Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 08:41 PM EDT

PDB ID	:	8UOT
EMDB ID	:	EMD-42438
Title	:	Composite map of PICdeltaTFIIK form1
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2023-10-20
Resolution	:	3.70 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:

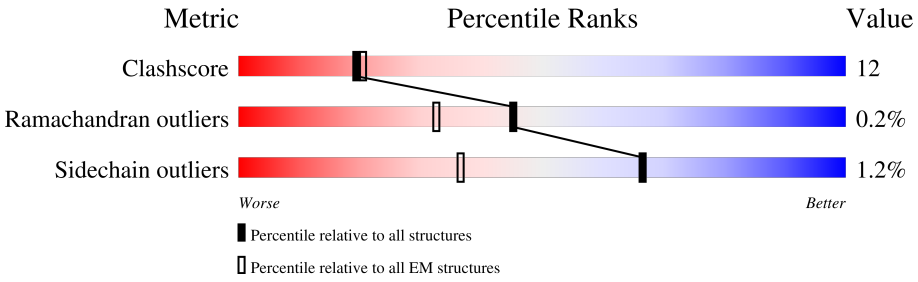
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	778	63% 33%
2	1	642	51% 13% 35%
3	2	513	8% 60% 26% 13%
4	4	338	65% 21% 14%
5	6	461	51% 25% 23%
6	7	843	48% 23% 28%
7	M	345	12% 59% 21% 19%
8	A	1733	61% 20% 18%

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Mol	Chain	Length	Quality of chain
9	B	1224	72% 22% 5%
10	C	318	58% 21% 17%
11	D	221	16% 56% 19% 24%
12	E	215	67% 30%
13	F	155	40% 16% 44%
14	G	171	63% 33%
15	H	146	62% 28% 8%
16	I	122	56% 34% 7%
17	J	70	59% 29% 6%
18	K	120	67% 20% 8%
19	L	70	37% 17% 6% 37%
20	Q	735	23% 6% 71%
21	P	400	31% 14% 55%
22	S	309	35% 17% 47%
23	O	240	52% 22% 25%
24	U	286	6% 23% 11% 63%
25	V	122	23% 62% 20% 15%
26	W	482	38% 13% 49%
27	X	328	34% 14% 51%
28	5	72	12% 61% 28% 8%
29	N	64	52% 42% 6%
30	T	64	61% 33% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	SF4	0	801	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 70523 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 General transcription and DNA repair factor IIH helicase subunit XPD/RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	417	Total	C	N	O	S	0	0
			3382	2139	587	640	16		

- Molecule 3 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	445	Total	C	N	O	S	0	0
			3546	2291	585	654	16		

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	292	Total	C	N	O	S	0	0
			2267	1449	376	428	14		

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	355	Total	C	N	O	S	0	0
			2786	1765	481	512	28		

- Molecule 6 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	608	Total	C	N	O	S	0	0
			4889	3110	847	906	26		

- Molecule 7 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	279	Total	C	N	O	S	0	0
			2175	1382	373	403	17		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1425	Total	C	N	O	S	0	0
			11167	7036	1948	2121	62		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1166	Total	C	N	O	S	0	0
			9227	5823	1619	1729	56		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	168	Total	C	N	O	S	0	0
			1331	822	237	270	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	171	Total	C	N	O	S	0	0
			1335	858	221	248	8		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 20 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 21 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	179	Total	C	N	O	S	0	0
			1484	941	258	279	6		

- Molecule 22 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	164	Total	C	N	O	S	0	0
			1294	809	230	247	8		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 24 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

- Molecule 25 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 26 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	247	Total	C	N	O	S	0	0
			2010	1275	347	381	7		

- Molecule 27 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	160	Total	C	N	O	S	0	0
			1288	826	212	245	5		

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	66	Total	C	N	O	S	0	0
			498	314	89	93	2		

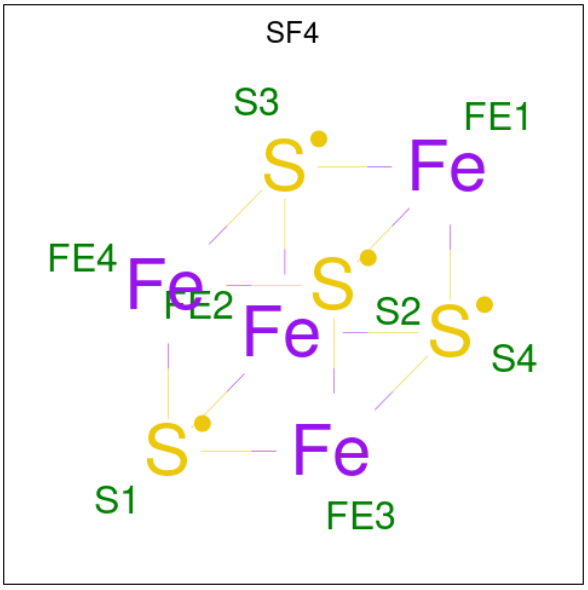
- Molecule 29 is a DNA chain called non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	N	64	Total	C	N	O	P	0	0
			1307	630	228	386	63		

- Molecule 30 is a DNA chain called template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	64	Total	C	N	O	P	0	0
			1314	630	240	380	64		

- Molecule 31 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
31	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
32	4	1	Total Zn 1 1	0
32	6	4	Total Zn 4 4	0
32	M	1	Total Zn 1 1	0
32	A	2	Total Zn 2 2	0
32	B	1	Total Zn 1 1	0
32	C	1	Total Zn 1 1	0
32	I	2	Total Zn 2 2	0
32	J	1	Total Zn 1 1	0
32	L	1	Total Zn 1 1	0
32	S	1	Total Zn 1 1	0

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

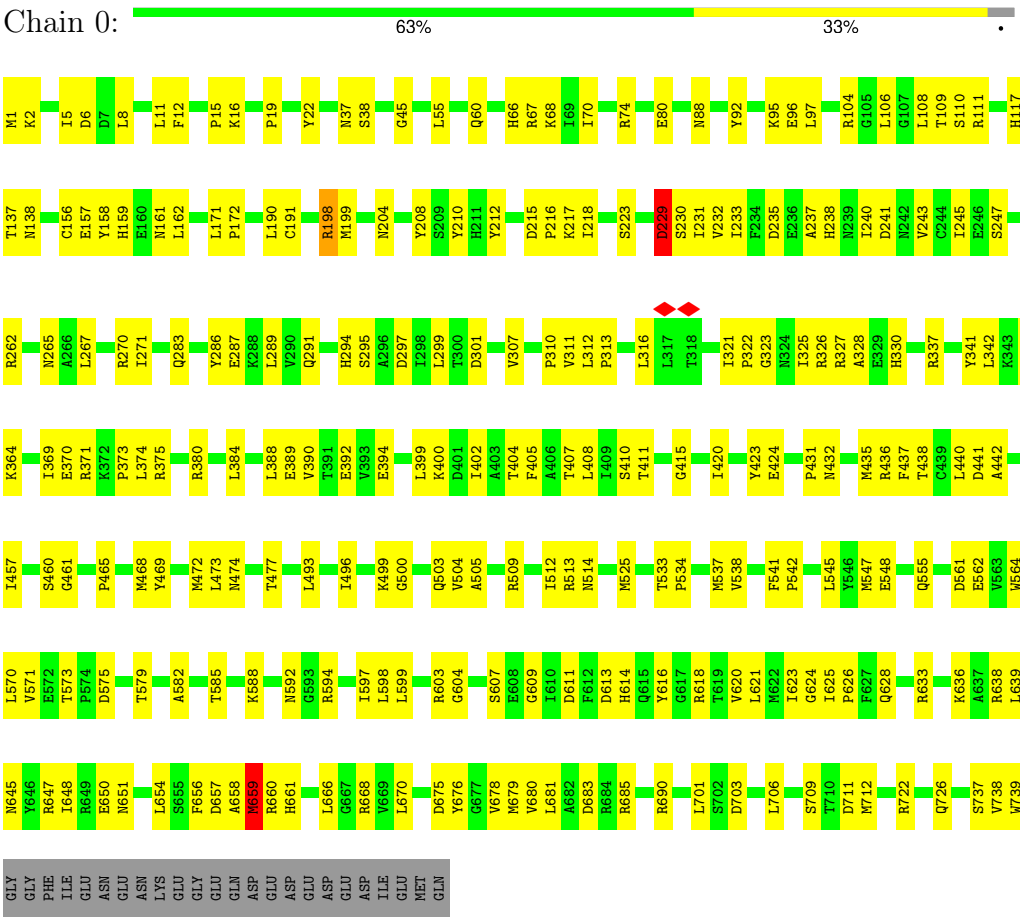
Mol	Chain	Residues	Atoms	AltConf
33	7	1	Total Mg 1 1	0
33	A	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

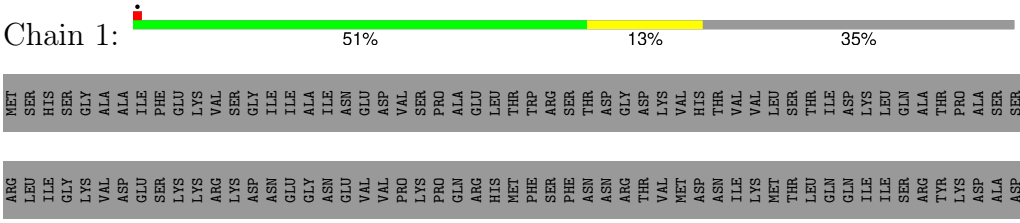
• Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD/RAD3

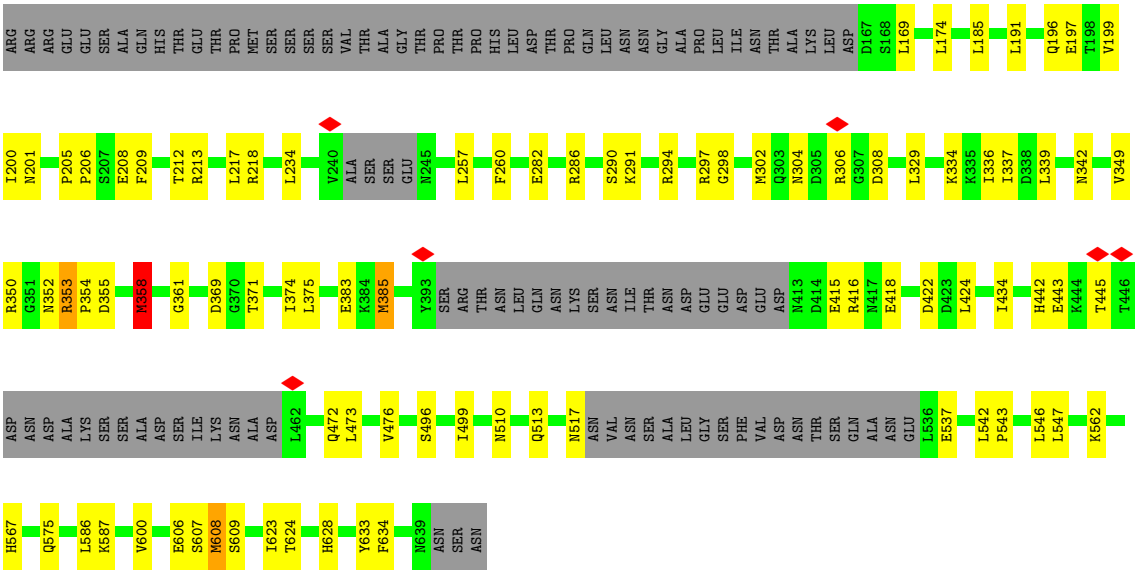
Chain 0:



• Molecule 2: General transcription and DNA repair factor IIH subunit TFB1

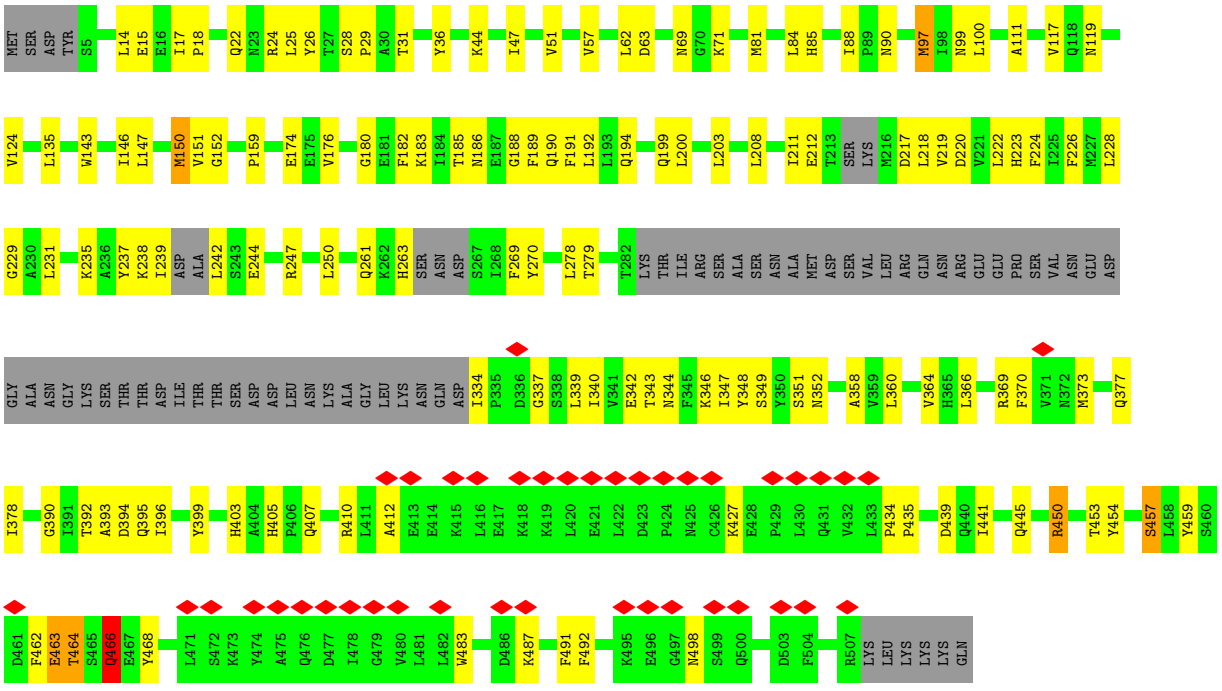
Chain 1:





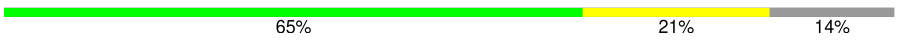
• Molecule 3: General transcription and DNA repair factor IIH subunit TFB2

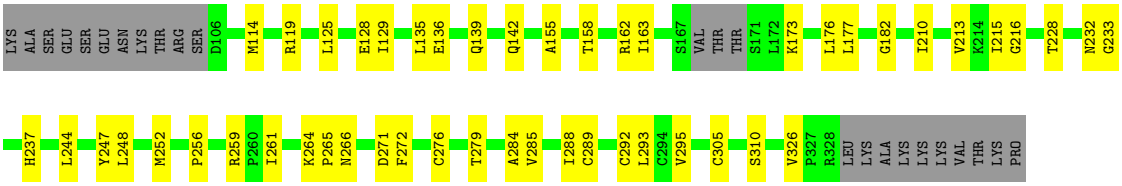
Chain 2:



• Molecule 4: General transcription and DNA repair factor IIH subunit TFB4

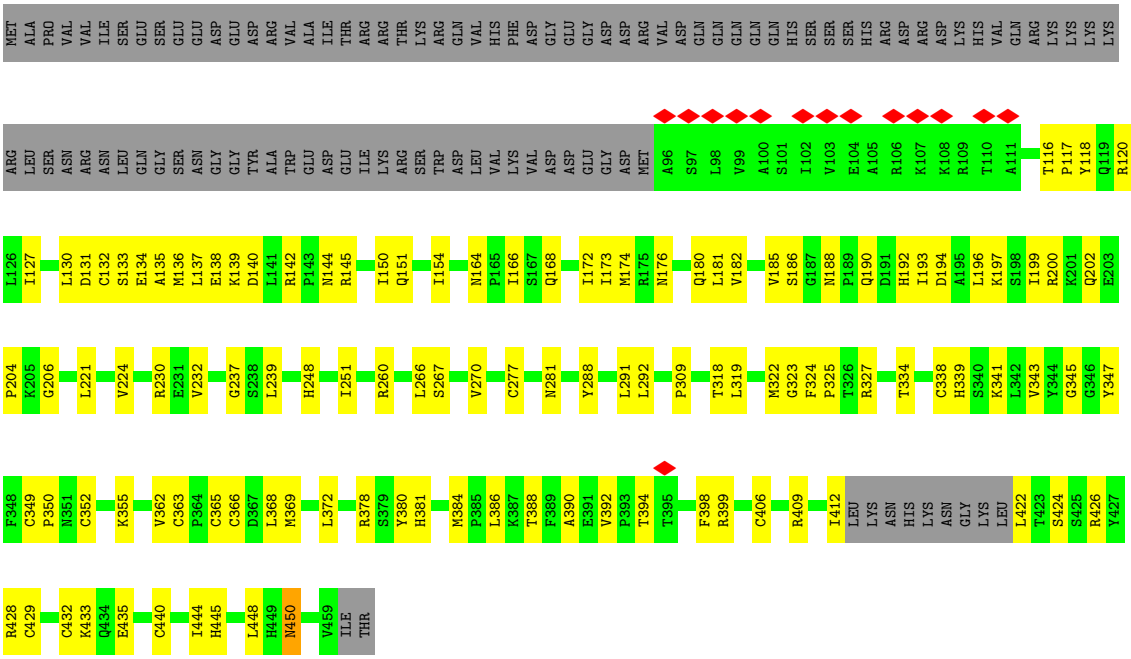
Chain 4:





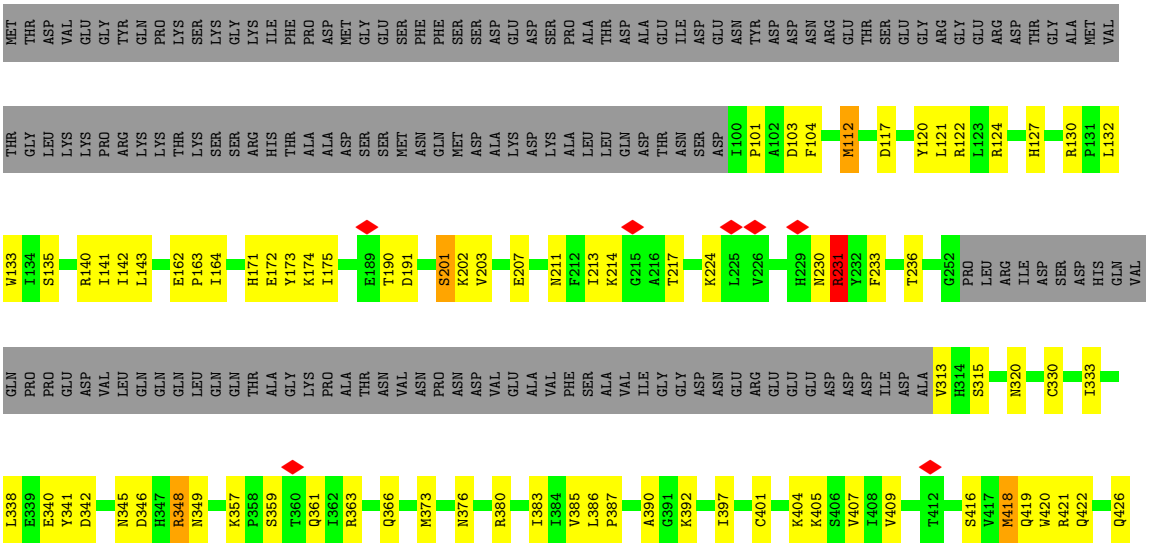
• Molecule 5: General transcription and DNA repair factor IIH subunit SSL1

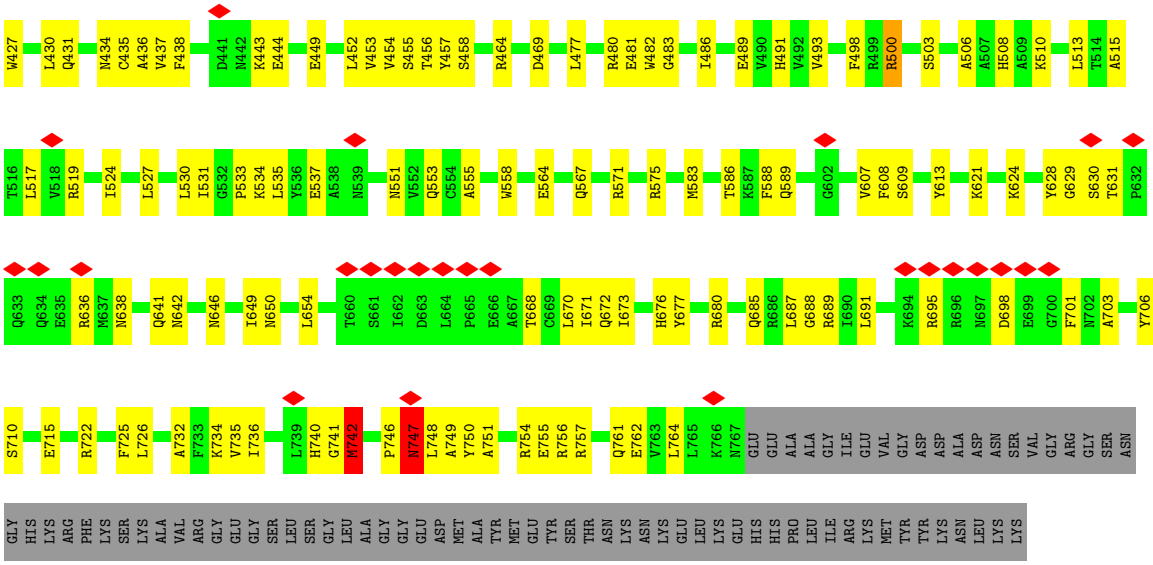
Chain 6:



• Molecule 6: General transcription and DNA repair factor IIH helicase subunit XPB

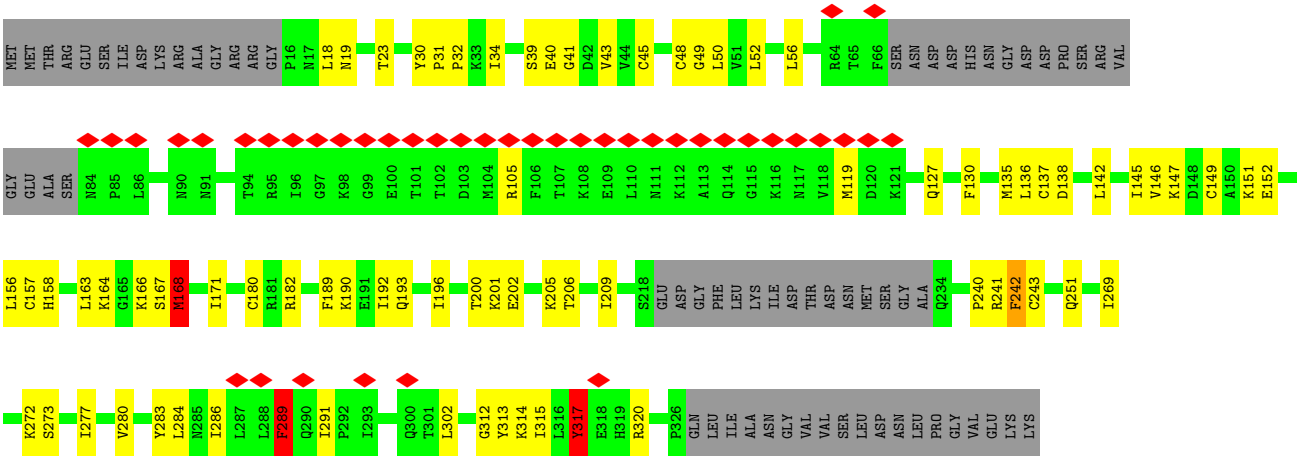
Chain 7:





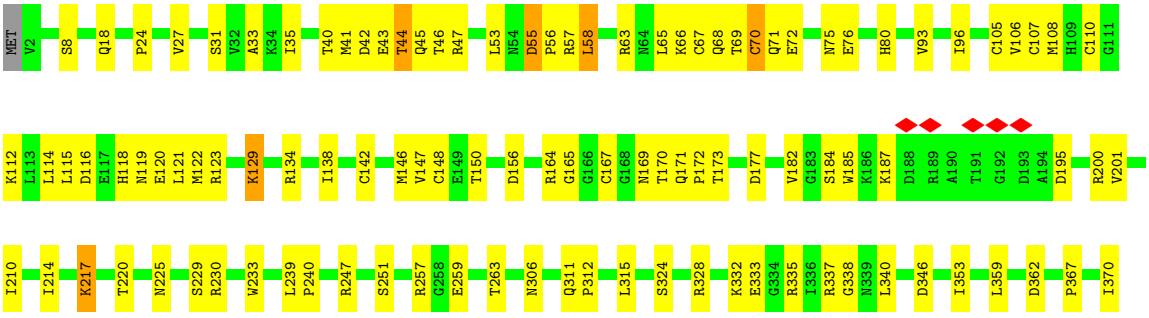
• Molecule 7: Transcription initiation factor IIB

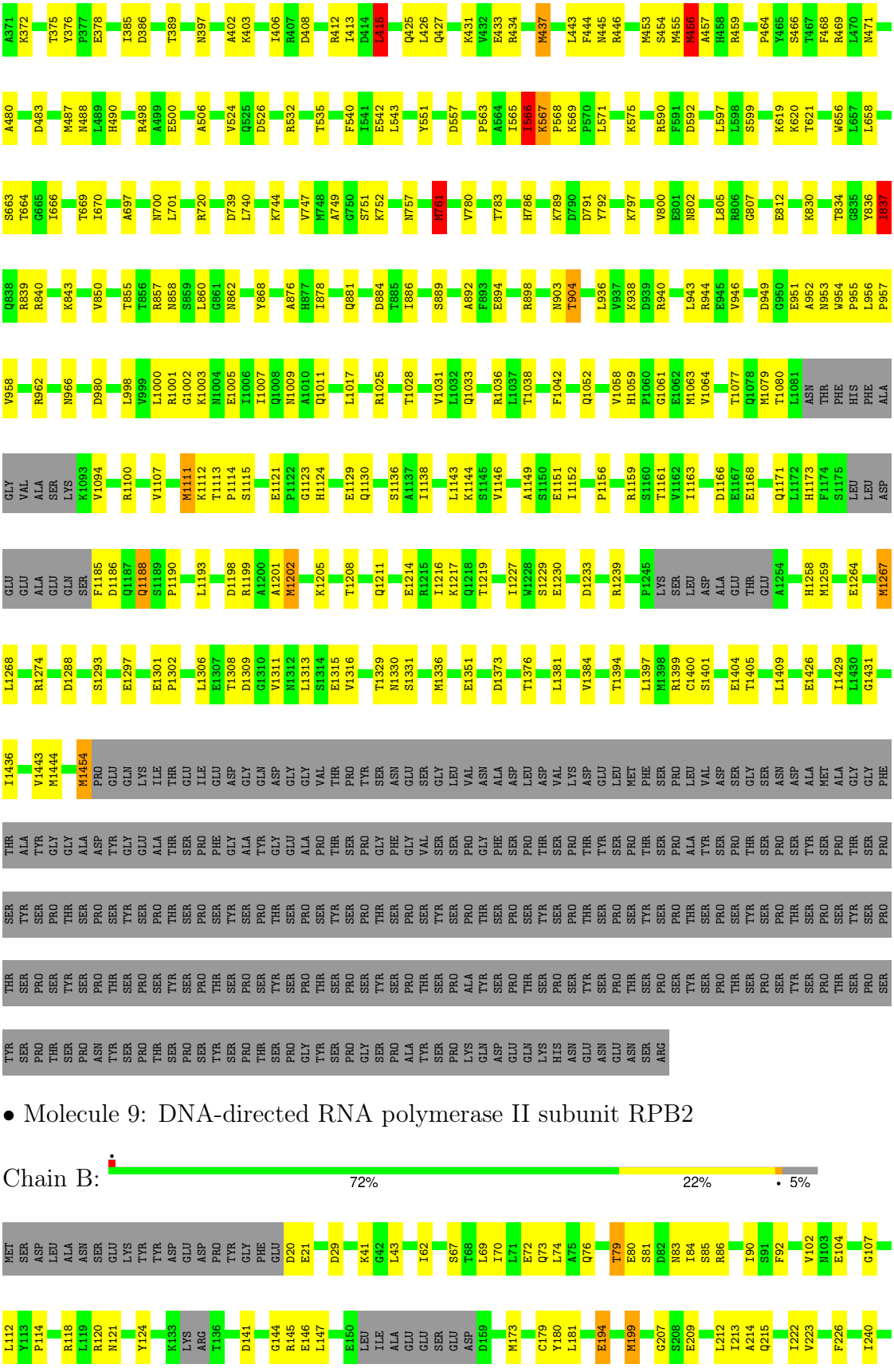
Chain M:



• Molecule 8: DNA-directed RNA polymerase II subunit RPB1

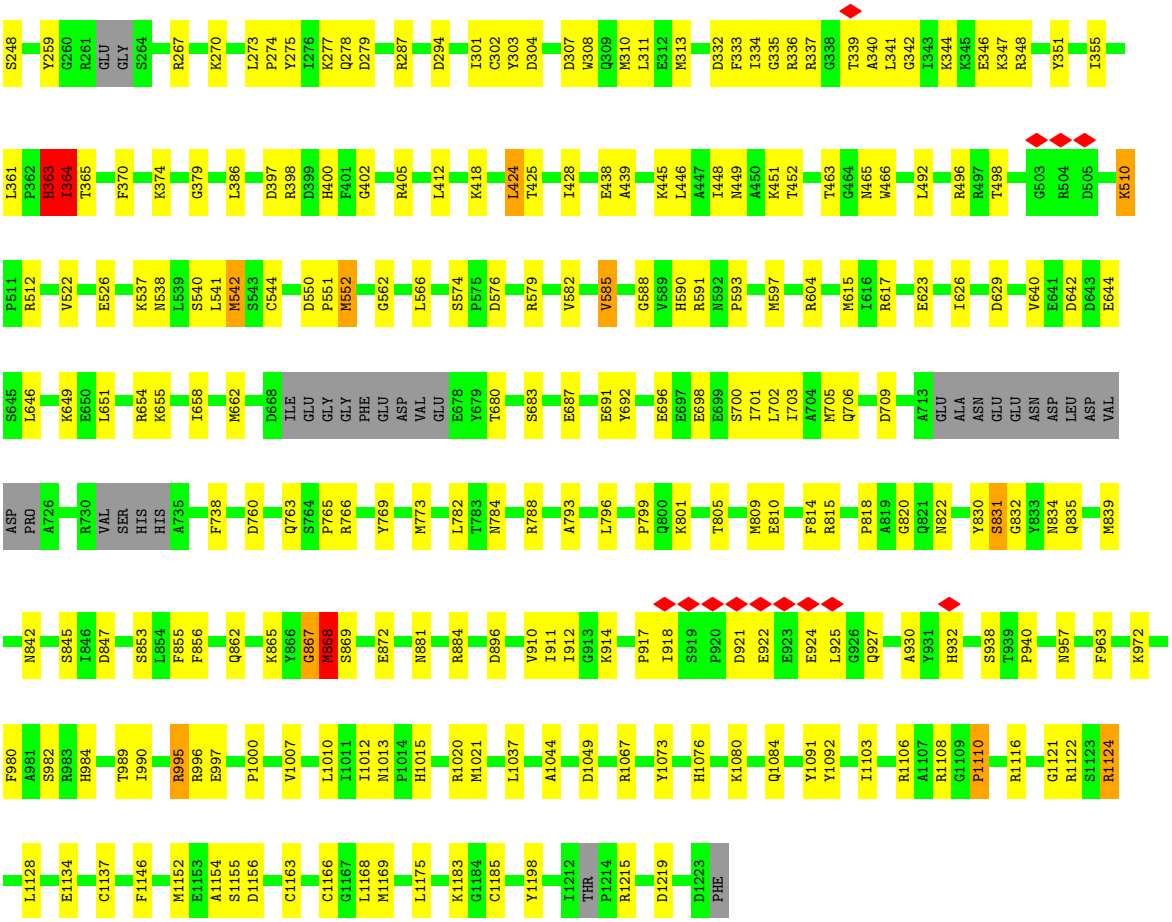
Chain A:





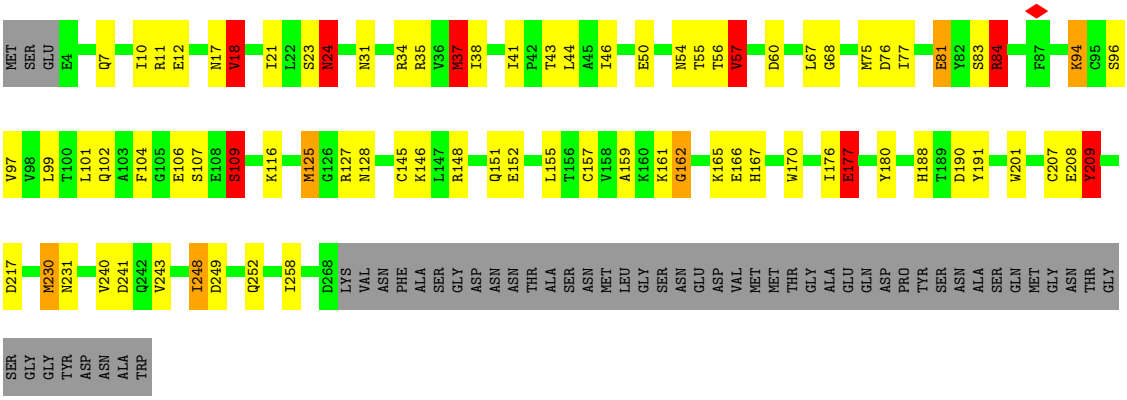
• Molecule 9: DNA-directed RNA polymerase II subunit RPB2

Chain B:



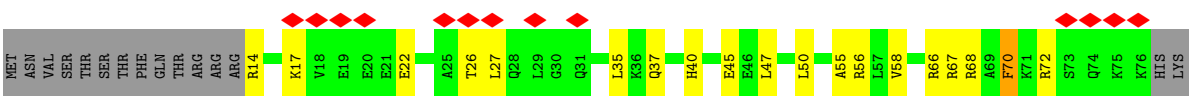
• Molecule 10: DNA-directed RNA polymerase II subunit RPB3

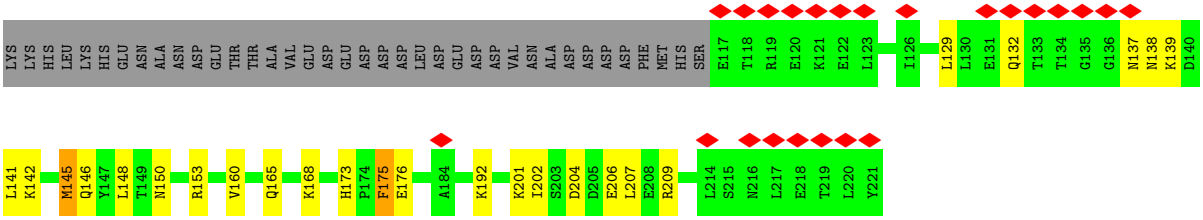
Chain C:



• Molecule 11: DNA-directed RNA polymerase II subunit RPB4

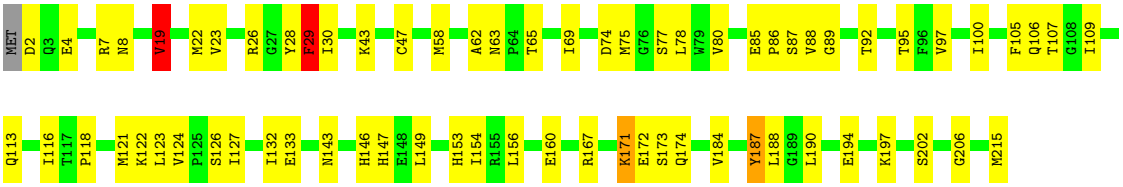
Chain D:





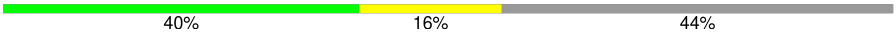
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC1

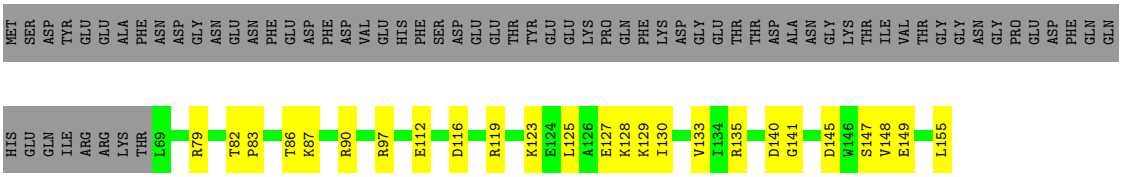
Chain E:



• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC2

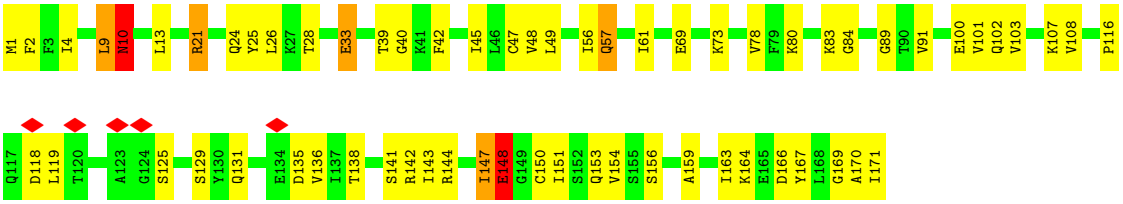
Chain F:





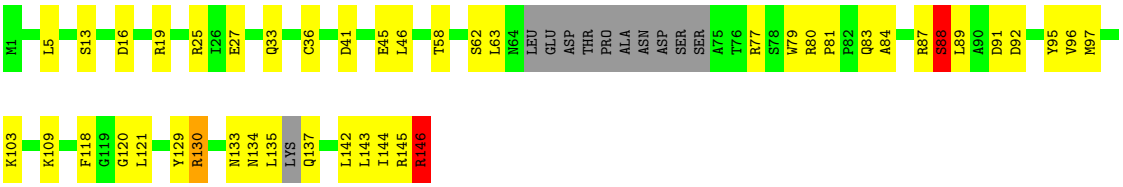
• Molecule 14: DNA-directed RNA polymerase II subunit RPB7

Chain G:



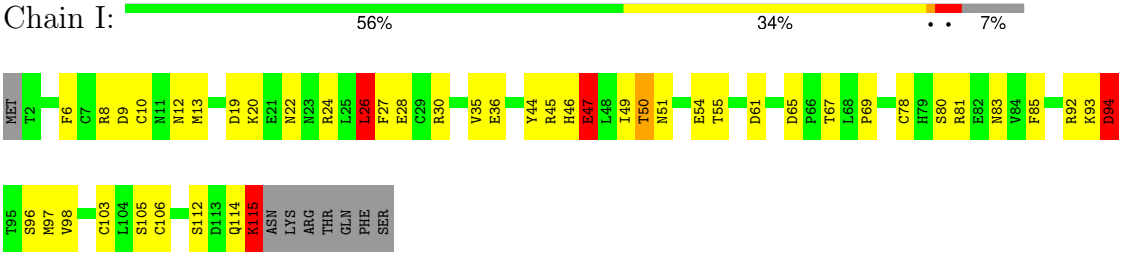
• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



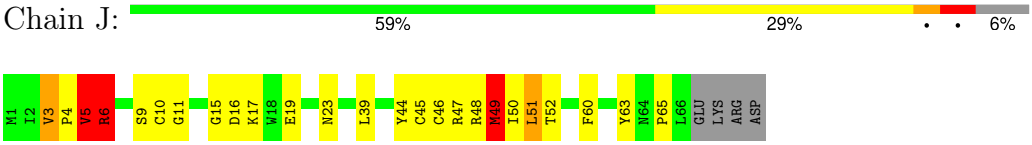
• Molecule 16: DNA-directed RNA polymerase II subunit RPB9

Chain I:



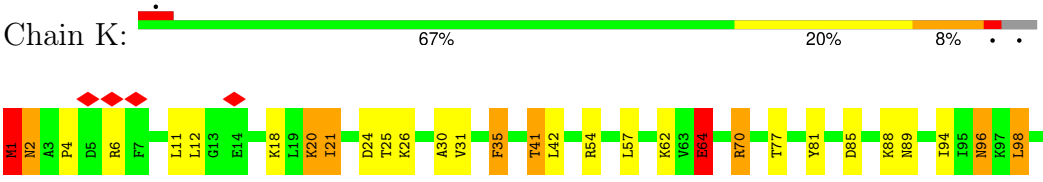
• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



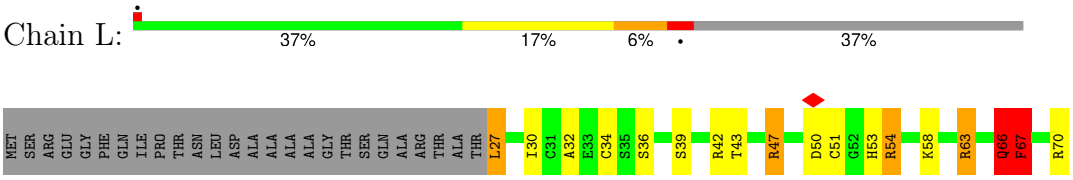
• Molecule 18: DNA-directed RNA polymerase II subunit RPB11

Chain K:



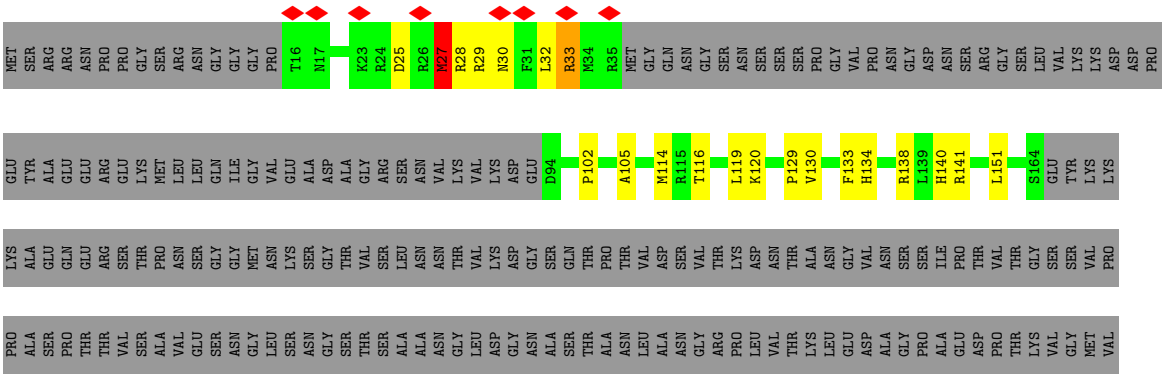
• Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC4

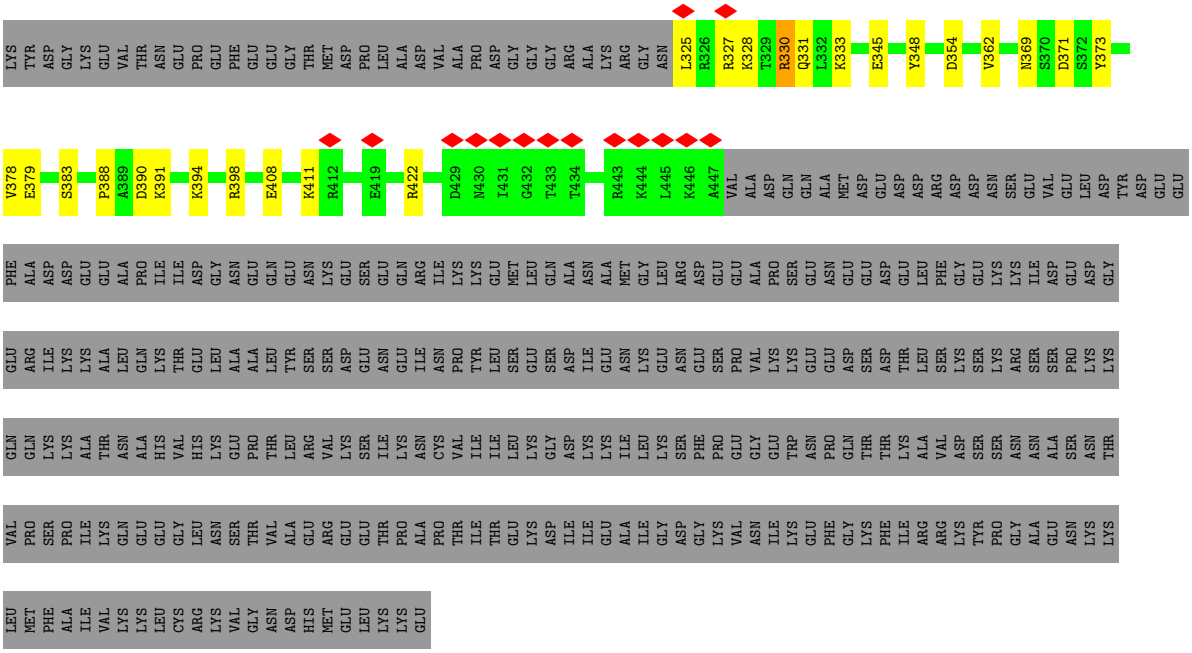
Chain L:



• Molecule 20: Transcription initiation factor IIF subunit alpha

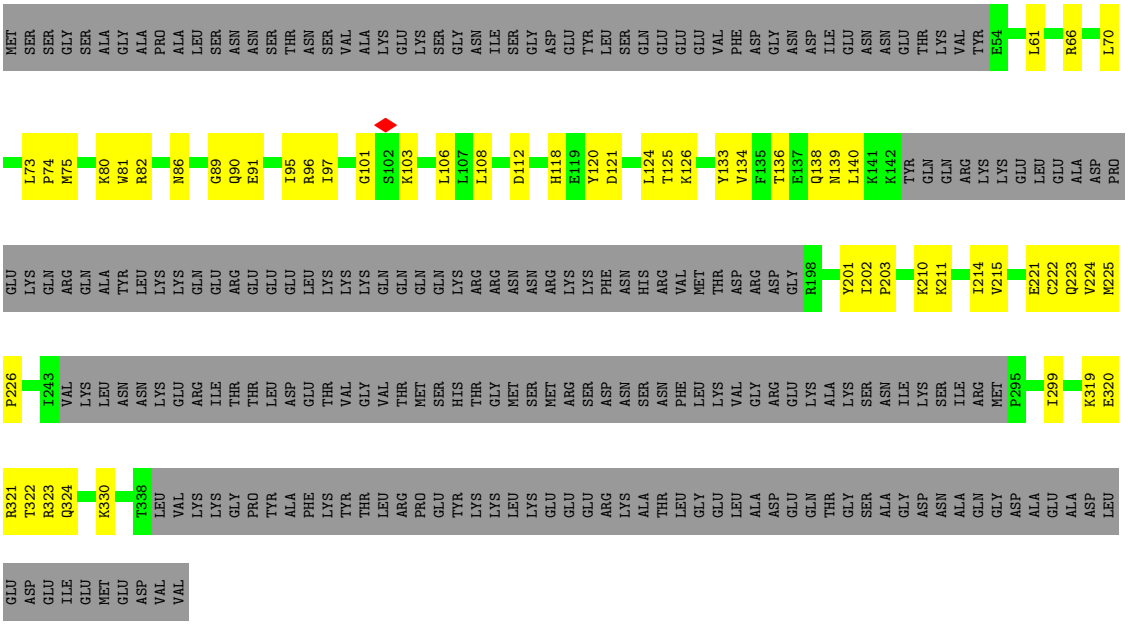
Chain Q:





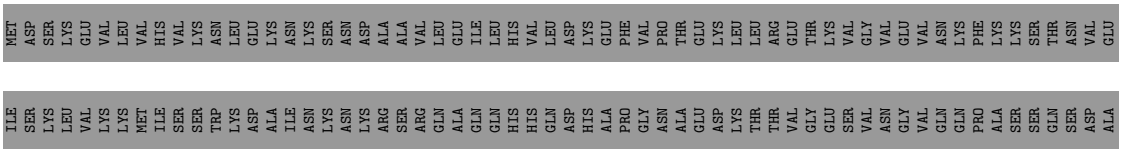
• Molecule 21: Transcription initiation factor IIF subunit beta

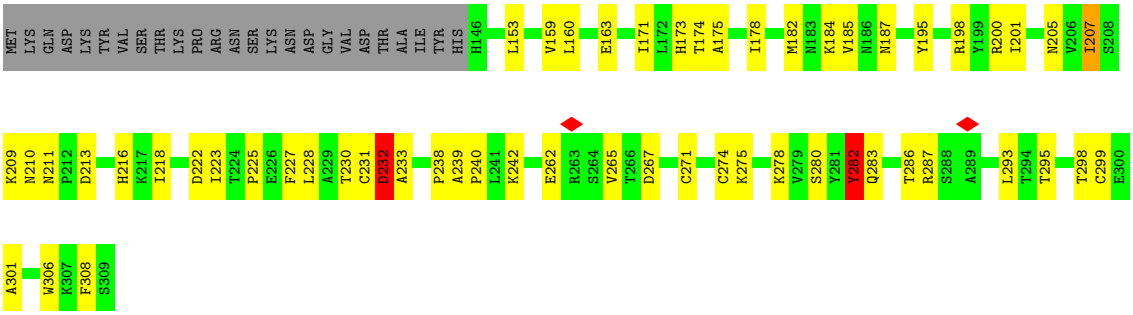
Chain P:



• Molecule 22: Transcription elongation factor S-II

Chain S:



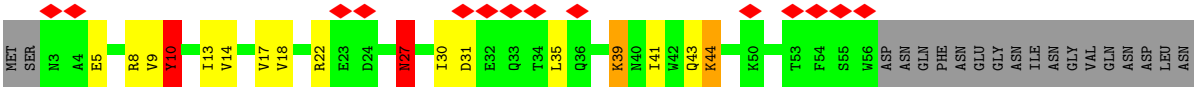


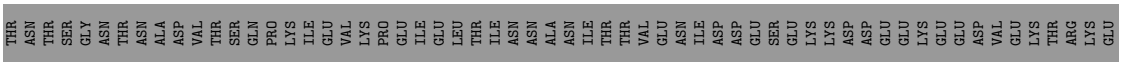
• Molecule 23: TATA-box-binding protein

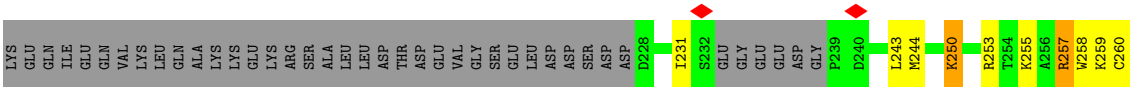
Chain O:

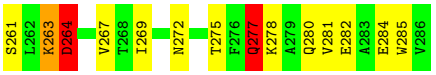
• Molecule 24: Transcription initiation factor IIA large subunit

Chain U:



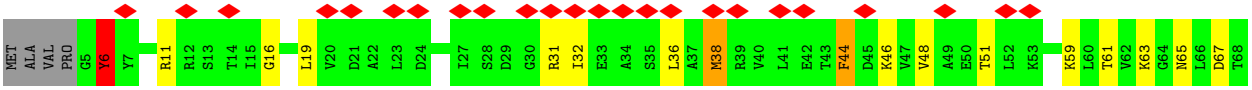


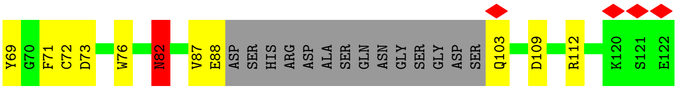




• Molecule 25: Transcription initiation factor IIA subunit 2

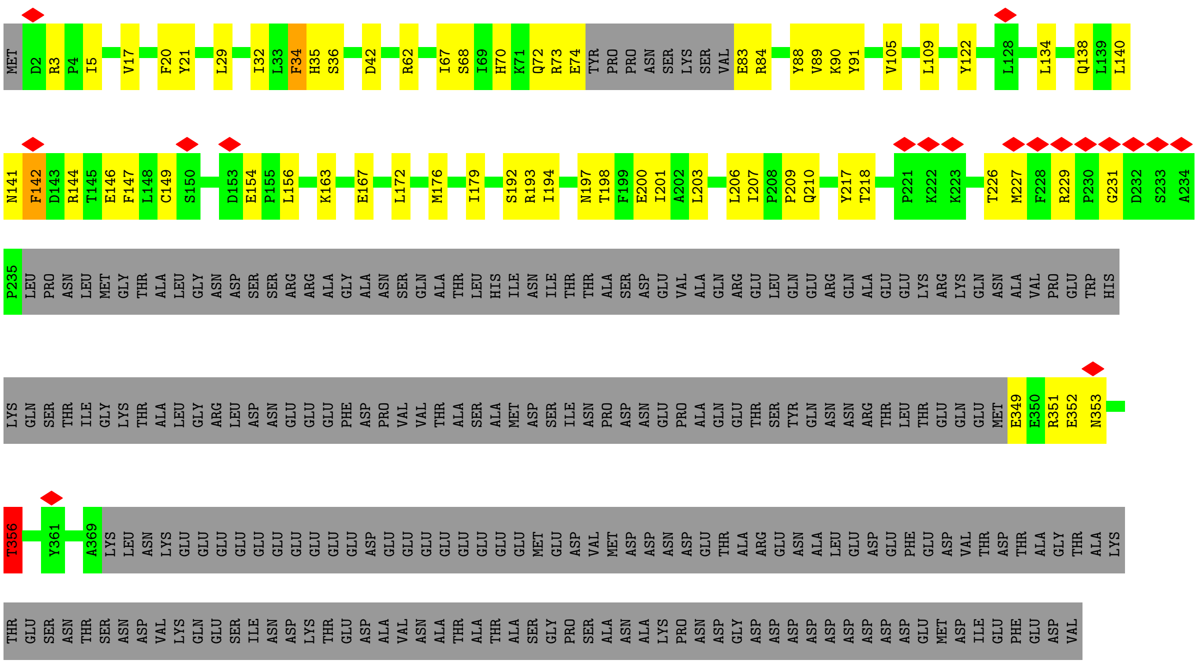
Chain V:





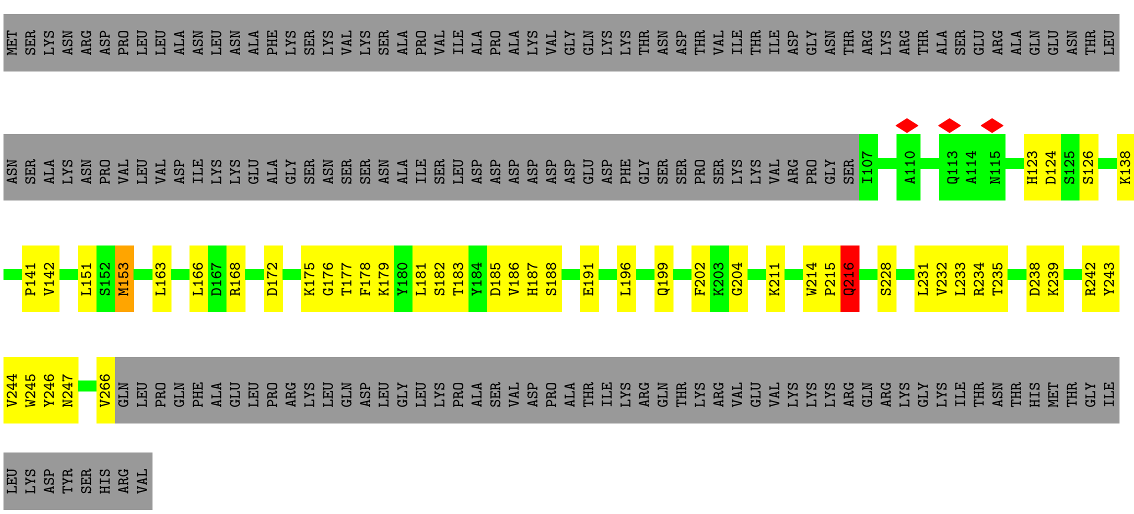
• Molecule 26: Transcription initiation factor IIE subunit alpha

Chain W:



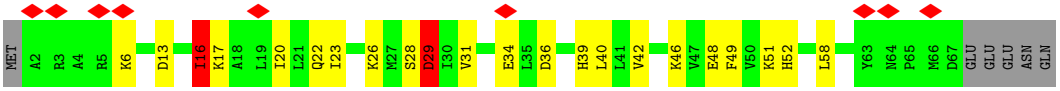
• Molecule 27: Transcription initiation factor IIE subunit beta

Chain X:



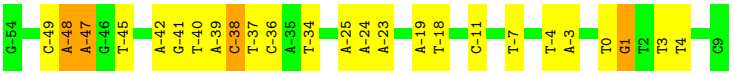
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



• Molecule 29: non-template DNA strand

• Molecule 30: template DNA strand



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.57	11/6209 (0.2%)	0.98	15/8384 (0.2%)
2	1	0.41	3/3434 (0.1%)	0.64	9/4624 (0.2%)
3	2	0.69	14/3611 (0.4%)	1.15	23/4881 (0.5%)
4	4	0.35	0/2305	0.52	0/3117
5	6	0.61	5/2843 (0.2%)	0.96	8/3845 (0.2%)
6	7	0.55	13/4992 (0.3%)	0.83	19/6754 (0.3%)
7	M	1.14	5/2204 (0.2%)	1.94	17/2963 (0.6%)
8	A	0.75	26/11368 (0.2%)	0.94	50/15383 (0.3%)
9	B	0.81	13/9402 (0.1%)	0.95	29/12680 (0.2%)
10	C	1.46	26/2124 (1.2%)	1.91	53/2879 (1.8%)
11	D	0.37	0/1339	0.71	6/1793 (0.3%)
12	E	1.17	14/1788 (0.8%)	2.12	23/2406 (1.0%)
13	F	0.65	0/717	0.72	0/967
14	G	0.66	4/1363 (0.3%)	1.05	9/1840 (0.5%)
15	H	1.02	5/1097 (0.5%)	1.24	9/1484 (0.6%)
16	I	0.81	3/945 (0.3%)	1.16	18/1273 (1.4%)
17	J	1.66	10/549 (1.8%)	2.36	16/738 (2.2%)
18	K	2.14	17/942 (1.8%)	2.37	40/1272 (3.1%)
19	L	2.92	10/354 (2.8%)	5.07	19/468 (4.1%)
20	Q	0.40	0/1648	0.63	3/2226 (0.1%)
21	P	0.35	0/1511	0.57	0/2035
22	S	0.75	5/1317 (0.4%)	0.95	8/1778 (0.4%)
23	O	1.33	13/1449 (0.9%)	2.95	20/1952 (1.0%)
24	U	0.95	10/898 (1.1%)	1.69	22/1212 (1.8%)
25	V	0.92	4/822 (0.5%)	1.42	13/1109 (1.2%)
26	W	0.81	6/2045 (0.3%)	2.10	15/2757 (0.5%)
27	X	0.60	4/1312 (0.3%)	0.87	8/1767 (0.5%)
28	5	0.95	5/502 (1.0%)	1.44	11/677 (1.6%)
29	N	1.17	5/1464 (0.3%)	1.29	8/2258 (0.4%)
30	T	1.33	12/1475 (0.8%)	1.21	8/2274 (0.4%)
All	All	0.86	243/72029 (0.3%)	1.29	479/97796 (0.5%)

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	1	2
3	2	1	1
6	7	2	2
7	M	0	6
8	A	2	11
9	B	0	8
10	C	1	6
11	D	0	2
12	E	1	4
13	F	0	1
14	G	3	4
15	H	2	2
16	I	2	1
17	J	1	2
18	K	3	4
19	L	0	4
22	S	0	4
23	O	1	1
24	U	2	2
25	V	1	2
26	W	0	1
27	X	0	1
28	5	1	1
All	All	24	72

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	64	GLU	CD-OE2	41.17	1.71	1.25
7	M	317	TYR	CG-CD2	40.27	1.91	1.39
23	O	224	TYR	CG-CD2	36.22	1.86	1.39
19	L	67	PHE	CG-CD2	28.28	1.81	1.38
9	B	194	GLU	CD-OE2	28.03	1.56	1.25
19	L	67	PHE	CB-CG	-27.81	1.04	1.51
7	M	317	TYR	CG-CD1	-25.79	1.05	1.39
26	W	34	PHE	CG-CD2	25.54	1.77	1.38
18	K	64	GLU	CD-OE1	-23.28	1.00	1.25
10	C	209	TYR	CG-CD2	21.72	1.67	1.39
12	E	29	PHE	CG-CD2	20.49	1.69	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	177	GLU	CG-CD	-20.23	1.21	1.51
19	L	47	ARG	CB-CG	-19.58	0.99	1.52
10	C	209	TYR	CG-CD1	-19.28	1.14	1.39
9	B	194	GLU	CD-OE1	-18.41	1.05	1.25
19	L	47	ARG	CD-NE	-16.60	1.18	1.46
25	V	82	ASN	CG-ND2	16.53	1.74	1.32
12	E	19	VAL	CB-CG2	16.05	1.86	1.52
6	7	231	ARG	CG-CD	-15.92	1.12	1.51
10	C	84	ARG	NE-CZ	-15.70	1.12	1.33
1	0	659	MET	CG-SD	-15.58	1.40	1.81
30	T	-38	DC	C2-O2	-15.53	1.10	1.24
15	H	146	ARG	CG-CD	-15.42	1.13	1.51
3	2	150	MET	CG-SD	-15.12	1.41	1.81
15	H	88	SER	CB-OG	-14.68	1.23	1.42
8	A	1267	MET	CG-SD	-14.42	1.43	1.81
5	6	450	ASN	CG-ND2	14.19	1.68	1.32
9	B	662	MET	CB-CG	-14.02	1.06	1.51
22	S	282	TYR	CG-CD2	13.96	1.57	1.39
27	X	216	GLN	CD-NE2	13.91	1.67	1.32
17	J	6	ARG	CB-CG	-13.86	1.15	1.52
1	0	547	MET	CB-CG	-13.75	1.07	1.51
18	K	31	VAL	CB-CG2	-13.39	1.24	1.52
10	C	18	VAL	CB-CG1	-13.22	1.25	1.52
8	A	1188	GLN	CD-OE1	-13.18	0.94	1.24
10	C	18	VAL	CB-CG2	13.13	1.80	1.52
19	L	63	ARG	CD-NE	-13.09	1.24	1.46
19	L	63	ARG	CB-CG	-13.08	1.17	1.52
5	6	202	GLN	CD-NE2	13.05	1.65	1.32
12	E	19	VAL	CB-CG1	-12.84	1.25	1.52
8	A	1188	GLN	CD-NE2	12.83	1.65	1.32
18	K	1	MET	CA-C	12.80	1.86	1.52
18	K	1	MET	N-CA	-12.77	1.20	1.46
8	A	217	LYS	CD-CE	-12.73	1.19	1.51
23	O	224	TYR	CG-CD1	-12.60	1.22	1.39
12	E	29	PHE	CG-CD1	-12.09	1.20	1.38
8	A	1202	MET	CB-CG	-12.08	1.12	1.51
10	C	177	GLU	CB-CG	-12.05	1.29	1.52
28	5	16	ILE	CB-CG2	11.99	1.90	1.52
17	J	5	VAL	CB-CG2	11.93	1.77	1.52
30	T	-47	DA	N3-C4	-11.90	1.27	1.34
30	T	-48	DA	N9-C4	-11.81	1.30	1.37
22	S	282	TYR	CG-CD1	-11.75	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	5	VAL	CB-CG1	-11.69	1.28	1.52
5	6	202	GLN	CD-OE1	-11.43	0.98	1.24
12	E	29	PHE	CA-C	11.43	1.82	1.52
18	K	1	MET	C-N	11.43	1.60	1.34
9	B	199	MET	CG-SD	-11.28	1.51	1.81
1	0	659	MET	CB-CG	11.27	1.87	1.51
25	V	38	MET	CA-CB	-11.24	1.29	1.53
23	O	236	GLU	CB-CG	-11.12	1.31	1.52
12	E	75	MET	CG-SD	-11.07	1.52	1.81
17	J	49	MET	CG-SD	-11.05	1.52	1.81
9	B	194	GLU	CG-CD	-11.01	1.35	1.51
26	W	34	PHE	CG-CD1	-10.97	1.22	1.38
10	C	84	ARG	CB-CG	10.94	1.82	1.52
8	A	837	ILE	CB-CG2	10.90	1.86	1.52
24	U	250	LYS	CB-CG	-10.86	1.23	1.52
18	K	64	GLU	CG-CD	10.85	1.68	1.51
5	6	450	ASN	CG-OD1	-10.76	1.00	1.24
3	2	97	MET	CG-SD	-10.71	1.53	1.81
10	C	57	VAL	CB-CG2	10.65	1.75	1.52
14	G	33	GLU	CB-CG	-10.62	1.31	1.52
18	K	70	ARG	CG-CD	-10.61	1.25	1.51
23	O	224	TYR	CB-CG	-10.45	1.35	1.51
26	W	356	THR	CB-CG2	10.38	1.86	1.52
23	O	104	MET	CA-CB	-10.14	1.31	1.53
17	J	6	ARG	NE-CZ	-10.02	1.20	1.33
23	O	221	GLU	CB-CG	-10.02	1.33	1.52
23	O	224	TYR	CD1-CE1	-9.75	1.24	1.39
24	U	39	LYS	CE-NZ	-9.54	1.25	1.49
26	W	34	PHE	CB-CG	-9.50	1.35	1.51
3	2	97	MET	CB-CG	-9.48	1.21	1.51
22	S	232	ASP	CA-C	9.37	1.77	1.52
17	J	49	MET	CB-CG	-9.27	1.21	1.51
10	C	84	ARG	CZ-NH1	9.15	1.45	1.33
7	M	168	MET	CB-CG	-9.13	1.22	1.51
6	7	747	ASN	CA-C	9.10	1.76	1.52
10	C	94	LYS	CE-NZ	-8.96	1.26	1.49
30	T	-47	DA	C2-N3	-8.65	1.25	1.33
8	A	415	LEU	CG-CD2	8.64	1.83	1.51
12	E	29	PHE	CA-CB	-8.62	1.34	1.53
30	T	-48	DA	N9-C8	-8.59	1.30	1.37
30	T	-48	DA	C8-N7	-8.51	1.25	1.31
12	E	29	PHE	N-CA	-8.50	1.29	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	81	MET	CA-CB	8.49	1.72	1.53
12	E	75	MET	CB-CG	-8.47	1.24	1.51
19	L	63	ARG	NE-CZ	-8.44	1.22	1.33
3	2	463	GLU	C-N	8.29	1.53	1.34
3	2	150	MET	CA-CB	8.29	1.72	1.53
10	C	37	MET	CA-C	8.28	1.74	1.52
17	J	6	ARG	CG-CD	-8.27	1.31	1.51
8	A	837	ILE	CB-CG1	-8.23	1.31	1.54
24	U	277	GLN	CB-CG	-8.20	1.30	1.52
1	0	346	MET	CB-CG	-8.18	1.25	1.51
8	A	437	MET	CG-SD	-8.15	1.59	1.81
18	K	2	ASN	CA-C	8.10	1.74	1.52
1	0	659	MET	CA-CB	-8.09	1.36	1.53
3	2	373	MET	CB-CG	-8.07	1.25	1.51
1	0	659	MET	SD-CE	-7.97	1.33	1.77
6	7	418	MET	CG-SD	-7.96	1.60	1.81
10	C	230	MET	CG-SD	-7.96	1.60	1.81
1	0	346	MET	CG-SD	7.92	2.01	1.81
3	2	150	MET	CB-CG	-7.92	1.26	1.51
8	A	761	MET	CG-SD	-7.90	1.60	1.81
28	5	16	ILE	CB-CG1	-7.88	1.31	1.54
26	W	34	PHE	CD1-CE1	-7.86	1.23	1.39
15	H	88	SER	CA-CB	-7.83	1.41	1.52
8	A	217	LYS	CG-CD	-7.77	1.26	1.52
22	S	231	CYS	C-N	7.72	1.51	1.34
10	C	81	GLU	CG-CD	-7.71	1.40	1.51
16	I	26	LEU	CG-CD2	7.70	1.80	1.51
10	C	24	ASN	CA-C	7.69	1.73	1.52
9	B	597	MET	CA-CB	7.62	1.70	1.53
17	J	49	MET	CA-CB	-7.57	1.37	1.53
18	K	103	THR	CB-OG1	-7.55	1.28	1.43
6	7	418	MET	CA-C	7.51	1.72	1.52
29	N	38	DG	C5-C6	-7.42	1.34	1.42
8	A	456	MET	CG-SD	-7.37	1.61	1.81
3	2	487	LYS	CA-C	7.35	1.72	1.52
2	1	358	MET	CA-C	7.34	1.72	1.52
23	O	236	GLU	CG-CD	-7.32	1.41	1.51
30	T	-48	DA	C2-N3	-7.31	1.26	1.33
9	B	194	GLU	CB-CG	7.31	1.66	1.52
28	5	16	ILE	CA-C	7.31	1.72	1.52
3	2	373	MET	CG-SD	-7.30	1.62	1.81
6	7	112	MET	CA-CB	7.15	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	T	-47	DA	C5-C4	7.13	1.43	1.38
1	0	659	MET	N-CA	-7.13	1.32	1.46
6	7	742	MET	N-CA	-7.12	1.32	1.46
12	E	22	MET	CG-SD	-7.03	1.62	1.81
24	U	250	LYS	CG-CD	-6.98	1.28	1.52
24	U	27	ASN	CG-ND2	6.90	1.50	1.32
8	A	904	THR	CB-OG1	-6.89	1.29	1.43
27	X	216	GLN	CD-OE1	-6.86	1.08	1.24
7	M	168	MET	CA-CB	6.85	1.69	1.53
2	1	608	MET	CA-C	6.84	1.70	1.52
30	T	-48	DA	C6-N6	6.84	1.39	1.33
12	E	22	MET	SD-CE	-6.73	1.40	1.77
18	K	21	ILE	CB-CG1	-6.73	1.35	1.54
8	A	837	ILE	CA-C	6.71	1.70	1.52
29	N	47	DT	N3-C4	-6.68	1.33	1.38
12	E	22	MET	CB-CG	-6.65	1.30	1.51
8	A	415	LEU	CG-CD1	-6.65	1.27	1.51
14	G	10	ASN	CA-CB	-6.63	1.35	1.53
16	I	93	LYS	C-N	-6.62	1.18	1.34
19	L	47	ARG	CA-CB	6.59	1.68	1.53
8	A	456	MET	CA-CB	-6.57	1.39	1.53
8	A	1454	MET	CA-CB	-6.57	1.39	1.53
10	C	177	GLU	CA-CB	-6.54	1.39	1.53
8	A	415	LEU	CA-CB	-6.53	1.38	1.53
29	N	0	DA	N9-C4	-6.40	1.34	1.37
6	7	231	ARG	CD-NE	-6.38	1.35	1.46
6	7	112	MET	CB-CG	-6.38	1.30	1.51
3	2	463	GLU	CG-CD	-6.36	1.42	1.51
8	A	1454	MET	CB-CG	-6.35	1.31	1.51
9	B	542	MET	SD-CE	-6.35	1.42	1.77
28	5	28	SER	C-N	6.32	1.48	1.34
24	U	250	LYS	CD-CE	6.29	1.67	1.51
26	W	356	THR	CA-C	6.26	1.69	1.52
10	C	24	ASN	CG-OD1	-6.24	1.10	1.24
6	7	418	MET	N-CA	-6.21	1.33	1.46
3	2	457	SER	C-O	-6.21	1.11	1.23
1	0	547	MET	CG-SD	-6.20	1.65	1.81
10	C	37	MET	N-CA	-6.20	1.33	1.46
23	O	224	TYR	CA-CB	6.19	1.67	1.53
9	B	542	MET	CA-CB	-6.16	1.40	1.53
30	T	-47	DA	N9-C4	-6.13	1.34	1.37
12	E	28	TYR	C-N	-6.13	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	552	MET	CG-SD	-6.11	1.65	1.81
9	B	552	MET	CA-C	6.09	1.68	1.52
7	M	168	MET	CG-SD	-6.08	1.65	1.81
15	H	146	ARG	CD-NE	-6.05	1.36	1.46
17	J	6	ARG	CZ-NH1	6.04	1.40	1.33
18	K	70	ARG	CB-CG	6.02	1.68	1.52
27	X	153	MET	CA-CB	-6.00	1.40	1.53
10	C	109	SER	CB-OG	-6.00	1.34	1.42
10	C	24	ASN	N-CA	-5.99	1.34	1.46
28	5	16	ILE	N-CA	-5.95	1.34	1.46
24	U	250	LYS	CA-CB	5.87	1.66	1.53
1	0	346	MET	CA-CB	-5.86	1.41	1.53
24	U	277	GLN	CA-CB	-5.85	1.41	1.53
14	G	10	ASN	N-CA	-5.84	1.34	1.46
8	A	217	LYS	N-CA	-5.84	1.34	1.46
10	C	177	GLU	CD-OE2	5.84	1.32	1.25
6	7	112	MET	CA-C	5.82	1.68	1.52
23	O	221	GLU	CD-OE1	5.79	1.32	1.25
19	L	67	PHE	CD1-CE1	-5.77	1.27	1.39
18	K	30	ALA	C-N	5.76	1.47	1.34
10	C	57	VAL	CB-CG1	-5.75	1.40	1.52
29	N	48	DT	N1-C2	-5.73	1.33	1.38
9	B	1137	CYS	CB-SG	-5.70	1.72	1.81
23	O	236	GLU	CA-C	5.68	1.67	1.52
8	A	1188	GLN	CG-CD	5.65	1.64	1.51
14	G	148	GLU	CB-CG	-5.65	1.41	1.52
16	I	94	ASP	N-CA	-5.63	1.35	1.46
30	T	-48	DA	C6-N1	-5.63	1.31	1.35
24	U	27	ASN	CB-CG	-5.61	1.38	1.51
5	6	450	ASN	CB-CG	5.58	1.63	1.51
12	E	29	PHE	CD1-CE1	-5.57	1.28	1.39
10	C	230	MET	CB-CG	-5.55	1.33	1.51
18	K	64	GLU	CB-CG	-5.51	1.41	1.52
6	7	742	MET	CA-CB	-5.48	1.41	1.53
30	T	-48	DA	N3-C4	-5.48	1.31	1.34
10	C	248	ILE	CG1-CD1	-5.43	1.12	1.50
8	A	1454	MET	CG-SD	5.42	1.95	1.81
8	A	455	MET	C-N	-5.41	1.21	1.34
23	O	104	MET	N-CA	-5.38	1.35	1.46
2	1	607	SER	C-N	5.37	1.46	1.34
3	2	97	MET	SD-CE	-5.36	1.47	1.77
27	X	216	GLN	CB-CG	-5.33	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	24	ASN	CG-ND2	5.26	1.46	1.32
8	A	837	ILE	N-CA	-5.23	1.35	1.46
15	H	145	ARG	C-N	5.21	1.46	1.34
29	N	38	DG	C6-N1	5.14	1.43	1.39
19	L	66	GLN	CD-NE2	5.14	1.45	1.32
6	7	430	LEU	C-N	-5.14	1.22	1.34
9	B	542	MET	CG-SD	-5.13	1.67	1.81
6	7	201	SER	CB-OG	-5.13	1.35	1.42
24	U	39	LYS	CG-CD	-5.12	1.35	1.52
3	2	464	THR	N-CA	-5.12	1.36	1.46
8	A	656	TRP	CB-CG	-5.09	1.41	1.50
18	K	2	ASN	CB-CG	-5.07	1.39	1.51
22	S	232	ASP	N-CA	-5.06	1.36	1.46
25	V	38	MET	CG-SD	-5.06	1.68	1.81
8	A	8	SER	C-N	-5.05	1.22	1.34
25	V	6	TYR	CG-CD2	5.05	1.45	1.39
1	0	346	MET	N-CA	-5.04	1.36	1.46
18	K	70	ARG	CD-NE	-5.04	1.37	1.46
23	O	221	GLU	CD-OE2	-5.03	1.20	1.25
18	K	31	VAL	CA-C	5.03	1.66	1.52
10	C	248	ILE	CA-CB	-5.02	1.43	1.54
17	J	3	VAL	CB-CG1	-5.01	1.42	1.52

