS:HE3	2.10	0.51
2:B:651:TYR:HB2	19:U:460:TYR:CZ	2.44	0.51
5:E:36:THR:HG1	5:E:39:GLU:CD	2.13	0.51
5:E:67:ASP:OD2	5:E:69:THR:OG1	2.22	0.51
16:Q:768:VAL:HG13	16:Q:769:LEU:HG	1.91	0.51
1:A:922:PHE:N	1:A:1052:ARG:HH11	2.09	0.51
4:D:63:LYS:HD3	7:G:103:PRO:HA	1.92	0.51
17:R:581:ALA:O	17:R:585:ASN:ND2	2.43	0.51
24:Z:568:VAL:HG13	24:Z:570:VAL:HG13	1.91	0.51
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.39	0.51
7:G:118:GLU:HG2	7:G:129:LYS:O	2.11	0.51
24:Z:206:THR:OG1	24:Z:207:ASP:N	2.43	0.51
24:Z:232:GLN:HE21	24:Z:252:GLN:HB2	1.75	0.51
24:Z:454:HIS:HE2	24:Z:463:PHE:HE2	1.58	0.51
1:A:43:TYR:HB3	1:A:45:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ASP:O	1:A:697:LYS:N	2.39	0.51
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.92	0.51
13:M:1443:LEU:HD13	13:M:1473:LEU:HD22	1.92	0.51
9:I:81:THR:HG23	9:I:96:PHE:CE1	2.45	0.51
13:M:1473:LEU:HD11	13:M:1484:ILE:HD12	1.92	0.51
14:N:34:DC:H2"	14:N:35:DA:H8	1.76	0.51
24:Z:470:LYS:HD2	24:Z:472:PHE:CZ	2.46	0.51
24:Z:745:VAL:HG11	24:Z:750:LEU:HD21	1.92	0.51
2:B:851:ASP:HB2	12:L:15:MET:HG2	1.91	0.51
2:B:997:GLY:HA2	20:V:131:MET:HG2	1.91	0.51
4:D:123:GLU:OE1	4:D:123:GLU:N	2.44	0.51
16:Q:513:PHE:HB2	21:W:213:TYR:HE1	1.75	0.51
22:X:248:ASN:OD1	22:X:249:ILE:HG13	2.10	0.51
24:Z:478:VAL:HG22	24:Z:490:GLY:O	2.11	0.51
1:A:927:GLU:HG3	1:A:943:LEU:HD11	1.92	0.51
2:B:993:LYS:HG2	2:B:1018:TYR:OH	2.11	0.51
2:B:1007:ASN:N	2:B:1007:ASN:OD1	2.42	0.51
16:Q:744:ARG:HG2	16:Q:748:PRO:HA	1.93	0.51
17:R:417:LEU:N	17:R:420:THR:O	2.40	0.51
20:V:193:HIS:H	20:V:197:PRO:HA	1.73	0.51
21:W:17:ASP:HB2	21:W:41:ASP:HB3	1.93	0.51
21:W:22:VAL:HG23	21:W:37:THR:HG22	1.92	0.51
1:A:428:ASP:OD1	1:A:430:ARG:NH1	2.44	0.51
2:B:177:CYS:SG	2:B:737:ILE:HD11	2.50	0.51
5:E:84:ILE:HG12	5:E:114:ALA:HA	1.92	0.51
16:Q:530:TYR:HD2	16:Q:533:CYS:HB2	1.76	0.51
16:Q:682:ASP:OD1	16:Q:683:VAL:N	2.43	0.51
18:T:36:DC:C2	18:T:37:DC:C5	2.99	0.51
23:Y:45:ASN:HD21	23:Y:48:MET:HB2	1.75	0.51
24:Z:478:VAL:O	24:Z:489:THR:HG23	2.11	0.51
1:A:120:ASP:O	1:A:122:ASN:ND2	2.44	0.51
1:A:419:ILE:HD12	1:A:440:LEU:HD23	1.92	0.51
1:A:1474:LEU:HB2	6:F:105:ILE:HG12	1.93	0.51
2:B:624:PRO:HA	2:B:663:GLU:O	2.09	0.51
7:G:46:ILE:HD11	7:G:77:PHE:CB	2.40	0.51
16:Q:244:ASN:HD22	20:V:69:GLN:HA	1.76	0.51
17:R:493:GLU:O	17:R:496:VAL:HG22	2.11	0.51
21:W:110:TRP:H	21:W:123:THR:HG23	1.76	0.51
24:Z:312:ASP:O	24:Z:315:ARG:HG2	2.11	0.51
1:A:44:PRO:HG2	1:A:285:LYS:HD3	1.93	0.51
1:A:725:LEU:HD23	1:A:733:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:GLY:HA2	5:E:178:PRO:HD2	1.93	0.51
1:A:1423:ASP:OD2	1:A:1423:ASP:N	2.38	0.51
16:Q:815:ARG:O	16:Q:818:SER:OG	2.25	0.51
17:R:454:LYS:NZ	17:R:458:ALA:HB2	2.26	0.51
21:W:44:VAL:HB	21:W:60:LEU:HB2	1.93	0.51
21:W:231:HIS:ND1	21:W:251:SER:HB3	2.26	0.51
22:X:252:ILE:HG13	22:X:253:LEU:N	2.26	0.51
23:Y:40:LEU:HD21	23:Y:52:CYS:SG	2.51	0.51
1:A:410:ASN:HD22	1:A:430:ARG:HD2	1.76	0.50
1:A:1288:ILE:HA	1:A:1291:ASN:ND2	2.27	0.50
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.29	0.50
2:B:56:GLN:HG2	2:B:91:ILE:HG22	1.92	0.50
5:E:21:CYS:O	5:E:26:TYR:HB2	2.11	0.50
7:G:91:GLN:HA	7:G:139:GLN:NE2	2.26	0.50
16:Q:93:TYR:HB3	16:Q:113:ALA:HB2	1.93	0.50
17:R:564:ASN:ND2	20:V:136:TYR:C	2.64	0.50
19:U:373:LEU:HD23	19:U:375:PHE:H	1.76	0.50
21:W:159:ASP:OD2	21:W:161:LYS:HE3	2.11	0.50
21:W:295:ASP:OD2	21:W:297:GLU:HB2	2.11	0.50
24:Z:436:LEU:HB3	24:Z:454:HIS:CE1	2.45	0.50
2:B:848:LEU:HD23	2:B:865:VAL:HG13	1.93	0.50
16:Q:106:LYS:O	16:Q:110:ILE:HG12	2.12	0.50
16:Q:880:GLN:HB2	16:Q:884:LYS:HZ3	1.75	0.50
21:W:116:PRO:HD3	21:W:156:TYR:HB3	1.92	0.50
24:Z:215:VAL:HG12	24:Z:227:VAL:HG23	1.94	0.50
1:A:202:TRP:HE3	1:A:212:LYS:HB2	1.76	0.50
1:A:471:GLY:O	1:A:521:VAL:HG23	2.12	0.50
1:A:1177:TYR:CE1	1:A:1210:TRP:HB3	2.46	0.50
1:A:1302:GLU:C	1:A:1304:ILE:H	2.15	0.50
4:D:37:VAL:HG21	7:G:2:PHE:HD2	1.75	0.50
13:M:1398:LEU:HD23	13:M:1400:ILE:HG23	1.93	0.50
13:M:1494:PHE:HE2	13:M:1504:VAL:HG12	1.75	0.50
23:Y:63:MET:SD	23:Y:72:SER:HB2	2.51	0.50
1:A:140:ARG:O	1:A:144:VAL:HG13	2.11	0.50
1:A:383:SER:HB3	11:K:2:ASN:HD21	1.76	0.50
1:A:1180:ASN:CG	1:A:1182:GLN:HE21	2.14	0.50
2:B:130:LYS:HB3	2:B:142:THR:HG23	1.94	0.50
4:D:61:PHE:O	4:D:65:LEU:HG	2.11	0.50
16:Q:38:HIS:CE1	16:Q:73:LEU:HD22	2.47	0.50
16:Q:164:PRO:HA	16:Q:167:LEU:HB2	1.93	0.50
16:Q:310:TYR:CE2	16:Q:342:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:635:ILE:O	16:Q:639:VAL:HG22	2.11	0.50
17:R:441:PHE:HA	24:Z:776:PRO:O	2.11	0.50
4:D:33:LEU:HB2	4:D:36:GLU:HB2	1.93	0.50
14:N:39:DA:C6	14:N:40:DG:C6	3.00	0.50
15:P:39:A:H2'	15:P:40:A:C8	2.47	0.50
16:Q:163:ILE:HB	16:Q:164:PRO:HD3	1.94	0.50
16:Q:841:LEU:HD23	16:Q:844:LYS:HD3	1.93	0.50
17:R:404:GLU:O	17:R:428:LEU:HA	2.11	0.50
24:Z:440:ILE:HA	24:Z:450:ILE:HD11	1.94	0.50
1:A:123:ASN:HD22	1:A:125:LYS:HD3	1.75	0.50
1:A:738:GLU:OE2	1:A:797:ARG:NH1	2.45	0.50
2:B:169:ARG:NH2	20:V:139:THR:O	2.43	0.50
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.45	0.50
2:B:1142:ASN:O	2:B:1144:THR:HG22	2.10	0.50
3:C:9:VAL:HG11	11:K:105:PHE:HD1	1.75	0.50
5:E:47:LYS:O	5:E:53:PRO:HD2	2.11	0.50
5:E:64:HIS:HB2	5:E:70:ASP:OD1	2.12	0.50
15:P:38:G:N3	15:P:39:A:C8	2.80	0.50
18:T:37:DC:H2"	18:T:38:DG:C8	2.46	0.50
1:A:324:GLY:O	1:A:325:LEU:HD22	2.12	0.50
1:A:1147:SER:OG	1:A:1351:ASP:OD1	2.29	0.50
16:Q:166:LEU:HA	16:Q:169:LYS:NZ	2.26	0.50
16:Q:837:GLU:O	16:Q:840:GLU:HG3	2.11	0.50
17:R:414:VAL:HG22	17:R:423:ASN:HB3	1.94	0.50
1:A:651:SER:O	1:A:655:ILE:HG12	2.11	0.50
13:M:1347:MET:HB2	13:M:1372:LYS:HE3	1.94	0.50
16:Q:288:VAL:HG13	16:Q:289:GLN:HG3	1.93	0.50
24:Z:444:ASP:HB3	24:Z:448:ILE:HA	1.93	0.50
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.93	0.49
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.76	0.49
7:G:46:ILE:HD11	7:G:77:PHE:HB3	1.94	0.49
14:N:39:DA:H2'	14:N:40:DG:C8	2.47	0.49
16:Q:163:ILE:O	16:Q:166:LEU:HG	2.12	0.49
21:W:258:VAL:O	21:W:267:VAL:HG22	2.11	0.49
1:A:833:PRO:HB2	2:B:677:MET:SD	2.52	0.49
2:B:649:ASN:OD1	2:B:649:ASN:N	2.46	0.49
2:B:728:MET:SD	2:B:942:LYS:HB3	2.52	0.49
3:C:86:ARG:NH1	24:Z:716:PRO:O	2.45	0.49
4:D:133:ASP:O	4:D:137:LYS:HG2	2.12	0.49
5:E:177:ASP:O	5:E:181:ARG:HG3	2.11	0.49
16:Q:524:LEU:HD11	16:Q:537:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:735:GLU:OE1	16:Q:738:GLN:HB2	2.13	0.49
17:R:403:ALA:HB3	17:R:428:LEU:HD13	1.93	0.49
21:W:65:LEU:HG	21:W:85:ASP:HB3	1.94	0.49
22:X:233:THR:HG22	22:X:236:THR:HG23	1.94	0.49
24:Z:529:ASP:HB3	24:Z:553:LEU:HD23	1.94	0.49
1:A:290:LEU:HD13	1:A:306:ASP:CG	2.33	0.49
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.93	0.49
2:B:218:THR:HG22	2:B:236:TRP:HD1	1.77	0.49
10:J:22:LEU:HD22	17:R:563:ILE:HG21	1.94	0.49
16:Q:743:ALA:O	16:Q:746:VAL:HG22	2.12	0.49
16:Q:829:ALA:HA	16:Q:832:ARG:HD2	1.94	0.49
1:A:742:ASN:O	1:A:746:ASN:ND2	2.45	0.49
2:B:237:VAL:HG11	2:B:369:VAL:HG22	1.94	0.49
20:V:126:LYS:HE3	20:V:126:LYS:HA	1.94	0.49
24:Z:470:LYS:HB3	24:Z:472:PHE:HE2	1.78	0.49
24:Z:588:ASP:HB3	24:Z:594:ILE:HG13	1.95	0.49
24:Z:735:GLU:HG3	24:Z:735:GLU:O	2.13	0.49
1:A:316:THR:HA	1:A:319:ASP:O	2.11	0.49
1:A:428:ASP:OD1	1:A:430:ARG:HG3	2.11	0.49
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.47	0.49
1:A:1295:ASP:OD2	1:A:1295:ASP:N	2.46	0.49
4:D:44:ARG:HA	4:D:47:GLN:OE1	2.12	0.49
16:Q:183:LEU:O	16:Q:187:LYS:HG2	2.13	0.49
17:R:363:ARG:HE	17:R:446:GLU:HG2	1.78	0.49
17:R:410:GLU:HA	17:R:424:LYS:HA	1.93	0.49
17:R:416:GLN:HE21	17:R:421:ARG:CZ	2.26	0.49
17:R:471:GLU:O	17:R:474:LYS:HG3	2.13	0.49
2:B:537:GLN:HG3	2:B:538:PRO:HD2	1.93	0.49
2:B:626:LEU:HD13	2:B:698:ILE:HG12	1.94	0.49
14:N:35:DA:H2"	14:N:36:DG:H8	1.75	0.49
16:Q:68:ARG:NE	16:Q:89:LEU:HD12	2.27	0.49
19:U:443:TRP:HE1	19:U:449:SER:HG	1.58	0.49
21:W:228:LEU:HD11	21:W:259:TRP:CZ3	2.48	0.49
1:A:587:THR:HG22	1:A:588:GLY:N	2.27	0.49
7:G:151:ARG:HG3	24:Z:477:HIS:NE2	2.26	0.49
13:M:1374:SER:HB2	13:M:1377:ILE:HD13	1.93	0.49
13:M:1485:GLU:OE1	13:M:1497:ARG:NE	2.34	0.49
16:Q:750:ASP:HB3	16:Q:753:LEU:HG	1.93	0.49
21:W:108:ASP:HB3	21:W:125:THR:HG23	1.95	0.49
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.43	0.49
2:B:130:LYS:NZ	2:B:429:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:VAL:HG11	7:G:44:PHE:CZ	2.48	0.49
7:G:110:ARG:HD2	7:G:113:ILE:HB	1.95	0.49
12:L:16:ILE:HG13	12:L:26:ASN:O	2.13	0.49
17:R:416:GLN:HG2	17:R:421:ARG:HB3	1.95	0.49
19:U:453:GLY:HA2	20:V:185:ASP:OD2	2.12	0.49
22:X:242:GLY:O	22:X:243:LYS:HE2	2.13	0.49
24:Z:257:ILE:O	24:Z:260:MET:HG2	2.13	0.49
1:A:54:LEU:O	1:A:61:ARG:NH2	2.45	0.49
1:A:496:PHE:HB2	2:B:791:GLU:O	2.12	0.49
1:A:963:ARG:O	1:A:967:ARG:HG3	2.13	0.49
1:A:1000:LEU:O	1:A:1059:ARG:NH1	2.45	0.49
2:B:22:TRP:CZ2	2:B:679:PRO:HG3	2.48	0.49
2:B:824:ASP:O	2:B:872:THR:HG23	2.13	0.49
13:M:783:GLY:N	13:M:797:ALA:O	2.46	0.49
17:R:358:GLU:HA	17:R:361:ARG:NE	2.27	0.49
17:R:389:ILE:O	17:R:400:TYR:HD1	1.95	0.49
24:Z:199:LYS:HG2	24:Z:210:LEU:HD21	1.93	0.49
24:Z:426:VAL:HG21	24:Z:468:LEU:HD13	1.95	0.49
1:A:926:ASN:O	1:A:930:LEU:HG	2.13	0.49
1:A:1007:ILE:HD12	1:A:1007:ILE:HA	1.63	0.49
2:B:792:ASP:CG	2:B:975:ARG:HH22	2.16	0.49
14:N:37:DG:N2	18:T:12:DC:C2	2.77	0.49
16:Q:128:GLN:HA	16:Q:158:GLN:NE2	2.26	0.49
16:Q:129:ASN:OD1	16:Q:132:LEU:HD13	2.12	0.49
17:R:416:GLN:HA	17:R:421:ARG:HA	1.94	0.49
1:A:1311:LEU:HD22	1:A:1332:GLN:HG2	1.95	0.48
2:B:431:LEU:HD23	2:B:431:LEU:H	1.77	0.48
2:B:679:PRO:HG2	2:B:680:ASP:H	1.78	0.48
2:B:816:GLU:OE2	2:B:869:LYS:HE3	2.13	0.48
2:B:1120:ASN:HD22	2:B:1145:GLN:HB3	1.77	0.48
4:D:108:ALA:N	4:D:128:GLN:OE1	2.46	0.48
16:Q:764:LEU:HD22	16:Q:785:GLU:OE1	2.12	0.48
17:R:563:ILE:O	17:R:566:ARG:HG2	2.13	0.48
21:W:35:VAL:O	21:W:47:TRP:N	2.44	0.48
21:W:231:HIS:ND1	21:W:235:VAL:HG22	2.26	0.48
1:A:84:HIS:H	1:A:84:HIS:CD2	2.31	0.48
1:A:1073:GLU:HG3	1:A:1074:SER:N	2.28	0.48
1:A:1087:VAL:HG23	1:A:1400:LEU:HD21	1.95	0.48
2:B:92:TYR:HD1	19:U:506:ALA:HB3	1.79	0.48
2:B:420:GLN:C	2:B:422:PHE:H	2.17	0.48
2:B:910:THR:OG1	2:B:911:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:90:THR:HG23	7:G:99:THR:HA	1.95	0.48
8:H:11:ASP:OD1	8:H:11:ASP:N	2.46	0.48
8:H:36:LYS:CE	16:Q:709:ARG:HH12	2.26	0.48
9:I:96:PHE:HA	9:I:111:TYR:O	2.13	0.48
16:Q:663:PHE:HB3	16:Q:690:ILE:HG23	1.95	0.48
21:W:204:LEU:HD22	21:W:216:ILE:HG22	1.95	0.48
23:Y:33:CYS:SG	23:Y:36:CYS:N	2.85	0.48
1:A:1359:SER:O	1:A:1359:SER:OG	2.16	0.48
1:A:1400:LEU:O	1:A:1404:THR:HG23	2.14	0.48
8:H:13:LYS:HG3	8:H:31:GLU:HG2	1.95	0.48
14:N:4:DT:OP2	14:N:4:DT:H71	2.13	0.48
16:Q:188:LYS:HB3	16:Q:191:ARG:NH1	2.29	0.48
16:Q:236:VAL:O	16:Q:240:VAL:HG23	2.13	0.48
16:Q:454:LEU:HB3	16:Q:477:SER:OG	2.13	0.48
16:Q:855:LYS:O	16:Q:858:LYS:HG3	2.13	0.48
23:Y:56:SER:HA	24:Z:271:ALA:HA	1.96	0.48
24:Z:436:LEU:HD13	24:Z:454:HIS:CD2	2.49	0.48
24:Z:746:ASP:OD1	24:Z:747:ARG:N	2.46	0.48
2:B:299:GLU:HA	2:B:302:LYS:HD3	1.95	0.48
3:C:74:THR:HG23	3:C:128:ILE:O	2.14	0.48
5:E:114:ALA:O	5:E:117:SER:OG	2.23	0.48
16:Q:80:LYS:O	16:Q:84:THR:HG23	2.13	0.48
16:Q:268:ASN:HB3	16:Q:271:VAL:HG12	1.95	0.48
16:Q:854:GLN:HB2	16:Q:855:LYS:NZ	2.28	0.48
19:U:522:THR:O	19:U:524:LYS:N	2.46	0.48
20:V:97:ASN:ND2	20:V:98:VAL:O	2.46	0.48
21:W:89:ARG:HA	21:W:101:SER:HA	1.94	0.48
1:A:111:CYS:SG	1:A:114:CYS:HB2	2.54	0.48
1:A:330:GLN:C	1:A:332:SER:H	2.17	0.48
1:A:733:LEU:HB2	9:I:106:ASP:HB2	1.96	0.48
17:R:576:GLU:O	17:R:580:VAL:HG13	2.14	0.48
24:Z:548:GLY:CA	24:Z:562:ASN:HA	2.44	0.48
24:Z:615:ARG:HB2	24:Z:616:HIS:CD2	2.49	0.48
4:D:76:ASN:O	4:D:79:THR:OG1	2.31	0.48
7:G:49:THR:OG1	7:G:50:THR:N	2.47	0.48
15:P:40:A:C2	18:T:32:DT:N3	2.81	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:NZ	2.29	0.48
24:Z:342:ALA:HB1	24:Z:346:ARG:NH2	2.28	0.48
1:A:86:GLY:C	1:A:255:VAL:HG12	2.34	0.48
1:A:606:HIS:CG	1:A:607:SER:N	2.82	0.48
1:A:922:PHE:N	1:A:1052:ARG:HD2	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:THR:HG23	1:A:1214:VAL:HG22	1.94	0.48
1:A:1218:ARG:HH22	1:A:1253:GLU:HA	1.77	0.48
16:Q:211:LEU:HB2	16:Q:213:LYS:HE3	1.94	0.48
16:Q:346:GLY:HA2	16:Q:349:GLN:HE21	1.79	0.48
16:Q:423:GLU:OE1	22:X:231:TRP:NE1	2.43	0.48
16:Q:568:TRP:CE2	16:Q:592:LEU:HD13	2.49	0.48
17:R:366:ARG:HH22	24:Z:773:SER:H	1.62	0.48
18:T:7:DA:H2"	18:T:8:DG:C8	2.48	0.48
21:W:76:LEU:HG	21:W:78:ILE:HG23	1.95	0.48
21:W:130:VAL:HG22	21:W:151:ILE:HG13	1.95	0.48
24:Z:206:THR:HG23	24:Z:208:THR:H	1.79	0.48
2:B:425:ARG:HH21	2:B:427:LYS:HD3	1.78	0.48
16:Q:542:ARG:NH2	16:Q:574:LEU:HA	2.28	0.48
17:R:359:LEU:HD22	17:R:452:PHE:CE1	2.48	0.48
17:R:370:GLU:HA	17:R:373:CYS:SG	2.54	0.48
21:W:46:VAL:HG11	21:W:58:TRP:HD1	1.78	0.48
21:W:89:ARG:HG2	21:W:101:SER:OG	2.13	0.48
21:W:110:TRP:CD2	21:W:150:PHE:HZ	2.32	0.48
24:Z:310:ARG:CZ	24:Z:337:GLN:HB2	2.44	0.48
24:Z:366:TYR:HB2	24:Z:374:LYS:HA	1.95	0.48
1:A:104:MET:CE	1:A:193:ARG:HD2	2.44	0.48
1:A:488:VAL:O	1:A:491:PRO:HD2	2.14	0.48
1:A:1129:ASN:O	1:A:1131:SER:N	2.47	0.48
1:A:1263:ASN:N	1:A:1263:ASN:OD1	2.47	0.48
2:B:355:ASP:OD2	2:B:356:PHE:N	2.46	0.48
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.48
14:N:12:DG:C4	14:N:13:DG:C8	3.02	0.48
16:Q:153:HIS:HA	16:Q:169:LYS:HE3	1.96	0.48
16:Q:568:TRP:CZ2	16:Q:591:ILE:HB	2.48	0.48
16:Q:645:LYS:HD2	22:X:242:GLY:O	2.14	0.48
16:Q:835:ASP:O	16:Q:839:ARG:HG3	2.14	0.48
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.96	0.48
1:A:557:ARG:O	1:A:561:MET:HG3	2.14	0.48
1:A:1162:GLU:HG2	1:A:1163:HIS:N	2.29	0.48
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.95	0.48
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.49	0.48
7:G:38:CYS:SG	7:G:39:THR:N	2.87	0.48
7:G:82:GLY:N	7:G:147:ILE:O	2.34	0.48
7:G:101:ILE:N	7:G:104:MET:O	2.43	0.48
8:H:15:ILE:O	8:H:16:ASP:C	2.51	0.48
8:H:106:THR:OG1	8:H:107:GLU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:232:VAL:O	16:Q:236:VAL:HG22	2.13	0.48
16:Q:390:ASP:HB2	16:Q:392:GLU:OE1	2.14	0.48
16:Q:578:LYS:HB2	16:Q:580:GLU:HG3	1.94	0.48
16:Q:682:ASP:OD1	16:Q:683:VAL:HG13	2.14	0.48
16:Q:844:LYS:O	16:Q:848:GLU:HG3	2.14	0.48
17:R:359:LEU:HD11	17:R:386:PHE:CE2	2.49	0.48
19:U:443:TRP:HA	20:V:201:PRO:HA	1.95	0.48
21:W:237:ASN:ND2	21:W:279:GLY:HA2	2.21	0.48
21:W:248:VAL:HG13	21:W:282:TYR:OH	2.14	0.48
21:W:254:LYS:HB3	21:W:273:HIS:O	2.14	0.48
24:Z:426:VAL:HG13	24:Z:440:ILE:HD11	1.95	0.48
1:A:495:ASP:HB3	1:A:499:ASP:OD2	2.14	0.47
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.95	0.47
1:A:1245:CYS:O	1:A:1246:ILE:HD13	2.13	0.47
1:A:1416:ARG:O	1:A:1420:ASN:HB2	2.14	0.47
3:C:92:GLU:HG2	24:Z:711:ARG:CZ	2.43	0.47
16:Q:39:THR:OG1	16:Q:43:ILE:HD13	2.14	0.47
16:Q:576:LEU:CD2	16:Q:585:GLN:HE22	2.27	0.47
16:Q:850:GLU:O	16:Q:854:GLN:NE2	2.44	0.47
17:R:363:ARG:HA	17:R:386:PHE:O	2.14	0.47
17:R:485:TYR:OH	17:R:489:ASP:OD2	2.32	0.47
1:A:141:LEU:HB2	1:A:236:LEU:O	2.14	0.47
2:B:108:MET:HE2	2:B:113:ALA:HB2	1.96	0.47
2:B:166:LEU:HG	2:B:170:ASP:HB2	1.96	0.47
2:B:320:PHE:O	2:B:323:SER:OG	2.31	0.47
2:B:719:SER:OG	2:B:720:PRO:HD3	2.13	0.47
2:B:768:ARG:HG3	2:B:771:GLU:OE2	2.15	0.47
7:G:109:SER:HB2	24:Z:503:PHE:CE2	2.48	0.47
16:Q:128:GLN:NE2	20:V:86:LEU:HD13	2.26	0.47
16:Q:336:ALA:HB1	16:Q:339:SER:OG	2.14	0.47
16:Q:358:GLU:O	16:Q:361:SER:OG	2.32	0.47
16:Q:689:HIS:HA	16:Q:692:VAL:HG12	1.96	0.47
16:Q:753:LEU:O	16:Q:757:VAL:HG13	2.14	0.47
1:A:46:THR:HB	1:A:58:MET:HB2	1.96	0.47
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.95	0.47
1:A:1177:TYR:HD2	9:I:28:GLU:OE1	1.97	0.47
2:B:44:LEU:HD23	2:B:155:MET:CE	2.44	0.47
5:E:2:ASP:OD2	5:E:3:ASP:N	2.47	0.47
10:J:64:PRO:HG2	10:J:65:LEU:H	1.78	0.47
21:W:191:MET:HB2	21:W:209:SER:HB3	1.96	0.47
1:A:10:ASP:O	2:B:1130:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG13	1:A:429:LEU:HD11	1.97	0.47
1:A:514:GLU:OE1	2:B:1101:GLN:HB2	2.14	0.47
1:A:527:THR:HG22	1:A:532:ARG:O	2.14	0.47
1:A:760:LEU:HD22	1:A:764:ASN:HD22	1.79	0.47
1:A:1060:LEU:HA	1:A:1060:LEU:HD23	1.60	0.47
1:A:1083:PRO:HD2	6:F:58:THR:HG21	1.96	0.47
3:C:2:PRO:HB3	11:K:54:PRO:CD	2.44	0.47
5:E:78:GLU:OE1	5:E:78:GLU:N	2.48	0.47
8:H:45:ILE:HA	8:H:45:ILE:HD12	1.68	0.47
16:Q:143:ASP:N	16:Q:143:ASP:OD1	2.44	0.47
21:W:112:LEU:HB3	21:W:121:LEU:HD11	1.96	0.47
24:Z:626:CYS:HB3	24:Z:629:LEU:HD12	1.95	0.47
2:B:313:GLU:HG2	2:B:316:VAL:HG12	1.95	0.47
2:B:680:ASP:O	2:B:684:GLU:HG2	2.14	0.47
4:D:93:HIS:HB3	4:D:96:GLU:OE1	2.14	0.47
7:G:4:HIS:CG	7:G:73:LYS:HE3	2.50	0.47
16:Q:172:ILE:HG22	16:Q:176:LYS:HZ1	1.79	0.47
16:Q:786:LEU:HD21	16:Q:820:LEU:HB3	1.96	0.47
17:R:363:ARG:HG3	17:R:447:PHE:CZ	2.49	0.47
17:R:587:LYS:O	17:R:588:ASN:ND2	2.48	0.47
1:A:199:TYR:CE2	1:A:215:LEU:HD13	2.49	0.47
7:G:119:PHE:HA	7:G:128:TYR:CD1	2.49	0.47
15:P:39:A:H2'	15:P:39:A:N3	2.29	0.47
16:Q:68:ARG:HE	16:Q:86:LEU:HD13	1.80	0.47
1:A:70:ARG:HD2	2:B:1131:ARG:HH12	1.79	0.47
1:A:416:ALA:HA	1:A:448:ARG:HA	1.97	0.47
1:A:513:ALA:O	1:A:517:GLU:HG2	2.14	0.47
1:A:1027:ASP:HB3	1:A:1030:SER:HB3	1.96	0.47
1:A:1177:TYR:CD2	9:I:28:GLU:OE1	2.68	0.47
2:B:170:ASP:N	2:B:170:ASP:OD1	2.43	0.47
2:B:1007:ASN:O	2:B:1011:ILE:HG13	2.14	0.47
14:N:12:DG:C6	14:N:13:DG:C6	3.02	0.47
16:Q:76:ARG:HH11	16:Q:76:ARG:HG3	1.80	0.47
16:Q:366:LYS:HG3	16:Q:369:LYS:HZ3	1.79	0.47
16:Q:721:LEU:HD11	20:V:31:CYS:HA	1.97	0.47
16:Q:737:LYS:HE3	16:Q:760:VAL:HG22	1.96	0.47
21:W:11:GLN:HB3	21:W:298:ILE:HB	1.97	0.47
24:Z:479:LYS:HD3	24:Z:521:CYS:HB2	1.96	0.47
1:A:724:GLU:OE1	1:A:724:GLU:N	2.47	0.47
1:A:951:GLU:HG2	1:A:1007:ILE:HD11	1.97	0.47
1:A:1236:ASN:O	1:A:1240:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1415:THR:O	1:A:1419:VAL:HG22	2.14	0.47
2:B:255:ARG:CD	2:B:307:GLU:HG3	2.44	0.47
2:B:347:MET:HG3	2:B:347:MET:O	2.15	0.47
4:D:62:MET:O	4:D:66:ASN:ND2	2.47	0.47
16:Q:167:LEU:HD21	16:Q:189:ALA:HB2	1.96	0.47
16:Q:373:ASN:HB2	16:Q:376:GLU:HG2	1.96	0.47
16:Q:750:ASP:OD1	16:Q:752:VAL:N	2.48	0.47
19:U:394:TYR:C	20:V:172:ARG:HH21	2.18	0.47
1:A:621:ILE:HG23	1:A:621:ILE:O	2.14	0.47
1:A:831:LEU:HB3	1:A:835:GLU:HG3	1.97	0.47
2:B:84:TYR:HA	2:B:132:VAL:HA	1.97	0.47
4:D:79:THR:O	4:D:82:SER:OG	2.33	0.47
7:G:147:ILE:HG23	7:G:159:ALA:HB1	1.96	0.47
15:P:38:G:C2'	15:P:39:A:H8	2.24	0.47
16:Q:347:LEU:HB2	16:Q:363:CYS:SG	2.54	0.47
16:Q:411:ASP:HB3	16:Q:415:TRP:CZ3	2.50	0.47
16:Q:624:LYS:HA	16:Q:627:ARG:HE	1.79	0.47
16:Q:712:TYR:O	16:Q:713:LYS:HG3	2.15	0.47
16:Q:833:LYS:O	16:Q:836:GLU:HG3	2.15	0.47
17:R:573:VAL:O	17:R:576:GLU:HG3	2.15	0.47
21:W:5:TYR:CE1	21:W:303:CYS:HB3	2.50	0.47
24:Z:433:LEU:HD13	24:Z:461:LEU:HD13	1.96	0.47
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	1.97	0.47
2:B:690:CYS:SG	2:B:693:TYR:CZ	3.08	0.47
2:B:1136:GLU:CB	2:B:1143:LYS:HG2	2.44	0.47
7:G:113:ILE:HG22	7:G:114:PRO:O	2.15	0.47
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.97	0.47
9:I:84:HIS:CD2	9:I:125:GLU:OE1	2.68	0.47
16:Q:7:GLU:OE2	16:Q:18:GLU:HB3	2.14	0.47
16:Q:716:ASN:HB3	16:Q:719:VAL:HG22	1.96	0.47
20:V:96:PRO:HA	20:V:97:ASN:HA	1.57	0.47
24:Z:521:CYS:HB3	24:Z:523:GLU:OE1	2.15	0.47
1:A:71:CYS:HB3	1:A:74:CYS:O	2.15	0.46
1:A:239:GLU:HG3	1:A:240:PRO:HD2	1.96	0.46
1:A:1184:THR:C	1:A:1186:VAL:N	2.64	0.46
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
5:E:3:ASP:OD1	5:E:47:LYS:HD2	2.15	0.46
5:E:82:VAL:HG12	5:E:110:MET:CB	2.45	0.46
8:H:112:LEU:HA	8:H:112:LEU:HD23	1.59	0.46
12:L:16:ILE:HD12	12:L:27:GLU:OE2	2.16	0.46
13:M:848:VAL:O	13:M:883:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:DT:H2"	14:N:43:DG:C8	2.51	0.46
21:W:215:LYS:HG2	21:W:227:THR:HG22	1.97	0.46
23:Y:22:VAL:HB	23:Y:84:VAL:HG12	1.97	0.46
