



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:21 AM JST

PDB ID : 7EGB / pdb_00007egb
EMDB ID : EMD-31111
Title : TFIID-based holo PIC on SCP promoter
Authors : Chen, X.; Wu, Z.; Hou, H.; Qi, Y.; Wang, X.; Li, J.; Xu, Y.
Deposited on : 2021-03-24
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

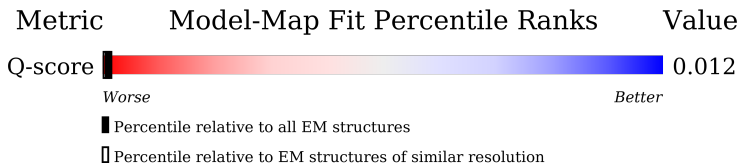
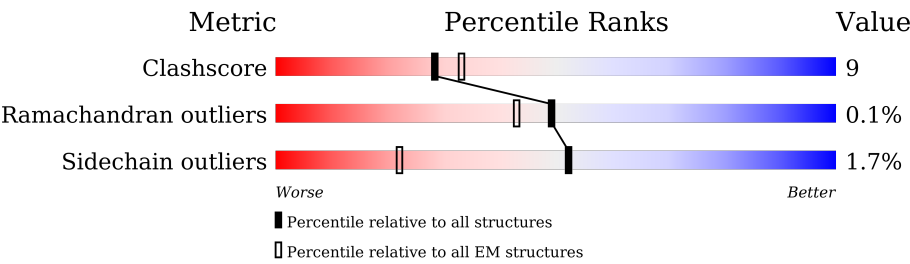
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	309	69% 53% 22% 24%
2	1	548	27% 40% 8% 52%
3	2	395	32% 68% 15% 17%
4	3	308	17% 65% 19% 15%

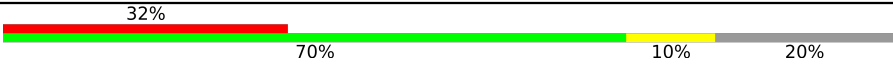
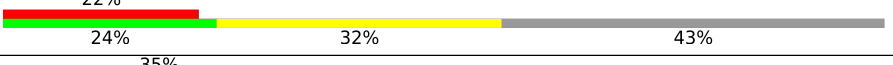
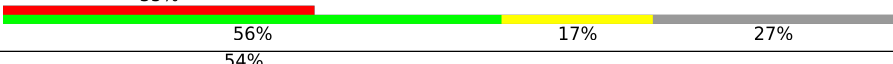
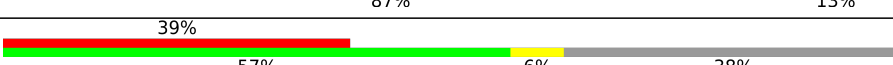
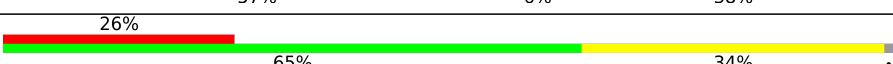
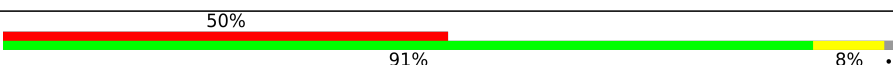
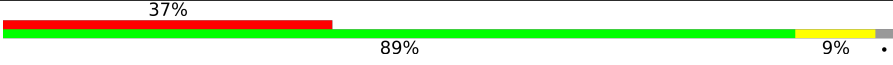
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Mol	Chain	Length	Quality of chain
5	4	462	
6	5	71	
7	6	782	
8	7	760	
9	8	346	
10	9	323	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	
23	Q	376	

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Mol	Chain	Length	Quality of chain
24	R	316	
25	S	517	
26	T	249	
27	U	439	
28	V	291	
29	X	94	
30	Y	69	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 112409 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	236	Total	C	N	O	S	0	0
			1932	1211	336	373	12		

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	329	Total	C	N	O	S	0	0
			2567	1621	440	479	27		

- Molecule 4 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	394	Total	C	N	O	S	0	0
			3189	2068	552	557	12		

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 8 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	298	Total	C	N	O	S	0	0
			2376	1537	404	423	12		

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	281	Total	C	N	O	S	0	0
			2293	1465	394	416	18		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	559	Total	C	N	O	S	0	0
			4580	2924	795	834	27		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	160	Total	C	N	O	S	0	0
			1337	834	249	251	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total	C	N	O	S	0	0
			4376	2774	759	822	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
18	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 22 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 23 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	252	Total	C	N	O	S	0	0
			1953	1224	346	366	17		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	108	Total	C	N	O	S	0	0
			872	558	153	159	2		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 29 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	69	Total	C	N	O	P	0	0
			1429	672	279	409	69		

- Molecule 30 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	69	Total	C	N	O	P	0	0
			1400	664	248	419	69		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1423	Total	C	N	O	S	0	0
			11274	7092	2016	2094	72		

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1135	Total	C	N	O	S	0	0
			9068	5735	1596	1673	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	q	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	r	128	Total	C	N	O	S	0	0
			1050	656	178	212	4		

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	79	Total	C	N	O	S	0	0
			636	406	108	117	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	u	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	v	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			928	571	166	180	11		

- Molecule 43 is a protein called RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	64	Total	C	N	O	S	0	0
			507	328	86	87	6		

- Molecule 44 is a protein called RNA_pol_L_2 domain-containing protein.

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

- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			373	231	72	64	6		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

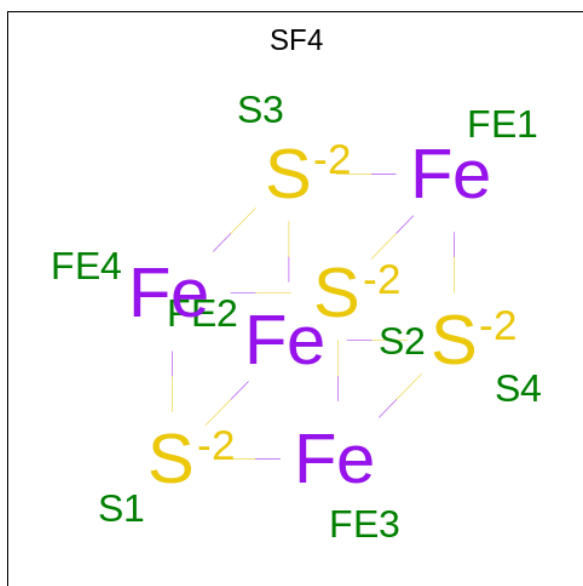
Mol	Chain	Residues	Atoms		AltConf
46	0	2	Total	Zn	0
			2	2	
46	2	3	Total	Zn	0
			3	3	
46	3	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
46	R	1	Total 1	Zn 1	0
46	U	1	Total 1	Zn 1	0
46	o	2	Total 2	Zn 2	0
46	p	1	Total 1	Zn 1	0
46	q	1	Total 1	Zn 1	0
46	w	2	Total 2	Zn 2	0
46	x	1	Total 1	Zn 1	0
46	z	1	Total 1	Zn 1	0

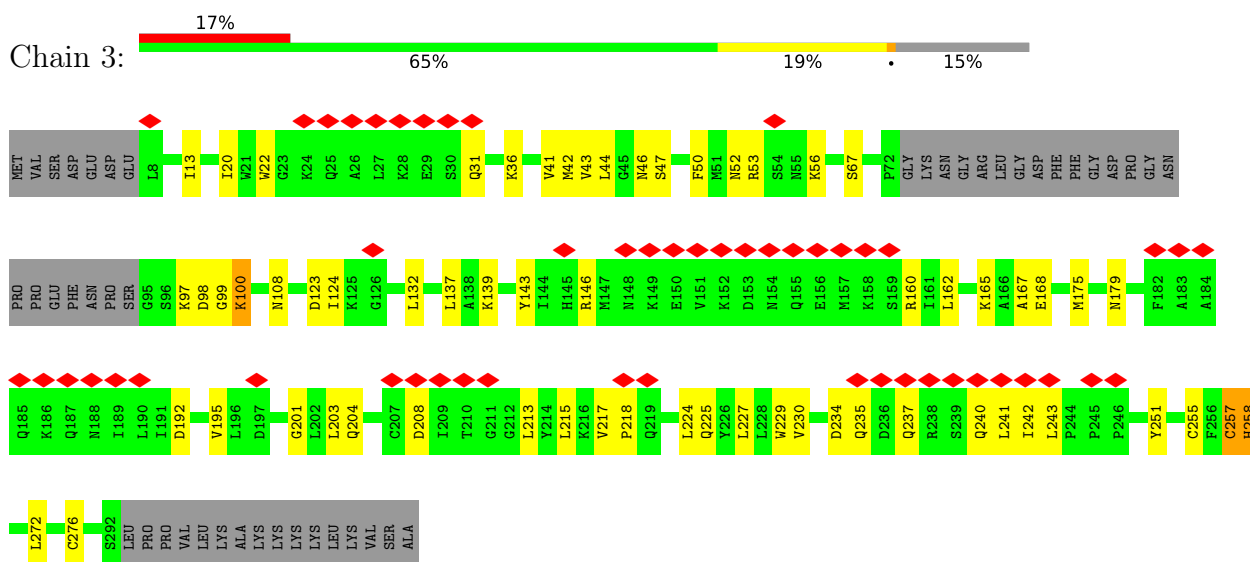
- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



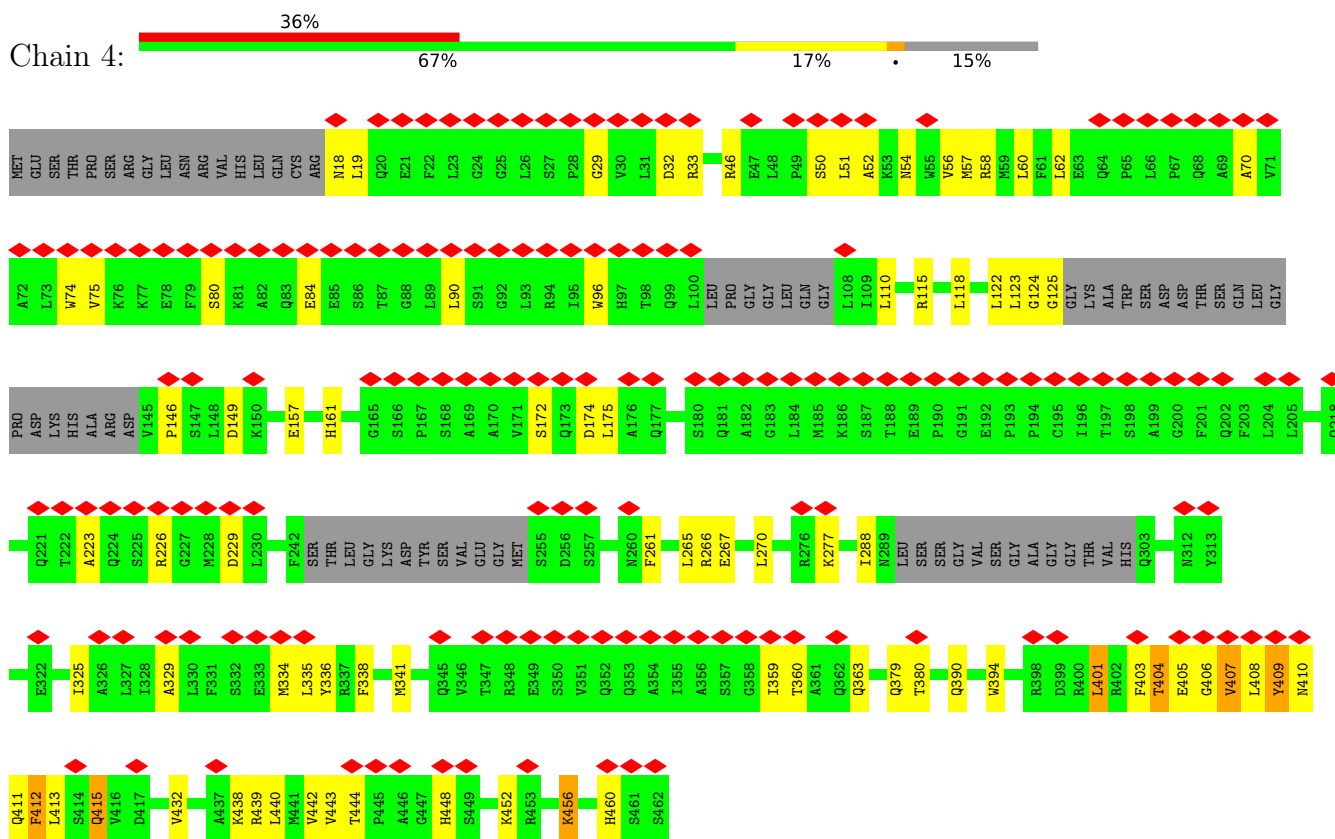
Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total 8	Fe 4	S 4	0

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

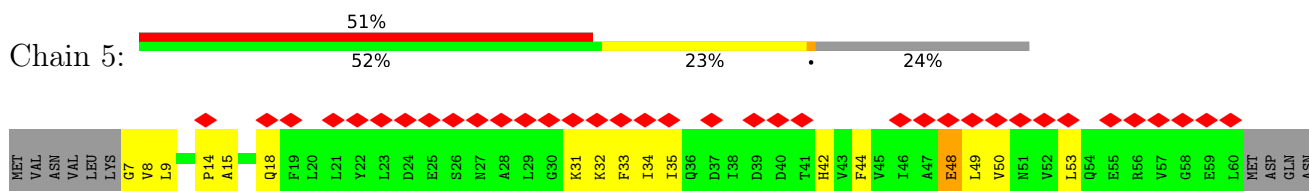
Mol	Chain	Residues	Atoms		AltConf
48	o	1	Total	Mg	0
			1	1	



• Molecule 5: General transcription factor IIH subunit 4



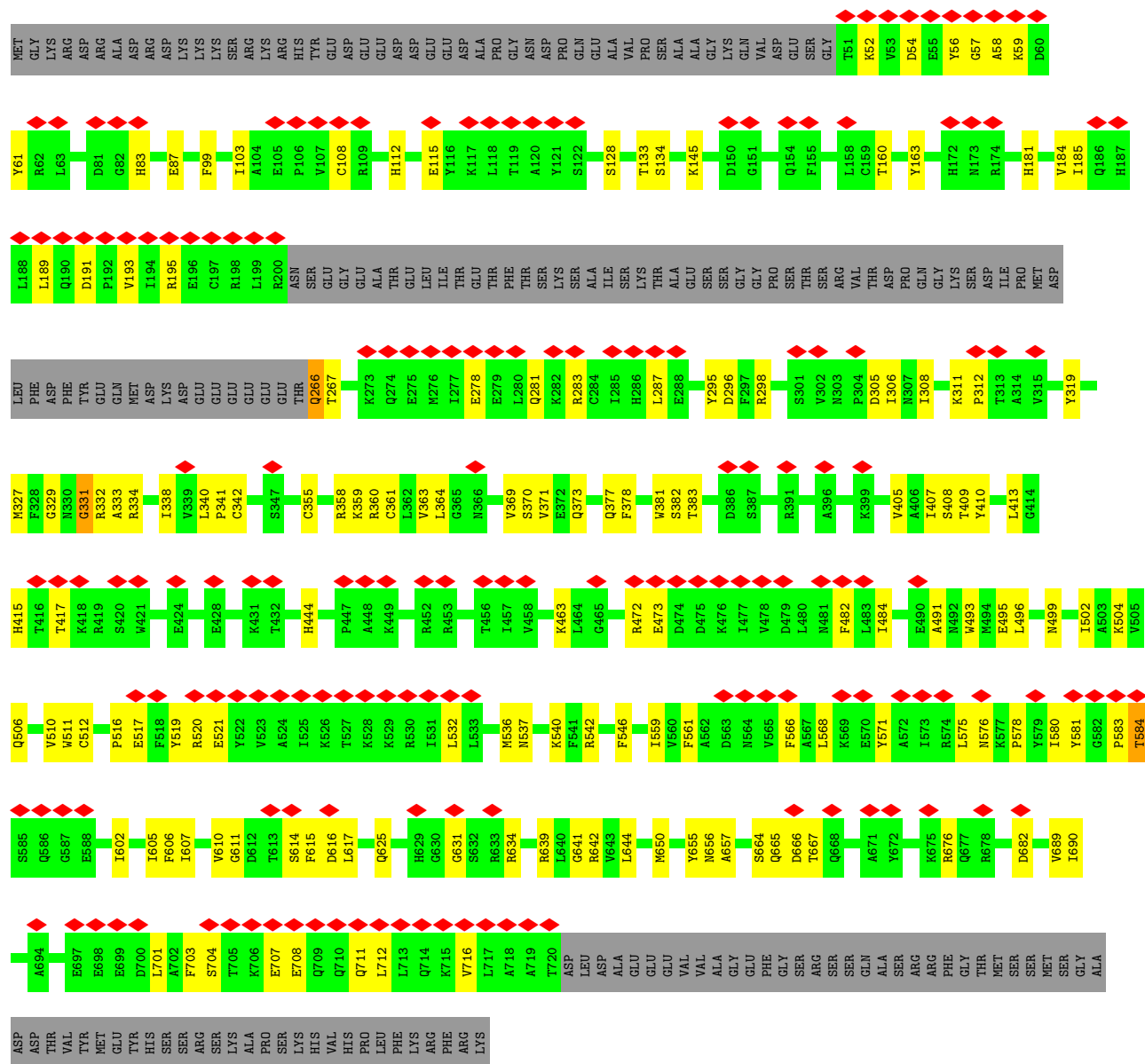
• Molecule 6: General transcription factor IIH subunit 5



ALA
PHE
SER
LEU
THR
GLN
LYS

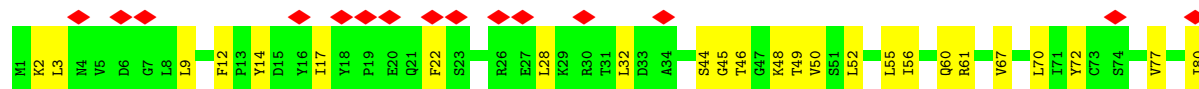
• Molecule 7: General transcription and DNA repair factor IIIH helicase subunit XPB

Chain 6: 

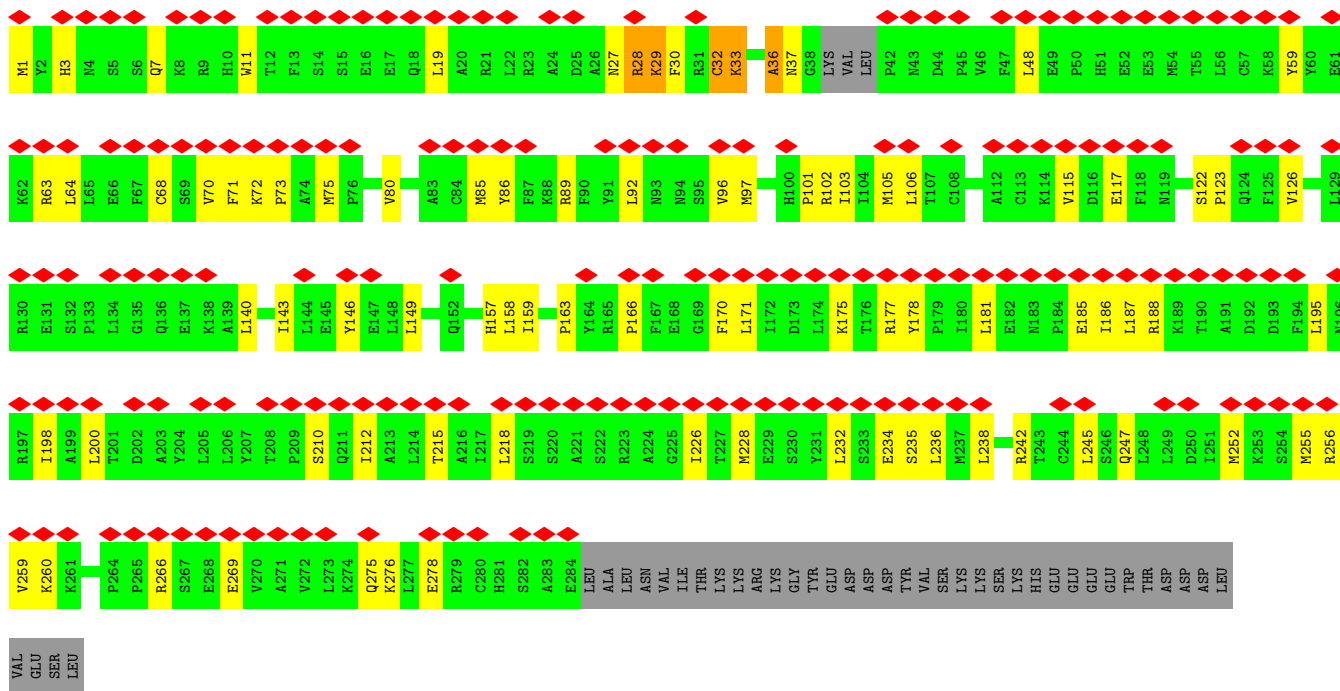


• Molecule 8: General transcription and DNA repair factor IIIH helicase subunit XPD

Chain 7: 



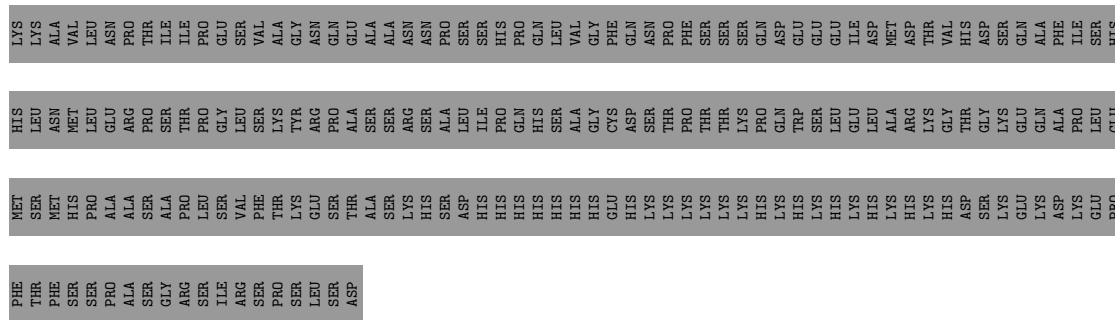
- Molecule 10: Cyclin-H



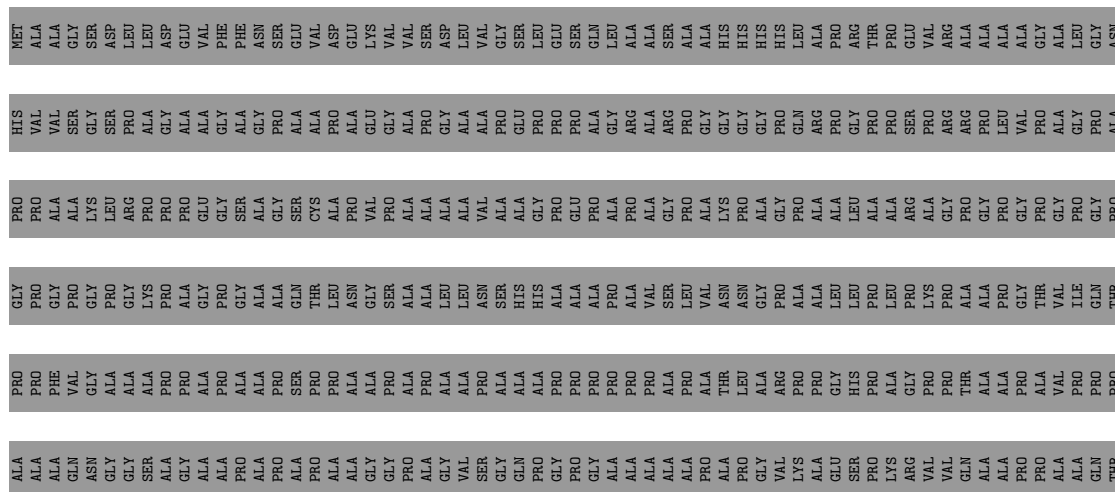
- Molecule 11: Transcription initiation factor TFIID subunit 1

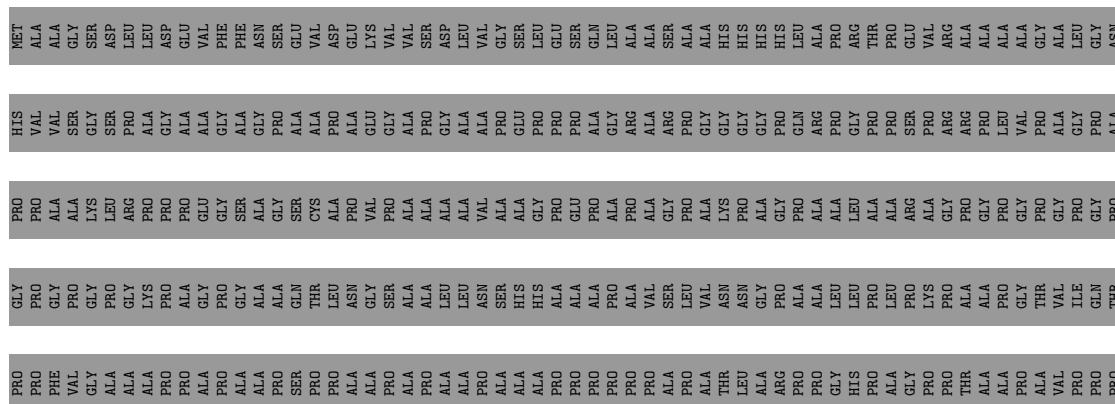






Chain D: 7% 12% 85%



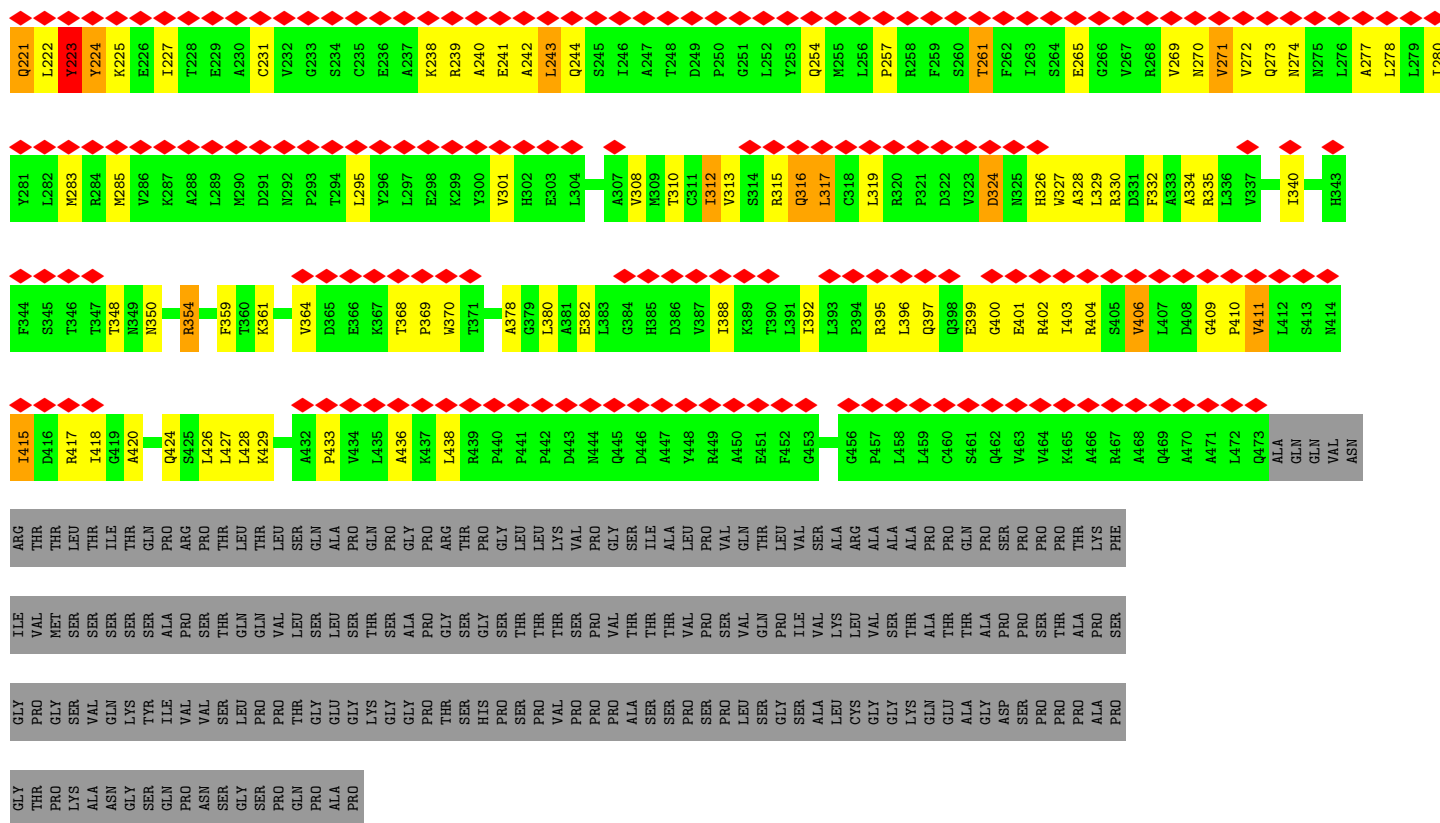


K1081	A1082	F1083	L1084	K1085
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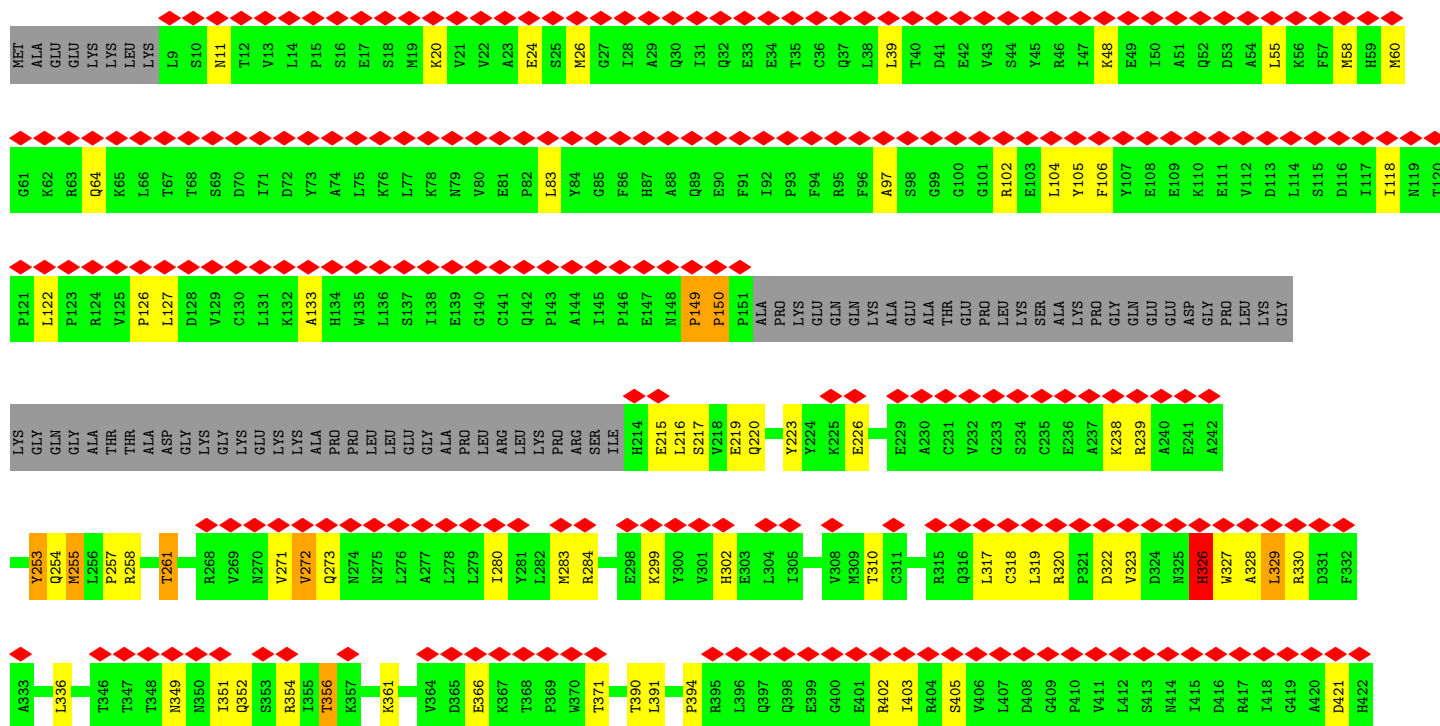
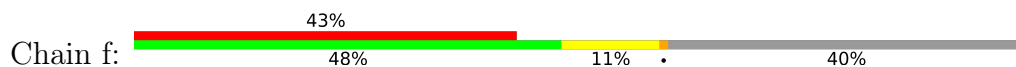
Chain E:

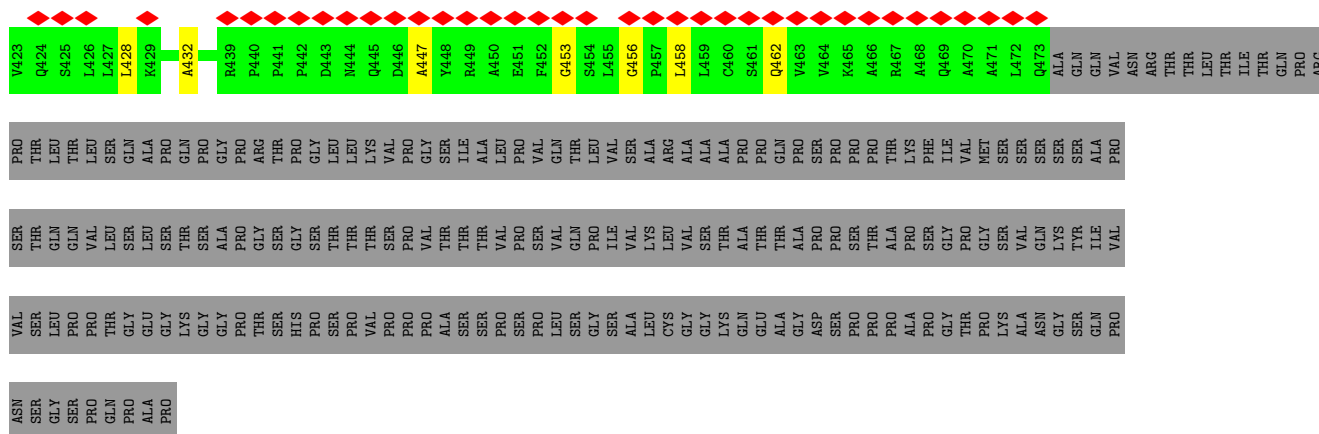
[illegible]