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W	34	PHE	CB-CG-CD1	84.09	179.66	120.80
23	O	224	TYR	CB-CG-CD1	78.29	167.97	121.00
23	O	224	TYR	CB-CG-CD2	-59.20	85.48	121.00
19	L	67	PHE	CB-CG-CD2	-55.53	81.93	120.80
23	O	224	TYR	CG-CD1-CE1	52.04	162.93	121.30
7	M	317	TYR	CB-CG-CD1	50.05	151.03	121.00
10	C	84	ARG	NE-CZ-NH1	-49.22	95.69	120.30
7	M	317	TYR	CB-CG-CD2	-48.45	91.93	121.00
12	E	29	PHE	CB-CG-CD1	46.33	153.23	120.80
1	0	659	MET	CG-SD-CE	45.67	173.27	100.20
3	2	97	MET	CG-SD-CE	44.17	170.87	100.20
19	L	63	ARG	NE-CZ-NH1	-42.77	98.92	120.30
7	M	317	TYR	CG-CD1-CE1	42.17	155.04	121.30
26	W	34	PHE	CB-CG-CD2	-41.84	91.51	120.80
19	L	67	PHE	CB-CG-CD1	41.49	149.85	120.80
12	E	29	PHE	CB-CG-CD2	-41.36	91.85	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	317	TYR	CD1-CG-CD2	-40.24	73.63	117.90
17	J	6	ARG	NE-CZ-NH1	-39.66	100.47	120.30
19	L	63	ARG	NE-CZ-NH2	38.20	139.40	120.30
18	K	64	GLU	OE1-CD-OE2	-36.93	78.98	123.30
26	W	34	PHE	CG-CD1-CE1	34.43	158.68	120.80
12	E	29	PHE	N-CA-CB	33.84	171.52	110.60
23	O	104	MET	CA-CB-CG	33.49	170.23	113.30
9	B	194	GLU	OE1-CD-OE2	-32.57	84.21	123.30
19	L	63	ARG	CD-NE-CZ	31.63	167.88	123.60
23	O	224	TYR	CD1-CG-CD2	-31.48	83.28	117.90
1	0	346	MET	CA-CB-CG	30.24	164.71	113.30
5	6	202	GLN	CG-CD-OE1	29.17	179.94	121.60
6	7	231	ARG	CG-CD-NE	26.96	168.41	111.80
9	B	194	GLU	CG-CD-OE1	26.21	170.73	118.30
12	E	29	PHE	CG-CD1-CE1	25.92	149.31	120.80
12	E	75	MET	CA-CB-CG	25.91	157.35	113.30
18	K	1	MET	N-CA-CB	25.90	157.22	110.60
8	A	217	LYS	CD-CE-NZ	25.67	170.75	111.70
5	6	450	ASN	CB-CG-OD1	25.14	171.88	121.60
19	L	67	PHE	CG-CD1-CE1	25.10	148.41	120.80
12	E	22	MET	CA-CB-CG	25.09	155.95	113.30
1	0	547	MET	CA-CB-CG	24.99	155.78	113.30
24	U	250	LYS	CB-CG-CD	24.24	174.62	111.60
8	A	1454	MET	CA-CB-CG	23.73	153.64	113.30
18	K	21	ILE	CB-CG1-CD1	23.60	179.99	113.90
9	B	199	MET	CA-CB-CG	23.44	153.15	113.30
26	W	34	PHE	CD1-CG-CD2	-23.18	88.17	118.30
10	C	209	TYR	CD1-CG-CD2	-22.94	92.67	117.90
8	A	1267	MET	CG-SD-CE	22.57	136.32	100.20
19	L	63	ARG	CA-CB-CG	22.44	162.77	113.40
14	G	10	ASN	N-CA-CB	22.16	150.49	110.60
15	H	146	ARG	CG-CD-NE	22.16	158.34	111.80
23	O	104	MET	N-CA-CB	22.16	150.48	110.60
19	L	67	PHE	CD1-CG-CD2	-22.04	89.64	118.30
12	E	29	PHE	CD1-CG-CD2	-22.00	89.71	118.30
12	E	75	MET	CB-CG-SD	21.49	176.88	112.40
7	M	168	MET	CB-CG-SD	21.27	176.22	112.40
10	C	177	GLU	CB-CG-CD	21.05	171.02	114.20
9	B	199	MET	CB-CG-SD	20.58	174.15	112.40
3	2	373	MET	CG-SD-CE	20.45	132.91	100.20
10	C	209	TYR	CB-CG-CD2	-20.23	108.86	121.00
18	K	64	GLU	CG-CD-OE1	19.78	157.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	64	GLU	CB-CG-CD	-19.69	61.03	114.20
7	M	317	TYR	CD1-CE1-CZ	-18.62	103.05	119.80
9	B	542	MET	CA-CB-CG	18.45	144.67	113.30
10	C	177	GLU	CA-CB-CG	18.33	153.72	113.40
7	M	168	MET	CA-CB-CG	-18.20	82.36	113.30
1	0	659	MET	N-CA-CB	17.93	142.88	110.60
10	C	18	VAL	CG1-CB-CG2	-17.90	82.26	110.90
26	W	356	THR	CA-CB-CG2	-17.73	87.57	112.40
3	2	97	MET	CA-CB-CG	17.71	143.40	113.30
1	0	547	MET	CB-CG-SD	17.64	165.31	112.40
17	J	49	MET	CA-CB-CG	17.49	143.04	113.30
12	E	19	VAL	CG1-CB-CG2	-17.27	83.26	110.90
25	V	82	ASN	OD1-CG-ND2	-17.17	82.41	121.90
5	6	450	ASN	OD1-CG-ND2	-17.07	82.64	121.90
15	H	146	ARG	CB-CG-CD	16.85	155.42	111.60
12	E	28	TYR	C-N-CA	16.40	162.71	121.70
24	U	39	LYS	CD-CE-NZ	16.37	149.36	111.70
1	0	659	MET	CA-CB-CG	-16.33	85.54	113.30
6	7	112	MET	CB-CG-SD	16.29	161.27	112.40
17	J	49	MET	CG-SD-CE	16.18	126.09	100.20
17	J	6	ARG	NE-CZ-NH2	16.14	128.37	120.30
3	2	150	MET	CB-CG-SD	16.02	160.45	112.40
22	S	282	TYR	CD1-CG-CD2	-15.95	100.35	117.90
9	B	662	MET	CA-CB-CG	15.90	140.33	113.30
3	2	150	MET	CA-CB-CG	-15.84	86.37	113.30
24	U	277	GLN	CA-CB-CG	15.81	148.18	113.40
24	U	264	ASP	CB-CG-OD2	15.69	132.42	118.30
6	7	231	ARG	CA-CB-CG	15.63	147.78	113.40
28	5	29	ASP	CB-CG-OD1	15.60	132.34	118.30
25	V	6	TYR	CB-CG-CD2	-15.45	111.73	121.00
1	0	346	MET	N-CA-CB	15.36	138.24	110.60
23	O	221	GLU	CA-CB-CG	15.19	146.82	113.40
3	2	373	MET	CB-CG-SD	15.00	157.39	112.40
8	A	217	LYS	CB-CG-CD	14.90	150.35	111.60
10	C	37	MET	CG-SD-CE	-14.73	76.63	100.20
8	A	415	LEU	CB-CG-CD1	14.64	135.88	111.00
12	E	22	MET	CB-CG-SD	14.63	156.28	112.40
17	J	5	VAL	CG1-CB-CG2	-14.62	87.52	110.90
10	C	94	LYS	CD-CE-NZ	14.60	145.28	111.70
28	5	16	ILE	CG1-CB-CG2	-14.47	79.57	111.40
1	0	547	MET	CB-CA-C	14.46	139.32	110.40
25	V	82	ASN	CB-CG-ND2	-14.43	82.06	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	1	MET	CA-CB-CG	-14.35	88.91	113.30
8	A	837	ILE	CG1-CB-CG2	-14.22	80.12	111.40
6	7	112	MET	CG-SD-CE	-14.18	77.51	100.20
27	X	216	GLN	CG-CD-NE2	-14.09	82.89	116.70
6	7	418	MET	CG-SD-CE	14.08	122.73	100.20
24	U	264	ASP	CB-CG-OD1	-13.89	105.80	118.30
10	C	84	ARG	CB-CG-CD	-13.88	75.50	111.60
28	5	16	ILE	CA-CB-CG1	13.87	137.34	111.00
10	C	209	TYR	CG-CD1-CE1	13.83	132.37	121.30
25	V	38	MET	CB-CG-SD	13.72	153.57	112.40
18	K	70	ARG	CD-NE-CZ	-13.68	104.45	123.60
27	X	216	GLN	OE1-CD-NE2	-13.67	90.47	121.90
17	J	6	ARG	CB-CG-CD	13.64	147.06	111.60
18	K	64	GLU	CA-CB-CG	13.60	143.32	113.40
14	G	33	GLU	CA-CB-CG	13.53	143.17	113.40
5	6	202	GLN	OE1-CD-NE2	-13.49	90.86	121.90
24	U	27	ASN	CB-CG-OD1	13.39	148.39	121.60
27	X	216	GLN	CG-CD-OE1	13.31	148.23	121.60
9	B	194	GLU	CG-CD-OE2	-13.27	91.76	118.30
8	A	217	LYS	CA-CB-CG	-13.14	84.50	113.40
9	B	597	MET	CA-CB-CG	-13.12	90.99	113.30
18	K	31	VAL	CA-CB-CG2	12.99	130.39	110.90
3	2	463	GLU	O-C-N	12.96	143.44	122.70
10	C	84	ARG	CG-CD-NE	12.89	138.86	111.80
10	C	248	ILE	CB-CG1-CD1	12.82	149.79	113.90
25	V	38	MET	CA-CB-CG	12.70	134.89	113.30
8	A	456	MET	CA-CB-CG	12.70	134.88	113.30
19	L	30	ILE	CA-CB-CG1	-12.67	86.93	111.00
8	A	437	MET	CA-CB-CG	-12.61	91.86	113.30
10	C	84	ARG	CD-NE-CZ	12.34	140.88	123.60
10	C	209	TYR	CD1-CE1-CZ	-12.33	108.70	119.80
3	2	463	GLU	CA-C-N	-12.32	90.08	117.20
10	C	57	VAL	CG1-CB-CG2	-12.10	91.55	110.90
12	E	29	PHE	CB-CA-C	-12.07	86.25	110.40
10	C	248	ILE	CA-CB-CG1	12.00	133.79	111.00
23	O	104	MET	CG-SD-CE	11.93	119.28	100.20
18	K	64	GLU	CG-CD-OE2	-11.92	94.45	118.30
10	C	84	ARG	NH1-CZ-NH2	-11.86	106.35	119.40
24	U	27	ASN	CB-CG-ND2	-11.82	88.34	116.70
3	2	150	MET	CG-SD-CE	11.81	119.09	100.20
8	A	1188	GLN	OE1-CD-NE2	-11.79	94.78	121.90
3	2	81	MET	CA-CB-CG	-11.74	93.33	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	418	MET	CB-CG-SD	11.62	147.26	112.40
19	L	30	ILE	CB-CG1-CD1	11.59	146.35	113.90
10	C	209	TYR	CB-CG-CD1	11.51	127.91	121.00
5	6	202	GLN	CG-CD-NE2	-11.51	89.08	116.70
15	H	146	ARG	NE-CZ-NH1	-11.50	114.55	120.30
12	E	19	VAL	CA-CB-CG1	11.49	128.14	110.90
18	K	21	ILE	CA-CB-CG1	-11.47	89.20	111.00
5	6	450	ASN	CB-CG-ND2	-11.43	89.26	116.70
23	O	236	GLU	CB-CA-C	-11.39	87.62	110.40
9	B	662	MET	CB-CA-C	11.34	133.08	110.40
18	K	21	ILE	CG1-CB-CG2	-11.28	86.58	111.40
8	A	837	ILE	CA-CB-CG1	11.15	132.19	111.00
18	K	20	LYS	CA-CB-CG	11.14	137.90	113.40
16	I	93	LYS	C-N-CA	11.03	149.28	121.70
26	W	356	THR	OG1-CB-CG2	-11.03	84.63	110.00
16	I	94	ASP	CB-CG-OD1	11.01	128.21	118.30
18	K	70	ARG	CG-CD-NE	10.98	134.85	111.80
24	U	10	TYR	CB-CG-CD2	-10.97	114.42	121.00
19	L	63	ARG	CB-CG-CD	10.97	140.12	111.60
19	L	67	PHE	CB-CA-C	10.97	132.34	110.40
15	H	88	SER	CA-CB-OG	10.85	140.51	111.20
10	C	18	VAL	CA-CB-CG1	10.79	127.08	110.90
18	K	1	MET	C-N-CA	-10.76	94.80	121.70
2	1	358	MET	CB-CA-C	-10.54	89.32	110.40
8	A	1202	MET	N-CA-CB	-10.51	91.69	110.60
8	A	217	LYS	CG-CD-CE	10.49	143.36	111.90
18	K	70	ARG	NE-CZ-NH1	10.39	125.49	120.30
8	A	1202	MET	CB-CA-C	10.36	131.12	110.40
3	2	463	GLU	C-N-CA	-10.33	95.87	121.70
17	J	6	ARG	CA-CB-CG	10.33	136.12	113.40
17	J	49	MET	CB-CG-SD	10.25	143.14	112.40
9	B	662	MET	N-CA-CB	-10.21	92.22	110.60
14	G	9	LEU	C-N-CA	10.21	147.22	121.70
6	7	742	MET	N-CA-CB	10.19	128.94	110.60
6	7	747	ASN	N-CA-C	-10.19	83.50	111.00
10	C	230	MET	CG-SD-CE	10.19	116.50	100.20
23	O	221	GLU	CG-CD-OE2	10.17	138.64	118.30
8	A	437	MET	CG-SD-CE	10.17	116.47	100.20
8	A	1188	GLN	CG-CD-OE1	10.12	141.85	121.60
23	O	221	GLU	N-CA-CB	-10.12	92.38	110.60
1	0	346	MET	CB-CG-SD	-10.12	82.04	112.40
1	0	346	MET	CB-CA-C	-10.06	90.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	39	LYS	CG-CD-CE	9.97	141.81	111.90
12	E	19	VAL	CA-CB-CG2	-9.94	95.99	110.90
12	E	29	PHE	CA-CB-CG	-9.86	90.24	113.90
10	C	12	GLU	N-CA-CB	9.86	128.34	110.60
8	A	415	LEU	CA-CB-CG	9.85	137.94	115.30
2	1	358	MET	CA-CB-CG	9.83	130.02	113.30
25	V	6	TYR	CB-CG-CD1	9.83	126.90	121.00
14	G	33	GLU	CB-CA-C	9.81	130.03	110.40
9	B	662	MET	CG-SD-CE	-9.80	84.52	100.20
7	M	317	TYR	CA-CB-CG	-9.74	94.89	113.40
24	U	277	GLN	N-CA-CB	-9.70	93.14	110.60
27	X	216	GLN	CB-CG-CD	9.68	136.75	111.60
18	K	70	ARG	CB-CG-CD	-9.67	86.47	111.60
7	M	242	PHE	CB-CG-CD2	-9.63	114.06	120.80
17	J	5	VAL	CA-CB-CG1	9.56	125.24	110.90
24	U	250	LYS	CA-CB-CG	-9.55	92.40	113.40
22	S	232	ASP	CB-CG-OD1	-9.55	109.71	118.30
8	A	1188	GLN	CG-CD-NE2	-9.53	93.84	116.70
25	V	44	PHE	CB-CG-CD2	-9.51	114.14	120.80
23	O	236	GLU	CB-CG-CD	9.45	139.70	114.20
24	U	27	ASN	CA-CB-CG	9.42	134.12	113.40
10	C	24	ASN	CA-CB-CG	-9.40	92.71	113.40
8	A	1202	MET	CA-CB-CG	9.39	129.27	113.30
8	A	415	LEU	CB-CG-CD2	-9.39	95.03	111.00
9	B	542	MET	CB-CA-C	9.35	129.10	110.40
9	B	542	MET	CG-SD-CE	9.34	115.15	100.20
11	D	175	PHE	CB-CG-CD2	-9.31	114.28	120.80
26	W	142	PHE	CB-CG-CD2	-9.28	114.30	120.80
25	V	38	MET	CG-SD-CE	9.26	115.02	100.20
23	O	221	GLU	CG-CD-OE1	-9.19	99.92	118.30
15	H	146	ARG	NE-CZ-NH2	9.18	124.89	120.30
18	K	20	LYS	N-CA-CB	-9.18	94.08	110.60
16	I	26	LEU	CB-CG-CD2	-9.11	95.52	111.00
10	C	177	GLU	OE1-CD-OE2	-9.09	112.39	123.30
8	A	217	LYS	N-CA-CB	9.07	126.93	110.60
22	S	232	ASP	N-CA-C	-9.06	86.52	111.00
12	E	29	PHE	CD1-CE1-CZ	-9.05	109.24	120.10
10	C	24	ASN	N-CA-CB	9.02	126.84	110.60
23	O	104	MET	CB-CA-C	-8.98	92.43	110.40
10	C	18	VAL	CA-CB-CG2	-8.93	97.51	110.90
9	B	194	GLU	CB-CG-CD	-8.92	90.12	114.20
3	2	373	MET	CB-CA-C	-8.91	92.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	153	MET	CA-CB-CG	8.88	128.40	113.30
24	U	277	GLN	CG-CD-OE1	-8.84	103.92	121.60
28	5	16	ILE	N-CA-CB	8.84	131.13	110.80
8	A	1267	MET	CB-CG-SD	8.83	138.90	112.40
26	W	356	THR	CB-CA-C	-8.82	87.80	111.60
25	V	44	PHE	CB-CG-CD1	8.76	126.93	120.80
28	5	29	ASP	CB-CG-OD2	-8.74	110.43	118.30
15	H	146	ARG	N-CA-CB	8.74	126.33	110.60
8	A	1454	MET	CB-CG-SD	-8.73	86.22	112.40
8	A	415	LEU	N-CA-CB	-8.72	92.96	110.40
22	S	282	TYR	CD1-CE1-CZ	-8.68	111.99	119.80
27	X	216	GLN	CA-CB-CG	8.66	132.45	113.40
24	U	277	GLN	CB-CG-CD	8.62	134.02	111.60
18	K	20	LYS	CG-CD-CE	8.62	137.76	111.90
1	0	547	MET	N-CA-CB	-8.62	95.09	110.60
10	C	84	ARG	NE-CZ-NH2	8.62	124.61	120.30
10	C	230	MET	CB-CG-SD	8.56	138.09	112.40
22	S	231	CYS	C-N-CA	-8.54	100.34	121.70
17	J	5	VAL	CA-CB-CG2	-8.54	98.09	110.90
22	S	282	TYR	CG-CD1-CE1	8.53	128.12	121.30
22	S	282	TYR	CB-CG-CD2	-8.52	115.89	121.00
8	A	456	MET	CB-CG-SD	8.48	137.85	112.40
7	M	283	TYR	CB-CG-CD2	-8.44	115.94	121.00
15	H	88	SER	CB-CA-C	8.43	126.11	110.10
18	K	42	LEU	CB-CG-CD1	8.41	125.29	111.00
1	0	658	ALA	C-N-CA	8.35	142.57	121.70
10	C	209	TYR	N-CA-CB	8.32	125.58	110.60
16	I	94	ASP	CA-CB-CG	-8.31	95.11	113.40
23	O	224	TYR	CA-CB-CG	-8.29	97.65	113.40
8	A	904	THR	N-CA-CB	-8.29	94.55	110.30
8	A	761	MET	CA-CB-CG	8.21	127.26	113.30
19	L	67	PHE	N-CA-CB	-8.21	95.82	110.60
18	K	103	THR	N-CA-CB	-8.14	94.83	110.30
3	2	97	MET	N-CA-CB	8.12	125.22	110.60
16	I	47	GLU	N-CA-CB	8.12	125.22	110.60
8	A	1454	MET	N-CA-CB	-8.09	96.04	110.60
5	6	450	ASN	CA-CB-CG	7.98	130.96	113.40
10	C	37	MET	CB-CA-C	-7.90	94.61	110.40
2	1	608	MET	N-CA-C	-7.84	89.82	111.00
5	6	202	GLN	CB-CG-CD	7.84	131.97	111.60
17	J	51	LEU	CA-CB-CG	7.80	133.24	115.30
17	J	51	LEU	CB-CA-C	-7.80	95.38	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	837	ILE	N-CA-CB	7.79	128.71	110.80
26	W	20	PHE	CB-CG-CD2	-7.75	115.38	120.80
6	7	741	GLY	C-N-CA	7.70	140.96	121.70
10	C	81	GLU	N-CA-CB	-7.64	96.84	110.60
10	C	209	TYR	CA-CB-CG	-7.64	98.88	113.40
8	A	437	MET	CB-CG-SD	7.60	135.20	112.40
18	K	20	LYS	CB-CA-C	7.59	125.58	110.40
23	O	224	TYR	CD1-CE1-CZ	-7.59	112.97	119.80
10	C	230	MET	N-CA-CB	-7.54	97.02	110.60
15	H	146	ARG	CD-NE-CZ	-7.54	113.05	123.60
18	K	64	GLU	CB-CA-C	7.53	125.45	110.40
24	U	264	ASP	N-CA-CB	7.52	124.13	110.60
2	1	385	MET	CB-CA-C	7.51	125.42	110.40
10	C	24	ASN	CB-CA-C	-7.48	95.44	110.40
10	C	24	ASN	N-CA-C	-7.47	90.82	111.00
20	Q	27	MET	CG-SD-CE	-7.47	88.24	100.20
8	A	415	LEU	CD1-CG-CD2	-7.46	88.13	110.50
14	G	148	GLU	CA-CB-CG	7.42	129.73	113.40
10	C	230	MET	CA-CB-CG	-7.42	100.68	113.30
6	7	418	MET	CB-CA-C	-7.37	95.67	110.40
16	I	20	LYS	CD-CE-NZ	7.29	128.47	111.70
16	I	50	THR	CA-CB-CG2	7.28	122.59	112.40
18	K	2	ASN	N-CA-C	-7.27	91.37	111.00
10	C	57	VAL	CA-CB-CG2	-7.26	100.01	110.90
29	N	6	DA	O4'-C4'-C3'	-7.25	101.60	104.50
8	A	761	MET	CB-CG-SD	7.25	134.14	112.40
10	C	81	GLU	CB-CA-C	7.23	124.86	110.40
6	7	231	ARG	CB-CA-C	7.19	124.78	110.40
14	G	10	ASN	CA-CB-CG	7.18	129.20	113.40
16	I	26	LEU	CD1-CG-CD2	-7.17	88.99	110.50
10	C	57	VAL	CB-CA-C	7.16	125.01	111.40
18	K	21	ILE	N-CA-C	-7.14	91.73	111.00
3	2	466	GLN	CB-CG-CD	7.13	130.14	111.60
18	K	31	VAL	CG1-CB-CG2	7.13	122.31	110.90
8	A	761	MET	CG-SD-CE	7.13	111.61	100.20
3	2	466	GLN	CA-CB-CG	7.09	129.00	113.40
2	1	607	SER	C-N-CA	-7.03	104.12	121.70
26	W	20	PHE	CB-CG-CD1	7.02	125.71	120.80
25	V	82	ASN	CA-CB-CG	6.96	128.72	113.40
22	S	282	TYR	CB-CA-C	6.95	124.29	110.40
2	1	608	MET	CA-CB-CG	6.93	125.09	113.30
3	2	487	LYS	CB-CA-C	-6.92	96.57	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	94	ASP	N-CA-CB	6.91	123.04	110.60
18	K	31	VAL	N-CA-CB	6.91	126.70	111.50
16	I	115	LYS	CB-CG-CD	6.86	129.43	111.60
9	B	542	MET	CB-CG-SD	-6.86	91.83	112.40
3	2	373	MET	N-CA-CB	6.85	122.93	110.60
23	O	221	GLU	CB-CG-CD	6.84	132.68	114.20
18	K	1	MET	CB-CA-C	-6.84	96.72	110.40
8	A	455	MET	CA-CB-CG	6.80	124.86	113.30
3	2	487	LYS	CA-CB-CG	-6.78	98.49	113.40
18	K	1	MET	CA-C-O	-6.76	105.90	120.10
18	K	30	ALA	C-N-CA	-6.75	104.83	121.70
26	W	356	THR	CA-CB-OG1	6.75	123.17	109.00
9	B	552	MET	CB-CG-SD	6.74	132.63	112.40
24	U	10	TYR	CB-CG-CD1	6.74	125.05	121.00
7	M	242	PHE	CB-CG-CD1	6.71	125.50	120.80
6	7	742	MET	CG-SD-CE	-6.71	89.46	100.20
30	T	1	DG	O4'-C4'-C3'	-6.71	101.82	104.50
24	U	27	ASN	CB-CA-C	6.71	123.81	110.40
6	7	747	ASN	N-CA-CB	6.69	122.65	110.60
9	B	542	MET	N-CA-CB	-6.67	98.59	110.60
20	Q	27	MET	N-CA-CB	-6.67	98.59	110.60
10	C	17	ASN	C-N-CA	6.63	138.28	121.70
29	N	47	DT	C6-N1-C2	6.62	124.61	121.30
18	K	41	THR	C-N-CA	6.60	138.20	121.70
7	M	283	TYR	CB-CG-CD1	6.59	124.95	121.00
8	A	1202	MET	CG-SD-CE	-6.59	89.65	100.20
23	O	104	MET	CB-CG-SD	-6.57	92.68	112.40
1	0	547	MET	CG-SD-CE	6.57	110.70	100.20
24	U	250	LYS	CG-CD-CE	-6.57	92.20	111.90
28	5	16	ILE	CA-CB-CG2	-6.56	97.79	110.90
3	2	373	MET	CA-CB-CG	-6.52	102.22	113.30
10	C	75	MET	CA-CB-CG	6.51	124.38	113.30
28	5	16	ILE	N-CA-C	-6.51	93.41	111.00
8	A	58	LEU	CA-CB-CG	6.51	130.27	115.30
18	K	31	VAL	N-CA-C	-6.51	93.43	111.00
28	5	29	ASP	CA-CB-CG	-6.50	99.11	113.40
16	I	47	GLU	CA-CB-CG	6.45	127.60	113.40
10	C	12	GLU	CB-CA-C	-6.45	97.50	110.40
3	2	487	LYS	N-CA-C	-6.45	93.60	111.00
9	B	424	LEU	CB-CG-CD1	-6.44	100.05	111.00
9	B	79	THR	C-N-CA	6.43	137.79	121.70
12	E	29	PHE	N-CA-C	-6.41	93.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	358	MET	N-CA-C	-6.38	93.76	111.00
6	7	583	MET	CA-CB-CG	6.38	124.15	113.30
30	T	-47	DA	C6-C5-N7	6.37	136.76	132.30
9	B	831	SER	C-N-CA	-6.37	108.93	122.30
10	C	109	SER	N-CA-CB	-6.34	100.98	110.50
24	U	277	GLN	CG-CD-NE2	6.34	131.92	116.70
29	N	52	DA	O4'-C1'-N9	6.32	112.42	108.00
19	L	66	GLN	CG-CD-NE2	-6.32	101.55	116.70
17	J	6	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
17	J	6	ARG	CD-NE-CZ	6.28	132.39	123.60
19	L	27	LEU	CA-CB-CG	6.25	129.69	115.30
27	X	151	LEU	CA-CB-CG	6.24	129.65	115.30
6	7	747	ASN	CB-CA-C	-6.24	97.93	110.40
18	K	35	PHE	CB-CG-CD2	-6.24	116.44	120.80
16	I	50	THR	N-CA-CB	-6.23	98.47	110.30
10	C	67	LEU	CB-CG-CD2	-6.21	100.44	111.00
3	2	487	LYS	CB-CG-CD	6.21	127.74	111.60
11	D	175	PHE	CB-CG-CD1	6.20	125.14	120.80
26	W	142	PHE	CB-CG-CD1	6.18	125.13	120.80
10	C	177	GLU	CG-CD-OE2	-6.18	105.94	118.30
7	M	168	MET	N-CA-C	-6.14	94.41	111.00
8	A	837	ILE	N-CA-C	-6.12	94.49	111.00
10	C	37	MET	N-CA-C	-6.12	94.49	111.00
9	B	868	MET	CA-CB-CG	6.10	123.67	113.30
29	N	37	DA	O4'-C4'-C3'	-6.10	102.06	104.50
23	O	236	GLU	N-CA-CB	6.09	121.56	110.60
1	0	229	ASP	N-CA-C	-6.06	94.65	111.00
24	U	263	LYS	C-N-CA	-6.05	106.57	121.70
6	7	230	ASN	C-N-CA	6.04	136.79	121.70
6	7	112	MET	N-CA-C	-6.03	94.71	111.00
20	Q	27	MET	CB-CA-C	6.02	122.44	110.40
25	V	82	ASN	CB-CG-OD1	5.99	133.59	121.60
27	X	153	MET	CB-CG-SD	-5.99	94.43	112.40
8	A	455	MET	C-N-CA	5.99	136.67	121.70
11	D	70	PHE	CB-CG-CD2	-5.98	116.62	120.80
8	A	70	CYS	CA-CB-SG	5.97	124.74	114.00
25	V	38	MET	CB-CA-C	5.93	122.26	110.40
10	C	23	SER	C-N-CA	5.91	136.48	121.70
16	I	50	THR	OG1-CB-CG2	5.90	123.58	110.00
16	I	47	GLU	CB-CG-CD	5.90	130.12	114.20
10	C	248	ILE	N-CA-CB	-5.88	97.29	110.80
12	E	75	MET	CG-SD-CE	-5.87	90.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	904	THR	CA-CB-CG2	5.87	120.62	112.40
10	C	24	ASN	CB-CG-OD1	5.87	133.33	121.60
6	7	112	MET	CA-CB-CG	-5.87	103.33	113.30
9	B	867	GLY	C-N-CA	5.86	136.34	121.70
26	W	34	PHE	CD1-CE1-CZ	-5.86	113.07	120.10
1	0	525	MET	CA-CB-CG	5.82	123.20	113.30
15	H	146	ARG	N-CA-C	5.81	126.68	111.00
2	1	358	MET	N-CA-CB	5.77	120.99	110.60
19	L	47	ARG	CD-NE-CZ	-5.74	115.56	123.60
29	N	48	DT	O4'-C4'-C3'	-5.74	102.20	104.50
8	A	837	ILE	CA-CB-CG2	-5.74	99.42	110.90
8	A	456	MET	CB-CA-C	5.74	121.88	110.40
18	K	1	MET	CA-C-N	5.74	129.83	117.20
12	E	187	TYR	CB-CG-CD1	5.73	124.44	121.00
16	I	94	ASP	CB-CG-OD2	-5.72	113.15	118.30
18	K	96	ASN	N-CA-CB	-5.71	100.32	110.60
28	5	29	ASP	OD1-CG-OD2	-5.71	112.45	123.30
18	K	103	THR	CA-CB-CG2	5.71	120.39	112.40
26	W	356	THR	N-CA-C	-5.67	95.70	111.00
8	A	415	LEU	CB-CA-C	5.63	120.90	110.20
29	N	36	DG	C3'-C2'-C1'	-5.62	95.75	102.50
7	M	167	SER	C-N-CA	5.62	135.75	121.70
6	7	418	MET	N-CA-C	-5.62	95.84	111.00
8	A	1107	VAL	C-N-CA	5.61	135.73	121.70
7	M	317	TYR	CZ-CE2-CD2	-5.59	114.77	119.80
10	C	81	GLU	OE1-CD-OE2	-5.58	116.60	123.30
8	A	903	ASN	C-N-CA	5.57	135.62	121.70
12	E	215	MET	CB-CA-C	-5.57	99.26	110.40
29	N	-3	DA	O4'-C1'-N9	5.56	111.89	108.00
19	L	63	ARG	N-CA-CB	5.53	120.55	110.60
2	1	385	MET	CA-CB-CG	5.52	122.69	113.30
9	B	585	VAL	CG1-CB-CG2	-5.51	102.08	110.90
3	2	373	MET	N-CA-C	-5.50	96.15	111.00
30	T	-34	DT	N3-C4-O4	5.50	123.20	119.90
14	G	148	GLU	CB-CG-CD	5.49	129.02	114.20
9	B	918	ILE	C-N-CA	5.49	135.42	121.70
12	E	19	VAL	N-CA-CB	5.49	123.57	111.50
30	T	-38	DC	N1-C2-O2	-5.47	115.62	118.90
9	B	173	MET	CB-CG-SD	-5.46	96.03	112.40
17	J	49	MET	N-CA-CB	-5.46	100.77	110.60
16	I	49	ILE	C-N-CA	5.46	135.34	121.70
12	E	58	MET	CA-CB-CG	5.45	122.57	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	T	-47	DA	C8-N9-C4	5.45	107.98	105.80
18	K	42	LEU	N-CA-C	5.43	125.67	111.00
10	C	125	MET	CA-CB-CG	5.43	122.53	113.30
14	G	148	GLU	N-CA-CB	5.42	120.36	110.60
12	E	22	MET	CB-CA-C	-5.42	99.56	110.40
24	U	264	ASP	CA-CB-CG	5.40	125.28	113.40
8	A	701	LEU	CA-CB-CG	5.39	127.70	115.30
30	T	-48	DA	C6-N1-C2	-5.38	115.37	118.60
18	K	98	LEU	CA-CB-CG	5.38	127.67	115.30
19	L	66	GLN	OE1-CD-NE2	-5.36	109.58	121.90
11	D	145	MET	CA-CB-CG	5.34	122.38	113.30
29	N	37	DA	C4'-C3'-C2'	-5.33	98.31	103.10
26	W	34	PHE	CA-CB-CG	-5.30	101.19	113.90
9	B	364	ILE	CG1-CB-CG2	-5.29	99.77	111.40
9	B	1021	MET	N-CA-CB	-5.26	101.14	110.60
10	C	57	VAL	N-CA-CB	-5.24	99.97	111.50
23	O	236	GLU	N-CA-C	-5.24	96.84	111.00
24	U	250	LYS	CB-CA-C	-5.24	99.92	110.40
9	B	1021	MET	CB-CA-C	5.23	120.86	110.40
11	D	145	MET	CB-CG-SD	5.23	128.10	112.40
25	V	38	MET	N-CA-CB	5.22	120.00	110.60
8	A	836	TYR	C-N-CA	-5.21	108.69	121.70
28	5	28	SER	C-N-CA	-5.20	108.70	121.70
11	D	27	LEU	CA-CB-CG	5.20	127.26	115.30
16	I	94	ASP	OD1-CG-OD2	-5.19	113.44	123.30
14	G	10	ASN	CB-CG-OD1	-5.17	111.27	121.60
30	T	-34	DT	C5-C4-O4	-5.17	121.28	124.90
17	J	5	VAL	C-N-CA	-5.15	108.82	121.70
3	2	100	LEU	CA-CB-CG	5.14	127.12	115.30
10	C	18	VAL	N-CA-CB	5.13	122.78	111.50
8	A	566	ILE	CG1-CB-CG2	-5.12	100.14	111.40
8	A	904	THR	OG1-CB-CG2	5.11	121.76	110.00
10	C	94	LYS	CG-CD-CE	-5.10	96.59	111.90
16	I	20	LYS	CA-CB-CG	-5.10	102.18	113.40
7	M	317	TYR	CB-CA-C	5.09	120.57	110.40
18	K	70	ARG	NE-CZ-NH2	-5.09	117.76	120.30
30	T	-47	DA	C2-N3-C4	5.08	113.14	110.60
8	A	1111	MET	CB-CG-SD	5.07	127.61	112.40
7	M	289	PHE	CB-CG-CD2	-5.05	117.26	120.80
28	5	58	LEU	CA-CB-CG	5.05	126.91	115.30
9	B	930	ALA	C-N-CA	5.04	134.31	121.70
18	K	2	ASN	CB-CG-OD1	-5.01	111.58	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	30	ILE	C-N-CA	5.00	134.21	121.70