24:Z:547:VAL:HG12	24:Z:563:MET:SD	2.54	0.46
1:A:866:LYS:HG3	1:A:1432:PHE:CD1	2.49	0.46
1:A:1162:GLU:O	1:A:1300:GLY:HA3	2.15	0.46
2:B:425:ARG:NH2	2:B:427:LYS:HD3	2.30	0.46
4:D:48:ASN:HB3	4:D:57:LEU:HD11	1.97	0.46
7:G:5:ILE:O	7:G:73:LYS:HD2	2.15	0.46
13:M:1362:LYS:HD3	13:M:1363:GLY:N	2.31	0.46
16:Q:211:LEU:HB2	16:Q:213:LYS:HZ2	1.80	0.46
16:Q:380:ILE:HB	16:Q:400:HIS:CE1	2.50	0.46
24:Z:571:ARG:H	24:Z:574:ALA:HB3	1.80	0.46
1:A:1474:LEU:HD12	6:F:105:ILE:HD11	1.97	0.46
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.61	0.46
11:K:7:PHE:CD2	11:K:11:LEU:HD12	2.50	0.46
13:M:1447:LEU:HA	13:M:1450:THR:HG22	1.97	0.46
15:P:43:C:H2'	15:P:44:A:O4'	2.16	0.46
16:Q:30:VAL:HA	16:Q:33:ILE:HG12	1.96	0.46
16:Q:830:ARG:HH21	16:Q:834:GLN:HG3	1.79	0.46
17:R:562:TYR:HB3	17:R:566:ARG:HH21	1.80	0.46
24:Z:340:PHE:HD2	24:Z:370:GLY:HA2	1.81	0.46
1:A:93:PRO:HG2	1:A:219:GLU:OE2	2.15	0.46
1:A:228:ILE:HG23	1:A:232:GLU:HG2	1.96	0.46
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.97	0.46
2:B:285:LEU:HD23	9:I:16:PHE:CZ	2.51	0.46
2:B:329:GLY:HA3	2:B:334:LYS:HB3	1.97	0.46
3:C:78:ILE:H	3:C:78:ILE:HG12	1.48	0.46
5:E:63:ALA:HB3	16:Q:880:GLN:HE22	1.80	0.46
5:E:153:LYS:O	5:E:157:THR:HG23	2.14	0.46
7:G:82:GLY:HA2	7:G:146:LYS:HE3	1.96	0.46
9:I:29:ASP:CB	9:I:34:ILE:HG13	2.45	0.46
16:Q:637:LYS:O	16:Q:641:ARG:HD3	2.15	0.46
21:W:151:ILE:HG23	21:W:165:SER:OG	2.15	0.46
1:A:1176:TYR:HD1	9:I:51:SER:O	1.99	0.46
1:A:1177:TYR:CE2	1:A:1210:TRP:HE3	2.34	0.46
1:A:1416:ARG:HD2	1:A:1434:GLU:OE2	2.15	0.46
2:B:566:LYS:HA	2:B:576:ILE:HD12	1.97	0.46
2:B:646:ARG:O	2:B:647:GLU:HG2	2.16	0.46
16:Q:386:ALA:HB1	16:Q:394:ARG:HG3	1.97	0.46
16:Q:452:GLU:OE1	16:Q:490:HIS:NE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:527:HIS:CE1	22:X:220:VAL:HB	2.51	0.46
16:Q:834:GLN:O	16:Q:838:GLU:HG2	2.15	0.46
1:A:609:HIS:HA	1:A:626:THR:HG21	1.98	0.46
1:A:1150:ASP:OD1	1:A:1150:ASP:N	2.48	0.46
1:A:1305:SER:OG	1:A:1306:LYS:N	2.48	0.46
2:B:26:CYS:O	2:B:30:ILE:HG12	2.15	0.46
8:H:67:ASP:OD1	8:H:67:ASP:N	2.46	0.46
9:I:17:CYS:SG	9:I:18:GLN:N	2.89	0.46
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.16	0.46
10:J:26:GLN:HA	17:R:566:ARG:HD2	1.98	0.46
16:Q:41:LEU:HD13	16:Q:75:TYR:HE2	1.81	0.46
16:Q:460:LEU:O	16:Q:464:LEU:HG	2.14	0.46
16:Q:855:LYS:HD3	16:Q:855:LYS:HA	1.59	0.46
17:R:574:GLU:HA	17:R:577:LYS:NZ	2.31	0.46
19:U:443:TRP:NE1	19:U:449:SER:OG	2.47	0.46
21:W:152:LEU:N	21:W:166:GLY:O	2.34	0.46
21:W:252:SER:HA	21:W:276:GLN:HB3	1.98	0.46
24:Z:182:VAL:O	24:Z:224:TYR:HB2	2.14	0.46
1:A:123:ASN:HB3	1:A:125:LYS:HG2	1.98	0.46
1:A:1547:SEP:HA	1:A:1548:PRO:HD3	1.78	0.46
2:B:133:ILE:HD12	2:B:139:GLN:HB3	1.98	0.46
2:B:548:TRP:CZ2	2:B:586:THR:HG21	2.51	0.46
7:G:111:HIS:ND1	24:Z:494:ARG:HB3	2.31	0.46
8:H:30:CYS:SG	8:H:56:PHE:HZ	2.39	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.16	0.46
16:Q:566:ASP:OD1	22:X:234:ARG:HD3	2.16	0.46
18:T:30:DG:H2'	18:T:31:DT:C6	2.50	0.46
19:U:469:ASN:HA	20:V:222:ARG:HA	1.98	0.46
21:W:46:VAL:CB	21:W:58:TRP:HB2	2.45	0.46
21:W:182:LEU:HD21	21:W:185:THR:OG1	2.16	0.46
21:W:233:SER:HB3	21:W:253:ASP:HB3	1.98	0.46
24:Z:571:ARG:HB2	24:Z:574:ALA:HB2	1.98	0.46
1:A:732:THR:HG23	1:A:735:GLN:OE1	2.14	0.46
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.56	0.46
1:A:1176:TYR:C	1:A:1177:TYR:HD1	2.19	0.46
16:Q:386:ALA:HB2	16:Q:393:LYS:CB	2.46	0.46
16:Q:563:ASP:O	16:Q:565:PRO:HD3	2.15	0.46
16:Q:803:MET:HE1	16:Q:807:LEU:HD11	1.98	0.46
24:Z:182:VAL:HG23	24:Z:225:ILE:HG13	1.98	0.46
24:Z:239:ILE:O	24:Z:242:VAL:HG22	2.15	0.46
24:Z:539:LEU:O	24:Z:578:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:CZ	1:A:220:ARG:NH1	2.84	0.46
5:E:126:ILE:H	5:E:126:ILE:HD12	1.81	0.46
6:F:57:MET:HB2	6:F:123:LEU:HD13	1.98	0.46
8:H:143:LEU:HD12	8:H:143:LEU:HA	1.62	0.46
10:J:25:LEU:HD23	17:R:567:ASN:HD21	1.81	0.46
16:Q:265:ASP:OD1	16:Q:268:ASN:HB2	2.16	0.46
16:Q:289:GLN:O	16:Q:293:LEU:HD23	2.16	0.46
16:Q:872:LYS:O	16:Q:875:LEU:HG	2.16	0.46
18:T:37:DC:H6	18:T:37:DC:H5'	1.81	0.46
18:T:41:DC:H4'	24:Z:283:ARG:NE	2.21	0.46
20:V:88:ASN:O	20:V:90:ASP:N	2.49	0.46
21:W:86:ALA:HB1	21:W:105:GLY:HA2	1.97	0.46
24:Z:705:LEU:HD21	24:Z:747:ARG:HD2	1.96	0.46
1:A:37:THR:O	1:A:37:THR:OG1	2.30	0.46
1:A:117:LEU:HD21	1:A:232:GLU:HG3	1.98	0.46
1:A:347:GLU:HA	1:A:352:GLY:HA3	1.98	0.46
1:A:753:GLY:O	1:A:757:GLN:HG2	2.16	0.46
1:A:1379:GLU:O	1:A:1379:GLU:HG2	2.16	0.46
3:C:60:HIS:HB3	3:C:61:ASP:H	1.33	0.46
16:Q:208:PHE:CD1	16:Q:213:LYS:HD2	2.51	0.46
16:Q:450:PRO:HB2	16:Q:452:GLU:HG2	1.98	0.46
19:U:378:LEU:HD23	19:U:382:LEU:O	2.16	0.46
24:Z:280:ARG:HG3	24:Z:386:VAL:HG13	1.98	0.46
24:Z:294:ASP:HB2	24:Z:306:LYS:HE2	1.98	0.46
24:Z:480:VAL:HG13	24:Z:487:GLY:H	1.81	0.46
1:A:465:HIS:HB3	1:A:1097:GLU:HG3	1.97	0.45
1:A:966:LEU:HA	1:A:966:LEU:HD23	1.74	0.45
1:A:971:PRO:O	1:A:972:THR:OG1	2.26	0.45
1:A:1117:VAL:HA	1:A:1136:THR:HG21	1.97	0.45
2:B:236:TRP:HB2	2:B:259:THR:HB	1.98	0.45
2:B:684:GLU:OE2	2:B:684:GLU:HA	2.16	0.45
12:L:52:LEU:HA	12:L:52:LEU:HD12	1.69	0.45
16:Q:620:ARG:NH1	16:Q:659:HIS:O	2.47	0.45
17:R:429:ARG:NE	17:R:431:GLY:O	2.42	0.45
21:W:13:GLN:H	21:W:297:GLU:HG2	1.80	0.45
22:X:253:LEU:O	22:X:256:VAL:HG12	2.16	0.45
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.99	0.45
1:A:124:PRO:HA	1:A:127:LYS:CG	2.45	0.45
1:A:1254:LYS:HD3	1:A:1254:LYS:HA	1.77	0.45
1:A:1298:LEU:HA	1:A:1298:LEU:HD23	1.77	0.45
2:B:121:SER:HA	2:B:153:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ARG:HD3	2:B:307:GLU:HG3	1.98	0.45
2:B:621:ILE:HD13	2:B:621:ILE:HG21	1.66	0.45
2:B:1006:VAL:HG22	20:V:130:TRP:CB	2.45	0.45
4:D:38:HIS:HB2	4:D:68:THR:OG1	2.16	0.45
11:K:71:ILE:HG21	11:K:71:ILE:HD13	1.61	0.45
16:Q:64:LEU:HA	16:Q:64:LEU:HD23	1.82	0.45
17:R:565:GLN:HA	17:R:568:ARG:CZ	2.47	0.45
20:V:38:SER:OG	20:V:39:LEU:N	2.49	0.45
21:W:7:ILE:HA	21:W:301:TYR:HA	1.98	0.45
21:W:233:SER:OG	21:W:252:SER:N	2.44	0.45
23:Y:35:ASN:ND2	23:Y:85:TYR:OH	2.49	0.45
24:Z:470:LYS:HB3	24:Z:472:PHE:CE2	2.51	0.45
1:A:189:PRO:HB2	1:A:201:GLU:H	1.81	0.45
1:A:989:ASN:O	1:A:993:ILE:HG13	2.16	0.45
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.99	0.45
2:B:317:ALA:O	2:B:321:ILE:HD12	2.15	0.45
2:B:681:ASP:OD2	2:B:681:ASP:N	2.50	0.45
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.62	0.45
14:N:12:DG:C4	14:N:13:DG:N7	2.84	0.45
1:A:1044:HIS:O	1:A:1048:THR:HG23	2.17	0.45
2:B:757:PRO:HB2	2:B:760:THR:HG22	1.99	0.45
3:C:92:GLU:HG2	24:Z:711:ARG:NH1	2.32	0.45
8:H:70:LEU:HD12	8:H:70:LEU:HA	1.76	0.45
9:I:73:SER:O	9:I:80:ARG:NH2	2.50	0.45
9:I:74:GLN:H	9:I:74:GLN:HG2	1.51	0.45
9:I:91:HIS:CD2	9:I:93:GLU:H	2.35	0.45
16:Q:474:PHE:CB	16:Q:503:LEU:HD13	2.46	0.45
16:Q:591:ILE:HG22	16:Q:592:LEU:HD12	1.97	0.45
23:Y:116:LYS:HD3	23:Y:116:LYS:HA	1.74	0.45
24:Z:469:ARG:NH2	24:Z:497:GLU:O	2.49	0.45
1:A:775:LYS:HD2	2:B:974:SER:HB3	1.97	0.45
2:B:332:LYS:HB3	2:B:332:LYS:HE3	1.57	0.45
2:B:388:TYR:HB2	2:B:504:THR:HG23	1.99	0.45
2:B:395:LEU:HA	2:B:395:LEU:HD23	1.67	0.45
3:C:44:ILE:HD13	3:C:44:ILE:HG21	1.48	0.45
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.50	0.45
21:W:235:VAL:HA	21:W:251:SER:HA	1.98	0.45
23:Y:66:PRO:HD3	23:Y:82:PRO:HG3	1.98	0.45
2:B:834:ARG:HH22	2:B:842:HIS:HA	1.80	0.45
14:N:12:DG:N1	18:T:38:DG:N2	2.64	0.45
16:Q:246:LYS:HD2	16:Q:246:LYS:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:620:ARG:HH22	16:Q:660:LYS:HA	1.81	0.45
17:R:388:ARG:HD3	17:R:445:GLN:HB2	1.99	0.45
17:R:570:TRP:CD1	20:V:133:LYS:HD2	2.43	0.45
20:V:103:ALA:O	20:V:107:LEU:HG	2.17	0.45
21:W:29:LYS:HE2	21:W:75:THR:HA	1.99	0.45
22:X:222:ARG:HA	22:X:225:VAL:HG22	1.97	0.45
23:Y:65:SER:O	23:Y:65:SER:OG	2.33	0.45
1:A:111:CYS:HG	1:A:114:CYS:HB2	1.81	0.45
1:A:825:ASN:ND2	1:A:835:GLU:OE1	2.47	0.45
1:A:1369:LEU:HD23	1:A:1369:LEU:HA	1.73	0.45
2:B:1134:THR:HG23	2:B:1134:THR:O	2.17	0.45
4:D:74:PHE:CE2	4:D:80:ILE:HG12	2.52	0.45
16:Q:763:ARG:HE	20:V:25:GLU:N	2.14	0.45
17:R:566:ARG:HA	17:R:569:GLU:OE1	2.16	0.45
21:W:56:LEU:HD21	21:W:59:SER:OG	2.16	0.45
24:Z:546:THR:HG22	24:Z:547:VAL:N	2.32	0.45
1:A:291:ARG:HG3	1:A:292:ARG:N	2.32	0.45
1:A:1226:LEU:HA	1:A:1230:GLN:NE2	2.31	0.45
2:B:357:CYS:SG	2:B:360:LYS:NZ	2.85	0.45
2:B:651:TYR:N	19:U:460:TYR:OH	2.49	0.45
2:B:714:PRO:CD	2:B:1001:PRO:HG3	2.47	0.45
2:B:1104:ARG:O	2:B:1108:PHE:HB3	2.16	0.45
3:C:45:ILE:HG22	3:C:165:ALA:HB1	1.98	0.45
4:D:32:LEU:HD23	4:D:32:LEU:HA	1.83	0.45
12:L:22:CYS:SG	12:L:39:CYS:SG	3.06	0.45
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.90	0.45
16:Q:123:ILE:HG23	16:Q:124:ILE:H	1.82	0.45
16:Q:134:ARG:HA	16:Q:134:ARG:HD2	1.76	0.45
16:Q:170:ALA:HB2	16:Q:185:TYR:HB2	1.99	0.45
17:R:402:VAL:HG23	17:R:451:GLU:HG2	1.98	0.45
20:V:190:ILE:O	20:V:190:ILE:HG13	2.17	0.45
21:W:64:GLN:OE1	21:W:89:ARG:NH2	2.48	0.45
24:Z:243:GLY:O	24:Z:246:ARG:HG2	2.17	0.45
2:B:319:ASN:HD21	2:B:332:LYS:HG2	1.82	0.45
8:H:64:LEU:HD23	8:H:64:LEU:HA	1.79	0.45
16:Q:386:ALA:HB2	16:Q:393:LYS:HB3	1.99	0.45
17:R:356:PRO:HB3	17:R:452:PHE:CB	2.47	0.45
1:A:557:ARG:HG3	1:A:558:GLY:N	2.27	0.45
2:B:479:LEU:O	2:B:483:ARG:HG3	2.17	0.45
5:E:185:ILE:HD12	5:E:209:VAL:HG21	1.98	0.45
16:Q:95:GLN:HG3	20:V:85:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:131:LEU:HD12	16:Q:155:VAL:HG22	1.98	0.45
16:Q:133:GLY:HA2	16:Q:136:CYS:SG	2.57	0.45
16:Q:200:VAL:HA	20:V:82:VAL:HG22	1.97	0.45
16:Q:380:ILE:HG21	16:Q:396:ILE:HD12	1.98	0.45
16:Q:568:TRP:CE3	16:Q:592:LEU:HB2	2.51	0.45
16:Q:736:CYS:O	16:Q:739:THR:HG22	2.17	0.45
23:Y:8:LYS:HE2	23:Y:27:GLN:NE2	2.32	0.45
24:Z:272:ASN:ND2	24:Z:384:GLU:HB2	2.32	0.45
24:Z:729:GLU:O	24:Z:747:ARG:NH2	2.50	0.45
1:A:74:CYS:SG	1:A:81:CYS:HB2	2.56	0.44
1:A:902:GLU:O	1:A:978:VAL:HA	2.17	0.44
1:A:1040:LEU:HA	1:A:1040:LEU:HD12	1.75	0.44
1:A:1118:THR:HG21	1:A:1135:LYS:HB2	1.99	0.44
1:A:1184:THR:O	1:A:1184:THR:OG1	2.28	0.44
2:B:655:ASP:O	2:B:659:SER:HB3	2.17	0.44
7:G:4:HIS:CD2	7:G:73:LYS:HE3	2.52	0.44
8:H:111:ARG:HA	8:H:128:ASP:HA	1.99	0.44
15:P:37:G:H2'	15:P:38:G:C8	2.52	0.44
20:V:75:LEU:HD12	20:V:75:LEU:HA	1.82	0.44
21:W:37:THR:HA	21:W:70:VAL:HG21	1.99	0.44
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.73	0.44
1:A:465:HIS:NE2	1:A:467:MET:HB2	2.31	0.44
2:B:67:LEU:HD13	2:B:420:GLN:OE1	2.17	0.44
4:D:93:HIS:CE1	4:D:94:LYS:HG3	2.52	0.44
14:N:44:DG:H2"	14:N:45:DG:C8	2.51	0.44
16:Q:716:ASN:OD1	16:Q:717:THR:N	2.50	0.44
17:R:428:LEU:HB2	17:R:437:PHE:CE2	2.52	0.44
23:Y:19:CYS:SG	23:Y:35:ASN:ND2	2.84	0.44
24:Z:280:ARG:HB2	24:Z:382:ILE:HG23	2.00	0.44
1:A:299:ALA:C	1:A:301:HIS:H	2.20	0.44
2:B:139:GLN:OE1	2:B:139:GLN:N	2.49	0.44
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.99	0.44
3:C:48:ASP:OD1	3:C:175:LYS:NZ	2.51	0.44
16:Q:667:ARG:HD3	16:Q:691:TYR:HE1	1.83	0.44
17:R:353:VAL:HG23	17:R:456:LYS:NZ	2.32	0.44
18:T:11:DC:H2"	18:T:12:DC:C6	2.51	0.44
21:W:203:GLN:OE1	21:W:204:LEU:HG	2.17	0.44
21:W:295:ASP:O	21:W:297:GLU:HG3	2.17	0.44
23:Y:76:ARG:HH11	23:Y:109:LYS:HD3	1.83	0.44
24:Z:639:LYS:HB2	24:Z:642:HIS:HB2	1.99	0.44
2:B:92:TYR:N	2:B:92:TYR:CD2	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.78	0.44
3:C:107:CYS:HB3	3:C:154:ARG:O	2.17	0.44
14:N:42:DT:C2	14:N:43:DG:C6	3.06	0.44
16:Q:415:TRP:HA	16:Q:418:LEU:HD12	2.00	0.44
16:Q:868:LYS:HD3	16:Q:868:LYS:HA	1.79	0.44
17:R:353:VAL:HG11	17:R:472:ILE:HD12	1.99	0.44
24:Z:258:LYS:HB3	24:Z:258:LYS:HE2	1.73	0.44
24:Z:614:ILE:HA	24:Z:624:LEU:HA	1.98	0.44
1:A:59:ASP:OD2	1:A:61:ARG:HB2	2.18	0.44
1:A:1124:LEU:HA	1:A:1124:LEU:HD12	1.67	0.44
1:A:1168:LYS:HA	1:A:1168:LYS:HD2	1.89	0.44
2:B:652:SER:N	2:B:655:ASP:OD1	2.38	0.44
2:B:737:ILE:HD12	2:B:737:ILE:HA	1.79	0.44
5:E:97:GLU:OE1	5:E:97:GLU:N	2.50	0.44
5:E:99:ILE:O	5:E:99:ILE:HG13	2.18	0.44
7:G:30:LEU:HD12	7:G:30:LEU:HA	1.72	0.44
16:Q:841:LEU:HA	16:Q:844:LYS:HG2	1.99	0.44
20:V:193:HIS:HB3	20:V:196:LYS:O	2.18	0.44
24:Z:479:LYS:O	24:Z:519:GLN:HG2	2.17	0.44
24:Z:489:THR:HB	24:Z:505:ASP:OD2	2.17	0.44
1:A:602:CYS:SG	1:A:652:LEU:HD13	2.57	0.44
1:A:982:ASN:HD22	1:A:985:ARG:HB2	1.83	0.44
2:B:897:ARG:CB	2:B:900:GLU:HG3	2.48	0.44
8:H:40:ILE:O	8:H:123:MET:HA	2.17	0.44
15:P:40:A:H2'	15:P:41:C:H6	1.77	0.44
17:R:366:ARG:HH12	24:Z:775:TPO:HA	1.83	0.44
1:A:249:ILE:HG13	1:A:249:ILE:O	2.16	0.44
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.70	0.44
5:E:37:LEU:HD21	5:E:41:LYS:HZ3	1.82	0.44
14:N:31:DC:H2"	14:N:32:DA:H8	1.80	0.44
16:Q:847:GLN:O	16:Q:851:LEU:HG	2.17	0.44
20:V:127:VAL:HG23	20:V:128:VAL:N	2.32	0.44
21:W:65:LEU:HD12	21:W:84:LEU:C	2.38	0.44
24:Z:242:VAL:HG23	24:Z:245:LEU:HB2	2.00	0.44
1:A:198:LEU:O	1:A:215:LEU:HD12	2.18	0.44
2:B:650:ASN:C	19:U:460:TYR:CE2	2.91	0.44
13:M:540:GLY:HA2	13:M:560:GLU:H	1.83	0.44
16:Q:128:GLN:HA	16:Q:158:GLN:HE22	1.82	0.44
16:Q:750:ASP:OD1	16:Q:753:LEU:N	2.40	0.44
16:Q:870:GLU:HA	16:Q:873:LYS:NZ	2.32	0.44
17:R:455:TRP:O	17:R:459:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:171:ILE:HG23	21:W:187:GLU:HG2	1.99	0.44
21:W:253:ASP:OD1	21:W:253:ASP:N	2.51	0.44
24:Z:499:PHE:HB3	24:Z:512:LYS:HD2	2.00	0.44
1:A:365:THR:HG22	1:A:366:VAL:N	2.31	0.44
1:A:676:ILE:HD12	1:A:676:ILE:HG23	1.76	0.44
1:A:1467:GLY:C	1:A:1469:GLY:H	2.21	0.44
2:B:1151:MET:HE2	2:B:1151:MET:HB2	1.71	0.44
6:F:105:ILE:HG21	6:F:105:ILE:HD13	1.63	0.44
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.80	0.44
14:N:37:DG:C2	18:T:12:DC:N3	2.86	0.44
15:P:39:A:N1	15:P:40:A:C6	2.86	0.44
16:Q:527:HIS:CD2	16:Q:530:TYR:HB2	2.53	0.44
16:Q:677:THR:HG22	16:Q:679:ASP:H	1.83	0.44
20:V:182:THR:HA	20:V:185:ASP:OD2	2.17	0.44
21:W:17:ASP:OD2	21:W:40:LEU:HB3	2.17	0.44
1:A:488:VAL:O	1:A:488:VAL:HG12	2.18	0.43
1:A:812:LYS:HE2	9:I:77:THR:HG23	1.99	0.43
1:A:1484:MET:N	1:A:1484:MET:SD	2.91	0.43
2:B:332:LYS:HZ1	2:B:333:GLU:HB2	1.83	0.43
2:B:556:ILE:HD12	2:B:556:ILE:HA	1.59	0.43
4:D:60:VAL:HG11	7:G:44:PHE:HZ	1.83	0.43
5:E:58:LEU:HD23	5:E:58:LEU:H	1.81	0.43
5:E:61:LEU:HA	5:E:61:LEU:HD12	1.77	0.43
7:G:151:ARG:HH11	24:Z:477:HIS:CD2	2.36	0.43
8:H:11:ASP:HB3	8:H:55:LYS:HG2	2.00	0.43
16:Q:513:PHE:HB2	21:W:213:TYR:CE1	2.53	0.43
16:Q:530:TYR:CE2	16:Q:532:ASP:HB2	2.53	0.43
21:W:191:MET:HG3	21:W:211:ASP:HB3	1.99	0.43
1:A:539:GLN:O	1:A:540:ASP:C	2.56	0.43
2:B:705:GLY:O	2:B:709:SER:HB3	2.18	0.43
4:D:93:HIS:HE1	4:D:94:LYS:HE3	1.83	0.43
7:G:131:MET:SD	7:G:131:MET:N	2.92	0.43
10:J:60:LEU:HD23	10:J:60:LEU:HA	1.79	0.43
13:M:1398:LEU:HD11	13:M:1415:TYR:CD1	2.53	0.43
13:M:1435:CYS:SG	13:M:1442:LYS:HG2	2.58	0.43
16:Q:120:ALA:HB1	16:Q:130:HIS:HE1	1.83	0.43
16:Q:538:GLY:HA2	16:Q:553:TRP:HE3	1.83	0.43
18:T:47:DG:H2"	18:T:48:DG:H5'	1.99	0.43
20:V:106:LYS:HA	20:V:106:LYS:HD2	1.87	0.43
21:W:281:LYS:HD2	21:W:281:LYS:HA	1.80	0.43
24:Z:389:THR:O	24:Z:393:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:593:ASN:HB3	24:Z:595:HIS:CE1	2.54	0.43
1:A:75:ALA:O	2:B:1131:ARG:NH1	2.52	0.43
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.18	0.43
2:B:1173:SER:O	2:B:1173:SER:OG	2.36	0.43
4:D:137:LYS:HA	4:D:137:LYS:HD3	1.83	0.43
9:I:53:ILE:HA	9:I:53:ILE:HD13	1.70	0.43
13:M:1476:TYR:CE2	13:M:1483:ARG:HD3	2.54	0.43
16:Q:218:ARG:HD3	16:Q:238:LEU:HD11	2.00	0.43
16:Q:710:LYS:HB2	16:Q:712:TYR:CE1	2.52	0.43
24:Z:188:GLU:OE1	24:Z:188:GLU:N	2.51	0.43
24:Z:420:PHE:HE1	24:Z:470:LYS:HG2	1.83	0.43
24:Z:464:PRO:HD2	24:Z:467:GLU:HB3	1.99	0.43
1:A:106:VAL:O	1:A:110:VAL:HG22	2.19	0.43
1:A:818:GLU:OE2	17:R:599:CYS:HA	2.18	0.43
1:A:996:ILE:HD13	1:A:996:ILE:HA	1.62	0.43
2:B:83:ARG:HH22	2:B:133:ILE:CG2	2.31	0.43
2:B:399:LEU:HA	2:B:399:LEU:HD23	1.80	0.43
2:B:576:ILE:HD12	2:B:576:ILE:HA	1.79	0.43
5:E:55:ARG:HA	5:E:58:LEU:CD2	2.48	0.43
16:Q:68:ARG:NH1	16:Q:82:GLN:HE22	2.16	0.43
16:Q:503:LEU:HG	16:Q:507:TYR:CE2	2.53	0.43
1:A:413:TYR:OH	1:A:450:MET:O	2.32	0.43
2:B:472:ARG:HA	2:B:472:ARG:HD2	1.92	0.43
2:B:497:LYS:HG3	2:B:498:PRO:CD	2.46	0.43
2:B:553:LEU:HA	2:B:553:LEU:HD12	1.73	0.43
5:E:3:ASP:OD1	5:E:49:SER:OG	2.20	0.43
5:E:27:LEU:HD12	5:E:27:LEU:HA	1.77	0.43
5:E:72:MET:HB2	5:E:72:MET:HE3	1.77	0.43
7:G:104:MET:HG3	7:G:157:ILE:O	2.19	0.43
16:Q:268:ASN:HD22	16:Q:271:VAL:HG12	1.84	0.43
16:Q:456:ASN:OD1	20:V:48:PHE:HA	2.18	0.43
16:Q:772:GLU:HB3	16:Q:774:SER:OG	2.18	0.43
16:Q:877:GLN:OE1	16:Q:881:TYR:CE1	2.72	0.43
17:R:359:LEU:HD22	17:R:452:PHE:HE1	1.84	0.43
17:R:456:LYS:NZ	17:R:466:LEU:HD13	2.33	0.43
21:W:40:LEU:HA	21:W:66:GLY:HA3	2.01	0.43
21:W:152:LEU:HD12	21:W:167:ALA:O	2.19	0.43
21:W:252:SER:HB3	21:W:276:GLN:OE1	2.18	0.43
24:Z:291:ALA:HB2	24:Z:307:MET:HG2	2.00	0.43
24:Z:502:LEU:HD21	24:Z:511:LEU:HD22	2.00	0.43
24:Z:557:THR:O	24:Z:558:PHE:CD1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:520:VAL:HG13	2:B:520:VAL:O	2.19	0.43
7:G:91:GLN:HB3	7:G:98:PHE:HD2	1.83	0.43
13:M:1037:ILE:H	13:M:1055:GLY:HA2	1.84	0.43
13:M:1341:LYS:HA	13:M:1341:LYS:HD2	1.85	0.43
14:N:10:DG:H2"	14:N:11:DC:C6	2.54	0.43
16:Q:69:ILE:H	16:Q:69:ILE:HD12	1.84	0.43
16:Q:239:ALA:O	16:Q:243:LEU:HG	2.17	0.43
16:Q:464:LEU:HB2	16:Q:466:ASN:HD22	1.84	0.43
16:Q:527:HIS:HD2	16:Q:530:TYR:HB2	1.83	0.43
16:Q:691:TYR:HB3	16:Q:699:SER:OG	2.19	0.43
23:Y:29:GLU:HG3	23:Y:45:ASN:O	2.19	0.43
24:Z:200:PHE:HA	24:Z:210:LEU:HD13	2.00	0.43
24:Z:540:VAL:HB	24:Z:575:VAL:CG2	2.49	0.43
1:A:417:LYS:HE2	1:A:418:TYR:CE2	2.53	0.43
1:A:479:TRP:CD1	1:A:479:TRP:N	2.87	0.43
2:B:472:ARG:HH11	2:B:472:ARG:HD3	1.65	0.43
2:B:679:PRO:HG2	2:B:680:ASP:N	2.33	0.43
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.00	0.43
3:C:94:CYS:SG	3:C:95:PRO:HD2	2.59	0.43
16:Q:762:GLN:O	16:Q:766:THR:HG22	2.18	0.43
1:A:37:THR:HG21	1:A:41:ILE:HD11	2.01	0.43
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.18	0.43
2:B:254:GLN:O	2:B:303:PRO:HB2	2.19	0.43
2:B:577:HIS:CE1	2:B:583:LEU:HD11	2.53	0.43
2:B:625:LEU:HA	2:B:625:LEU:HD23	1.87	0.43
2:B:866:ILE:HG23	2:B:866:ILE:HD12	1.57	0.43
2:B:1142:ASN:ND2	2:B:1145:GLN:HB2	2.27	0.43
7:G:151:ARG:HA	24:Z:477:HIS:CE1	2.54	0.43
8:H:15:ILE:HG23	8:H:16:ASP:N	2.33	0.43
11:K:12:LEU:HD23	11:K:12:LEU:HA	1.86	0.43
16:Q:380:ILE:HD12	16:Q:400:HIS:CE1	2.53	0.43
17:R:454:LYS:HA	17:R:454:LYS:HD2	1.77	0.43
2:B:100:GLU:HA	2:B:105:PRO:HB3	1.99	0.43
2:B:313:GLU:HG3	2:B:315:ASN:H	1.82	0.43
4:D:33:LEU:HD21	4:D:97:LEU:HD23	2.00	0.43
7:G:81:LYS:HG3	7:G:148:VAL:C	2.39	0.43
16:Q:471:LYS:O	16:Q:475:LEU:HD23	2.18	0.43
16:Q:484:GLU:HB2	16:Q:492:TYR:HB3	2.00	0.43
21:W:25:GLY:N	21:W:72:ILE:HD12	2.34	0.43
21:W:84:LEU:HD21	21:W:110:TRP:CZ3	2.53	0.43
21:W:231:HIS:CG	21:W:251:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HA	1:A:201:GLU:O	2.19	0.43
1:A:592:PHE:CD2	1:A:592:PHE:O	2.71	0.43
1:A:770:VAL:HG21	1:A:781:ILE:HD11	2.01	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.43
1:A:1006:PRO:O	1:A:1010:VAL:HG23	2.19	0.43
1:A:1551:ALA:O	13:M:1509:ARG:HD2	2.19	0.43
4:D:17:ALA:HB1	4:D:95:PHE:CZ	2.54	0.43
7:G:80:PHE:HB2	7:G:83:GLU:CD	2.40	0.43
16:Q:645:LYS:HE3	22:X:243:LYS:NZ	2.33	0.43
16:Q:651:ASN:HB3	20:V:37:ASN:HD21	1.82	0.43
16:Q:651:ASN:ND2	16:Q:682:ASP:OD2	2.52	0.43
16:Q:653:ILE:O	16:Q:656:VAL:HG22	2.19	0.43
17:R:378:PHE:CZ	17:R:382:VAL:HG11	2.54	0.43
18:T:35:DG:N2	18:T:36:DC:O2	2.51	0.43
19:U:459:VAL:HG23	19:U:494:HIS:C	2.39	0.43
24:Z:196:LEU:HD12	24:Z:196:LEU:HA	1.79	0.43
24:Z:478:VAL:O	24:Z:489:THR:HA	2.19	0.43
1:A:1132:LYS:H	1:A:1132:LYS:HG2	1.65	0.42
1:A:1463:LEU:HA	1:A:1463:LEU:HD12	1.59	0.42
2:B:501:LEU:HD12	2:B:505:LEU:HD12	2.01	0.42
2:B:1038:THR:HA	3:C:195:THR:HA	1.99	0.42
15:P:35:A:H5'	15:P:36:G:OP2	2.18	0.42