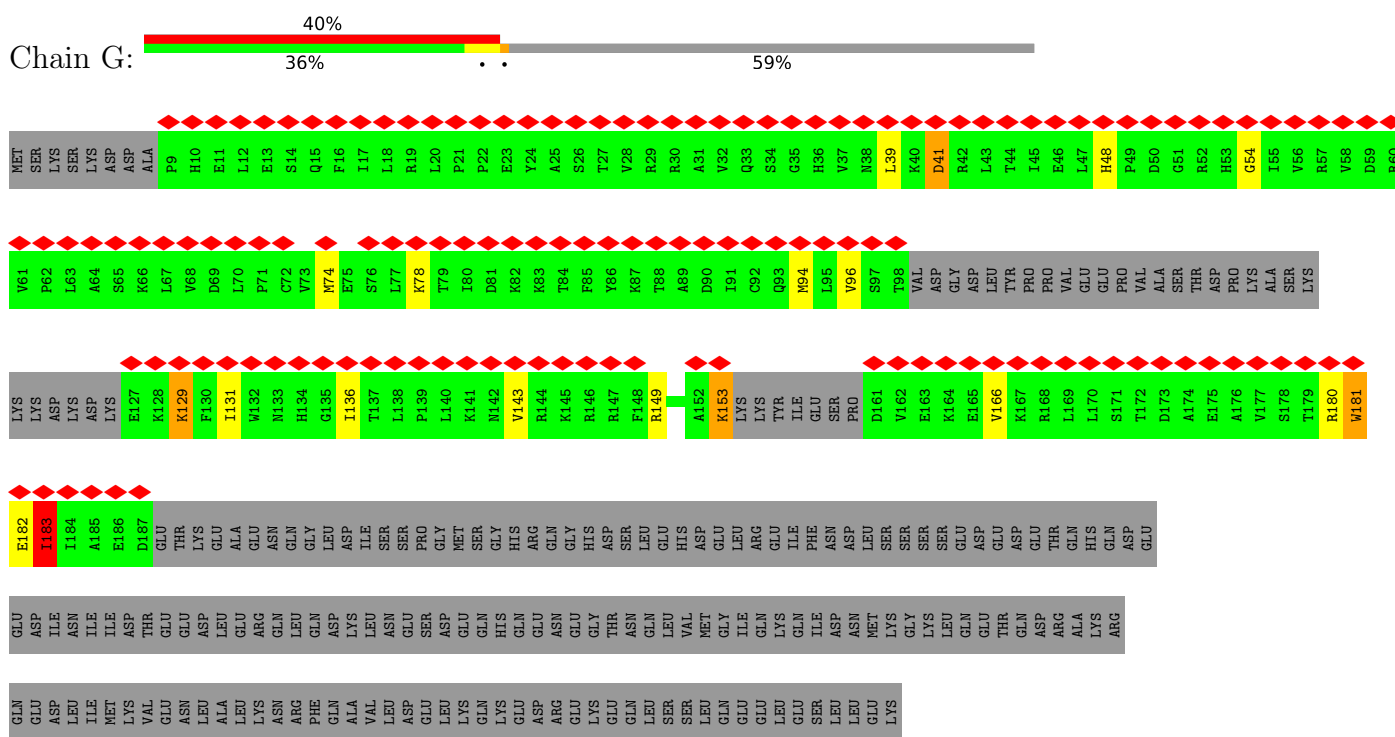


• Molecule 15: Transcription initiation factor TFIID subunit 6

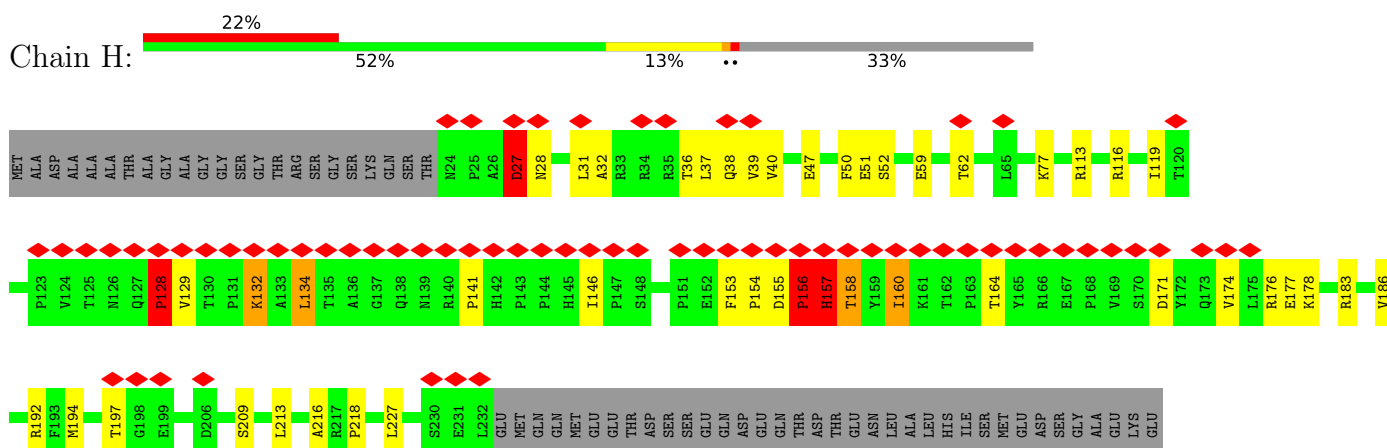




- Molecule 16: Transcription initiation factor TFIID subunit 7



- Molecule 17: Transcription initiation factor TFIID subunit 8



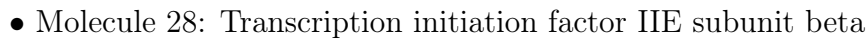
Chain O: 40% 70% 21% 9%



Chain T:



Chain U:



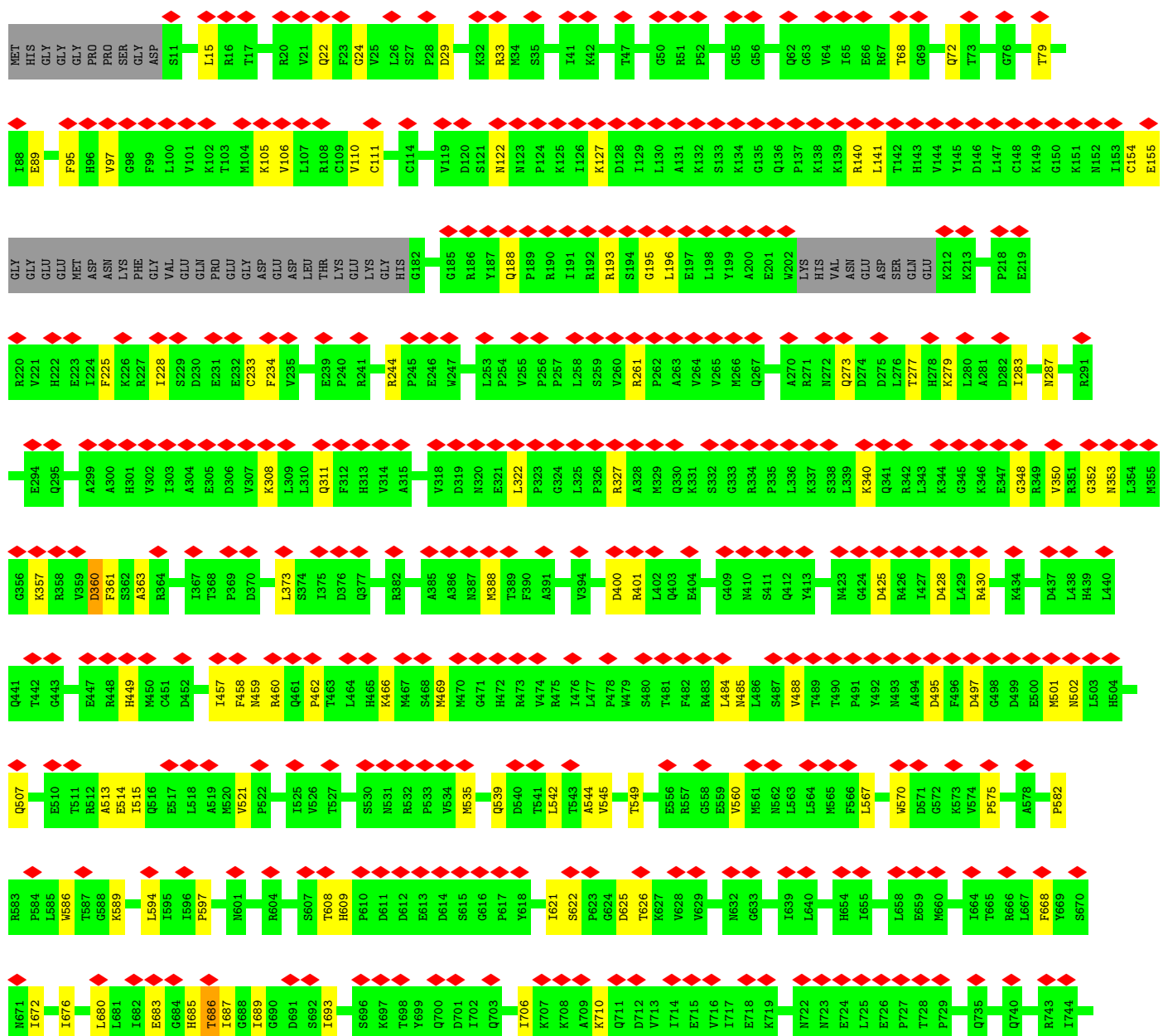
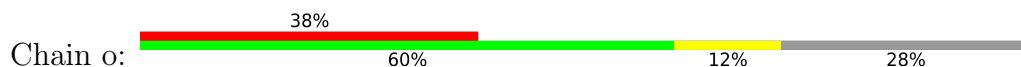
Chain V:





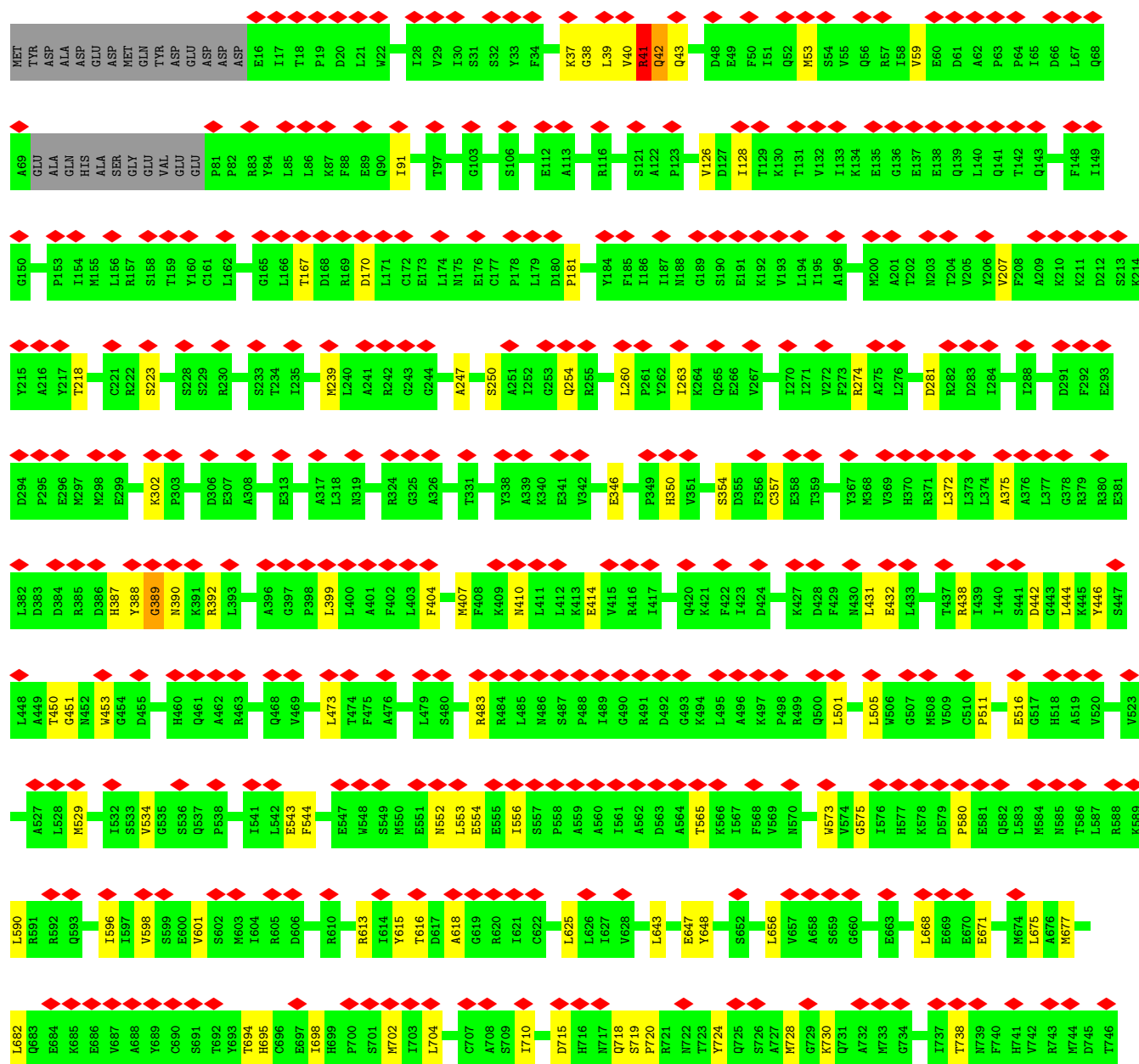
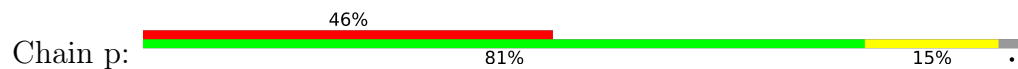


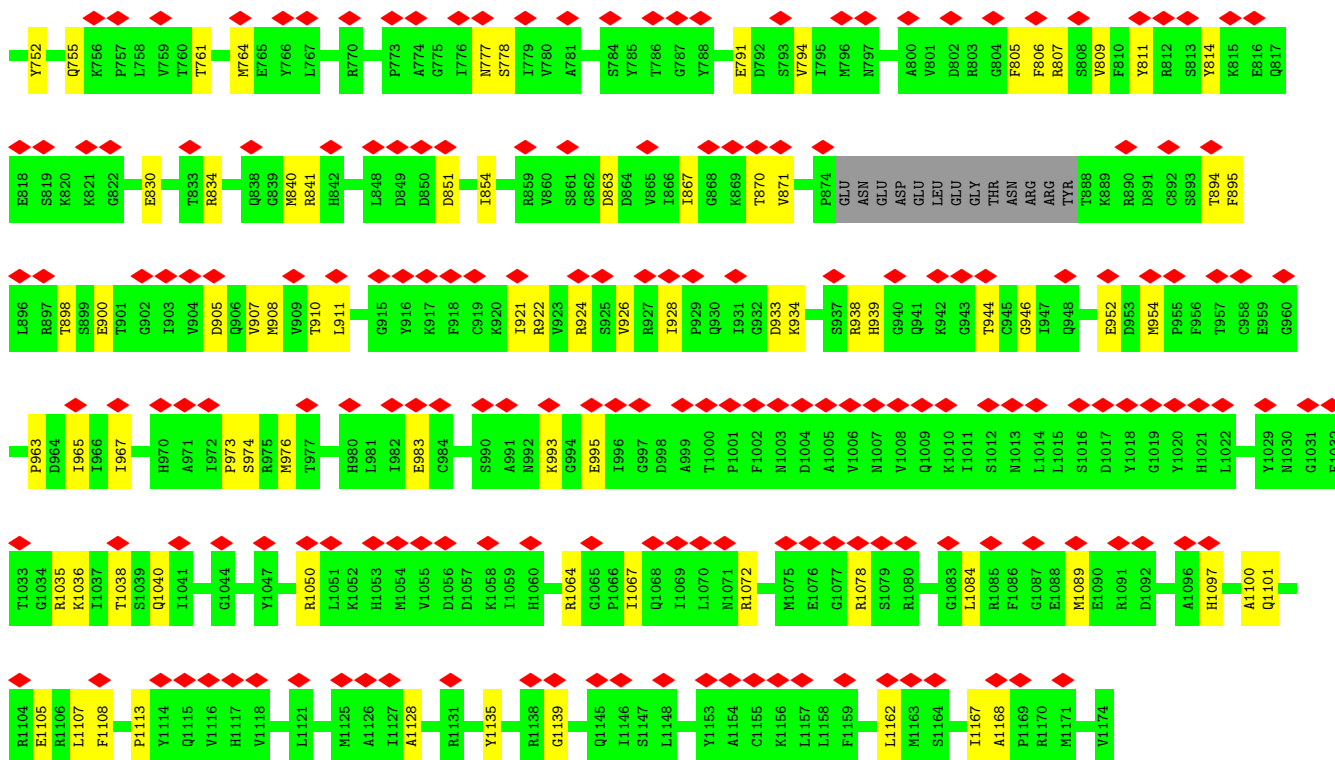
• Molecule 34: DNA-directed RNA polymerase II subunit RPB1



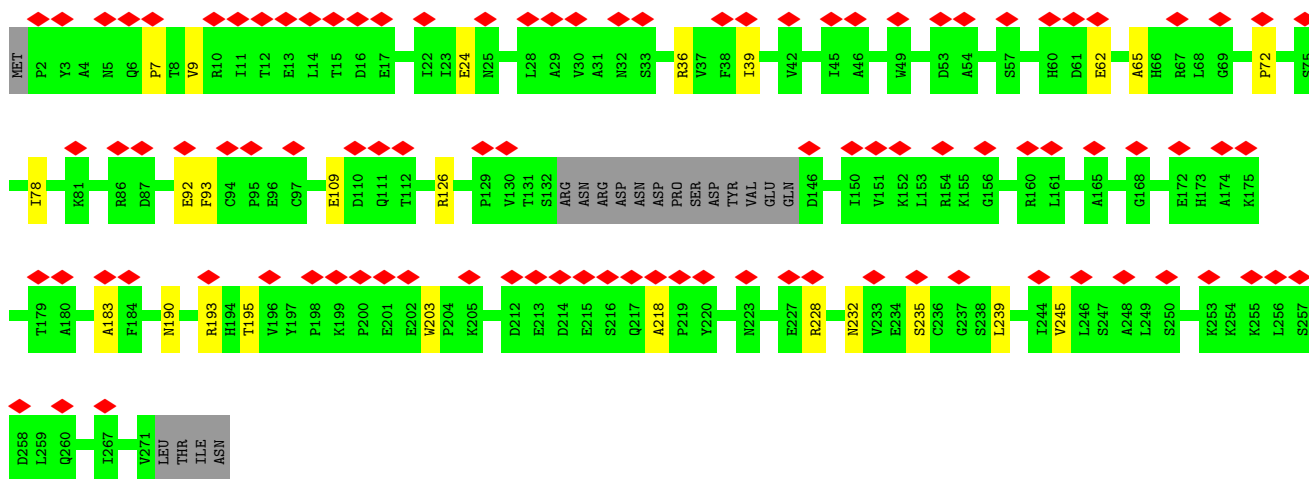
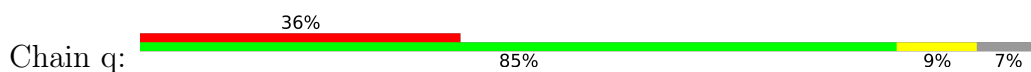


- Molecule 35: DNA-directed RNA polymerase subunit beta



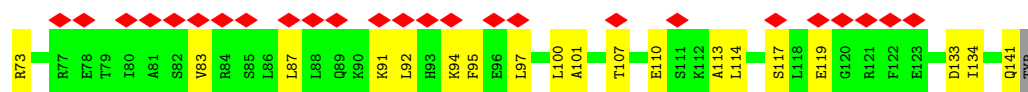


• Molecule 36: DNA-directed RNA polymerase II subunit RPB3

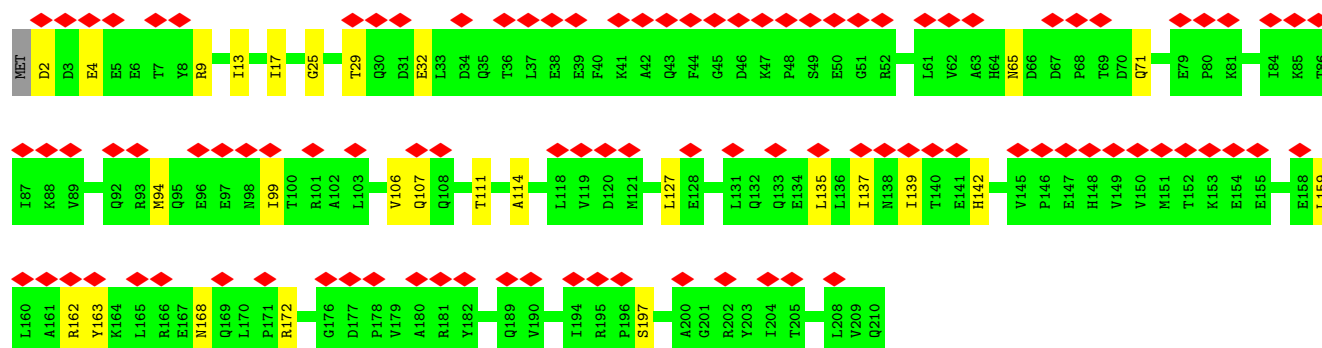
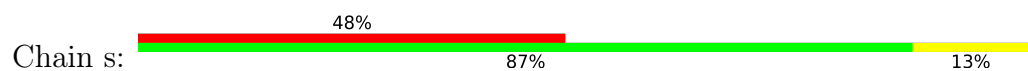


• Molecule 37: DNA-directed RNA polymerase II subunit RPB4

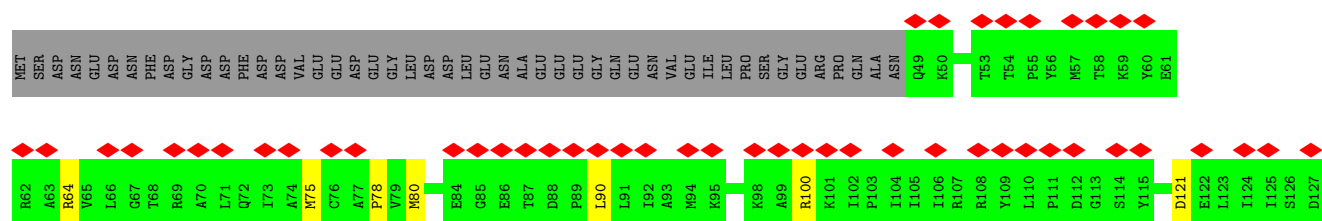
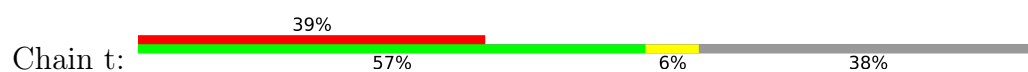




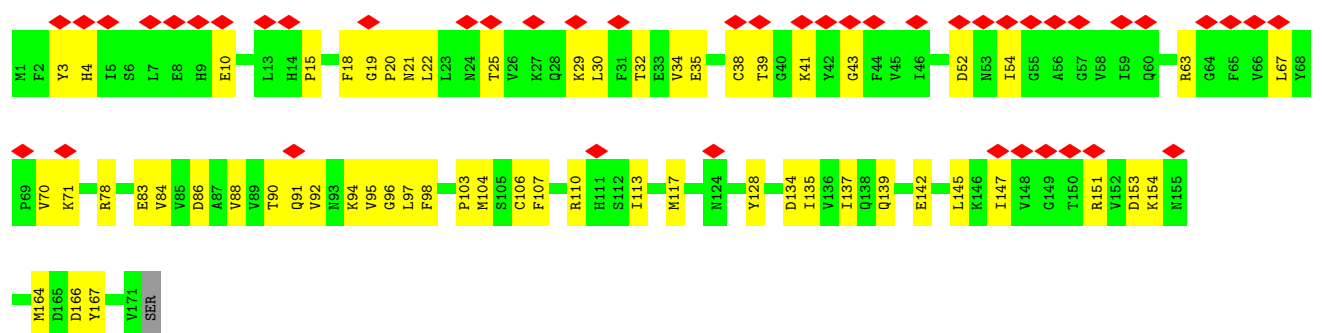
- Molecule 38: DNA-directed RNA polymerase II subunit E



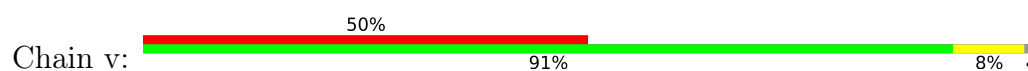
- Molecule 39: DNA-directed RNA polymerase II subunit F

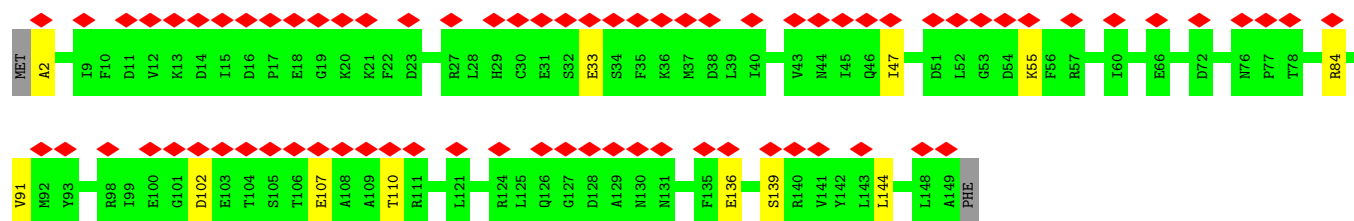


- Molecule 40: DNA-directed RNA polymerase II subunit RPB7

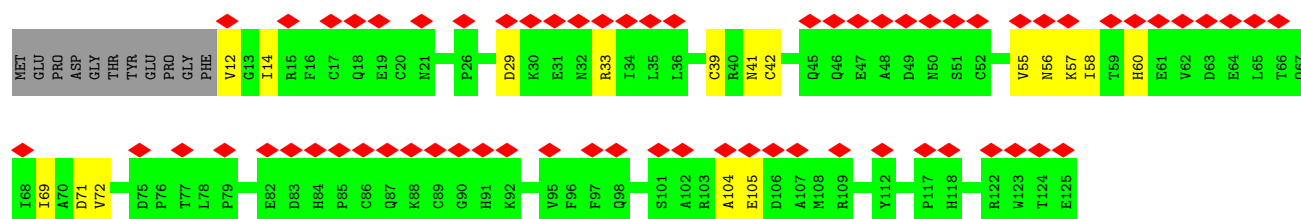
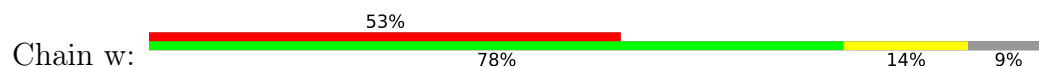


- Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

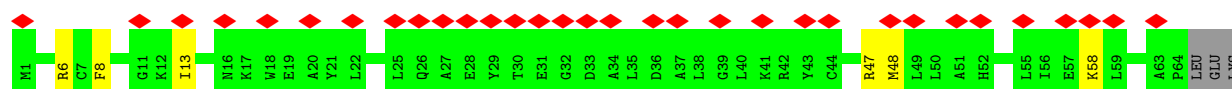
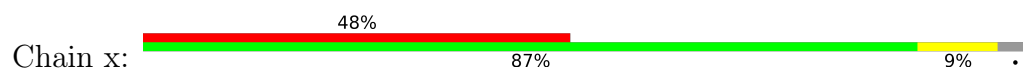




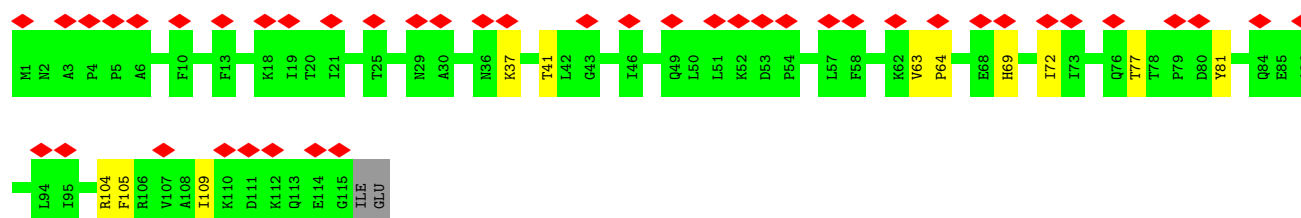
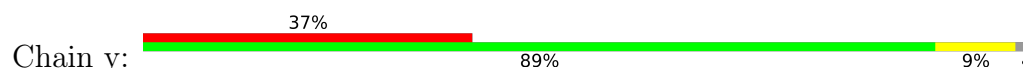
• Molecule 42: DNA-directed RNA polymerase II subunit RPB9



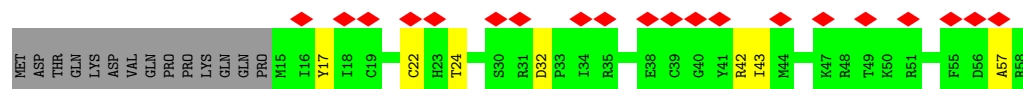
• Molecule 43: RPB10



• Molecule 44: RNA_pol_L_2 domain-containing protein



• Molecule 45: RPB12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.811	Depositor
Minimum map value	-4.382	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.39	0/1965	0.62	0/2646
2	1	0.23	0/2210	0.39	0/2975
3	2	0.16	0/2624	0.28	0/3555
4	3	0.30	0/2103	0.47	1/2846 (0.0%)
5	4	0.31	0/3262	0.51	2/4418 (0.0%)
6	5	0.34	0/433	0.60	0/585
7	6	0.29	0/4994	0.48	2/6745 (0.0%)
8	7	0.21	0/5875	0.37	1/7955 (0.0%)
9	8	0.35	0/2434	0.55	1/3300 (0.0%)
10	9	0.46	0/2342	0.72	6/3159 (0.2%)
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.69	6/10836 (0.1%)
13	D	0.54	0/1350	0.81	2/1805 (0.1%)
13	d	0.48	0/1321	0.71	2/1772 (0.1%)
14	E	0.45	1/4482 (0.0%)	0.72	3/6069 (0.0%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.65	1/3201 (0.0%)	1.07	13/4347 (0.3%)
15	f	0.47	1/3140 (0.0%)	0.80	6/4268 (0.1%)
16	G	0.68	0/1190	0.94	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	1.00	14/2285 (0.6%)
18	I	0.21	0/981	0.41	0/1332
18	i	0.21	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.73	0/775	0.96	0/1049
20	L	0.68	0/630	1.13	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.25	0/816	0.43	0/1105
22	P	0.16	0/1448	0.28	0/1948
23	Q	0.18	0/945	0.35	0/1274
24	R	0.23	0/1983	0.38	0/2679
25	S	0.12	0/896	0.25	0/1213
26	T	0.20	0/1817	0.39	1/2445 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	U	0.41	0/1545	0.68	1/2075 (0.0%)
28	V	0.24	0/1380	0.58	0/1854
29	X	0.28	0/1607	0.58	0/2481
30	Y	0.29	0/1565	0.59	0/2410
31	c	0.48	0/1035	0.67	0/1406
32	k	0.29	0/799	0.53	1/1070 (0.1%)
33	m	0.85	0/733	1.18	1/977 (0.1%)
34	o	0.37	8/11479 (0.1%)	0.55	21/15496 (0.1%)
35	p	0.40	6/9249 (0.1%)	0.39	7/12482 (0.1%)
36	q	0.15	0/2102	0.29	0/2857
37	r	0.14	0/1064	0.22	0/1428
38	s	0.29	1/1752 (0.1%)	0.53	3/2366 (0.1%)
39	t	0.16	0/646	0.27	0/871
40	u	0.20	0/1382	0.28	0/1874
41	v	0.14	0/1207	0.28	0/1628
42	w	0.23	0/949	0.41	0/1284
43	x	0.16	0/516	0.25	0/696
44	y	0.22	0/939	0.37	0/1271
45	z	0.17	0/378	0.28	0/500
All	All	0.41	23/114954 (0.0%)	0.62	103/155974 (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	0	0	1
26	T	0	1
27	U	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	p	704	LEU	C-N	20.97	1.56	1.33
35	p	806	PHE	C-N	16.04	1.56	1.33
35	p	928	ILE	C-N	13.37	1.50	1.33
34	o	388	MET	C-N	12.26	1.50	1.33
34	o	1466	ALA	C-N	12.03	1.51	1.33
34	o	1424	THR	C-N	11.09	1.50	1.33
34	o	449	HIS	C-N	10.82	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	s	139	ILE	C-N	10.47	1.47	1.34
35	p	534	VAL	C-N	8.85	1.45	1.32
17	H	28	ASN	C-O	-7.50	1.15	1.24
17	H	27	ASP	C-O	-7.10	1.15	1.24
34	o	893	GLU	C-N	7.09	1.45	1.33
34	o	1082	HIS	C-N	-6.68	1.24	1.33
17	H	31	LEU	C-O	-6.57	1.16	1.24
34	o	833	PRO	C-O	-6.52	1.16	1.24
12	B	61	ASN	C-O	-5.90	1.18	1.24
14	E	524	LEU	C-O	5.77	1.30	1.24
14	e	445	LYS	C-O	5.64	1.30	1.24
15	F	395	ARG	C-O	5.59	1.31	1.24
34	o	685	HIS	C-O	-5.51	1.17	1.23
35	p	451	GLY	C-N	-5.50	1.25	1.33
15	f	217	SER	CA-CB	-5.06	1.45	1.53
35	p	618	ALA	C-N	5.02	1.41	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	o	1082	HIS	CA-C-N	16.32	136.59	119.78
34	o	1082	HIS	C-N-CA	16.32	136.59	119.78
38	s	139	ILE	O-C-N	-15.11	106.61	121.87
34	o	1483	GLY	N-CA-C	14.43	129.23	112.50
17	H	156	PRO	N-CA-C	-13.59	90.10	111.03
34	o	893	GLU	O-C-N	-12.22	109.04	121.87
34	o	1082	HIS	O-C-N	-11.76	104.49	121.54
34	o	1481	LYS	N-CA-C	-11.57	99.53	112.72
38	s	139	ILE	CA-C-N	11.13	136.63	120.38
38	s	139	ILE	C-N-CA	11.13	136.63	120.38
34	o	1466	ALA	O-C-N	9.82	134.98	123.30
12	B	491	HIS	N-CA-C	-9.54	100.88	111.28
34	o	1424	THR	CA-C-N	-9.37	107.16	121.87
34	o	1424	THR	C-N-CA	-9.37	107.16	121.87
34	o	1424	THR	O-C-N	9.17	133.69	123.33
15	f	149	PRO	O-C-N	8.91	125.41	121.31
34	o	893	GLU	CA-C-N	8.56	135.07	121.98
34	o	893	GLU	C-N-CA	8.56	135.07	121.98
14	E	756	THR	N-CA-C	-8.36	103.22	113.50
17	H	32	ALA	N-CA-C	-8.19	102.31	111.07
15	F	224	TYR	N-CA-C	-7.99	101.53	111.75
17	H	27	ASP	N-CA-C	-7.85	102.81	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	6	331	GLY	O-C-N	7.63	131.70	122.84
15	F	223	TYR	CB-CA-C	-7.61	97.92	110.85
15	F	271	VAL	N-CA-C	-7.41	105.79	112.90
35	p	389	GLY	N-CA-C	-7.40	106.19	114.40
14	E	762	PRO	N-CA-C	7.30	124.12	114.27
17	H	157	HIS	CB-CA-C	-7.28	95.92	110.42
5	4	415	GLN	N-CA-C	7.20	119.13	111.28
11	A	715	PRO	N-CA-C	-7.09	100.11	111.03
17	H	128	PRO	CB-CA-C	7.05	123.19	111.56
7	6	581	TYR	CB-CA-C	-7.02	97.95	110.03
12	B	495	GLN	N-CA-C	-6.97	104.77	113.28
35	p	42	GLN	CB-CA-C	-6.92	100.39	111.39
5	4	412	PHE	CB-CA-C	6.88	123.19	110.11
32	k	180	PRO	N-CA-C	6.71	118.88	110.70
11	A	396	LEU	N-CA-C	-6.70	104.85	113.16
17	H	128	PRO	CA-N-CD	-6.65	102.69	112.00
15	f	326	HIS	N-CA-C	-6.63	104.29	112.38
15	f	319	LEU	N-CA-C	-6.57	103.94	112.68
4	3	97	LYS	O-C-N	6.47	128.98	122.12
11	A	467	ILE	N-CA-C	-6.46	103.96	111.00
11	A	1205	PHE	CA-CB-CG	-6.30	107.50	113.80
9	8	165	PRO	CB-CA-C	-6.25	102.99	112.11
17	H	156	PRO	CA-C-O	-6.17	114.62	121.23
15	F	218	VAL	N-CA-C	-6.14	104.36	110.62
19	J	148	ASP	CA-C-N	6.13	125.86	119.05
19	J	148	ASP	C-N-CA	6.13	125.86	119.05
10	9	29	LYS	CA-C-N	-6.07	112.14	120.28
10	9	29	LYS	C-N-CA	-6.07	112.14	120.28
17	H	27	ASP	CA-C-O	-6.03	114.03	120.42
13	D	995	GLU	CB-CA-C	-6.02	101.42	110.88
17	H	158	THR	N-CA-C	-5.98	104.84	111.36
15	f	255	MET	N-CA-C	-5.91	104.93	114.09
15	F	223	TYR	N-CA-C	-5.86	104.97	111.36
17	H	156	PRO	CB-CA-C	-5.84	104.28	111.64
15	F	316	GLN	CB-CA-C	5.82	120.27	110.79
17	H	128	PRO	N-CA-CB	-5.79	97.17	103.25
26	T	144	GLN	O-C-N	-5.73	115.37	122.82
12	B	583	GLU	CB-CA-C	-5.70	101.33	110.79
15	F	310	THR	CB-CA-C	5.67	120.20	110.79
15	f	150	PRO	N-CA-C	5.65	117.59	110.70
15	F	330	ARG	N-CA-C	-5.65	105.12	111.28
12	B	181	GLY	CA-C-O	-5.65	118.25	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	p	41	ARG	N-CA-C	-5.62	105.77	113.30
12	B	264	GLU	N-CA-C	-5.59	106.12	113.17
34	o	1487	PRO	N-CA-CB	-5.57	96.87	103.00
15	F	244	GLN	N-CA-C	-5.55	105.23	111.28
15	F	324	ASP	N-CA-C	-5.53	105.35	111.71
10	9	36	ALA	CB-CA-C	-5.52	102.21	110.88
33	m	71	LYS	CB-CA-C	5.48	119.89	110.79
34	o	1466	ALA	CA-C-N	-5.48	110.67	121.41
34	o	1466	ALA	C-N-CA	-5.48	110.67	121.41
15	F	272	VAL	N-CA-C	-5.47	105.04	110.62
14	E	270	ASP	CB-CA-C	5.44	119.18	110.09
13	D	958	LYS	N-CA-C	-5.44	105.35	111.28
10	9	37	ASN	CB-CA-C	5.37	119.71	110.79
34	o	1482	TYR	N-CA-CB	-5.37	102.33	111.20
35	p	38	GLY	CA-C-O	-5.36	115.78	122.65
17	H	156	PRO	N-CA-CB	-5.32	98.48	103.27
34	o	834	THR	CB-CA-C	-5.31	101.82	110.85
16	G	183	ILE	N-CA-C	-5.31	102.67	109.30
35	p	928	ILE	O-C-N	-5.31	115.05	121.10
10	9	33	LYS	N-CA-C	-5.29	105.52	111.28
34	o	360	ASP	CB-CA-C	-5.28	101.22	112.63
17	H	134	LEU	CB-CA-C	-5.26	110.49	116.54
15	f	329	LEU	N-CA-C	-5.24	106.58	112.87
12	B	491	HIS	CB-CA-C	5.24	119.48	110.79
8	7	593	GLY	CA-C-O	-5.23	117.15	122.59
34	o	1482	TYR	CA-CB-CG	5.19	123.23	113.90
20	L	106	ARG	N-CA-C	-5.16	107.01	113.15
11	A	1067	GLN	CB-CA-C	5.11	119.27	110.79
13	d	942	ALA	CA-C-N	-5.10	113.44	120.28
13	d	942	ALA	C-N-CA	-5.10	113.44	120.28
10	9	30	PHE	CB-CA-C	-5.07	102.37	110.79
17	H	51	GLU	CB-CA-C	-5.06	100.45	109.71
34	o	1473	LEU	O-C-N	-5.05	117.28	123.30
15	F	241	GLU	N-CA-C	-5.05	105.77	111.28
15	F	438	LEU	N-CA-C	5.04	118.51	111.30
34	o	686	THR	CA-C-O	-5.02	115.89	121.51
35	p	392	ARG	CA-C-O	-5.01	115.58	121.44
27	U	167	ALA	CA-C-O	-5.00	115.56	120.82
35	p	42	GLN	N-CA-C	-5.00	103.28	111.04

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	126	GLN	Mainchain
26	T	144	GLN	Mainchain
27	U	78	VAL	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	0	1932	0	1905	86	0
2	1	2167	0	2175	35	0
3	2	2567	0	2539	49	0
4	3	2066	0	2097	89	0
5	4	3189	0	3243	131	0
6	5	428	0	434	45	0
7	6	4890	0	4949	214	0
8	7	5751	0	5794	115	0
9	8	2376	0	2402	73	0
10	9	2293	0	2315	76	0
11	A	4580	0	4502	97	0
12	B	7796	0	7751	113	0
13	D	1337	0	1358	44	0
13	d	1307	0	1318	16	0
14	E	4376	0	4256	78	0
14	e	4327	0	4197	64	0
15	F	3143	0	3093	103	0
15	f	3081	0	3012	70	0
16	G	1171	0	1222	17	0
17	H	1633	0	1621	42	0
18	I	959	0	969	13	0
18	i	967	0	977	10	0
19	J	720	0	719	12	0
19	j	759	0	759	14	0
20	L	622	0	620	21	0
20	l	876	0	893	10	0
21	O	806	0	818	22	0
22	P	1422	0	1514	29	0
23	Q	930	0	888	31	0
24	R	1953	0	1987	30	0
25	S	872	0	848	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	T	1788	0	1819	40	0
27	U	1520	0	1520	88	0
28	V	1357	0	1381	78	0
29	X	1429	0	770	13	0
30	Y	1400	0	775	9	0
31	c	1011	0	975	17	0
32	k	785	0	818	7	0
33	m	724	0	744	26	0
34	o	11274	0	11406	175	0
35	p	9068	0	9112	157	0
36	q	2059	0	2007	18	0
37	r	1050	0	1033	30	0
38	s	1721	0	1737	18	0
39	t	636	0	665	18	0
40	u	1351	0	1358	65	0
41	v	1186	0	1147	9	0
42	w	928	0	861	16	0
43	x	507	0	523	7	0
44	y	920	0	942	11	0
45	z	373	0	378	6	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0
46	x	1	0	0	0	0
46	z	1	0	0	0	0
47	7	8	0	0	0	0
48	o	1	0	0	0	0
All	All	112409	0	111146	2117	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 9.