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	659	MET	CA
3	2	466	GLN	CA
6	7	231	ARG	CA
6	7	742	MET	CA
8	A	217	LYS	CA
8	A	904	THR	CB
10	C	84	ARG	CA
12	E	29	PHE	CA
14	G	10	ASN	CA
14	G	33	GLU	CA
14	G	148	GLU	CA
15	H	88	SER	CA
15	H	146	ARG	CA
16	I	50	THR	CB
16	I	94	ASP	CA
17	J	6	ARG	CA
18	K	1	MET	CA
18	K	64	GLU	CA
18	K	103	THR	CB
23	O	104	MET	CA
24	U	27	ASN	CA
24	U	264	ASP	CA
25	V	38	MET	CA
28	5	29	ASP	CA

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	159	HIS	Sidechain
1	0	229	ASP	Sidechain
3	2	466	GLN	Sidechain
28	5	29	ASP	Sidechain
6	7	231	ARG	Sidechain
6	7	746	PRO	Peptide
8	A	1079	MET	Peptide
8	A	1188	GLN	Sidechain
8	A	1404	GLU	Peptide

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Mol	Chain	Res	Type	Group
8	A	259	GLU	Peptide
8	A	44	THR	Peptide
8	A	454	SER	Peptide
8	A	524	VAL	Peptide
8	A	55	ASP	Peptide
8	A	566	ILE	Peptide
8	A	567	LYS	Peptide
8	A	65	LEU	Peptide
9	B	1110	PRO	Peptide
9	B	333	PHE	Peptide
9	B	363	HIS	Peptide
9	B	510	LYS	Peptide
9	B	551	PRO	Peptide
9	B	832	GLY	Peptide
9	B	868	MET	Peptide
9	B	922	GLU	Peptide
10	C	177	GLU	Sidechain
10	C	209	TYR	Sidechain
10	C	24	ASN	Sidechain
10	C	81	GLU	Sidechain
10	C	83	SER	Peptide
10	C	84	ARG	Sidechain
11	D	175	PHE	Sidechain
11	D	70	PHE	Sidechain
12	E	171	LYS	Peptide
12	E	172	GLU	Sidechain
12	E	29	PHE	Sidechain
12	E	63	ASN	Sidechain
13	F	127	GLU	Peptide
14	G	10	ASN	Sidechain
14	G	147	ILE	Peptide
14	G	148	GLU	Sidechain
14	G	9	LEU	Peptide
15	H	146	ARG	Sidechain
15	H	81	PRO	Peptide
16	I	94	ASP	Sidechain
17	J	4	PRO	Peptide
17	J	6	ARG	Sidechain
18	K	2	ASN	Sidechain
18	K	64	GLU	Sidechain
18	K	70	ARG	Sidechain
18	K	96	ASN	Sidechain

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Mol	Chain	Res	Type	Group
19	L	47	ARG	Sidechain
19	L	58	LYS	Peptide
19	L	66	GLN	Sidechain
19	L	67	PHE	Sidechain
7	M	242	PHE	Sidechain
7	M	269	ILE	Peptide
7	M	289	PHE	Sidechain
7	M	30	TYR	Peptide
7	M	31	PRO	Peptide
7	M	317	TYR	Sidechain
23	O	236	GLU	Sidechain
22	S	207	ILE	Peptide
22	S	209	LYS	Peptide
22	S	232	ASP	Sidechain
22	S	282	TYR	Sidechain
24	U	10	TYR	Sidechain
24	U	27	ASN	Sidechain
25	V	6	TYR	Sidechain
25	V	82	ASN	Sidechain
26	W	142	PHE	Sidechain
27	X	216	GLN	Sidechain

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	6091	0	6154	189	0
2	1	3382	0	3436	63	0
3	2	3546	0	3593	88	0
4	4	2267	0	2323	54	0
5	6	2786	0	2804	93	0
6	7	4889	0	4875	133	0
7	M	2175	0	2283	53	0
8	A	11167	0	11187	277	0
9	B	9227	0	9201	209	0
10	C	2086	0	2043	74	0
11	D	1331	0	1345	35	0
12	E	1752	0	1775	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	F	705	0	731	16	0
14	G	1335	0	1345	38	0
15	H	1080	0	1049	37	0
16	I	927	0	879	39	0
17	J	540	0	552	24	0
18	K	924	0	933	31	0
19	L	352	0	374	17	0
20	Q	1619	0	1452	38	0
21	P	1484	0	1480	40	0
22	S	1294	0	1289	40	0
23	O	1422	0	1500	48	0
24	U	885	0	866	32	0
25	V	815	0	822	33	0
26	W	2010	0	2026	54	0
27	X	1288	0	1307	37	0
28	5	498	0	506	22	0
29	N	1307	0	730	24	0
30	T	1314	0	725	21	0
31	0	8	0	0	3	0
32	4	1	0	0	0	0
32	6	4	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	M	1	0	0	0	0
32	S	1	0	0	0	0
33	7	1	0	0	0	0
33	A	1	0	0	0	0
All	All	70523	0	69585	1729	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 12.