16:Q:689:HIS:HB2	20:V:35:TYR:HE1	1.84	0.42
16:Q:725:ARG:NE	20:V:31:CYS:SG	2.92	0.42
16:Q:729:LYS:HB2	16:Q:732:LYS:CD	2.46	0.42
16:Q:750:ASP:OD1	16:Q:753:LEU:HG	2.18	0.42
21:W:9:PHE:CE2	21:W:54:LEU:HB3	2.54	0.42
24:Z:261:THR:O	24:Z:264:LEU:HG	2.18	0.42
24:Z:492:ILE:HA	24:Z:502:LEU:HA	1.99	0.42
24:Z:602:VAL:HG21	24:Z:636:PHE:HE2	1.83	0.42
24:Z:705:LEU:HD12	24:Z:724:VAL:HG11	2.01	0.42
1:A:130:LEU:HD11	1:A:235:VAL:HG13	2.01	0.42
1:A:510:GLU:OE1	2:B:1101:GLN:NE2	2.52	0.42
1:A:639:ILE:HG21	1:A:639:ILE:HD13	1.81	0.42
1:A:1179:PRO:HA	1:A:1209:PRO:CB	2.49	0.42
1:A:1323:THR:HG22	1:A:1329:LYS:HD2	2.01	0.42
2:B:568:PHE:CE1	2:B:573:TRP:HB2	2.54	0.42
3:C:67:ARG:NH1	10:J:2:ILE:HG23	2.33	0.42
3:C:75:SER:HB3	3:C:79:VAL:HB	2.01	0.42
4:D:22:PHE:HB2	4:D:27:GLU:OE1	2.18	0.42
16:Q:508:GLU:OE2	16:Q:540:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:163:LEU:HB2	21:W:177:ILE:HG23	2.00	0.42
24:Z:439:LYS:O	24:Z:452:PRO:HA	2.19	0.42
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.52	0.42
1:A:1177:TYR:CE2	1:A:1210:TRP:CE3	3.06	0.42
2:B:186:ILE:HG21	2:B:186:ILE:HD13	1.74	0.42
3:C:268:GLN:HG3	3:C:269:SER:N	2.34	0.42
4:D:16:ASP:H	4:D:21:ILE:CG2	2.32	0.42
4:D:122:PHE:HD1	4:D:126:GLU:CD	2.23	0.42
16:Q:182:ALA:O	16:Q:186:TYR:CD2	2.72	0.42
16:Q:365:GLU:HG2	16:Q:369:LYS:NZ	2.34	0.42
16:Q:745:HIS:HB2	21:W:20:TRP:CH2	2.53	0.42
20:V:196:LYS:O	20:V:198:ARG:N	2.49	0.42
21:W:135:VAL:HG23	21:W:136:GLU:HG2	2.01	0.42
21:W:170:GLY:HA2	21:W:193:ILE:HG13	2.01	0.42
24:Z:525:ALA:O	24:Z:552:ARG:NH1	2.49	0.42
1:A:104:MET:HE1	1:A:193:ARG:HD2	2.01	0.42
1:A:338:SER:OG	1:A:341:GLN:HG2	2.20	0.42
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.55	0.42
1:A:421:ARG:HE	1:A:427:ILE:HD11	1.85	0.42
1:A:461:GLN:O	1:A:463:THR:N	2.52	0.42
1:A:1137:PRO:O	1:A:1341:VAL:HG23	2.20	0.42
7:G:127:CYS:SG	7:G:138:GLN:HB3	2.60	0.42
14:N:35:DA:H2"	14:N:36:DG:C8	2.53	0.42
16:Q:611:TRP:HZ2	16:Q:631:ARG:HH11	1.65	0.42
16:Q:880:GLN:HE21	16:Q:884:LYS:CE	2.32	0.42
17:R:578:ALA:HA	20:V:127:VAL:HB	2.01	0.42
1:A:427:ILE:N	1:A:427:ILE:HD12	2.35	0.42
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.85	0.42
1:A:820:ARG:HH11	1:A:820:ARG:HD3	1.66	0.42
1:A:1343:LEU:HD12	1:A:1343:LEU:HA	1.76	0.42
2:B:319:ASN:ND2	2:B:332:LYS:HG2	2.34	0.42
2:B:544:PHE:CE2	2:B:548:TRP:NE1	2.81	0.42
2:B:544:PHE:CZ	2:B:548:TRP:NE1	2.87	0.42
2:B:574:VAL:O	2:B:574:VAL:HG22	2.20	0.42
2:B:841:ARG:HD3	2:B:841:ARG:HA	1.77	0.42
13:M:1408:LEU:HD23	13:M:1408:LEU:H	1.84	0.42
13:M:1490:THR:OG1	13:M:1493:GLY:N	2.53	0.42
14:N:37:DG:C6	18:T:12:DC:N4	2.79	0.42
15:P:37:G:C2'	15:P:38:G:H8	2.33	0.42
16:Q:62:LYS:HA	16:Q:62:LYS:HD3	1.74	0.42
16:Q:240:VAL:HG11	20:V:72:HIS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:598:GLN:HA	16:Q:599:SER:HA	1.76	0.42
16:Q:719:VAL:HG23	16:Q:720:VAL:N	2.35	0.42
17:R:581:ALA:CB	20:V:127:VAL:HG21	2.48	0.42
21:W:11:GLN:HE21	21:W:54:LEU:HD23	1.85	0.42
21:W:288:LYS:HA	21:W:288:LYS:HD3	1.77	0.42
1:A:503:LEU:O	1:A:503:LEU:HD23	2.19	0.42
1:A:909:LEU:O	1:A:910:LYS:HG2	2.20	0.42
1:A:932:ARG:HD3	8:H:106:THR:O	2.19	0.42
1:A:1166:LEU:HA	1:A:1166:LEU:HD23	1.84	0.42
1:A:1401:LEU:O	1:A:1405:MET:HG3	2.19	0.42
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.71	0.42
2:B:428:ASP:OD1	2:B:429:PHE:N	2.52	0.42
2:B:638:ARG:HH21	2:B:639:HIS:CE1	2.38	0.42
2:B:1125:MET:HE3	2:B:1156:LYS:HG2	2.02	0.42
3:C:263:LEU:HD13	11:K:19:ILE:HD13	2.00	0.42
5:E:96:GLU:OE1	5:E:96:GLU:N	2.52	0.42
7:G:106:CYS:SG	7:G:159:ALA:HB3	2.59	0.42
11:K:101:LEU:HA	11:K:101:LEU:HD12	1.85	0.42
14:N:12:DG:C6	18:T:38:DG:N2	2.87	0.42
14:N:14:DC:OP2	24:Z:186:ILE:HD12	2.19	0.42
16:Q:384:LEU:HD11	16:Q:393:LYS:O	2.20	0.42
16:Q:542:ARG:HD2	16:Q:554:PHE:HE2	1.83	0.42
16:Q:553:TRP:HA	16:Q:556:GLU:OE1	2.19	0.42
17:R:397:LYS:O	24:Z:777:MET:HE3	2.19	0.42
17:R:429:ARG:HB2	17:R:434:GLN:HB3	2.02	0.42
17:R:492:ILE:H	17:R:492:ILE:HD12	1.83	0.42
22:X:250:PHE:HA	22:X:253:LEU:HB3	2.02	0.42
23:Y:18:LEU:HD23	23:Y:18:LEU:HA	1.86	0.42
24:Z:178:ASN:OD1	24:Z:179:LEU:N	2.47	0.42
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.52	0.42
2:B:235:ILE:HD12	2:B:235:ILE:HG23	1.64	0.42
2:B:479:LEU:HD23	2:B:479:LEU:HA	1.79	0.42
2:B:557:SER:O	2:B:559:ALA:N	2.53	0.42
2:B:666:ASP:N	2:B:666:ASP:OD1	2.48	0.42
2:B:1062:ARG:CZ	2:B:1065:GLY:H	2.32	0.42
5:E:27:LEU:HD13	5:E:65:ASN:ND2	2.35	0.42
13:M:1421:SER:OG	13:M:1424:ARG:NH2	2.53	0.42
21:W:228:LEU:HD11	21:W:259:TRP:CE3	2.54	0.42
24:Z:450:ILE:O	24:Z:462:GLU:HA	2.20	0.42
1:A:361:PHE:HA	1:A:388:MET:HE2	2.02	0.42
1:A:362:SER:O	1:A:388:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:933:THR:OG1	1:A:934:LEU:HG	2.19	0.42
1:A:965:VAL:O	1:A:968:VAL:HG22	2.19	0.42
2:B:355:ASP:N	2:B:355:ASP:OD2	2.52	0.42
3:C:131:THR:HG22	3:C:147:ASP:OD1	2.20	0.42
3:C:172:GLU:HG2	11:K:10:PHE:CE1	2.54	0.42
4:D:100:LEU:HD11	4:D:118:LEU:HD21	2.01	0.42
5:E:61:LEU:HD23	16:Q:884:LYS:HG2	2.02	0.42
16:Q:188:LYS:HA	16:Q:191:ARG:HG2	2.01	0.42
16:Q:310:TYR:OH	20:V:67:GLU:OE2	2.36	0.42
16:Q:773:LYS:HE2	16:Q:827:HIS:HE1	1.84	0.42
20:V:49:ILE:HG22	22:X:227:ARG:HG3	2.01	0.42
21:W:83:SER:HB3	21:W:85:ASP:OD1	2.20	0.42
22:X:221:THR:O	22:X:225:VAL:HG22	2.19	0.42
1:A:374:SER:OG	1:A:375:ILE:N	2.53	0.42
1:A:621:ILE:HG21	1:A:621:ILE:HD13	1.78	0.42
1:A:1417:HIS:HA	1:A:1421:ARG:NH1	2.35	0.42
2:B:44:LEU:HD23	2:B:155:MET:HE2	2.01	0.42
2:B:839:GLY:O	2:B:891:ASP:HB2	2.20	0.42
7:G:119:PHE:HA	7:G:128:TYR:CE1	2.54	0.42
8:H:132:LEU:HA	8:H:132:LEU:HD23	1.81	0.42
16:Q:132:LEU:HD11	20:V:85:ASP:HA	2.01	0.42
16:Q:211:LEU:HB2	16:Q:213:LYS:CE	2.49	0.42
16:Q:639:VAL:HA	16:Q:642:ASN:OD1	2.20	0.42
16:Q:652:GLY:O	16:Q:656:VAL:HG13	2.20	0.42
17:R:414:VAL:HA	17:R:423:ASN:HB3	2.02	0.42
17:R:429:ARG:NH2	17:R:431:GLY:O	2.51	0.42
17:R:452:PHE:HD2	17:R:453:MET:CE	2.33	0.42
20:V:47:LYS:HA	20:V:47:LYS:HD3	1.75	0.42
21:W:108:ASP:OD1	21:W:126:HIS:ND1	2.53	0.42
21:W:214:ILE:HD12	21:W:228:LEU:HD23	2.02	0.42
21:W:231:HIS:CE1	21:W:249:SER:HG	2.38	0.42
24:Z:490:GLY:HA3	24:Z:503:PHE:O	2.20	0.42
24:Z:526:SER:OG	24:Z:527:GLY:N	2.53	0.42
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.77	0.42
1:A:680:LEU:HD12	1:A:680:LEU:HA	1.85	0.42
1:A:828:LEU:HD12	1:A:828:LEU:HA	1.85	0.42
2:B:53:MET:HB3	2:B:57:ARG:HH21	1.84	0.42
2:B:583:LEU:O	2:B:587:LEU:HD23	2.20	0.42
2:B:847:LYS:HE3	2:B:864:ASP:OD2	2.20	0.42
3:C:113:ARG:HD2	3:C:113:ARG:HA	1.90	0.42
5:E:64:HIS:ND1	5:E:65:ASN:N	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASN:N	10:J:16:ASN:OD1	2.24	0.42
12:L:35:ARG:HH21	12:L:40:GLY:HA3	1.83	0.42
15:P:27:A:O2'	15:P:28:A:O5'	2.36	0.42
16:Q:152:PHE:HD1	16:Q:172:ILE:HD11	1.83	0.42
17:R:452:PHE:O	17:R:456:LYS:HG2	2.20	0.42
20:V:121:SER:O	20:V:121:SER:OG	2.37	0.42
21:W:155:ALA:O	21:W:163:LEU:HG	2.20	0.42
24:Z:176:ASP:OD2	24:Z:176:ASP:N	2.53	0.42
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.54	0.41
1:A:636:ILE:HG23	1:A:636:ILE:HD12	1.66	0.41
1:A:832:THR:HG23	1:A:833:PRO:HD2	2.02	0.41
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.52	0.41
2:B:309:PHE:CD2	9:I:40:ARG:NE	2.88	0.41
2:B:835:GLU:OE1	2:B:835:GLU:N	2.53	0.41
2:B:1116:VAL:HG11	2:B:1125:MET:HE3	2.02	0.41
5:E:10:LEU:HD23	5:E:10:LEU:HA	1.79	0.41
7:G:111:HIS:CD2	24:Z:501:ILE:HD13	2.54	0.41
9:I:31:GLU:OE1	9:I:31:GLU:N	2.53	0.41
16:Q:707:CYS:SG	16:Q:708:LEU:N	2.93	0.41
16:Q:744:ARG:HG3	16:Q:753:LEU:HD12	2.02	0.41
17:R:563:ILE:HD12	17:R:566:ARG:HD2	2.02	0.41
18:T:6:DC:H1'	18:T:7:DA:C8	2.55	0.41
20:V:51:TYR:CD1	20:V:52:PRO:HD2	2.55	0.41
23:Y:14:ARG:NH1	24:Z:300:GLN:OE1	2.53	0.41
1:A:321:GLU:HG2	1:A:327:ARG:NH2	2.35	0.41
1:A:912:SER:O	1:A:914:LYS:N	2.54	0.41
1:A:1216:LEU:HA	1:A:1216:LEU:HD23	1.86	0.41
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.84	0.41
2:B:544:PHE:O	2:B:547:GLU:N	2.48	0.41
2:B:679:PRO:CG	2:B:680:ASP:N	2.84	0.41
2:B:993:LYS:HD3	20:V:131:MET:SD	2.60	0.41
5:E:37:LEU:O	5:E:41:LYS:HG3	2.20	0.41
5:E:166:ARG:NH1	5:E:168:ASN:HB3	2.35	0.41
7:G:24:ASN:O	7:G:28:GLN:HG2	2.20	0.41
9:I:109:ARG:HD3	9:I:124:THR:CG2	2.46	0.41
16:Q:858:LYS:HA	16:Q:861:GLU:HG3	2.03	0.41
24:Z:199:LYS:HG3	24:Z:203:TYR:HD2	1.84	0.41
1:A:993:ILE:HD13	1:A:993:ILE:HG21	1.81	0.41
1:A:1217:ASP:OD2	1:A:1218:ARG:N	2.53	0.41
2:B:199:LYS:HB3	2:B:199:LYS:HE2	1.87	0.41
2:B:566:LYS:HG2	2:B:576:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:ILE:HG22	2:B:601:VAL:HB	2.01	0.41
2:B:739:ASN:N	2:B:739:ASN:OD1	2.53	0.41
4:D:112:LYS:HE3	4:D:112:LYS:HB2	1.74	0.41
13:M:758:TYR:N	13:M:920:ILE:O	2.49	0.41
16:Q:215:GLU:HG2	16:Q:216:LYS:NZ	2.35	0.41
16:Q:431:LEU:HD23	16:Q:431:LEU:HA	1.83	0.41
16:Q:791:ARG:HH12	21:W:87:HIS:CD2	2.38	0.41
17:R:397:LYS:HA	17:R:397:LYS:HD2	1.85	0.41
17:R:402:VAL:HB	17:R:455:TRP:HB2	2.02	0.41
17:R:485:TYR:HD1	17:R:487:PHE:CE1	2.38	0.41
21:W:25:GLY:HA3	21:W:31:ASN:C	2.40	0.41
1:A:140:ARG:NH2	1:A:234:PHE:O	2.50	0.41
1:A:561:MET:SD	11:K:58:PHE:HA	2.59	0.41
1:A:1165:THR:HG22	1:A:1297:THR:H	1.85	0.41
1:A:1255:LEU:HD12	1:A:1255:LEU:N	2.34	0.41
2:B:105:PRO:HG2	19:U:512:THR:CA	2.37	0.41
3:C:64:ILE:HG23	3:C:64:ILE:HD12	1.70	0.41
3:C:166:LYS:HE2	3:C:166:LYS:HB3	1.74	0.41
4:D:41:LEU:HB3	4:D:65:LEU:CD2	2.50	0.41
4:D:84:ARG:HG3	4:D:97:LEU:HD11	2.02	0.41
6:F:90:LEU:HA	6:F:90:LEU:HD23	1.82	0.41
10:J:49:LEU:HD23	10:J:49:LEU:HA	1.82	0.41
16:Q:345:PHE:O	16:Q:349:GLN:HG2	2.20	0.41
16:Q:537:LEU:HB3	16:Q:553:TRP:CZ3	2.55	0.41
16:Q:572:GLY:O	16:Q:576:LEU:HG	2.20	0.41
16:Q:851:LEU:O	16:Q:855:LYS:HG2	2.21	0.41
21:W:8:LEU:HD13	21:W:288:LYS:HE3	2.01	0.41
22:X:246:SER:HA	22:X:249:ILE:HD12	2.02	0.41
24:Z:439:LYS:H	24:Z:453:LYS:H	1.66	0.41
24:Z:548:GLY:HA3	24:Z:562:ASN:HA	2.01	0.41
24:Z:593:ASN:HB3	24:Z:595:HIS:HE1	1.84	0.41
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.03	0.41
1:A:618:TYR:HB3	1:A:621:ILE:O	2.21	0.41
1:A:1321:ILE:O	1:A:1328:PHE:O	2.38	0.41
2:B:305:LEU:HD12	2:B:305:LEU:HA	1.74	0.41
3:C:259:LEU:HA	3:C:259:LEU:HD12	1.81	0.41
5:E:39:GLU:O	5:E:43:GLN:HB2	2.20	0.41
10:J:30:THR:HG22	10:J:33:ASP:HB2	2.02	0.41
11:K:109:ILE:HD13	11:K:109:ILE:HA	1.88	0.41
16:Q:202:LEU:HD21	16:Q:233:GLY:HA3	2.02	0.41
16:Q:424:GLN:HB2	22:X:231:TRP:CZ3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:37:DC:C4	18:T:38:DG:C6	3.08	0.41
21:W:84:LEU:HD23	21:W:84:LEU:HA	1.77	0.41
1:A:725:LEU:HD21	1:A:736:THR:HG23	2.02	0.41
2:B:186:ILE:O	2:B:187:ILE:HD13	2.20	0.41
2:B:322:GLY:CA	2:B:339:ALA:HB2	2.50	0.41
2:B:422:PHE:HB3	2:B:429:PHE:CB	2.50	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.01	0.41
2:B:937:SER:OG	2:B:938:ARG:N	2.53	0.41
4:D:110:GLU:O	4:D:114:LEU:HD23	2.21	0.41
5:E:36:THR:OG1	5:E:39:GLU:OE1	2.29	0.41
13:M:623:LYS:O	13:M:627:ASP:N	2.51	0.41
16:Q:285:TYR:HA	16:Q:288:VAL:HG12	2.01	0.41
16:Q:720:VAL:HG21	16:Q:743:ALA:HB2	2.01	0.41
16:Q:733:LEU:HA	16:Q:733:LEU:HD23	1.72	0.41
17:R:507:PRO:HA	17:R:508:ASN:HA	1.49	0.41
21:W:46:VAL:CG2	21:W:58:TRP:HB2	2.51	0.41
24:Z:601:LYS:HG3	24:Z:611:GLU:OE2	2.20	0.41
24:Z:736:LEU:HA	24:Z:736:LEU:HD23	1.79	0.41
1:A:46:THR:OG1	1:A:47:THR:N	2.53	0.41
1:A:626:THR:O	1:A:627:LYS:HB3	2.21	0.41
1:A:849:ASP:HA	1:A:852:VAL:HG22	2.03	0.41
1:A:875:TYR:OH	6:F:61:GLU:OE2	2.28	0.41
2:B:273:PHE:CG	2:B:284:ILE:HG23	2.56	0.41
2:B:312:GLN:OE1	9:I:40:ARG:NH2	2.54	0.41
5:E:111:THR:O	5:E:114:ALA:N	2.52	0.41
7:G:7:LEU:HB2	7:G:72:TYR:CE2	2.55	0.41
13:M:1354:ASP:O	13:M:1372:LYS:HG2	2.20	0.41
13:M:1474:LEU:HD21	13:M:1511:PHE:CE1	2.55	0.41
17:R:440:GLU:HG3	17:R:441:PHE:CE1	2.55	0.41
21:W:27:ASN:ND2	21:W:74:HIS:O	2.53	0.41
24:Z:192:THR:OG1	24:Z:244:ASN:ND2	2.54	0.41
1:A:151:LYS:O	1:A:152:ASN:ND2	2.53	0.41
1:A:954:ARG:HH11	1:A:954:ARG:HD2	1.74	0.41
1:A:1290:SER:O	1:A:1294:THR:HG23	2.21	0.41
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.84	0.41
3:C:34:ILE:HG21	3:C:34:ILE:HD13	1.80	0.41
5:E:17:ILE:HD13	5:E:17:ILE:HA	1.87	0.41
5:E:60:VAL:HG23	5:E:74:VAL:HB	2.03	0.41
5:E:185:ILE:HG21	5:E:185:ILE:HD13	1.67	0.41
7:G:81:LYS:HE2	7:G:149:GLY:HA2	2.03	0.41
8:H:96:VAL:HA	8:H:116:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:235:LEU:HD23	16:Q:261:ALA:HB2	2.02	0.41
16:Q:468:GLY:O	16:Q:472:LYS:HG2	2.20	0.41
16:Q:790:HIS:NE2	16:Q:817:CYS:SG	2.94	0.41
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.69	0.41
1:A:120:ASP:O	1:A:122:ASN:N	2.54	0.41
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.78	0.41
1:A:419:ILE:HD13	1:A:419:ILE:HG21	1.70	0.41
1:A:421:ARG:NE	1:A:427:ILE:HD11	2.36	0.41
1:A:461:GLN:O	1:A:461:GLN:NE2	2.53	0.41
1:A:497:ASP:HB3	2:B:792:ASP:HB3	2.01	0.41
1:A:596:ILE:HG21	1:A:596:ILE:HD13	1.76	0.41
1:A:738:GLU:OE1	1:A:797:ARG:HD3	2.21	0.41
1:A:1121:VAL:N	1:A:1122:PRO:CD	2.84	0.41
1:A:1164:THR:O	1:A:1298:LEU:N	2.53	0.41
2:B:19:PRO:C	2:B:21:LEU:N	2.74	0.41
2:B:222:ARG:HH11	2:B:222:ARG:HD3	1.72	0.41
2:B:889:LYS:HB2	2:B:889:LYS:HE2	1.46	0.41
2:B:1010:LYS:HE3	20:V:130:TRP:CH2	2.56	0.41
3:C:246:LEU:HA	3:C:246:LEU:HD23	1.87	0.41
7:G:14:HIS:O	7:G:16:ARG:N	2.54	0.41
7:G:50:THR:HG22	7:G:73:LYS:HB3	2.03	0.41
7:G:92:VAL:H	7:G:139:GLN:HE21	1.68	0.41
11:K:93:ASP:OD1	11:K:94:LEU:N	2.53	0.41
15:P:40:A:C2	15:P:41:C:C4	3.08	0.41
16:Q:258:LEU:HD23	16:Q:258:LEU:HA	1.90	0.41
16:Q:858:LYS:O	16:Q:861:GLU:HG3	2.21	0.41
17:R:388:ARG:HG2	17:R:443:SER:HB2	2.03	0.41
17:R:390:GLY:HA2	17:R:400:TYR:CD1	2.55	0.41
17:R:582:GLU:HA	17:R:585:ASN:HD21	1.85	0.41
21:W:196:LEU:HD13	21:W:205:LEU:HD11	2.01	0.41
21:W:222:ALA:O	21:W:223:ASN:ND2	2.54	0.41
24:Z:389:THR:HG23	24:Z:391:SER:H	1.85	0.41
24:Z:491:LEU:HD23	24:Z:491:LEU:HA	1.83	0.41
24:Z:562:ASN:ND2	24:Z:566:LYS:HG3	2.33	0.41
1:A:33:ARG:H	1:A:33:ARG:HG2	1.69	0.41
1:A:102:LYS:HE2	1:A:138:LYS:NZ	2.36	0.41
1:A:117:LEU:O	1:A:119:VAL:N	2.53	0.41
1:A:455:ILE:HD12	1:A:520:MET:HE1	2.03	0.41
1:A:939:VAL:O	1:A:943:LEU:HD12	2.21	0.41
1:A:1090:LEU:HD23	1:A:1090:LEU:HA	1.79	0.41
2:B:650:ASN:C	19:U:460:TYR:HE2	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:SER:HB2	7:G:125:PRO:HD2	2.03	0.41
8:H:6:PHE:CZ	8:H:37:MET:SD	3.14	0.41
11:K:103:GLU:O	11:K:107:VAL:HG13	2.20	0.41
12:L:18:ILE:HD11	12:L:47:LYS:HG3	2.02	0.41
16:Q:218:ARG:HH11	16:Q:238:LEU:CD2	2.33	0.41
16:Q:467:LEU:HD12	16:Q:506:LEU:HG	2.02	0.41
16:Q:790:HIS:CD2	16:Q:817:CYS:SG	3.14	0.41
18:T:37:DC:H5'	18:T:37:DC:C6	2.56	0.41
18:T:39:DC:H2"	18:T:40:DT:H72	2.02	0.41
21:W:5:TYR:CD1	21:W:303:CYS:HB3	2.56	0.41
21:W:250:SER:OG	21:W:277:VAL:HG23	2.21	0.41
1:A:217:SER:O	1:A:220:ARG:N	2.53	0.40
1:A:812:LYS:O	1:A:813:ASP:HB2	2.21	0.40
1:A:1177:TYR:HH	1:A:1282:ASP:HA	1.86	0.40
1:A:1212:LEU:CD1	1:A:1285:LEU:HD13	2.48	0.40
1:A:1376:LYS:O	1:A:1380:ARG:HG3	2.21	0.40
1:A:1481:LYS:HA	7:G:20:PRO:HA	2.03	0.40
2:B:123:PRO:HB2	2:B:148:PHE:HE1	1.86	0.40
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.02	0.40
16:Q:18:GLU:N	16:Q:18:GLU:OE1	2.53	0.40
16:Q:274:HIS:HA	16:Q:277:ASN:HD21	1.84	0.40
16:Q:296:PHE:CE1	16:Q:305:GLN:HB2	2.56	0.40
16:Q:398:LYS:HE2	16:Q:421:ILE:HG21	2.03	0.40
24:Z:525:ALA:CB	24:Z:552:ARG:HH22	2.31	0.40
1:A:99:PHE:O	1:A:103:THR:HG23	2.21	0.40
1:A:247:TRP:N	1:A:247:TRP:CD1	2.87	0.40
1:A:539:GLN:C	1:A:541:THR:N	2.74	0.40
1:A:991:GLN:HA	1:A:996:ILE:HG12	2.04	0.40
1:A:1222:THR:C	1:A:1225:LYS:H	2.23	0.40
1:A:1288:ILE:HA	1:A:1291:ASN:HD21	1.86	0.40
2:B:583:LEU:N	2:B:583:LEU:HD12	2.36	0.40
4:D:35:SER:OG	4:D:72:SER:HA	2.21	0.40
7:G:110:ARG:HG2	7:G:119:PHE:CZ	2.56	0.40
7:G:152:VAL:HA	7:G:157:ILE:HA	2.03	0.40
16:Q:238:LEU:HD12	16:Q:238:LEU:HA	1.96	0.40
16:Q:393:LYS:HB3	16:Q:393:LYS:HE3	1.70	0.40
18:T:21:DT:H6	18:T:21:DT:H2'	1.67	0.40
21:W:251:SER:HG	21:W:255:SER:HG	1.68	0.40
24:Z:551:VAL:HG21	24:Z:632:ASN:OD1	2.20	0.40
24:Z:571:ARG:HB2	24:Z:574:ALA:CB	2.51	0.40
1:A:92:LYS:CD	1:A:307:VAL:HG11	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:VAL:HG21	1:A:1435:THR:HG23	2.03	0.40
1:A:413:TYR:O	1:A:449:HIS:CD2	2.67	0.40
1:A:713:VAL:CG2	1:A:817:PRO:HD3	2.45	0.40
1:A:1150:ASP:OD2	1:A:1153:ARG:HG3	2.21	0.40
1:A:1182:GLN:O	1:A:1192:TRP:CE2	2.73	0.40
1:A:1261:ILE:C	1:A:1262:MET:HE3	2.41	0.40
2:B:157:ARG:NH2	2:B:177:CYS:O	2.54	0.40
2:B:665:ILE:HA	2:B:665:ILE:HD12	1.78	0.40
2:B:833:THR:HG22	2:B:835:GLU:OE1	2.22	0.40
5:E:101:ARG:HA	5:E:126:ILE:O	2.20	0.40
7:G:110:ARG:NH2	7:G:117:MET:O	2.55	0.40
8:H:125:LEU:HD12	8:H:125:LEU:HA	1.79	0.40
11:K:80:ASP:N	11:K:80:ASP:OD1	2.32	0.40
12:L:13:GLN:HA	12:L:14:PRO:HD3	1.88	0.40
14:N:42:DT:H6	14:N:42:DT:H2'	1.71	0.40
16:Q:3:ARG:HB3	16:Q:4:GLY:H	1.67	0.40
16:Q:153:HIS:CE1	16:Q:156:LEU:HD12	2.56	0.40
16:Q:333:THR:HG21	16:Q:347:LEU:HD12	2.02	0.40
16:Q:415:TRP:CZ3	16:Q:440:ILE:HG12	2.57	0.40
17:R:392:GLY:HA2	17:R:397:LYS:O	2.20	0.40
17:R:587:LYS:HE2	17:R:587:LYS:HB2	1.93	0.40
20:V:282:ALA:C	20:V:284:GLU:H	2.25	0.40
21:W:243:ASP:OD2	21:W:243:ASP:N	2.54	0.40
21:W:254:LYS:HG2	21:W:275:ASP:C	2.42	0.40
23:Y:93:LEU:HD23	23:Y:93:LEU:HA	1.87	0.40
24:Z:260:MET:N	24:Z:260:MET:SD	2.94	0.40
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.85	0.40
1:A:135:GLY:O	1:A:137:PRO:HD3	2.21	0.40
1:A:538:VAL:O	1:A:539:GLN:HG2	2.22	0.40
1:A:1182:GLN:C	1:A:1192:TRP:HE1	2.18	0.40
2:B:84:TYR:CB	2:B:132:VAL:HA	2.52	0.40
2:B:95:LYS:HA	2:B:95:LYS:HD2	1.92	0.40
2:B:332:LYS:HD2	2:B:332:LYS:C	2.41	0.40
2:B:388:TYR:H	2:B:504:THR:CG2	2.27	0.40
2:B:620:ARG:HH11	2:B:620:ARG:HD2	1.69	0.40
2:B:791:GLU:O	2:B:792:ASP:HB2	2.21	0.40
5:E:25:GLY:O	5:E:65:ASN:HB2	2.22	0.40
13:M:1429:HIS:CE1	13:M:1460:TYR:HH	2.37	0.40
16:Q:24:LEU:HD11	16:Q:56:LYS:NZ	2.36	0.40
16:Q:95:GLN:OE1	20:V:83:THR:OG1	2.38	0.40
16:Q:689:HIS:HB2	20:V:35:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:14:ALA:CB	21:W:298:ILE:HG13	2.52	0.40
24:Z:200:PHE:HB2	24:Z:210:LEU:HD22	2.02	0.40
24:Z:420:PHE:CE1	24:Z:470:LYS:HG2	2.56	0.40
1:A:29:ASP:O	1:A:33:ARG:HG2	2.21	0.40
1:A:955:GLU:OE1	1:A:1010:VAL:HG22	2.22	0.40
1:A:1163:HIS:CD2	1:A:1297:THR:HG23	2.57	0.40
2:B:50:PHE:HA	2:B:54:SER:HB3	2.02	0.40
2:B:242:ARG:NH2	2:B:252:ILE:HD12	2.37	0.40
9:I:14:ILE:HG23	9:I:23:MET:HG3	2.03	0.40
16:Q:386:ALA:HB1	16:Q:394:ARG:CG	2.51	0.40
16:Q:636:TYR:CE2	16:Q:652:GLY:HA3	2.56	0.40
18:T:1:DG:H2"	18:T:2:DC:C6	2.56	0.40
21:W:172:ILE:O	21:W:186:LEU:N	2.54	0.40
21:W:273:HIS:CE1	21:W:291:SER:HG	2.39	0.40
24:Z:501:ILE:HA	24:Z:511:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1984 (71%)	1281 (91%)	117 (8%)	10 (1%)	22	57
2	B	1112/1251 (89%)	998 (90%)	105 (9%)	9 (1%)	19	54
3	C	254/275 (92%)	232 (91%)	19 (8%)	3 (1%)	13	44
4	D	124/142 (87%)	118 (95%)	6 (5%)	0	100	100
5	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	29	64
6	F	76/127 (60%)	70 (92%)	6 (8%)	0	100	100
7	G	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
8	H	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	I	114/125 (91%)	104 (91%)	10 (9%)	0	100 100
10	J	64/67 (96%)	60 (94%)	2 (3%)	2 (3%)	4 23
11	K	113/117 (97%)	107 (95%)	6 (5%)	0	100 100
12	L	45/58 (78%)	39 (87%)	6 (13%)	0	100 100
13	M	976/1729 (56%)	903 (92%)	72 (7%)	1 (0%)	51 83
16	Q	888/1179 (75%)	836 (94%)	52 (6%)	0	100 100
17	R	240/713 (34%)	225 (94%)	14 (6%)	1 (0%)	34 69
19	U	117/666 (18%)	88 (75%)	21 (18%)	8 (7%)	1 7
20	V	234/531 (44%)	199 (85%)	31 (13%)	4 (2%)	9 36
21	W	298/305 (98%)	268 (90%)	30 (10%)	0	100 100
22	X	41/531 (8%)	41 (100%)	0	0	100 100
23	Y	114/121 (94%)	109 (96%)	5 (4%)	0	100 100
24	Z	497/1087 (46%)	460 (93%)	36 (7%)	1 (0%)	47 79
All	All	7238/11540 (63%)	6624 (92%)	573 (8%)	41 (1%)	29 59