All (2117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:308:ILE:CG2	7:6:358:ARG:HA	1.25	1.62
6:5:33:PHE:CE1	6:5:49:LEU:HD12	1.44	1.51
6:5:31:LYS:HB3	12:B:540:LYS:NZ	1.31	1.39
4:3:50:PHE:CZ	5:4:118:LEU:HD11	1.57	1.37
6:5:31:LYS:CB	12:B:540:LYS:HZ3	1.37	1.37
3:2:174:LEU:HD13	8:7:533:ASP:OD1	1.26	1.36
6:5:15:ALA:HB2	7:6:516:PRO:CB	1.53	1.36
27:U:139:LEU:HD22	40:u:151:ARG:CD	1.58	1.30
1:0:85:ARG:HH22	1:0:139:LYS:C	1.40	1.27
26:T:192:GLU:OE2	28:V:76:GLY:HA3	1.36	1.24
1:0:85:ARG:NH1	1:0:140:LEU:HG	1.51	1.23
27:U:139:LEU:CD2	40:u:151:ARG:HD2	1.71	1.21
4:3:50:PHE:CZ	5:4:118:LEU:CD1	2.25	1.18
7:6:308:ILE:HG21	7:6:358:ARG:HA	1.25	1.18
7:6:308:ILE:CG2	7:6:358:ARG:CA	2.21	1.17
6:5:15:ALA:HB1	7:6:516:PRO:HA	1.27	1.17
1:0:21:LEU:HD22	1:0:69:ASP:OD2	1.43	1.16
34:o:1482:TYR:HB2	39:t:80:MET:SD	1.85	1.16
5:4:334:MET:SD	7:6:56:TYR:CD2	2.38	1.15
6:5:15:ALA:CB	7:6:516:PRO:HA	1.75	1.15
10:9:242:ARG:HB2	34:o:1008:LYS:HZ2	1.08	1.15
7:6:319:TYR:OH	7:6:495:GLU:HG2	1.44	1.15
1:0:85:ARG:HH22	1:0:140:LEU:N	1.46	1.14
4:3:50:PHE:HZ	5:4:118:LEU:CD1	1.58	1.12
6:5:31:LYS:CB	12:B:540:LYS:NZ	2.02	1.12
4:3:229:TRP:CZ3	5:4:58:ARG:NH1	2.17	1.11
6:5:33:PHE:CE1	6:5:49:LEU:CD1	2.34	1.10
1:0:85:ARG:NH2	1:0:139:LYS:C	2.08	1.10
7:6:305:ASP:HA	7:6:359:LYS:CE	1.81	1.09
6:5:33:PHE:HE1	6:5:49:LEU:CD1	1.66	1.09
7:6:305:ASP:HA	7:6:359:LYS:HE3	1.12	1.09
10:9:242:ARG:HB3	34:o:1008:LYS:HZ1	1.09	1.09
7:6:308:ILE:HG22	7:6:358:ARG:HA	1.14	1.09
6:5:15:ALA:CB	7:6:516:PRO:HB3	1.83	1.08
11:A:1200:THR:O	11:A:1204:GLU:HG2	1.52	1.08
35:p:40:VAL:HG21	35:p:181:PRO:HB2	1.31	1.08
13:D:1002:ARG:NH2	26:T:182:HIS:CB	2.17	1.07
1:0:83:ASN:OD1	1:0:140:LEU:HD11	1.53	1.07
10:9:242:ARG:CB	34:o:1008:LYS:NZ	2.17	1.07
6:5:15:ALA:CB	7:6:516:PRO:CA	2.33	1.06
7:6:341:PRO:HD3	7:6:491:ALA:HB3	1.36	1.06
6:5:15:ALA:CB	7:6:516:PRO:CB	2.34	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:298:ARG:HG2	7:6:331:GLY:O	1.57	1.05
6:5:15:ALA:HB2	7:6:516:PRO:CA	1.86	1.04
1:0:84:LYS:HA	1:0:136:ASN:ND2	1.72	1.04
7:6:311:LYS:HE3	7:6:383:THR:HG22	1.38	1.03
34:o:1483:GLY:HA2	39:t:80:MET:HE1	1.40	1.02
13:D:1002:ARG:NH2	26:T:182:HIS:CG	2.27	1.02
1:0:5:GLY:HA3	1:0:10:LYS:HB2	1.37	1.01
11:A:339:ALA:HB3	11:A:355:VAL:HG21	1.42	1.01
5:4:334:MET:SD	7:6:56:TYR:CE2	2.55	0.99
7:6:305:ASP:CA	7:6:359:LYS:HE3	1.93	0.98
19:J:192:LYS:N	19:J:192:LYS:HE3	1.78	0.98
11:A:725:CYS:SG	11:A:725:CYS:O	2.22	0.97
26:T:192:GLU:OE2	28:V:76:GLY:CA	2.13	0.97
10:9:242:ARG:HB2	34:o:1008:LYS:NZ	1.78	0.96
10:9:242:ARG:HB3	34:o:1008:LYS:NZ	1.78	0.95
7:6:308:ILE:HG22	7:6:358:ARG:CA	1.88	0.95
10:9:242:ARG:CB	34:o:1008:LYS:HZ2	1.80	0.94
6:5:15:ALA:HB2	7:6:516:PRO:HB3	0.96	0.93
1:0:27:GLY:HA3	1:0:70:LYS:HD3	1.51	0.92
7:6:306:ILE:CG1	7:6:359:LYS:HA	1.99	0.92
1:0:85:ARG:HH12	1:0:140:LEU:HG	1.34	0.91
4:3:229:TRP:CE3	5:4:58:ARG:NE	2.38	0.91
7:6:306:ILE:HG12	7:6:359:LYS:HA	1.52	0.91
24:R:51:GLU:C	35:p:841:ARG:HH21	1.77	0.91
1:0:21:LEU:CD2	1:0:69:ASP:OD2	2.18	0.91
13:D:1002:ARG:NH2	26:T:182:HIS:HB2	1.83	0.91
13:D:1002:ARG:HH22	26:T:182:HIS:CB	1.82	0.91
5:4:412:PHE:HB2	5:4:439:ARG:HB3	1.52	0.91
5:4:442:VAL:HG21	6:5:44:PHE:HZ	1.35	0.90
4:3:108:ASN:OD1	5:4:123:LEU:HD13	1.69	0.90
39:t:78:PRO:HG2	40:u:18:PHE:O	1.70	0.90
34:o:1483:GLY:HA2	39:t:80:MET:CE	2.02	0.90
7:6:54:ASP:HB2	7:6:58:ALA:HB3	1.53	0.89
14:E:365:ARG:HD3	14:E:757:GLY:HA3	1.54	0.89
3:2:174:LEU:CD1	8:7:533:ASP:OD1	2.18	0.89
4:3:229:TRP:CE3	5:4:58:ARG:CZ	2.55	0.89
16:G:153:LYS:HD3	16:G:153:LYS:H	1.35	0.89
34:o:79:THR:HA	35:p:1072:ARG:NH2	1.88	0.89
7:6:298:ARG:HG3	7:6:331:GLY:HA3	1.56	0.88
4:3:50:PHE:CG	5:4:122:LEU:HD12	2.07	0.88
4:3:229:TRP:CZ3	5:4:58:ARG:CZ	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1005:HIS:CD2	34:o:1007:ILE:HG22	2.09	0.87
1:0:83:ASN:CG	1:0:140:LEU:CD1	2.47	0.87
27:U:53:LYS:HD2	28:V:166:ILE:HD11	1.56	0.87
5:4:438:LYS:HE2	12:B:621:ALA:CB	2.04	0.87
7:6:502:ILE:HG23	7:6:644:LEU:HB3	1.55	0.87
26:T:153:TYR:CE1	35:p:432:GLU:HB3	2.10	0.87
11:A:511:LEU:H	11:A:511:LEU:HD22	1.37	0.87
5:4:442:VAL:HG21	6:5:44:PHE:CZ	2.09	0.87
6:5:35:ILE:O	12:B:539:ARG:HD3	1.75	0.86
6:5:15:ALA:HB1	7:6:516:PRO:CA	2.02	0.86
7:6:506:GLN:NE2	7:6:655:TYR:CD2	2.45	0.85
7:6:305:ASP:HB3	7:6:359:LYS:HZ1	1.42	0.85
34:o:79:THR:HA	35:p:1072:ARG:HH22	1.41	0.85
11:A:475:LEU:HD11	15:f:351:ILE:HD11	1.57	0.85
7:6:308:ILE:HG23	7:6:358:ARG:HA	1.52	0.85
7:6:308:ILE:O	7:6:358:ARG:HG2	1.77	0.84
14:e:508:LYS:HB3	14:e:512:ASP:HB2	1.59	0.84
7:6:311:LYS:HE3	7:6:383:THR:CG2	2.06	0.84
27:U:77:ARG:HG3	27:U:78:VAL:H	1.42	0.84
24:R:51:GLU:O	35:p:841:ARG:NH2	2.09	0.84
7:6:311:LYS:NZ	7:6:382:SER:C	2.37	0.83
11:A:1065:GLU:OE1	11:A:1065:GLU:HA	1.78	0.83
5:4:448:HIS:O	5:4:452:LYS:HG2	1.78	0.83
4:3:50:PHE:CE2	5:4:118:LEU:HD11	2.12	0.82
9:8:94:MET:HE3	9:8:152:LYS:HD2	1.60	0.82
40:u:41:LYS:O	40:u:78:ARG:NH2	2.11	0.82
7:6:311:LYS:HZ2	7:6:383:THR:N	1.76	0.82
1:0:83:ASN:ND2	1:0:140:LEU:CD1	2.43	0.82
22:P:206:GLU:OE1	22:P:236:LYS:NZ	2.13	0.82
10:9:126:VAL:HG11	10:9:140:LEU:HB2	1.62	0.82
11:A:821:ARG:CZ	11:A:821:ARG:HA	2.10	0.81
33:m:77:ARG:HH11	33:m:77:ARG:HG2	1.45	0.81
27:U:139:LEU:HD23	40:u:151:ARG:HH11	1.45	0.81
15:f:447:ALA:HA	15:f:456:GLY:HA3	1.61	0.81
34:o:911:PRO:O	34:o:963:ARG:NH2	2.14	0.81
7:6:266:GLN:N	7:6:266:GLN:HE21	1.79	0.81
14:E:327:ASN:HD22	14:E:327:ASN:H	1.29	0.81
5:4:438:LYS:CE	12:B:621:ALA:H	1.94	0.80
7:6:332:ARG:HB2	7:6:334:ARG:HH12	1.46	0.80
7:6:506:GLN:NE2	7:6:655:TYR:CE2	2.50	0.80
1:0:83:ASN:CG	1:0:140:LEU:HD11	2.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:305:ASP:HB3	7:6:359:LYS:NZ	1.96	0.80
10:9:36:ALA:HB2	40:u:20:PRO:CG	2.12	0.80
7:6:319:TYR:HE2	7:6:499:ASN:HD22	1.27	0.80
39:t:78:PRO:HG2	40:u:18:PHE:C	2.07	0.80
4:3:100:LYS:HD2	5:4:124:GLY:H	1.47	0.79
6:5:31:LYS:HB3	12:B:540:LYS:HZ3	0.68	0.79
7:6:332:ARG:HB2	7:6:334:ARG:NH1	1.97	0.79
13:D:963:ARG:HB2	13:D:983:ARG:HH21	1.46	0.79
15:F:324:ASP:HA	15:F:327:TRP:HB3	1.62	0.79
4:3:56:LYS:NZ	4:3:143:TYR:OH	2.16	0.79
14:e:747:LEU:HD23	14:e:747:LEU:H	1.47	0.79
34:o:1477:ALA:HA	40:u:22:LEU:HD11	1.64	0.79
15:F:273:GLN:NE2	15:F:273:GLN:H	1.81	0.79
5:4:415:GLN:HB2	5:4:439:ARG:NH2	1.98	0.79
14:E:774:MET:HE2	14:E:774:MET:H	1.46	0.79
39:t:78:PRO:CG	40:u:18:PHE:O	2.30	0.79
5:4:335:LEU:O	7:6:58:ALA:HA	1.83	0.79
6:5:18:GLN:OE1	7:6:520:ARG:HD3	1.83	0.79
34:o:902:GLU:OE2	34:o:985:ARG:NH2	2.16	0.79
1:0:83:ASN:OD1	1:0:140:LEU:CD1	2.31	0.78
7:6:319:TYR:OH	7:6:495:GLU:CG	2.28	0.78
34:o:22:GLN:NE2	34:o:1446:GLY:O	2.17	0.78
7:6:311:LYS:NZ	7:6:383:THR:N	2.32	0.78
15:F:274:ASN:ND2	15:F:316:GLN:HA	1.99	0.78
13:D:1002:ARG:CZ	26:T:182:HIS:CD2	2.67	0.78
5:4:456:LYS:O	5:4:460:HIS:CD2	2.37	0.78
33:m:31:LEU:HD23	33:m:31:LEU:H	1.47	0.78
15:F:429:LYS:O	15:F:433:PRO:HD2	1.85	0.77
27:U:151:THR:HG23	27:U:153:ARG:HD3	1.65	0.77
7:6:502:ILE:CG2	7:6:644:LEU:HB3	2.15	0.77
7:6:342:CYS:SG	7:6:641:GLY:O	2.43	0.77
1:0:85:ARG:HH22	1:0:140:LEU:CA	1.98	0.77
4:3:46:ASN:OD1	5:4:123:LEU:HD22	1.85	0.77
1:0:85:ARG:NH2	1:0:140:LEU:N	2.26	0.77
37:r:94:LYS:NZ	40:u:3:TYR:OH	2.17	0.77
1:0:84:LYS:CA	1:0:136:ASN:ND2	2.48	0.76
4:3:240:GLN:NE2	5:4:51:LEU:HD21	2.00	0.76
34:o:1005:HIS:HD2	34:o:1007:ILE:HG22	1.50	0.76
13:D:1002:ARG:HH22	26:T:182:HIS:HB3	1.50	0.76
6:5:33:PHE:CZ	6:5:49:LEU:HD12	2.17	0.76
35:p:752:TYR:CD2	35:p:807:ARG:HB3	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:371:VAL:HG23	7:6:407:ILE:HG22	1.68	0.76
7:6:370:SER:HB2	7:6:614:SER:HB3	1.67	0.75
39:t:75:MET:HE3	40:u:15:PRO:HG2	1.67	0.75
39:t:78:PRO:HD2	40:u:18:PHE:HB2	1.67	0.75
8:7:711:ASP:OD1	8:7:715:GLN:NE2	2.20	0.75
35:p:926:VAL:HG21	36:q:62:GLU:HG3	1.69	0.75
34:o:1242:ASP:HA	34:o:1262:MET:HE2	1.68	0.75
34:o:513:ALA:HB2	39:t:90:LEU:HD21	1.69	0.75
7:6:56:TYR:C	7:6:58:ALA:H	1.95	0.75
15:F:359:PHE:HB3	15:F:380:LEU:HG	1.69	0.75
5:4:334:MET:HB2	7:6:56:TYR:CB	2.17	0.74
13:D:1002:ARG:HH21	26:T:182:HIS:HB2	1.51	0.74
4:3:47:SER:HA	5:4:122:LEU:HD11	1.69	0.74
41:v:2:ALA:O	41:v:84:ARG:NH2	2.20	0.74
7:6:306:ILE:HB	7:6:358:ARG:O	1.86	0.74
27:U:48:MET:HE2	27:U:52:LEU:HB2	1.69	0.74
37:r:87:LEU:HD11	37:r:100:LEU:HD11	1.70	0.74
34:o:279:LYS:O	34:o:283:ILE:HD12	1.87	0.74
7:6:281:GLN:HG2	7:6:482:PHE:HB2	1.69	0.74
7:6:298:ARG:HG2	7:6:331:GLY:C	2.13	0.74
6:5:33:PHE:HE1	6:5:49:LEU:HD12	0.84	0.73
10:9:36:ALA:HB2	40:u:20:PRO:HG3	1.69	0.73
21:O:3:TYR:HB3	21:O:5:LEU:CD1	2.18	0.73
11:A:463:PRO:HG2	15:F:218:VAL:O	1.86	0.73
15:F:217:SER:N	15:F:220:GLN:HB2	2.02	0.73
11:A:639:LEU:HD11	11:A:774:ARG:HG2	1.70	0.73
35:p:387:HIS:CE1	35:p:671:GLU:OE2	2.42	0.73
44:y:77:THR:OG1	44:y:81:TYR:O	2.04	0.73
5:4:438:LYS:HE2	12:B:621:ALA:HB3	1.70	0.73
7:6:319:TYR:HE2	7:6:499:ASN:ND2	1.87	0.73
4:3:50:PHE:CD2	5:4:122:LEU:HD12	2.24	0.73
5:4:415:GLN:HB2	5:4:439:ARG:HH21	1.52	0.73
24:R:51:GLU:C	35:p:841:ARG:NH2	2.47	0.73
6:5:31:LYS:HB3	12:B:540:LYS:CE	2.17	0.73
8:7:231:VAL:HG13	8:7:454:VAL:HG23	1.70	0.73
1:0:23:VAL:HG21	1:0:73:GLU:HG3	1.71	0.72
7:6:312:PRO:O	8:7:514:ILE:HG21	1.89	0.72
7:6:615:PHE:HB3	7:6:617:LEU:HG	1.70	0.72
7:6:536:MET:HG2	7:6:571:TYR:HE1	1.52	0.72
28:V:131:GLU:HG3	28:V:140:LYS:HA	1.72	0.72
11:A:463:PRO:HG3	15:F:222:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:85:ARG:NH2	1:0:139:LYS:O	2.23	0.72
7:6:341:PRO:HG2	7:6:496:LEU:HD12	1.72	0.72
7:6:278:GLU:HG3	7:6:482:PHE:HE1	1.54	0.72
28:V:197:LYS:HG3	28:V:198:LYS:HG3	1.72	0.72
6:5:34:ILE:O	12:B:539:ARG:NH2	2.22	0.72
35:p:59:VAL:HG21	35:p:91:ILE:HD11	1.70	0.72
37:r:67:TYR:OH	40:u:86:ASP:OD1	2.06	0.72
15:F:418:ILE:H	15:F:418:ILE:HD12	1.54	0.72
7:6:341:PRO:CD	7:6:491:ALA:HB3	2.19	0.71
7:6:512:CYS:O	7:6:665:GLN:HG3	1.89	0.71
11:A:488:ALA:HB1	15:f:271:VAL:HG23	1.71	0.71
11:A:468:PHE:CE1	15:F:221:GLN:HG3	2.25	0.71
4:3:160:ARG:NH2	4:3:234:ASP:OD1	2.23	0.71
1:0:120:LYS:O	1:0:124:ILE:HD12	1.91	0.71
7:6:311:LYS:HB3	7:6:383:THR:HG23	1.71	0.71
22:P:239:ARG:NH1	23:Q:314:LEU:O	2.23	0.71
6:5:31:LYS:CG	12:B:540:LYS:HZ3	2.02	0.70
35:p:40:VAL:HG21	35:p:181:PRO:CB	2.15	0.70
4:3:272:LEU:O	4:3:272:LEU:HD23	1.90	0.70
5:4:334:MET:SD	7:6:56:TYR:HD2	2.14	0.70
27:U:23:ARG:HD2	27:U:31:ALA:HB1	1.73	0.70
35:p:254:GLN:OE1	35:p:254:GLN:N	2.24	0.70
14:E:258:ASN:H	14:E:258:ASN:ND2	1.89	0.70
34:o:322:LEU:O	34:o:327:ARG:NH2	2.23	0.70
11:A:353:LEU:HD21	15:f:272:VAL:HG21	1.72	0.70
12:B:241:PRO:HG2	12:B:496:MET:HE1	1.72	0.70
7:6:519:TYR:HE2	7:6:666:ASP:CB	2.05	0.70
27:U:139:LEU:CD2	40:u:151:ARG:HH11	2.04	0.70
3:2:109:THR:OG1	3:2:148:SER:OG	2.06	0.70
4:3:67:SER:O	4:3:139:LYS:NZ	2.24	0.70
4:3:98:ASP:O	5:4:125:GLY:HA3	1.91	0.70
13:D:1002:ARG:NH2	26:T:182:HIS:CD2	2.59	0.70
7:6:191:ASP:O	7:6:195:ARG:NH1	2.25	0.70
14:e:274:TYR:HB3	14:e:367:ALA:HB2	1.72	0.70
4:3:242:ILE:HD11	5:4:75:VAL:C	2.17	0.70
5:4:404:THR:HG22	6:5:9:LEU:H	1.56	0.70
7:6:502:ILE:HG23	7:6:644:LEU:O	1.92	0.69
28:V:234:GLU:OE1	28:V:238:LYS:NZ	2.25	0.69
11:A:339:ALA:CB	11:A:355:VAL:HG21	2.22	0.69
5:4:29:GLY:O	5:4:33:ARG:NE	2.24	0.69
7:6:611:GLY:O	7:6:642:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:373:LEU:O	34:o:485:ASN:ND2	2.25	0.69
12:B:490:SER:HA	12:B:493:TRP:HB2	1.75	0.69
27:U:36:ILE:HD11	28:V:163:LEU:HD22	1.74	0.69
2:1:468:VAL:HG21	2:1:525:ILE:HD11	1.74	0.69
4:3:237:GLN:NE2	5:4:50:SER:O	2.25	0.69
15:F:217:SER:H	15:F:220:GLN:HB2	1.56	0.69
6:5:31:LYS:CB	12:B:540:LYS:HZ1	1.99	0.69
8:7:252:THR:HG22	8:7:432:ILE:HG22	1.74	0.69
11:A:568:SER:HB2	12:B:389:ASN:HB2	1.74	0.69
15:F:274:ASN:HB2	15:F:317:LEU:H	1.58	0.69
24:R:51:GLU:HB3	35:p:841:ARG:NH2	2.08	0.69
27:U:75:ARG:H	27:U:91:TYR:HB2	1.55	0.69
27:U:145:PHE:HD2	27:U:146:ASP:N	1.90	0.69
40:u:21:ASN:O	40:u:25:THR:OG1	2.05	0.69
7:6:493:TRP:CZ3	7:6:644:LEU:HD11	2.28	0.69
8:7:637:LEU:HD11	8:7:648:GLU:HA	1.74	0.69
9:8:125:LEU:HD21	9:8:195:ASP:HB3	1.75	0.69
40:u:97:LEU:HD23	40:u:113:ILE:HD11	1.75	0.69
27:U:24:GLY:HA2	28:V:209:GLN:HG2	1.75	0.68
27:U:139:LEU:HD22	40:u:151:ARG:HD2	0.75	0.68
5:4:334:MET:HB2	7:6:56:TYR:HB2	1.74	0.68
9:8:43:ILE:HD13	9:8:87:ILE:HG13	1.73	0.68
14:e:645:GLY:H	14:e:675:LEU:HD11	1.59	0.68
35:p:752:TYR:CE2	35:p:807:ARG:HG2	2.28	0.68
14:E:426:ARG:HH11	14:E:640:ASN:HD22	1.42	0.68
35:p:388:TYR:C	35:p:390:ASN:N	2.49	0.68
9:8:226:PHE:HB3	9:8:231:THR:HG22	1.76	0.68
39:t:100:ARG:NH2	39:t:121:ASP:O	2.26	0.68
15:F:83:LEU:CD1	15:F:83:LEU:H	2.07	0.68
28:V:141:PRO:HB2	28:V:144:ASN:HB3	1.76	0.68
34:o:1248:ASN:ND2	34:o:1254:LYS:O	2.26	0.68
11:A:463:PRO:HD3	15:F:222:LEU:HB2	1.74	0.68
3:2:75:ASP:OD2	8:7:722:ARG:NH2	2.26	0.68
3:2:75:ASP:OD1	8:7:722:ARG:NH2	2.28	0.67
4:3:46:ASN:OD1	5:4:123:LEU:CD2	2.42	0.67
5:4:60:LEU:HD13	5:4:118:LEU:HD23	1.76	0.67
15:f:447:ALA:CA	15:f:456:GLY:HA3	2.23	0.67
32:k:191:VAL:HG13	32:k:200:ILE:HD13	1.74	0.67
10:9:238:LEU:HB3	10:9:245:LEU:HB2	1.76	0.67
27:U:136:PHE:O	27:U:137:THR:OG1	2.12	0.67
29:X:-27:DA:H2'	29:X:-26:DA:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:88:LEU:CD2	3:2:131:LEU:HD21	2.24	0.67
7:6:519:TYR:HE2	7:6:666:ASP:HB2	1.59	0.67
24:R:23:LEU:HD12	24:R:32:MET:HE2	1.74	0.67
1:0:55:LYS:C	1:0:57:ASN:H	2.02	0.67
5:4:438:LYS:HE3	12:B:621:ALA:H	1.58	0.67
8:7:72:TYR:OH	8:7:234:ASP:OD2	2.12	0.67
22:P:239:ARG:CD	23:Q:317:GLU:HG3	2.25	0.67
35:p:814:TYR:OH	35:p:900:GLU:OE1	2.13	0.67
4:3:229:TRP:HE3	5:4:58:ARG:NE	1.92	0.67
9:8:158:LEU:HD12	9:8:173:VAL:HB	1.76	0.67
15:f:239:ARG:HD3	15:f:284:ARG:HH11	1.60	0.67
37:r:18:SER:O	37:r:117:SER:OG	2.08	0.67
7:6:311:LYS:HB3	7:6:383:THR:CG2	2.24	0.67
8:7:60:GLN:OE1	8:7:61:ARG:NH1	2.28	0.67
8:7:382:LEU:O	8:7:385:THR:OG1	2.11	0.67
19:j:123:LEU:C	19:j:125:ASP:H	2.03	0.67
11:A:396:LEU:HD21	15:f:394:PRO:HB2	1.77	0.67
21:O:51:ARG:NH2	23:Q:20:ASP:OD2	2.27	0.67
4:3:229:TRP:CE3	5:4:58:ARG:CD	2.78	0.67
27:U:48:MET:HA	27:U:48:MET:HE3	1.75	0.67
36:q:193:ARG:NH2	36:q:218:ALA:O	2.26	0.67
7:6:319:TYR:CE2	7:6:499:ASN:ND2	2.62	0.66
10:9:218:LEU:HD12	10:9:252:MET:HE1	1.77	0.66
11:A:511:LEU:HD22	11:A:511:LEU:N	2.11	0.66
14:E:365:ARG:HD3	14:E:757:GLY:CA	2.24	0.66
27:U:20:TYR:O	27:U:23:ARG:NH2	2.27	0.66
1:0:106:VAL:O	1:0:110:THR:HG23	1.95	0.66
13:D:963:ARG:HB2	13:D:983:ARG:NH2	2.10	0.66
16:G:129:LYS:O	16:G:129:LYS:NZ	2.23	0.66
34:o:1483:GLY:CA	39:t:80:MET:HE1	2.22	0.66
36:q:109:GLU:OE1	36:q:109:GLU:N	2.28	0.66
1:0:85:ARG:NH1	1:0:140:LEU:CG	2.45	0.66
4:3:98:ASP:HB3	5:4:125:GLY:C	2.21	0.66
8:7:238:ASN:ND2	8:7:662:GLN:OE1	2.29	0.66
9:8:40:ILE:HG12	9:8:90:VAL:HG22	1.76	0.66
9:8:113:HIS:CD2	9:8:308:PRO:HD3	2.31	0.66
4:3:240:GLN:HE21	5:4:51:LEU:HD21	1.61	0.66
6:5:31:LYS:HB2	12:B:540:LYS:NZ	2.06	0.66
8:7:571:THR:OG1	8:7:576:GLU:OE1	2.08	0.66
20:L:79:ASP:OD1	20:L:79:ASP:N	2.25	0.66
1:0:295:ARG:HD2	9:8:163:GLY:HA3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:137:MET:SD	3:2:139:CYS:N	2.67	0.66
30:Y:28:DT:H2'	30:Y:29:DA:C8	2.30	0.66
34:o:1428:MET:SD	34:o:1455:SER:OG	2.51	0.66
4:3:43:VAL:HG11	4:3:224:LEU:HD21	1.78	0.65
10:9:177:ARG:NH2	10:9:235:SER:O	2.30	0.65
11:A:1168:TYR:HB2	16:G:180:ARG:HB3	1.79	0.65
7:6:298:ARG:HG3	7:6:331:GLY:CA	2.24	0.65
17:H:40:VAL:HG11	19:J:130:ILE:HG12	1.77	0.65
27:U:72:ILE:HG22	27:U:94:ILE:HA	1.78	0.65
28:V:144:ASN:HA	28:V:173:GLU:HB2	1.78	0.65
35:p:388:TYR:C	35:p:390:ASN:H	2.03	0.65
35:p:752:TYR:HE2	35:p:807:ARG:HD2	1.61	0.65
41:v:91:VAL:HG22	41:v:144:LEU:CD2	2.25	0.65
1:0:307:GLN:OE1	10:9:247:GLN:NE2	2.30	0.65
28:V:158:HIS:O	28:V:162:GLY:N	2.29	0.65
22:P:208:ARG:HH22	23:Q:346:LYS:CG	2.10	0.65
24:R:128:ILE:HG23	24:R:183:VAL:HG11	1.77	0.65
20:l:141:LYS:HE2	33:m:79:GLY:HA2	1.76	0.65
3:2:377:ASP:O	3:2:380:HIS:NE2	2.30	0.65
4:3:229:TRP:CE3	5:4:58:ARG:HD2	2.31	0.65
28:V:227:SER:HB3	28:V:230:GLU:HB2	1.77	0.65
35:p:677:MET:H	35:p:682:LEU:HD22	1.62	0.65
5:4:438:LYS:HE3	12:B:621:ALA:N	2.10	0.65
42:w:60:HIS:ND1	42:w:60:HIS:O	2.30	0.65
15:f:320:ARG:NH1	15:f:320:ARG:HB3	2.12	0.65
1:0:27:GLY:CA	1:0:70:LYS:HD3	2.26	0.64
7:6:506:GLN:HB2	7:6:655:TYR:HD2	1.62	0.64
28:V:78:LEU:HD21	28:V:124:LEU:HD22	1.80	0.64
11:A:970:ASN:OD1	11:A:970:ASN:N	2.21	0.64
15:F:83:LEU:HD12	15:F:83:LEU:N	2.12	0.64
19:j:123:LEU:O	19:j:125:ASP:N	2.30	0.64
37:r:14:GLU:OE1	37:r:14:GLU:N	2.31	0.64
5:4:409:TYR:HB2	5:4:412:PHE:CZ	2.33	0.64
7:6:305:ASP:CB	7:6:359:LYS:NZ	2.59	0.64
12:B:361:ARG:HD2	12:B:367:GLU:HB2	1.80	0.64
13:D:1004:ALA:HB1	21:O:4:GLN:HB2	1.79	0.64
14:E:522:ASP:HB2	14:E:526:ARG:HG2	1.80	0.64
34:o:122:ASN:O	34:o:127:LYS:NZ	2.30	0.64
34:o:140:ARG:NH1	34:o:234:PHE:O	2.30	0.64
37:r:87:LEU:HB3	37:r:97:LEU:HD22	1.79	0.64
7:6:306:ILE:N	7:6:358:ARG:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:513:ASP:OD1	8:7:516:VAL:N	2.29	0.64
22:P:186:ARG:NH1	22:P:244:LEU:O	2.31	0.64
24:R:26:ASP:OD1	34:o:430:ARG:NH2	2.30	0.64
4:3:168:GLU:N	4:3:168:GLU:OE1	2.31	0.64
5:4:172:SER:OG	5:4:267:GLU:OE2	2.13	0.64
27:U:76:MET:HE3	27:U:88:ARG:HD2	1.80	0.64
34:o:687:ILE:HD12	34:o:765:ASN:HB2	1.78	0.64
7:6:311:LYS:CE	7:6:383:THR:HG22	2.23	0.64
11:A:821:ARG:HA	11:A:821:ARG:NH1	2.11	0.64
2:1:195:SER:O	2:1:199:THR:OG1	2.05	0.64
12:B:583:GLU:CD	12:B:583:GLU:H	2.06	0.63
34:o:589:LYS:NZ	34:o:625:ASP:OD2	2.23	0.63
4:3:100:LYS:HE2	5:4:123:LEU:H	1.62	0.63
7:6:287:LEU:HD23	7:6:287:LEU:O	1.98	0.63
35:p:407:MET:HE1	35:p:444:LEU:HG	1.80	0.63
35:p:910:THR:HG22	35:p:911:LEU:H	1.62	0.63
36:q:24:GLU:OE2	36:q:228:ARG:NH1	2.31	0.63
7:6:517:GLU:O	7:6:521:GLU:OE1	2.16	0.63
9:8:134:LEU:HD11	9:8:192:VAL:HA	1.81	0.63
13:D:1002:ARG:CZ	26:T:182:HIS:CG	2.81	0.63
22:P:297:LYS:NZ	22:P:323:GLU:OE2	2.31	0.63
22:P:239:ARG:HD3	23:Q:317:GLU:HG3	1.80	0.63
5:4:172:SER:OG	5:4:174:ASP:OD1	2.15	0.63
9:8:13:GLU:OE1	9:8:32:LYS:NZ	2.31	0.63
7:6:108:CYS:SG	7:6:682:ASP:HB3	2.39	0.63
7:6:266:GLN:HG2	7:6:267:THR:HG23	1.81	0.63
8:7:343:ARG:O	8:7:346:VAL:HG12	1.99	0.63
15:F:92:ILE:HG13	15:F:93:PRO:HD3	1.81	0.63
35:p:777:ASN:O	43:x:47:ARG:NH1	2.32	0.63
3:2:87:LEU:HD22	3:2:232:LEU:HD12	1.81	0.63
3:2:112:LYS:O	3:2:147:ASN:ND2	2.32	0.62
11:A:342:ARG:HG2	11:A:342:ARG:O	1.99	0.62
15:F:223:TYR:C	15:F:225:LYS:N	2.51	0.62
24:R:273:GLU:O	24:R:277:ILE:HD12	1.98	0.62
27:U:145:PHE:HD2	27:U:146:ASP:H	1.47	0.62
34:o:1471:PHE:O	39:t:64:ARG:NH1	2.32	0.62
13:d:884:GLU:HA	13:d:887:LYS:HE3	1.82	0.62
14:e:277:ASP:OD1	14:e:277:ASP:N	2.32	0.62
1:0:71:GLU:OE2	8:7:335:ARG:NH1	2.32	0.62
22:P:208:ARG:HH22	23:Q:346:LYS:HG3	1.63	0.62
27:U:100:VAL:O	27:U:104:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:9:VAL:HG11	44:y:105:PHE:CD1	2.35	0.62
7:6:371:VAL:HG23	7:6:407:ILE:CG2	2.29	0.62
11:A:468:PHE:HE1	15:F:221:GLN:HG3	1.63	0.62
9:8:284:ILE:HA	9:8:288:GLN:HE21	1.65	0.62
15:F:335:ARG:NE	15:F:382:GLU:OE1	2.33	0.62
37:r:29:ALA:HB3	40:u:3:TYR:CE2	2.33	0.62
7:6:342:CYS:SG	7:6:641:GLY:C	2.82	0.62
7:6:373:GLN:HB2	7:6:616:ASP:HB2	1.80	0.62
14:E:613:ALA:HB2	14:E:620:LEU:HD11	1.81	0.62
29:X:7:DA:H61	30:Y:-7:DT:H3	1.47	0.62
19:j:176:MET:HE1	33:m:75:ILE:HD11	1.82	0.62
33:m:77:ARG:HH11	33:m:77:ARG:CG	2.10	0.62
4:3:53:ARG:HG2	5:4:46:ARG:NH2	2.15	0.62
9:8:30:ARG:HH21	9:8:35:ASN:HB2	1.63	0.62
22:P:208:ARG:NH2	23:Q:346:LYS:HG2	2.15	0.62
7:6:340:LEU:HD23	7:6:491:ALA:HB2	1.81	0.62
7:6:512:CYS:C	7:6:665:GLN:HG3	2.25	0.62
13:D:1004:ALA:CB	21:O:4:GLN:HB2	2.30	0.62
37:r:119:GLU:OE1	37:r:119:GLU:N	2.33	0.62
38:s:168:ASN:OD1	38:s:172:ARG:NH2	2.33	0.62
24:R:54:THR:HA	35:p:895:PHE:H	1.64	0.62
8:7:405:THR:O	8:7:409:THR:OG1	2.16	0.61
35:p:752:TYR:CE2	35:p:807:ARG:CG	2.83	0.61
38:s:9:ARG:O	38:s:13:ILE:HD12	1.99	0.61
1:0:83:ASN:ND2	1:0:140:LEU:HD12	2.14	0.61
3:2:379:LEU:HD22	3:2:381:CYS:O	1.99	0.61
6:5:32:LYS:HD3	12:B:540:LYS:HA	1.80	0.61
9:8:132:TRP:CD1	10:9:1:MET:HE3	2.35	0.61
34:o:1375:ARG:NH1	34:o:1379:GLU:OE1	2.31	0.61
2:1:432:THR:O	2:1:435:SER:OG	2.10	0.61
3:2:75:ASP:CG	8:7:722:ARG:NH2	2.57	0.61
4:3:229:TRP:HE3	5:4:58:ARG:CD	2.12	0.61
7:6:56:TYR:C	7:6:58:ALA:N	2.57	0.61
17:H:50:PHE:HD1	19:J:193:TYR:O	1.82	0.61
27:U:25:PHE:O	28:V:217:GLN:NE2	2.33	0.61
31:c:18:CYS:O	31:c:23:TRP:HB2	2.01	0.61
7:6:128:SER:HG	7:6:163:TYR:HH	1.45	0.61
7:6:473:GLU:OE1	7:6:473:GLU:N	2.33	0.61
7:6:532:LEU:HD11	7:6:566:PHE:CE2	2.35	0.61
8:7:2:LYS:HB3	8:7:9:LEU:HD11	1.81	0.61
37:r:29:ALA:HB3	40:u:3:TYR:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:422:LEU:HD22	4:3:225:GLN:HE22	1.66	0.61
7:6:537:ASN:OD1	7:6:540:LYS:HB3	2.00	0.61
3:2:357:VAL:HG13	3:2:366:VAL:HG23	1.83	0.61
1:0:265:MET:SD	1:0:268:ARG:NE	2.73	0.61
7:6:128:SER:OG	7:6:163:TYR:OH	2.17	0.61
13:D:1011:ALA:HB2	21:O:96:VAL:HG21	1.81	0.61
35:p:794:VAL:HG13	35:p:965:ILE:HG23	1.82	0.61
7:6:369:VAL:CG1	7:6:615:PHE:HA	2.30	0.61
9:8:79:ASP:OD2	9:8:80:ALA:N	2.33	0.61
28:V:121:THR:O	28:V:125:VAL:HG23	2.01	0.61
17:H:192:ARG:NH1	17:H:209:SER:O	2.34	0.61
36:q:78:ILE:HD11	36:q:126:ARG:HB3	1.83	0.61
43:x:8:PHE:CD2	43:x:48:MET:HE1	2.36	0.61
7:6:532:LEU:HD11	7:6:566:PHE:CD2	2.36	0.61
9:8:213:LEU:HD13	9:8:225:ILE:HG12	1.82	0.61
5:4:265:LEU:CD1	5:4:270:LEU:HD12	2.31	0.60
7:6:369:VAL:HG11	7:6:615:PHE:HA	1.83	0.60
10:9:215:THR:HA	10:9:252:MET:HE3	1.83	0.60
14:E:754:THR:O	14:E:755:ALA:HB3	2.01	0.60
24:R:51:GLU:HB3	35:p:841:ARG:HH22	1.65	0.60
33:m:31:LEU:HD23	33:m:31:LEU:N	2.16	0.60
38:s:29:THR:HG23	38:s:32:GLU:H	1.65	0.60
4:3:229:TRP:HZ3	5:4:58:ARG:HH11	1.44	0.60
7:6:266:GLN:N	7:6:266:GLN:NE2	2.49	0.60
7:6:281:GLN:NE2	7:6:482:PHE:O	2.35	0.60
8:7:44:SER:OG	8:7:46:THR:O	2.16	0.60
10:9:68:CYS:HB3	10:9:80:VAL:HG22	1.84	0.60
15:F:90:GLU:H	15:F:90:GLU:CD	2.08	0.60
28:V:77:VAL:O	28:V:81:ILE:HG12	2.01	0.60
7:6:305:ASP:CA	7:6:359:LYS:CE	2.66	0.60
8:7:372:LEU:HD11	8:7:404:ALA:HB1	1.84	0.60
10:9:86:TYR:OH	10:9:158:LEU:O	2.18	0.60
28:V:174:ALA:HB1	28:V:180:LYS:HZ1	1.67	0.60
34:o:805:ARG:NH2	35:p:671:GLU:O	2.33	0.60
34:o:1290:SER:HB2	35:p:250:SER:HB2	1.83	0.60
37:r:29:ALA:HB1	40:u:4:HIS:O	2.01	0.60
15:F:218:VAL:HB	17:H:164:THR:HB	1.83	0.60
3:2:242:SER:O	3:2:245:SER:OG	2.17	0.60
7:6:189:LEU:O	7:6:195:ARG:NH1	2.33	0.60
9:8:267:ASP:OD2	9:8:297:ASN:ND2	2.31	0.60
15:F:223:TYR:HB2	17:H:157:HIS:NE2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:f:330:ARG:HH22	15:f:371:THR:HB	1.66	0.60
34:o:29:ASP:OD2	34:o:33:ARG:NH2	2.34	0.60
34:o:261:ARG:HD2	34:o:261:ARG:O	2.02	0.60
35:p:302:LYS:CE	42:w:14:ILE:HD12	2.32	0.60
40:u:10:GLU:HG2	40:u:67:LEU:HD12	1.84	0.60
14:e:257:GLU:H	14:e:257:GLU:CD	2.10	0.60
8:7:609:ASP:OD1	8:7:669:ARG:NH2	2.34	0.60
12:B:27:LYS:HE3	12:B:490:SER:HB3	1.84	0.60
15:F:114:LEU:HB2	17:H:52:SER:H	1.66	0.60
28:V:171:ILE:HD13	28:V:177:ASN:HB3	1.83	0.60
2:1:130:ASP:OD2	2:1:463:HIS:NE2	2.33	0.59
5:4:18:ASN:OD1	5:4:19:LEU:N	2.35	0.59
8:7:628:THR:O	8:7:628:THR:HG22	2.02	0.59
10:9:48:LEU:HD23	10:9:276:LYS:HE3	1.84	0.59
29:X:24:DA:H2'	29:X:25:DG:C8	2.37	0.59
35:p:354:SER:OG	35:p:357:CYS:SG	2.59	0.59
2:1:471:LEU:HD12	2:1:472:LEU:HD22	1.84	0.59
8:7:461:LEU:HD23	8:7:464:LEU:CD2	2.32	0.59
9:8:137:ASP:OD2	9:8:139:LYS:NZ	2.35	0.59
27:U:36:ILE:HG21	27:U:48:MET:HE1	1.84	0.59
8:7:462:SER:OG	8:7:463:PRO:HD2	2.02	0.59
11:A:1193:ALA:HB3	16:G:166:VAL:HG21	1.83	0.59
26:T:141:LEU:CD2	35:p:53:MET:SD	2.90	0.59
37:r:70:ARG:NH2	40:u:142:GLU:OE2	2.35	0.59
28:V:163:LEU:HG	28:V:201:LEU:HD21	1.85	0.59
35:p:752:TYR:HE2	35:p:807:ARG:CD	2.14	0.59
5:4:438:LYS:HE2	12:B:621:ALA:HB2	1.82	0.59
7:6:707:GLU:O	7:6:711:GLN:OE1	2.20	0.59
14:e:562:SER:OG	14:e:564:ASP:OD1	2.21	0.59
15:f:349:ASN:HB3	15:f:351:ILE:HG13	1.84	0.59
36:q:9:VAL:HG11	44:y:105:PHE:HD1	1.68	0.59
4:3:195:VAL:HG12	4:3:203:LEU:HD23	1.85	0.59
6:5:48:GLU:HG3	6:5:49:LEU:HG	1.84	0.59
7:6:415:HIS:NE2	7:6:417:THR:OG1	2.35	0.59
34:o:1424:THR:HB	34:o:1428:MET:HB3	1.84	0.59
3:2:345:CYS:O	3:2:349:GLN:N	2.36	0.59
7:6:108:CYS:SG	7:6:682:ASP:CG	2.86	0.59
8:7:262:ASN:O	8:7:266:LEU:HD23	2.03	0.59
17:H:194:MET:HE1	15:f:226:GLU:HG3	1.84	0.59
24:R:52:TRP:CE2	35:p:841:ARG:HG2	2.37	0.59
27:U:15:LYS:NZ	27:U:94:ILE:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:88:PHE:C	33:m:88:PHE:CD1	2.81	0.59
11:A:475:LEU:HD13	15:f:349:ASN:OD1	2.02	0.59
12:B:203:LYS:HD3	12:B:237:MET:HE3	1.83	0.59
34:o:1173:THR:OG1	42:w:56:ASN:OD1	2.18	0.59
1:0:53:LEU:HB3	1:0:57:ASN:HB2	1.84	0.59
3:2:88:LEU:HD22	3:2:131:LEU:HD21	1.84	0.59
4:3:50:PHE:HZ	5:4:118:LEU:HD13	1.62	0.59
7:6:519:TYR:CE2	7:6:666:ASP:CB	2.86	0.59
15:F:312:ILE:HG13	15:F:334:ALA:CB	2.33	0.59
7:6:56:TYR:O	7:6:58:ALA:N	2.35	0.59
8:7:664:VAL:HG22	8:7:677:MET:HG2	1.83	0.59
14:E:586:TYR:HB3	14:E:605:HIS:HB3	1.85	0.59
31:c:99:PHE:HB2	31:c:100:PRO:HD3	1.83	0.59
13:d:967:MET:HA	13:d:967:MET:HE2	1.85	0.59
35:p:867:ILE:HB	35:p:894:THR:HG22	1.85	0.59
1:0:83:ASN:HD21	1:0:140:LEU:HD13	1.67	0.58
4:3:242:ILE:HD13	5:4:74:TRP:C	2.27	0.58
33:m:67:GLU:HA	33:m:67:GLU:OE1	2.02	0.58
7:6:625:GLN:OE1	7:6:639:ARG:NH1	2.36	0.58
9:8:26:VAL:HG22	9:8:41:LYS:HG3	1.84	0.58
35:p:274:ARG:NH2	35:p:281:ASP:OD1	2.36	0.58
9:8:118:MET:HE2	9:8:203:LEU:HD22	1.84	0.58
26:T:80:GLU:OE2	26:T:81:HIS:N	2.35	0.58
35:p:752:TYR:CE2	35:p:807:ARG:HD2	2.38	0.58
7:6:341:PRO:HG3	7:6:493:TRP:CD1	2.38	0.58
7:6:580:ILE:HG23	7:6:584:THR:HG21	1.84	0.58
27:U:77:ARG:HG3	27:U:78:VAL:N	2.16	0.58
35:p:407:MET:HE1	35:p:444:LEU:CD2	2.33	0.58
36:q:7:PRO:O	44:y:104:ARG:NH1	2.37	0.58
1:0:5:GLY:HA3	1:0:10:LYS:CB	2.25	0.58
15:F:207:ARG:HD2	15:F:207:ARG:N	2.18	0.58
35:p:910:THR:HG22	35:p:911:LEU:N	2.18	0.58
41:v:102:ASP:OD2	41:v:110:THR:OG1	2.21	0.58
1:0:35:VAL:HG13	1:0:58:PHE:CE2	2.39	0.58
1:0:84:LYS:HA	1:0:136:ASN:CG	2.28	0.58
35:p:223:SER:HG	35:p:350:HIS:CE1	2.19	0.58
5:4:404:THR:H	6:5:8:VAL:HG13	1.68	0.58
31:c:21:LEU:HD12	31:c:21:LEU:C	2.29	0.58
14:e:484:LEU:HD21	14:e:504:LEU:HD21	1.85	0.58
8:7:240:ASP:OD1	8:7:241:ASN:N	2.37	0.58
34:o:111:CYS:SG	34:o:188:GLN:NE2	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:415:GLN:CB	5:4:439:ARG:HH21	2.16	0.58
7:6:306:ILE:HG13	7:6:360:ARG:N	2.18	0.58
12:B:769:LYS:O	12:B:769:LYS:HG3	2.03	0.58
12:B:837:LEU:HD22	17:H:213:LEU:HD22	1.86	0.58
17:H:171:ASP:HB3	17:H:174:VAL:HG12	1.85	0.58
5:4:407:VAL:N	5:4:443:VAL:O	2.37	0.57
34:o:1482:TYR:CB	39:t:80:MET:SD	2.78	0.57
35:p:755:GLN:HE22	43:x:48:MET:HE2	1.68	0.57
2:1:417:LYS:HA	2:1:421:VAL:HG23	1.85	0.57
10:9:85:MET:HE3	10:9:89:ARG:HE	1.69	0.57
11:A:334:THR:HA	11:A:489:GLN:O	2.04	0.57
11:A:470:ILE:O	11:A:470:ILE:HG22	2.02	0.57
4:3:241:LEU:HD23	4:3:243:LEU:HD11	1.86	0.57
11:A:340:GLU:N	11:A:497:PRO:HG2	2.19	0.57
11:A:1063:LYS:HD3	11:A:1063:LYS:C	2.29	0.57
12:B:560:TYR:CD2	12:B:581:ILE:HD11	2.39	0.57
15:f:320:ARG:CB	15:f:320:ARG:HH11	2.18	0.57
35:p:399:LEU:HB3	35:p:453:TRP:CZ2	2.39	0.57
2:1:422:LEU:HD22	4:3:225:GLN:NE2	2.18	0.57
5:4:266:ARG:HE	5:4:277:LYS:HZ2	1.51	0.57
5:4:438:LYS:CE	12:B:621:ALA:N	2.64	0.57
13:D:995:GLU:HG2	26:T:186:MET:HE1	1.85	0.57
27:U:70:LYS:HE2	28:V:226:ASP:HA	1.86	0.57
15:f:219:GLU:OE1	15:f:219:GLU:N	2.25	0.57
4:3:52:ASN:OD1	4:3:53:ARG:N	2.37	0.57
10:9:175:LYS:NZ	10:9:185:GLU:OE2	2.29	0.57
15:F:335:ARG:HH21	15:F:378:ALA:HB1	1.69	0.57
25:S:142:ASN:OD1	25:S:143:TRP:N	2.37	0.57
28:V:192:VAL:HG21	28:V:203:PHE:HB3	1.86	0.57
14:e:513:LEU:HD21	14:e:527:ILE:HG23	1.86	0.57
35:p:643:LEU:HD11	35:p:656:LEU:HD11	1.87	0.57
1:0:1:MET:SD	8:7:345:ARG:HD3	2.45	0.57
14:E:522:ASP:O	14:E:524:LEU:N	2.37	0.57
14:e:257:GLU:CD	14:e:257:GLU:N	2.63	0.57
7:6:278:GLU:CG	7:6:482:PHE:HE1	2.16	0.57
9:8:258:HIS:HB3	9:8:269:LEU:HD21	1.85	0.57
15:F:83:LEU:CD1	15:F:83:LEU:N	2.67	0.57
15:F:315:ARG:CZ	15:F:369:PRO:HB3	2.35	0.57
27:U:137:THR:HB	27:U:140:GLU:OE1	2.04	0.57
28:V:148:LYS:HG3	28:V:149:LYS:HE2	1.87	0.57
34:o:1245:CYS:O	34:o:1246:ILE:HD13	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:166:ASP:OD1	40:u:167:TYR:N	2.37	0.57
12:B:27:LYS:CE	12:B:490:SER:HB3	2.35	0.57
17:H:156:PRO:HB3	17:H:160:ILE:HB	1.87	0.57
28:V:149:LYS:HA	28:V:152:LEU:HD12	1.87	0.57
40:u:38:CYS:SG	40:u:39:THR:N	2.78	0.57
28:V:86:LYS:NZ	28:V:140:LYS:HD2	2.20	0.57
3:2:261:SER:OG	3:2:265:GLN:O	2.23	0.56
9:8:58:THR:HG23	9:8:157:GLY:HA3	1.87	0.56
11:A:402:PHE:HA	11:A:407:GLN:NE2	2.20	0.56
11:A:851:ASP:OD1	11:A:851:ASP:N	2.38	0.56
12:B:820:ASP:OD1	12:B:820:ASP:N	2.37	0.56
14:e:636:HIS:HD2	14:e:638:ASN:H	1.53	0.56
11:A:929:THR:HG22	11:A:954:ALA:HA	1.86	0.56
27:U:14:LEU:HD11	27:U:194:THR:HG23	1.87	0.56
27:U:160:GLU:OE2	27:U:162:GLU:N	2.38	0.56
29:X:-30:DA:H2''	29:X:-29:DT:H5'	1.87	0.56
34:o:193:ARG:NH1	34:o:195:GLY:O	2.38	0.56
1:0:1:MET:SD	8:7:345:ARG:CD	2.93	0.56
1:0:20:LYS:HE3	1:0:62:LEU:HD13	1.87	0.56
3:2:59:ARG:NH2	3:2:166:GLU:OE1	2.38	0.56
4:3:215:LEU:HD22	4:3:230:VAL:HG21	1.87	0.56
7:6:444:HIS:O	7:6:472:ARG:NH1	2.39	0.56
14:E:345:MET:HE3	14:E:346:PRO:HD2	1.88	0.56
15:F:81:GLU:HB3	15:F:83:LEU:HD13	1.85	0.56
15:F:418:ILE:HD12	15:F:418:ILE:N	2.20	0.56
21:O:62:LEU:HA	21:O:76:LEU:HD23	1.87	0.56
31:c:12:VAL:HG23	15:f:118:ILE:HA	1.85	0.56
35:p:346:GLU:OE1	35:p:346:GLU:N	2.38	0.56
12:B:61:ASN:O	12:B:130:VAL:HG23	2.06	0.56
28:V:234:GLU:HB3	28:V:238:LYS:HZ3	1.69	0.56
13:d:960:GLU:HG2	13:d:963:ARG:HH21	1.71	0.56
35:p:42:GLN:HE22	35:p:483:ARG:HG2	1.70	0.56
35:p:302:LYS:HE2	42:w:14:ILE:HD12	1.86	0.56
7:6:361:CYS:SG	7:6:405:VAL:HG13	2.46	0.56
12:B:259:ASP:HB3	12:B:262:MET:O	2.06	0.56
13:d:910:LEU:HD11	20:l:88:ALA:HB2	1.87	0.56
34:o:672:ILE:HG23	34:o:676:ILE:HD13	1.88	0.56
35:p:91:ILE:HD13	35:p:126:VAL:HG12	1.87	0.56
41:v:33:GLU:OE2	41:v:55:LYS:NZ	2.38	0.56
1:0:84:LYS:CB	1:0:136:ASN:ND2	2.68	0.56
7:6:504:LYS:O	7:6:657:ALA:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:506:GLN:HB2	7:6:655:TYR:CD2	2.39	0.56
8:7:725:ALA:O	8:7:726:GLN:HB2	2.05	0.56
9:8:144:LEU:HG	9:8:154:ALA:HB2	1.88	0.56
10:9:72:LYS:HB3	10:9:73:PRO:HD3	1.86	0.56
20:L:113:VAL:O	20:L:114:LYS:C	2.49	0.56
20:L:119:HIS:NE2	20:L:123:GLN:OE1	2.38	0.56
7:6:519:TYR:CE2	7:6:666:ASP:HB2	2.41	0.56
8:7:664:VAL:HG21	8:7:679:PHE:CE1	2.40	0.56
15:f:223:TYR:HD2	15:f:255:MET:HE1	1.71	0.56
37:r:100:LEU:HD12	37:r:101:ALA:N	2.21	0.56
24:R:43:ASP:OD1	35:p:1064:ARG:NH2	2.39	0.56
35:p:694:THR:HG22	35:p:695:HIS:CE1	2.41	0.56
35:p:764:MET:HE1	35:p:938:ARG:NH1	2.21	0.56
7:6:278:GLU:HG3	7:6:482:PHE:CE1	2.39	0.56
21:O:29:THR:HG23	21:O:32:LEU:H	1.69	0.56
26:T:192:GLU:OE2	28:V:76:GLY:N	2.39	0.56
14:e:527:ILE:HG22	14:e:527:ILE:O	2.05	0.56
34:o:1453:GLY:O	34:o:1457:ASN:ND2	2.35	0.56
2:1:456:ASP:OD1	2:1:457:ILE:HD12	2.06	0.56
7:6:281:GLN:CG	7:6:482:PHE:HB2	2.35	0.56
28:V:155:LEU:HD21	28:V:204:ASN:H	1.70	0.56
7:6:87:GLU:OE2	7:6:145:LYS:NZ	2.40	0.55
15:F:312:ILE:HG13	15:F:334:ALA:HB3	1.88	0.55
13:d:917:ILE:HD11	13:d:1063:LEU:HD13	1.87	0.55
15:F:265:GLU:OE2	15:F:265:GLU:HA	2.06	0.55
28:V:147:ASP:HB3	28:V:150:ALA:H	1.71	0.55
28:V:213:ASP:O	28:V:217:GLN:N	2.39	0.55
34:o:621:ILE:HG23	34:o:621:ILE:O	2.06	0.55
11:A:401:ASN:H	11:A:401:ASN:HD22	1.53	0.55
11:A:675:ASP:OD1	16:G:78:LYS:NZ	2.37	0.55
27:U:76:MET:HG2	27:U:88:ARG:HB3	1.89	0.55
7:6:308:ILE:HG23	7:6:358:ARG:HG2	1.88	0.55
7:6:311:LYS:HZ1	7:6:382:SER:C	2.15	0.55
24:R:27:TYR:HB3	24:R:52:TRP:CE2	2.41	0.55
27:U:30:HIS:CD2	27:U:62:VAL:HG13	2.41	0.55
15:f:352:GLN:O	15:f:356:THR:OG1	2.25	0.55
20:l:99:ALA:HB1	20:l:111:LEU:HD11	1.87	0.55
35:p:752:TYR:CE2	35:p:807:ARG:CD	2.89	0.55
35:p:934:LYS:HG3	35:p:944:THR:HG22	1.87	0.55
4:3:242:ILE:C	4:3:243:LEU:HD12	2.31	0.55
14:E:468:ASN:ND2	15:F:128:ASP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:87:HIS:HB2	18:I:45:ARG:HE	1.71	0.55
28:V:148:LYS:HB3	28:V:183:LYS:HE3	1.86	0.55
15:f:253:TYR:O	15:f:254:GLN:HB3	2.06	0.55
34:o:1347:LEU:HB3	38:s:137:ILE:CD1	2.37	0.55
34:o:1411:LEU:O	34:o:1421:ARG:NH2	2.39	0.55
8:7:606:GLU:O	8:7:666:ARG:NH2	2.39	0.55
37:r:29:ALA:O	37:r:94:LYS:NZ	2.39	0.55
37:r:110:GLU:O	37:r:114:LEU:HD23	2.07	0.55
7:6:519:TYR:CE2	7:6:666:ASP:HB3	2.42	0.55
10:9:198:ILE:HD11	10:9:255:MET:SD	2.45	0.55
12:B:248:SER:OG	12:B:322:MET:SD	2.65	0.55
35:p:939:HIS:NE2	35:p:983:GLU:OE1	2.35	0.55
7:6:308:ILE:HG21	7:6:358:ARG:CA	2.10	0.55
15:F:71:ILE:HD11	18:I:35:VAL:HG13	1.89	0.55
15:f:280:ILE:O	15:f:284:ARG:HG3	2.05	0.55
34:o:15:LEU:HD22	40:u:63:ARG:HD2	1.88	0.55
35:p:260:LEU:HB2	35:p:263:ILE:HD12	1.89	0.55
35:p:952:GLU:OE2	36:q:39:ILE:HG22	2.07	0.55
2:1:486:LEU:O	2:1:490:VAL:HG23	2.06	0.55
8:7:420:PRO:HA	8:7:431:PRO:HB3	1.89	0.55
10:9:64:LEU:HB2	10:9:105:MET:HG3	1.89	0.55
11:A:355:VAL:O	11:A:355:VAL:HG23	2.07	0.55
11:A:1052:ARG:HD2	11:A:1052:ARG:O	2.07	0.55
14:E:561:SER:HB2	14:E:588:VAL:HB	1.88	0.55
15:F:406:VAL:HG11	15:F:420:ALA:HB2	1.88	0.55
23:Q:15:ARG:HA	23:Q:18:ILE:HD12	1.89	0.55
28:V:170:ASP:HA	28:V:173:GLU:HG2	1.89	0.55
4:3:229:TRP:CZ3	5:4:58:ARG:HD2	2.42	0.55
9:8:78:LEU:N	9:8:90:VAL:O	2.40	0.55
24:R:173:VAL:O	24:R:175:ARG:NH1	2.40	0.55
27:U:32:LEU:O	27:U:36:ILE:HG12	2.07	0.55