All (1729) 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)
26:W:34:PHE:CD2	26:W:34:PHE:CG	1.77	1.65
23:O:224:TYR:CD2	23:O:224:TYR:CG	1.86	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:67:PHE:CD2	19:L:67:PHE:CG	1.81	1.60
10:C:57:VAL:CB	10:C:57:VAL:CG2	1.75	1.59
17:J:5:VAL:CB	17:J:5:VAL:CG2	1.77	1.59
10:C:18:VAL:CB	10:C:18:VAL:CG2	1.80	1.58
7:M:317:TYR:CD2	7:M:317:TYR:CG	1.91	1.58
16:I:26:LEU:CD2	16:I:26:LEU:CG	1.80	1.56
8:A:415:LEU:CD2	8:A:415:LEU:CG	1.83	1.54
10:C:37:MET:CA	10:C:37:MET:C	1.74	1.53
26:W:356:THR:CB	26:W:356:THR:CG2	1.86	1.52
10:C:84:ARG:CG	10:C:84:ARG:CB	1.82	1.52
8:A:837:ILE:CB	8:A:837:ILE:CG2	1.86	1.51
22:S:232:ASP:CA	22:S:232:ASP:C	1.77	1.51
6:7:747:ASN:CA	6:7:747:ASN:C	1.76	1.50
12:E:19:VAL:CB	12:E:19:VAL:CG2	1.86	1.49
1:0:659:MET:CB	1:0:659:MET:CG	1.87	1.48
12:E:29:PHE:CA	12:E:29:PHE:C	1.82	1.48
1:0:346:MET:CG	1:0:346:MET:SD	2.01	1.48
1:0:346:MET:SD	1:0:346:MET:HB2	1.54	1.47
5:6:450:ASN:CG	5:6:450:ASN:ND2	1.68	1.46
28:5:16:ILE:CG2	28:5:16:ILE:CB	1.90	1.46
19:L:67:PHE:CD2	19:L:67:PHE:CB	1.95	1.46
27:X:216:GLN:CD	27:X:216:GLN:NE2	1.67	1.45
18:K:1:MET:CA	18:K:1:MET:C	1.86	1.42
19:L:67:PHE:CD2	19:L:67:PHE:HB2	1.46	1.42
10:C:84:ARG:CB	10:C:84:ARG:CD	2.00	1.39
25:V:82:ASN:ND2	25:V:82:ASN:CG	1.74	1.38
10:C:18:VAL:CG2	10:C:18:VAL:CG1	2.05	1.32
7:M:317:TYR:CD2	7:M:317:TYR:CD1	1.90	1.31
8:A:837:ILE:CG2	8:A:837:ILE:CG1	2.08	1.30
28:5:16:ILE:CG2	28:5:16:ILE:CG1	2.10	1.29
18:K:64:GLU:CD	18:K:64:GLU:OE2	1.70	1.28
12:E:19:VAL:CG2	12:E:19:VAL:CG1	2.12	1.27
1:0:346:MET:SD	1:0:346:MET:CB	2.22	1.26
17:J:5:VAL:CG2	17:J:5:VAL:CG1	2.14	1.25
28:5:16:ILE:CG2	28:5:16:ILE:HG12	1.67	1.24
8:A:837:ILE:CG2	8:A:837:ILE:HG12	1.67	1.24
23:O:224:TYR:CD2	23:O:224:TYR:CB	2.21	1.23
8:A:415:LEU:CD2	8:A:415:LEU:CD1	2.20	1.20
26:W:34:PHE:CD2	26:W:34:PHE:CB	2.25	1.18
10:C:18:VAL:CG2	10:C:18:VAL:HG13	1.75	1.17
1:0:659:MET:CG	1:0:659:MET:CA	2.22	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:34:PHE:CD2	26:W:34:PHE:CD1	2.11	1.13
16:I:26:LEU:CD2	16:I:26:LEU:CD1	2.26	1.12
10:C:57:VAL:CG2	10:C:57:VAL:CG1	2.27	1.12
27:X:216:GLN:NE2	27:X:216:GLN:CG	2.11	1.12
26:W:356:THR:CG2	26:W:356:THR:CA	2.29	1.10
12:E:29:PHE:C	12:E:29:PHE:CB	2.19	1.10
12:E:19:VAL:CG2	12:E:19:VAL:HG13	1.80	1.10
5:6:450:ASN:ND2	5:6:450:ASN:OD1	1.84	1.08
10:C:84:ARG:CD	10:C:84:ARG:HB3	1.85	1.06
25:V:82:ASN:ND2	25:V:82:ASN:CB	2.19	1.05
7:M:45:CYS:HB3	7:M:48:CYS:SG	1.97	1.05
23:O:224:TYR:CD2	23:O:224:TYR:CD1	2.10	1.05
6:7:747:ASN:C	6:7:747:ASN:N	2.11	1.05
5:6:406:CYS:HB3	5:6:440:CYS:SG	2.00	1.01
7:M:317:TYR:CD2	7:M:317:TYR:CB	2.44	1.01
23:O:224:TYR:CD2	23:O:224:TYR:HB2	1.94	1.01
10:C:84:ARG:CB	10:C:84:ARG:HD3	1.89	1.00
1:0:659:MET:CB	1:0:659:MET:SD	2.50	0.99
26:W:34:PHE:CD2	26:W:34:PHE:HB3	1.97	0.99
22:S:232:ASP:C	22:S:232:ASP:N	2.16	0.97
8:A:415:LEU:CD2	8:A:415:LEU:CB	2.43	0.96
18:K:64:GLU:OE2	18:K:64:GLU:OE1	1.80	0.96
8:A:415:LEU:CD2	8:A:415:LEU:HD13	1.95	0.95
10:C:37:MET:C	10:C:37:MET:CB	2.35	0.95
19:L:27:LEU:N	19:L:39:SER:HG	1.62	0.95
25:V:82:ASN:ND2	25:V:82:ASN:OD1	1.96	0.95
17:J:5:VAL:CG2	17:J:5:VAL:HG13	1.94	0.94
16:I:26:LEU:CD2	16:I:26:LEU:CB	2.45	0.94
27:X:216:GLN:NE2	27:X:216:GLN:OE1	2.00	0.92
5:6:450:ASN:ND2	5:6:450:ASN:CB	2.33	0.91
12:E:29:PHE:C	12:E:29:PHE:HB2	1.89	0.90
17:J:5:VAL:CG2	17:J:5:VAL:CA	2.49	0.89
10:C:18:VAL:CG2	10:C:18:VAL:CA	2.50	0.89
10:C:57:VAL:CG2	10:C:57:VAL:CA	2.50	0.89
12:E:19:VAL:CG2	12:E:19:VAL:CA	2.51	0.88
26:W:356:THR:CG2	26:W:356:THR:OG1	2.19	0.88
24:U:39:LYS:HG3	24:U:43:GLN:HE22	1.38	0.88
19:L:34:CYS:HB3	19:L:51:CYS:SG	2.14	0.88
7:M:317:TYR:CD2	7:M:317:TYR:HD1	1.90	0.87
10:C:84:ARG:HB3	10:C:84:ARG:NE	1.89	0.87
10:C:37:MET:C	10:C:37:MET:N	2.27	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:454:TYR:CZ	3:2:483:TRP:HB2	2.11	0.86
12:E:29:PHE:C	12:E:29:PHE:N	2.30	0.85
8:A:107:CYS:SG	8:A:148:CYS:HB2	2.16	0.85
16:I:26:LEU:CD2	16:I:26:LEU:HD13	2.06	0.85
1:0:659:MET:CG	1:0:659:MET:HA	2.07	0.85
19:L:67:PHE:CD2	19:L:67:PHE:CD1	2.26	0.84
5:6:338:CYS:SG	5:6:339:HIS:CE1	2.71	0.83
6:7:747:ASN:C	6:7:747:ASN:CB	2.48	0.82
8:A:837:ILE:CG2	8:A:837:ILE:CA	2.58	0.82
28:5:16:ILE:CG2	28:5:16:ILE:CA	2.58	0.81
18:K:1:MET:C	18:K:1:MET:CB	2.49	0.80
29:N:38:DG:N1	30:T:-38:DC:O2	2.15	0.79
8:A:107:CYS:HB3	8:A:110:CYS:SG	2.22	0.79
10:C:177:GLU:HG3	10:C:231:ASN:HB3	1.65	0.79
10:C:252:GLN:HB3	18:K:98:LEU:HD11	1.63	0.79
7:M:317:TYR:CD2	7:M:317:TYR:HB3	2.17	0.78
10:C:18:VAL:HG13	10:C:18:VAL:HG22	1.62	0.78
9:B:1169:MET:SD	9:B:1169:MET:N	2.57	0.78
8:A:110:CYS:HB3	8:A:167:CYS:SG	2.24	0.77
28:5:16:ILE:HG12	28:5:16:ILE:HG21	1.65	0.77
10:C:57:VAL:CG2	10:C:57:VAL:HG13	2.15	0.76
19:L:34:CYS:CB	19:L:51:CYS:SG	2.74	0.76
5:6:429:CYS:HB3	5:6:432:CYS:SG	2.25	0.75
21:P:106:LEU:HB3	21:P:120:TYR:HB2	1.68	0.75
18:K:1:MET:C	18:K:1:MET:N	2.38	0.75
9:B:344:LYS:HG2	9:B:348:ARG:HG2	1.68	0.74
28:5:16:ILE:CG1	28:5:16:ILE:HG21	2.17	0.74
26:W:356:THR:CG2	26:W:356:THR:HA	2.17	0.74
3:2:459:TYR:OH	3:2:498:ASN:OD1	2.06	0.74
1:0:134:ARG:O	1:0:138:ASN:HB2	1.88	0.73
8:A:367:PRO:HB3	8:A:466:SER:HA	1.69	0.73
14:G:138:THR:H	14:G:141:SER:HB3	1.53	0.72
8:A:837:ILE:HG12	8:A:837:ILE:HG21	1.71	0.72
12:E:19:VAL:HG13	12:E:19:VAL:HG22	1.71	0.72
8:A:567:LYS:HE2	15:H:97:MET:HB2	1.72	0.72
23:O:93:GLU:H	25:V:72:CYS:H	1.38	0.72
8:A:346:ASP:H	9:B:1154:ALA:HB1	1.55	0.71
9:B:680:THR:H	9:B:683:SER:HB2	1.56	0.71
11:D:50:LEU:HD11	14:G:2:PHE:HB2	1.72	0.71
22:S:232:ASP:C	22:S:232:ASP:CB	2.59	0.71
3:2:337:GLY:H	3:2:351:SER:HB3	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:589:GLN:HG2	6:7:748:LEU:HB3	1.72	0.71
8:A:72:GLU:HB3	8:A:76:GLU:HB2	1.72	0.71
1:0:503:GLN:HB3	6:7:361:GLN:HB2	1.73	0.70
8:A:311:GLN:HG2	8:A:312:PRO:HD3	1.73	0.70
11:D:66:ARG:HH12	11:D:67:ARG:HH21	1.39	0.70
8:A:837:ILE:HG12	8:A:837:ILE:HG23	1.67	0.70
19:L:67:PHE:HB2	19:L:67:PHE:HD2	1.43	0.70
6:7:527:LEU:HA	6:7:530:LEU:HB2	1.74	0.70
1:0:571:VAL:HG11	2:1:375:LEU:HD13	1.75	0.69
15:H:135:LEU:O	15:H:137:GLN:N	2.26	0.69
3:2:352:ASN:ND2	3:2:370:PHE:O	2.26	0.69
15:H:95:TYR:HB3	15:H:144:ILE:HB	1.74	0.69
10:C:18:VAL:CG1	10:C:18:VAL:HG21	2.20	0.69
8:A:837:ILE:CG1	8:A:837:ILE:HG21	2.19	0.68
12:E:29:PHE:HA	12:E:65:THR:HG22	1.74	0.68
1:0:659:MET:CA	1:0:659:MET:HG3	2.21	0.68
17:J:10:CYS:SG	17:J:11:GLY:N	2.66	0.68
5:6:131:ASP:HA	5:6:174:MET:HB3	1.76	0.68
3:2:427:LYS:HG2	6:7:740:HIS:HA	1.75	0.68
8:A:464:PRO:HB3	18:K:4:PRO:HD2	1.76	0.68
13:F:125:LEU:HA	13:F:130:ILE:HD11	1.76	0.68
27:X:196:LEU:HB3	27:X:246:TYR:HB2	1.75	0.67
8:A:1059:HIS:ND1	13:F:86:THR:OG1	2.27	0.67
25:V:82:ASN:ND2	25:V:82:ASN:HB3	2.08	0.67
26:W:149:CYS:HB3	26:W:154:GLU:H	1.60	0.67
7:M:272:LYS:HE2	23:O:191:PRO:HD3	1.75	0.66
8:A:1171:GLN:HE22	22:S:207:ILE:HD13	1.61	0.66
9:B:799:PRO:HB2	9:B:818:PRO:HG2	1.77	0.66
10:C:56:THR:HA	10:C:151:GLN:HG2	1.77	0.66
9:B:287:ARG:NH2	9:B:294:ASP:OD1	2.29	0.66
28:5:16:ILE:HG12	28:5:16:ILE:HG23	1.73	0.66
1:0:493:LEU:HB3	1:0:678:VAL:HG12	1.76	0.66
5:6:450:ASN:HD22	5:6:450:ASN:CA	2.07	0.66
9:B:277:LYS:HZ2	9:B:336:ARG:H	1.44	0.66
10:C:54:ASN:ND2	10:C:60:ASP:OD1	2.26	0.66
2:1:624:THR:O	2:1:628:HIS:ND1	2.28	0.66
7:M:241:ARG:NH1	9:B:107:GLY:O	2.29	0.65
21:P:124:LEU:HD23	21:P:222:CYS:HB3	1.76	0.65
25:V:72:CYS:SG	25:V:73:ASP:N	2.67	0.65
2:1:209:PHE:O	2:1:213:ARG:NH1	2.29	0.65
16:I:6:PHE:HA	16:I:13:MET:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:187:ASN:HB2	22:S:228:LEU:HD11	1.77	0.65
8:A:1000:LEU:HB2	8:A:1011:GLN:HB2	1.77	0.65
20:Q:105:ALA:H	21:P:89:GLY:HA2	1.62	0.65
3:2:347:ILE:HD11	3:2:378:ILE:HG13	1.78	0.65
13:F:133:VAL:HG12	13:F:147:SER:HA	1.78	0.65
1:0:538:VAL:HG12	1:0:598:LEU:HB2	1.79	0.65
6:7:464:ARG:HD2	29:N:44:DT:H4'	1.78	0.65
9:B:72:GLU:O	20:Q:330:ARG:NH2	2.30	0.65
17:J:5:VAL:HG13	17:J:5:VAL:HG22	1.79	0.65
22:S:265:VAL:HG12	22:S:280:SER:HB3	1.78	0.65
27:X:216:GLN:NE2	27:X:216:GLN:HG3	2.08	0.65
8:A:700:ASN:O	16:I:115:LYS:NZ	2.25	0.65
11:D:50:LEU:HD13	11:D:55:ALA:HB2	1.78	0.65
15:H:80:ARG:HH12	18:K:57:LEU:HD22	1.61	0.65
28:5:48:GLU:O	28:5:52:HIS:ND1	2.27	0.65
1:0:156:CYS:CB	31:0:801:SF4:S1	2.84	0.65
1:0:162:LEU:HB3	1:0:198:ARG:HH22	1.62	0.65
8:A:565:ILE:HB	8:A:567:LYS:HB2	1.77	0.65
8:A:1138:ILE:HD11	8:A:1316:VAL:HG12	1.79	0.65
9:B:445:LYS:NZ	9:B:449:ASN:OD1	2.30	0.65
2:1:472:GLN:HE22	4:4:41:ASP:HB2	1.62	0.64
8:A:830:LYS:NZ	8:A:1077:THR:O	2.28	0.64
8:A:1152:ILE:HG22	16:I:44:TYR:H	1.62	0.64
8:A:1173:HIS:HA	22:S:200:ARG:HH22	1.62	0.64
8:A:1193:LEU:HD11	8:A:1264:GLU:HB3	1.79	0.64
20:Q:119:LEU:HD23	21:P:133:TYR:HB2	1.79	0.64
9:B:74:LEU:O	9:B:86:ARG:NH1	2.31	0.64
11:D:67:ARG:HD2	11:D:129:LEU:HD22	1.79	0.64
22:S:283:GLN:HB2	22:S:293:LEU:HD13	1.80	0.64
1:0:108:LEU:HB3	1:0:208:TYR:HB3	1.78	0.64
6:7:688:GLY:HA2	6:7:691:LEU:HB2	1.80	0.64
7:M:18:LEU:HD13	8:A:66:LYS:HB2	1.79	0.64
8:A:840:ARG:NH1	8:A:1384:VAL:O	2.31	0.64
6:7:456:THR:HG23	6:7:458:SER:H	1.63	0.64
9:B:76:GLN:OE1	20:Q:330:ARG:NH1	2.31	0.64
3:2:151:VAL:HG11	3:2:358:ALA:HB1	1.79	0.63
15:H:83:GLN:O	15:H:87:ARG:NH1	2.31	0.63
21:P:96:ARG:NH2	21:P:103:LYS:O	2.31	0.63
8:A:894:GLU:O	8:A:898:ARG:HB3	1.98	0.63
8:A:1161:THR:HG21	8:A:1166:ASP:HB2	1.79	0.63
9:B:259:TYR:O	9:B:267:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:51:ASN:HA	16:I:92:ARG:HH22	1.63	0.63
6:7:421:ARG:NH1	6:7:435:CYS:SG	2.72	0.63
7:M:286:ILE:HD11	7:M:291:ILE:HB	1.81	0.63
3:2:14:LEU:O	3:2:22:GLN:NE2	2.31	0.63
6:7:163:PRO:HA	6:7:173:TYR:HA	1.79	0.63
8:A:42:ASP:O	8:A:45:GLN:NE2	2.32	0.63
3:2:454:TYR:OH	3:2:483:TRP:HB2	1.97	0.63
26:W:17:VAL:HG21	26:W:29:LEU:HD13	1.79	0.63
9:B:1076:HIS:O	10:C:31:ASN:ND2	2.31	0.63
15:H:62:SER:OG	15:H:63:LEU:N	2.32	0.63
20:Q:105:ALA:HB3	21:P:89:GLY:H	1.63	0.63
4:4:289:CYS:HB3	4:4:292:CYS:SG	2.38	0.63
26:W:227:MET:SD	26:W:229:ARG:NH1	2.70	0.63
3:2:407:GLN:HG3	3:2:410:ARG:HH21	1.63	0.63
7:M:138:ASP:HB3	9:B:451:LYS:HG3	1.81	0.63
22:S:271:CYS:HB3	22:S:274:CYS:SG	2.38	0.63
6:7:366:GLN:NE2	6:7:390:ALA:O	2.32	0.62
1:0:641:PHE:O	1:0:645:ASN:ND2	2.31	0.62
8:A:551:TYR:O	18:K:62:LYS:NZ	2.31	0.62
24:U:10:TYR:HA	24:U:13:ILE:HG12	1.81	0.62
3:2:190:GLN:HG3	3:2:395:GLN:HE21	1.65	0.62
9:B:41:LYS:NZ	9:B:544:CYS:SG	2.71	0.62
1:0:472:MET:HG3	1:0:473:LEU:HG	1.80	0.62
9:B:793:ALA:HB3	9:B:856:PHE:HB2	1.81	0.62
22:S:198:ARG:NH2	22:S:227:PHE:O	2.31	0.62
26:W:3:ARG:HH11	26:W:5:ILE:HG23	1.64	0.62
8:A:108:MET:N	8:A:108:MET:SD	2.69	0.62
18:K:1:MET:C	18:K:1:MET:HG2	2.19	0.62
21:P:319:LYS:NZ	21:P:324:GLN:O	2.32	0.62
20:Q:29:ARG:HA	20:Q:32:LEU:HB2	1.82	0.62
3:2:238:LYS:NZ	3:2:239:ILE:O	2.33	0.62
3:2:352:ASN:HD21	3:2:369:ARG:HG3	1.65	0.62
2:1:606:GLU:HA	2:1:609:SER:HB3	1.82	0.62
3:2:22:GLN:OE1	3:2:85:HIS:ND1	2.31	0.62
9:B:336:ARG:NH1	9:B:339:THR:O	2.30	0.62
9:B:397:ASP:OD2	9:B:400:HIS:N	2.33	0.62
20:Q:27:MET:HA	20:Q:30:ASN:HB2	1.81	0.62
27:X:204:GLY:HA3	27:X:243:TYR:HB3	1.82	0.62
1:0:352:ILE:HB	1:0:420:ILE:HB	1.80	0.61
10:C:84:ARG:HB3	10:C:84:ARG:HE	1.65	0.61
27:X:234:ARG:HD3	27:X:239:LYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:152:GLY:HA2	3:2:182:PHE:HE2	1.64	0.61
8:A:386:ASP:N	8:A:386:ASP:OD1	2.33	0.61
19:L:42:ARG:HG3	19:L:43:THR:HG23	1.81	0.61
1:0:117:HIS:ND1	1:0:156:CYS:SG	2.71	0.61
2:1:174:LEU:HD12	2:1:217:LEU:HB3	1.83	0.61
12:E:154:ILE:HD11	12:E:197:LYS:HD3	1.82	0.61
8:A:535:THR:HG23	8:A:575:LYS:HG2	1.81	0.61
9:B:104:GLU:OE2	19:L:54:ARG:NH1	2.33	0.61
9:B:839:MET:HG2	9:B:1012:ILE:HG22	1.83	0.61
21:P:320:GLU:O	21:P:323:ARG:NH1	2.32	0.61
1:0:505:ALA:H	6:7:359:SER:HA	1.65	0.61
1:0:670:LEU:HD12	1:0:675:ASP:HB3	1.83	0.61
5:6:450:ASN:ND2	5:6:450:ASN:CA	2.63	0.61
8:A:445:ASN:HB3	8:A:488:ASN:HB2	1.83	0.61
21:P:86:ASN:OD1	21:P:90:GLN:NE2	2.34	0.61
8:A:68:GLN:NE2	8:A:70:CYS:SG	2.73	0.61
9:B:801:LYS:O	17:J:52:THR:OG1	2.18	0.61
1:0:106:LEU:HD12	1:0:199:MET:HG3	1.82	0.61
3:2:392:THR:HG22	3:2:394:ASP:H	1.66	0.61
3:2:453:THR:OG1	28:5:51:LYS:NZ	2.33	0.61
3:2:457:SER:O	3:2:492:PHE:CE2	2.53	0.61
5:6:139:LYS:HD3	5:6:144:ASN:HB3	1.82	0.61
9:B:911:ILE:HG13	9:B:912:ILE:HG12	1.81	0.61
11:D:153:ARG:HH22	11:D:160:VAL:HA	1.65	0.61
24:U:18:VAL:O	24:U:22:ARG:NH1	2.34	0.61
1:0:513:ARG:NH1	1:0:514:ASN:OD1	2.34	0.61
10:C:84:ARG:CZ	18:K:11:LEU:HD11	2.31	0.61
1:0:571:VAL:HG21	2:1:375:LEU:HD22	1.82	0.60
3:2:340:ILE:HB	3:2:348:TYR:HB2	1.82	0.60
5:6:327:ARG:HA	5:6:347:TYR:HA	1.83	0.60
8:A:670:ILE:HD13	9:B:1067:ARG:HE	1.64	0.60
8:A:1151:GLU:OE2	16:I:45:ARG:NH1	2.34	0.60
8:A:116:ASP:O	8:A:118:HIS:ND1	2.34	0.60
10:C:37:MET:C	10:C:37:MET:HB3	2.18	0.60
8:A:75:ASN:HA	9:B:1116:ARG:HH22	1.66	0.60
8:A:1208:THR:OG1	8:A:1211:GLN:OE1	2.19	0.60
9:B:69:LEU:HB3	9:B:90:ILE:HG13	1.84	0.60
11:D:138:ASN:HB2	11:D:141:LEU:HB3	1.83	0.60
14:G:1:MET:N	14:G:80:LYS:O	2.34	0.60
6:7:761:GLN:HA	6:7:764:LEU:HB2	1.82	0.60
9:B:84:ILE:O	9:B:86:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:241:ASP:N	10:C:241:ASP:OD1	2.32	0.60
14:G:89:GLY:HA3	14:G:103:VAL:HG22	1.82	0.60
24:U:257:ARG:O	24:U:259:LYS:NZ	2.34	0.60
8:A:1397:LEU:HB2	8:A:1426:GLU:HG3	1.84	0.60
22:S:223:ILE:HG22	22:S:225:PRO:HD2	1.82	0.60
1:0:287:GLU:O	1:0:291:GLN:NE2	2.34	0.60
8:A:1230:GLU:OE2	22:S:205:ASN:ND2	2.35	0.60
18:K:64:GLU:OE2	18:K:64:GLU:CG	2.48	0.60
15:H:83:GLN:HA	18:K:54:ARG:HH22	1.67	0.60
22:S:232:ASP:N	22:S:233:ALA:N	2.49	0.60
6:7:642:ASN:HB3	6:7:649:ILE:HG13	1.83	0.60
17:J:9:SER:OG	17:J:10:CYS:N	2.35	0.60
4:4:232:ASN:O	4:4:259:ARG:NH1	2.35	0.60
1:0:624:GLY:HA2	1:0:683:ASP:HB2	1.83	0.60
9:B:213:ILE:O	9:B:215:GLN:NE2	2.33	0.60
24:U:250:LYS:H	24:U:261:SER:HG	1.47	0.60
29:N:38:DG:H22	30:T:-38:DC:H1'	1.67	0.60
6:7:130:ARG:NH1	6:7:201:SER:O	2.35	0.59
5:6:221:LEU:O	5:6:230:ARG:NH1	2.35	0.59
8:A:147:VAL:HA	8:A:170:THR:HA	1.84	0.59
8:A:590:ARG:NH2	8:A:621:THR:OG1	2.35	0.59
8:A:862:ASN:HD22	12:E:174:GLN:HA	1.66	0.59
8:A:1443:VAL:HG12	14:G:61:ILE:HD13	1.82	0.59
14:G:47:CYS:SG	14:G:48:VAL:N	2.75	0.59
26:W:73:ARG:NH1	30:T:-23:DA:OP1	2.35	0.59
1:0:424:GLU:N	1:0:432:ASN:O	2.35	0.59
2:1:339:LEU:HD23	2:1:342:ASN:HD22	1.67	0.59
6:7:673:ILE:HG22	6:7:708:LEU:HD12	1.84	0.59
7:M:19:ASN:OD1	8:A:63:ARG:NH1	2.34	0.59
8:A:739:ASP:OD2	15:H:19:ARG:NH1	2.29	0.59
9:B:363:HIS:O	9:B:365:THR:N	2.35	0.59
1:0:104:ARG:NH1	1:0:172:PRO:O	2.34	0.59
6:7:320:ASN:ND2	6:7:503:SER:O	2.35	0.59
7:M:23:THR:HA	7:M:32:PRO:HG3	1.83	0.59
9:B:997:GLU:O	10:C:35:ARG:NH1	2.35	0.59
16:I:8:ARG:NH1	16:I:9:ASP:OD1	2.36	0.59
22:S:227:PHE:HA	22:S:230:THR:HG23	1.84	0.59
5:6:116:THR:HG23	5:6:120:ARG:HH22	1.66	0.59
8:A:120:GLU:OE1	8:A:123:ARG:NH1	2.36	0.59
24:U:260:CYS:HB2	24:U:281:VAL:HB	1.84	0.59
14:G:167:TYR:HA	14:G:170:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N:15:DT:H2"	29:N:16:DA:H5"	1.85	0.59
1:0:67:ARG:NH2	1:0:230:SER:O	2.36	0.59
8:A:1100:ARG:NH2	8:A:1351:GLU:OE2	2.36	0.59
9:B:308:TRP:O	9:B:311:LEU:N	2.35	0.59
10:C:125:MET:SD	10:C:127:ARG:NE	2.76	0.59
1:0:415:GLY:O	1:0:440:LEU:N	2.36	0.58
2:1:212:THR:OG1	2:1:213:ARG:NH1	2.36	0.58
8:A:406:ILE:HB	8:A:431:LYS:HB2	1.84	0.58
8:A:1115:SER:OG	8:A:1330:ASN:ND2	2.36	0.58
9:B:74:LEU:HA	9:B:85:SER:HA	1.84	0.58
5:6:362:VAL:HA	5:6:369:MET:HA	1.85	0.58
8:A:415:LEU:CD1	8:A:415:LEU:HD21	2.29	0.58
1:0:618:ARG:NH1	1:0:675:ASP:OD1	2.36	0.58
6:7:431:GLN:OE1	6:7:434:ASN:ND2	2.36	0.58
6:7:754:ARG:HE	6:7:757:ARG:HH21	1.51	0.58
8:A:568:PRO:HD2	15:H:46:LEU:HD13	1.83	0.58
16:I:78:CYS:SG	16:I:106:CYS:HB3	2.43	0.58
8:A:884:ASP:OD2	8:A:1025:ARG:NE	2.34	0.58
24:U:22:ARG:HH21	24:U:35:LEU:HD13	1.68	0.58
1:0:223:SER:O	1:0:452:ARG:NH2	2.35	0.58
6:7:340:GLU:OE1	6:7:376:ASN:ND2	2.37	0.58
9:B:102:VAL:HB	9:B:112:LEU:HD13	1.86	0.58
16:I:26:LEU:CD2	16:I:26:LEU:HB3	2.32	0.58
2:1:434:ILE:HA	5:6:118:TYR:HA	1.86	0.58
8:A:1033:GLN:O	8:A:1036:ARG:NH1	2.37	0.58
9:B:277:LYS:HE2	9:B:278:GLN:HE22	1.67	0.58
21:P:299:ILE:HD11	21:P:322:THR:HG22	1.85	0.58
8:A:949:ASP:OD1	8:A:949:ASP:N	2.36	0.58
4:4:64:HIS:NE2	4:4:71:ASN:O	2.35	0.58
7:M:317:TYR:HA	7:M:320:ARG:HH12	1.69	0.58
8:A:1094:VAL:HG23	8:A:1113:THR:HG21	1.85	0.58
15:H:87:ARG:HB3	15:H:89:LEU:HG	1.85	0.58
1:0:460:SER:OG	1:0:461:GLY:N	2.37	0.58
10:C:162:GLY:HA3	10:C:170:TRP:CE2	2.39	0.58
22:S:213:ASP:HA	22:S:216:HIS:HD1	1.69	0.58
1:0:156:CYS:HB3	31:0:801:SF4:S1	2.43	0.58
3:2:219:VAL:O	3:2:223:HIS:ND1	2.29	0.58
23:O:95:ASN:HB3	23:O:98:ARG:HB2	1.86	0.58
2:1:196:GLN:O	2:1:200:ILE:HB	2.04	0.57
3:2:194:GLN:O	3:2:199:GLN:NE2	2.36	0.57
5:6:116:THR:O	5:6:120:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:357:LYS:NZ	6:7:426:GLN:O	2.36	0.57
8:A:663:SER:OG	8:A:664:THR:N	2.36	0.57
8:A:1005:GLU:OE2	8:A:1009:ASN:ND2	2.36	0.57
9:B:346:GLU:HG2	9:B:347:LYS:HG2	1.86	0.57
9:B:1037:LEU:O	17:J:47:ARG:NH1	2.37	0.57
20:Q:388:PRO:HB3	21:P:82:ARG:HG2	1.85	0.57
24:U:30:ILE:HG12	25:V:31:ARG:HH12	1.68	0.57
9:B:302:CYS:SG	9:B:303:TYR:N	2.77	0.57
9:B:1155:SER:OG	9:B:1156:ASP:N	2.36	0.57
11:D:22:GLU:HG2	14:G:83:LYS:HE2	1.86	0.57
18:K:1:MET:C	18:K:1:MET:CG	2.72	0.57
3:2:393:ALA:HA	3:2:396:ILE:HD12	1.86	0.57
21:P:138:GLN:HG2	21:P:211:LYS:HB3	1.86	0.57
1:0:636:LYS:HA	1:0:639:LEU:HD12	1.86	0.57
5:6:139:LYS:O	5:6:142:ARG:NH1	2.37	0.57
9:B:921:ASP:OD1	9:B:927:GLN:NE2	2.37	0.57
10:C:96:SER:OG	10:C:97:VAL:N	2.37	0.57
25:V:87:VAL:O	25:V:103:GLN:N	2.37	0.57
1:0:38:SER:HA	1:0:477:THR:HB	1.87	0.57
8:A:565:ILE:HB	8:A:567:LYS:HE3	1.87	0.57
10:C:57:VAL:HG13	10:C:57:VAL:HG22	1.86	0.57
1:0:436:ARG:HH12	2:1:352:ASN:HB3	1.70	0.57
6:7:124:ARG:NH2	6:7:203:VAL:O	2.37	0.57
6:7:141:ILE:HD11	6:7:175:ILE:HG13	1.85	0.57
8:A:886:ILE:O	8:A:944:ARG:NH2	2.37	0.57
16:I:54:GLU:HG2	16:I:55:THR:HG23	1.87	0.57
12:E:147:HIS:HE1	12:E:149:LEU:HD13	1.69	0.57
16:I:26:LEU:HD13	16:I:26:LEU:HD22	1.82	0.57
22:S:160:LEU:HA	22:S:163:GLU:HG3	1.86	0.57
26:W:34:PHE:HB3	26:W:34:PHE:HD2	1.64	0.57
4:4:162:ARG:NH1	5:6:406:CYS:O	2.37	0.57
8:A:406:ILE:HG12	8:A:412:ARG:HG2	1.87	0.57
9:B:822:ASN:O	17:J:48:ARG:NH1	2.37	0.57
14:G:116:PRO:HD3	14:G:163:ILE:HG13	1.86	0.57
6:7:668:THR:HG21	6:7:695:ARG:HH21	1.70	0.57
8:A:359:LEU:O	8:A:471:ASN:ND2	2.31	0.57
25:V:87:VAL:HG12	25:V:88:GLU:HG3	1.87	0.57
1:0:388:LEU:HB3	1:0:390:VAL:HG13	1.87	0.57
13:F:79:ARG:NH1	13:F:145:ASP:O	2.33	0.57
26:W:109:LEU:HB3	26:W:172:LEU:HD13	1.86	0.57
27:X:186:VAL:HG13	27:X:191:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:5:ILE:HB	1:0:8:LEU:HB3	1.87	0.56
1:0:496:ILE:HD11	1:0:701:LEU:HD21	1.87	0.56
2:1:510:ASN:ND2	4:4:264:LYS:O	2.38	0.56
6:7:567:GLN:O	6:7:571:ARG:NE	2.35	0.56
14:G:100:GLU:HB3	14:G:107:LYS:HD2	1.84	0.56
16:I:96:SER:OG	16:I:97:MET:N	2.37	0.56
1:0:496:ILE:HD12	1:0:706:LEU:HA	1.87	0.56
6:7:491:HIS:O	6:7:519:ARG:NH1	2.38	0.56
7:M:127:GLN:HA	7:M:130:PHE:HB2	1.87	0.56
9:B:259:TYR:HE2	9:B:270:LYS:HB2	1.70	0.56
11:D:67:ARG:NH1	11:D:132:GLN:OE1	2.38	0.56
1:0:22:TYR:OH	1:0:751:ARG:NH1	2.38	0.56
1:0:104:ARG:NH2	1:0:171:LEU:O	2.36	0.56
1:0:135:ARG:NH1	1:0:392:GLU:OE2	2.38	0.56
1:0:289:LEU:HD22	1:0:321:ILE:HG13	1.87	0.56
1:0:364:LYS:NZ	1:0:370:GLU:OE2	2.37	0.56
6:7:207:GLU:OE2	6:7:211:ASN:ND2	2.39	0.56
8:A:1199:ARG:NH1	8:A:1233:ASP:O	2.39	0.56
9:B:805:THR:O	9:B:1044:ALA:N	2.34	0.56
11:D:145:MET:HA	11:D:148:LEU:HD12	1.87	0.56
12:E:97:VAL:HA	12:E:100:ILE:HD12	1.87	0.56
16:I:78:CYS:SG	16:I:106:CYS:CB	2.93	0.56
21:P:134:VAL:HG13	21:P:215:VAL:HG23	1.85	0.56
24:U:260:CYS:O	24:U:280:GLN:NE2	2.38	0.56
1:0:496:ILE:HA	1:0:681:LEU:HB2	1.88	0.56
3:2:146:ILE:HD13	3:2:159:PRO:HB3	1.87	0.56
7:M:43:VAL:HG23	7:M:52:LEU:HB2	1.88	0.56
8:A:114:LEU:HD12	8:A:142:CYS:HB2	1.86	0.56
9:B:1166:CYS:HB3	9:B:1168:LEU:HD23	1.87	0.56
20:Q:379:GLU:HA	21:P:66:ARG:HH12	1.69	0.56
3:2:176:VAL:O	3:2:180:GLY:N	2.39	0.56
7:M:202:GLU:HA	7:M:205:LYS:HD2	1.87	0.56
9:B:43:LEU:O	9:B:496:ARG:NH2	2.39	0.56
13:F:130:ILE:HB	13:F:148:VAL:HG11	1.86	0.56
1:0:283:GLN:OE1	1:0:327:ARG:NH2	2.37	0.56
5:6:224:VAL:O	5:6:230:ARG:NH2	2.37	0.56
8:A:881:GLN:NE2	8:A:957:PRO:O	2.39	0.56
8:A:1205:LYS:O	8:A:1274:ARG:NH2	2.38	0.56
1:0:621:LEU:HD13	1:0:680:VAL:HG21	1.87	0.56
3:2:124:VAL:HA	3:2:237:TYR:HD1	1.70	0.56
4:4:182:GLY:N	4:4:215:ILE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:685:GLN:OE1	6:7:689:ARG:NH2	2.39	0.56
7:M:273:SER:OG	23:O:188:GLU:O	2.23	0.56
14:G:116:PRO:HG3	14:G:164:LYS:HA	1.87	0.56
8:A:66:LYS:HD2	8:A:69:THR:H	1.70	0.56
8:A:1121:GLU:HG3	8:A:1123:GLY:H	1.71	0.56
9:B:313:MET:HG2	9:B:386:LEU:HD11	1.88	0.56
10:C:166:GLU:O	18:K:6:ARG:NH1	2.39	0.56
5:6:380:TYR:O	5:6:384:MET:N	2.38	0.56
12:E:118:PRO:HA	12:E:121:MET:HG3	1.87	0.56
14:G:154:VAL:O	14:G:156:SER:N	2.39	0.56
27:X:163:LEU:HD12	27:X:166:LEU:HD12	1.87	0.56
1:0:380:ARG:NH1	1:0:380:ARG:O	2.39	0.56
3:2:69:ASN:HB3	4:4:261:ILE:HG22	1.88	0.56
8:A:134:ARG:NH2	8:A:220:THR:O	2.38	0.56
8:A:1159:ARG:NH1	8:A:1186:ASP:OD1	2.39	0.56
9:B:810:GLU:HB2	9:B:815:ARG:HH22	1.71	0.56
23:O:193:LEU:HD22	23:O:206:ILE:HD12	1.86	0.56
1:0:407:THR:O	1:0:411:THR:OG1	2.21	0.55
1:0:571:VAL:HG22	1:0:599:LEU:HD12	1.87	0.55
1:0:1:MET:N	1:0:12:PHE:O	2.37	0.55
1:0:337:ARG:HE	1:0:369:ILE:HD11	1.71	0.55
1:0:609:GLY:H	1:0:668:ARG:HH12	1.53	0.55
18:K:12:LEU:HB2	18:K:18:LYS:HD3	1.88	0.55
2:1:510:ASN:OD1	2:1:513:GLN:NE2	2.39	0.55
5:6:135:ALA:O	5:6:145:ARG:NH1	2.39	0.55
6:7:638:ASN:OD1	6:7:641:GLN:NE2	2.39	0.55
9:B:73:GLN:HA	20:Q:330:ARG:HH22	1.70	0.55
9:B:209:GLU:OE2	9:B:788:ARG:NH2	2.38	0.55
9:B:310:MET:SD	9:B:310:MET:N	2.78	0.55
9:B:365:THR:HG21	9:B:370:PHE:HB2	1.87	0.55
10:C:207:CYS:SG	10:C:208:GLU:N	2.80	0.55
10:C:249:ASP:O	10:C:252:GLN:NE2	2.40	0.55
8:A:56:PRO:O	8:A:66:LYS:NZ	2.36	0.55
8:A:119:ASN:HB3	8:A:122:MET:HG3	1.88	0.55
11:D:139:LYS:HD2	11:D:142:LYS:HD2	1.88	0.55
15:H:118:PHE:N	15:H:121:LEU:O	2.40	0.55
23:O:224:TYR:HB2	23:O:224:TYR:HD2	1.66	0.55
28:5:23:ILE:HA	28:5:26:LYS:HZ3	1.70	0.55
6:7:676:HIS:O	6:7:722:ARG:NH1	2.39	0.55
17:J:19:GLU:O	17:J:23:ASN:ND2	2.40	0.55
2:1:205:PRO:HB2	2:1:208:GLU:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:378:ARG:O	5:6:381:HIS:NE2	2.39	0.55
22:S:160:LEU:HD23	22:S:173:HIS:HD2	1.72	0.55
18:K:1:MET:CA	18:K:1:MET:O	2.51	0.55
20:Q:116:THR:HA	21:P:136:THR:HA	1.88	0.55
23:O:72:ALA:O	23:O:123:VAL:N	2.38	0.55
1:0:722:ARG:NH2	5:6:267:SER:O	2.39	0.55
3:2:24:ARG:HE	3:2:219:VAL:HG21	1.71	0.55
5:6:345:GLY:O	5:6:355:LYS:NZ	2.39	0.55
8:A:40:THR:HG22	8:A:53:LEU:HD13	1.89	0.55
8:A:802:ASN:ND2	8:A:807:GLY:O	2.39	0.55
8:A:1211:GLN:HA	8:A:1214:GLU:HG3	1.89	0.55
9:B:341:LEU:HB3	9:B:344:LYS:HD2	1.89	0.55
12:E:74:ASP:N	12:E:74:ASP:OD1	2.38	0.55
12:E:202:SER:N	12:E:206:GLY:O	2.39	0.55
16:I:112:SER:O	16:I:114:GLN:NE2	2.40	0.55
1:0:500:GLY:N	1:0:504:VAL:O	2.39	0.55
1:0:643:ARG:HA	1:0:648:ILE:H	1.72	0.55
3:2:228:LEU:HD23	3:2:231:LEU:HD12	1.89	0.55
4:4:285:VAL:HA	5:6:323:GLY:HA2	1.89	0.55
9:B:604:ARG:NH1	9:B:615:MET:SD	2.78	0.55
9:B:862:GLN:O	9:B:914:LYS:NZ	2.36	0.55
17:J:45:CYS:SG	17:J:46:CYS:N	2.80	0.55
22:S:295:THR:OG1	22:S:308:PHE:O	2.24	0.55
28:5:17:LYS:HG3	28:5:40:LEU:HD11	1.87	0.55
7:M:163:LEU:O	7:M:166:LYS:NZ	2.40	0.55
16:I:61:ASP:OD1	16:I:61:ASP:N	2.39	0.55
23:O:74:VAL:HG22	23:O:155:PHE:HA	1.89	0.55
26:W:134:LEU:O	26:W:138:GLN:NE2	2.39	0.55
27:X:211:LYS:NZ	27:X:215:PRO:O	2.39	0.55
1:0:628:GLN:NE2	1:0:657:ASP:OD2	2.40	0.54
8:A:415:LEU:CD2	8:A:415:LEU:CA	2.84	0.54
8:A:855:THR:OG1	8:A:857:ARG:NH1	2.40	0.54
9:B:277:LYS:HA	9:B:337:ARG:HH21	1.72	0.54
20:Q:141:ARG:NH1	20:Q:345:GLU:O	2.40	0.54
2:1:567:HIS:ND1	2:1:575:GLN:OE1	2.38	0.54
8:A:375:THR:OG1	8:A:376:TYR:N	2.39	0.54
15:H:16:ASP:HB3	15:H:25:ARG:HB2	1.89	0.54
24:U:278:LYS:HG3	25:V:59:LYS:HD3	1.89	0.54
1:0:640:GLU:OE1	1:0:643:ARG:NH2	2.39	0.54
8:A:346:ASP:OD2	9:B:1106:ARG:NH1	2.40	0.54
9:B:842:ASN:ND2	9:B:845:SER:OG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:46:ILE:HG23	10:C:68:GLY:HA2	1.89	0.54
11:D:67:ARG:HG3	11:D:129:LEU:HD13	1.88	0.54
20:Q:141:ARG:NH1	20:Q:348:TYR:O	2.39	0.54
1:0:375:ARG:NE	1:0:410:SER:O	2.36	0.54
1:0:573:THR:OG1	1:0:575:ASP:O	2.23	0.54
3:2:63:ASP:OD1	3:2:71:LYS:NZ	2.40	0.54
3:2:399:TYR:O	3:2:403:HIS:ND1	2.38	0.54
4:4:216:GLY:O	4:4:237:HIS:NE2	2.33	0.54
6:7:631:THR:O	6:7:636:ARG:NH2	2.41	0.54
7:M:182:ARG:O	9:B:869:SER:OG	2.25	0.54
8:A:55:ASP:HA	8:A:58:LEU:HD23	1.89	0.54
9:B:334:ILE:HG13	9:B:335:GLY:H	1.72	0.54
9:B:526:GLU:OE2	9:B:538:ASN:N	2.41	0.54
10:C:37:MET:N	10:C:38:ILE:N	2.55	0.54
1:0:80:GLU:HG2	2:1:336:ILE:HG22	1.88	0.54
1:0:666:LEU:HD12	1:0:679:MET:HG3	1.90	0.54
6:7:407:VAL:HG13	6:7:452:LEU:HD12	1.89	0.54
8:A:850:VAL:HG13	8:A:1061:GLY:H	1.73	0.54
9:B:304:ASP:OD2	9:B:307:ASP:N	2.35	0.54
17:J:17:LYS:HB3	17:J:39:LEU:HD21	1.87	0.54
27:X:216:GLN:CG	27:X:216:GLN:HE21	2.14	0.54
30:T:0:DT:H2"	30:T:1:DG:C8	2.43	0.54
1:0:60:GLN:O	1:0:66:HIS:ND1	2.40	0.54
3:2:26:TYR:OH	3:2:84:LEU:O	2.23	0.54
16:I:78:CYS:SG	16:I:105:SER:OG	2.65	0.54
22:S:184:LYS:NZ	22:S:195:TYR:O	2.41	0.54
1:0:212:TYR:HA	1:0:218:ILE:HG13	1.88	0.54
1:0:656:PHE:O	1:0:659:MET:HG3	2.07	0.54
8:A:962:ARG:O	8:A:966:ASN:ND2	2.40	0.54
8:A:1168:GLU:O	8:A:1171:GLN:NE2	2.33	0.54
27:X:202:PHE:O	27:X:245:TRP:NE1	2.41	0.54
1:0:294:HIS:H	1:0:297:ASP:HB2	1.72	0.54
5:6:334:THR:O	5:6:343:VAL:N	2.38	0.54
5:6:428:ARG:HA	5:6:435:GLU:HA	1.89	0.54
6:7:383:ILE:O	6:7:535:LEU:N	2.35	0.54
6:7:449:GLU:O	6:7:480:ARG:NH2	2.40	0.54
9:B:1106:ARG:NH2	9:B:1110:PRO:O	2.41	0.54
5:6:130:LEU:O	5:6:174:MET:N	2.41	0.54
6:7:330:CYS:HA	6:7:333:ILE:HG12	1.89	0.54
8:A:18:GLN:O	9:B:1215:ARG:N	2.40	0.54
9:B:881:ASN:HA	9:B:932:HIS:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:N:-9:DG:H2"	29:N:-8:DG:C8	2.42	0.54
1:0:162:LEU:HD21	1:0:190:LEU:HB3	1.89	0.54
1:0:643:ARG:O	1:0:647:ARG:NH1	2.41	0.54
9:B:463:THR:HG22	9:B:465:ASN:H	1.73	0.54
9:B:996:ARG:HE	9:B:1007:VAL:HG11	1.73	0.54
14:G:144:ARG:O	14:G:169:GLY:N	2.40	0.54
26:W:42:ASP:OD1	26:W:210:GLN:NE2	2.41	0.54
5:6:394:THR:HA	5:6:398:PHE:HZ	1.73	0.53
8:A:372:LYS:NZ	8:A:397:ASN:O	2.36	0.53
8:A:597:LEU:HD21	15:H:103:LYS:HG2	1.90	0.53
1:0:603:ARG:NH2	1:0:626:PRO:O	2.41	0.53
3:2:342:GLU:HG3	3:2:344:ASN:H	1.73	0.53
8:A:251:SER:OG	8:A:257:ARG:NH2	2.35	0.53
10:C:76:ASP:OD2	10:C:128:ASN:N	2.33	0.53
15:H:58:THR:HB	15:H:143:LEU:HB2	1.89	0.53
15:H:118:PHE:HB2	15:H:121:LEU:HB2	1.91	0.53
15:H:135:LEU:HB3	15:H:137:GLN:HB3	1.90	0.53
26:W:163:LYS:NZ	26:W:167:GLU:OE2	2.40	0.53
30:T:-42:DA:H2'	30:T:-41:DG:C8	2.42	0.53
6:7:164:ILE:N	6:7:172:GLU:O	2.41	0.53
8:A:425:GLN:HE22	8:A:427:GLN:HB2	1.74	0.53
1:0:570:LEU:O	1:0:599:LEU:N	2.39	0.53
3:2:364:VAL:HG22	3:2:378:ILE:HG12	1.90	0.53
12:E:19:VAL:CG1	12:E:19:VAL:HG21	2.27	0.53
17:J:5:VAL:CG2	17:J:5:VAL:N	2.72	0.53
22:S:278:LYS:HD2	22:S:301:ALA:HB2	1.90	0.53
27:X:235:THR:OG1	27:X:238:ASP:O	2.24	0.53
28:5:22:GLN:OE1	28:5:26:LYS:NZ	2.41	0.53
29:N:42:DT:H2"	29:N:43:DT:H5"	1.91	0.53
1:0:588:LYS:O	1:0:592:ASN:ND2	2.41	0.53
9:B:924:GLU:HG2	9:B:925:LEU:HD12	1.90	0.53
26:W:17:VAL:HA	26:W:21:TYR:HD2	1.72	0.53
5:6:277:CYS:O	5:6:281:ASN:HB2	2.09	0.53
8:A:567:LYS:HD2	15:H:95:TYR:CG	2.44	0.53
9:B:835:GLN:OE1	9:B:835:GLN:N	2.38	0.53
9:B:1010:LEU:HD11	9:B:1092:TYR:HE2	1.74	0.53
10:C:57:VAL:HG21	17:J:60:PHE:HB3	1.89	0.53
17:J:16:ASP:N	17:J:16:ASP:OD1	2.39	0.53
3:2:90:ASN:O	3:2:97:MET:N	2.40	0.53
16:I:45:ARG:HH21	16:I:47:GLU:H	1.57	0.53
24:U:41:ILE:HG23	24:U:44:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:104:ARG:O	1:0:204:ASN:N	2.41	0.53
1:0:323:GLY:HA2	1:0:326:ARG:HB2	1.89	0.53
5:6:168:GLN:HB3	5:6:185:VAL:HB	1.91	0.53
24:U:263:LYS:HA	24:U:278:LYS:HA	1.91	0.53
1:0:423:TYR:HB3	1:0:431:PRO:HB3	1.91	0.53
3:2:441:ILE:O	3:2:445:GLN:N	2.42	0.53
6:7:489:GLU:OE1	6:7:491:HIS:NE2	2.38	0.53
8:A:116:ASP:OD2	8:A:164:ARG:NH1	2.42	0.53
8:A:542:GLU:OE1	8:A:543:LEU:N	2.42	0.53
9:B:273:LEU:HD12	9:B:274:PRO:HD2	1.89	0.53
20:Q:371:ASP:OD1	20:Q:371:ASP:N	2.38	0.53
5:6:248:HIS:HA	5:6:251:ILE:HD12	1.91	0.53
6:7:443:LYS:HD2	6:7:469:ASP:HB3	1.90	0.53
8:A:173:THR:HG1	8:A:184:SER:HG	1.50	0.53
13:F:112:GLU:OE1	13:F:123:LYS:NZ	2.39	0.53
14:G:4:ILE:HD12	14:G:49:LEU:HD11	1.89	0.53
17:J:5:VAL:CG1	17:J:5:VAL:HG21	2.30	0.53
27:X:228:SER:O	27:X:247:ASN:ND2	2.42	0.53
7:M:48:CYS:SG	7:M:49:GLY:N	2.82	0.52
8:A:408:ASP:N	8:A:408:ASP:OD1	2.42	0.52
8:A:1394:THR:HB	8:A:1399:ARG:HD3	1.91	0.52
16:I:45:ARG:HE	16:I:46:HIS:H	1.57	0.52
22:S:238:PRO:HB2	22:S:240:PRO:HD2	1.90	0.52
27:X:168:ARG:HA	27:X:181:LEU:HB3	1.91	0.52
1:0:447:LYS:NZ	1:0:474:ASN:O	2.43	0.52
5:6:392:VAL:HG22	5:6:426:ARG:HB2	1.92	0.52
11:D:56:ARG:NH1	11:D:145:MET:O	2.42	0.52
21:P:133:TYR:HB3	21:P:214:ILE:HD11	1.90	0.52
22:S:239:ALA:HA	22:S:242:LYS:HD3	1.91	0.52
1:0:534:PRO:HA	5:6:239:LEU:HB3	1.92	0.52
3:2:117:VAL:HG13	3:2:119:ASN:H	1.73	0.52
5:6:412:ILE:O	5:6:422:LEU:N	2.43	0.52
6:7:553:GLN:N	6:7:703:ALA:O	2.38	0.52
8:A:951:GLU:OE2	8:A:953:ASN:N	2.36	0.52
9:B:562:GLY:O	9:B:590:HIS:ND1	2.42	0.52
1:0:67:ARG:NE	1:0:229:ASP:O	2.37	0.52
1:0:259:ARG:NH2	1:0:394:GLU:O	2.41	0.52
4:4:305:CYS:HB3	4:4:310:SER:H	1.75	0.52
5:6:197:LYS:HD2	5:6:200:ARG:HH21	1.75	0.52
6:7:101:PRO:HD2	6:7:120:TYR:HD1	1.74	0.52
8:A:182:VAL:HG12	8:A:201:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:35:LEU:HA	11:D:47:LEU:HB2	1.91	0.52
4:4:228:THR:O	4:4:233:GLY:N	2.38	0.52
14:G:10:ASN:HB3	14:G:69:GLU:OE2	2.09	0.52
2:1:185:LEU:HA	2:1:191:LEU:HD23	1.92	0.52
9:B:640:VAL:HA	9:B:651:LEU:HA	1.92	0.52
2:1:234:LEU:HB3	2:1:297:ARG:HG3	1.92	0.52
4:4:176:LEU:HD22	4:4:210:ILE:HG23	1.91	0.52
6:7:340:GLU:OE2	6:7:380:ARG:NH1	2.42	0.52
7:M:164:LYS:HE2	30:T:-11:DC:H3'	1.91	0.52
9:B:74:LEU:HD11	9:B:141:ASP:H	1.75	0.52
10:C:101:LEU:O	10:C:102:GLN:NE2	2.43	0.52
24:U:39:LYS:O	24:U:43:GLN:NE2	2.43	0.52
2:1:257:LEU:HD13	2:1:260:PHE:HD2	1.75	0.52
3:2:29:PRO:HB3	3:2:111:ALA:HB2	1.91	0.52
9:B:709:ASP:OD1	9:B:709:ASP:N	2.41	0.52
12:E:106:GLN:HG2	12:E:107:THR:HG23	1.91	0.52
14:G:56:ILE:HG13	14:G:57:GLN:H	1.74	0.52
20:Q:25:ASP:HB2	20:Q:29:ARG:NH1	2.25	0.52
21:P:121:ASP:N	21:P:225:MET:O	2.42	0.52
26:W:90:LYS:NZ	26:W:231:GLY:O	2.37	0.52
1:0:642:MET:HB2	1:0:648:ILE:HD12	1.92	0.52
2:1:169:LEU:O	2:1:218:ARG:NH2	2.36	0.52
8:A:1002:GLY:HA3	8:A:1007:ILE:HG21	1.91	0.52
9:B:67:SER:OG	9:B:92:PHE:N	2.36	0.52
9:B:307:ASP:OD1	9:B:308:TRP:N	2.42	0.52
5:6:260:ARG:HH21	5:6:281:ASN:HB3	1.75	0.52
6:7:103:ASP:OD1	6:7:103:ASP:N	2.42	0.52
6:7:567:GLN:OE1	6:7:571:ARG:NH2	2.43	0.52
23:O:61:SER:HB3	23:O:228:GLU:HG3	1.92	0.52
1:0:561:ASP:HA	1:0:564:TRP:HD1	1.74	0.51
5:6:188:ASN:HD21	5:6:190:GLN:HB3	1.75	0.51
6:7:387:PRO:O	6:7:392:LYS:NZ	2.43	0.51
6:7:671:ILE:HA	6:7:706:TYR:HB2	1.92	0.51
9:B:80:GLU:HG2	9:B:83:ASN:HB2	1.91	0.51
23:O:107:ARG:HH11	24:U:285:TRP:HE1	1.56	0.51
26:W:35:HIS:HA	26:W:207:ILE:HB	1.91	0.51
9:B:830:TYR:CZ	9:B:1000:PRO:HD3	2.45	0.51
15:H:13:SER:OG	15:H:27:GLU:OE2	2.28	0.51
1:0:570:LEU:N	1:0:597:ILE:O	2.39	0.51
4:4:78:ALA:HA	4:4:83:ILE:HA	1.90	0.51
8:A:239:LEU:HD12	8:A:240:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:889:SER:HG	8:A:892:ALA:H	1.55	0.51
9:B:146:GLU:HG2	9:B:147:LEU:H	1.74	0.51
9:B:687:GLU:N	9:B:687:GLU:OE1	2.43	0.51
20:Q:325:LEU:O	20:Q:327:ARG:NH2	2.44	0.51
24:U:244:MET:HB3	24:U:267:VAL:HG23	1.92	0.51
5:6:450:ASN:HD22	5:6:450:ASN:C	2.12	0.51
6:7:517:LEU:HD12	6:7:524:ILE:HD11	1.92	0.51
8:A:1229:SER:OG	8:A:1233:ASP:OD2	2.27	0.51
15:H:5:LEU:HD23	15:H:135:LEU:HD21	1.92	0.51
26:W:122:TYR:HB3	26:W:156:LEU:HD12	1.92	0.51
6:7:236:THR:O	6:7:313:VAL:N	2.43	0.51
7:M:277:ILE:HA	7:M:280:VAL:HG22	1.91	0.51
8:A:566:ILE:HB	15:H:96:VAL:HG13	1.91	0.51
8:A:886:ILE:HD11	8:A:943:LEU:HB3	1.92	0.51
8:A:1444:MET:HB2	13:F:133:VAL:HG23	1.93	0.51
9:B:73:GLN:O	9:B:86:ARG:N	2.37	0.51
9:B:342:GLY:H	9:B:344:LYS:HZ3	1.57	0.51
3:2:261:GLN:HA	3:2:269:PHE:HA	1.92	0.51
4:4:139:GLN:HB2	4:4:142:GLN:HE22	1.75	0.51
4:4:248:LEU:HD22	4:4:252:MET:HG3	1.93	0.51
6:7:392:LYS:HG2	6:7:513:LEU:HD22	1.93	0.51
8:A:43:GLU:HG2	8:A:44:THR:HG23	1.92	0.51
11:D:139:LYS:HZ2	11:D:142:LYS:HB2	1.76	0.51
23:O:129:GLU:OE1	23:O:220:ARG:NH1	2.44	0.51
23:O:170:ILE:HD12	23:O:238:ARG:HA	1.92	0.51
7:M:145:ILE:HD12	9:B:865:LYS:HB3	1.93	0.51
7:M:189:PHE:HA	7:M:192:ILE:HD12	1.93	0.51
9:B:120:ARG:NH2	9:B:957:ASN:O	2.44	0.51
11:D:202:ILE:HG21	11:D:207:LEU:HD13	1.92	0.51
25:V:48:VAL:HA	25:V:51:THR:HG22	1.92	0.51
10:C:37:MET:CA	10:C:38:ILE:N	2.65	0.51
11:D:35:LEU:HD12	11:D:47:LEU:H	1.76	0.51
12:E:23:VAL:HG13	12:E:78:LEU:HD21	1.93	0.51
3:2:242:LEU:O	3:2:247:ARG:NH2	2.43	0.51
5:6:124:ARG:NH1	5:6:164:ASN:OD1	2.42	0.51
6:7:421:ARG:NH2	6:7:435:CYS:O	2.41	0.51
12:E:124:VAL:HG13	12:E:132:ILE:HB	1.93	0.51
29:N:7:DA:H2'	29:N:8:DA:C8	2.46	0.51
6:7:162:GLU:O	6:7:174:LYS:N	2.44	0.51
7:M:206:THR:HA	7:M:209:ILE:HG12	1.93	0.51
8:A:1227:ILE:HB	8:A:1239:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:116:PRO:HD2	14:G:119:LEU:HD22	1.93	0.51
14:G:142:ARG:HE	14:G:171:ILE:HG21	1.74	0.51
27:X:187:HIS:N	27:X:191:GLU:OE1	2.39	0.51
1:0:542:PRO:HB3	1:0:626:PRO:HA	1.93	0.50
5:6:150:ILE:HG21	5:6:200:ARG:HG2	1.93	0.50
6:7:385:VAL:HG21	6:7:517:LEU:HD22	1.92	0.50
8:A:446:ARG:HD2	8:A:480:ALA:HB2	1.93	0.50
16:I:105:SER:OG	16:I:106:CYS:N	2.44	0.50
23:O:138:LYS:HG2	23:O:141:ARG:HH12	1.76	0.50
1:0:70:ILE:N	1:0:231:ILE:O	2.37	0.50
3:2:189:PHE:HA	3:2:192:LEU:HD12	1.91	0.50
8:A:376:TYR:OH	8:A:498:ARG:NH1	2.43	0.50
15:H:118:PHE:O	15:H:120:GLY:N	2.45	0.50
16:I:80:SER:HG	16:I:103:CYS:HG	1.58	0.50
23:O:92:ALA:HB3	25:V:76:TRP:HA	1.93	0.50
29:N:-9:DG:H2"	29:N:-8:DG:H8	1.76	0.50
1:0:613:ASP:H	1:0:616:TYR:HB2	1.77	0.50
2:1:353:ARG:NH1	2:1:354:PRO:O	2.43	0.50
6:7:190:THR:OG1	6:7:213:ILE:O	2.29	0.50
20:Q:373:TYR:HB3	21:P:70:LEU:HD11	1.93	0.50
1:0:307:VAL:HG22	1:0:400:LYS:HG2	1.94	0.50
1:0:613:ASP:OD1	1:0:613:ASP:N	2.43	0.50
4:4:27:THR:HB	4:4:176:LEU:HA	1.94	0.50
8:A:1080:THR:HA	22:S:286:THR:HG23	1.93	0.50
9:B:615:MET:SD	9:B:615:MET:N	2.84	0.50
9:B:822:ASN:HB3	9:B:1091:TYR:HD1	1.77	0.50
5:6:140:ASP:N	5:6:140:ASP:OD1	2.44	0.50
5:6:196:LEU:HA	5:6:199:ILE:HD12	1.93	0.50
8:A:565:ILE:HD11	8:A:571:LEU:HD13	1.92	0.50
19:L:66:GLN:HG3	19:L:67:PHE:N	2.27	0.50
30:T:-4:DT:H2"	30:T:-3:DA:C8	2.46	0.50
5:6:221:LEU:HD22	5:6:230:ARG:HB3	1.92	0.50
8:A:146:MET:N	8:A:146:MET:SD	2.85	0.50
9:B:522:VAL:HG21	9:B:537:LYS:HD3	1.94	0.50
1:0:722:ARG:NH1	5:6:291:LEU:O	2.45	0.50
5:6:186:SER:HB3	5:6:192:HIS:CE1	2.47	0.50
6:7:629:GLY:HA3	30:T:-45:DT:H5"	1.93	0.50
9:B:702:LEU:HD23	9:B:738:PHE:HA	1.92	0.50
9:B:995:ARG:HH12	10:C:165:LYS:HG3	1.77	0.50
23:O:91:ASN:HB3	25:V:71:PHE:N	2.27	0.50
25:V:6:TYR:HB2	25:V:46:LYS:NZ	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:509:ARG:HB2	1:0:512:ILE:HG12	1.92	0.50
1:0:711:ASP:OD1	1:0:712:MET:N	2.45	0.50
6:7:383:ILE:N	6:7:533:PRO:O	2.39	0.50
9:B:1219:ASP:N	9:B:1219:ASP:OD1	2.44	0.50
10:C:55:THR:HB	10:C:152:GLU:H	1.77	0.50
10:C:99:LEU:HB2	10:C:157:CYS:HB2	1.93	0.50
29:N:38:DG:C6	30:T:-38:DC:O2	2.64	0.50
2:1:302:MET:HG3	2:1:304:ASN:H	1.75	0.50
2:1:546:LEU:HD11	2:1:600:VAL:HG22	1.92	0.50
8:A:68:GLN:HE21	8:A:80:HIS:CE1	2.30	0.50
9:B:629:ASP:OD1	9:B:629:ASP:N	2.41	0.50
15:H:91:ASP:OD1	15:H:91:ASP:N	2.43	0.50
2:1:496:SER:HA	2:1:499:ILE:HD12	1.93	0.49
5:6:429:CYS:O	5:6:433:LYS:N	2.44	0.49
6:7:575:ARG:NH2	29:N:49:DG:N3	2.59	0.49
8:A:46:THR:OG1	8:A:47:ARG:N	2.45	0.49
9:B:921:ASP:O	9:B:927:GLN:NE2	2.45	0.49
11:D:55:ALA:HA	11:D:58:VAL:HG22	1.93	0.49
12:E:126:SER:OG	12:E:127:ILE:N	2.45	0.49
4:4:25:LEU:HD13	4:4:163:ILE:HG21	1.93	0.49
4:4:87:TYR:HB2	4:4:125:LEU:HD21	1.93	0.49
6:7:401:CYS:O	6:7:404:LYS:NZ	2.38	0.49
8:A:697:ALA:HB1	16:I:97:MET:HG3	1.93	0.49
9:B:796:LEU:HA	9:B:853:SER:HA	1.94	0.49
21:P:202:ILE:HD12	21:P:203:PRO:HD2	1.93	0.49
26:W:140:LEU:HA	26:W:147:PHE:HA	1.94	0.49
1:0:216:PRO:HB3	1:0:312:LEU:HD13	1.94	0.49
1:0:322:PRO:HG3	1:0:373:PRO:HG3	1.95	0.49
1:0:371:ARG:NE	1:0:410:SER:O	2.45	0.49
4:4:139:GLN:OE1	4:4:142:GLN:NE2	2.45	0.49
5:6:270:VAL:N	5:6:288:TYR:OH	2.38	0.49
6:7:477:LEU:HG	6:7:482:TRP:HZ2	1.77	0.49
9:B:763:GLN:HG2	9:B:765:PRO:HD2	1.95	0.49
9:B:862:GLN:HB3	9:B:963:PHE:HD1	1.78	0.49
5:6:426:ARG:HB3	5:6:435:GLU:HB3	1.94	0.49
6:7:419:GLN:O	6:7:422:GLN:NE2	2.45	0.49
8:A:483:ASP:OD1	8:A:483:ASP:N	2.41	0.49
8:A:783:THR:HG21	8:A:797:LYS:HA	1.93	0.49
9:B:1103:ILE:O	9:B:1122:ARG:NH2	2.44	0.49
1:0:133:CYS:O	1:0:137:THR:OG1	2.26	0.49
1:0:346:MET:SD	1:0:346:MET:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:469:TYR:HA	1:0:472:MET:HG2	1.94	0.49
1:0:568:LEU:O	1:0:597:ILE:N	2.45	0.49
3:2:349:SER:OG	3:2:351:SER:OG	2.29	0.49
6:7:613:TYR:OH	6:7:762:GLU:OE2	2.31	0.49
7:M:241:ARG:NH2	9:B:104:GLU:O	2.46	0.49
8:A:540:PHE:HB3	8:A:571:LEU:HD23	1.95	0.49
12:E:62:ALA:O	12:E:77:SER:OG	2.25	0.49
26:W:74:GLU:O	26:W:84:ARG:NH2	2.45	0.49
26:W:349:GLU:HG2	26:W:352:GLU:HG3	1.93	0.49
1:0:438:THR:HB	1:0:638:ARG:HH12	1.75	0.49
6:7:346:ASP:OD2	6:7:348:ARG:NH2	2.46	0.49
8:A:172:PRO:HB2	8:A:184:SER:H	1.77	0.49
28:5:46:LYS:HA	28:5:49:PHE:HD2	1.77	0.49
1:0:555:GLN:NE2	2:1:298:GLY:O	2.46	0.49
5:6:127:ILE:HB	5:6:232:VAL:HG22	1.95	0.49
8:A:567:LYS:HD2	15:H:95:TYR:CD2	2.47	0.49
8:A:1124:HIS:CG	8:A:1130:GLN:HG2	2.47	0.49
9:B:275:TYR:HB3	9:B:337:ARG:HD2	1.95	0.49
20:Q:378:VAL:O	21:P:66:ARG:NH2	2.46	0.49
23:O:90:ARG:HG3	24:U:231:ILE:HG13	1.93	0.49
2:1:537:GLU:HB3	5:6:341:LYS:HB2	1.95	0.49
6:7:104:PHE:HZ	6:7:117:ASP:HB3	1.77	0.49
7:M:157:CYS:SG	7:M:158:HIS:N	2.82	0.49
8:A:744:LYS:HA	8:A:747:VAL:HG12	1.94	0.49
8:A:1308:THR:OG1	8:A:1309:ASP:N	2.45	0.49
9:B:644:GLU:HG3	9:B:646:LEU:H	1.77	0.49
15:H:33:GLN:HG3	15:H:36:CYS:H	1.77	0.49
24:U:269:ILE:N	24:U:272:ASN:O	2.41	0.49
29:N:-5:DA:N6	30:T:4:DT:O4	2.45	0.49
3:2:36:TYR:HD1	3:2:47:ILE:HD11	1.77	0.49
5:6:134:GLU:OE2	5:6:206:GLY:N	2.46	0.49
8:A:333:GLU:HA	8:A:338:GLY:HA3	1.95	0.49
8:A:340:LEU:HB3	8:A:1429:ILE:HG22	1.95	0.49
8:A:658:LEU:HB2	9:B:831:SER:HB3	1.95	0.49
1:0:109:THR:OG1	1:0:110:SER:N	2.42	0.49
2:1:472:GLN:HG2	4:4:38:THR:HG22	1.95	0.49
6:7:457:TYR:O	6:7:500:ARG:NH2	2.45	0.49
7:M:137:CYS:SG	7:M:138:ASP:N	2.85	0.49
9:B:402:GLY:O	9:B:405:ARG:NH1	2.42	0.49
14:G:13:LEU:HD22	14:G:26:LEU:HD21	1.94	0.49
14:G:166:ASP:N	14:G:166:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:188:SER:N	27:X:191:GLU:OE1	2.44	0.49
9:B:332:ASP:N	9:B:332:ASP:OD1	2.44	0.48
22:S:299:CYS:HB2	22:S:306:TRP:HZ3	1.78	0.48
1:0:111:ARG:NE	31:0:801:SF4:S2	2.81	0.48
8:A:592:ASP:OD1	8:A:592:ASP:N	2.40	0.48
8:A:943:LEU:HA	8:A:946:VAL:HG12	1.95	0.48
9:B:112:LEU:HD23	9:B:124:TYR:HD1	1.78	0.48
9:B:574:SER:HB3	9:B:591:ARG:HH21	1.78	0.48
13:F:140:ASP:OD1	13:F:141:GLY:N	2.47	0.48
26:W:70:HIS:HB2	26:W:88:TYR:HE1	1.77	0.48
3:2:88:ILE:N	3:2:99:ASN:O	2.37	0.48
6:7:676:HIS:NE2	29:N:48:DT:OP1	2.46	0.48
8:A:170:THR:HG21	8:A:187:LYS:HG2	1.94	0.48
10:C:180:TYR:OH	10:C:188:HIS:ND1	2.40	0.48
22:S:280:SER:OG	22:S:298:THR:O	2.32	0.48
23:O:70:ILE:N	23:O:126:ALA:O	2.44	0.48
28:5:36:ASP:OD2	28:5:39:HIS:ND1	2.36	0.48
1:0:541:PHE:HA	1:0:623:ILE:HB	1.94	0.48
6:7:500:ARG:H	6:7:500:ARG:HD3	1.77	0.48
8:A:469:ARG:HD3	8:A:469:ARG:HA	1.61	0.48
9:B:760:ASP:N	9:B:760:ASP:OD1	2.42	0.48
9:B:839:MET:N	9:B:989:THR:O	2.46	0.48
9:B:1121:GLY:HA3	9:B:1124:ARG:HE	1.78	0.48
11:D:142:LYS:HA	11:D:145:MET:SD	2.53	0.48
28:5:13:ASP:HB3	28:5:16:ILE:HG22	1.95	0.48
3:2:339:LEU:HD13	3:2:403:HIS:HB3	1.95	0.48
5:6:172:ILE:HG12	5:6:181:LEU:HA	1.94	0.48
8:A:156:ASP:OD1	8:A:156:ASP:N	2.47	0.48
8:A:868:TYR:CE1	8:A:1064:VAL:HG11	2.48	0.48
8:A:1288:ASP:HA	8:A:1302:PRO:HA	1.94	0.48
12:E:80:VAL:HA	12:E:109:ILE:HB	1.94	0.48
16:I:65:ASP:OD2	16:I:67:THR:N	2.46	0.48
19:L:34:CYS:SG	19:L:36:SER:OG	2.64	0.48
20:Q:120:LYS:HB3	20:Q:394:LYS:HA	1.95	0.48
23:O:107:ARG:HG2	25:V:69:TYR:HE1	1.77	0.48
26:W:349:GLU:O	26:W:353:ASN:ND2	2.47	0.48
1:0:722:ARG:HD3	5:6:292:LEU:HA	1.94	0.48