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ASP
1	A	1185	VAL
1	A	1468	THR
2	B	19	PRO
3	C	93	PHE
13	M	1330	PRO
17	R	507	PRO
19	U	506	ALA
19	U	508	HIS
20	V	238	PRO
24	Z	760	GLY
1	A	1435	THR
19	U	481	GLY
19	U	521	LYS
2	B	20	ASP
2	B	142	THR
2	B	1004	ASP
10	J	28	GLU
19	U	463	PRO

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Mol	Chain	Res	Type
19	U	513	LEU
19	U	516	ALA
19	U	523	GLN
20	V	228	GLU
20	V	249	ASP
20	V	291	ASN
1	A	300	ALA
1	A	696	SER
2	B	950	ARG
1	A	495	ASP
1	A	1130	ILE
2	B	679	PRO
2	B	834	ARG
3	C	60	HIS
3	C	92	GLU
2	B	650	ASN
2	B	1001	PRO
1	A	478	PRO
5	E	45	GLY
8	H	17	PRO
10	J	64	PRO
1	A	980	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1245/1761 (71%)	1226 (98%)	19 (2%)	65	85
2	B	986/1084 (91%)	949 (96%)	37 (4%)	33	66
3	C	235/252 (93%)	228 (97%)	7 (3%)	41	71
4	D	109/126 (86%)	108 (99%)	1 (1%)	78	91
5	E	191/192 (100%)	189 (99%)	2 (1%)	76	90
6	F	68/111 (61%)	67 (98%)	1 (2%)	65	85
7	G	146/153 (95%)	143 (98%)	3 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	130/131 (99%)	122 (94%)	8 (6%)	18 49
9	I	104/112 (93%)	101 (97%)	3 (3%)	42 72
10	J	55/56 (98%)	54 (98%)	1 (2%)	59 82
11	K	104/106 (98%)	103 (99%)	1 (1%)	76 90
12	L	43/55 (78%)	40 (93%)	3 (7%)	15 45
13	M	154/1524 (10%)	154 (100%)	0	100 100
16	Q	761/1011 (75%)	755 (99%)	6 (1%)	81 92
17	R	168/625 (27%)	166 (99%)	2 (1%)	71 88
19	U	63/590 (11%)	63 (100%)	0	100 100
20	V	144/462 (31%)	141 (98%)	3 (2%)	53 79
21	W	255/260 (98%)	254 (100%)	1 (0%)	91 96
22	X	40/467 (9%)	40 (100%)	0	100 100
23	Y	102/105 (97%)	102 (100%)	0	100 100
24	Z	434/939 (46%)	432 (100%)	2 (0%)	88 94
All	All	5537/10122 (55%)	5437 (98%)	100 (2%)	61 82