29:X:-28:DA:H2'	29:X:-27:DA:C8	2.42	0.55
37:r:133:ASP:OD1	37:r:134:ILE:N	2.39	0.55
5:4:409:TYR:HB2	5:4:412:PHE:HZ	1.72	0.54
14:e:610:ARG:HD3	14:e:619:PRO:HG3	1.89	0.54
1:0:83:ASN:HD21	1:0:140:LEU:CD1	2.18	0.54
28:V:89:HIS:NE2	28:V:138:ALA:O	2.38	0.54
34:o:350:VAL:HG12	34:o:1435:THR:HG21	1.89	0.54
34:o:507:GLN:N	35:p:1105:GLU:OE2	2.38	0.54
7:6:83:HIS:ND1	7:6:115:GLU:OE2	2.40	0.54
12:B:544:LEU:HD23	12:B:590:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:261:ARG:NH1	34:o:277:THR:OG1	2.40	0.54
1:0:307:GLN:CD	10:9:247:GLN:HE21	2.16	0.54
8:7:133:LYS:O	8:7:137:LEU:HD23	2.08	0.54
14:E:524:LEU:O	14:E:527:ILE:HG12	2.08	0.54
28:V:170:ASP:OD1	28:V:171:ILE:N	2.40	0.54
34:o:850:THR:O	34:o:854:THR:HG23	2.07	0.54
1:0:85:ARG:NH2	1:0:140:LEU:HA	2.22	0.54
4:3:108:ASN:HD21	5:4:123:LEU:HD22	1.71	0.54
5:4:80:SER:O	5:4:84:GLU:OE1	2.25	0.54
13:d:911:GLN:NE2	20:l:69:GLU:OE2	2.41	0.54
14:e:646:SER:OG	14:e:647:ALA:N	2.40	0.54
7:6:583:PRO:O	7:6:584:THR:C	2.49	0.54
8:7:309:VAL:HG12	8:7:309:VAL:O	2.06	0.54
8:7:365:VAL:HG22	8:7:365:VAL:O	2.08	0.54
14:E:645:GLY:H	14:E:675:LEU:HD11	1.73	0.54
14:e:368:ASN:ND2	14:e:701:GLY:HA3	2.23	0.54
1:0:85:ARG:HH12	1:0:140:LEU:N	2.06	0.54
4:3:100:LYS:HB2	5:4:124:GLY:O	2.07	0.54
4:3:242:ILE:CD1	5:4:75:VAL:C	2.81	0.54
5:4:401:LEU:HD12	6:5:50:VAL:HG22	1.90	0.54
5:4:415:GLN:CA	5:4:439:ARG:HH21	2.21	0.54
7:6:306:ILE:CB	7:6:358:ARG:O	2.55	0.54
4:3:44:LEU:HD21	4:3:162:LEU:HD13	1.89	0.54
7:6:664:SER:O	7:6:667:THR:OG1	2.25	0.54
11:A:489:GLN:NE2	11:A:489:GLN:H	2.04	0.54
12:B:66:ASN:HD21	12:B:119:PRO:HB3	1.73	0.54
19:j:123:LEU:C	19:j:125:ASP:N	2.66	0.54
35:p:851:ASP:OD2	45:z:17:TYR:OH	2.24	0.54
40:u:92:VAL:HG23	40:u:139:GLN:HG2	1.89	0.54
8:7:437:CYS:SG	8:7:438:MET:N	2.81	0.54
13:D:995:GLU:CG	26:T:186:MET:HE1	2.38	0.54
14:E:563:GLU:HG2	14:E:587:PRO:HG3	1.90	0.54
33:m:110:LEU:N	33:m:110:LEU:HD23	2.23	0.54
35:p:128:ILE:HG21	35:p:431:LEU:HD21	1.90	0.54
14:E:474:THR:HG22	15:F:61:GLY:HA2	1.89	0.54
15:F:83:LEU:H	15:F:83:LEU:HD12	1.71	0.54
24:R:133:ASN:OD1	24:R:134:ILE:N	2.40	0.54
35:p:501:LEU:HD12	35:p:505:LEU:HD12	1.90	0.54
7:6:298:ARG:CG	7:6:331:GLY:CA	2.87	0.53
7:6:306:ILE:CB	7:6:359:LYS:HA	2.37	0.53
8:7:17:ILE:HD11	8:7:22:PHE:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:19:LEU:HG	10:9:92:LEU:HD11	1.89	0.53
12:B:345:CYS:HA	12:B:348:GLN:HE21	1.73	0.53
35:p:738:THR:HG21	43:x:58:LYS:HG3	1.90	0.53
6:5:32:LYS:HB3	12:B:540:LYS:HG3	1.90	0.53
8:7:80:ILE:HD11	8:7:206:VAL:HB	1.89	0.53
8:7:114:ASN:C	8:7:114:ASN:HD22	2.15	0.53
13:D:922:GLN:NE2	20:L:71:ASP:OD2	2.41	0.53
14:E:299:ASP:OD2	14:E:607:ARG:NH2	2.38	0.53
15:F:335:ARG:HD2	15:F:382:GLU:HB2	1.90	0.53
15:F:433:PRO:HA	15:F:436:ALA:HB3	1.90	0.53
14:E:653:LEU:HB2	14:E:663:ARG:HB2	1.91	0.53
15:F:86:PHE:CD1	15:F:86:PHE:N	2.75	0.53
21:O:16:GLN:NE2	21:O:20:ASP:OD2	2.40	0.53
24:R:222:LEU:CD2	24:R:277:ILE:HD13	2.38	0.53
28:V:156:ASP:O	28:V:160:GLN:HG2	2.08	0.53
29:X:8:DT:H3	30:Y:-8:DA:H61	1.55	0.53
1:0:83:ASN:CG	1:0:140:LEU:HD12	2.34	0.53
3:2:88:LEU:HD23	3:2:131:LEU:HD21	1.91	0.53
4:3:195:VAL:CG1	4:3:203:LEU:HD23	2.38	0.53
7:6:308:ILE:HG12	7:6:355:CYS:HA	1.91	0.53
7:6:341:PRO:HG3	7:6:493:TRP:NE1	2.23	0.53
8:7:28:LEU:HD22	8:7:55:LEU:HD23	1.91	0.53
12:B:628:ILE:O	12:B:644:GLN:NE2	2.41	0.53
14:E:781:VAL:HG13	15:F:62:LYS:HD3	1.90	0.53
28:V:175:LEU:HB2	28:V:180:LYS:HE2	1.91	0.53
15:f:390:THR:HG23	15:f:391:LEU:HD22	1.89	0.53
34:o:582:PRO:HD2	41:v:47:ILE:HD12	1.90	0.53
12:B:629:ARG:NH1	12:B:658:ASP:OD2	2.37	0.53
35:p:40:VAL:CG2	35:p:181:PRO:HB2	2.21	0.53
35:p:410:ASN:O	35:p:414:GLU:OE1	2.26	0.53
24:R:286:ARG:HD2	24:R:290:ARG:HH22	1.73	0.53
34:o:1347:LEU:HB3	38:s:137:ILE:HD13	1.90	0.53
7:6:369:VAL:CG1	7:6:616:ASP:H	2.22	0.53
13:D:954:GLU:O	13:D:955:LYS:C	2.49	0.53
22:P:239:ARG:NH1	23:Q:314:LEU:C	2.66	0.53
2:1:127:LEU:HD12	2:1:467:ALA:HA	1.91	0.53
12:B:937:THR:HG23	12:B:939:ASN:H	1.74	0.53
15:F:403:ILE:O	15:F:406:VAL:HG22	2.08	0.53
17:H:156:PRO:HB3	17:H:160:ILE:HD12	1.90	0.53
14:e:747:LEU:HG	14:e:747:LEU:O	2.09	0.53
15:f:283:MET:HG3	15:f:329:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:44:LEU:HD22	4:3:227:LEU:HB3	1.91	0.53
12:B:808:PRO:HA	12:B:864:ASN:HB3	1.91	0.53
22:P:206:GLU:HB3	22:P:207:PRO:HD3	1.91	0.53
25:S:109:LYS:O	25:S:149:LEU:N	2.37	0.53
34:o:233:CYS:SG	34:o:244:ARG:NH1	2.81	0.53
1:0:255:THR:HG22	10:9:3:HIS:CE1	2.43	0.53
3:2:121:SER:OG	3:2:127:HIS:NE2	2.39	0.53
8:7:115:LEU:HD13	8:7:191:PRO:HB2	1.91	0.53
9:8:75:ILE:HA	9:8:152:LYS:HD3	1.91	0.53
16:G:149:ARG:O	16:G:149:ARG:HG3	2.08	0.53
25:S:43:ASN:OD1	25:S:44:GLN:N	2.43	0.53
15:f:318:CYS:SG	15:f:326:HIS:HB3	2.49	0.53
5:4:438:LYS:HE2	12:B:621:ALA:H	1.73	0.52
8:7:488:VAL:HG23	8:7:488:VAL:O	2.09	0.52
22:P:208:ARG:NH2	23:Q:346:LYS:CG	2.70	0.52
15:f:447:ALA:O	15:f:453:GLY:HA2	2.09	0.52
5:4:265:LEU:HD12	5:4:270:LEU:HD12	1.90	0.52
8:7:289:VAL:HG22	8:7:324:ARG:NH1	2.23	0.52
12:B:489:GLN:OE1	12:B:489:GLN:N	2.34	0.52
35:p:625:LEU:HD13	35:p:675:LEU:HD21	1.91	0.52
35:p:718:GLN:HG2	35:p:720:PRO:HD2	1.90	0.52
38:s:111:THR:HG23	38:s:114:ALA:H	1.74	0.52
11:A:828:GLU:HA	11:A:831:LYS:HB2	1.91	0.52
13:D:910:LEU:HD11	20:L:88:ALA:HB2	1.91	0.52
16:G:181:TRP:CE3	16:G:181:TRP:O	2.63	0.52
35:p:552:ASN:OD1	35:p:553:LEU:N	2.42	0.52
35:p:910:THR:HG23	45:z:42:ARG:O	2.09	0.52
15:F:223:TYR:O	15:F:224:TYR:C	2.52	0.52
19:J:137:TYR:OH	19:J:141:ARG:NH2	2.43	0.52
21:O:1:MET:H3	21:O:38:LEU:HD13	1.75	0.52
28:V:179:GLN:O	28:V:183:LYS:HB2	2.10	0.52
4:3:108:ASN:CG	5:4:123:LEU:HD13	2.34	0.52
5:4:32:ASP:OD1	5:4:33:ARG:N	2.42	0.52
7:6:363:VAL:HG21	7:6:378:PHE:HE2	1.75	0.52
9:8:167:ARG:HH21	9:8:167:ARG:HG2	1.74	0.52
10:9:275:GLN:O	10:9:278:GLU:HG3	2.10	0.52
27:U:141:ALA:HB1	40:u:107:PHE:CE2	2.45	0.52
40:u:52:ASP:N	40:u:71:LYS:O	2.42	0.52
3:2:54:ARG:NH2	3:2:245:SER:O	2.42	0.52
4:3:50:PHE:CZ	5:4:118:LEU:HD12	2.38	0.52
12:B:571:LEU:HD21	12:B:619:MET:HE1	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:607:ARG:NH1	18:i:87:PRO:O	2.43	0.52
34:o:459:ASN:OD1	34:o:460:ARG:N	2.42	0.52
35:p:613:ARG:NH1	35:p:615:TYR:OH	2.41	0.52
35:p:794:VAL:O	35:p:946:GLY:N	2.43	0.52
3:2:337:GLU:O	3:2:340:ASN:ND2	2.38	0.52
7:6:568:LEU:HD11	7:6:606:PHE:HB3	1.90	0.52
8:7:393:ASP:OD1	8:7:394:PHE:N	2.42	0.52
9:8:213:LEU:HA	9:8:224:ARG:HD2	1.92	0.52
11:A:339:ALA:HA	11:A:497:PRO:HG3	1.91	0.52
14:E:522:ASP:OD1	14:E:522:ASP:N	2.43	0.52
14:E:562:SER:OG	14:E:564:ASP:OD1	2.28	0.52
14:E:746:ASP:OD1	14:E:746:ASP:N	2.42	0.52
27:U:128:LYS:O	27:U:162:GLU:HB3	2.10	0.52
5:4:335:LEU:O	7:6:59:LYS:N	2.42	0.52
5:4:408:LEU:HD11	5:4:440:LEU:HB3	1.92	0.52
7:6:463:LYS:O	7:6:484:ILE:HG23	2.10	0.52
15:F:39:LEU:HD11	18:I:51:LEU:HD21	1.92	0.52
15:F:273:GLN:H	15:F:273:GLN:CD	2.17	0.52
24:R:107:MET:O	24:R:112:ARG:NH2	2.43	0.52
1:0:85:ARG:NH2	1:0:140:LEU:CA	2.68	0.52
7:6:342:CYS:SG	7:6:641:GLY:HA3	2.49	0.52
13:D:959:ASP:HB3	13:D:983:ARG:NH1	2.25	0.52
14:E:278:ASP:OD1	14:E:278:ASP:N	2.43	0.52
19:J:114:THR:HB	19:J:117:VAL:HB	1.92	0.52
27:U:183:GLN:NE2	28:V:211:SER:O	2.42	0.52
14:e:423:PRO:HG2	14:e:426:ARG:HB2	1.91	0.52
15:f:320:ARG:NH1	15:f:320:ARG:CB	2.73	0.52
7:6:311:LYS:CE	7:6:383:THR:CG2	2.85	0.52
7:6:377:GLN:OE1	7:6:381:TRP:NE1	2.40	0.52
8:7:709:THR:HG22	8:7:710:VAL:N	2.25	0.52
10:9:181:LEU:HD13	10:9:226:ILE:HG21	1.92	0.52
11:A:338:VAL:HG12	11:A:497:PRO:HD3	1.91	0.52
22:P:205:ARG:HB3	23:Q:376:TRP:CZ3	2.45	0.52
41:v:91:VAL:HG22	41:v:144:LEU:HD23	1.91	0.52
2:1:412:GLU:OE1	2:1:412:GLU:N	2.43	0.51
2:1:503:THR:OG1	2:1:533:TYR:OH	2.01	0.51
6:5:31:LYS:HB2	12:B:540:LYS:HZ1	1.67	0.51
10:9:7:GLN:HG3	10:9:89:ARG:NH2	2.25	0.51
12:B:90:THR:O	12:B:968:ARG:NH2	2.43	0.51
12:B:656:GLU:HG2	12:B:661:ALA:HB3	1.92	0.51
17:H:52:SER:O	19:J:194:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:48:MET:O	27:U:52:LEU:N	2.42	0.51
28:V:97:LEU:HG	28:V:101:GLU:CD	2.35	0.51
8:7:126:PHE:CE2	8:7:128:LYS:HB2	2.46	0.51
10:9:59:TYR:CZ	10:9:63:ARG:HD2	2.45	0.51
12:B:66:ASN:OD1	12:B:187:ARG:NH1	2.43	0.51
13:D:997:ALA:O	13:D:1001:GLN:HG3	2.10	0.51
31:c:33:LEU:HD13	19:j:197:MET:HE1	1.90	0.51
14:e:500:THR:HG22	14:e:502:LYS:H	1.76	0.51
14:e:595:PRO:HD2	14:e:639:SER:HB3	1.91	0.51
34:o:1016:LEU:O	34:o:1020:LEU:HG	2.10	0.51
3:2:87:LEU:HD11	3:2:229:LYS:HG2	1.91	0.51
4:3:108:ASN:ND2	5:4:123:LEU:HD22	2.26	0.51
4:3:165:LYS:NZ	4:3:167:ALA:O	2.38	0.51
14:E:256:HIS:HB3	14:E:259:GLU:HG2	1.93	0.51
14:E:304:LYS:NZ	14:E:335:GLU:O	2.42	0.51
21:O:57:ASN:OD1	21:O:58:PHE:N	2.44	0.51
26:T:153:TYR:HE1	35:p:432:GLU:HB3	1.69	0.51
34:o:485:ASN:O	34:o:488:VAL:HG22	2.10	0.51
44:y:63:VAL:HG23	44:y:63:VAL:O	2.10	0.51
7:6:181:HIS:O	7:6:184:VAL:HG12	2.10	0.51
7:6:296:ASP:HA	7:6:332:ARG:HB3	1.93	0.51
13:D:873:LEU:HD21	20:L:92:ILE:HD11	1.91	0.51
26:T:146:ASP:O	26:T:147:LYS:HB2	2.09	0.51
42:w:69:ILE:HG22	42:w:71:ASP:H	1.74	0.51
14:E:601:VAL:HG21	14:E:642:VAL:HG11	1.92	0.51
31:c:21:LEU:HD12	31:c:21:LEU:O	2.11	0.51
9:8:268:LEU:O	9:8:272:ILE:HG12	2.11	0.51
11:A:510:ILE:HB	11:A:511:LEU:HD13	1.92	0.51
12:B:983:ARG:HH11	12:B:983:ARG:HG3	1.75	0.51
16:G:181:TRP:CD2	16:G:181:TRP:C	2.87	0.51
34:o:1172:ASN:HA	42:w:58:ILE:HD12	1.93	0.51
35:p:834:ARG:HG2	35:p:840:MET:HE2	1.93	0.51
27:U:110:MET:O	27:U:114:ILE:HG12	2.11	0.51
27:U:139:LEU:HD23	40:u:151:ARG:NH1	2.20	0.51
27:U:141:ALA:CB	40:u:107:PHE:CD2	2.94	0.51
27:U:184:ILE:HG23	27:U:187:ILE:HB	1.91	0.51
34:o:1139:LEU:HD13	34:o:1341:VAL:HA	1.91	0.51
35:p:529:MET:HE1	35:p:698:ILE:HD12	1.91	0.51
35:p:938:ARG:NH2	35:p:983:GLU:OE2	2.38	0.51
7:6:108:CYS:SG	7:6:682:ASP:CB	2.99	0.51
7:6:298:ARG:CG	7:6:331:GLY:C	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:341:PRO:HG2	7:6:496:LEU:CD1	2.41	0.51
7:6:502:ILE:HG23	7:6:644:LEU:CB	2.36	0.51
15:F:238:LYS:O	15:F:239:ARG:C	2.54	0.51
24:R:53:ARG:O	24:R:54:THR:C	2.54	0.51
28:V:87:THR:O	28:V:91:ARG:HG2	2.11	0.51
13:d:916:LYS:NZ	13:d:1070:GLU:OE2	2.42	0.51
33:m:28:ARG:HH21	33:m:31:LEU:HD21	1.76	0.51
33:m:52:GLU:OE1	33:m:52:GLU:N	2.40	0.51
5:4:338:PHE:N	5:4:341:MET:O	2.44	0.51
11:A:395:ASP:OD1	11:A:395:ASP:N	2.41	0.51
12:B:529:VAL:HG11	12:B:560:TYR:HB2	1.91	0.51
14:E:423:PRO:HG2	14:E:426:ARG:HB2	1.92	0.51
24:R:222:LEU:HD21	24:R:277:ILE:HD13	1.92	0.51
15:f:24:GLU:HG2	20:l:145:THR:HG21	1.93	0.51
44:y:105:PHE:CE2	44:y:109:ILE:HD11	2.45	0.51
8:7:284:GLU:HG2	8:7:385:THR:HG21	1.93	0.51
12:B:274:LEU:HG	12:B:278:LYS:HE2	1.93	0.51
2:1:471:LEU:HD13	2:1:475:PHE:HE2	1.75	0.50
3:2:204:GLU:OE1	3:2:209:THR:OG1	2.29	0.50
5:4:405:GLU:O	5:4:444:THR:HG22	2.11	0.50
12:B:739:ASN:ND2	12:B:782:ASN:OD1	2.44	0.50
12:B:983:ARG:HG3	12:B:983:ARG:NH1	2.26	0.50
1:0:304:LEU:HD11	10:9:170:PHE:HZ	1.76	0.50
8:7:3:LEU:O	8:7:9:LEU:HD12	2.11	0.50
26:T:228:ILE:HG23	26:T:229:HIS:N	2.26	0.50
27:U:74:CYS:HA	27:U:91:TYR:O	2.11	0.50
33:m:77:ARG:CG	33:m:77:ARG:NH1	2.73	0.50
40:u:39:THR:O	40:u:43:GLY:N	2.42	0.50
1:0:85:ARG:HH22	1:0:140:LEU:HA	1.72	0.50
2:1:471:LEU:HD13	2:1:475:PHE:CE2	2.47	0.50
7:6:281:GLN:CD	7:6:482:PHE:HB2	2.36	0.50
8:7:118:HIS:HB3	8:7:121:VAL:HG22	1.93	0.50
11:A:1200:THR:C	11:A:1204:GLU:HG2	2.31	0.50
12:B:780:LYS:O	17:H:183:ARG:NH1	2.44	0.50
20:L:126:MET:HE3	20:L:128:ILE:HD11	1.93	0.50
31:c:77:LEU:HD23	31:c:77:LEU:O	2.11	0.50
9:8:207:LEU:HD11	9:8:268:LEU:HD21	1.93	0.50
12:B:202:TRP:HB2	12:B:238:LEU:HB3	1.92	0.50
15:F:71:ILE:HD12	18:I:38:GLN:HE21	1.76	0.50
17:H:113:ARG:O	17:H:116:ARG:NH1	2.44	0.50
20:L:93:GLU:O	20:L:97:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:97:LEU:HD21	40:u:128:TYR:CE1	2.46	0.50
1:0:55:LYS:C	1:0:57:ASN:N	2.69	0.50
11:A:1163:ARG:HB3	16:G:183:ILE:HG22	1.92	0.50
15:F:273:GLN:CD	15:F:273:GLN:N	2.70	0.50
14:e:650:THR:HG22	14:e:666:THR:HG22	1.93	0.50
35:p:809:VAL:HG11	35:p:811:TYR:CE2	2.46	0.50
5:4:438:LYS:CE	12:B:621:ALA:HB2	2.42	0.50
7:6:363:VAL:HG21	7:6:378:PHE:CE2	2.47	0.50
26:T:141:LEU:HD21	35:p:53:MET:SD	2.51	0.50
34:o:863:ARG:NH2	34:o:1415:THR:OG1	2.44	0.50
8:7:377:GLU:OE1	8:7:377:GLU:N	2.44	0.50
14:E:481:ASP:OD1	14:E:481:ASP:N	2.41	0.50
34:o:1382:LEU:HD23	34:o:1398:LEU:HD13	1.93	0.50
5:4:390:GLN:HE21	5:4:394:TRP:NE1	2.09	0.50
6:5:15:ALA:CA	7:6:516:PRO:HB3	2.39	0.50
7:6:306:ILE:HB	7:6:358:ARG:C	2.36	0.50
10:9:85:MET:O	10:9:89:ARG:HG3	2.11	0.50
14:e:527:ILE:O	14:e:527:ILE:CG2	2.59	0.50
34:o:95:PHE:N	34:o:311:GLN:OE1	2.43	0.50
1:0:129:ASN:O	1:0:130:LYS:C	2.55	0.50
2:1:136:VAL:HG11	2:1:502:VAL:HG12	1.92	0.50
8:7:284:GLU:HA	8:7:287:ARG:HG2	1.94	0.50
12:B:152:LEU:HD23	12:B:155:PRO:HB3	1.94	0.50
12:B:598:ARG:HH11	12:B:619:MET:HE3	1.77	0.50
27:U:30:HIS:CE1	27:U:62:VAL:HG22	2.47	0.50
14:e:474:THR:OG1	14:e:546:VAL:O	2.28	0.50
35:p:601:VAL:HG22	35:p:616:THR:HG23	1.93	0.50
3:2:89:GLU:OE2	3:2:132:LYS:NZ	2.42	0.49
4:3:13:ILE:HD13	4:3:41:VAL:HG13	1.94	0.49
9:8:97:ASP:HA	9:8:144:LEU:HA	1.94	0.49
12:B:818:THR:OG1	12:B:819:LEU:N	2.44	0.49
34:o:521:VAL:HG13	34:o:535:MET:HE1	1.93	0.49
34:o:1424:THR:O	34:o:1429:LYS:HE3	2.12	0.49
2:1:481:VAL:HG23	2:1:483:THR:HG23	1.94	0.49
9:8:174:VAL:O	9:8:179:ARG:NH2	2.31	0.49
13:D:995:GLU:CB	26:T:186:MET:HE1	2.41	0.49
13:D:1002:ARG:NH2	26:T:179:ASP:OD1	2.45	0.49
19:J:139:LEU:HB3	19:J:144:PHE:HB3	1.93	0.49
28:V:110:ASP:OD1	28:V:114:LYS:HD3	2.12	0.49
14:e:586:TYR:HB3	14:e:605:HIS:HB3	1.94	0.49
34:o:1144:LEU:HD23	34:o:1144:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:258:PRO:HG2	1:0:301:PHE:CG	2.47	0.49
3:2:69:ARG:HH21	8:7:563:ARG:HE	1.58	0.49
7:6:306:ILE:CA	7:6:358:ARG:O	2.60	0.49
7:6:340:LEU:CD2	7:6:491:ALA:HB2	2.41	0.49
22:P:249:LYS:HB3	23:Q:312:GLU:OE1	2.12	0.49
22:P:292:ILE:HG12	29:X:-29:DT:H5"	1.93	0.49
29:X:-27:DA:H2'	29:X:-26:DA:H8	1.76	0.49
3:2:291:CYS:SG	3:2:294:CYS:N	2.82	0.49
8:7:674:TYR:HB2	8:7:724:MET:HG3	1.95	0.49
12:B:882:HIS:HE1	17:H:216:ALA:HB1	1.77	0.49
13:D:959:ASP:O	13:D:983:ARG:NH2	2.44	0.49
22:P:239:ARG:CD	23:Q:317:GLU:CG	2.90	0.49
28:V:227:SER:O	28:V:231:GLU:HG2	2.12	0.49
34:o:196:LEU:HD11	34:o:308:LYS:HD2	1.94	0.49
34:o:683:GLU:O	35:p:1038:THR:HB	2.13	0.49
34:o:1173:THR:HG22	34:o:1214:VAL:HG23	1.94	0.49
34:o:1242:ASP:O	34:o:1262:MET:N	2.46	0.49
35:p:404:PHE:HA	35:p:407:MET:HE3	1.94	0.49
35:p:407:MET:HE1	35:p:444:LEU:CG	2.43	0.49
35:p:907:VAL:HG22	35:p:921:ILE:HG12	1.94	0.49
5:4:406:GLY:HA2	5:4:444:THR:HA	1.93	0.49
7:6:578:PRO:HG3	7:6:602:ILE:HD11	1.94	0.49
8:7:134:CYS:O	8:7:138:THR:HG22	2.12	0.49
27:U:139:LEU:CD2	40:u:151:ARG:CD	2.54	0.49
34:o:469:MET:O	35:p:1097:HIS:NE2	2.46	0.49
2:1:374:LEU:HD12	2:1:374:LEU:O	2.13	0.49
3:2:206:ARG:HG2	8:7:589:GLU:HA	1.94	0.49
5:4:379:GLN:OE1	7:6:112:HIS:HE1	1.96	0.49
28:V:113:LEU:HA	28:V:116:LYS:HE2	1.94	0.49
34:o:363:ALA:O	35:p:1084:LEU:HD11	2.11	0.49
34:o:1382:LEU:HD23	34:o:1398:LEU:CD1	2.42	0.49
35:p:501:LEU:HD11	35:p:511:PRO:HA	1.95	0.49
5:4:335:LEU:C	7:6:58:ALA:HA	2.37	0.49
7:6:444:HIS:ND1	7:6:634:ARG:HD2	2.26	0.49
21:O:73:THR:O	21:O:73:THR:HG22	2.12	0.49
34:o:196:LEU:HD11	34:o:308:LYS:CD	2.42	0.49
34:o:196:LEU:HD11	34:o:308:LYS:CE	2.42	0.49
35:p:1035:ARG:NH1	35:p:1036:LYS:O	2.44	0.49
40:u:134:ASP:OD1	40:u:135:ILE:N	2.45	0.49
3:2:63:VAL:HG11	3:2:88:LEU:HD11	1.95	0.49
3:2:87:LEU:HD11	3:2:229:LYS:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:285:THR:O	3:2:297:LYS:NZ	2.46	0.49
13:D:997:ALA:HB1	21:O:1:MET:HA	1.94	0.49
15:F:257:PRO:O	15:F:261:THR:OG1	2.26	0.49
16:G:94:MET:HE3	16:G:96:VAL:HG22	1.94	0.49
42:w:29:ASP:O	42:w:33:ARG:N	2.40	0.49
1:0:125:TYR:O	1:0:129:ASN:HB2	2.13	0.49
8:7:45:GLY:O	8:7:48:LYS:NZ	2.44	0.49
9:8:20:GLU:HG3	9:8:25:THR:HG22	1.94	0.49
11:A:927:VAL:O	11:A:933:ASN:ND2	2.44	0.49
14:E:589:TRP:CE3	15:F:60:MET:HG3	2.48	0.49
14:E:634:ARG:HG3	14:E:675:LEU:HB2	1.95	0.49
22:P:205:ARG:NH2	23:Q:376:TRP:CD1	2.81	0.49
23:Q:18:ILE:HD11	23:Q:46:TRP:CZ3	2.48	0.49
19:j:176:MET:O	19:j:178:GLY:N	2.43	0.49
34:o:350:VAL:CG1	34:o:1435:THR:HG21	2.43	0.49
1:0:4:GLN:OE1	1:0:10:LYS:HD3	2.13	0.49
13:D:995:GLU:HB3	26:T:186:MET:HE1	1.95	0.49
15:F:312:ILE:HG22	15:F:313:VAL:HG13	1.94	0.49
22:P:239:ARG:HD3	23:Q:317:GLU:CG	2.43	0.49
31:c:119:GLU:HG3	14:e:790:LEU:HD11	1.95	0.49
13:d:1080:TYR:OH	14:e:606:ASP:OD2	2.26	0.49
15:f:97:ALA:HB2	15:f:106:PHE:HE1	1.77	0.49
34:o:1218:ARG:NH2	34:o:1252:ALA:O	2.46	0.49
2:1:440:LEU:HD11	4:3:218:PRO:CD	2.43	0.48
5:4:360:THR:HG22	5:4:363:GLN:OE1	2.13	0.48
7:6:295:TYR:HB3	7:6:333:ALA:O	2.13	0.48
8:7:81:GLU:O	8:7:84:ILE:HG22	2.13	0.48
8:7:310:LEU:HG	8:7:409:THR:HG21	1.95	0.48
8:7:637:LEU:HD13	8:7:651:PHE:CD2	2.47	0.48
20:L:113:VAL:O	20:L:116:VAL:N	2.46	0.48
26:T:43:LEU:HD12	26:T:55:SER:O	2.13	0.48
28:V:176:PRO:O	28:V:178:SER:N	2.46	0.48
33:m:57:LEU:HA	33:m:57:LEU:HD23	1.73	0.48
34:o:1251:ASN:OD1	34:o:1252:ALA:N	2.46	0.48
37:r:55:GLN:NE2	37:r:56:GLU:O	2.46	0.48
4:3:100:LYS:HD3	5:4:123:LEU:HA	1.95	0.48
5:4:329:ALA:HB1	7:6:56:TYR:CE1	2.48	0.48
11:A:337:ARG:HH11	11:A:338:VAL:H	1.61	0.48
11:A:569:ASN:HB3	11:A:572:TYR:HD2	1.78	0.48
14:E:481:ASP:HB3	14:E:787:ARG:HH22	1.77	0.48
27:U:99:LEU:O	27:U:103:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:1:MET:HG3	15:f:126:PRO:HB3	1.93	0.48
33:m:69:THR:HG22	33:m:73:MET:HE2	1.94	0.48
40:u:83:GLU:OE2	40:u:147:ILE:HD12	2.13	0.48
1:0:303:GLY:O	10:9:210:SER:HB2	2.13	0.48
2:1:488:GLU:O	2:1:491:VAL:HG22	2.13	0.48
7:6:342:CYS:SG	7:6:641:GLY:CA	3.01	0.48
7:6:373:GLN:OE1	7:6:616:ASP:HA	2.12	0.48
7:6:511:TRP:CD1	7:6:689:VAL:HG13	2.48	0.48
9:8:61:ARG:HD3	9:8:159:ALA:H	1.78	0.48
10:9:96:VAL:HG13	10:9:101:PRO:CG	2.43	0.48
10:9:195:LEU:HA	10:9:198:ILE:HG22	1.95	0.48
10:9:234:GLU:C	10:9:236:LEU:H	2.20	0.48
11:A:639:LEU:O	11:A:643:ILE:HG13	2.13	0.48
15:F:409:GLY:O	15:F:417:ARG:NH2	2.47	0.48
27:U:76:MET:HB2	27:U:90:ASN:OD1	2.13	0.48
28:V:117:GLN:O	28:V:121:THR:OG1	2.18	0.48
34:o:225:PHE:HA	34:o:228:ILE:HD12	1.96	0.48
7:6:516:PRO:O	7:6:520:ARG:HG3	2.13	0.48
8:7:115:LEU:HD12	8:7:115:LEU:O	2.13	0.48
8:7:243:CYS:SG	8:7:443:ALA:HB3	2.53	0.48
14:E:732:ASP:OD1	14:E:734:THR:OG1	2.31	0.48
16:G:48:HIS:HD2	16:G:54:GLY:HA2	1.78	0.48
14:e:720:SER:OG	14:e:721:ARG:N	2.47	0.48
14:e:747:LEU:H	14:e:747:LEU:CD2	2.22	0.48
34:o:1178:ASP:OD2	34:o:1260:ARG:NH2	2.45	0.48
7:6:542:ARG:NH1	7:6:704:SER:HB3	2.28	0.48
14:e:556:ASN:HA	14:e:572:LEU:HB2	1.96	0.48
14:e:651:VAL:HG13	14:e:665:PHE:HB2	1.95	0.48
34:o:904:GLN:NE2	34:o:981:CYS:O	2.42	0.48
4:3:20:ILE:H	4:3:20:ILE:HD12	1.79	0.48
10:9:146:TYR:HD1	10:9:149:LEU:HD23	1.78	0.48
11:A:475:LEU:O	15:f:354:ARG:NH2	2.47	0.48
20:L:104:ARG:HD2	20:L:104:ARG:HA	1.49	0.48
27:U:44:LYS:HG3	27:U:89:HIS:CD2	2.48	0.48
28:V:234:GLU:HB3	28:V:238:LYS:NZ	2.28	0.48
14:e:724:GLU:OE1	14:e:789:ASN:ND2	2.46	0.48
15:f:254:GLN:O	15:f:258:ARG:NH2	2.47	0.48
34:o:502:ASN:OD1	35:p:1084:LEU:HD13	2.13	0.48
34:o:542:LEU:O	34:o:545:VAL:HG12	2.14	0.48
34:o:686:THR:HG21	35:p:1040:GLN:O	2.14	0.48
34:o:928:ARG:NH2	41:v:107:GLU:OE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:63:PHE:HB2	1:0:69:ASP:OD1	2.13	0.48
5:4:174:ASP:OD1	5:4:175:LEU:N	2.45	0.48
5:4:456:LYS:HD2	5:4:456:LYS:HA	1.50	0.48
11:A:338:VAL:HG13	11:A:360:SER:HB2	1.96	0.48
13:D:1068:GLU:OE2	14:E:582:LYS:NZ	2.45	0.48
14:E:467:LEU:HD11	15:F:132:LYS:HD3	1.94	0.48
14:E:693:VAL:HB	14:E:707:LEU:HB2	1.94	0.48
15:F:316:GLN:NE2	15:F:319:LEU:O	2.45	0.48
26:T:58:LEU:HD11	26:T:62:LEU:HD23	1.96	0.48
31:c:26:VAL:HG23	19:j:195:LEU:HB3	1.96	0.48
14:e:589:TRP:HB3	15:f:60:MET:HE3	1.96	0.48
32:k:173:CYS:SG	32:k:179:MET:O	2.72	0.48
35:p:830:GLU:OE2	35:p:870:THR:OG1	2.21	0.48
35:p:1108:PHE:CE1	35:p:1113:PRO:HA	2.49	0.48
42:w:12:VAL:CG1	42:w:55:VAL:CG1	2.92	0.48
2:1:456:ASP:OD1	2:1:456:ASP:N	2.47	0.48
4:3:31:GLN:OE1	4:3:36:LYS:NZ	2.42	0.48
7:6:615:PHE:CD2	7:6:617:LEU:HD21	2.49	0.48
9:8:59:ALA:HB1	9:8:87:ILE:HD11	1.95	0.48
11:A:824:ARG:HB3	11:A:863:VAL:HG12	1.95	0.48
12:B:135:TRP:HA	12:B:138:VAL:HG12	1.95	0.48
12:B:560:TYR:HD2	12:B:581:ILE:HD11	1.78	0.48
12:B:636:VAL:HG23	12:B:638:ARG:HB3	1.96	0.48
14:E:256:HIS:HB3	14:E:259:GLU:CG	2.43	0.48
14:E:703:MET:HE2	14:E:761:LEU:HD21	1.95	0.48
17:H:39:VAL:HG12	17:H:119:ILE:HG12	1.96	0.48
17:H:155:ASP:O	17:H:156:PRO:C	2.55	0.48
14:e:693:VAL:HB	14:e:707:LEU:HB2	1.94	0.48
36:q:92:GLU:O	36:q:93:PHE:CG	2.67	0.48
37:r:33:LEU:O	37:r:37:VAL:HG23	2.13	0.48
37:r:114:LEU:CD1	40:u:84:VAL:HG21	2.43	0.48
3:2:348:CYS:O	4:3:146:ARG:NH2	2.45	0.48
7:6:305:ASP:HA	7:6:359:LYS:CD	2.44	0.48
7:6:631:GLY:HA2	7:6:676:ARG:HB2	1.95	0.48
10:9:106:LEU:HB3	10:9:143:ILE:HD11	1.96	0.48
11:A:575:PRO:HD3	12:B:608:ASN:HD22	1.79	0.48
32:k:191:VAL:HG13	32:k:200:ILE:CD1	2.41	0.48
34:o:689:ILE:O	34:o:693:ILE:HG12	2.14	0.48
34:o:1415:THR:HG22	34:o:1416:ARG:N	2.29	0.48
35:p:598:VAL:CG2	35:p:601:VAL:HG23	2.44	0.48
1:0:275:VAL:HG21	1:0:293:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:136:SER:O	8:7:142:VAL:HG21	2.13	0.48
11:A:485:ILE:HB	15:f:310:THR:HG23	1.94	0.48
12:B:570:GLU:HA	12:B:625:LEU:HA	1.95	0.48
12:B:781:TYR:O	17:H:176:ARG:NH2	2.47	0.48
27:U:30:HIS:NE2	27:U:62:VAL:HA	2.28	0.48
14:e:234:ALA:HB2	14:e:648:ASP:HB2	1.96	0.48
14:e:633:THR:O	14:e:634:ARG:NH2	2.45	0.48
34:o:775:LYS:HD2	35:p:974:SER:HB3	1.96	0.48
35:p:718:GLN:OE1	35:p:976:MET:HE3	2.14	0.48
37:r:15:GLU:OE2	40:u:78:ARG:NH1	2.47	0.48
39:t:78:PRO:HG2	40:u:19:GLY:HA3	1.96	0.48
40:u:30:LEU:O	40:u:34:VAL:HG22	2.14	0.48
5:4:261:PHE:O	5:4:265:LEU:HD23	2.14	0.47
5:4:329:ALA:CB	7:6:56:TYR:CZ	2.97	0.47
11:A:821:ARG:HA	11:A:821:ARG:NE	2.25	0.47
14:E:696:TRP:HA	14:E:703:MET:HA	1.96	0.47
15:F:317:LEU:N	15:F:317:LEU:CD2	2.77	0.47
27:U:49:LEU:O	27:U:53:LYS:HA	2.15	0.47
15:f:39:LEU:HD22	18:i:47:VAL:HG13	1.95	0.47
15:f:257:PRO:O	15:f:261:THR:OG1	2.31	0.47
34:o:1454:VAL:HG12	34:o:1458:ILE:HD12	1.95	0.47
5:4:379:GLN:OE1	7:6:112:HIS:CE1	2.67	0.47
5:4:415:GLN:N	5:4:439:ARG:HH21	2.12	0.47
7:6:575:LEU:O	7:6:576:ASN:OD1	2.31	0.47
9:8:142:ASN:ND2	9:8:155:ASP:OD1	2.47	0.47
13:D:959:ASP:HB3	13:D:983:ARG:CZ	2.43	0.47
20:L:106:ARG:O	20:L:106:ARG:HG2	2.14	0.47
22:P:297:LYS:HG2	22:P:298:PRO:HD3	1.96	0.47
34:o:1357:THR:O	38:s:142:HIS:NE2	2.45	0.47
1:0:28:HIS:HB3	1:0:30:LEU:HG	1.96	0.47
2:1:422:LEU:HD13	4:3:225:GLN:NE2	2.29	0.47
3:2:253:GLY:N	3:2:310:LEU:HD21	2.29	0.47
4:3:192:ASP:OD1	4:3:213:LEU:N	2.45	0.47
17:H:197:THR:HB	15:f:238:LYS:HG2	1.96	0.47
30:Y:30:DT:H2'	30:Y:31:DA:C8	2.49	0.47
34:o:1468:THR:HG21	35:p:1101:GLN:HG3	1.96	0.47
35:p:438:ARG:NH2	35:p:442:ASP:OD2	2.47	0.47
37:r:73:ARG:O	37:r:141:GLN:NE2	2.44	0.47
4:3:123:ASP:OD1	4:3:124:ILE:N	2.45	0.47
8:7:617:ALA:HB2	8:7:676:LEU:HD21	1.97	0.47
10:9:178:TYR:CE1	10:9:228:MET:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:501:THR:O	11:A:502:LEU:C	2.58	0.47
14:E:774:MET:HE2	14:E:774:MET:N	2.23	0.47
15:F:90:GLU:CD	15:F:90:GLU:N	2.72	0.47
30:Y:-14:DT:H2'	30:Y:-13:DG:C8	2.49	0.47
34:o:462:PRO:HB2	35:p:1089:MET:HE1	1.96	0.47
34:o:484:LEU:HD11	34:o:501:MET:SD	2.54	0.47
34:o:1479:LYS:HB3	34:o:1479:LYS:HE2	1.75	0.47
35:p:738:THR:HG21	43:x:58:LYS:CG	2.44	0.47
3:2:357:VAL:CG1	3:2:366:VAL:HG23	2.45	0.47
9:8:61:ARG:HH11	9:8:158:LEU:HA	1.78	0.47
10:9:32:CYS:SG	10:9:33:LYS:N	2.87	0.47
12:B:859:ARG:HA	12:B:859:ARG:HD2	1.80	0.47
18:I:63:LYS:NZ	18:I:69:ASP:OD1	2.47	0.47
38:s:25:GLY:O	38:s:65:ASN:ND2	2.47	0.47
8:7:373:ARG:O	8:7:405:THR:OG1	2.24	0.47
9:8:136:ARG:NH1	9:8:160:LYS:HD3	2.29	0.47
12:B:329:LEU:HB3	12:B:342:THR:HG23	1.95	0.47
12:B:564:LEU:HB2	12:B:581:ILE:HD13	1.97	0.47
12:B:953:LEU:HD12	12:B:979:PHE:HE2	1.79	0.47
14:E:232:HIS:HD1	14:E:313:SER:HG	1.58	0.47
27:U:114:ILE:O	27:U:174:ARG:NH2	2.47	0.47
28:V:103:LEU:HA	28:V:106:THR:HG22	1.96	0.47
13:d:922:GLN:NE2	20:l:71:ASP:OD2	2.47	0.47
15:f:102:ARG:HD3	20:l:151:ARG:HG3	1.96	0.47
15:f:328:ALA:C	15:f:330:ARG:N	2.72	0.47
35:p:167:THR:HG23	35:p:170:ASP:H	1.78	0.47
35:p:898:THR:HG23	35:p:1078:ARG:O	2.14	0.47
43:x:6:ARG:HD3	43:x:13:ILE:HD13	1.95	0.47
3:2:175:THR:HG23	8:7:592:ARG:HA	1.97	0.47
4:3:42:MET:SD	4:3:108:ASN:ND2	2.87	0.47
5:4:410:ASN:HA	5:4:440:LEU:HD23	1.96	0.47
8:7:52:LEU:HD21	8:7:232:VAL:HG11	1.96	0.47
8:7:77:VAL:HA	8:7:80:ILE:HG22	1.97	0.47
9:8:45:LEU:HD11	9:8:86:ASN:HB3	1.96	0.47
9:8:62:GLU:OE2	9:8:157:GLY:N	2.48	0.47
10:9:101:PRO:O	10:9:105:MET:HB2	2.14	0.47
11:A:1165:LEU:HB2	11:A:1191:ILE:HG12	1.97	0.47
14:E:651:VAL:HB	14:E:665:PHE:HB2	1.95	0.47
15:F:317:LEU:N	15:F:317:LEU:HD23	2.29	0.47
15:F:415:ILE:O	15:F:415:ILE:HG12	2.14	0.47
18:I:119:ARG:NH1	18:I:120:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:141:ALA:CB	40:u:107:PHE:CE2	2.97	0.47
13:d:1061:ARG:NH1	18:i:119:ARG:O	2.48	0.47
15:f:330:ARG:NH1	15:f:371:THR:O	2.47	0.47
35:p:905:ASP:N	35:p:922:ARG:O	2.42	0.47
7:6:536:MET:HG2	7:6:571:TYR:CE1	2.42	0.47
11:A:730:PHE:CD1	11:A:730:PHE:N	2.82	0.47
15:F:223:TYR:C	15:F:225:LYS:H	2.23	0.47
17:H:27:ASP:OD1	17:H:27:ASP:N	2.48	0.47
20:l:129:PRO:HB2	33:m:56:ILE:HG23	1.97	0.47
34:o:33:ARG:NH1	35:p:1139:GLY:O	2.47	0.47
40:u:104:MET:HE1	40:u:106:CYS:HB2	1.96	0.47
42:w:12:VAL:HG13	42:w:55:VAL:CG1	2.45	0.47
4:3:44:LEU:HD21	4:3:162:LEU:CD1	2.45	0.47
9:8:167:ARG:HG2	9:8:167:ARG:NH2	2.30	0.47
11:A:397:LEU:HD21	15:f:361:LYS:HB3	1.97	0.47
15:F:424:GLN:O	15:F:428:LEU:HG	2.15	0.47
20:L:104:ARG:HA	20:L:104:ARG:HH21	1.79	0.47
21:O:3:TYR:HB3	21:O:5:LEU:HD13	1.96	0.47
14:e:717:LEU:HD22	14:e:726:LEU:HD11	1.97	0.47
15:f:149:PRO:HA	15:f:150:PRO:HD3	1.83	0.47
4:3:229:TRP:CH2	5:4:58:ARG:NH1	2.79	0.47
8:7:28:LEU:O	8:7:32:LEU:HD23	2.15	0.47
12:B:71:ARG:HD3	12:B:73:TYR:CE1	2.50	0.47
15:F:411:VAL:HG13	15:F:411:VAL:O	2.15	0.47
23:Q:321:SER:OG	23:Q:322:ASP:N	2.48	0.47
27:U:179:ARG:HA	27:U:182:GLU:HG2	1.96	0.47
28:V:225:VAL:HG13	28:V:226:ASP:OD2	2.15	0.47
15:f:58:MET:HE3	15:f:64:GLN:HA	1.97	0.47
34:o:466:LYS:O	35:p:1097:HIS:NE2	2.47	0.47
35:p:207:VAL:HG11	35:p:375:ALA:CB	2.45	0.47
35:p:993:LYS:NZ	35:p:995:GLU:OE1	2.44	0.47
37:r:83:VAL:O	37:r:87:LEU:HD23	2.15	0.47
7:6:703:PHE:N	7:6:708:GLU:OE1	2.42	0.46
15:F:215:GLU:O	15:F:254:GLN:NE2	2.39	0.46
24:R:128:ILE:HG23	24:R:183:VAL:CG1	2.44	0.46
33:m:67:GLU:O	33:m:71:LYS:HG2	2.14	0.46
35:p:724:TYR:HB3	35:p:728:MET:HE3	1.97	0.46
1:0:264:GLU:HG2	1:0:265:MET:N	2.30	0.46
5:4:404:THR:O	6:5:8:VAL:HG22	2.15	0.46
7:6:295:TYR:O	7:6:332:ARG:CA	2.63	0.46
10:9:11:TRP:CZ3	10:9:89:ARG:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:E:730:SER:OG	14:E:732:ASP:OD1	2.33	0.46
26:T:141:LEU:HD22	35:p:53:MET:SD	2.55	0.46
27:U:36:ILE:HG21	27:U:48:MET:CE	2.45	0.46
34:o:458:PHE:HE2	34:o:484:LEU:HD11	1.80	0.46
34:o:913:ASN:OD1	34:o:963:ARG:NH1	2.48	0.46
41:v:91:VAL:HG22	41:v:144:LEU:HD22	1.98	0.46
4:3:13:ILE:HG21	4:3:41:VAL:HG13	1.97	0.46
7:6:185:ILE:HG22	7:6:189:LEU:HD13	1.97	0.46
11:A:638:PRO:HB3	16:G:39:LEU:HD23	1.95	0.46
16:G:41:ASP:OD1	16:G:41:ASP:N	2.48	0.46
18:I:38:GLN:HA	18:I:41:GLU:HB2	1.98	0.46
27:U:14:LEU:HD13	27:U:197:VAL:HG22	1.96	0.46
27:U:140:GLU:OE1	27:U:140:GLU:N	2.48	0.46
28:V:86:LYS:HZ1	28:V:140:LYS:HD2	1.79	0.46
28:V:129:LYS:HA	28:V:129:LYS:HE3	1.97	0.46
14:e:238:GLN:O	14:e:242:PRO:HD2	2.16	0.46
15:f:327:TRP:O	15:f:330:ARG:HB2	2.16	0.46
40:u:29:LYS:O	40:u:32:THR:OG1	2.32	0.46
1:0:31:CYS:SG	1:0:34:CYS:HB2	2.55	0.46
7:6:54:ASP:HB2	7:6:58:ALA:CB	2.36	0.46
7:6:605:ILE:HD12	7:6:607:ILE:HD11	1.96	0.46
11:A:592:SER:OG	11:A:695:GLY:O	2.31	0.46
14:E:321:LEU:HB3	14:E:330:TRP:HB2	1.98	0.46
34:o:1200:PRO:HG2	34:o:1204:VAL:HG22	1.96	0.46
34:o:1203:ASP:OD2	34:o:1244:ASN:ND2	2.44	0.46
42:w:39:CYS:SG	42:w:42:CYS:HB3	2.56	0.46
3:2:175:THR:HA	8:7:591:GLY:O	2.16	0.46
4:3:53:ARG:HD2	5:4:46:ARG:HH12	1.81	0.46
6:5:32:LYS:HB2	12:B:540:LYS:O	2.16	0.46
7:6:493:TRP:CZ3	7:6:644:LEU:CD1	2.98	0.46
14:E:277:ASP:O	14:E:280:ARG:HG2	2.15	0.46
14:E:690:ASP:OD1	14:E:690:ASP:N	2.43	0.46
31:c:80:LEU:HB3	19:j:119:PHE:CZ	2.50	0.46
15:f:326:HIS:ND1	15:f:326:HIS:N	2.64	0.46
34:o:609:HIS:ND1	34:o:626:THR:HG23	2.31	0.46
34:o:1479:LYS:HG2	34:o:1482:TYR:OH	2.16	0.46
2:1:320:ARG:HH21	3:2:179:PRO:HA	1.81	0.46
7:6:656:ASN:OD1	7:6:657:ALA:N	2.49	0.46
9:8:64:LYS:NZ	10:9:117:GLU:OE2	2.43	0.46
13:D:871:THR:HG21	13:D:910:LEU:HD12	1.98	0.46
14:E:245:VAL:HG13	14:E:282:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:145:PHE:CD2	40:u:98:PHE:HZ	2.33	0.46
13:d:1084:LEU:HB3	18:i:99:ARG:HH21	1.81	0.46
8:7:361:LEU:O	8:7:365:VAL:HG12	2.16	0.46
14:E:646:SER:OG	14:E:647:ALA:N	2.49	0.46
15:F:418:ILE:H	15:F:418:ILE:CD1	2.26	0.46
20:L:106:ARG:NH1	20:L:115:ASP:OD2	2.48	0.46
24:R:44:ARG:HH11	35:p:1067:ILE:HD13	1.79	0.46
34:o:1165:THR:O	34:o:1166:LEU:C	2.57	0.46
35:p:553:LEU:HD23	35:p:556:ILE:HD11	1.98	0.46
36:q:72:PRO:HD3	43:x:13:ILE:HD11	1.98	0.46
1:0:27:GLY:HA3	1:0:70:LYS:CD	2.34	0.46
1:0:37:LEU:O	1:0:40:VAL:HG12	2.16	0.46
5:4:406:GLY:O	6:5:7:GLY:N	2.49	0.46
7:6:703:PHE:HA	7:6:708:GLU:HB2	1.97	0.46
8:7:137:LEU:O	8:7:142:VAL:HG11	2.15	0.46
12:B:559:LYS:HB2	12:B:559:LYS:NZ	2.31	0.46
28:V:96:PRO:HB3	28:V:136:LYS:HD2	1.98	0.46
34:o:340:LYS:HE2	34:o:1436:VAL:HG11	1.98	0.46
34:o:1344:MET:CE	38:s:137:ILE:CG2	2.94	0.46
45:z:22:CYS:SG	45:z:24:THR:OG1	2.69	0.46
3:2:382:CYS:HB3	3:2:385:CYS:HB3	1.96	0.46
9:8:177:TRP:CD1	9:8:215:GLY:H	2.34	0.46
10:9:218:LEU:HD11	10:9:232:LEU:HD21	1.98	0.46
24:R:39:LEU:HD11	34:o:425:ASP:HB2	1.98	0.46
24:R:178:LYS:HB3	26:T:155:PRO:HB2	1.98	0.46
25:S:127:PHE:CE2	26:T:21:VAL:HG21	2.51	0.46
26:T:31:TRP:HD1	26:T:62:LEU:HD21	1.81	0.46
14:e:281:VAL:HG11	14:e:297:MET:HB3	1.98	0.46
34:o:24:GLY:O	35:p:1168:ALA:HB3	2.16	0.46
34:o:1162:GLU:O	34:o:1300:GLY:HA3	2.16	0.46
3:2:87:LEU:HD13	3:2:228:TYR:HD2	1.80	0.46
7:6:306:ILE:HB	7:6:359:LYS:HA	1.96	0.46
8:7:460:THR:HB	8:7:661:ALA:HB1	1.98	0.46
10:9:171:LEU:O	10:9:175:LYS:HG3	2.15	0.46
10:9:255:MET:O	10:9:259:VAL:HG23	2.15	0.46
11:A:404:MET:O	11:A:408:LEU:HB2	2.16	0.46
11:A:475:LEU:HD23	11:A:480:TRP:HE1	1.81	0.46
12:B:184:ASN:ND2	12:B:184:ASN:N	2.62	0.46
28:V:97:LEU:O	28:V:137:TYR:HE1	1.99	0.46
14:e:519:GLU:O	14:e:519:GLU:HG3	2.16	0.46
37:r:70:ARG:NH2	40:u:88:VAL:HG22	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:u:110:ARG:HA	40:u:113:ILE:HD12	1.97	0.46
2:1:524:HIS:ND1	3:2:270:SER:OG	2.38	0.45
8:7:109:LEU:HD12	8:7:207:TYR:CD2	2.52	0.45
9:8:134:LEU:HD22	9:8:162:PHE:HB3	1.98	0.45
12:B:559:LYS:HB2	12:B:559:LYS:HZ3	1.80	0.45
17:H:132:LYS:HD2	17:H:132:LYS:HA	1.69	0.45
17:H:156:PRO:CA	17:H:160:ILE:HB	2.46	0.45
22:P:205:ARG:NH2	23:Q:376:TRP:CE2	2.85	0.45
27:U:179:ARG:HH21	27:U:183:GLN:HG3	1.81	0.45
27:U:181:ASN:O	27:U:185:GLU:HG3	2.16	0.45
15:f:405:SER:O	15:f:405:SER:OG	2.34	0.45
34:o:1261:ILE:HG22	34:o:1262:MET:N	2.30	0.45
35:p:128:ILE:CG2	35:p:431:LEU:HD21	2.45	0.45
1:0:21:LEU:HD21	1:0:29:THR:HG23	1.98	0.45
1:0:32:GLU:OE1	1:0:32:GLU:N	2.46	0.45
2:1:472:LEU:HD12	2:1:476:TRP:CD1	2.51	0.45
4:3:201:GLY:O	4:3:204:GLN:HG2	2.17	0.45
5:4:401:LEU:HG	6:5:53:LEU:HD23	1.97	0.45
9:8:11:ARG:HH11	9:8:33:ASN:HD22	1.64	0.45
10:9:96:VAL:HG13	10:9:101:PRO:HG3	1.98	0.45
10:9:256:ARG:O	10:9:260:LYS:HG3	2.17	0.45
12:B:568:VAL:HG22	12:B:628:ILE:HG23	1.98	0.45
15:F:47:ILE:HD13	18:I:19:MET:HE1	1.96	0.45
21:O:64:THR:HG22	21:O:65:TYR:N	2.31	0.45
26:T:30:GLN:O	26:T:62:LEU:HD11	2.16	0.45
27:U:112:ARG:O	27:U:115:GLU:HG2	2.16	0.45
28:V:176:PRO:C	28:V:178:SER:H	2.24	0.45
15:f:326:HIS:O	15:f:330:ARG:HG2	2.15	0.45
35:p:596:ILE:O	35:p:596:ILE:HG22	2.15	0.45
35:p:694:THR:HG22	35:p:695:HIS:ND1	2.31	0.45
35:p:809:VAL:HG11	35:p:811:TYR:CZ	2.51	0.45
4:3:98:ASP:HB3	5:4:125:GLY:O	2.15	0.45
5:4:52:ALA:HB1	5:4:90:LEU:HD21	1.99	0.45
7:6:54:ASP:CB	7:6:58:ALA:HB3	2.36	0.45
8:7:107:LEU:HD12	8:7:195:ALA:HB1	1.98	0.45
10:9:186:ILE:H	10:9:186:ILE:HD12	1.79	0.45
11:A:1063:LYS:HD3	11:A:1063:LYS:O	2.16	0.45
22:P:227:GLU:OE1	22:P:318:ARG:NH2	2.46	0.45
27:U:54:PHE:CE1	28:V:195:PRO:HG3	2.52	0.45
40:u:153:ASP:OD1	40:u:154:LYS:N	2.50	0.45
42:w:58:ILE:HD12	42:w:58:ILE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:w:69:ILE:O	42:w:72:VAL:HG22	2.15	0.45
45:z:32:ASP:OD1	45:z:32:ASP:N	2.50	0.45
3:2:242:SER:N	3:2:245:SER:OG	2.50	0.45
8:7:600:ALA:HB1	8:7:659:HIS:HD2	1.82	0.45
14:E:327:ASN:HD22	14:E:327:ASN:N	2.07	0.45
15:F:47:ILE:HD11	18:I:43:ALA:HB2	1.98	0.45
34:o:910:LYS:N	34:o:911:PRO:HD2	2.32	0.45
34:o:1483:GLY:HA2	39:t:80:MET:HE2	1.93	0.45
44:y:105:PHE:CD2	44:y:109:ILE:HD11	2.51	0.45
3:2:199:ILE:CG2	3:2:222:ILE:HD11	2.47	0.45
5:4:336:TYR:CD2	7:6:61:TYR:CE2	3.04	0.45
10:9:218:LEU:HB2	10:9:252:MET:HE1	1.99	0.45
14:E:327:ASN:H	14:E:327:ASN:ND2	2.05	0.45
34:o:400:ASP:OD1	34:o:401:ARG:N	2.49	0.45
35:p:908:MET:HE2	45:z:43:ILE:HG23	1.98	0.45
40:u:90:THR:OG1	40:u:91:GLN:OE1	2.11	0.45
1:0:1:MET:SD	8:7:345:ARG:HD2	2.57	0.45
2:1:400:ILE:H	2:1:400:ILE:HD12	1.82	0.45