9:B:424:LEU:HD11	9:B:449:ASN:HB3	1.96	0.48
23:O:105:ARG:O	25:V:69:TYR:OH	2.22	0.48
5:6:190:GLN:NE2	5:6:194:ASP:OD1	2.46	0.48
6:7:363:ARG:NH1	6:7:390:ALA:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:687:LEU:HD22	6:7:726:LEU:HD13	1.95	0.48
8:A:18:GLN:HB3	9:B:1215:ARG:HB2	1.96	0.48
13:F:116:ASP:OD2	13:F:119:ARG:N	2.35	0.48
22:S:159:VAL:HG23	22:S:160:LEU:HD12	1.94	0.48
23:O:98:ARG:HH11	30:T:-7:DT:H4'	1.78	0.48
26:W:140:LEU:HD12	26:W:144:ARG:HA	1.95	0.48
26:W:198:THR:HG23	26:W:201:ILE:HD12	1.95	0.48
1:0:570:LEU:HD12	1:0:582:ALA:HB1	1.96	0.48
1:0:603:ARG:HG2	1:0:661:HIS:HD2	1.79	0.48
2:1:434:ILE:HB	5:6:117:PRO:HG2	1.96	0.48
4:4:289:CYS:HB3	4:4:293:LEU:H	1.78	0.48
6:7:558:TRP:HE1	6:7:735:VAL:HA	1.77	0.48
8:A:328:ARG:HH11	8:A:335:ARG:HH12	1.59	0.48
9:B:424:LEU:HD12	9:B:424:LEU:HA	1.57	0.48
23:O:196:ARG:HG2	23:O:203:VAL:HG22	1.94	0.48
24:U:280:GLN:HB2	25:V:61:THR:HG23	1.96	0.48
27:X:231:LEU:HB2	27:X:245:TRP:HB2	1.95	0.48
1:0:651:ASN:HA	1:0:654:LEU:HD12	1.95	0.48
6:7:438:PHE:HB3	6:7:455:SER:HB3	1.94	0.48
6:7:698:ASP:OD1	6:7:698:ASP:N	2.47	0.48
9:B:698:GLU:HA	9:B:701:ILE:HG12	1.95	0.48
26:W:35:HIS:CG	26:W:209:PRO:HG3	2.48	0.48
1:0:384:LEU:O	1:0:388:LEU:HB2	2.13	0.48
5:6:182:VAL:HG21	5:6:199:ILE:HD11	1.96	0.48
7:M:190:LYS:NZ	7:M:302:LEU:O	2.47	0.48
8:A:112:LYS:NZ	8:A:148:CYS:SG	2.71	0.48
9:B:809:MET:HB2	9:B:814:PHE:HB3	1.95	0.48
26:W:68:SER:N	26:W:88:TYR:O	2.47	0.48
2:1:371:THR:HA	2:1:374:ILE:HG12	1.96	0.47
3:2:412:ALA:HB2	3:2:434:PRO:HG3	1.94	0.47
6:7:624:LYS:HE3	6:7:650:ASN:H	1.79	0.47
8:A:858:ASN:OD1	8:A:862:ASN:N	2.47	0.47
13:F:86:THR:OG1	13:F:87:LYS:N	2.48	0.47
14:G:25:TYR:O	14:G:28:THR:OG1	2.29	0.47
15:H:146:ARG:HH11	15:H:146:ARG:HD2	1.59	0.47
16:I:45:ARG:HE	16:I:46:HIS:N	2.12	0.47
20:Q:134:HIS:HB2	20:Q:354:ASP:HB2	1.95	0.47
22:S:175:ALA:HA	22:S:178:ILE:HG12	1.96	0.47
5:6:197:LYS:HG2	5:6:200:ARG:HE	1.79	0.47
8:A:332:LYS:H	8:A:337:ARG:HD3	1.79	0.47
8:A:1000:LEU:N	8:A:1011:GLN:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:847:ASP:HB3	10:C:167:HIS:CE1	2.49	0.47
9:B:855:PHE:HB2	9:B:972:LYS:HD2	1.96	0.47
12:E:87:SER:OG	12:E:88:VAL:N	2.47	0.47
15:H:97:MET:HG2	15:H:118:PHE:CD2	2.49	0.47
30:T:-41:DG:H2"	30:T:-40:DT:H5"	1.95	0.47
5:6:444:ILE:HA	5:6:448:LEU:HB2	1.96	0.47
8:A:40:THR:OG1	8:A:41:MET:N	2.48	0.47
9:B:277:LYS:NZ	9:B:336:ARG:H	2.10	0.47
9:B:279:ASP:N	9:B:279:ASP:OD1	2.47	0.47
9:B:301:ILE:HD13	9:B:379:GLY:HA2	1.96	0.47
9:B:361:LEU:HD23	9:B:374:LYS:HD3	1.96	0.47
10:C:11:ARG:HD2	10:C:21:ILE:HD11	1.96	0.47
15:H:129:TYR:CZ	15:H:130:ARG:HD2	2.49	0.47
23:O:159:ASN:ND2	29:N:4:DA:N3	2.62	0.47
26:W:72:GLN:NE2	26:W:218:THR:O	2.33	0.47
27:X:232:VAL:HA	27:X:244:VAL:HG12	1.97	0.47
2:1:542:LEU:HB2	2:1:547:LEU:HD12	1.97	0.47
6:7:373:MET:HA	6:7:380:ARG:HD2	1.97	0.47
6:7:383:ILE:HB	6:7:534:LYS:HA	1.96	0.47
6:7:515:ALA:HB3	6:7:685:GLN:HE22	1.79	0.47
9:B:69:LEU:HD12	9:B:69:LEU:HA	1.77	0.47
9:B:425:THR:HA	9:B:428:ILE:HG22	1.97	0.47
9:B:1049:ASP:OD1	9:B:1049:ASP:N	2.37	0.47
1:0:500:GLY:O	1:0:709:SER:OG	2.30	0.47
8:A:378:GLU:OE2	8:A:434:ARG:NH2	2.43	0.47
8:A:658:LEU:HD13	9:B:831:SER:HB3	1.97	0.47
8:A:843:LYS:NZ	8:A:1401:SER:O	2.48	0.47
9:B:540:SER:OG	9:B:541:LEU:N	2.46	0.47
1:0:585:THR:OG1	2:1:383:GLU:OE2	2.32	0.47
9:B:248:SER:H	9:B:418:LYS:HZ1	1.61	0.47
11:D:56:ARG:HD2	11:D:148:LEU:HB3	1.96	0.47
21:P:140:LEU:H	21:P:210:LYS:HD2	1.79	0.47
26:W:176:MET:HA	26:W:179:ILE:HG22	1.96	0.47
2:1:199:VAL:HG11	2:1:206:PRO:HG3	1.97	0.47
2:1:633:TYR:HB3	4:4:326:VAL:HG21	1.95	0.47
3:2:44:LYS:NZ	4:4:67:PHE:O	2.43	0.47
8:A:148:CYS:N	8:A:169:ASN:O	2.42	0.47
8:A:150:THR:HA	8:A:165:GLY:HA3	1.96	0.47
8:A:1159:ARG:NH2	8:A:1185:PHE:O	2.38	0.47
9:B:79:THR:HB	9:B:81:SER:H	1.79	0.47
12:E:43:LYS:HE3	12:E:47:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:92:THR:O	12:E:95:THR:OG1	2.27	0.47
12:E:143:ASN:HD22	12:E:146:HIS:CE1	2.33	0.47
16:I:30:ARG:NH1	20:Q:422:ARG:O	2.48	0.47
21:P:70:LEU:HB3	21:P:221:GLU:HG2	1.96	0.47
22:S:218:ILE:HD12	22:S:222:ASP:HB2	1.97	0.47
23:O:107:ARG:NH1	25:V:67:ASP:O	2.47	0.47
23:O:154:ASP:N	23:O:154:ASP:OD1	2.48	0.47
6:7:120:TYR:O	6:7:122:ARG:NH1	2.48	0.47
7:M:50:LEU:HA	8:A:413:ILE:HA	1.95	0.47
8:A:1229:SER:OG	8:A:1230:GLU:N	2.47	0.47
8:A:1309:ASP:N	8:A:1309:ASP:OD1	2.46	0.47
8:A:1329:THR:HG22	8:A:1331:SER:H	1.79	0.47
26:W:356:THR:HA	26:W:356:THR:HG22	1.96	0.47
1:0:575:ASP:O	1:0:579:THR:OG1	2.32	0.47
2:1:355:ASP:HB2	2:1:358:MET:HG3	1.97	0.47
8:A:500:GLU:OE2	9:B:1146:PHE:N	2.44	0.47
8:A:889:SER:HA	8:A:1297:GLU:HG3	1.96	0.47
9:B:29:ASP:HB3	9:B:658:ILE:HD13	1.97	0.47
9:B:214:ALA:HB3	9:B:498:THR:HG22	1.96	0.47
11:D:68:ARG:HB3	11:D:72:ARG:NH1	2.30	0.47
23:O:232:PRO:O	23:O:236:GLU:HG2	2.15	0.47
25:V:82:ASN:HB3	25:V:82:ASN:HD22	1.79	0.47
1:0:659:MET:CG	1:0:659:MET:C	2.84	0.47
3:2:462:PHE:CD2	3:2:468:TYR:HD1	2.33	0.47
4:4:136:GLU:HA	4:4:139:GLN:HE21	1.80	0.47
5:6:352:CYS:SG	5:6:366:CYS:HB3	2.55	0.47
6:7:143:LEU:HD23	6:7:171:HIS:HB2	1.97	0.47
14:G:39:THR:HG23	14:G:42:PHE:H	1.79	0.47
21:P:75:MET:N	21:P:75:MET:SD	2.85	0.47
24:U:253:ARG:HH11	24:U:255:LYS:HA	1.80	0.47
27:X:142:VAL:O	27:X:178:PHE:N	2.47	0.47
27:X:196:LEU:HA	27:X:199:GLN:HG2	1.97	0.47
5:6:237:GLY:HA2	5:6:266:LEU:HB2	1.97	0.46
6:7:132:LEU:HB2	6:7:201:SER:HA	1.96	0.46
6:7:710:SER:N	6:7:715:GLU:OE1	2.48	0.46
8:A:35:ILE:H	8:A:35:ILE:HD12	1.81	0.46
8:A:599:SER:O	8:A:599:SER:OG	2.30	0.46
8:A:700:ASN:HD21	16:I:98:VAL:HG22	1.80	0.46
8:A:1400:CYS:HB2	8:A:1405:THR:HG23	1.97	0.46
23:O:112:THR:HB	23:O:124:THR:HG23	1.96	0.46
3:2:462:PHE:HD2	3:2:468:TYR:CD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:191:ASP:OD1	6:7:191:ASP:N	2.47	0.46
8:A:1114:PRO:HB2	8:A:1311:VAL:HB	1.97	0.46
9:B:1156:ASP:HB3	9:B:1198:TYR:H	1.80	0.46
11:D:56:ARG:HH22	11:D:145:MET:HB2	1.80	0.46
12:E:118:PRO:O	12:E:122:LYS:N	2.48	0.46
1:0:210:TYR:OH	1:0:235:ASP:O	2.32	0.46
3:2:434:PRO:HA	3:2:435:PRO:HD3	1.81	0.46
8:A:791:ASP:OD1	8:A:792:TYR:N	2.48	0.46
5:6:190:GLN:HA	5:6:193:ILE:HD12	1.98	0.46
11:D:165:GLN:HA	11:D:168:LYS:HD3	1.97	0.46
12:E:109:ILE:HA	12:E:133:GLU:HG2	1.97	0.46
20:Q:129:PRO:O	20:Q:133:PHE:HB2	2.15	0.46
24:U:284:GLU:H	25:V:65:ASN:HA	1.80	0.46
1:0:1:MET:HB2	1:0:15:PRO:HA	1.96	0.46
1:0:259:ARG:HG2	1:0:262:ARG:HH12	1.80	0.46
8:A:31:SER:O	9:B:1183:LYS:NZ	2.35	0.46
8:A:443:LEU:HB3	8:A:490:HIS:HB2	1.98	0.46
8:A:958:VAL:HG21	8:A:1052:GLN:HB3	1.96	0.46
23:O:195:TYR:CE2	23:O:197:MET:HB3	2.51	0.46
24:U:282:GLU:HB2	25:V:63:LYS:HG3	1.98	0.46
25:V:11:ARG:HA	25:V:16:GLY:HA3	1.98	0.46
30:T:3:DT:H4'	30:T:4:DT:H5'	1.97	0.46
1:0:252:LEU:HB2	1:0:435:MET:HB2	1.96	0.46
1:0:322:PRO:HG2	1:0:325:ILE:HG12	1.98	0.46
1:0:604:GLY:O	1:0:607:SER:OG	2.30	0.46
3:2:244:GLU:HA	3:2:247:ARG:HE	1.80	0.46
5:6:134:GLU:HA	5:6:137:LEU:HD12	1.98	0.46
5:6:386:LEU:HD23	5:6:445:HIS:HA	1.97	0.46
8:A:362:ASP:O	8:A:459:ARG:N	2.39	0.46
8:A:860:LEU:O	12:E:174:GLN:NE2	2.37	0.46
8:A:1028:THR:HA	8:A:1031:VAL:HG12	1.97	0.46
12:E:86:PRO:HA	12:E:113:GLN:HB2	1.97	0.46
12:E:171:LYS:O	12:E:173:SER:N	2.48	0.46
14:G:101:VAL:N	14:G:108:VAL:O	2.47	0.46
18:K:57:LEU:HG	18:K:77:THR:HA	1.97	0.46
27:X:216:GLN:HG3	27:X:216:GLN:HE21	1.77	0.46
4:4:284:ALA:O	5:6:324:PHE:N	2.46	0.46
6:7:127:HIS:HA	6:7:202:LYS:HG2	1.97	0.46
8:A:956:LEU:HD23	8:A:956:LEU:HA	1.81	0.46
11:D:26:THR:HG22	11:D:201:LYS:HG2	1.97	0.46
12:E:4:GLU:OE1	12:E:8:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:T:-25:DA:H2"	30:T:-24:DA:N7	2.30	0.46
1:0:158:TYR:HB3	1:0:191:CYS:N	2.31	0.46
1:0:301:ASP:OD1	1:0:301:ASP:N	2.49	0.46
2:1:587:LYS:HA	2:1:587:LYS:HD3	1.74	0.46
8:A:367:PRO:HG2	8:A:370:ILE:HG12	1.97	0.46
8:A:666:ILE:O	8:A:669:THR:N	2.48	0.46
9:B:336:ARG:HH22	9:B:340:ALA:HA	1.81	0.46
16:I:13:MET:N	16:I:13:MET:SD	2.89	0.46
22:S:182:MET:HA	22:S:185:VAL:HG22	1.98	0.46
29:N:3:DT:H6	29:N:3:DT:H2'	1.54	0.46
5:6:120:ARG:HA	5:6:309:PRO:HA	1.98	0.46
5:6:133:SER:H	5:6:136:MET:HE2	1.81	0.46
8:A:1156:PRO:HA	8:A:1190:PRO:HB2	1.98	0.46
10:C:84:ARG:HB3	10:C:84:ARG:HD3	1.74	0.46
10:C:148:ARG:HH12	17:J:65:PRO:HD2	1.80	0.46
22:S:201:ILE:O	22:S:205:ASN:ND2	2.43	0.46
4:4:28:VAL:HG11	4:4:57:LEU:HD21	1.97	0.46
6:7:133:TRP:HB2	6:7:142:ILE:HB	1.98	0.46
7:M:251:GLN:HE21	7:M:289:PHE:HE2	1.64	0.46
8:A:225:ASN:O	8:A:229:SER:N	2.38	0.46
8:A:402:ALA:HA	8:A:434:ARG:HA	1.98	0.46
8:A:433:GLU:OE2	9:B:1108:ARG:NH2	2.48	0.46
8:A:456:MET:HB2	8:A:456:MET:HE2	1.81	0.46
8:A:1431:GLY:HA3	9:B:1152:MET:HE2	1.98	0.46
9:B:784:ASN:OD1	9:B:784:ASN:N	2.43	0.46
21:P:120:TYR:HA	21:P:226:PRO:HA	1.98	0.46
24:U:9:VAL:HG11	24:U:275:THR:HG21	1.96	0.46
24:U:14:VAL:HA	24:U:17:VAL:HG22	1.98	0.46
1:0:245:ILE:HG23	1:0:638:ARG:HH21	1.79	0.45
2:1:282:GLU:OE2	2:1:286:ARG:NH2	2.34	0.45
3:2:462:PHE:CE2	3:2:491:PHE:CE2	3.03	0.45
6:7:101:PRO:HG2	6:7:121:LEU:HA	1.97	0.45
6:7:416:SER:HA	6:7:419:GLN:HG2	1.98	0.45
6:7:621:LYS:HD2	6:7:621:LYS:HA	1.79	0.45
8:A:24:PRO:HA	8:A:27:VAL:HG12	1.98	0.45
8:A:1216:ILE:HD12	8:A:1219:THR:HB	1.97	0.45
10:C:167:HIS:NE2	19:L:70:ARG:O	2.49	0.45
23:O:196:ARG:HH21	29:N:3:DT:P	2.39	0.45
1:0:499:LYS:HE2	1:0:709:SER:HB2	1.97	0.45
4:4:26:LEU:HB3	4:4:73:VAL:HA	1.98	0.45
6:7:489:GLU:HB3	6:7:491:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:33:ALA:HA	8:A:57:ARG:HH21	1.80	0.45
8:A:147:VAL:HG23	8:A:170:THR:HG22	1.97	0.45
9:B:76:GLN:NE2	20:Q:328:LYS:O	2.49	0.45
9:B:449:ASN:O	9:B:452:THR:OG1	2.29	0.45
11:D:173:HIS:HB3	11:D:176:GLU:HB3	1.99	0.45
21:P:112:ASP:OD1	21:P:118:HIS:NE2	2.49	0.45
25:V:109:ASP:OD1	25:V:109:ASP:N	2.49	0.45
1:0:241:ASP:OD1	1:0:241:ASP:N	2.49	0.45
1:0:271:ILE:HD13	1:0:328:ALA:HB1	1.97	0.45
1:0:310:PRO:HB3	1:0:404:THR:HG23	1.97	0.45
5:6:388:THR:HA	5:6:445:HIS:HE1	1.81	0.45
6:7:341:TYR:OH	6:7:349:ASN:OD1	2.32	0.45
9:B:223:VAL:HG22	9:B:240:ILE:HD11	1.99	0.45
9:B:834:ASN:N	9:B:835:GLN:OE1	2.47	0.45
10:C:217:ASP:N	10:C:217:ASP:OD1	2.49	0.45
16:I:81:ARG:HD3	16:I:81:ARG:HA	1.61	0.45
1:0:342:LEU:HD12	1:0:402:ILE:HD11	1.97	0.45
2:1:562:LYS:HG2	5:6:365:CYS:HA	1.99	0.45
9:B:1134:GLU:OE1	9:B:1134:GLU:N	2.43	0.45
9:B:1166:CYS:SG	9:B:1185:CYS:HB2	2.57	0.45
20:Q:25:ASP:HA	20:Q:28:ARG:HB3	1.97	0.45
1:0:232:VAL:HB	1:0:456:VAL:HA	1.98	0.45
1:0:499:LYS:HA	1:0:505:ALA:HA	1.99	0.45
2:1:290:SER:HA	2:1:308:ASP:H	1.80	0.45
2:1:334:LYS:HB3	2:1:336:ILE:HG12	1.99	0.45
2:1:369:ASP:N	2:1:369:ASP:OD1	2.48	0.45
3:2:185:THR:OG1	3:2:188:GLY:N	2.39	0.45
5:6:349:CYS:SG	5:6:352:CYS:N	2.85	0.45
9:B:1084:GLN:NE2	10:C:190:ASP:O	2.38	0.45
28:5:20:ILE:HG23	28:5:31:VAL:HG21	1.99	0.45
1:0:215:ASP:OD1	1:0:217:LYS:NZ	2.39	0.45
1:0:380:ARG:HH22	1:0:384:LEU:HD13	1.82	0.45
2:1:510:ASN:ND2	4:4:266:ASN:O	2.50	0.45
6:7:436:ALA:HB1	6:7:444:GLU:HG2	1.98	0.45
7:M:147:LYS:HD3	7:M:151:LYS:HE3	1.98	0.45
8:A:590:ARG:NH2	8:A:620:LYS:O	2.49	0.45
14:G:45:ILE:HA	14:G:78:VAL:HG12	1.99	0.45
23:O:93:GLU:H	25:V:72:CYS:N	2.11	0.45
24:U:243:LEU:HD22	25:V:112:ARG:HH21	1.82	0.45
26:W:200:GLU:HG3	26:W:203:LEU:HD12	1.99	0.45
2:1:205:PRO:HA	2:1:206:PRO:HD3	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:364:ILE:HG22	9:B:585:VAL:HG23	1.99	0.45
11:D:192:LYS:HZ2	11:D:204:ASP:N	2.15	0.45
23:O:67:LEU:HA	23:O:162:GLY:HA2	1.99	0.45
23:O:73:THR:HA	23:O:122:VAL:HA	1.99	0.45
23:O:207:PHE:CG	23:O:211:LYS:HB2	2.52	0.45
26:W:91:TYR:CD2	26:W:197:ASN:HB2	2.51	0.45
1:0:405:PHE:HE1	1:0:437:PHE:HB2	1.82	0.45
1:0:618:ARG:HH12	1:0:676:TYR:H	1.65	0.45
4:4:60:PHE:CZ	4:4:248:LEU:HB2	2.52	0.45
5:6:125:SER:HB3	5:6:230:ARG:HA	1.98	0.45
10:C:35:ARG:HH21	18:K:41:THR:HB	1.81	0.45
20:Q:30:ASN:O	20:Q:33:ARG:NH1	2.49	0.45
26:W:67:ILE:HG13	26:W:89:VAL:HG22	1.99	0.45
1:0:88:ASN:HA	2:1:416:ARG:HH22	1.82	0.45
8:A:453:MET:N	8:A:453:MET:SD	2.90	0.45
8:A:1198:ASP:O	8:A:1202:MET:HB2	2.17	0.45
9:B:222:ILE:HD12	9:B:222:ILE:HA	1.83	0.45
23:O:69:ASN:ND2	23:O:124:THR:OG1	2.49	0.45
28:5:31:VAL:HA	28:5:42:VAL:HA	1.99	0.45
3:2:219:VAL:HA	3:2:222:LEU:HD12	1.99	0.45
5:6:343:VAL:HB	5:6:355:LYS:HZ3	1.82	0.45
6:7:482:TRP:O	6:7:508:HIS:ND1	2.46	0.45
8:A:951:GLU:OE2	8:A:952:ALA:N	2.50	0.45
8:A:1111:MET:HE2	8:A:1114:PRO:HG3	1.99	0.45
8:A:1373:ASP:HA	8:A:1376:THR:HG22	1.99	0.45
9:B:20:ASP:OD1	9:B:21:GLU:N	2.49	0.45
9:B:769:TYR:O	9:B:773:MET:HG3	2.17	0.45
11:D:206:GLU:HG2	11:D:209:ARG:HE	1.82	0.45
12:E:85:GLU:OE2	12:E:89:GLY:N	2.42	0.45
16:I:19:ASP:HB3	16:I:24:ARG:H	1.82	0.45
23:O:93:GLU:H	25:V:71:PHE:HA	1.82	0.45
3:2:235:LYS:HB2	3:2:237:TYR:CZ	2.52	0.44
4:4:244:LEU:HA	4:4:247:TYR:HB2	1.99	0.44
6:7:534:LYS:HD2	6:7:537:GLU:HB2	1.99	0.44
6:7:642:ASN:O	6:7:646:ASN:HB3	2.17	0.44
7:M:34:ILE:HG22	7:M:45:CYS:HA	1.98	0.44
1:0:157:GLU:O	1:0:161:ASN:ND2	2.49	0.44
1:0:283:GLN:HE22	1:0:286:TYR:HD2	1.64	0.44
1:0:311:VAL:HG12	1:0:408:LEU:HD23	1.99	0.44
1:0:465:PRO:HG2	1:0:468:MET:HB2	1.99	0.44
4:4:173:LYS:HB3	4:4:256:PRO:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:420:TRP:HH2	6:7:452:LEU:HD11	1.80	0.44
8:A:1397:LEU:HD13	8:A:1429:ILE:HD11	1.99	0.44
9:B:550:ASP:OD2	9:B:552:MET:HB2	2.18	0.44
9:B:566:LEU:HG	9:B:588:GLY:HA2	1.98	0.44
23:O:184:SER:N	23:O:194:ILE:O	2.50	0.44
24:U:18:VAL:HB	24:U:22:ARG:HH12	1.83	0.44
26:W:105:VAL:HG22	27:X:266:VAL:HG21	2.00	0.44
6:7:349:ASN:ND2	6:7:481:GLU:O	2.49	0.44
8:A:886:ILE:O	8:A:940:ARG:NH1	2.48	0.44
8:A:936:LEU:HD12	8:A:936:LEU:HA	1.81	0.44
14:G:21:ARG:HB2	14:G:24:GLN:HE22	1.82	0.44
16:I:27:PHE:N	16:I:36:GLU:O	2.50	0.44
20:Q:130:VAL:HG12	21:P:61:LEU:HD23	1.98	0.44
27:X:175:LYS:HB2	27:X:177:THR:HG23	1.98	0.44
1:0:74:ARG:HH21	1:0:237:ALA:HA	1.82	0.44
1:0:625:ILE:HD11	1:0:685:ARG:HB2	1.99	0.44
21:P:73:LEU:HD12	21:P:74:PRO:HD2	1.98	0.44
27:X:185:ASP:OD1	27:X:185:ASP:N	2.41	0.44
27:X:187:HIS:HA	27:X:214:TRP:CD2	2.52	0.44
1:0:533:THR:HG21	1:0:537:MET:HB2	1.98	0.44
3:2:224:PHE:HE1	3:2:242:LEU:HD11	1.82	0.44
3:2:261:GLN:NE2	3:2:263:HIS:O	2.48	0.44
4:4:292:CYS:SG	4:4:293:LEU:N	2.90	0.44
8:A:1149:ALA:HB1	16:I:45:ARG:HH22	1.82	0.44
9:B:579:ARG:NH2	9:B:623:GLU:OE2	2.47	0.44
14:G:91:VAL:HG22	14:G:101:VAL:HG22	2.00	0.44
26:W:62:ARG:HH21	26:W:67:ILE:HB	1.82	0.44
1:0:95:LYS:NZ	1:0:96:GLU:OE2	2.51	0.44
1:0:562:GLU:HA	1:0:565:LYS:HD2	1.99	0.44
1:0:611:ASP:HA	1:0:668:ARG:HB3	1.98	0.44
4:4:27:THR:O	4:4:177:LEU:N	2.44	0.44
6:7:555:ALA:HB1	6:7:736:ILE:HD12	1.99	0.44
8:A:757:ASN:O	8:A:761:MET:HG3	2.18	0.44
10:C:10:ILE:HG21	18:K:112:GLN:HG3	1.99	0.44
10:C:258:ILE:HD11	18:K:35:PHE:CE1	2.53	0.44
12:E:19:VAL:CG2	12:E:19:VAL:N	2.80	0.44
12:E:156:LEU:HD21	12:E:197:LYS:HB2	2.00	0.44
1:0:690:ARG:NH1	1:0:703:ASP:OD1	2.45	0.44
4:4:271:ASP:OD1	4:4:271:ASP:N	2.51	0.44
5:6:399:ARG:NH2	5:6:433:LYS:O	2.50	0.44
6:7:628:TYR:HD1	6:7:630:SER:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:270:LYS:HB3	9:B:279:ASP:HB2	1.98	0.44
9:B:576:ASP:OD1	9:B:576:ASP:N	2.49	0.44
20:Q:25:ASP:HB2	20:Q:29:ARG:HH12	1.82	0.44
20:Q:114:MET:HA	21:P:138:GLN:HA	2.00	0.44
20:Q:138:ARG:HB3	20:Q:140:HIS:NE2	2.33	0.44
26:W:147:PHE:HB2	26:W:156:LEU:HB2	1.99	0.44
2:1:634:PHE:HA	4:4:326:VAL:HG11	1.99	0.44
5:6:363:CYS:HB3	5:6:368:LEU:H	1.83	0.44
6:7:190:THR:HG21	6:7:214:LYS:HA	1.99	0.44
8:A:353:ILE:HG22	8:A:468:PHE:HB2	2.00	0.44
9:B:1163:CYS:SG	9:B:1166:CYS:N	2.79	0.44
10:C:101:LEU:HB3	10:C:155:LEU:HB2	2.00	0.44
21:P:139:ASN:HA	21:P:210:LYS:HD2	1.99	0.44
23:O:116:PHE:CE1	29:N:7:DA:H2"	2.53	0.44
26:W:73:ARG:HA	26:W:83:GLU:HA	1.99	0.44
27:X:141:PRO:HB3	27:X:179:LYS:HB3	2.00	0.44
1:0:325:ILE:HD13	1:0:373:PRO:HB3	1.99	0.44
1:0:633:ARG:HA	1:0:636:LYS:HE3	2.00	0.44
2:1:422:ASP:OD1	2:1:422:ASP:N	2.50	0.44
3:2:360:LEU:HD13	3:2:366:LEU:HD21	2.00	0.44
6:7:483:GLY:HA2	6:7:508:HIS:HD1	1.83	0.44
6:7:750:TYR:HA	6:7:755:GLU:HB3	2.00	0.44
8:A:740:LEU:HD13	8:A:740:LEU:HA	1.85	0.44
10:C:240:VAL:HA	10:C:243:VAL:HG12	1.99	0.44
11:D:146:GLN:O	11:D:150:ASN:HB2	2.18	0.44
20:Q:102:PRO:HB2	21:P:91:GLU:HB3	2.00	0.44
29:N:47:DT:N3	30:T:-47:DA:C2	2.86	0.44
3:2:217:ASP:HB3	3:2:220:ASP:HB2	1.99	0.43
3:2:463:GLU:HB3	3:2:464:THR:H	1.36	0.43
5:6:409:ARG:HH21	5:6:412:ILE:HD11	1.83	0.43
7:M:146:VAL:HG22	7:M:180:CYS:HA	1.98	0.43
8:A:532:ARG:HD2	8:A:749:ALA:HB2	2.00	0.43
8:A:1063:MET:HE1	8:A:1436:ILE:HD12	2.00	0.43
8:A:1306:LEU:HA	8:A:1306:LEU:HD23	1.75	0.43
8:A:1313:LEU:HD23	8:A:1313:LEU:HA	1.83	0.43
8:A:1336:MET:HG3	8:A:1381:LEU:HD13	2.00	0.43
10:C:148:ARG:NH1	17:J:63:TYR:O	2.51	0.43
12:E:187:TYR:HD2	12:E:188:LEU:HD22	1.83	0.43
14:G:125:SER:HB3	14:G:129:SER:H	1.82	0.43
14:G:150:CYS:HA	14:G:159:ALA:HA	1.99	0.43
21:P:330:LYS:HA	21:P:330:LYS:HD3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:31:ASP:OD1	24:U:31:ASP:N	2.49	0.43
24:U:250:LYS:N	24:U:261:SER:OG	2.32	0.43
29:N:34:DA:H2'	29:N:35:DT:C6	2.52	0.43
1:0:1:MET:SD	1:0:2:LYS:N	2.92	0.43
1:0:341:TYR:O	1:0:344:THR:OG1	2.31	0.43
1:0:533:THR:HG22	1:0:567:LYS:HE2	2.00	0.43
6:7:482:TRP:N	6:7:506:ALA:O	2.50	0.43
8:A:954:TRP:HE3	8:A:955:PRO:HD2	1.82	0.43
9:B:179:CYS:SG	9:B:180:TYR:N	2.90	0.43
14:G:151:ILE:HD13	26:W:134:LEU:HD13	2.00	0.43
29:N:18:DA:C8	29:N:19:DT:H72	2.53	0.43
1:0:337:ARG:HH21	1:0:369:ILE:HD11	1.82	0.43
8:A:938:LYS:HD2	8:A:938:LYS:HA	1.84	0.43
8:A:1214:GLU:HA	8:A:1217:LYS:HB3	2.00	0.43
9:B:820:GLY:N	9:B:1091:TYR:OH	2.38	0.43
18:K:24:ASP:OD1	18:K:25:THR:N	2.51	0.43
22:S:210:ASN:HA	22:S:211:ASN:HA	1.67	0.43
23:O:72:ALA:HA	23:O:157:ILE:HA	1.99	0.43
26:W:42:ASP:OD2	26:W:217:TYR:OH	2.32	0.43
27:X:216:GLN:NE2	27:X:216:GLN:CB	2.78	0.43
28:5:34:GLU:HA	28:5:40:LEU:HD23	1.99	0.43
1:0:45:GLY:HA3	1:0:670:LEU:HD23	2.01	0.43
1:0:237:ALA:HB1	1:0:240:ILE:HB	2.00	0.43
1:0:238:HIS:O	1:0:660:ARG:NH1	2.52	0.43
2:1:415:GLU:HA	2:1:418:GLU:HB2	2.00	0.43
2:1:472:GLN:NE2	4:4:38:THR:HA	2.33	0.43
4:4:79:TYR:N	4:4:82:GLY:O	2.51	0.43
23:O:93:GLU:N	25:V:72:CYS:H	2.12	0.43
24:U:17:VAL:HB	25:V:44:PHE:HE1	1.84	0.43
28:5:48:GLU:HA	28:5:51:LYS:HB2	2.01	0.43
1:0:722:ARG:O	1:0:726:GLN:NE2	2.36	0.43
3:2:435:PRO:HA	3:2:439:ASP:H	1.83	0.43
3:2:454:TYR:CZ	3:2:483:TRP:CB	2.94	0.43
7:M:201:LYS:HD2	29:N:1:DT:O5'	2.18	0.43
8:A:426:LEU:HD12	8:A:426:LEU:HA	1.87	0.43
8:A:868:TYR:CD2	8:A:1058:VAL:HG21	2.53	0.43
9:B:351:TYR:CZ	9:B:355:ILE:HD11	2.53	0.43
9:B:386:LEU:HA	9:B:386:LEU:HD12	1.78	0.43
10:C:7:GLN:HA	18:K:104:ASN:ND2	2.33	0.43
14:G:102:GLN:HB2	14:G:107:LYS:NZ	2.33	0.43
15:H:130:ARG:HG2	15:H:134:ASN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:81:TYR:OH	18:K:89:ASN:ND2	2.51	0.43
1:0:327:ARG:HB2	1:0:330:HIS:CG	2.53	0.43
3:2:143:TRP:HA	3:2:146:ILE:HG22	2.01	0.43
3:2:224:PHE:HE2	3:2:250:LEU:HB2	1.84	0.43
8:A:93:VAL:HA	8:A:96:ILE:HG12	2.00	0.43
8:A:225:ASN:N	8:A:229:SER:OG	2.45	0.43
8:A:444:PHE:CE2	8:A:487:MET:HG3	2.54	0.43
11:D:137:ASN:N	11:D:137:ASN:OD1	2.51	0.43
12:E:26:ARG:NH2	12:E:187:TYR:O	2.47	0.43
17:J:48:ARG:HG3	17:J:49:MET:N	2.34	0.43
17:J:50:ILE:HD13	17:J:50:ILE:HA	1.74	0.43
19:L:32:ALA:HB3	19:L:34:CYS:SG	2.59	0.43
22:S:232:ASP:CA	22:S:233:ALA:N	2.67	0.43
4:4:288:ILE:HG23	5:6:322:MET:HG2	2.00	0.43
6:7:747:ASN:C	6:7:747:ASN:H	2.16	0.43
7:M:168:MET:SD	7:M:171:ILE:HD11	2.59	0.43
8:A:670:ILE:HG22	8:A:805:LEU:HD21	2.00	0.43
15:H:130:ARG:HD3	15:H:130:ARG:H	1.83	0.43
23:O:128:SER:OG	23:O:130:ASP:OD1	2.27	0.43
28:5:31:VAL:HG22	28:5:42:VAL:HG23	1.99	0.43
1:0:37:ASN:HB2	1:0:477:THR:HG22	2.01	0.43
1:0:261:THR:O	1:0:265:ASN:ND2	2.52	0.43
2:1:517:ASN:N	2:1:517:ASN:OD1	2.50	0.43
5:6:132:CYS:HB2	5:6:204:PRO:HB3	2.01	0.43
7:M:284:LEU:HD21	7:M:313:TYR:HA	2.01	0.43
7:M:312:GLY:HA2	7:M:315:ILE:HG22	2.00	0.43
8:A:177:ASP:N	8:A:177:ASP:OD1	2.52	0.43
8:A:200:ARG:NH1	26:W:227:MET:HG3	2.34	0.43
9:B:834:ASN:N	9:B:834:ASN:OD1	2.52	0.43
9:B:982:SER:OG	9:B:984:HIS:N	2.44	0.43
12:E:190:LEU:HD12	12:E:194:GLU:HB2	2.01	0.43
13:F:90:ARG:HD2	13:F:155:LEU:HD11	2.00	0.43
15:H:130:ARG:HB2	15:H:133:ASN:HB3	2.00	0.43
23:O:183:SER:HB2	23:O:193:LEU:HD21	1.99	0.43
27:X:123:HIS:O	27:X:126:SER:OG	2.24	0.43
30:T:-37:DT:H1'	30:T:-36:DC:C4	2.54	0.43
1:0:537:MET:SD	1:0:621:LEU:HD23	2.59	0.43
1:0:609:GLY:H	1:0:668:ARG:NH1	2.16	0.43
1:0:659:MET:HG3	1:0:660:ARG:N	2.33	0.43
4:4:54:LEU:HD13	4:4:129:ILE:HD13	2.00	0.43
6:7:437:VAL:HG23	6:7:454:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:551:ASN:H	6:7:701:PHE:HE2	1.65	0.43
6:7:564:GLU:HG2	6:7:756:ARG:HB3	2.01	0.43
8:A:1143:LEU:HA	8:A:1146:VAL:HG22	2.01	0.43
8:A:1394:THR:O	8:A:1399:ARG:NE	2.51	0.43
9:B:121:ASN:HA	9:B:207:GLY:HA3	2.00	0.43
9:B:492:LEU:HD23	9:B:492:LEU:HA	1.82	0.43
9:B:655:LYS:HA	9:B:658:ILE:HG22	2.00	0.43
10:C:50:GLU:OE2	19:L:66:GLN:NE2	2.46	0.43
26:W:29:LEU:HA	26:W:32:ILE:HG12	2.01	0.43
1:0:243:VAL:O	1:0:247:SER:OG	2.28	0.43
1:0:571:VAL:HA	1:0:599:LEU:HB2	2.01	0.43
1:0:737:SER:OG	1:0:738:VAL:N	2.51	0.43
3:2:454:TYR:CE2	3:2:483:TRP:CG	3.07	0.43
6:7:342:ASP:HB3	6:7:345:ASN:HB2	2.01	0.43
6:7:385:VAL:HB	6:7:537:GLU:HG3	1.99	0.43
6:7:493:VAL:HA	6:7:498:PHE:HB3	2.01	0.43
8:A:415:LEU:CD2	8:A:415:LEU:HA	2.49	0.43
8:A:1144:LYS:HZ3	8:A:1268:LEU:HB3	1.82	0.43
8:A:1301:GLU:HA	8:A:1302:PRO:HD3	1.90	0.43
9:B:1080:LYS:HD2	10:C:188:HIS:HB2	2.01	0.43
11:D:14:ARG:HH21	11:D:17:LYS:HZ1	1.66	0.43
13:F:128:LYS:HD2	13:F:149:GLU:HA	2.01	0.43
15:H:142:LEU:HD12	15:H:142:LEU:HA	1.76	0.43
22:S:267:ASP:OD1	22:S:267:ASP:N	2.49	0.43
4:4:213:VAL:HG11	4:4:248:LEU:HD11	2.01	0.42
5:6:398:PHE:HE1	5:6:424:SER:HG	1.65	0.42
7:M:142:LEU:HD13	7:M:146:VAL:HG11	2.01	0.42
8:A:1293:SER:HB3	8:A:1297:GLU:H	1.84	0.42
11:D:37:GLN:HB2	11:D:45:GLU:HB3	2.01	0.42
3:2:135:LEU:HD21	3:2:270:TYR:HB3	2.01	0.42
6:7:233:PHE:HB3	6:7:315:SER:HB2	2.01	0.42
6:7:609:SER:HB2	6:7:673:ILE:HD11	2.01	0.42
7:M:119:MET:SD	7:M:119:MET:N	2.92	0.42
8:A:105:CYS:HA	8:A:142:CYS:SG	2.59	0.42
9:B:212:LEU:HD23	9:B:212:LEU:HA	1.83	0.42
9:B:867:GLY:HA2	9:B:868:MET:SD	2.59	0.42
10:C:18:VAL:CG2	10:C:18:VAL:N	2.82	0.42
11:D:139:LYS:HA	11:D:142:LYS:HD2	2.00	0.42
12:E:2:ASP:O	12:E:7:ARG:NH1	2.38	0.42
14:G:84:GLY:N	14:G:147:ILE:O	2.41	0.42
15:H:25:ARG:NH1	15:H:41:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:92:ASP:OD1	15:H:92:ASP:N	2.45	0.42
16:I:28:GLU:HB3	16:I:35:VAL:HG23	2.01	0.42
30:T:-4:DT:H6	30:T:-4:DT:H2'	1.66	0.42
1:0:16:LYS:HD2	2:1:424:LEU:HA	2.01	0.42
3:2:147:LEU:HD23	3:2:147:LEU:HA	1.86	0.42
4:4:272:PHE:HB2	5:6:372:LEU:HD22	2.01	0.42
8:A:980:ASP:OD1	8:A:980:ASP:N	2.35	0.42
8:A:1258:HIS:NE2	8:A:1259:MET:SD	2.92	0.42
9:B:644:GLU:HG3	9:B:646:LEU:HB2	2.01	0.42
9:B:701:ILE:HD12	9:B:703:ILE:HD11	2.02	0.42
10:C:107:SER:OG	10:C:109:SER:O	2.38	0.42
24:U:244:MET:H	25:V:112:ARG:NH2	2.17	0.42
27:X:124:ASP:N	27:X:124:ASP:OD1	2.52	0.42
27:X:168:ARG:O	27:X:181:LEU:N	2.39	0.42
30:T:-19:DA:H2'	30:T:-18:DT:C6	2.55	0.42
1:0:534:PRO:HB3	5:6:239:LEU:HD22	2.02	0.42
2:1:442:HIS:ND1	2:1:443:GLU:O	2.41	0.42
6:7:341:TYR:HE2	6:7:405:LYS:HD2	1.85	0.42
8:A:445:ASN:OD1	8:A:446:ARG:N	2.52	0.42
8:A:805:LEU:HD12	8:A:805:LEU:HA	1.76	0.42
9:B:62:ILE:HD11	9:B:418:LYS:HB2	2.02	0.42
22:S:153:LEU:HD23	22:S:153:LEU:HA	1.88	0.42
1:0:545:LEU:HD13	2:1:361:GLY:HA3	2.01	0.42
3:2:47:ILE:O	3:2:51:VAL:HB	2.20	0.42
3:2:191:PHE:HZ	3:2:203:LEU:HG	1.85	0.42
3:2:454:TYR:HH	3:2:483:TRP:HD1	1.65	0.42
4:4:24:SER:HA	4:4:173:LYS:HB2	2.02	0.42
7:M:152:GLU:OE1	9:B:868:MET:N	2.44	0.42
8:A:115:LEU:HB3	8:A:122:MET:HG2	2.01	0.42
8:A:119:ASN:HD21	8:A:121:LEU:HB3	1.85	0.42
8:A:337:ARG:HH21	8:A:839:ARG:NE	2.17	0.42
8:A:1003:LYS:HD3	8:A:1003:LYS:HA	1.85	0.42
9:B:118:ARG:NH1	9:B:788:ARG:HE	2.18	0.42
9:B:438:GLU:HA	9:B:439:ALA:HA	1.76	0.42
9:B:706:GLN:HB2	9:B:709:ASP:HB3	2.02	0.42
9:B:910:VAL:HG21	9:B:938:SER:HB3	2.02	0.42
12:E:43:LYS:HA	12:E:43:LYS:HD2	1.85	0.42
12:E:100:ILE:HG23	12:E:105:PHE:HB2	2.02	0.42
20:Q:408:GLU:HA	20:Q:411:LYS:HE2	2.01	0.42
23:O:153:THR:HG22	23:O:154:ASP:H	1.85	0.42
3:2:211:ILE:HD12	3:2:211:ILE:HA	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:586:THR:OG1	6:7:756:ARG:NH2	2.50	0.42
7:M:156:LEU:HD23	7:M:156:LEU:HA	1.88	0.42
7:M:193:GLN:HG3	7:M:200:THR:HG22	2.00	0.42
8:A:68:GLN:HG3	8:A:80:HIS:CD2	2.54	0.42
8:A:1315:GLU:OE1	8:A:1315:GLU:N	2.52	0.42
9:B:763:GLN:HB3	9:B:766:ARG:HG2	2.01	0.42
16:I:26:LEU:HD23	16:I:35:VAL:HG21	2.01	0.42
20:Q:151:LEU:HA	21:P:201:TYR:CZ	2.55	0.42
3:2:239:ILE:HG12	3:2:247:ARG:HG2	2.01	0.42
4:4:266:ASN:OD1	4:4:266:ASN:N	2.52	0.42
5:6:166:ILE:HD12	5:6:166:ILE:HG23	1.86	0.42
6:7:124:ARG:NH2	6:7:201:SER:O	2.46	0.42
6:7:124:ARG:O	6:7:127:HIS:ND1	2.32	0.42
6:7:224:LYS:HE2	6:7:338:LEU:HG	2.02	0.42
8:A:171:GLN:OE1	8:A:171:GLN:N	2.53	0.42
8:A:834:THR:HA	8:A:837:ILE:HG22	2.01	0.42
21:P:95:ILE:HD12	21:P:95:ILE:HA	1.95	0.42
22:S:160:LEU:HD23	22:S:173:HIS:CD2	2.53	0.42
23:O:69:ASN:HD21	23:O:125:GLY:H	1.68	0.42
25:V:6:TYR:HD2	25:V:46:LYS:HZ2	1.68	0.42
26:W:36:SER:HB2	26:W:206:LEU:HD12	2.01	0.42
3:2:174:GLU:O	3:2:183:LYS:N	2.52	0.42
6:7:135:SER:HB3	6:7:140:ARG:HB2	2.02	0.42
6:7:691:LEU:HD23	6:7:691:LEU:HA	1.92	0.42
8:A:565:ILE:HD11	8:A:571:LEU:HB2	2.02	0.42
8:A:780:VAL:HG13	8:A:789:LYS:HZ1	1.85	0.42
8:A:1017:LEU:HA	8:A:1017:LEU:HD23	1.88	0.42
9:B:1128:LEU:HD13	9:B:1128:LEU:HA	1.85	0.42
12:E:123:LEU:HD23	12:E:123:LEU:H	1.85	0.42
21:P:320:GLU:OE2	21:P:321:ARG:NH2	2.53	0.42
26:W:17:VAL:HG13	26:W:21:TYR:HB2	2.02	0.42
27:X:238:ASP:N	27:X:238:ASP:OD1	2.52	0.42
4:4:155:ALA:O	4:4:158:THR:OG1	2.30	0.42
6:7:190:THR:OG1	6:7:217:THR:OG1	2.30	0.42
6:7:349:ASN:HD21	6:7:508:HIS:HE1	1.66	0.42
8:A:403:LYS:O	8:A:415:LEU:HB2	2.20	0.42
8:A:567:LYS:HB2	8:A:567:LYS:HE3	1.87	0.42
9:B:872:GLU:HG2	9:B:917:PRO:HD3	2.01	0.42
10:C:176:ILE:HD12	10:C:176:ILE:HA	1.95	0.42
12:E:69:ILE:HD13	12:E:69:ILE:HA	1.90	0.42
18:K:85:ASP:HA	18:K:88:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:379:GLU:HB2	20:Q:383:SER:HB2	2.01	0.42
25:V:6:TYR:HB2	25:V:46:LYS:HZ2	1.85	0.42
26:W:349:GLU:OE2	26:W:351:ARG:NE	2.53	0.42
27:X:138:LYS:HA	27:X:138:LYS:HD2	1.87	0.42
30:T:-40:DT:H2"	30:T:-39:DA:H5"	2.02	0.42
1:0:313:PRO:HA	1:0:316:LEU:HD12	2.01	0.42
3:2:17:ILE:HA	3:2:18:PRO:HD3	1.96	0.42
3:2:346:LYS:HD3	3:2:377:GLN:HG3	2.01	0.42
4:4:26:LEU:HB2	4:4:64:HIS:CE1	2.55	0.42
6:7:534:LYS:HE3	6:7:534:LYS:HB3	1.92	0.42
8:A:563:PRO:HD2	15:H:79:TRP:CD1	2.55	0.42
9:B:412:LEU:HB3	9:B:466:TRP:CZ2	2.55	0.42
10:C:94:LYS:HA	10:C:94:LYS:HD3	1.85	0.42
13:F:135:ARG:HE	13:F:135:ARG:HB2	1.64	0.42
21:P:223:GLN:NE2	21:P:224:VAL:O	2.53	0.42
1:0:270:ARG:NH2	1:0:389:GLU:O	2.53	0.41
1:0:548:GLU:HB3	2:1:371:THR:HG21	2.02	0.41
2:1:349:VAL:O	2:1:350:ARG:NE	2.53	0.41
3:2:200:LEU:HD22	3:2:278:LEU:HD12	2.01	0.41
3:2:242:LEU:HD23	3:2:247:ARG:HG3	2.02	0.41
3:2:334:ILE:HG22	3:2:405:HIS:CE1	2.54	0.41
8:A:457:ALA:HB3	8:A:506:ALA:HA	2.02	0.41
9:B:805:THR:OG1	9:B:809:MET:SD	2.69	0.41
12:E:4:GLU:O	12:E:8:ASN:ND2	2.36	0.41
17:J:44:TYR:HA	17:J:47:ARG:HB3	2.02	0.41
20:Q:369:ASN:N	20:Q:369:ASN:OD1	2.49	0.41
21:P:108:LEU:HB3	21:P:118:HIS:HA	2.01	0.41
1:0:19:PRO:HG3	1:0:739:TRP:CD2	2.55	0.41
4:4:135:LEU:O	4:4:139:GLN:HG3	2.20	0.41
5:6:325:PRO:HB3	5:6:350:PRO:HD3	2.02	0.41
8:A:172:PRO:HB3	8:A:185:TRP:CD2	2.54	0.41
8:A:567:LYS:HD3	8:A:567:LYS:HA	1.85	0.41
8:A:800:VAL:HG13	8:A:812:GLU:HB3	2.02	0.41
8:A:876:ALA:O	8:A:878:ILE:N	2.48	0.41
9:B:424:LEU:HD11	9:B:449:ASN:CB	2.49	0.41
9:B:700:SER:O	9:B:700:SER:OG	2.33	0.41
9:B:910:VAL:HA	9:B:940:PRO:HA	2.01	0.41
9:B:1073:TYR:CE1	9:B:1080:LYS:HG2	2.55	0.41
10:C:10:ILE:N	18:K:108:GLU:OE2	2.40	0.41
10:C:77:ILE:HD11	10:C:161:LYS:HD2	2.01	0.41
12:E:156:LEU:HD12	12:E:160:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:130:ARG:O	15:H:133:ASN:N	2.54	0.41
20:Q:390:ASP:OD1	20:Q:391:LYS:N	2.52	0.41
21:P:126:LYS:HD2	21:P:126:LYS:HA	1.73	0.41
23:O:124:THR:OG1	23:O:125:GLY:N	2.53	0.41
24:U:5:GLU:O	24:U:8:ARG:HG3	2.20	0.41
29:N:-1:DC:H2"	29:N:0:DA:H5'	2.02	0.41
2:1:234:LEU:O	2:1:297:ARG:NE	2.53	0.41
3:2:57:VAL:HG11	3:2:62:LEU:HD21	2.01	0.41
4:4:77:ALA:HB2	4:4:86:LEU:HD11	2.02	0.41
5:6:136:MET:N	5:6:136:MET:SD	2.92	0.41
5:6:151:GLN:HA	5:6:154:ILE:HD12	2.00	0.41
6:7:588:PHE:HB3	6:7:749:ALA:HB3	2.01	0.41
7:M:314:LYS:HB2	7:M:314:LYS:HE2	1.83	0.41
8:A:210:ILE:HD12	8:A:210:ILE:HA	1.94	0.41
8:A:372:LYS:HZ3	18:K:1:MET:C	2.24	0.41
8:A:1025:ARG:HD3	8:A:1025:ARG:HA	1.81	0.41
9:B:766:ARG:HH12	9:B:1020:ARG:HH11	1.68	0.41
9:B:896:ASP:OD1	9:B:896:ASP:N	2.50	0.41
10:C:41:ILE:HD13	10:C:41:ILE:HA	1.91	0.41
12:E:153:HIS:CE1	12:E:184:VAL:HG21	2.55	0.41
26:W:192:SER:OG	26:W:193:ARG:N	2.54	0.41
1:0:97:LEU:HD23	1:0:97:LEU:HA	1.85	0.41
2:1:445:THR:OG1	4:4:279:THR:O	2.38	0.41
6:7:748:LEU:HB2	6:7:751:ALA:HB2	2.02	0.41
16:I:69:PRO:HB2	16:I:85:PHE:CE1	2.56	0.41
21:P:97:ILE:HD11	21:P:101:GLY:HA2	2.02	0.41
1:0:342:LEU:HD23	1:0:342:LEU:HA	1.89	0.41
2:1:336:ILE:HG13	2:1:337:ILE:HG12	2.02	0.41
3:2:186:ASN:ND2	3:2:390:GLY:O	2.32	0.41
6:7:386:LEU:HB2	6:7:392:LYS:HZ2	1.86	0.41
6:7:436:ALA:HB3	6:7:453:VAL:HG22	2.02	0.41
6:7:555:ALA:HA	6:7:734:LYS:HG2	2.03	0.41
6:7:608:PHE:HE2	6:7:670:LEU:HD11	1.84	0.41
7:M:149:CYS:SG	9:B:869:SER:HB3	2.61	0.41
7:M:240:PRO:HA	7:M:243:CYS:SG	2.60	0.41
8:A:1136:SER:HB2	8:A:1274:ARG:HH21	1.85	0.41
1:0:11:LEU:HB3	1:0:92:TYR:HE2	1.86	0.41
1:0:267:LEU:HD23	1:0:267:LEU:HA	1.93	0.41
1:0:399:LEU:HA	1:0:402:ILE:HG22	2.03	0.41
1:0:650:GLU:OE1	1:0:650:GLU:N	2.54	0.41
4:4:86:LEU:HA	4:4:128:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:197:LYS:HA	5:6:200:ARG:HG3	2.03	0.41
9:B:446:LEU:O	9:B:449:ASN:HB2	2.20	0.41
9:B:510:LYS:O	9:B:512:ARG:N	2.54	0.41
14:G:151:ILE:HG13	14:G:153:GLN:HE22	1.86	0.41
18:K:94:ILE:HA	18:K:94:ILE:HD13	1.84	0.41
20:Q:362:VAL:HB	20:Q:398:ARG:HH21	1.85	0.41
20:Q:379:GLU:N	20:Q:383:SER:O	2.53	0.41
21:P:125:THR:H	21:P:222:CYS:HA	1.86	0.41
22:S:171:ILE:HA	22:S:174:THR:HG22	2.03	0.41
24:U:264:ASP:H	24:U:277:GLN:C	2.24	0.41
1:0:233:ILE:HG22	1:0:457:ILE:HB	2.03	0.41
2:1:291:LYS:HA	2:1:294:ARG:HG3	2.02	0.41
3:2:229:GLY:O	3:2:279:THR:OG1	2.27	0.41
3:2:343:THR:HG21	6:7:732:ALA:HB1	2.02	0.41
3:2:454:TYR:HH	3:2:483:TRP:HB2	1.86	0.41
4:4:87:TYR:HA	4:4:88:PRO:HA	1.87	0.41
6:7:409:VAL:HG22	6:7:486:ILE:HB	2.03	0.41
7:M:241:ARG:CZ	9:B:107:GLY:H	2.33	0.41
7:M:313:TYR:O	7:M:317:TYR:HB2	2.20	0.41
8:A:557:ASP:HA	18:K:26:LYS:HD3	2.02	0.41
8:A:1111:MET:HB2	8:A:1114:PRO:HB3	2.03	0.41
8:A:1198:ASP:OD2	8:A:1201:ALA:N	2.50	0.41
9:B:70:ILE:O	20:Q:331:GLN:NE2	2.45	0.41
9:B:226:PHE:HZ	9:B:398:ARG:HD3	1.86	0.41
9:B:642:ASP:HA	9:B:649:LYS:HE3	2.02	0.41
18:K:104:ASN:O	18:K:107:THR:OG1	2.33	0.41
27:X:172:ASP:HB3	27:X:176:GLY:H	1.86	0.41
1:0:538:VAL:HG23	1:0:620:VAL:HG13	2.02	0.41
1:0:573:THR:OG1	1:0:579:THR:OG1	2.31	0.41
3:2:454:TYR:CE1	3:2:483:TRP:HB2	2.55	0.41
4:4:114:MET:HG3	4:4:119:ARG:HB2	2.02	0.41
5:6:118:TYR:HB2	5:6:120:ARG:CZ	2.51	0.41
8:A:230:ARG:HB2	8:A:233:TRP:CD2	2.54	0.41
8:A:569:LYS:HE2	8:A:569:LYS:HB3	1.92	0.41
8:A:1409:LEU:HD23	8:A:1409:LEU:HA	1.76	0.41
9:B:582:VAL:HG22	9:B:626:ILE:HB	2.02	0.41
14:G:131:GLN:HG3	14:G:136:VAL:HG22	2.02	0.41
27:X:233:LEU:O	27:X:242:ARG:N	2.53	0.41
29:N:47:DT:C4	30:T:-47:DA:N1	2.88	0.41
1:0:111:ARG:NE	1:0:133:CYS:SG	2.94	0.41
1:0:295:SER:O	1:0:299:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:441:ASP:OD1	1:0:442:ALA:N	2.52	0.41
2:1:329:LEU:HD22	2:1:383:GLU:HB3	2.03	0.41
4:4:264:LYS:HA	4:4:265:PRO:HD3	1.90	0.41
5:6:176:ASN:HA	5:6:206:GLY:HA3	2.03	0.41
6:7:397:ILE:HD13	6:7:427:TRP:HB2	2.03	0.41
6:7:672:GLN:HB2	6:7:707:SER:HA	2.03	0.41
8:A:67:CYS:SG	8:A:71:GLN:N	2.94	0.41
8:A:112:LYS:HE3	8:A:165:GLY:HA2	2.03	0.41
8:A:138:ILE:HD13	8:A:138:ILE:HA	1.94	0.41
8:A:195:ASP:OD1	8:A:195:ASP:N	2.48	0.41
8:A:306:ASN:N	8:A:324:SER:OG	2.54	0.41
8:A:337:ARG:HH21	8:A:839:ARG:CZ	2.34	0.41
8:A:526:ASP:OD1	8:A:526:ASP:N	2.54	0.41
8:A:1129:GLU:OE1	8:A:1129:GLU:N	2.45	0.41
9:B:240:ILE:HD13	9:B:240:ILE:HA	1.92	0.41
9:B:593:PRO:HG2	9:B:617:ARG:NH2	2.35	0.41
9:B:654:ARG:HA	9:B:654:ARG:HD3	1.83	0.41
9:B:696:GLU:OE1	9:B:696:GLU:N	2.54	0.41
9:B:980:PHE:CE2	9:B:990:ILE:HD11	2.55	0.41
10:C:191:TYR:HD2	10:C:201:TRP:CE2	2.39	0.41
11:D:40:HIS:CG	14:G:73:LYS:HD2	2.56	0.41
11:D:56:ARG:NH2	11:D:145:MET:HB2	2.36	0.41
12:E:167:ARG:HD3	12:E:167:ARG:HA	1.72	0.41
13:F:129:LYS:HE2	13:F:129:LYS:HB3	1.93	0.41
16:I:83:ASN:N	16:I:83:ASN:OD1	2.53	0.41
18:K:18:LYS:HA	18:K:18:LYS:HD2	1.91	0.41
21:P:80:LYS:HB3	21:P:81:TRP:HD1	1.86	0.41
25:V:11:ARG:HH12	25:V:19:LEU:HD13	1.85	0.41
26:W:141:ASN:HD21	26:W:146:GLU:H	1.69	0.41
26:W:198:THR:H	26:W:201:ILE:HB	1.85	0.41
29:N:24:DT:H2”	29:N:25:DT:C5	2.56	0.41
1:0:70:ILE:HD12	1:0:232:VAL:HG22	2.02	0.41
2:1:543:PRO:HG2	2:1:546:LEU:HB3	2.03	0.41
4:4:276:CYS:HA	4:4:295:VAL:HG23	2.03	0.41
5:6:388:THR:HA	5:6:445:HIS:CE1	2.56	0.41
6:7:510:LYS:HB3	6:7:531:ILE:HG22	2.03	0.41
6:7:607:VAL:O	6:7:654:LEU:N	2.52	0.41
6:7:677:TYR:O	6:7:722:ARG:NH1	2.54	0.41
8:A:720:ARG:HH12	22:S:262:GLU:HG2	1.85	0.41
8:A:752:LYS:HA	8:A:752:LYS:HD2	1.75	0.41
9:B:412:LEU:HD23	9:B:412:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:691:GLU:OE2	9:B:692:TYR:N	2.54	0.41
9:B:1175:LEU:HD23	9:B:1175:LEU:HA	1.88	0.41
17:J:19:GLU:OE1	17:J:19:GLU:N	2.48	0.41
26:W:109:LEU:HD23	26:W:109:LEU:HA	1.84	0.41
27:X:182:SER:OG	27:X:183:THR:N	2.53	0.41
30:T:-49:DC:H2"	30:T:-48:DA:C8	2.56	0.41
1:0:68:LYS:O	1:0:231:ILE:N	2.47	0.40
1:0:374:LEU:HG	1:0:410:SER:HB3	2.03	0.40
1:0:613:ASP:HB2	1:0:614:HIS:ND1	2.36	0.40
3:2:25:LEU:HD21	3:2:226:PHE:HE2	1.86	0.40
5:6:173:ILE:O	5:6:180:GLN:N	2.40	0.40
7:M:39:SER:OG	7:M:40:GLU:OE1	2.33	0.40
7:M:135:MET:SD	9:B:448:ILE:HG12	2.61	0.40
8:A:315:LEU:HD23	8:A:315:LEU:H	1.86	0.40
8:A:1038:THR:O	8:A:1042:PHE:HB2	2.21	0.40
9:B:445:LYS:HE2	9:B:445:LYS:HB2	1.92	0.40
9:B:1013:ASN:OD1	9:B:1015:HIS:ND1	2.41	0.40
10:C:145:CYS:SG	10:C:146:LYS:N	2.94	0.40
11:D:40:HIS:ND1	14:G:73:LYS:HD2	2.37	0.40
13:F:82:THR:HA	13:F:83:PRO:HD3	1.91	0.40
13:F:97:ARG:HD2	13:F:97:ARG:HA	1.91	0.40
25:V:32:ILE:HG23	25:V:36:LEU:HD22	2.03	0.40
28:5:20:ILE:HD13	28:5:23:ILE:HD12	2.02	0.40
29:N:2:DA:H1'	29:N:3:DT:H5'	2.03	0.40
2:1:197:GLU:HA	2:1:201:ASN:HB2	2.03	0.40
5:6:138:GLU:HB2	5:6:145:ARG:HD2	2.04	0.40
5:6:390:ALA:O	5:6:428:ARG:N	2.46	0.40
8:A:998:LEU:HB3	8:A:1001:ARG:NH1	2.36	0.40
8:A:1161:THR:HG23	8:A:1239:ARG:NH2	2.35	0.40
8:A:1173:HIS:CG	8:A:1227:ILE:HG23	2.55	0.40
9:B:144:GLY:HA2	9:B:145:ARG:HA	1.83	0.40
9:B:782:LEU:HD23	9:B:782:LEU:HA	1.88	0.40
10:C:97:VAL:HG12	10:C:159:ALA:HB3	2.03	0.40
14:G:39:THR:OG1	14:G:40:GLY:N	2.55	0.40
14:G:118:ASP:OD1	14:G:118:ASP:N	2.43	0.40
14:G:135:ASP:HB2	14:G:143:ILE:HD12	2.02	0.40
15:H:45:GLU:OE2	15:H:46:LEU:HG	2.21	0.40
23:O:184:SER:HB3	23:O:194:ILE:HB	2.03	0.40
27:X:187:HIS:HA	27:X:214:TRP:CG	2.56	0.40
1:0:55:LEU:HD12	1:0:55:LEU:HA	1.85	0.40
2:1:586:LEU:HD22	2:1:623:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:15:GLU:HG3	3:2:84:LEU:HD23	2.04	0.40
3:2:28:SER:O	3:2:31:THR:OG1	2.34	0.40
3:2:212:GLU:HA	3:2:218:LEU:HD21	2.03	0.40
5:6:139:LYS:HB3	5:6:142:ARG:HH22	1.86	0.40
7:M:41:GLY:HA2	7:M:56:LEU:HB2	2.04	0.40
8:A:106:VAL:HG21	8:A:214:ILE:HD12	2.03	0.40
8:A:251:SER:HA	8:A:257:ARG:HA	2.03	0.40
8:A:385:ILE:O	8:A:389:THR:OG1	2.26	0.40
8:A:786:HIS:ND1	9:B:703:ILE:HB	2.35	0.40
8:A:1161:THR:HG22	8:A:1163:ILE:H	1.85	0.40
9:B:114:PRO:HG3	9:B:181:LEU:HD11	2.02	0.40
9:B:566:LEU:HD23	9:B:566:LEU:HA	1.83	0.40
9:B:989:THR:OG1	9:B:990:ILE:N	2.54	0.40
10:C:104:PHE:HB3	10:C:106:GLU:HG2	2.03	0.40
12:E:29:PHE:HB2	12:E:30:ILE:N	2.35	0.40
16:I:10:CYS:O	16:I:12:ASN:N	2.54	0.40
22:S:198:ARG:NH2	22:S:228:LEU:O	2.54	0.40
22:S:271:CYS:HB3	22:S:275:LYS:N	2.36	0.40
22:S:282:TYR:CG	22:S:283:GLN:N	2.89	0.40
24:U:253:ARG:HB3	24:U:258:TRP:CD1	2.56	0.40
26:W:91:TYR:HB3	26:W:194:ILE:HD11	2.03	0.40
2:1:473:LEU:HA	2:1:476:VAL:HG12	2.04	0.40
3:2:208:LEU:HA	3:2:211:ILE:HG22	2.03	0.40
6:7:608:PHE:HD2	6:7:670:LEU:HD21	1.87	0.40
6:7:680:ARG:HH11	6:7:725:PHE:HB2	1.85	0.40
7:M:136:LEU:HD22	7:M:196:ILE:HD11	2.03	0.40
8:A:187:LYS:HE2	26:W:226:THR:HB	2.03	0.40
8:A:247:ARG:NH1	8:A:263:THR:OG1	2.51	0.40
9:B:274:PRO:HA	9:B:275:TYR:HA	1.78	0.40
9:B:342:GLY:H	9:B:344:LYS:NZ	2.18	0.40
9:B:498:THR:OG1	9:B:537:LYS:HG3	2.21	0.40
15:H:46:LEU:HD23	15:H:46:LEU:HA	1.94	0.40
16:I:19:ASP:OD1	16:I:22:ASN:N	2.35	0.40
19:L:51:CYS:HB3	19:L:53:HIS:ND1	2.36	0.40
1:0:6:ASP:OD1	1:0:6:ASP:N	2.54	0.40
5:6:318:THR:OG1	5:6:319:LEU:N	2.53	0.40
8:A:118:HIS:HA	8:A:123:ARG:NH2	2.37	0.40
8:A:129:LYS:HB3	8:A:134:ARG:HD3	2.02	0.40
8:A:751:SER:OG	8:A:752:LYS:N	2.54	0.40
10:C:34:ARG:HD3	10:C:176:ILE:HG21	2.03	0.40
10:C:43:THR:OG1	10:C:44:LEU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:201:LYS:HA	11:D:201:LYS:HD2	1.84	0.40
12:E:88:VAL:HG11	12:E:116:ILE:HG23	2.04	0.40
17:J:3:VAL:HG21	17:J:15:GLY:HA2	2.02	0.40
19:L:50:ASP:OD1	19:L:50:ASP:N	2.47	0.40
28:5:6:LYS:HA	28:5:6:LYS:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	750/778 (96%)	708 (94%)	41 (6%)	1 (0%)	48 78
2	1	407/642 (63%)	389 (96%)	18 (4%)	0	100 100
3	2	435/513 (85%)	413 (95%)	20 (5%)	2 (0%)	25 57
4	4	286/338 (85%)	276 (96%)	10 (4%)	0	100 100
5	6	351/461 (76%)	333 (95%)	18 (5%)	0	100 100
6	7	604/843 (72%)	575 (95%)	28 (5%)	1 (0%)	44 72
7	M	273/345 (79%)	240 (88%)	33 (12%)	0	100 100
8	A	1417/1733 (82%)	1248 (88%)	168 (12%)	1 (0%)	48 78
9	B	1150/1224 (94%)	981 (85%)	166 (14%)	3 (0%)	37 67
10	C	263/318 (83%)	225 (86%)	35 (13%)	3 (1%)	12 43
11	D	164/221 (74%)	153 (93%)	11 (7%)	0	100 100
12	E	212/215 (99%)	191 (90%)	20 (9%)	1 (0%)	25 57
13	F	85/155 (55%)	77 (91%)	8 (9%)	0	100 100
14	G	169/171 (99%)	145 (86%)	23 (14%)	1 (1%)	22 54
15	H	129/146 (88%)	104 (81%)	23 (18%)	2 (2%)	8 37
16	I	112/122 (92%)	97 (87%)	15 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
18	K	113/120 (94%)	103 (91%)	10 (9%)	0	100	100
19	L	42/70 (60%)	25 (60%)	17 (40%)	0	100	100
20	Q	208/735 (28%)	191 (92%)	17 (8%)	0	100	100
21	P	173/400 (43%)	160 (92%)	13 (8%)	0	100	100
22	S	162/309 (52%)	142 (88%)	20 (12%)	0	100	100
23	O	179/240 (75%)	165 (92%)	14 (8%)	0	100	100
24	U	101/286 (35%)	97 (96%)	4 (4%)	0	100	100
25	V	100/122 (82%)	96 (96%)	4 (4%)	0	100	100
26	W	241/482 (50%)	234 (97%)	7 (3%)	0	100	100
27	X	158/328 (48%)	148 (94%)	10 (6%)	0	100	100
28	5	64/72 (89%)	60 (94%)	4 (6%)	0	100	100
All	All	8412/11459 (73%)	7633 (91%)	764 (9%)	15 (0%)	45	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	B	364	ILE
10	C	84	ARG
1	0	659	MET
6	7	742	MET
12	E	29	PHE
14	G	57	GLN
15	H	88	SER
3	2	466	GLN
9	B	363	HIS
10	C	24	ASN
8	A	1112	LYS
9	B	705	MET
3	2	450	ARG
15	H	84	ALA
10	C	162	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	684/707 (97%)	681 (100%)	3 (0%)	89 93
2	1	389/589 (66%)	384 (99%)	5 (1%)	65 77
3	2	394/468 (84%)	391 (99%)	3 (1%)	79 85
4	4	259/300 (86%)	259 (100%)	0	100 100
5	6	322/418 (77%)	322 (100%)	0	100 100
6	7	540/737 (73%)	533 (99%)	7 (1%)	65 77
7	M	245/299 (82%)	242 (99%)	3 (1%)	67 79
8	A	1235/1520 (81%)	1224 (99%)	11 (1%)	75 84
9	B	1000/1061 (94%)	994 (99%)	6 (1%)	84 90
10	C	233/274 (85%)	224 (96%)	9 (4%)	27 53
11	D	146/200 (73%)	146 (100%)	0	100 100
12	E	196/197 (100%)	194 (99%)	2 (1%)	73 82
13	F	77/137 (56%)	77 (100%)	0	100 100
14	G	151/152 (99%)	147 (97%)	4 (3%)	41 61
15	H	118/128 (92%)	113 (96%)	5 (4%)	25 51
16	I	108/116 (93%)	103 (95%)	5 (5%)	23 49
17	J	61/65 (94%)	57 (93%)	4 (7%)	14 41
18	K	99/102 (97%)	95 (96%)	4 (4%)	27 52
19	L	39/57 (68%)	37 (95%)	2 (5%)	20 47
20	Q	147/641 (23%)	143 (97%)	4 (3%)	40 61
21	P	166/363 (46%)	166 (100%)	0	100 100
22	S	141/274 (52%)	139 (99%)	2 (1%)	62 76
23	O	153/205 (75%)	151 (99%)	2 (1%)	65 77
24	U	99/260 (38%)	94 (95%)	5 (5%)	20 47
25	V	94/108 (87%)	92 (98%)	2 (2%)	48 67
26	W	224/429 (52%)	223 (100%)	1 (0%)	89 93
27	X	144/295 (49%)	142 (99%)	2 (1%)	62 76
28	5	53/66 (80%)	51 (96%)	2 (4%)	28 53
All	All	7517/10168 (74%)	7424 (99%)	93 (1%)	66 79