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	147	LEU
1	A	251	THR
1	A	301	HIS
1	A	382	ARG
1	A	476	ILE
1	A	539	GLN
1	A	571	ASP
1	A	605	THR
1	A	757	GLN
1	A	761	SER
1	A	819	SER
1	A	884	ASN
1	A	931	ARG
1	A	937	ASP
1	A	1030	SER
1	A	1074	SER
1	A	1210	TRP

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Mol	Chain	Res	Type
1	A	1286	ARG
2	B	20	ASP
2	B	83	ARG
2	B	90	GLN
2	B	92	TYR
2	B	115	LEU
2	B	147	THR
2	B	170	ASP
2	B	180	ASP
2	B	218	THR
2	B	236	TRP
2	B	267	VAL
2	B	331	THR
2	B	332	LYS
2	B	348	LEU
2	B	351	VAL
2	B	354	SER
2	B	359	THR
2	B	386	ASP
2	B	411	LEU
2	B	429	PHE
2	B	453	TRP
2	B	592	ARG
2	B	597	ILE
2	B	610	ARG
2	B	626	LEU
2	B	649	ASN
2	B	650	ASN
2	B	659	SER
2	B	715	ASP
2	B	731	GLN
2	B	738	THR
2	B	743	ARG
2	B	784	SER
2	B	931	ILE
2	B	1118	VAL
2	B	1148	LEU
2	B	1174	VAL
3	C	33	SER
3	C	63	PHE
3	C	74	THR
3	C	75	SER