26:T:220:ILE:HG13	26:T:221:GLY:H	1.82	0.45
10:9:7:GLN:HG3	10:9:89:ARG:HH21	1.81	0.45
16:G:129:LYS:HA	16:G:129:LYS:HD2	1.77	0.45
27:U:76:MET:CG	27:U:88:ARG:HB3	2.46	0.45
36:q:245:VAL:HG11	44:y:105:PHE:CZ	2.52	0.45
1:0:42:GLY:O	40:u:164:MET:CB	2.65	0.45
9:8:34:THR:O	9:8:34:THR:HG22	2.17	0.45
11:A:857:MET:HE3	11:A:858:ASP:H	1.81	0.45
27:U:69:ASP:OD1	27:U:69:ASP:N	2.39	0.45
27:U:112:ARG:HA	27:U:115:GLU:OE2	2.16	0.45
14:e:703:MET:HE2	14:e:703:MET:HB3	1.83	0.45
34:o:68:THR:HG23	34:o:68:THR:O	2.16	0.45
37:r:17:ALA:HB1	37:r:95:PHE:CE2	2.52	0.45
39:t:78:PRO:CD	40:u:18:PHE:HB2	2.44	0.45
3:2:112:LYS:N	3:2:142:GLU:O	2.41	0.45
4:3:242:ILE:CD1	5:4:75:VAL:N	2.80	0.45
10:9:266:ARG:HB2	10:9:269:GLU:HB3	1.98	0.45
11:A:1182:CYS:O	11:A:1182:CYS:SG	2.75	0.45
12:B:217:ASN:ND2	12:B:320:ALA:O	2.35	0.45
14:E:250:GLU:O	14:E:254:ASN:ND2	2.50	0.45
14:E:731:MET:HE3	14:E:731:MET:HB3	1.91	0.45
15:f:223:TYR:CD2	15:f:255:MET:HE1	2.52	0.45
34:o:1034:GLN:HE22	34:o:1038:THR:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:389:GLY:HA3	35:p:668:LEU:HG	1.99	0.45
37:r:91:LYS:C	37:r:92:LEU:HD22	2.42	0.45
2:1:457:ILE:HG22	2:1:461:LEU:HD13	1.98	0.45
7:6:546:PHE:HB2	7:6:701:LEU:HD11	1.99	0.45
10:9:102:ARG:HG3	10:9:103:ILE:HD12	1.99	0.45
22:P:239:ARG:HD3	23:Q:317:GLU:OE2	2.17	0.45
28:V:130:ILE:HD12	28:V:140:LYS:HG3	1.99	0.45
15:f:317:LEU:HD12	15:f:329:LEU:HD23	1.98	0.45
36:q:65:ALA:O	45:z:57:ALA:HB1	2.17	0.45
8:7:613:HIS:ND1	8:7:613:HIS:O	2.50	0.44
9:8:189:MET:HE2	9:8:189:MET:HB2	1.75	0.44
11:A:690:LEU:HD22	11:A:747:LEU:HD22	1.99	0.44
11:A:1053:PHE:HB2	11:A:1057:GLU:HB2	1.99	0.44
13:D:947:PHE:HE1	14:E:527:ILE:HD12	1.82	0.44
13:D:1007:THR:HG21	21:O:98:CYS:SG	2.57	0.44
15:F:328:ALA:O	15:F:332:PHE:N	2.50	0.44
14:e:245:VAL:HG12	14:e:282:LEU:HD11	1.99	0.44
14:e:268:HIS:O	14:e:268:HIS:CG	2.70	0.44
20:l:113:VAL:O	20:l:113:VAL:HG22	2.18	0.44
4:3:108:ASN:OD1	5:4:123:LEU:CD1	2.51	0.44
13:D:1080:TYR:OH	14:E:606:ASP:OD2	2.30	0.44
14:E:650:THR:HG22	14:E:666:THR:HG22	2.00	0.44
15:F:218:VAL:CA	17:H:164:THR:HB	2.48	0.44
15:F:221:GLN:O	15:F:224:TYR:HB3	2.17	0.44
15:F:361:LYS:HA	15:F:364:VAL:HG22	1.99	0.44
17:H:178:LYS:HA	17:H:178:LYS:HD3	1.82	0.44
17:H:186:VAL:HG21	15:f:220:GLN:HB3	1.97	0.44
19:J:124:GLU:O	19:J:125:ASP:HB3	2.17	0.44
13:d:860:VAL:HA	33:m:47:GLN:HG2	1.98	0.44
14:e:718:ARG:HA	14:e:718:ARG:HD3	1.76	0.44
34:o:1480:CYS:C	34:o:1482:TYR:H	2.23	0.44
35:p:710:ILE:HA	35:p:764:MET:HE2	1.99	0.44
1:0:97:ASP:O	1:0:101:GLU:OE1	2.36	0.44
5:4:325:ILE:H	5:4:325:ILE:HD12	1.82	0.44
13:D:1002:ARG:HH22	26:T:182:HIS:CG	2.18	0.44
15:F:426:LEU:C	15:F:426:LEU:HD23	2.42	0.44
22:P:251:LEU:HD21	23:Q:312:GLU:OE2	2.18	0.44
27:U:12:ALA:O	27:U:16:ARG:HG2	2.18	0.44
15:f:26:MET:HE3	15:f:26:MET:HB3	1.77	0.44
15:f:83:LEU:HD22	18:i:41:GLU:HG2	1.99	0.44
7:6:311:LYS:HZ1	7:6:383:THR:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:1011:ALA:HA	23:Q:330:ASP:OD2	2.17	0.44
15:f:105:TYR:O	19:j:217:PHE:N	2.51	0.44
18:i:16:ALA:HB2	18:i:40:LEU:HD11	2.00	0.44
35:p:218:THR:HG23	35:p:218:THR:O	2.18	0.44
35:p:1040:GLN:HG2	36:q:203:TRP:CZ2	2.53	0.44
1:0:85:ARG:CZ	1:0:140:LEU:HG	2.38	0.44
1:0:249:GLN:HA	1:0:250:PRO:HD3	1.85	0.44
4:3:235:GLN:O	4:3:235:GLN:NE2	2.47	0.44
5:4:438:LYS:CE	12:B:621:ALA:CB	2.86	0.44
15:F:218:VAL:CB	17:H:164:THR:HB	2.48	0.44
23:Q:22:ILE:HG22	23:Q:39:LEU:HD11	1.99	0.44
24:R:52:TRP:NE1	35:p:841:ARG:HG2	2.33	0.44
29:X:-23:DG:H2''	29:X:-22:DG:C8	2.52	0.44
34:o:495:ASP:C	34:o:495:ASP:OD1	2.60	0.44
34:o:769:MET:SD	35:p:973:PRO:HG3	2.57	0.44
34:o:1341:VAL:HG23	34:o:1341:VAL:O	2.17	0.44
6:5:9:LEU:HD11	6:5:42:HIS:HD2	1.83	0.44
8:7:329:PHE:O	8:7:333:LEU:HD23	2.17	0.44
9:8:224:ARG:HA	9:8:227:GLU:HG2	1.99	0.44
15:F:312:ILE:HG13	15:F:334:ALA:HB1	2.00	0.44
17:H:59:GLU:HA	17:H:62:THR:HG22	1.99	0.44
27:U:53:LYS:O	28:V:199:LYS:HE2	2.18	0.44
28:V:168:LEU:O	28:V:172:GLU:HG2	2.16	0.44
28:V:214:GLU:HA	28:V:217:GLN:HB3	1.99	0.44
13:d:871:THR:O	20:l:62:LYS:NZ	2.42	0.44
14:e:525:GLU:CD	14:e:525:GLU:N	2.76	0.44
14:e:542:HIS:CE1	14:e:568:ARG:HG3	2.53	0.44
34:o:495:ASP:OD1	34:o:497:ASP:OD1	2.36	0.44
34:o:893:GLU:OE1	38:s:197:SER:OG	2.34	0.44
34:o:1165:THR:HG23	34:o:1167:ARG:HB3	2.00	0.44
1:0:6:CYS:O	1:0:10:LYS:HE3	2.17	0.44
1:0:44:GLY:O	1:0:53:LEU:N	2.50	0.44
7:6:99:PHE:CZ	7:6:103:ILE:HD13	2.52	0.44
8:7:434:HIS:CB	8:7:632:ILE:HD11	2.48	0.44
8:7:475:PRO:HG3	8:7:478:MET:HE2	1.99	0.44
11:A:400:GLU:HG3	11:A:401:ASN:N	2.32	0.44
11:A:604:PRO:O	11:A:889:TYR:OH	2.34	0.44
12:B:328:ASN:HA	17:H:227:LEU:HD21	2.00	0.44
14:E:518:LYS:C	14:E:520:SER:H	2.25	0.44
24:R:27:TYR:HB3	24:R:52:TRP:CZ2	2.53	0.44
31:c:101:VAL:HG22	15:f:127:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:554:ASP:OD1	14:e:554:ASP:N	2.45	0.44
15:f:11:ASN:OD1	15:f:48:LYS:NZ	2.51	0.44
34:o:1171:ALA:N	34:o:1215:GLU:O	2.47	0.44
38:s:159:LEU:HD12	38:s:163:TYR:CD2	2.53	0.44
40:u:145:LEU:H	40:u:145:LEU:HD23	1.82	0.44
44:y:37:LYS:N	44:y:69:HIS:O	2.49	0.44
7:6:133:THR:HB	7:6:160:THR:HG21	2.00	0.44
7:6:610:VAL:HG22	7:6:615:PHE:CE1	2.53	0.44
10:9:163:PRO:HA	10:9:166:PRO:HG2	1.99	0.44
10:9:235:SER:O	10:9:236:LEU:HD12	2.18	0.44
12:B:766:LEU:HA	12:B:807:THR:HG21	2.00	0.44
24:R:245:VAL:HG23	24:R:245:VAL:O	2.17	0.44
28:V:78:LEU:O	28:V:82:VAL:HG23	2.18	0.44
29:X:-40:DA:H61	30:Y:40:DT:H3	1.65	0.44
31:c:24:ASP:CB	19:j:192:LYS:HD2	2.48	0.44
14:e:258:ASN:OD1	14:e:258:ASN:N	2.39	0.44
37:r:107:THR:HG23	37:r:110:GLU:H	1.83	0.44
3:2:87:LEU:HD23	3:2:87:LEU:O	2.18	0.44
10:9:218:LEU:CD1	10:9:252:MET:HE1	2.48	0.44
12:B:925:LYS:HD3	12:B:925:LYS:HA	1.78	0.44
14:E:377:LEU:HD21	14:E:422:PRO:HG2	2.00	0.44
15:F:370:TRP:CZ3	15:F:420:ALA:HA	2.53	0.44
21:O:48:LEU:HG	23:Q:366:ILE:HD11	2.00	0.44
26:T:94:THR:HG22	26:T:109:ILE:HG22	2.00	0.44
14:e:525:GLU:N	14:e:525:GLU:OE1	2.41	0.44
33:m:87:VAL:HG13	33:m:97:PHE:HE1	1.83	0.44
34:o:105:LYS:HD2	34:o:141:LEU:HD22	2.00	0.44
34:o:348:GLY:O	34:o:352:GLY:N	2.46	0.44
34:o:502:ASN:HB3	35:p:1084:LEU:HD13	2.00	0.44
34:o:1213:ARG:NH2	34:o:1215:GLU:OE2	2.51	0.44
35:p:37:LYS:O	35:p:41:ARG:HB2	2.18	0.44
42:w:104:ALA:O	42:w:105:GLU:HG2	2.18	0.44
1:0:246:TYR:CD1	9:8:119:LEU:HD21	2.53	0.43
3:2:369:VAL:HG13	3:2:370:ASP:N	2.32	0.43
5:4:157:GLU:O	5:4:161:HIS:ND1	2.51	0.43
5:4:288:ILE:H	5:4:288:ILE:HD12	1.83	0.43
7:6:615:PHE:HD2	7:6:617:LEU:HD21	1.82	0.43
10:9:185:GLU:O	10:9:188:ARG:HB3	2.18	0.43
11:A:401:ASN:HD22	11:A:401:ASN:N	2.14	0.43
15:F:218:VAL:HA	17:H:164:THR:HB	2.00	0.43
34:o:1366:PHE:HB2	34:o:1374:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:p:544:PHE:CE1	35:p:590:LEU:HD11	2.53	0.43
35:p:854:ILE:O	35:p:907:VAL:HG21	2.18	0.43
37:r:17:ALA:HB1	37:r:95:PHE:HE2	1.83	0.43
40:u:117:MET:HE3	40:u:137:ILE:HD13	1.99	0.43
7:6:408:SER:HB3	7:6:413:LEU:HD11	2.00	0.43
8:7:249:VAL:HG21	8:7:403:PHE:HB2	2.00	0.43
8:7:285:TYR:O	8:7:289:VAL:HG23	2.17	0.43
13:D:933:ARG:HD2	19:J:117:VAL:HG11	2.00	0.43
19:J:192:LYS:N	19:J:192:LYS:CE	2.66	0.43
34:o:273:GLN:HB3	34:o:277:THR:HG21	2.00	0.43
35:p:719:SER:OG	35:p:720:PRO:HD3	2.18	0.43
14:E:249:LEU:HD21	14:E:282:LEU:HD22	2.00	0.43
14:E:369:LYS:HA	14:E:369:LYS:HD3	1.74	0.43
15:F:270:ASN:HD22	15:F:270:ASN:HA	1.61	0.43
15:F:400:GLY:O	15:F:404:ARG:HG2	2.18	0.43
15:F:402:ARG:O	15:F:406:VAL:HG13	2.19	0.43
27:U:141:ALA:O	27:U:145:PHE:HB2	2.18	0.43
27:U:172:ASP:OD1	27:U:172:ASP:N	2.51	0.43
28:V:229:ASP:HA	28:V:232:LYS:HE2	1.99	0.43
28:V:231:GLU:OE1	28:V:231:GLU:HA	2.18	0.43
34:o:72:GLN:OE1	34:o:72:GLN:N	2.50	0.43
34:o:622:SER:OG	34:o:626:THR:HG22	2.17	0.43
34:o:786:ALA:O	34:o:787:VAL:HG23	2.19	0.43
35:p:529:MET:HE2	35:p:702:MET:HG3	2.00	0.43
1:0:64:GLU:OE1	8:7:345:ARG:NH2	2.51	0.43
7:6:308:ILE:HG22	7:6:358:ARG:CB	2.47	0.43
8:7:332:PHE:CZ	8:7:367:ILE:HG23	2.53	0.43
10:9:11:TRP:HE1	10:9:157:HIS:HD2	1.66	0.43
11:A:340:GLU:H	11:A:497:PRO:HG2	1.84	0.43
12:B:639:LYS:NZ	12:B:641:GLU:OE2	2.42	0.43
17:H:156:PRO:CB	17:H:160:ILE:HB	2.47	0.43
26:T:48:THR:OG1	26:T:51:ARG:O	2.33	0.43
27:U:104:LYS:HE3	27:U:191:LEU:HB2	2.01	0.43
29:X:-7:DC:H2"	29:X:-6:DG:C8	2.53	0.43
31:c:21:LEU:HD11	31:c:23:TRP:CD1	2.54	0.43
14:e:777:SER:O	14:e:777:SER:OG	2.34	0.43
34:o:1443:ALA:HB2	35:p:1167:ILE:HG23	2.01	0.43
35:p:761:THR:H	35:p:764:MET:HE3	1.82	0.43
38:s:71:GLN:HB2	38:s:99:ILE:HD12	1.99	0.43
1:0:85:ARG:HH12	1:0:140:LEU:H	1.66	0.43
7:6:133:THR:HG23	7:6:134:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:27:ASN:ND2	10:9:97:MET:HE1	2.34	0.43
12:B:594:SER:OG	12:B:595:LYS:N	2.52	0.43
12:B:653:LEU:HG	12:B:684:ILE:HG13	1.99	0.43
12:B:839:MET:HE1	12:B:843:LEU:HD13	2.00	0.43
14:E:476:VAL:HB	14:E:782:HIS:HB2	2.00	0.43
15:F:6:LYS:HE2	15:F:8:LYS:HG3	2.01	0.43
26:T:194:HIS:ND1	26:T:196:TYR:O	2.49	0.43
29:X:24:DA:H61	30:Y:-24:DT:H3	1.67	0.43
18:i:45:ARG:HG3	19:j:212:LYS:HB3	2.00	0.43
5:4:336:TYR:HD2	7:6:61:TYR:CE2	2.35	0.43
7:6:305:ASP:CB	7:6:359:LYS:HZ2	2.32	0.43
7:6:532:LEU:HD23	7:6:532:LEU:O	2.19	0.43
9:8:100:VAL:HG23	9:8:310:PRO:HG3	2.01	0.43
10:9:195:LEU:O	10:9:198:ILE:HG22	2.18	0.43
11:A:899:LYS:HE3	11:A:899:LYS:HB2	1.81	0.43
12:B:414:LEU:HB2	12:B:523:VAL:HG13	2.00	0.43
13:D:891:ILE:HG21	20:L:111:LEU:HB2	2.01	0.43
14:E:784:HIS:HB3	14:E:792:LEU:HB2	1.99	0.43
15:F:283:MET:HE1	15:F:308:VAL:HG12	2.00	0.43
16:G:181:TRP:O	16:G:181:TRP:CD2	2.72	0.43
24:R:25:GLU:OE1	24:R:46:ILE:HD12	2.18	0.43
14:e:447:THR:O	14:e:450:ARG:HB2	2.19	0.43
34:o:514:GLU:OE1	35:p:1101:GLN:HB2	2.19	0.43
34:o:1007:ILE:HD12	34:o:1007:ILE:HA	1.89	0.43
35:p:871:VAL:O	35:p:871:VAL:HG13	2.18	0.43
36:q:235:SER:OG	36:q:239:LEU:O	2.32	0.43
38:s:106:VAL:HG12	38:s:107:GLN:N	2.34	0.43
8:7:168:VAL:O	8:7:168:VAL:HG13	2.19	0.43
18:I:23:LEU:HD22	18:I:28:ILE:HD12	2.01	0.43
23:Q:18:ILE:HD11	23:Q:46:TRP:CH2	2.54	0.43
27:U:145:PHE:CD2	27:U:146:ASP:N	2.78	0.43
28:V:165:GLY:HA2	28:V:169:GLU:OE1	2.18	0.43
34:o:97:VAL:HG21	34:o:322:LEU:HD22	1.99	0.43
34:o:872:MET:O	34:o:879:VAL:HA	2.18	0.43
35:p:905:ASP:OD1	35:p:924:ARG:NH1	2.49	0.43
5:4:380:THR:HG23	5:4:380:THR:O	2.18	0.43
7:6:650:MET:SD	7:6:656:ASN:ND2	2.82	0.43
14:E:351:GLN:HG2	14:E:355:MET:HE2	2.01	0.43
26:T:58:LEU:CD1	26:T:62:LEU:HD23	2.49	0.43
28:V:184:ALA:O	28:V:189:ILE:HG23	2.19	0.43
14:e:436:ASP:N	14:e:436:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:t:78:PRO:HG2	40:u:19:GLY:CA	2.49	0.43
8:7:67:VAL:HG23	8:7:67:VAL:O	2.19	0.43
8:7:109:LEU:HD11	8:7:199:ILE:HD11	2.01	0.43
11:A:1165:LEU:HD22	11:A:1165:LEU:HA	1.88	0.43
14:E:280:ARG:HE	14:E:280:ARG:HB3	1.50	0.43
15:F:50:ILE:O	15:F:54:ALA:N	2.47	0.43
15:F:240:ALA:HA	15:F:243:LEU:HB2	1.99	0.43
18:I:21:GLN:HE22	18:I:24:LYS:HE2	1.84	0.43
28:V:109:LEU:HD23	28:V:109:LEU:H	1.84	0.43
34:o:428:ASP:OD2	34:o:430:ARG:NH1	2.51	0.43
38:s:94:MET:HE1	38:s:127:LEU:HD11	2.00	0.43
1:0:85:ARG:NH2	1:0:139:LYS:HB3	2.34	0.43
5:4:54:ASN:O	5:4:58:ARG:HG3	2.19	0.43
7:6:329:GLY:H	7:6:334:ARG:HD3	1.84	0.43
9:8:132:TRP:HD1	10:9:1:MET:HE3	1.82	0.43
9:8:174:VAL:CG1	9:8:179:ARG:HG3	2.48	0.43
11:A:470:ILE:O	15:f:299:LYS:NZ	2.49	0.43
12:B:496:MET:HE3	12:B:496:MET:HB2	1.84	0.43
13:D:963:ARG:HH11	13:D:983:ARG:HE	1.66	0.43
15:F:227:ILE:CD1	15:F:242:ALA:HA	2.49	0.43
20:L:122:ARG:HA	20:L:122:ARG:HD2	1.87	0.43
27:U:167:ALA:HB3	27:U:170:LYS:HZ2	1.84	0.43
31:c:66:VAL:HG21	19:j:151:ILE:HG23	2.01	0.43
31:c:124:ILE:HD11	15:f:133:ALA:HB1	2.00	0.43
35:p:1162:LEU:HB3	35:p:1167:ILE:HB	2.00	0.43
4:3:257:CYS:HB2	4:3:258:HIS:CD2	2.54	0.42
6:5:14:PRO:O	7:6:520:ARG:NH2	2.44	0.42
7:6:327:MET:HB2	7:6:338:ILE:HD11	1.99	0.42
8:7:354:PRO:HB2	8:7:355:PRO:HD3	2.00	0.42
9:8:79:ASP:HB3	9:8:90:VAL:HB	2.00	0.42
9:8:83:HIS:ND1	9:8:84:LYS:N	2.67	0.42
11:A:463:PRO:CB	15:F:221:GLN:HB3	2.49	0.42
11:A:1052:ARG:O	11:A:1052:ARG:CG	2.67	0.42
12:B:216:SER:OG	12:B:217:ASN:N	2.52	0.42
14:E:790:LEU:HD13	17:H:146:ILE:HG12	2.01	0.42
15:F:401:GLU:C	15:F:401:GLU:CD	2.87	0.42
27:U:145:PHE:CE1	40:u:107:PHE:HE1	2.37	0.42
32:k:179:MET:HB3	32:k:180:PRO:CD	2.49	0.42
34:o:154:CYS:SG	34:o:155:GLU:N	2.92	0.42
34:o:1239:PHE:HZ	34:o:1291:ASN:HD21	1.67	0.42
1:0:23:VAL:HG12	1:0:59:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:308:ASN:ND2	8:7:576:GLU:OE2	2.49	0.42
4:3:98:ASP:O	4:3:99:GLY:C	2.62	0.42
4:3:229:TRP:CZ3	5:4:58:ARG:CD	3.03	0.42
5:4:403:PHE:HA	6:5:8:VAL:HG13	2.01	0.42
7:6:193:VAL:HG11	7:6:283:ARG:CD	2.49	0.42
9:8:239:ASP:O	9:8:239:ASP:CG	2.62	0.42
11:A:727:THR:HG23	11:A:727:THR:O	2.19	0.42
20:L:120:LEU:O	20:L:125:ASN:N	2.52	0.42
24:R:195:PHE:CZ	24:R:199:LEU:HD11	2.55	0.42
25:S:50:ASP:OD1	25:S:53:ASN:ND2	2.52	0.42
27:U:44:LYS:HB2	27:U:47:ASP:OD1	2.19	0.42
35:p:1128:ALA:HB1	35:p:1135:TYR:HD1	1.84	0.42
1:0:116:ASP:OD1	1:0:117:ASN:N	2.51	0.42
1:0:305:PHE:N	1:0:305:PHE:CD1	2.85	0.42
2:1:303:ILE:HG22	2:1:307:PHE:CE2	2.54	0.42
5:4:70:ALA:HB1	5:4:74:TRP:CZ2	2.54	0.42
7:6:532:LEU:CD2	7:6:716:VAL:HG13	2.49	0.42
8:7:661:ALA:HA	8:7:664:VAL:HG12	2.02	0.42
9:8:94:MET:SD	9:8:146:ASP:HB3	2.59	0.42
10:9:218:LEU:HD12	10:9:252:MET:CE	2.49	0.42
10:9:218:LEU:CD2	10:9:228:MET:HE2	2.50	0.42
13:D:1071:ARG:HH22	18:I:82:SER:HA	1.83	0.42
14:E:521:ASP:OD1	14:E:521:ASP:N	2.53	0.42
17:H:154:PRO:HB2	17:H:158:THR:OG1	2.18	0.42
28:V:111:ILE:O	28:V:114:LYS:N	2.51	0.42
28:V:228:MET:O	28:V:232:LYS:HG3	2.20	0.42
15:f:447:ALA:CB	15:f:456:GLY:HA3	2.49	0.42
34:o:608:THR:HG23	34:o:771:VAL:HG13	2.00	0.42
4:3:175:MET:HE3	4:3:179:ASN:ND2	2.35	0.42
4:3:242:ILE:CD1	5:4:74:TRP:C	2.91	0.42
9:8:64:LYS:HD2	10:9:115:VAL:HG13	2.01	0.42
10:9:7:GLN:HE21	10:9:85:MET:HE2	1.84	0.42
10:9:181:LEU:HD21	10:9:187:LEU:CD1	2.49	0.42
11:A:639:LEU:O	11:A:639:LEU:CD1	2.67	0.42
15:F:324:ASP:CG	15:F:327:TRP:HD1	2.28	0.42
15:F:410:PRO:O	15:F:411:VAL:C	2.63	0.42
27:U:14:LEU:HD12	27:U:194:THR:HA	2.02	0.42
33:m:91:ARG:HG2	33:m:92:LYS:N	2.34	0.42
34:o:706:ILE:O	34:o:710:LYS:HG2	2.19	0.42
1:0:68:VAL:HG11	8:7:338:GLU:HG2	2.00	0.42
7:6:184:VAL:HG13	7:6:185:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:49:THR:HG23	8:7:50:VAL:N	2.34	0.42
10:9:71:PHE:CG	10:9:75:MET:HE3	2.55	0.42
14:E:613:ALA:HB3	14:E:616:HIS:HD2	1.83	0.42
14:e:513:LEU:CD2	14:e:527:ILE:HG23	2.49	0.42
14:e:667:GLY:O	14:e:692:ARG:NH2	2.52	0.42
34:o:1382:LEU:O	34:o:1385:VAL:HG22	2.18	0.42
41:v:136:GLU:O	41:v:139:SER:OG	2.31	0.42
2:1:374:LEU:HD12	2:1:374:LEU:C	2.45	0.42
7:6:559:ILE:HG22	7:6:561:PHE:CE1	2.55	0.42
7:6:703:PHE:CZ	7:6:712:LEU:HD12	2.55	0.42
9:8:231:THR:HG23	9:8:252:PHE:H	1.83	0.42
11:A:639:LEU:O	11:A:639:LEU:HD13	2.20	0.42
19:J:123:LEU:HD12	19:J:123:LEU:HA	1.73	0.42
15:f:428:LEU:HD13	15:f:458:LEU:CB	2.50	0.42
15:f:432:ALA:HB1	15:f:462:GLN:CB	2.49	0.42
34:o:875:TYR:HE2	34:o:1470:CYS:HG	1.67	0.42
35:p:1107:LEU:HD23	35:p:1107:LEU:HA	1.92	0.42
42:w:41:ASN:OD1	42:w:41:ASN:C	2.63	0.42
2:1:524:HIS:NE2	2:1:528:MET:SD	2.93	0.42
9:8:110:THR:OG1	9:8:113:HIS:ND1	2.33	0.42
9:8:182:GLU:HG2	9:8:183:LEU:N	2.33	0.42
14:E:466:PHE:HB2	14:E:796:ALA:HA	2.00	0.42
15:F:312:ILE:HG22	15:F:313:VAL:CG1	2.49	0.42
26:T:31:TRP:CD1	26:T:62:LEU:HD21	2.55	0.42
27:U:145:PHE:HE1	40:u:107:PHE:HE1	1.66	0.42
28:V:99:LEU:HD23	28:V:114:LYS:HZ2	1.83	0.42
28:V:187:ASP:HB2	28:V:189:ILE:HG22	2.02	0.42
14:e:332:ILE:HA	14:e:336:HIS:HD2	1.84	0.42
14:e:378:LYS:HZ3	14:e:378:LYS:HG2	1.61	0.42
32:k:179:MET:HB3	32:k:180:PRO:HD2	2.00	0.42
34:o:1287:CYS:HA	35:p:247:ALA:O	2.19	0.42
35:p:239:MET:HB2	35:p:372:LEU:HD21	2.01	0.42
35:p:565:THR:HG21	35:p:580:PRO:HG3	2.01	0.42
35:p:933:ASP:OD2	35:p:1050:ARG:NH2	2.51	0.42
36:q:190:ASN:ND2	36:q:195:THR:O	2.39	0.42
37:r:58:SER:OG	40:u:35:GLU:OE2	2.35	0.42
38:s:13:ILE:HD12	38:s:13:ILE:H	1.84	0.42
1:0:55:LYS:HG2	37:r:113:ALA:HB2	2.02	0.42
5:4:261:PHE:CZ	5:4:265:LEU:HD21	2.54	0.42
10:9:200:LEU:HD23	10:9:200:LEU:HA	1.83	0.42
15:F:68:THR:OG1	18:I:32:GLU:OE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:F:231:CYS:HB3	15:F:285:MET:HE2	2.02	0.42
15:F:396:LEU:HA	15:F:399:GLU:OE1	2.20	0.42
31:c:94:HIS:CD2	15:f:122:LEU:HD22	2.55	0.42
15:f:317:LEU:HG	15:f:330:ARG:HE	1.83	0.42
32:k:165:VAL:O	32:k:169:ALA:N	2.47	0.42
34:o:89:GLU:O	34:o:287:ASN:ND2	2.45	0.42
34:o:827:TYR:HH	34:o:839:HIS:CE1	2.36	0.42
2:1:496:ASN:HB3	2:1:536:LEU:HD11	2.01	0.42
4:3:53:ARG:HG3	5:4:46:ARG:CZ	2.49	0.42
5:4:336:TYR:CD2	7:6:61:TYR:HE2	2.37	0.42
5:4:413:LEU:O	5:4:439:ARG:NE	2.53	0.42
7:6:295:TYR:O	7:6:332:ARG:HA	2.20	0.42
10:9:198:ILE:HD11	10:9:255:MET:HG2	2.01	0.42
11:A:825:ILE:HD12	11:A:830:ILE:HD11	2.01	0.42
14:E:265:GLU:OE1	14:E:265:GLU:HA	2.20	0.42
14:E:508:LYS:HB3	14:E:512:ASP:HB2	2.02	0.42
27:U:188:TYR:O	27:U:191:LEU:HG	2.19	0.42
14:e:225:ILE:HD12	14:e:236:LEU:HB3	2.02	0.42
34:o:567:LEU:HB2	34:o:570:TRP:HB2	2.01	0.42
34:o:597:PRO:HD3	34:o:668:PHE:CD1	2.54	0.42
7:6:295:TYR:O	7:6:332:ARG:HB3	2.20	0.42
8:7:524:LEU:HD22	8:7:561:ILE:HD13	2.01	0.42
10:9:28:ARG:O	10:9:29:LYS:C	2.61	0.42
12:B:176:HIS:HE1	12:B:310:ASP:H	1.68	0.42
12:B:882:HIS:CE1	17:H:216:ALA:HB1	2.54	0.42
15:F:350:ASN:OD1	15:F:350:ASN:N	2.51	0.42
27:U:154:CYS:HB3	27:U:157:CYS:O	2.19	0.42
30:Y:-18:DC:H2'	30:Y:-17:DG:C8	2.55	0.42
34:o:106:VAL:O	34:o:110:VAL:HG12	2.19	0.42
34:o:823:VAL:HG22	34:o:835:GLU:HB3	2.02	0.42
34:o:1030:SER:OG	38:s:162:ARG:NE	2.47	0.42
35:p:573:TRP:NE1	35:p:575:GLY:O	2.51	0.42
4:3:208:ASP:OD2	4:3:251:TYR:OH	2.38	0.41
7:6:370:SER:HB2	7:6:614:SER:CB	2.46	0.41
8:7:111:SER:N	8:7:211:TYR:OH	2.52	0.41
9:8:64:LYS:HG3	10:9:159:ILE:HD11	2.01	0.41
9:8:143:LEU:HD22	9:8:151:LEU:HD21	2.02	0.41
11:A:464:TRP:CD1	11:A:464:TRP:C	2.96	0.41
14:E:476:VAL:HG11	14:E:794:ALA:HB3	2.02	0.41
20:L:113:VAL:C	20:L:115:ASP:N	2.75	0.41
20:L:120:LEU:HD23	20:L:128:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:15:VAL:HG12	25:S:16:VAL:N	2.34	0.41
27:U:188:TYR:O	27:U:192:ARG:HG2	2.19	0.41
28:V:90:GLN:HE22	28:V:176:PRO:HG3	1.84	0.41
15:f:55:LEU:HD13	18:i:28:ILE:HG12	2.01	0.41
15:f:320:ARG:HH11	15:f:320:ARG:HB2	1.83	0.41
34:o:1234:LYS:NZ	34:o:1297:THR:O	2.52	0.41
35:p:42:GLN:H	35:p:42:GLN:HG3	1.69	0.41
5:4:96:TRP:HB3	5:4:110:LEU:HD23	2.02	0.41
8:7:56:ILE:HD12	8:7:230:VAL:HG11	2.02	0.41
8:7:462:SER:OG	8:7:463:PRO:CD	2.66	0.41
9:8:231:THR:HG21	9:8:250:LYS:O	2.20	0.41
11:A:357:GLU:HB3	11:A:358:ASP:H	1.61	0.41
11:A:413:ASP:O	11:A:414:ILE:C	2.63	0.41
12:B:562:GLY:O	12:B:581:ILE:HG12	2.19	0.41
12:B:831:GLU:OE1	12:B:835:ARG:NH2	2.52	0.41
12:B:887:ARG:NH2	12:B:917:ASP:OD2	2.49	0.41
12:B:984:PRO:HG2	12:B:987:LEU:HD22	2.02	0.41
15:F:388:ILE:HA	15:F:392:ILE:HG12	2.03	0.41
19:J:124:GLU:H	19:J:124:GLU:HG2	1.64	0.41
20:L:83:MET:HB3	20:L:83:MET:HE3	1.61	0.41
22:P:189:ASN:HD21	23:Q:376:TRP:HE1	1.67	0.41
25:S:47:LEU:HD11	25:S:98:TRP:HB3	2.01	0.41
26:T:224:ASN:ND2	26:T:234:GLU:OE2	2.53	0.41
14:e:246:HIS:CD2	14:e:246:HIS:C	2.98	0.41
14:e:267:PHE:C	14:e:269:GLY:H	2.29	0.41
14:e:504:LEU:HD23	14:e:504:LEU:HA	1.90	0.41
32:k:130:PRO:HD3	33:m:35:GLU:HG2	2.02	0.41
34:o:1203:ASP:N	34:o:1203:ASP:OD1	2.51	0.41
34:o:1281:ASP:O	34:o:1285:LEU:HD13	2.19	0.41
35:p:446:TYR:CE1	35:p:450:THR:HG21	2.55	0.41
35:p:718:GLN:CD	35:p:976:MET:HE3	2.45	0.41
10:9:70:VAL:O	10:9:70:VAL:HG12	2.19	0.41
11:A:337:ARG:HD3	11:A:338:VAL:H	1.85	0.41
11:A:464:TRP:CD1	11:A:464:TRP:O	2.73	0.41
14:E:564:ASP:OD1	14:E:564:ASP:N	2.51	0.41
15:F:274:ASN:HB2	15:F:317:LEU:N	2.31	0.41
17:H:155:ASP:HB3	17:H:157:HIS:HB2	2.02	0.41
27:U:76:MET:HG3	27:U:89:HIS:C	2.45	0.41
29:X:13:DC:H2'	29:X:14:DA:C8	2.56	0.41
34:o:883:ILE:O	34:o:883:ILE:HG22	2.19	0.41
34:o:1129:ASN:O	34:o:1130:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:o:1437:ASP:O	34:o:1441:GLU:HG2	2.20	0.41
34:o:1466:ALA:O	35:p:1100:ALA:HB2	2.19	0.41
1:0:84:LYS:CB	1:0:136:ASN:HD21	2.33	0.41
8:7:354:PRO:HA	8:7:416:ILE:HD12	2.03	0.41
8:7:383:LEU:HD21	8:7:388:ILE:HD11	2.02	0.41
11:A:338:VAL:HG22	11:A:360:SER:HB2	2.03	0.41
11:A:353:LEU:HD22	15:f:273:GLN:HE22	1.85	0.41
12:B:102:ASN:OD1	12:B:102:ASN:N	2.54	0.41
12:B:319:TYR:O	12:B:353:GLN:NE2	2.49	0.41
17:H:38:GLN:HG2	17:H:62:THR:HG21	2.01	0.41
28:V:229:ASP:HA	28:V:232:LYS:HG3	2.02	0.41
15:f:104:LEU:HD22	19:j:216:TYR:HB2	2.02	0.41
34:o:497:ASP:OD1	34:o:497:ASP:C	2.64	0.41
34:o:544:ALA:CB	34:o:680:LEU:HD13	2.50	0.41
34:o:549:THR:O	34:o:549:THR:HG22	2.19	0.41
34:o:1137:PRO:HB2	34:o:1341:VAL:HG13	2.03	0.41
37:r:64:THR:HG22	40:u:103:PRO:HD3	2.01	0.41
2:1:422:LEU:HD21	4:3:224:LEU:HB3	2.01	0.41
7:6:510:VAL:HG22	7:6:690:ILE:HD12	2.03	0.41
9:8:61:ARG:HD2	9:8:157:GLY:O	2.21	0.41
12:B:55:PRO:HB3	12:B:60:LEU:HD22	2.02	0.41
13:D:918:SER:OG	20:L:74:GLU:OE1	2.37	0.41
25:S:121:ASN:ND2	35:p:543:GLU:HB3	2.36	0.41
27:U:74:CYS:SG	27:U:92:TYR:HA	2.60	0.41
27:U:145:PHE:CE1	40:u:98:PHE:CZ	3.09	0.41
14:e:690:ASP:OD1	14:e:690:ASP:N	2.53	0.41
33:m:90:ILE:HD12	33:m:90:ILE:HA	1.77	0.41
34:o:910:LYS:N	34:o:911:PRO:CD	2.83	0.41
35:p:388:TYR:O	35:p:389:GLY:C	2.57	0.41
4:3:175:MET:HE3	4:3:179:ASN:CG	2.45	0.41
5:4:359:ILE:HG22	5:4:360:THR:N	2.35	0.41
6:5:35:ILE:C	12:B:539:ARG:HD3	2.42	0.41
7:6:281:GLN:NE2	7:6:482:PHE:HB2	2.36	0.41
8:7:56:ILE:HG21	8:7:70:LEU:HD22	2.01	0.41
9:8:125:LEU:HG	9:8:129:HIS:CE1	2.56	0.41
10:9:122:SER:N	10:9:123:PRO:HD2	2.36	0.41
11:A:931:PRO:O	11:A:935:THR:OG1	2.25	0.41
12:B:487:LYS:O	12:B:487:LYS:CG	2.67	0.41
12:B:881:GLY:HA3	17:H:218:PRO:HB3	2.03	0.41
25:S:115:LYS:HD2	35:p:554:GLU:HB2	2.02	0.41
27:U:77:ARG:HG3	27:U:79:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:e:504:LEU:HD22	14:e:575:PHE:HZ	1.84	0.41
14:e:636:HIS:CD2	14:e:638:ASN:H	2.36	0.41
15:f:402:ARG:HH22	15:f:403:ILE:HD12	1.86	0.41
33:m:77:ARG:CZ	33:m:77:ARG:HB3	2.51	0.41
34:o:560:VAL:HG21	34:o:586:TRP:HB2	2.02	0.41
34:o:1430:CYS:O	34:o:1435:THR:OG1	2.38	0.41
4:3:217:VAL:O	4:3:217:VAL:HG23	2.20	0.41
5:4:146:PRO:HA	5:4:149:ASP:OD2	2.21	0.41
6:5:32:LYS:HE3	12:B:539:ARG:NH2	2.36	0.41
7:6:409:THR:O	7:6:413:LEU:HD13	2.19	0.41
8:7:225:LEU:O	8:7:227:ARG:NH1	2.53	0.41
8:7:272:ARG:HA	8:7:275:GLU:HG2	2.03	0.41
8:7:323:ILE:O	8:7:378:ARG:NH1	2.53	0.41
10:9:11:TRP:HE1	10:9:157:HIS:CD2	2.39	0.41
12:B:781:TYR:OH	17:H:177:GLU:OE1	2.27	0.41
12:B:957:MET:O	12:B:968:ARG:NH1	2.53	0.41
14:E:306:VAL:HA	14:E:338:TYR:HB3	2.03	0.41
15:F:396:LEU:HA	15:F:399:GLU:CD	2.46	0.41
15:F:426:LEU:O	15:F:429:LYS:HG2	2.21	0.41
28:V:192:VAL:HG13	28:V:194:ARG:HG2	2.03	0.41
35:p:42:GLN:HB2	35:p:43:GLN:H	1.56	0.41
44:y:64:PRO:HG3	44:y:72:ILE:HD12	2.02	0.41
1:0:85:ARG:NH1	1:0:140:LEU:N	2.68	0.41
7:6:281:GLN:NE2	7:6:482:PHE:CA	2.84	0.41
8:7:585:GLN:O	8:7:589:GLU:HG2	2.20	0.41
9:8:142:ASN:HD22	9:8:142:ASN:HA	1.69	0.41
11:A:1061:ARG:HD3	11:A:1061:ARG:HA	1.63	0.41
12:B:749:LEU:HA	12:B:752:THR:HG22	2.03	0.41
15:F:277:ALA:O	15:F:278:LEU:C	2.64	0.41
17:H:37:LEU:HD23	17:H:37:LEU:HA	1.88	0.41
17:H:47:GLU:OE1	17:H:113:ARG:NH2	2.54	0.41
24:R:296:ALA:N	24:R:297:PRO:HD2	2.36	0.41
14:e:525:GLU:CD	14:e:525:GLU:H	2.27	0.41
35:p:794:VAL:HG22	35:p:967:ILE:HG22	2.02	0.41
40:u:94:LYS:O	40:u:110:ARG:HD3	2.20	0.41
40:u:96:GLY:HA3	40:u:107:PHE:CE1	2.56	0.41
1:0:85:ARG:HH12	1:0:140:LEU:CG	2.19	0.41
3:2:379:LEU:O	3:2:379:LEU:HD23	2.21	0.41
4:3:42:MET:HE3	4:3:108:ASN:HA	2.02	0.41
4:3:46:ASN:OD1	5:4:123:LEU:HD23	2.20	0.41
7:6:193:VAL:HG11	7:6:283:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:364:LEU:HD23	7:6:410:TYR:CD1	2.56	0.41
8:7:72:TYR:HE1	8:7:83:VAL:HG21	1.86	0.41
8:7:427:THR:HG23	8:7:427:THR:O	2.21	0.41
9:8:101:ILE:HD12	9:8:145:LEU:HD21	2.02	0.41
10:9:72:LYS:HA	10:9:72:LYS:HD3	1.83	0.41
11:A:335:LYS:HE2	11:A:495:LEU:HB2	2.03	0.41
11:A:472:ASN:ND2	15:f:299:LYS:O	2.53	0.41
11:A:725:CYS:SG	11:A:734:LEU:HD12	2.61	0.41
12:B:366:ASP:OD1	12:B:500:THR:OG1	2.34	0.41
13:D:1004:ALA:HB2	21:O:3:TYR:O	2.21	0.41
14:E:239:LEU:HB3	14:E:307:LEU:HD21	2.03	0.41
14:E:651:VAL:HG21	14:E:686:THR:HG21	2.01	0.41
14:E:775:THR:CG2	14:E:778:THR:HB	2.51	0.41
15:F:370:TRP:CH2	15:F:402:ARG:HB3	2.56	0.41
20:L:110:THR:HG23	20:L:112:GLU:HG3	2.02	0.41
21:O:65:TYR:O	22:P:188:ARG:O	2.39	0.41
22:P:188:ARG:NH2	23:Q:321:SER:OG	2.54	0.41
22:P:189:ASN:CG	23:Q:376:TRP:HZ2	2.28	0.41
22:P:258:MET:N	22:P:315:ALA:O	2.54	0.41
28:V:166:ILE:HG22	28:V:167:LEU:H	1.86	0.41
15:f:20:LYS:HB3	15:f:20:LYS:HE2	1.83	0.41
34:o:539:GLN:NE2	35:p:791:GLU:OE2	2.53	0.41
34:o:575:PRO:HG3	34:o:594:LEU:HD11	2.02	0.41
34:o:1172:ASN:HB3	42:w:57:LYS:HA	2.03	0.41
35:p:387:HIS:O	35:p:390:ASN:HB2	2.20	0.41
35:p:387:HIS:NE2	35:p:671:GLU:OE2	2.54	0.41
35:p:473:LEU:HD22	35:p:730:LYS:O	2.20	0.41
37:r:60:VAL:HG22	40:u:103:PRO:HG3	2.02	0.41
3:2:186:ILE:HG12	3:2:211:LEU:HD12	2.03	0.41
4:3:255:CYS:HB2	4:3:276:CYS:N	2.36	0.41
7:6:52:LYS:O	7:6:59:LYS:HA	2.20	0.41
9:8:58:THR:HG23	9:8:157:GLY:CA	2.50	0.41
9:8:98:LEU:HD12	9:8:98:LEU:HA	1.89	0.41
10:9:198:ILE:HD13	10:9:212:ILE:HG23	2.03	0.41
12:B:267:HIS:HB3	12:B:277:LEU:HD11	2.03	0.41
12:B:987:LEU:HG	12:B:988:PRO:HD2	2.03	0.41
14:E:306:VAL:HG21	14:E:363:ALA:HA	2.03	0.41
16:G:74:MET:HE1	16:G:136:ILE:HD12	2.03	0.41
17:H:132:LYS:HE3	17:H:134:LEU:H	1.86	0.41
21:O:11:LEU:HD23	21:O:44:ILE:HD12	2.02	0.41
21:O:32:LEU:HD13	23:Q:32:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:145:PHE:CE2	40:u:98:PHE:HZ	2.39	0.41
27:U:191:LEU:HA	27:U:194:THR:OG1	2.21	0.41
28:V:149:LYS:HA	28:V:149:LYS:HD3	1.99	0.41
28:V:166:ILE:HG22	28:V:167:LEU:N	2.36	0.41
14:e:783:LEU:HD23	14:e:783:LEU:HA	1.93	0.41
15:f:83:LEU:HD11	18:i:42:PHE:HB2	2.03	0.41
19:j:173:HIS:HA	19:j:176:MET:HE3	2.02	0.41
33:m:70:HIS:HA	33:m:73:MET:HE3	2.02	0.41
33:m:93:ASP:OD1	33:m:93:ASP:C	2.64	0.41
33:m:106:MET:HE3	33:m:106:MET:HB3	1.88	0.41
34:o:360:ASP:O	34:o:361:PHE:C	2.63	0.41
34:o:544:ALA:HB2	34:o:680:LEU:HD13	2.03	0.41
35:p:863:ASP:H	35:p:1078:ARG:NH2	2.19	0.41
38:s:2:ASP:OD1	38:s:4:GLU:N	2.54	0.41
1:0:1:MET:HG3	8:7:345:ARG:NH1	2.36	0.40
5:4:62:LEU:O	5:4:115:ARG:NH2	2.54	0.40
5:4:223:ALA:HA	5:4:226:ARG:HG2	2.02	0.40
5:4:448:HIS:CD2	5:4:452:LYS:HE3	2.55	0.40
7:6:373:GLN:OE1	7:6:616:ASP:CA	2.69	0.40
8:7:618:VAL:HG11	8:7:664:VAL:HA	2.03	0.40
9:8:30:ARG:HE	9:8:35:ASN:HB2	1.85	0.40
9:8:71:HIS:CD2	9:8:72:PRO:HD2	2.56	0.40
9:8:257:LEU:HD23	9:8:260:ILE:HD12	2.03	0.40
12:B:464:ILE:HG12	12:B:513:LYS:HE2	2.02	0.40
15:F:114:LEU:HB2	17:H:52:SER:N	2.35	0.40
27:U:32:LEU:HD12	27:U:54:PHE:HZ	1.86	0.40
28:V:133:ILE:HG22	28:V:134:ASP:N	2.36	0.40
28:V:145:VAL:C	28:V:146:ARG:HD2	2.45	0.40
30:Y:28:DT:H2'	30:Y:29:DA:H8	1.82	0.40
13:d:963:ARG:HH22	13:d:964:GLU:HG2	1.86	0.40
34:o:353:ASN:O	34:o:357:LYS:HG3	2.21	0.40
34:o:876:ASP:OD2	34:o:880:ARG:NH2	2.54	0.40
34:o:962:ASP:HB3	34:o:1043:ILE:HG23	2.03	0.40
35:p:302:LYS:CE	42:w:14:ILE:CD1	2.98	0.40
35:p:516:GLU:OE1	35:p:516:GLU:N	2.54	0.40
4:3:242:ILE:HD13	5:4:75:VAL:N	2.36	0.40
5:4:401:LEU:HD22	5:4:401:LEU:HA	1.80	0.40
8:7:12:PHE:CE2	8:7:14:TYR:HB2	2.56	0.40
11:A:511:LEU:N	11:A:511:LEU:HD13	2.35	0.40
12:B:295:LEU:HD13	12:B:477:LEU:HD11	2.03	0.40
15:F:222:LEU:C	15:F:225:LYS:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:3:TYR:HB3	21:O:5:LEU:HD12	1.99	0.40
27:U:39:ARG:H	27:U:39:ARG:HG2	1.74	0.40
27:U:145:PHE:HE2	27:U:150:GLY:HA2	1.87	0.40
34:o:457:ILE:HD11	34:o:515:ILE:HG23	2.03	0.40
39:t:78:PRO:CG	40:u:18:PHE:C	2.87	0.40
40:u:54:ILE:HD12	40:u:70:VAL:HG22	2.04	0.40
2:1:219:GLU:O	2:1:223:ARG:HG2	2.22	0.40
2:1:407:ILE:HD12	4:3:22:TRP:CB	2.51	0.40
3:2:318:LEU:HD12	4:3:272:LEU:CD2	2.51	0.40
6:5:15:ALA:CA	7:6:516:PRO:CB	2.97	0.40
8:7:114:ASN:C	8:7:114:ASN:ND2	2.78	0.40
9:8:43:ILE:HG12	9:8:59:ALA:HB2	2.02	0.40
9:8:119:LEU:HD12	9:8:119:LEU:HA	1.89	0.40
11:A:1068:ARG:HD2	11:A:1068:ARG:C	2.46	0.40
13:D:1001:GLN:O	13:D:1002:ARG:C	2.62	0.40
13:D:1006:LEU:HD11	21:O:71:VAL:HG21	2.03	0.40
15:F:329:LEU:HA	15:F:332:PHE:HB3	2.02	0.40
26:T:179:ASP:OD1	26:T:179:ASP:N	2.54	0.40
27:U:145:PHE:CG	40:u:98:PHE:HZ	2.39	0.40
28:V:133:ILE:HG22	28:V:134:ASP:H	1.87	0.40
15:f:336:LEU:HA	15:f:336:LEU:HD12	1.88	0.40
33:m:84:GLU:H	33:m:84:GLU:HG3	1.42	0.40
35:p:954:MET:HE3	35:p:963:PRO:O	2.22	0.40
36:q:36:ARG:HD3	44:y:41:THR:OG1	2.20	0.40
1:0:84:LYS:HB3	1:0:136:ASN:ND2	2.36	0.40
1:0:294:HIS:ND1	1:0:298:GLN:OE1	2.53	0.40
3:2:115:GLU:OE1	3:2:115:GLU:N	2.54	0.40
5:4:229:ASP:OD1	5:4:229:ASP:N	2.54	0.40
7:6:311:LYS:NZ	7:6:383:THR:CA	2.85	0.40
8:7:46:THR:HG22	8:7:670:GLY:HA3	2.03	0.40
8:7:531:VAL:HG12	8:7:532:PRO:O	2.22	0.40
9:8:118:MET:HE1	9:8:199:VAL:CG1	2.51	0.40
11:A:925:ASP:N	11:A:925:ASP:OD1	2.52	0.40
12:B:492:MET:HE3	12:B:492:MET:HB2	1.85	0.40
12:B:544:LEU:HD22	12:B:625:LEU:HD22	2.02	0.40
13:D:966:LEU:HD22	13:D:966:LEU:HA	1.86	0.40
15:F:350:ASN:O	15:F:354:ARG:NH1	2.55	0.40
16:G:153:LYS:HD3	16:G:153:LYS:N	2.18	0.40
23:Q:19:GLU:O	23:Q:22:ILE:HG12	2.22	0.40
27:U:19:LYS:HA	27:U:22:ILE:HB	2.03	0.40
27:U:194:THR:O	27:U:195:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:75:PHE:O	28:V:78:LEU:HB3	2.22	0.40
13:d:1064:ILE:HD13	13:d:1064:ILE:HA	1.94	0.40
15:f:216:LEU:HD21	15:f:254:GLN:O	2.21	0.40
35:p:647:GLU:O	35:p:648:TYR:CG	2.74	0.40
35:p:715:ASP:OD1	35:p:715:ASP:N	2.54	0.40
36:q:183:ALA:HB3	36:q:232:ASN:HB3	2.04	0.40
38:s:17:ILE:HD11	38:s:135:LEU:HD21	2.03	0.40
1:0:13:LYS:N	1:0:13:LYS:HD3	2.36	0.40
5:4:412:PHE:HD1	5:4:439:ARG:O	2.05	0.40
8:7:101:LYS:C	8:7:102:LEU:HD12	2.46	0.40
11:A:472:ASN:ND2	15:f:302:HIS:ND1	2.70	0.40
11:A:620:LEU:HD11	11:A:766:ARG:HD3	2.02	0.40
12:B:203:LYS:HZ3	12:B:235:HIS:HB3	1.86	0.40
12:B:402:ILE:HD12	12:B:455:LEU:HD12	2.04	0.40
14:E:754:THR:O	14:E:755:ALA:CB	2.67	0.40
15:F:89:GLN:HE21	15:F:89:GLN:HB2	1.67	0.40
17:H:77:LYS:HE3	17:H:77:LYS:HB3	1.93	0.40
22:P:203:ARG:NH2	23:Q:344:ARG:NH2	2.69	0.40
23:Q:332:GLU:OE1	23:Q:332:GLU:N	2.49	0.40
28:V:146:ARG:NE	28:V:173:GLU:O	2.54	0.40
13:d:892:THR:OG1	13:d:893:GLU:OE1	2.33	0.40
18:i:78:ARG:HD3	18:i:78:ARG:HA	1.78	0.40
34:o:1482:TYR:N	34:o:1482:TYR:CD1	2.89	0.40
35:p:764:MET:HE1	35:p:938:ARG:HH11	1.85	0.40
35:p:778:SER:HG	35:p:805:PHE:HZ	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	232/309 (75%)	215 (93%)	17 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	253/548 (46%)	245 (97%)	8 (3%)	0	100	100
3	2	325/395 (82%)	313 (96%)	12 (4%)	0	100	100
4	3	259/308 (84%)	251 (97%)	8 (3%)	0	100	100
5	4	384/462 (83%)	367 (96%)	17 (4%)	0	100	100
6	5	52/71 (73%)	47 (90%)	4 (8%)	1 (2%)	6	28
7	6	601/782 (77%)	576 (96%)	23 (4%)	2 (0%)	36	65
8	7	710/760 (93%)	683 (96%)	26 (4%)	1 (0%)	48	75
9	8	294/346 (85%)	277 (94%)	17 (6%)	0	100	100
10	9	277/323 (86%)	268 (97%)	9 (3%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43	71
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
13	D	154/1085 (14%)	148 (96%)	6 (4%)	0	100	100
13	d	154/1085 (14%)	149 (97%)	5 (3%)	0	100	100
14	E	541/800 (68%)	517 (96%)	23 (4%)	1 (0%)	43	71
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	71
15	F	408/677 (60%)	389 (95%)	18 (4%)	1 (0%)	43	71
15	f	399/677 (59%)	380 (95%)	19 (5%)	0	100	100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
17	H	207/310 (67%)	189 (91%)	14 (7%)	4 (2%)	6	28
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100	100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100	100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100	100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	5	26
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100	100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100	100
21	O	97/109 (89%)	97 (100%)	0	0	100	100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
24	R	248/316 (78%)	246 (99%)	2 (1%)	0	100	100
25	S	104/517 (20%)	104 (100%)	0	0	100	100
26	T	218/249 (88%)	211 (97%)	6 (3%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	U	180/439 (41%)	152 (84%)	26 (14%)	2 (1%)	11	39
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100	100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100	100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100	100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100	100
34	o	1413/1970 (72%)	1369 (97%)	44 (3%)	0	100	100
35	p	1129/1174 (96%)	1089 (96%)	40 (4%)	0	100	100
36	q	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
37	r	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
39	t	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
40	u	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
41	v	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
42	w	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
43	x	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
44	y	113/117 (97%)	112 (99%)	1 (1%)	0	100	100
45	z	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
All	All	13465/22931 (59%)	12871 (96%)	577 (4%)	17 (0%)	49	75