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	198	ARG
1	0	594	ARG
1	0	659	MET
2	1	306	ARG
2	1	353	ARG
2	1	358	MET
2	1	385	MET
2	1	608	MET
3	2	150	MET
3	2	450	ARG
3	2	466	GLN
6	7	112	MET
6	7	231	ARG
6	7	348	ARG
6	7	418	MET
6	7	500	ARG
6	7	742	MET
6	7	747	ASN
7	M	105	ARG
7	M	168	MET
7	M	317	TYR
8	A	129	LYS
8	A	217	LYS
8	A	415	LEU
8	A	437	MET
8	A	456	MET
8	A	619	LYS
8	A	761	MET
8	A	837	ILE
8	A	904	THR
8	A	1267	MET
8	A	1454	MET
9	B	194	GLU
9	B	199	MET
9	B	542	MET
9	B	884	ARG
9	B	995	ARG
9	B	1124	ARG
10	C	18	VAL
10	C	24	ASN
10	C	37	MET
10	C	57	VAL
10	C	109	SER

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Mol	Chain	Res	Type
10	C	116	LYS
10	C	209	TYR
10	C	230	MET
10	C	248	ILE
12	E	19	VAL
12	E	29	PHE
14	G	10	ASN
14	G	21	ARG
14	G	33	GLU
14	G	148	GLU
15	H	77	ARG
15	H	88	SER
15	H	109	LYS
15	H	130	ARG
15	H	146	ARG
16	I	26	LEU
16	I	47	GLU
16	I	50	THR
16	I	94	ASP
16	I	115	LYS
17	J	5	VAL
17	J	6	ARG
17	J	49	MET
17	J	51	LEU
18	K	1	MET
18	K	20	LYS
18	K	21	ILE
18	K	103	THR
19	L	54	ARG
19	L	63	ARG
20	Q	27	MET
20	Q	33	ARG
20	Q	330	ARG
20	Q	333	LYS
22	S	282	TYR
22	S	287	ARG
23	O	221	GLU
23	O	236	GLU
24	U	27	ASN
24	U	44	LYS
24	U	257	ARG
24	U	264	ASP