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Mol	Chain	Res	Type
3	C	76	ASP
3	C	147	ASP
3	C	151	VAL
4	D	94	LYS
5	E	82	VAL
5	E	117	SER
6	F	123	LEU
7	G	21	ASN
7	G	37	THR
7	G	67	LEU
8	H	15	ILE
8	H	67	ASP
8	H	83	SER
8	H	95	LYS
8	H	96	VAL
8	H	113	SER
8	H	116	VAL
8	H	141	VAL
9	I	12	VAL
9	I	15	ARG
9	I	101	SER
10	J	47	ARG
11	K	99	SER
12	L	34	ILE
12	L	39	CYS
12	L	44	MET
16	Q	180	ARG
16	Q	191	ARG
16	Q	697	TYR
16	Q	707	CYS
16	Q	820	LEU
16	Q	858	LYS
17	R	422	THR
17	R	474	LYS
20	V	45	ASP
20	V	132	ARG
20	V	181	LYS
21	W	169	ASP
24	Z	176	ASP
24	Z	720	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	96	HIS
1	A	122	ASN
1	A	123	ASN
1	A	152	ASN
1	A	288	ASN
1	A	313	HIS
1	A	449	HIS
1	A	704	ASN
1	A	742	ASN
1	A	780	ASN
1	A	809	HIS
1	A	935	GLN
1	A	982	ASN
1	A	1005	HIS
1	A	1182	GLN
1	A	1230	GLN
2	B	52	GLN
2	B	175	ASN
2	B	319	ASN
2	B	471	ASN
2	B	631	GLN
2	B	649	ASN
2	B	1003	ASN
2	B	1040	GLN
2	B	1120	ASN
2	B	1142	ASN
3	C	60	HIS
3	C	114	HIS
3	C	262	GLN
4	D	34	ASN
4	D	48	ASN
4	D	66	ASN
4	D	76	ASN
4	D	129	GLN
5	E	107	GLN
5	E	168	ASN
7	G	93	ASN
7	G	139	GLN
8	H	131	ASN
9	I	84	HIS
9	I	91	HIS
11	K	49	GLN

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Mol	Chain	Res	Type
13	M	1352	GLN
16	Q	38	HIS
16	Q	40	GLN
16	Q	82	GLN
16	Q	105	ASN
16	Q	128	GLN
16	Q	161	ASN
16	Q	244	ASN
16	Q	268	ASN
16	Q	289	GLN
16	Q	294	HIS
16	Q	298	ASN
16	Q	305	GLN
16	Q	349	GLN
16	Q	359	ASN
16	Q	373	ASN
16	Q	407	GLN
16	Q	466	ASN
16	Q	502	ASN
16	Q	527	HIS
16	Q	561	ASN
16	Q	573	ASN
16	Q	585	GLN
16	Q	616	HIS
16	Q	706	ASN
16	Q	714	HIS
16	Q	877	GLN
16	Q	880	GLN
16	Q	887	ASN
17	R	416	GLN
17	R	432	ASN
17	R	484	ASN
17	R	585	ASN
17	R	588	ASN
20	V	37	ASN
20	V	69	GLN
20	V	72	HIS
20	V	97	ASN
20	V	122	GLN
20	V	193	HIS
21	W	11	GLN
21	W	15	HIS

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Mol	Chain	Res	Type
21	W	27	ASN
21	W	98	GLN
21	W	131	ASN
21	W	173	ASN
21	W	223	ASN
21	W	268	HIS
21	W	273	HIS
23	Y	27	GLN
24	Z	232	GLN
24	Z	251	ASN
24	Z	466	GLN
24	Z	519	GLN
24	Z	595	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	20/46 (43%)	7 (35%)	3 (15%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	29	C
15	P	30	C
15	P	31	G
15	P	36	G
15	P	37	G
15	P	39	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	28	A
15	P	36	G
15	P	38	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
24	TPO	Z	775	24	8,10,11	1.54	1 (12%)	10,14,16	1.99	1 (10%)
1	TPO	A	1525	1	8,10,11	1.60	1 (12%)	10,14,16	1.83	1 (10%)
1	SEP	A	1547	1	8,9,10	1.49	1 (12%)	8,12,14	1.39	2 (25%)

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
24	TPO	Z	775	24	-	1/9/11/13	-
1	TPO	A	1525	1	-	4/9/11/13	-
1	SEP	A	1547	1	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1525	TPO	P-O1P	3.41	1.61	1.50
24	Z	775	TPO	P-O1P	3.34	1.61	1.50
1	A	1547	SEP	P-O1P	3.25	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Z	775	TPO	P-OG1-CB	-5.85	105.53	123.21
1	A	1525	TPO	P-OG1-CB	-4.96	108.22	123.21
1	A	1547	SEP	P-OG-CB	-2.69	110.89	118.30
1	A	1547	SEP	OG-CB-CA	2.01	110.10	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1525	TPO	N-CA-CB-CG2
1	A	1525	TPO	N-CA-CB-OG1
1	A	1525	TPO	C-CA-CB-CG2
24	Z	775	TPO	C-CA-CB-CG2
1	A	1525	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	775	TPO	2	0
1	A	1525	TPO	1	0
1	A	1547	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	3
19	U	1
20	V	1
13	M	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	25.86
1	V	299:GLU	C	310:ASN	N	12.74
1	M	1334:ASN	C	1338:ILE	N	5.29
1	B	755:GLN	C	756:LYS	N	1.18
1	B	108:MET	C	109:MET	N	1.17
1	A	999:ARG	C	1000:LEU	N	1.15
1	B	94:SER	C	95:LYS	N	1.07

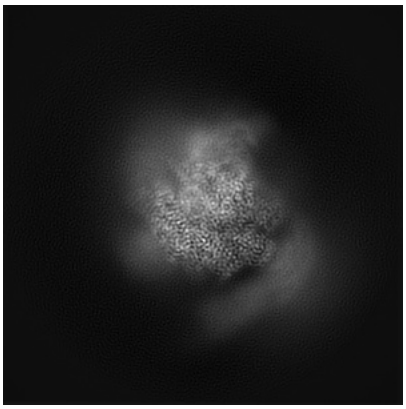
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10480. These allow visual inspection of the internal detail of the map and identification of artifacts.