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	128	PRO
14	e	522	ASP
19	j	124	GLU
7	6	584	THR
11	A	502	LEU
15	F	411	VAL
17	H	129	VAL
17	H	157	HIS
26	T	147	LYS
19	j	177	LYS
17	H	141	PRO
27	U	163	GLU

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Mol	Chain	Res	Type
8	7	726	GLN
27	U	78	VAL
7	6	57	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	216/283 (76%)	213 (99%)	3 (1%)	59	73
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	295 (100%)	0	100	100
4	3	234/272 (86%)	229 (98%)	5 (2%)	47	67
5	4	346/399 (87%)	337 (97%)	9 (3%)	40	64
6	5	48/64 (75%)	48 (100%)	0	100	100
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	88
8	7	624/664 (94%)	623 (100%)	1 (0%)	87	88
9	8	259/299 (87%)	258 (100%)	1 (0%)	84	84
10	9	256/296 (86%)	254 (99%)	2 (1%)	73	79
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9	32
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55	72
13	D	145/815 (18%)	139 (96%)	6 (4%)	27	55
13	d	146/815 (18%)	144 (99%)	2 (1%)	59	73
14	E	480/657 (73%)	467 (97%)	13 (3%)	39	63
14	e	475/657 (72%)	462 (97%)	13 (3%)	39	63
15	F	328/574 (57%)	303 (92%)	25 (8%)	12	37
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	60
16	G	132/322 (41%)	124 (94%)	8 (6%)	17	45
17	H	181/270 (67%)	173 (96%)	8 (4%)	25	54
18	I	106/235 (45%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	i	107/235 (46%)	107 (100%)	0	100	100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9	32
19	j	83/154 (54%)	82 (99%)	1 (1%)	63	75
20	L	71/141 (50%)	66 (93%)	5 (7%)	14	41
20	l	98/141 (70%)	97 (99%)	1 (1%)	68	76
21	O	90/98 (92%)	90 (100%)	0	100	100
22	P	154/293 (53%)	154 (100%)	0	100	100
23	Q	105/324 (32%)	105 (100%)	0	100	100
24	R	215/268 (80%)	214 (100%)	1 (0%)	81	83
25	S	93/448 (21%)	93 (100%)	0	100	100
26	T	196/218 (90%)	193 (98%)	3 (2%)	57	72
27	U	167/373 (45%)	163 (98%)	4 (2%)	43	65
28	V	150/261 (58%)	149 (99%)	1 (1%)	76	80
31	c	113/833 (14%)	111 (98%)	2 (2%)	51	70
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	71 (89%)	9 (11%)	5	21
34	o	1254/1748 (72%)	1247 (99%)	7 (1%)	78	81
35	p	993/1027 (97%)	991 (100%)	2 (0%)	87	88
36	q	234/252 (93%)	234 (100%)	0	100	100
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	191 (100%)	0	100	100
39	t	69/111 (62%)	69 (100%)	0	100	100
40	u	152/153 (99%)	151 (99%)	1 (1%)	76	80
41	v	129/131 (98%)	129 (100%)	0	100	100
42	w	103/112 (92%)	103 (100%)	0	100	100
43	x	53/56 (95%)	53 (100%)	0	100	100
44	y	104/106 (98%)	104 (100%)	0	100	100
45	z	41/55 (74%)	41 (100%)	0	100	100
All	All	12071/19766 (61%)	11862 (98%)	209 (2%)	52	71