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Mol	Chain	Res	Type
24	U	277	GLN
25	V	38	MET
25	V	82	ASN
26	W	356	THR
27	X	153	MET
27	X	216	GLN
28	5	16	ILE
28	5	29	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	291	GLN
1	0	628	GLN
2	1	513	GLN
3	2	405	HIS
3	2	407	GLN
4	4	139	GLN
4	4	142	GLN
5	6	192	HIS
5	6	202	GLN
5	6	450	ASN
8	A	68	GLN
8	A	503	GLN
8	A	966	ASN
8	A	1171	GLN
8	A	1330	ASN
12	E	146	HIS
17	J	23	ASN
18	K	89	ASN
24	U	43	GLN
24	U	280	GLN

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 18 ligands modelled in this entry, 17 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	$\#\|Z\| > 2$
31	SF4	0	801	1	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
31	SF4	0	801	1	-	-	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	0	801	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	E	1
16	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:TYR	C	29:PHE	N	1.20
1	I	93:LYS	C	94:ASP	N	1.18

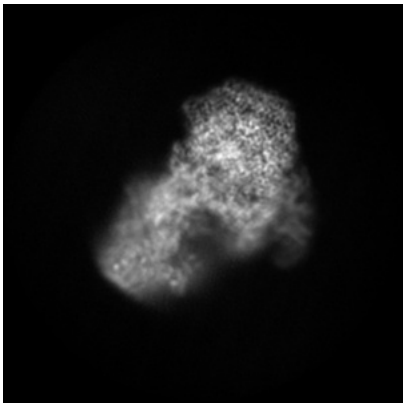
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42438. These allow visual inspection of the internal detail of the map and identification of artifacts.

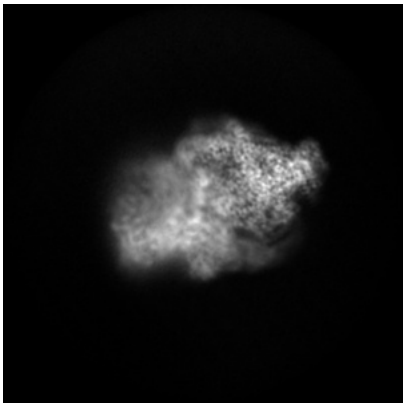
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

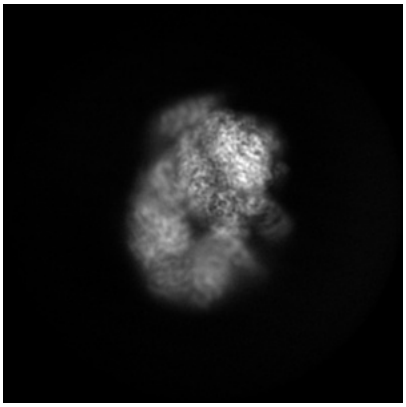
6.1.1 Primary map



X



Y

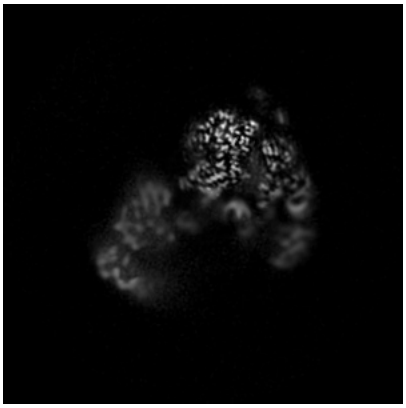


Z

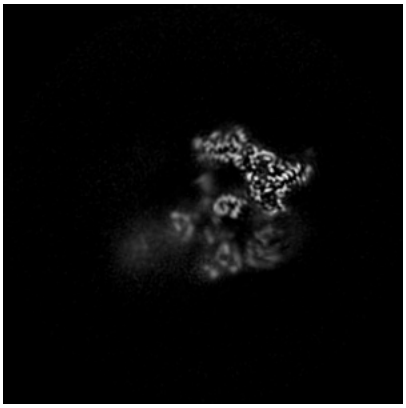
The images above show the map projected in three orthogonal directions.

6.2 Central slices

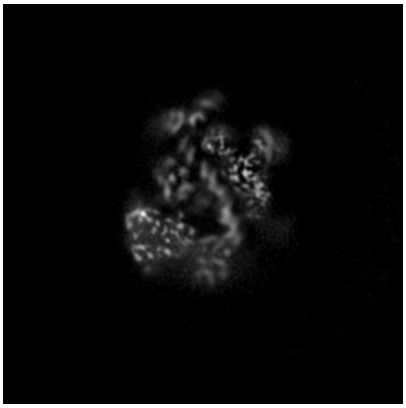
6.2.1 Primary map



X Index: 192



Y Index: 192

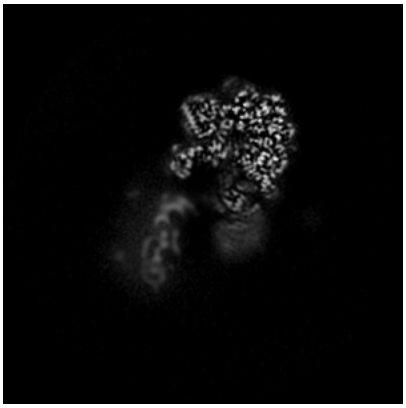


Z Index: 192

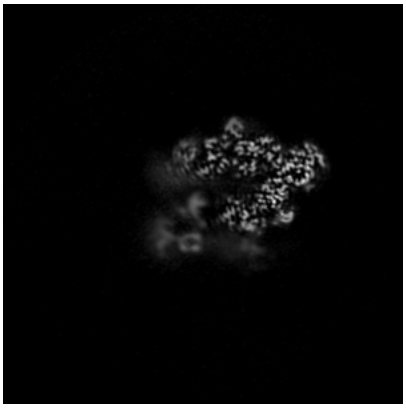
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

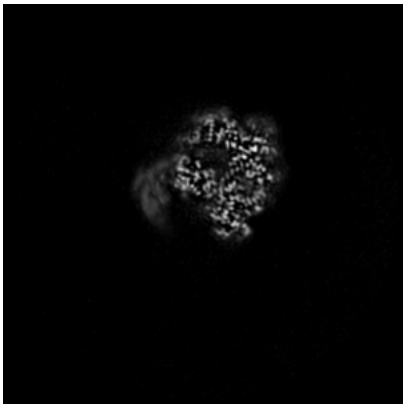
6.3.1 Primary map



X Index: 222



Y Index: 226

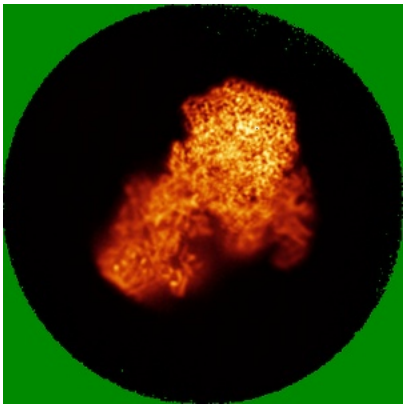


Z Index: 237

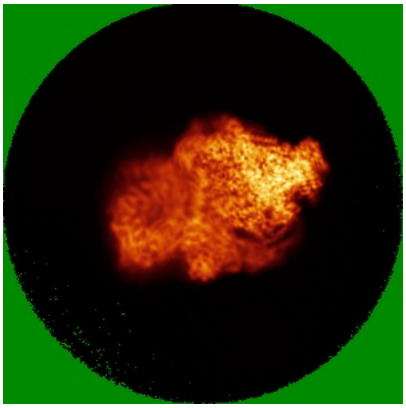
The images above show the largest variance slices of the map in three orthogonal directions.

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

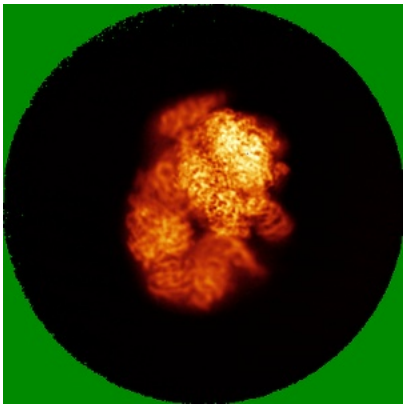
6.4.1 Primary map



X



Y

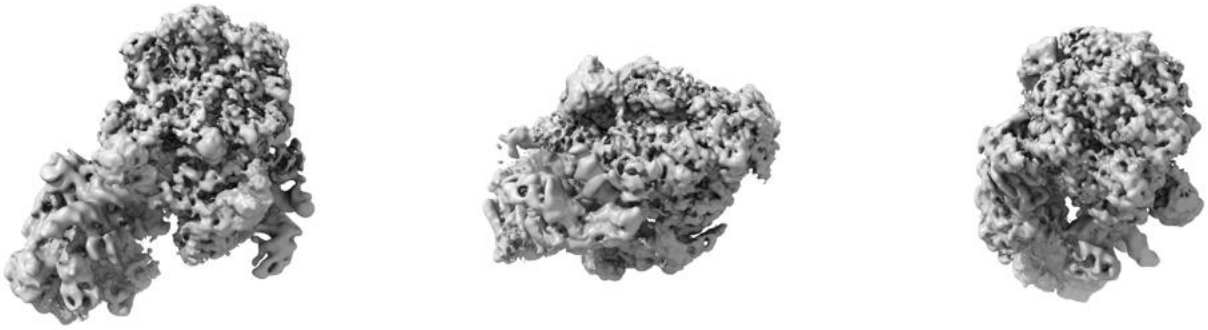


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

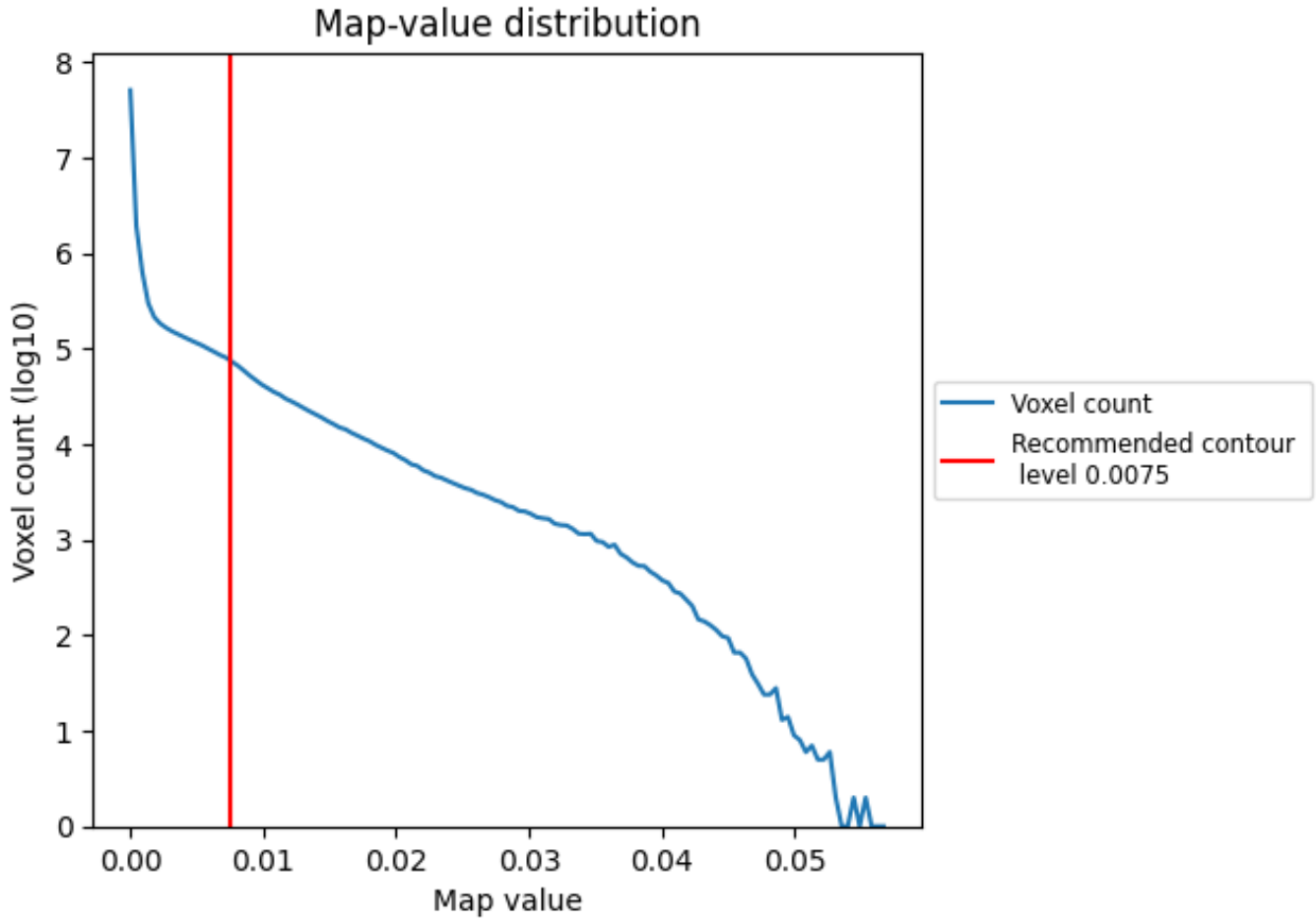
6.6 Mask visualisation (i)

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

7 Map analysis

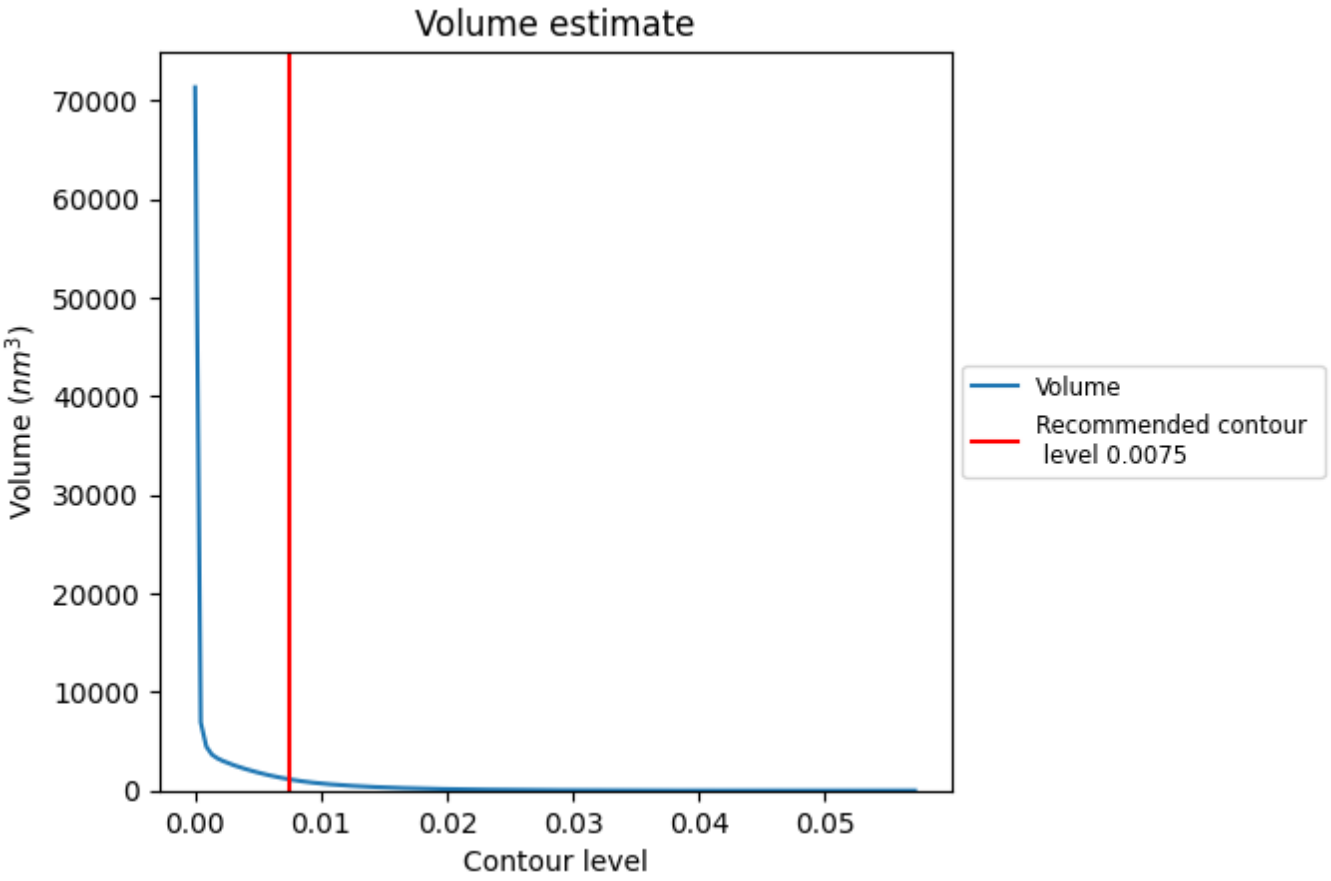
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

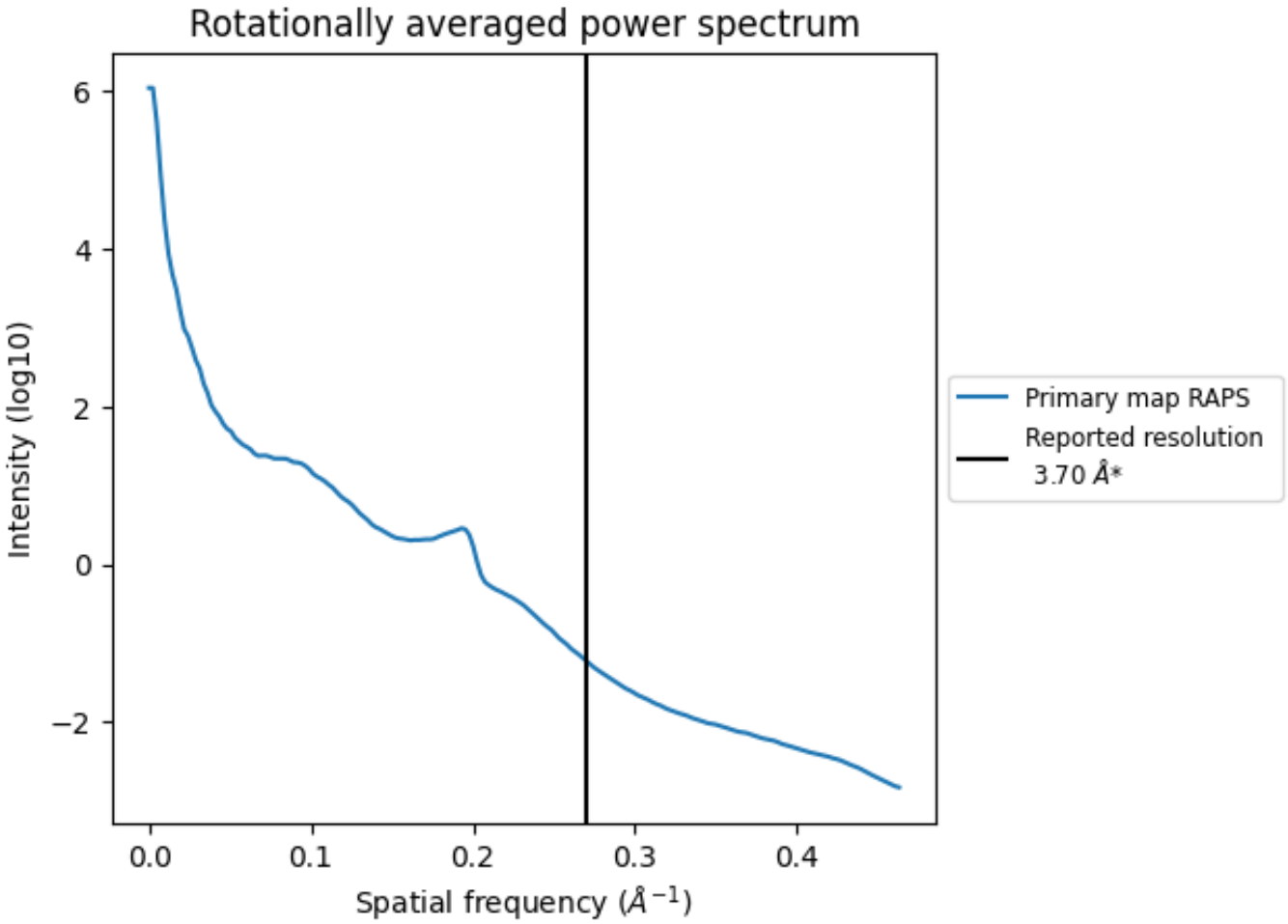
7.2 Volume estimate



The volume at the recommended contour level is 1139 nm^3; this corresponds to an approximate mass of 1029 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

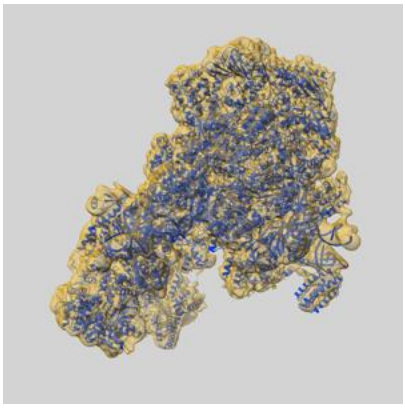
8 Fourier-Shell correlation

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

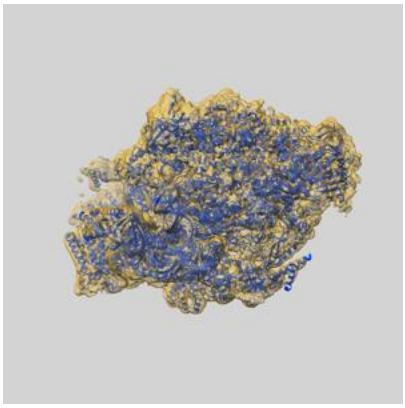
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42438 and PDB model 8UOT. Per-residue inclusion information can be found in section 3 on page 11.

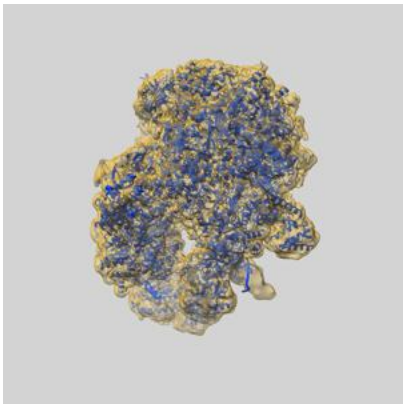
9.1 Map-model overlay



X



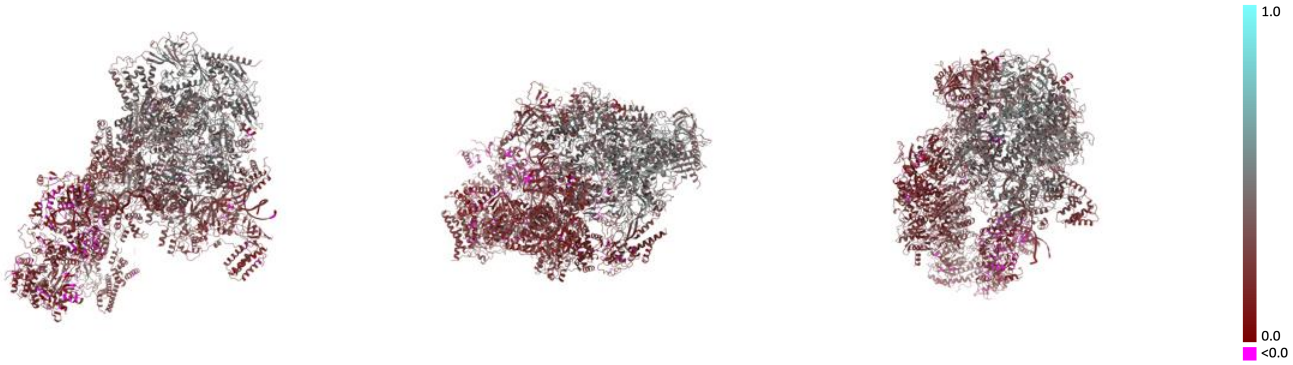
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075 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.

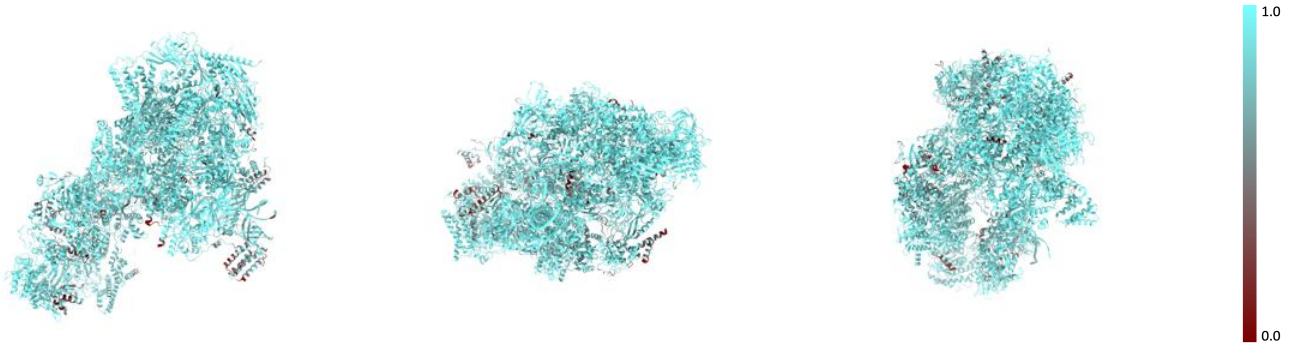
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

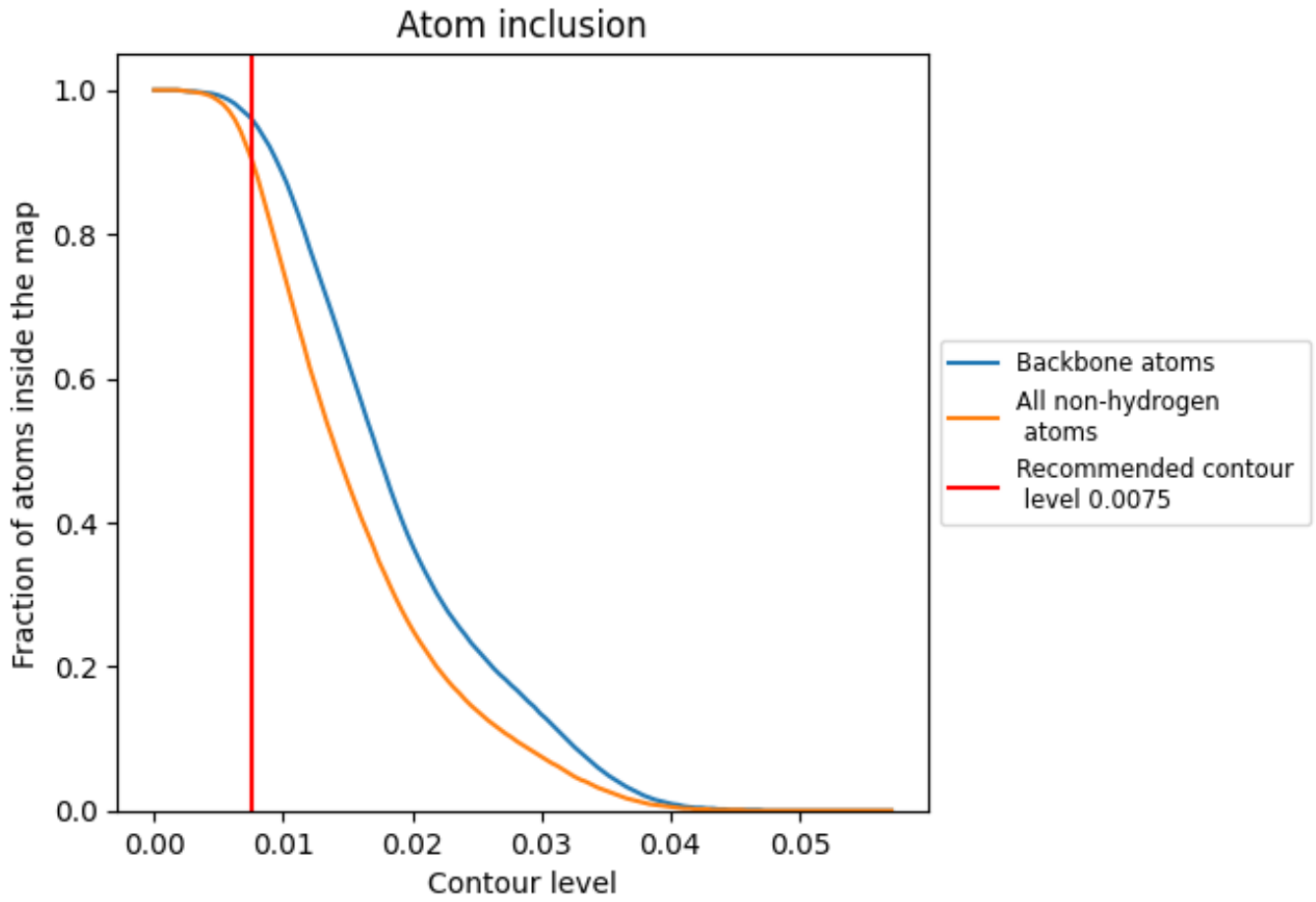
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0075).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9060	0.2830
0	0.9200	0.2170
1	0.8980	0.1910
2	0.8580	0.1420
4	0.9490	0.2030
5	0.7910	0.1450
6	0.9070	0.2150
7	0.8620	0.1250
A	0.9670	0.4060
B	0.9620	0.4160
C	0.9850	0.4380
D	0.6680	0.1900
E	0.9810	0.3840
F	0.9840	0.4120
G	0.8810	0.2580
H	0.9830	0.3960
I	0.9580	0.3660
J	0.9910	0.4450
K	0.9260	0.4160
L	0.9290	0.3280
M	0.7120	0.2540
N	0.8910	0.2000
O	0.8950	0.1660
P	0.9440	0.2340
Q	0.8490	0.2960
S	0.8970	0.2530
T	0.8770	0.2030
U	0.6830	0.1650
V	0.6290	0.1680
W	0.8390	0.1840
X	0.9310	0.1830