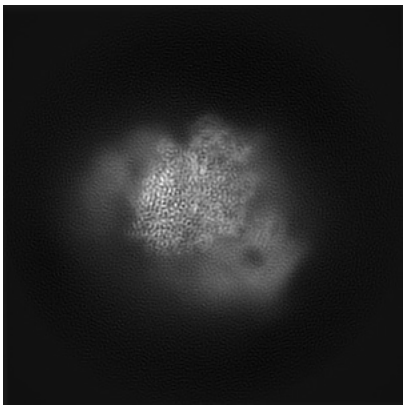
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

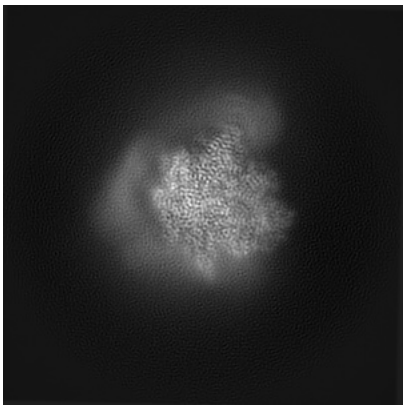
6.1.1 Primary map



X

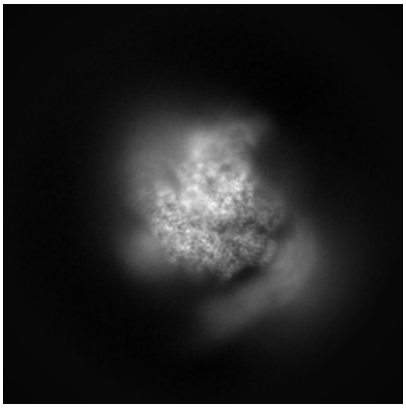


Y

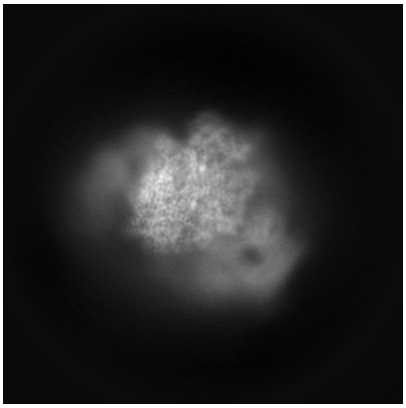


Z

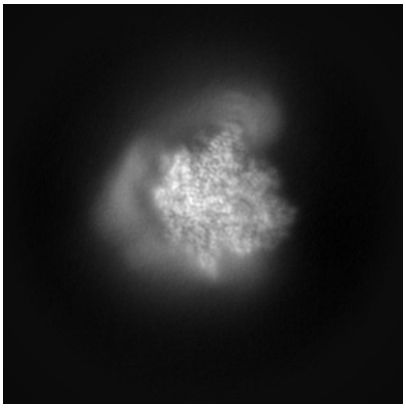
6.1.2 Raw map



X



Y

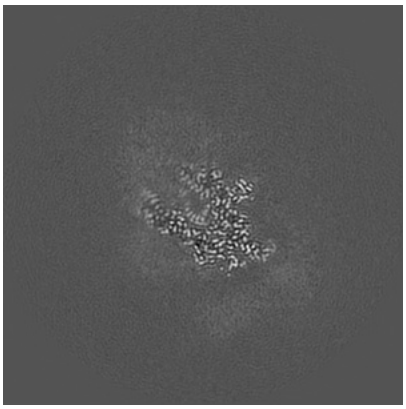


Z

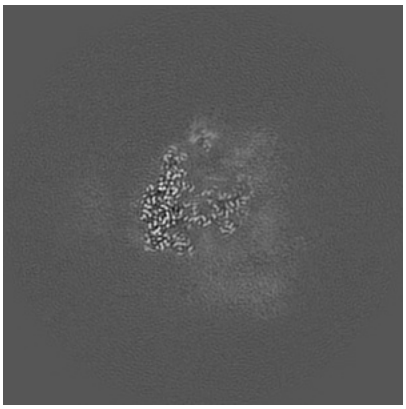
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

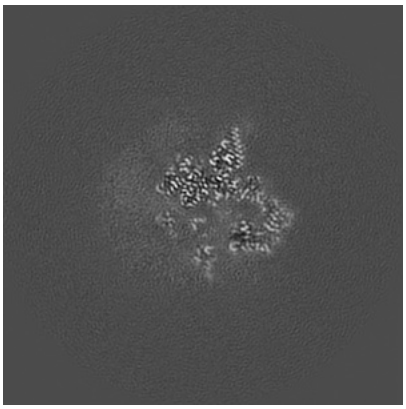
6.2.1 Primary map



X Index: 180

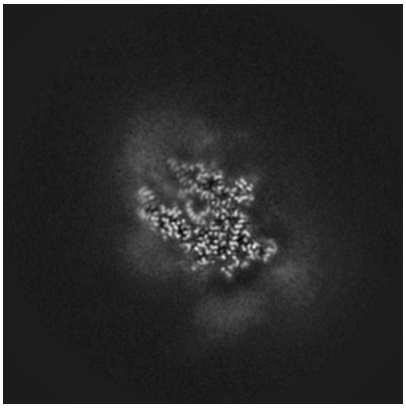


Y Index: 180

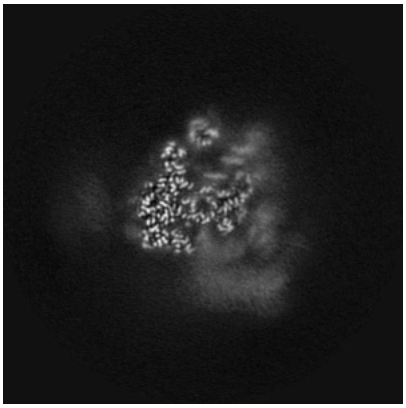


Z Index: 180

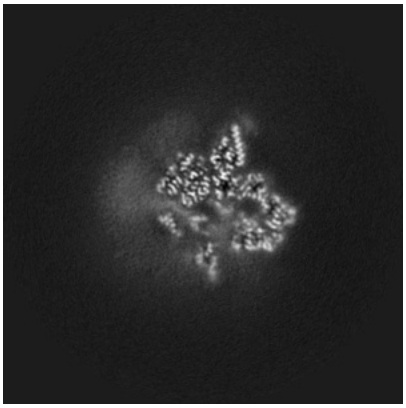
6.2.2 Raw map



X Index: 180



Y Index: 180

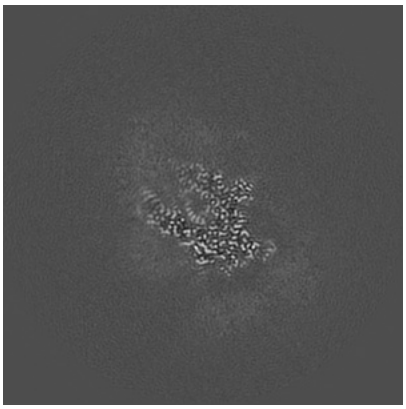


Z Index: 180

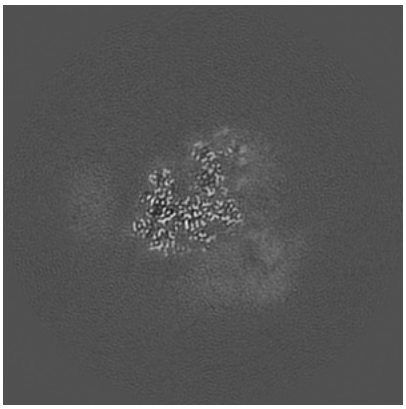
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

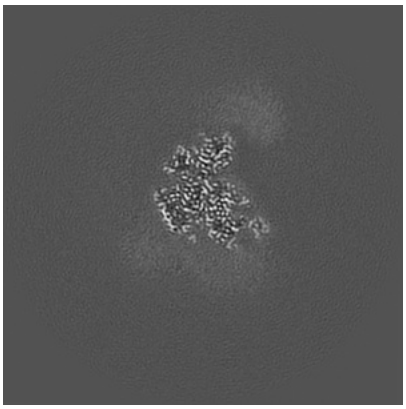
6.3.1 Primary map



X Index: 179

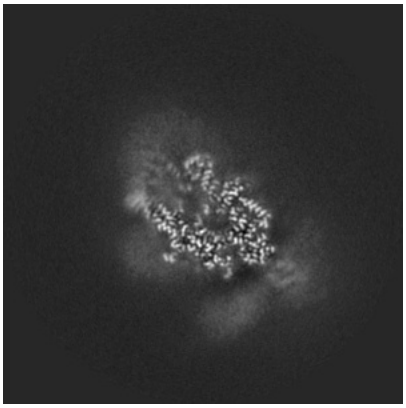


Y Index: 193

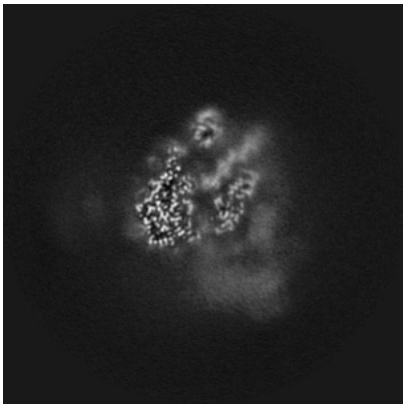


Z Index: 143

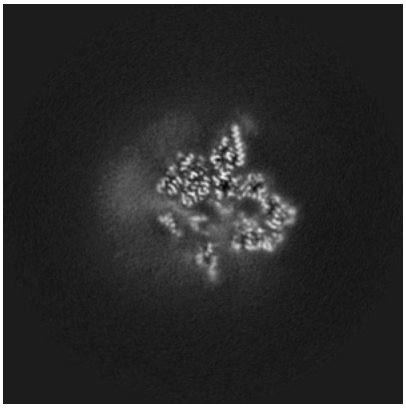
6.3.2 Raw map



X Index: 189



Y Index: 174



Z Index: 180

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

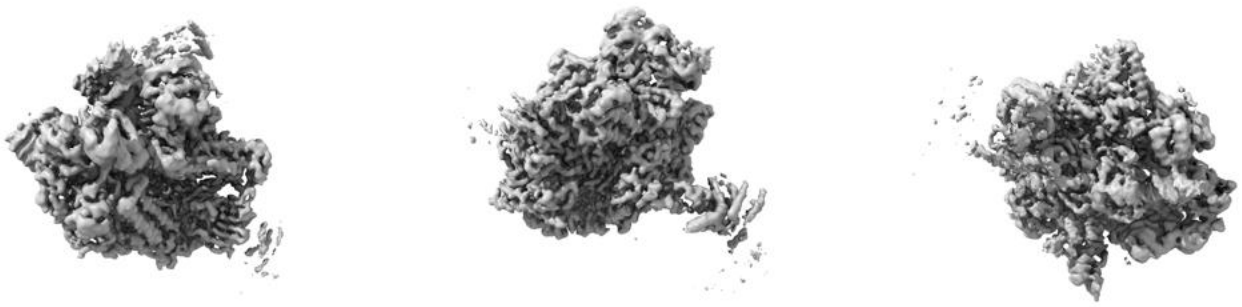
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

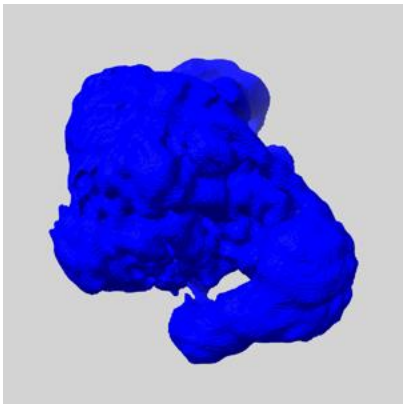
6.5 Mask visualisation

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

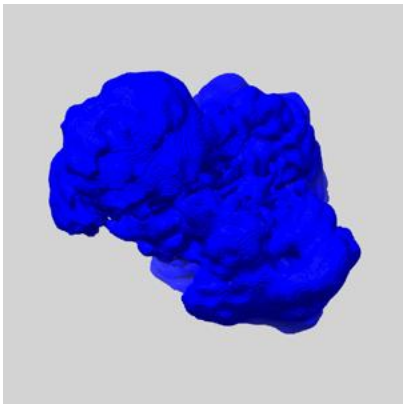
A mask typically either:

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

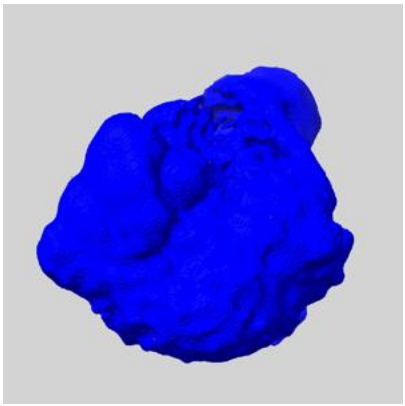
6.5.1 emd_10480_msk_1.map



X

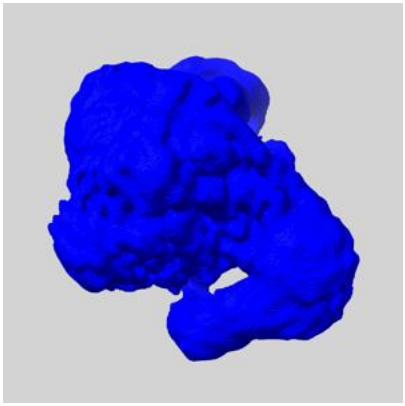


Y

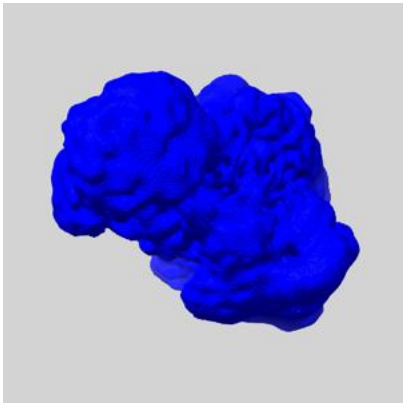


Z

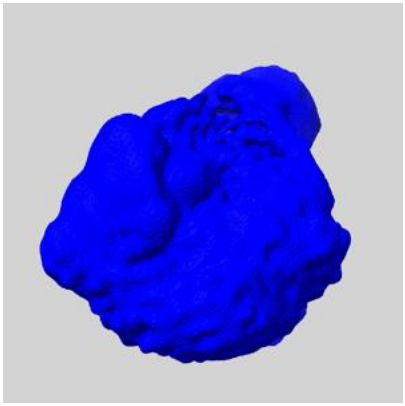
6.5.2 emd_10480_msk_2.map



X



Y

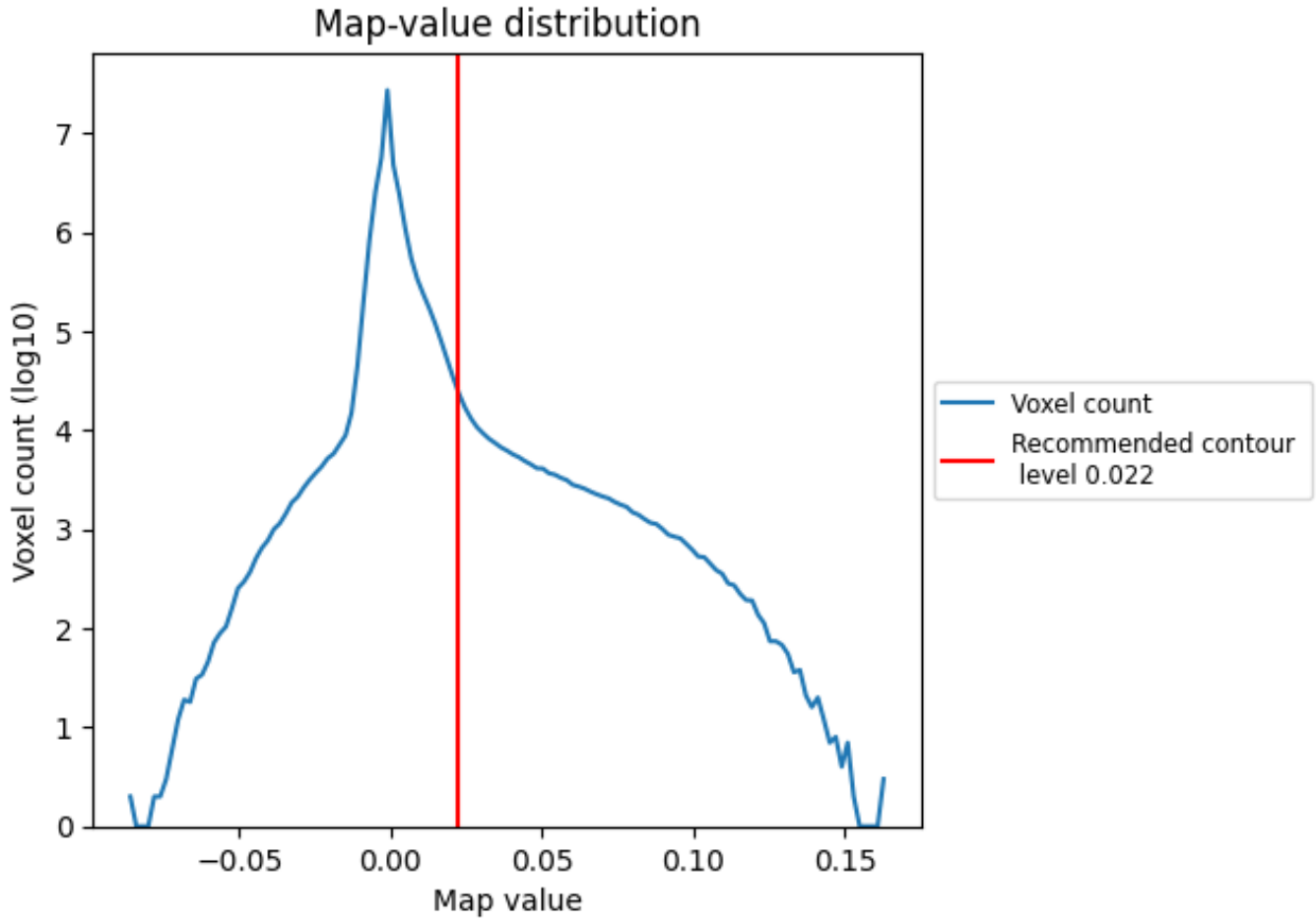


Z

7 Map analysis

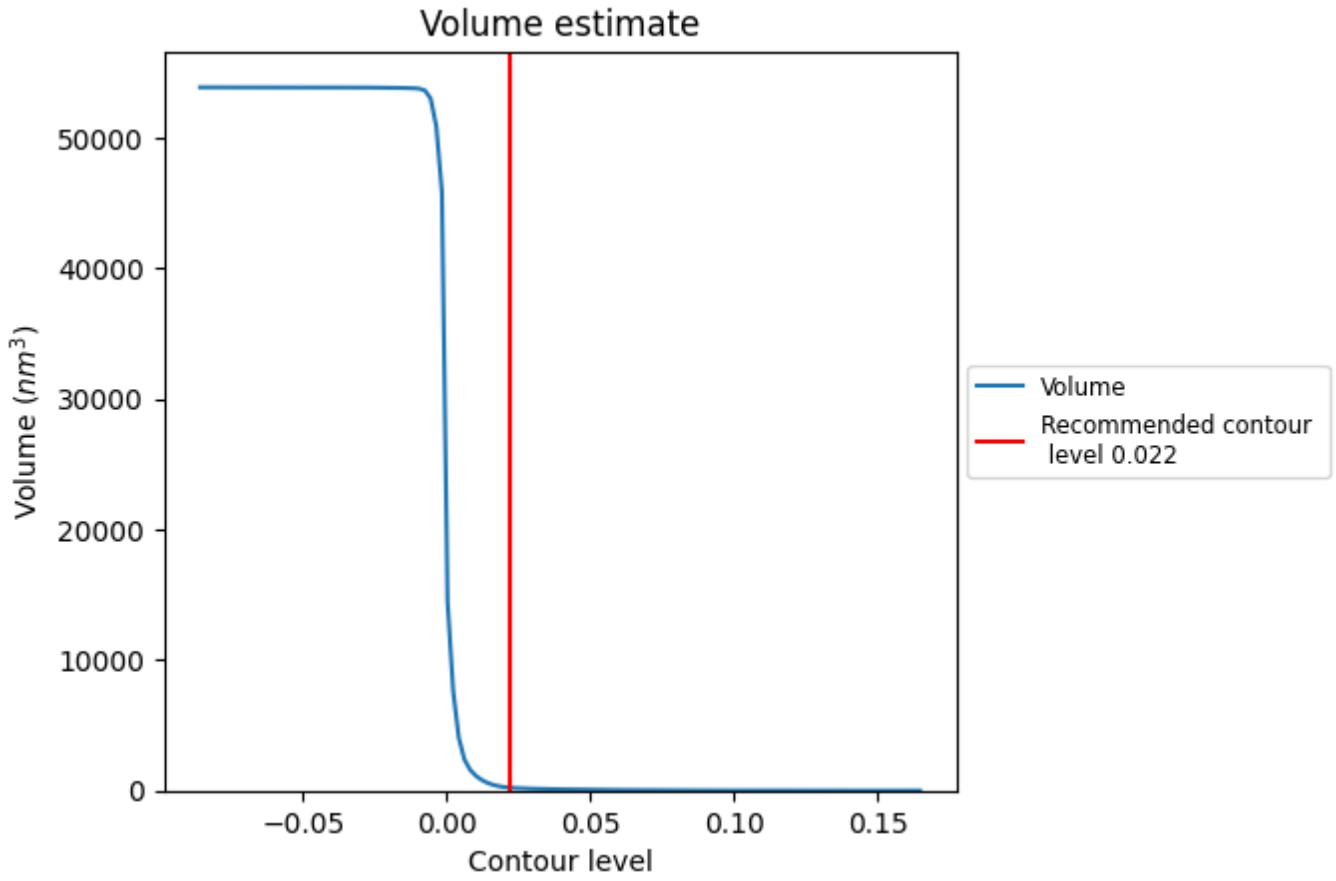
This section contains the results of statistical analysis of the map.