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	11	THR
1	0	28	HIS
1	0	53	LEU
4	3	100	LYS
4	3	132	LEU
4	3	137	LEU
4	3	257	CYS
4	3	258	HIS
5	4	56	VAL
5	4	57	MET
5	4	401	LEU
5	4	404	THR
5	4	407	VAL
5	4	409	TYR
5	4	411	GLN
5	4	432	VAL
5	4	456	LYS
7	6	266	GLN
8	7	563	ARG
9	8	164	SER
10	9	28	ARG
10	9	32	CYS
11	A	337	ARG
11	A	338	VAL
11	A	348	LEU
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	401	ASN
11	A	403	LEU
11	A	404	MET
11	A	408	LEU
11	A	415	ILE
11	A	416	TRP
11	A	419	GLU
11	A	470	ILE
11	A	475	LEU
11	A	481	GLU
11	A	483	ASN
11	A	491	MET
11	A	499	VAL
11	A	500	LEU

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Mol	Chain	Res	Type
11	A	501	THR
11	A	502	LEU
11	A	505	ASN
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	819	LYS
11	A	821	ARG
11	A	828	GLU
11	A	925	ASP
11	A	943	LYS
11	A	970	ASN
11	A	1052	ARG
11	A	1058	HIS
11	A	1062	TYR
11	A	1068	ARG
11	A	1073	GLN
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	71	ARG
12	B	140	GLU
12	B	184	ASN
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	559	LYS
12	B	603	LYS
12	B	640	VAL
12	B	746	SER
12	B	771	VAL
12	B	818	THR
12	B	987	LEU
13	D	948	GLU
13	D	952	GLN
13	D	953	ILE
13	D	966	LEU
13	D	1006	LEU

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Mol	Chain	Res	Type
13	D	1009	LEU
14	E	258	ASN
14	E	274	TYR
14	E	278	ASP
14	E	280	ARG
14	E	326	ASN
14	E	327	ASN
14	E	519	GLU
14	E	521	ASP
14	E	522	ASP
14	E	527	ILE
14	E	761	LEU
14	E	774	MET
14	E	775	THR
15	F	83	LEU
15	F	91	PHE
15	F	94	PHE
15	F	218	VAL
15	F	219	GLU
15	F	221	GLN
15	F	223	TYR
15	F	243	LEU
15	F	261	THR
15	F	269	VAL
15	F	271	VAL
15	F	280	ILE
15	F	295	LEU
15	F	301	VAL
15	F	312	ILE
15	F	317	LEU
15	F	326	HIS
15	F	340	ILE
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	397	GLN
15	F	406	VAL
15	F	415	ILE
15	F	427	LEU
16	G	41	ASP
16	G	129	LYS
16	G	131	ILE