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.

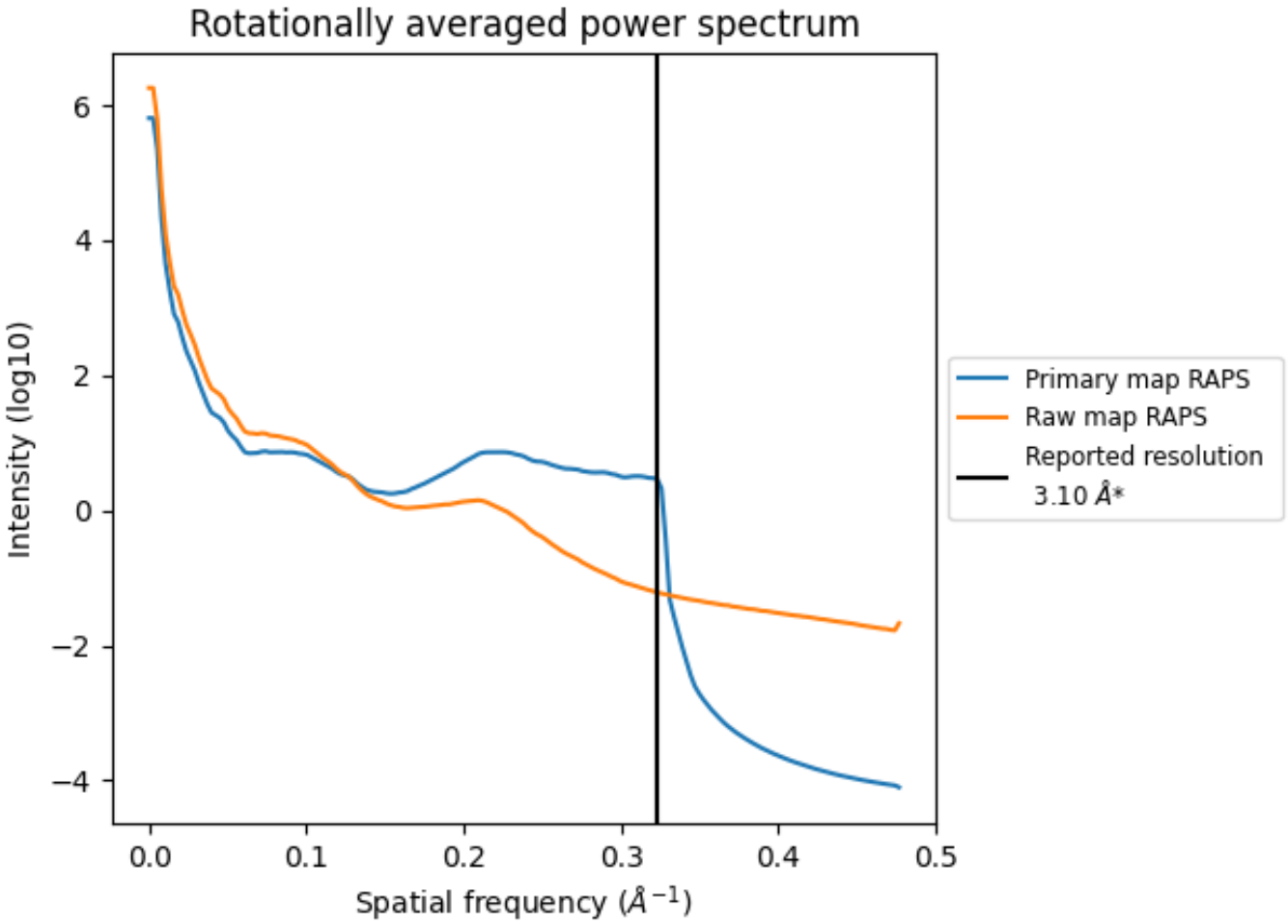
7.2 Volume estimate



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 202 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)

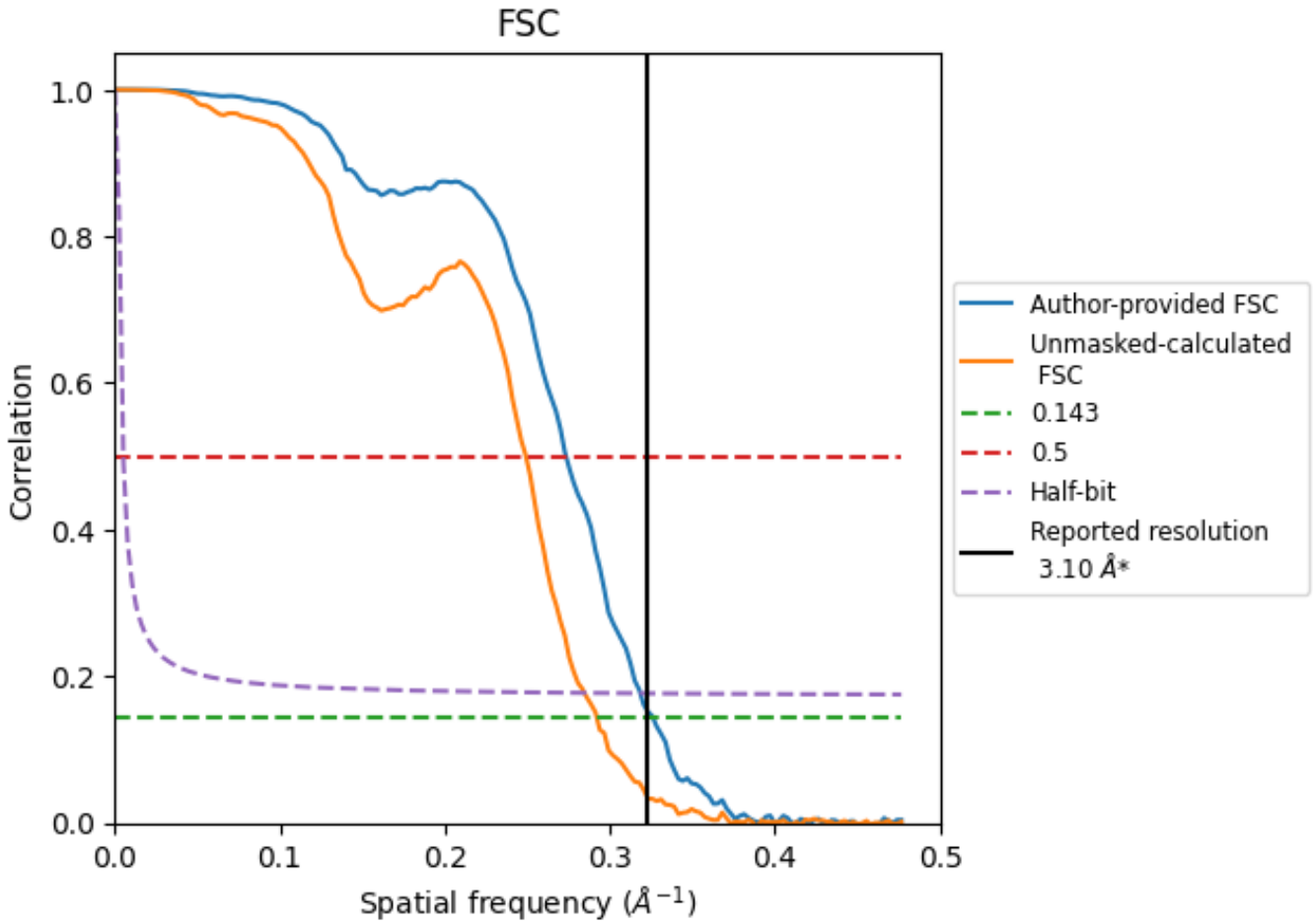


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

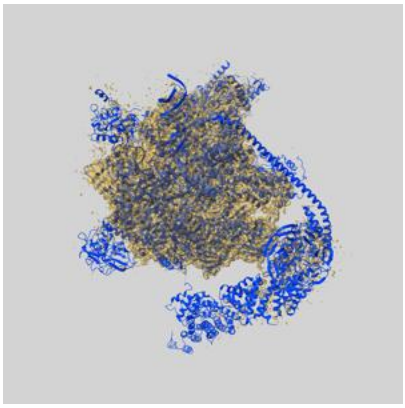
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.66	3.14
Unmasked-calculated*	3.42	4.01	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.1 by more than 10 %

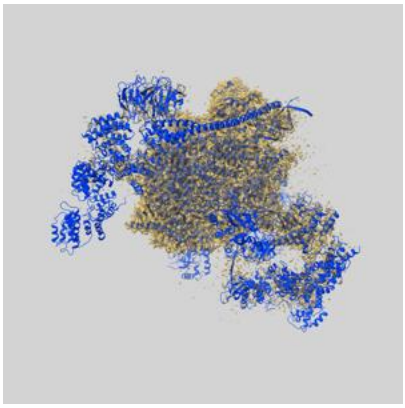
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10480 and PDB model 6TED. Per-residue inclusion information can be found in section 3 on page 9.

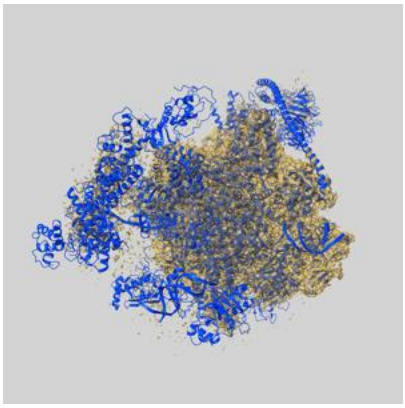
9.1 Map-model overlay



X



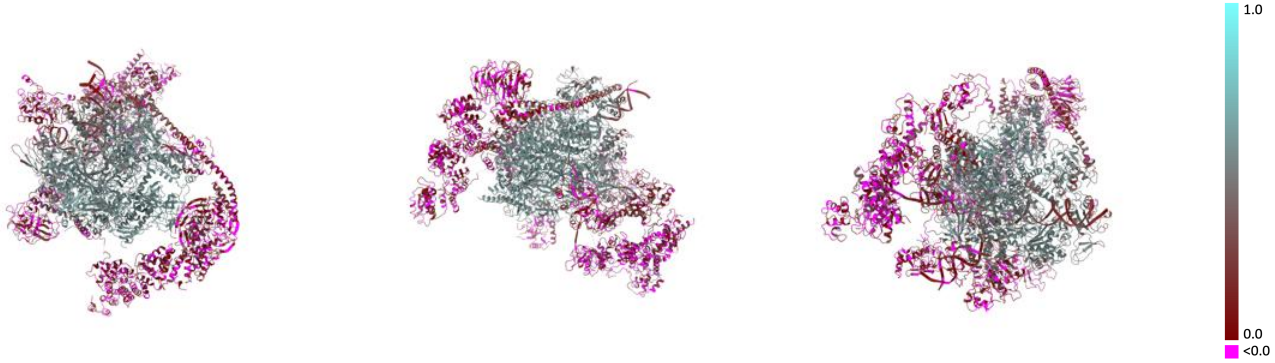
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

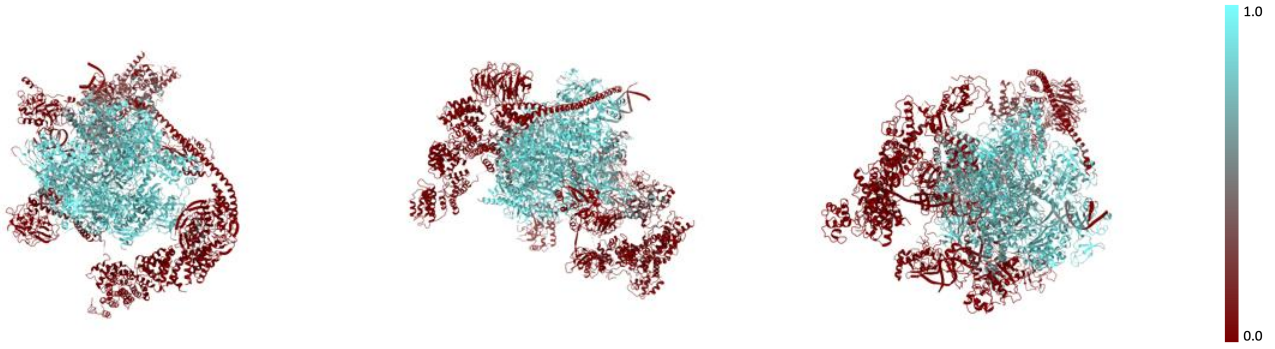
9.2 Q-score mapped to coordinate model



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.

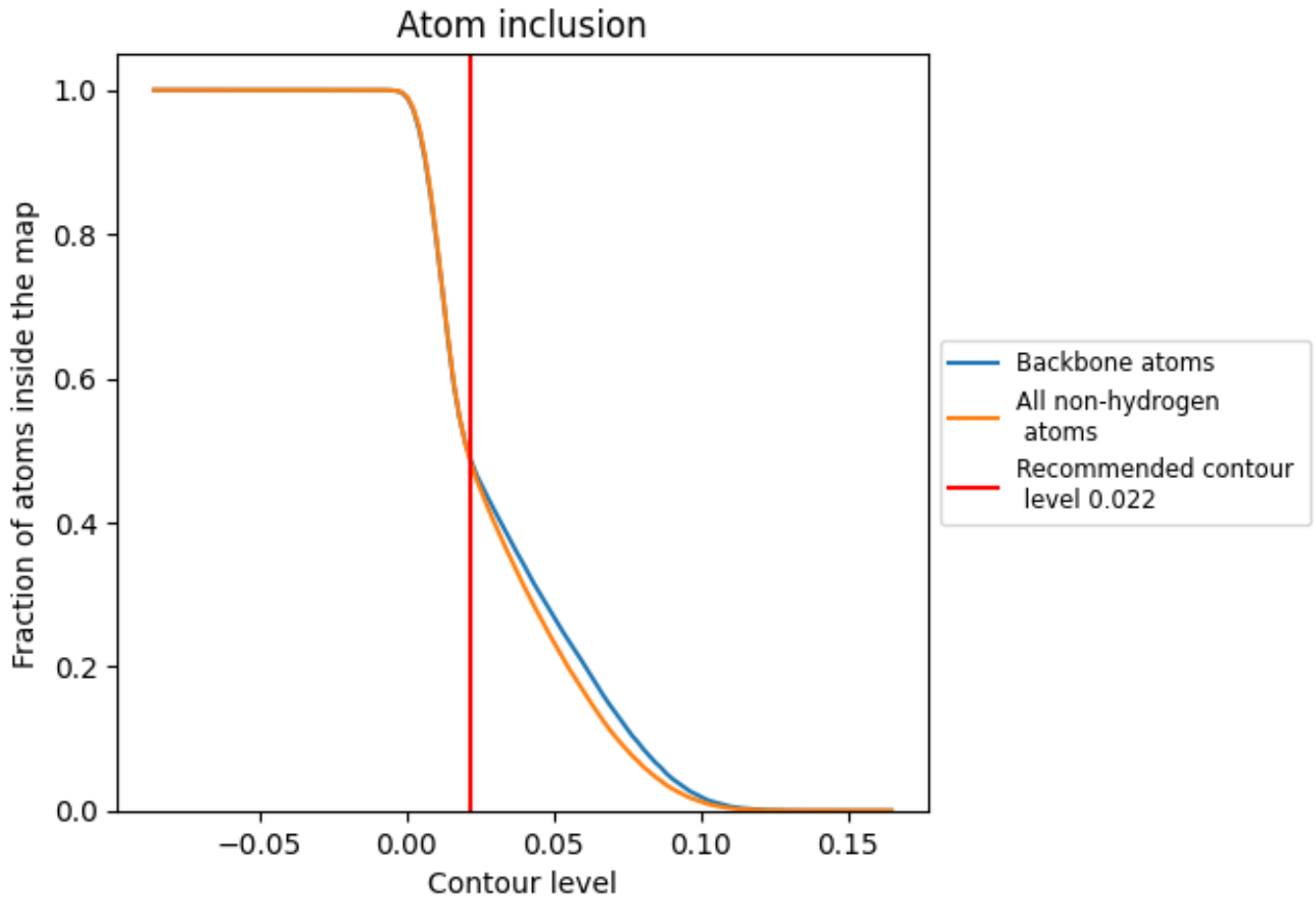
9.3 Atom inclusion mapped to coordinate model



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 48% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4806	0.3380
A	0.8491	0.5370
B	0.8820	0.5560
C	0.9108	0.5800
D	0.2725	0.1850
E	0.8535	0.5210
F	0.8962	0.5740
G	0.4391	0.3110
H	0.8513	0.5590
I	0.8472	0.5110
J	0.9180	0.5730
K	0.9211	0.5890
L	0.8480	0.5090
M	0.0153	0.0750
N	0.3467	0.2200
P	0.4248	0.2780
Q	0.0282	0.1020
R	0.0117	0.0880
T	0.5195	0.3100
U	0.0548	0.1140
V	0.0256	0.1270
W	0.0109	0.0430
X	0.0235	0.1060
Y	0.0056	0.0770
Z	0.0993	0.1660