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Mol	Chain	Res	Type
16	G	143	VAL
16	G	153	LYS
16	G	181	TRP
16	G	182	GLU
16	G	183	ILE
17	H	27	ASP
17	H	36	THR
17	H	128	PRO
17	H	132	LYS
17	H	153	PHE
17	H	156	PRO
17	H	157	HIS
17	H	160	ILE
19	J	116	LEU
19	J	123	LEU
19	J	156	SER
19	J	164	SER
19	J	174	CYS
19	J	177	LYS
19	J	192	LYS
20	L	79	ASP
20	L	104	ARG
20	L	108	SER
20	L	113	VAL
20	L	114	LYS
24	R	53	ARG
26	T	145	LEU
26	T	147	LYS
26	T	149	VAL
27	U	124	ARG
27	U	144	LEU
27	U	164	ASP
27	U	168	MET
28	V	189	ILE
31	c	24	ASP
31	c	106	VAL
13	d	950	LEU
13	d	951	ASP
14	e	243	LEU
14	e	258	ASN
14	e	268	HIS
14	e	270	ASP

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Mol	Chain	Res	Type
14	e	277	ASP
14	e	282	LEU
14	e	436	ASP
14	e	438	LEU
14	e	512	ASP
14	e	515	LEU
14	e	516	ILE
14	e	546	VAL
14	e	579	VAL
15	f	215	GLU
15	f	253	TYR
15	f	261	THR
15	f	272	VAL
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	366	GLU
15	f	421	ASP
19	j	114	THR
20	l	114	LYS
33	m	31	LEU
33	m	55	ASP
33	m	58	GLU
33	m	77	ARG
33	m	83	VAL
33	m	84	GLU
33	m	90	ILE
33	m	91	ARG
33	m	110	LEU
34	o	1291	ASN
34	o	1299	GLN
34	o	1474	LEU
34	o	1475	LEU
34	o	1482	TYR
34	o	1486	ILE
34	o	1487	PRO
35	p	39	LEU
35	p	41	ARG
40	u	95	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	ASN
1	0	45	ASN
1	0	83	ASN
1	0	136	ASN
2	1	384	HIS
2	1	420	GLN
2	1	537	HIS
3	2	227	HIS
3	2	293	GLN
3	2	317	HIS
4	3	9	ASN
4	3	240	GLN
5	4	54	ASN
5	4	211	GLN
5	4	218	GLN
5	4	390	GLN
5	4	458	GLN
5	4	460	HIS
6	5	36	GLN
6	5	42	HIS
7	6	112	HIS
7	6	281	GLN
7	6	330	ASN
7	6	498	ASN
7	6	506	GLN
7	6	551	HIS
7	6	598	HIS
7	6	638	GLN
7	6	677	GLN
7	6	709	GLN
8	7	560	ASN
8	7	723	GLN
9	8	129	HIS
9	8	130	GLN
9	8	288	GLN
9	8	306	GLN
10	9	3	HIS
10	9	18	GLN
10	9	142	GLN
10	9	247	GLN
11	A	401	ASN
11	A	472	ASN
11	A	489	GLN

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Mol	Chain	Res	Type
11	A	590	GLN
11	A	630	GLN
11	A	693	GLN
11	A	702	ASN
11	A	755	HIS
11	A	802	HIS
11	A	860	ASN
11	A	896	GLN
11	A	1073	GLN
12	B	30	HIS
12	B	36	ASN
12	B	176	HIS
12	B	183	GLN
12	B	235	HIS
12	B	348	GLN
12	B	432	HIS
12	B	439	HIS
12	B	450	GLN
12	B	509	ASN
12	B	577	HIS
12	B	644	GLN
12	B	652	GLN
12	B	750	GLN
12	B	813	ASN
12	B	864	ASN
12	B	882	HIS
12	B	908	GLN
12	B	912	ASN
12	B	963	HIS
13	D	875	GLN
13	D	912	ASN
13	D	925	ASN
13	D	936	GLN
13	D	956	GLN
13	D	1001	GLN
13	D	1053	GLN
14	E	254	ASN
14	E	256	HIS
14	E	258	ASN
14	E	327	ASN
14	E	351	GLN
14	E	616	HIS

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Mol	Chain	Res	Type
14	E	640	ASN
14	E	673	HIS
14	E	733	ASN
14	E	758	HIS
14	E	800	GLN
15	F	37	GLN
15	F	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	244	GLN
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
15	F	326	HIS
15	F	430	HIS
16	G	10	HIS
16	G	48	HIS
16	G	142	ASN
17	H	24	ASN
17	H	145	HIS
17	H	149	HIS
18	I	21	GLN
18	I	38	GLN
18	I	98	GLN
19	J	210	ASN
20	L	117	GLN
21	O	35	GLN
21	O	45	ASN
21	O	70	ASN
22	P	189	ASN
22	P	229	GLN
22	P	278	GLN
23	Q	343	HIS
24	R	116	ASN
25	S	32	ASN
26	T	143	GLN
26	T	144	GLN
27	U	64	ASN
27	U	143	GLN
27	U	183	GLN
28	V	83	ASN
28	V	90	GLN

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Mol	Chain	Res	Type
28	V	117	GLN
28	V	157	GLN
31	c	27	GLN
31	c	50	HIS
13	d	912	ASN
13	d	943	GLN
13	d	952	GLN
14	e	246	HIS
14	e	320	HIS
14	e	336	HIS
14	e	368	ASN
14	e	424	GLN
14	e	640	ASN
14	e	733	ASN
15	f	30	GLN
15	f	119	ASN
15	f	134	HIS
15	f	273	GLN
15	f	325	ASN
18	i	38	GLN
19	j	172	GLN
19	j	173	HIS
32	k	186	HIS
32	k	202	ASN
32	k	205	HIS
20	l	73	ASN
20	l	86	GLN
20	l	105	HIS
20	l	119	HIS
33	m	107	ASN
34	o	96	HIS
34	o	267	GLN
34	o	372	ASN
34	o	504	HIS
34	o	671	ASN
34	o	700	GLN
34	o	723	ASN
34	o	861	GLN
34	o	905	ASN
34	o	1032	GLN
34	o	1082	HIS
34	o	1093	GLN

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Mol	Chain	Res	Type
34	o	1291	ASN
34	o	1310	HIS
34	o	1445	HIS
35	p	42	GLN
35	p	98	HIS
35	p	111	ASN
35	p	145	GLN
35	p	188	ASN
35	p	420	GLN
35	p	913	GLN
36	q	66	HIS
36	q	260	GLN
36	q	265	HIS
37	r	38	HIS
38	s	65	ASN
38	s	92	GLN
38	s	133	GLN
40	u	28	GLN
44	y	44	ASN
44	y	49	GLN
44	y	55	GLN
44	y	89	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	SF4	7	1000	8	0,12,12	-	-	-		

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
47	SF4	7	1000	8	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

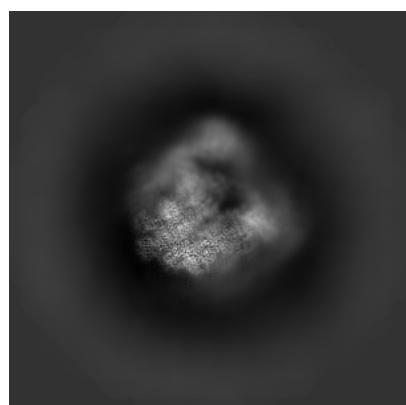
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31111. These allow visual inspection of the internal detail of the map and identification of artifacts.

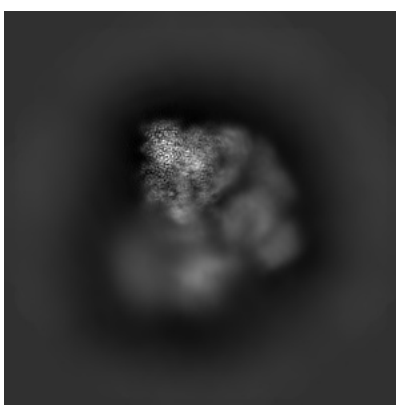
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

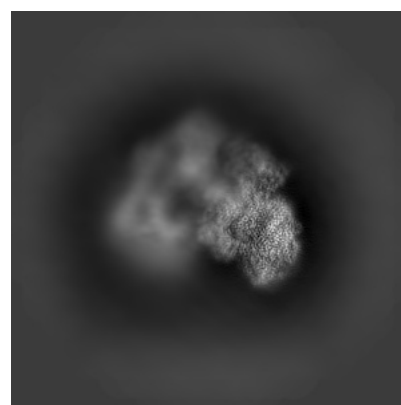
6.1.1 Primary map



X



Y

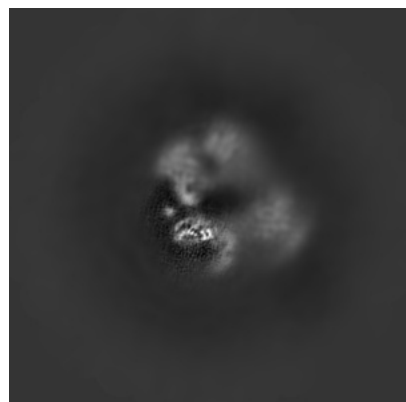


Z

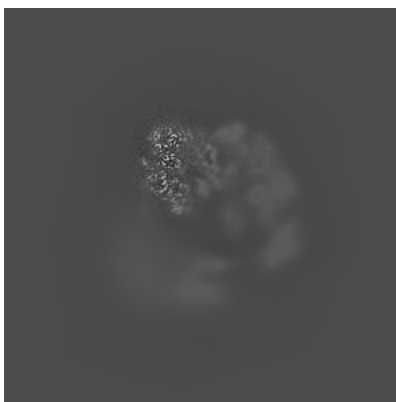
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

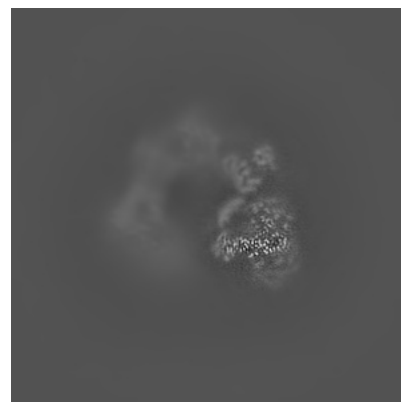
6.2.1 Primary map



X Index: 256



Y Index: 256

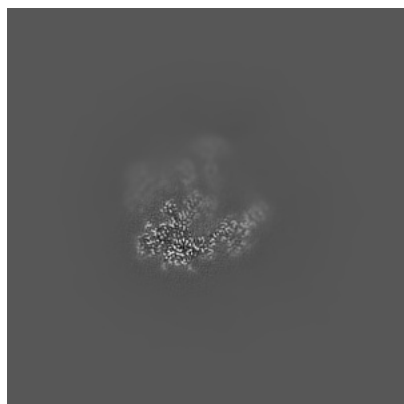


Z Index: 256

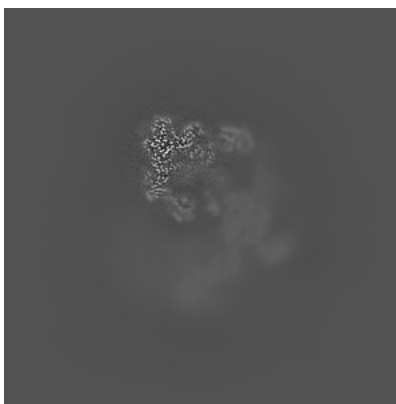
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

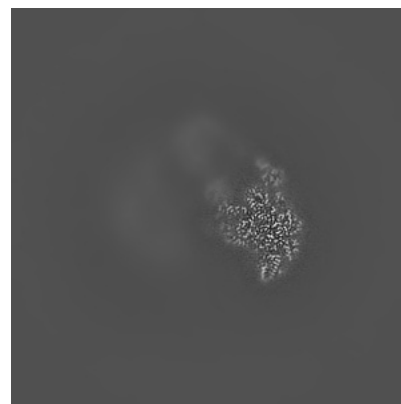
6.3.1 Primary map



X Index: 331



Y Index: 229

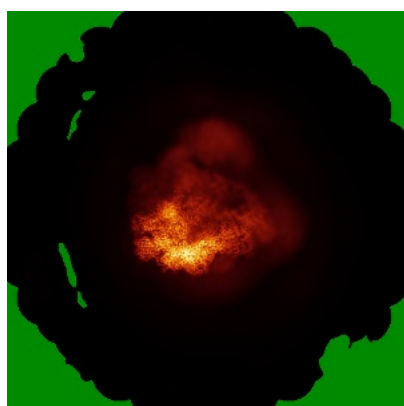


Z Index: 206

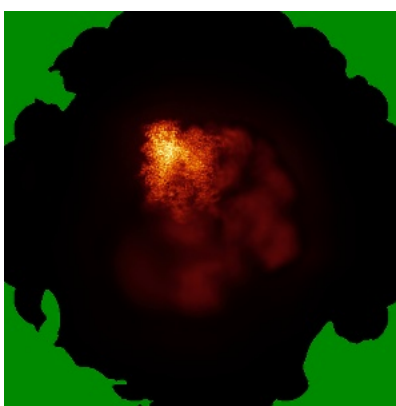
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

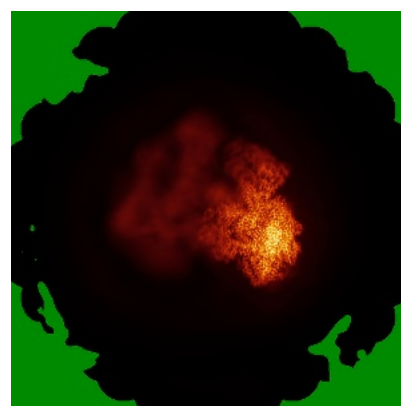
6.4.1 Primary map



X



Y

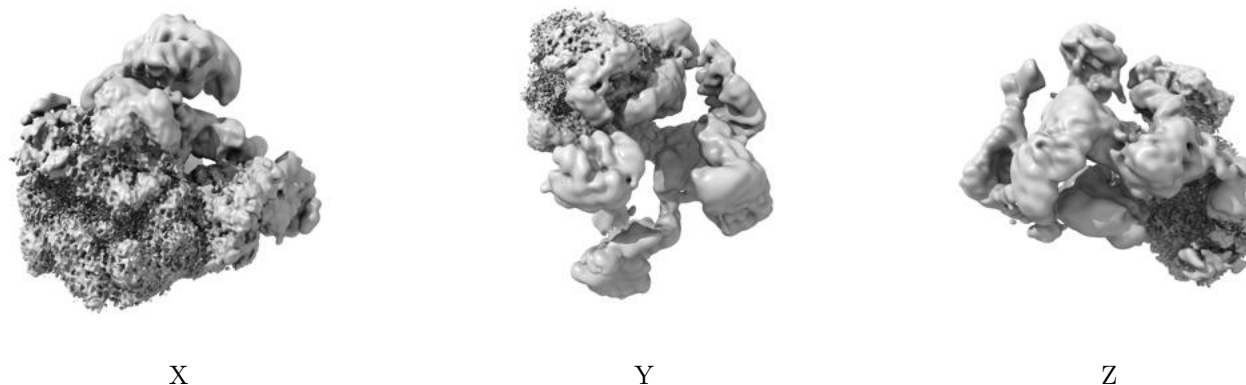


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

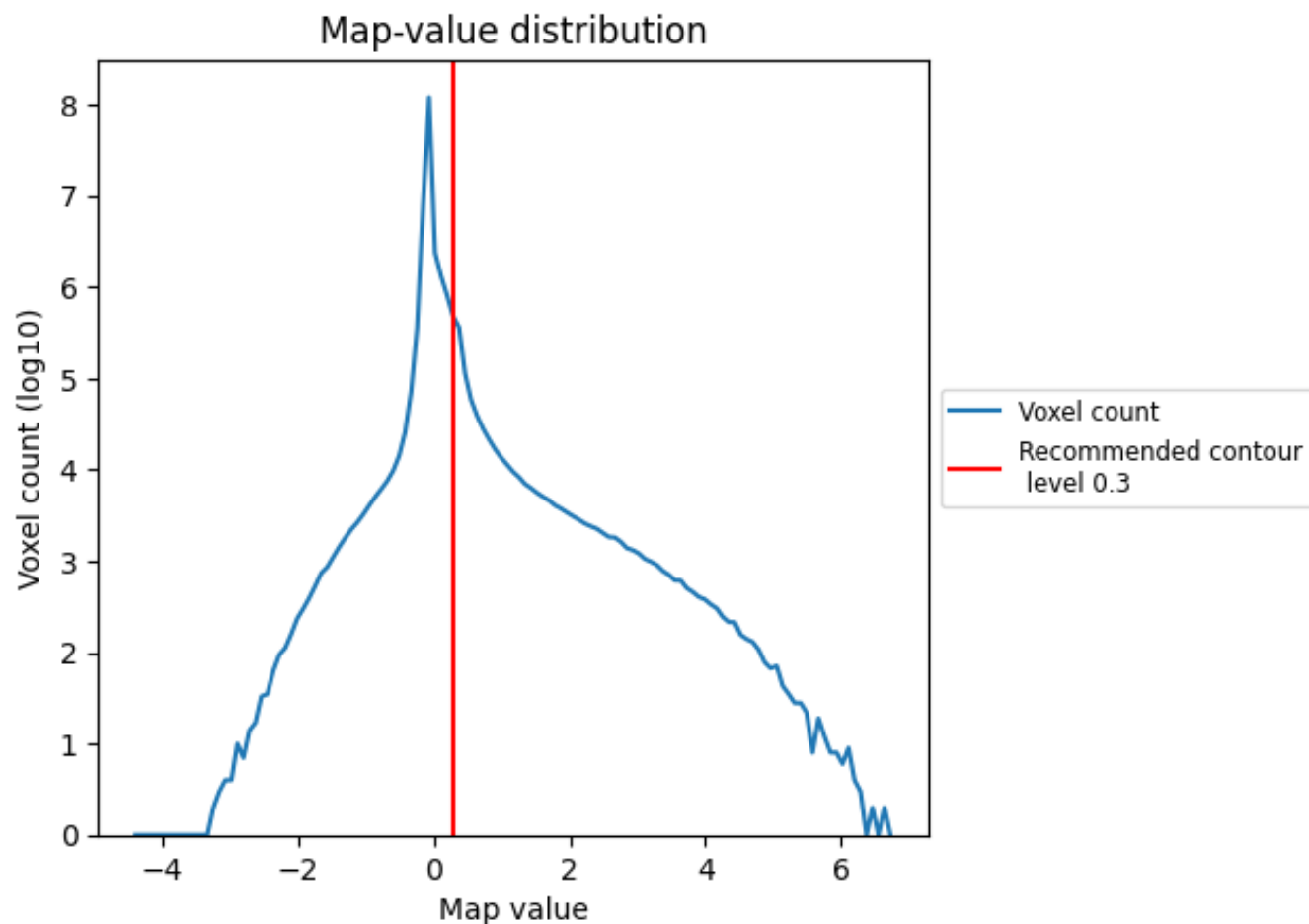
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

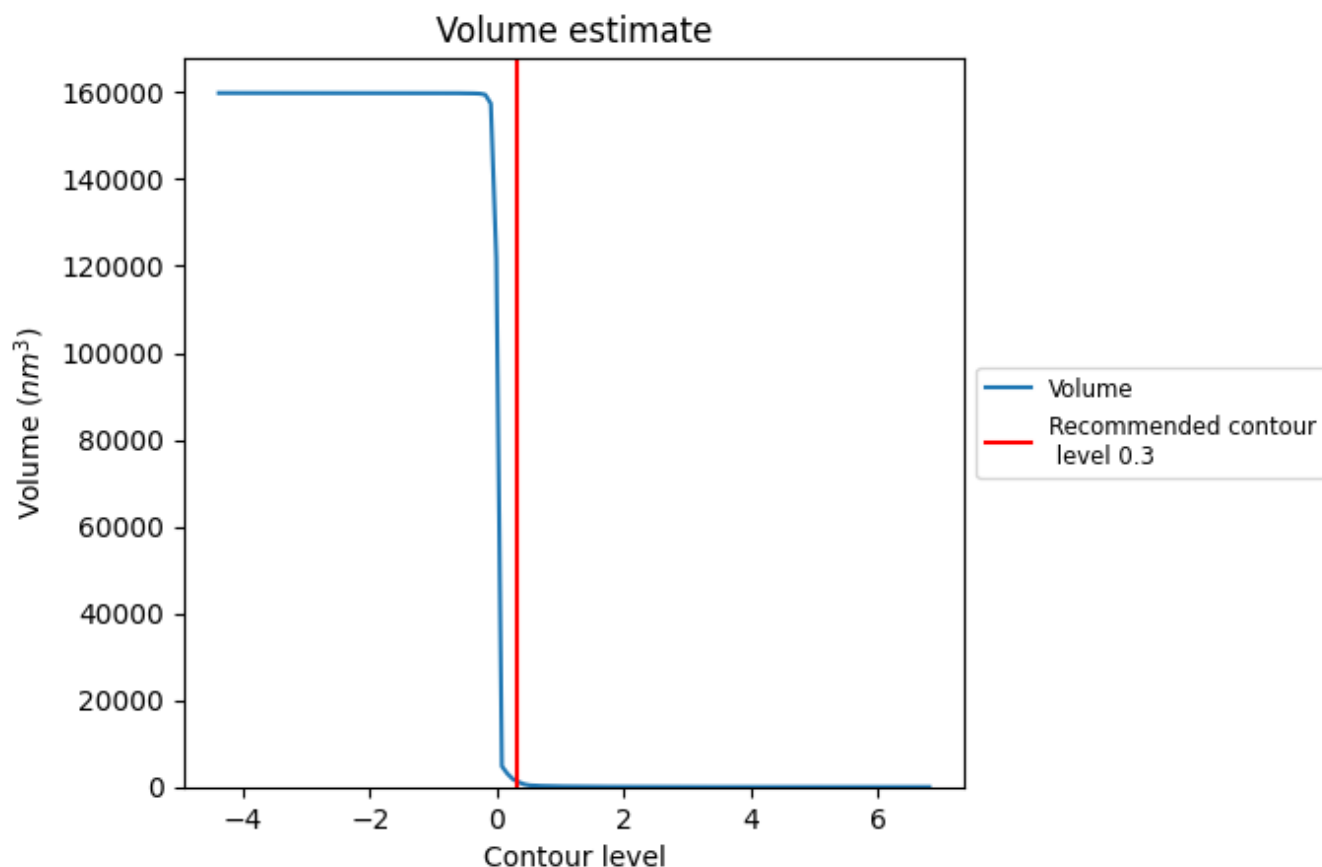
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

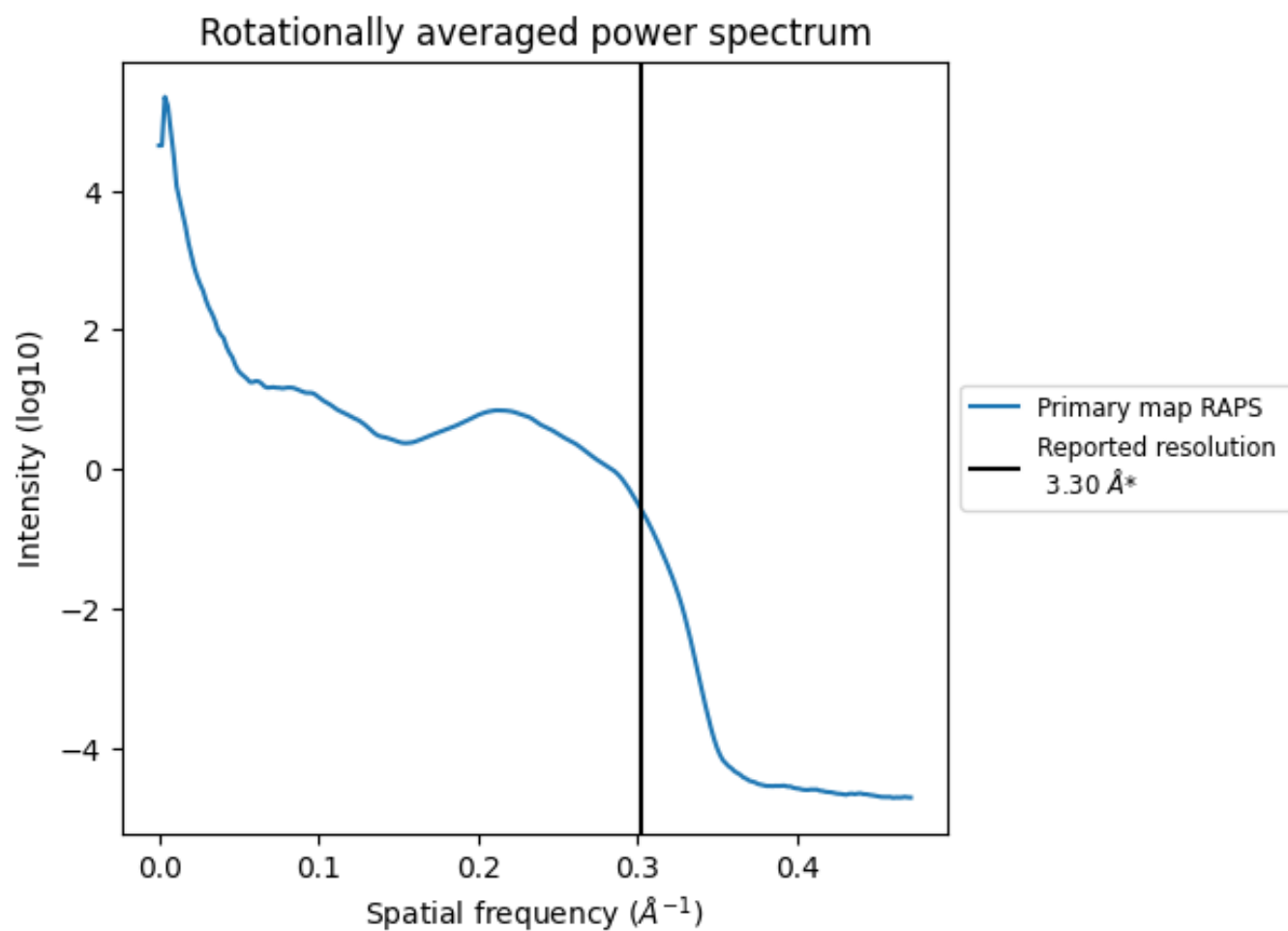
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1427 nm^3 ; this corresponds to an approximate mass of 1289 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

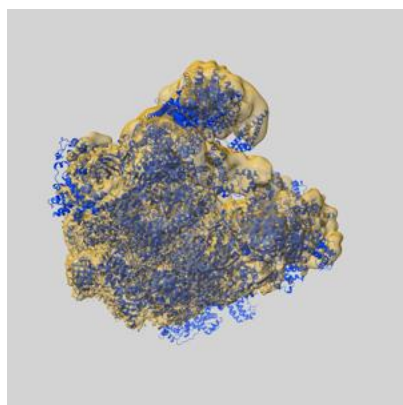
8 Fourier-Shell correlation

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

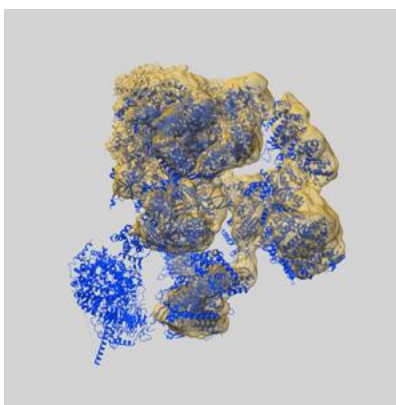
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31111 and PDB model 7EGB. Per-residue inclusion information can be found in section 3 on page 14.

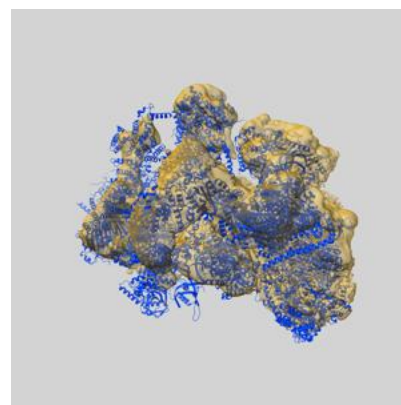
9.1 Map-model overlay [i](#)



X



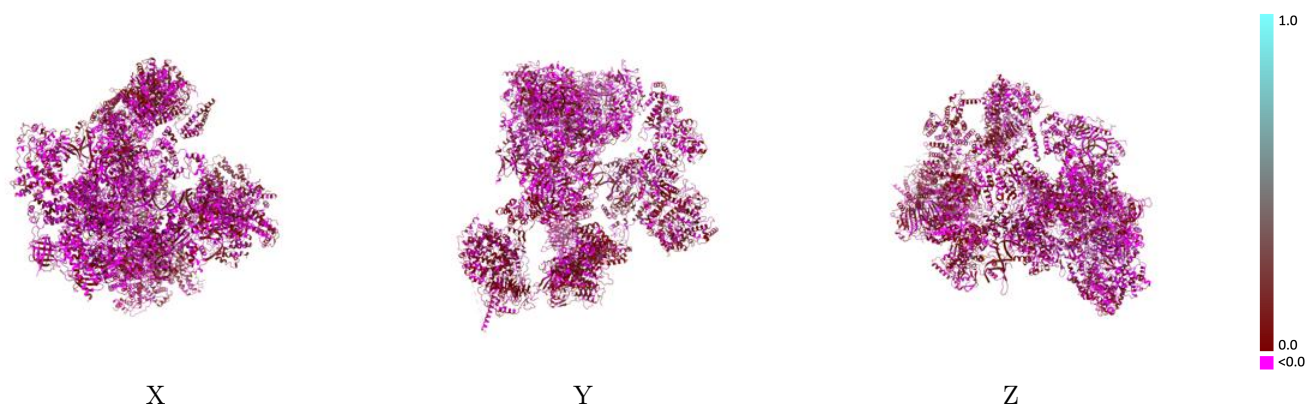
Y



Z

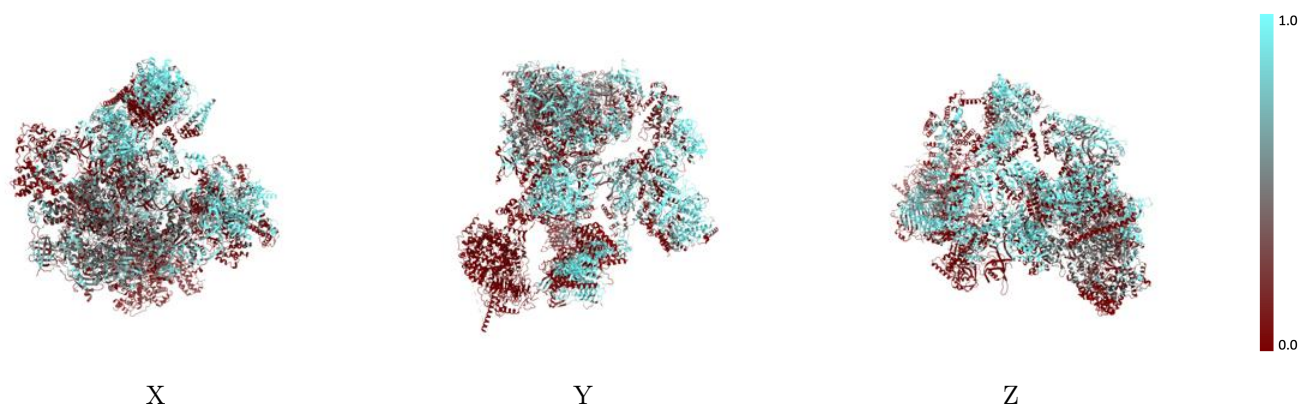
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



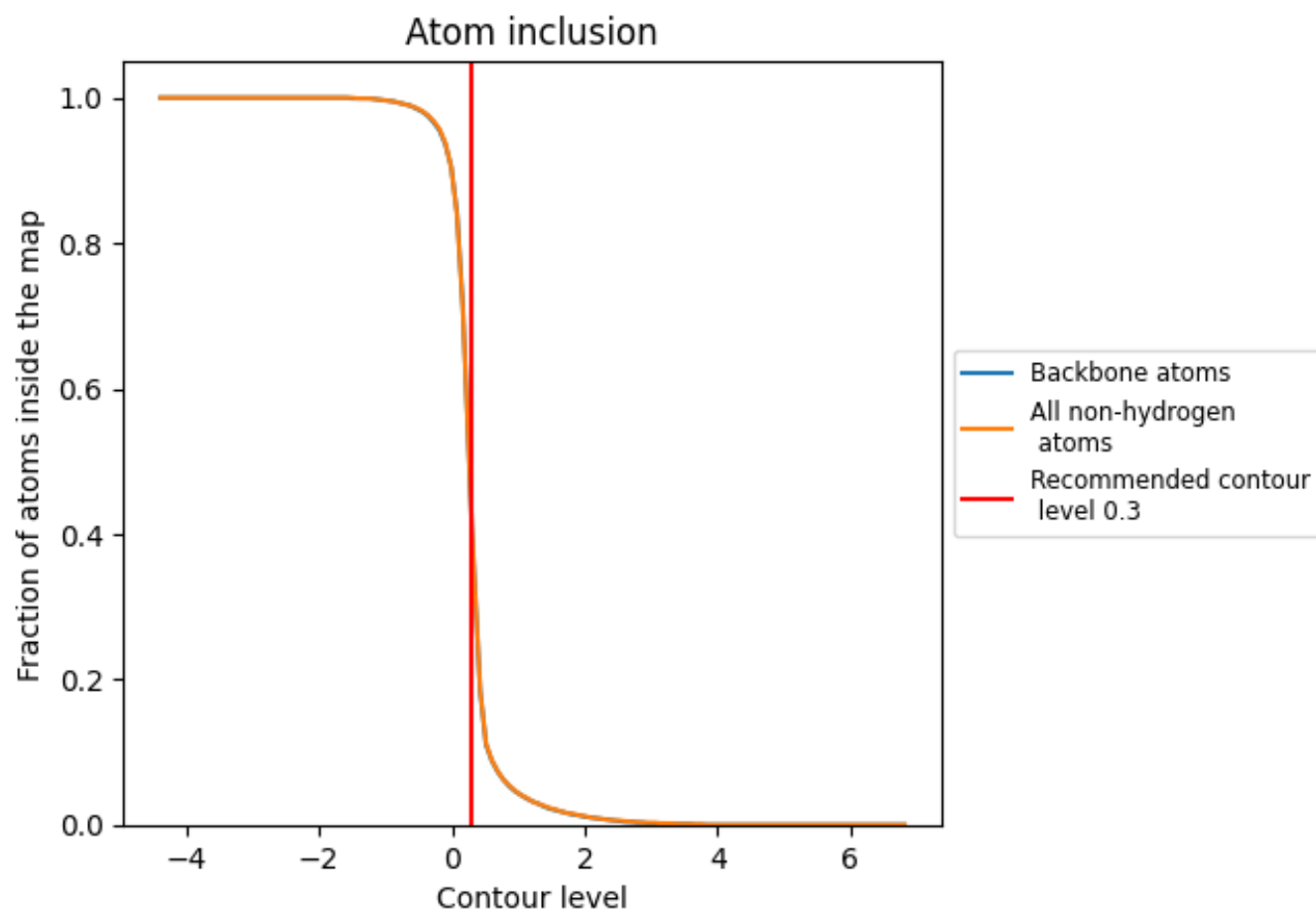
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 41% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4140	0.0120
0	0.0890	-0.0020
1	0.4320	0.0430
2	0.5810	0.0260
3	0.7830	0.0500
4	0.5720	0.0510
5	0.3110	-0.0010
6	0.6730	0.0420
7	0.5860	0.0310
8	0.1610	0.0120
9	0.2780	0.0070
A	0.1510	0.0250
B	0.6230	0.0280
D	0.5050	0.0280
E	0.4020	0.0310
F	0.3590	0.0460
G	0.0300	0.0170
H	0.6440	0.0390
I	0.4490	-0.0180
J	0.8020	0.0260
L	0.3170	-0.0230
O	0.5370	-0.0150
P	0.7170	-0.0160
Q	0.5570	0.0160
R	0.4940	-0.0010
S	0.5220	0.0290
T	0.4100	0.0270
U	0.4650	-0.0380
V	0.6180	0.0190
X	0.4470	0.0500
Y	0.4070	0.0480
c	0.0000	0.0340
d	0.0000	0.0100
e	0.0000	0.0340
f	0.2680	0.0380



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Chain	Atom inclusion	Q-score
i	 0.0000	 0.0300
j	 0.0000	 0.0070
k	 0.0000	 0.0130
l	 0.0000	 0.0230
m	 0.0000	 0.0150
o	 0.4030	 -0.0240
p	 0.4300	 -0.0300
q	 0.4700	 0.0000
r	 0.5270	 -0.0370
s	 0.4330	 -0.0260
t	 0.3740	 -0.0310
u	 0.6640	 -0.0100
v	 0.4060	 -0.0110
w	 0.3780	 -0.0350
x	 0.4220	 0.0140
y	 0.4850	 -0.0190
z	 0.4710	 0.0040